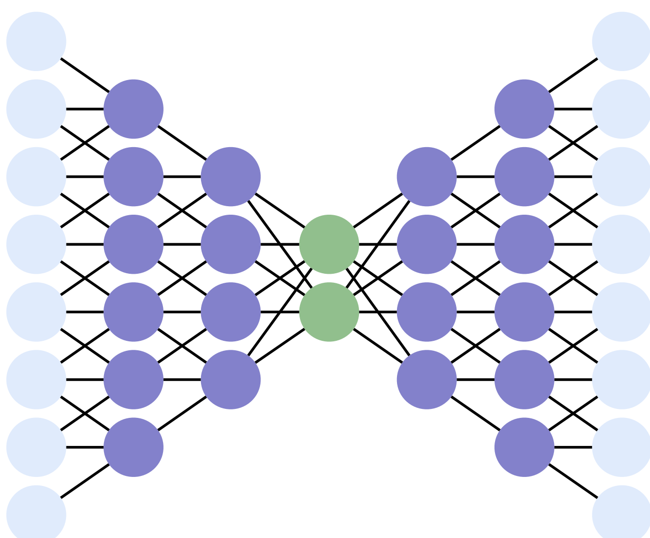
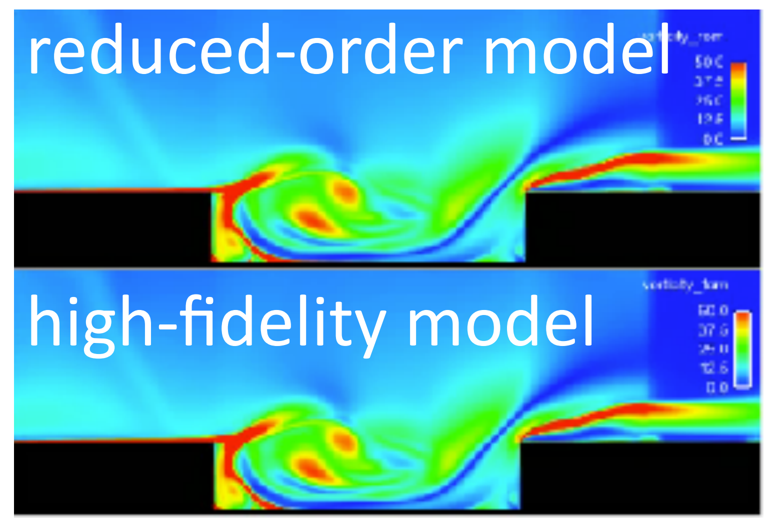
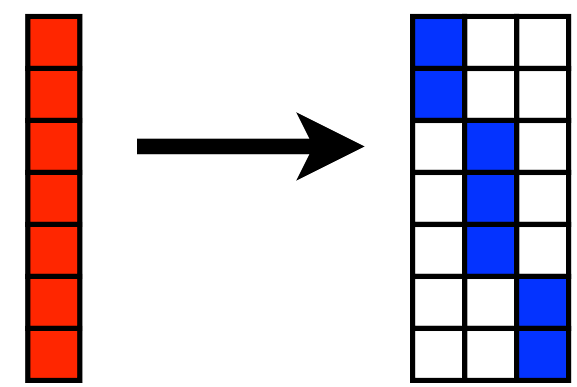
Convolutional autoencoders and LSTMs

Using deep learning to overcome Kolmogorov-width limitations and accurately model errors in nonlinear model reduction







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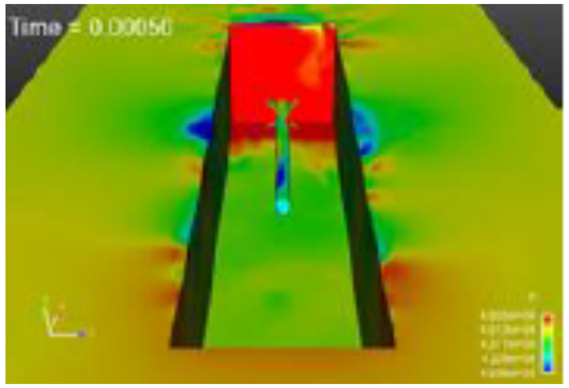
Mathematics of Reduced-Order Models

ICERM, Providence, Rhode Island

February 21, 2020

High-fidelity simulation

+ Indispensable in science and engineering
- Extreme-scale models required for high fidelity



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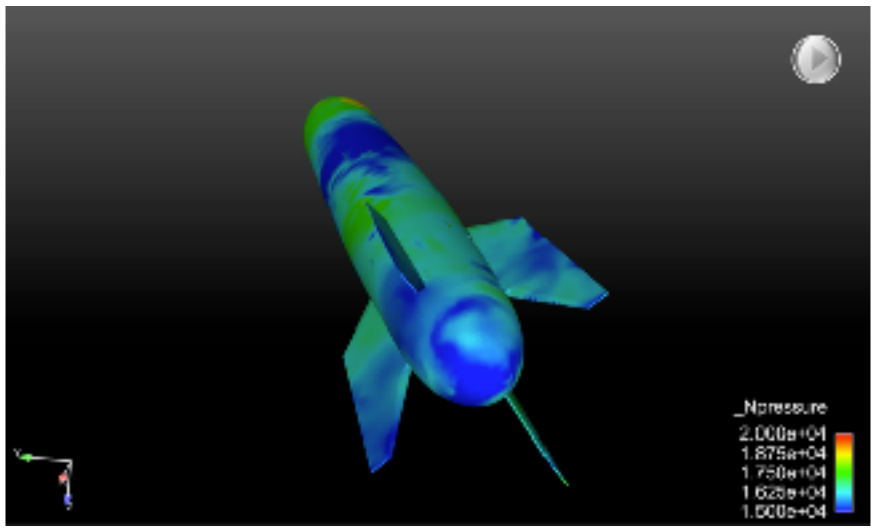
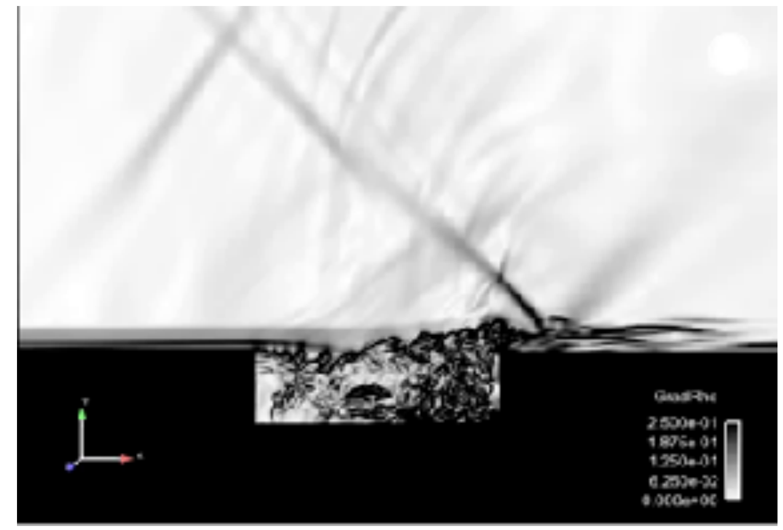




+ *High fidelity*: matches wind-tunnel experiments to within 5%
- *Extreme scale*: 100 million cells, 200,000 time steps
- *High simulation costs*: 6 weeks, 5000 cores

computational barrier

Many-query problems

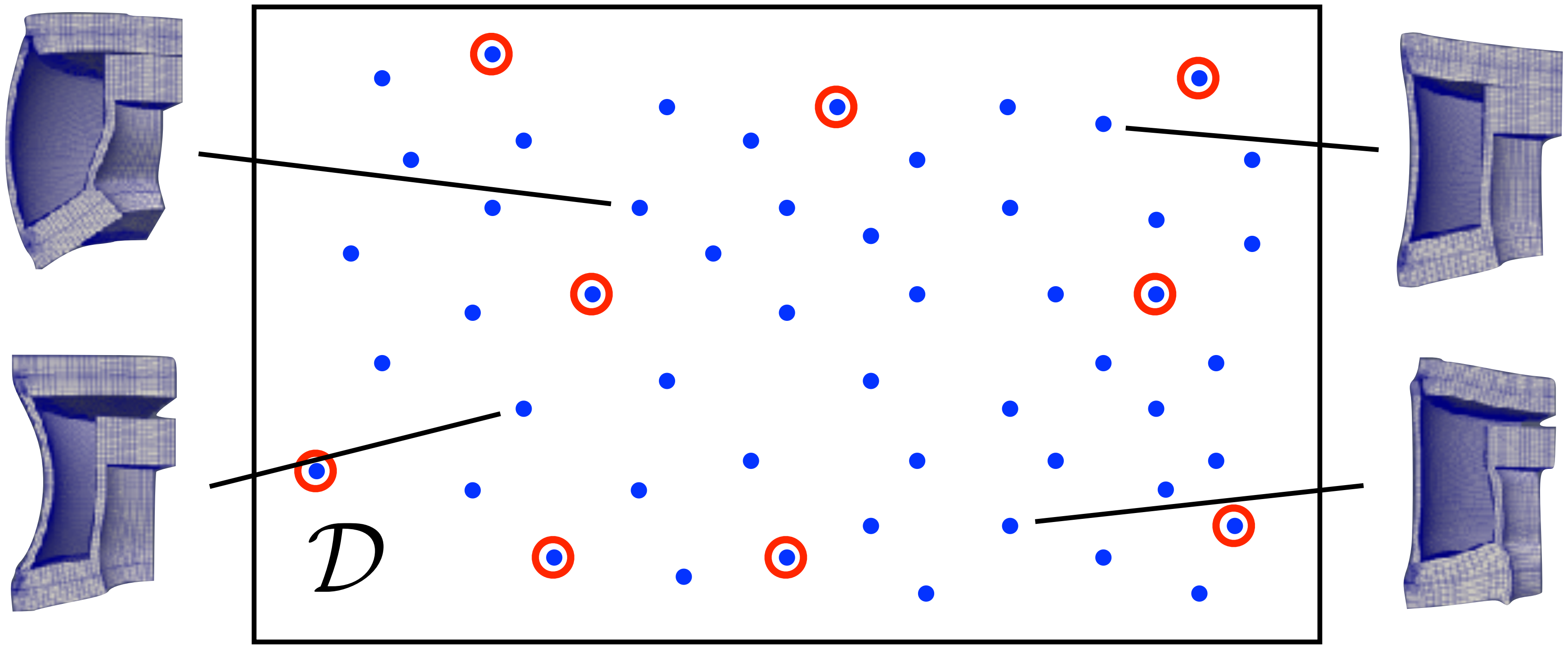
- uncertainty propagation
- Bayesian inference
- stochastic optimization

Goal: break computational barrier

Approach: exploit simulation data

$$\text{ODE:} \quad \frac{d\mathbf{x}}{dt} = \mathbf{f}(\mathbf{x}; t, \boldsymbol{\mu}), \quad \mathbf{x}(0, \boldsymbol{\mu}) = \mathbf{x}_0(\boldsymbol{\mu}), \quad t \in [0, T_{\text{final}}], \quad \boldsymbol{\mu} \in \mathcal{D}$$

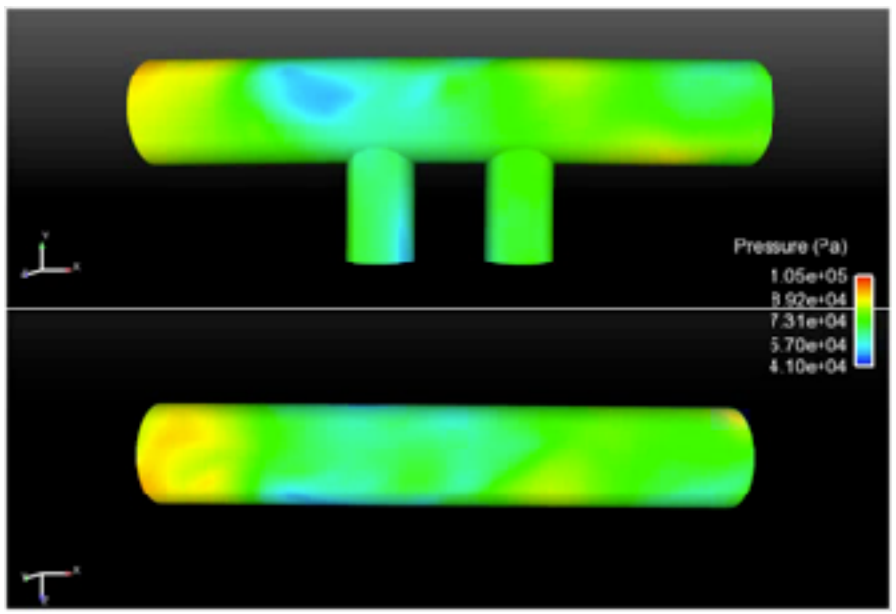
***Many-query problem**: solve ODE for $\boldsymbol{\mu} \in \mathcal{D}_{\text{query}}$*



***Idea**: exploit simulation data collected at a few points*

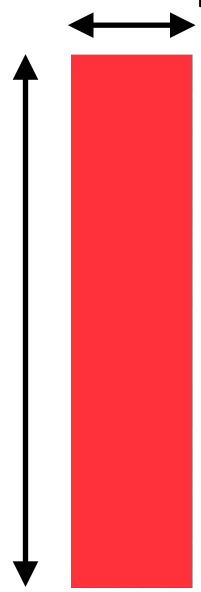
1. *Training:* Solve ODE for $\mu \in \mathcal{D}_{\text{training}}$ and collect simulation data
2. *Machine learning:* Identify structure in data
3. *Reduction:* Reduce the cost of solving ODE for $\mu \in \mathcal{D}_{\text{query}} \setminus \mathcal{D}_{\text{training}}$

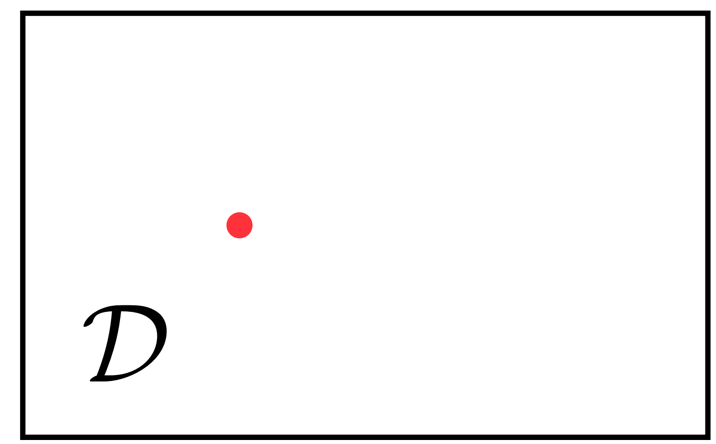
$$\text{ODE:} \quad \frac{d\mathbf{x}}{dt} = \mathbf{f}(\mathbf{x}; t, \mu)$$



number of time steps T

number of state variables N





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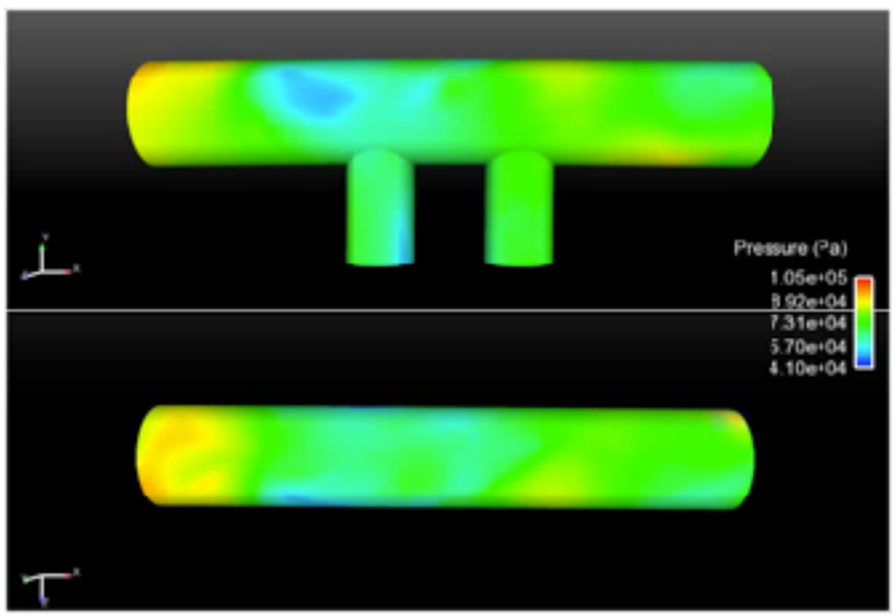
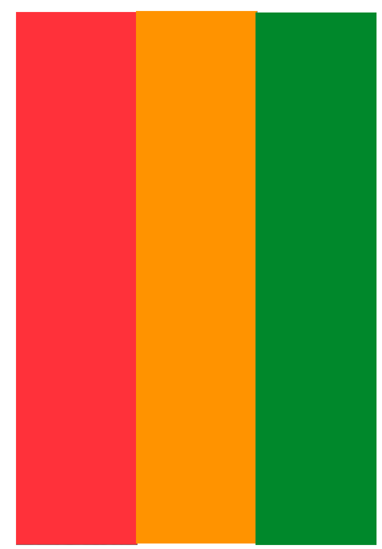
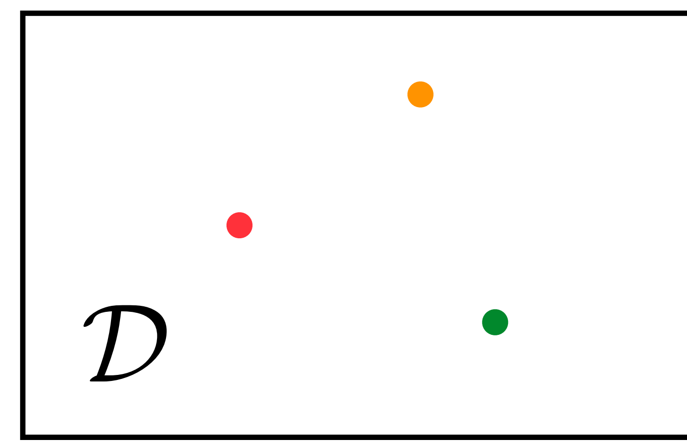


$\mathbf{X} =$ 



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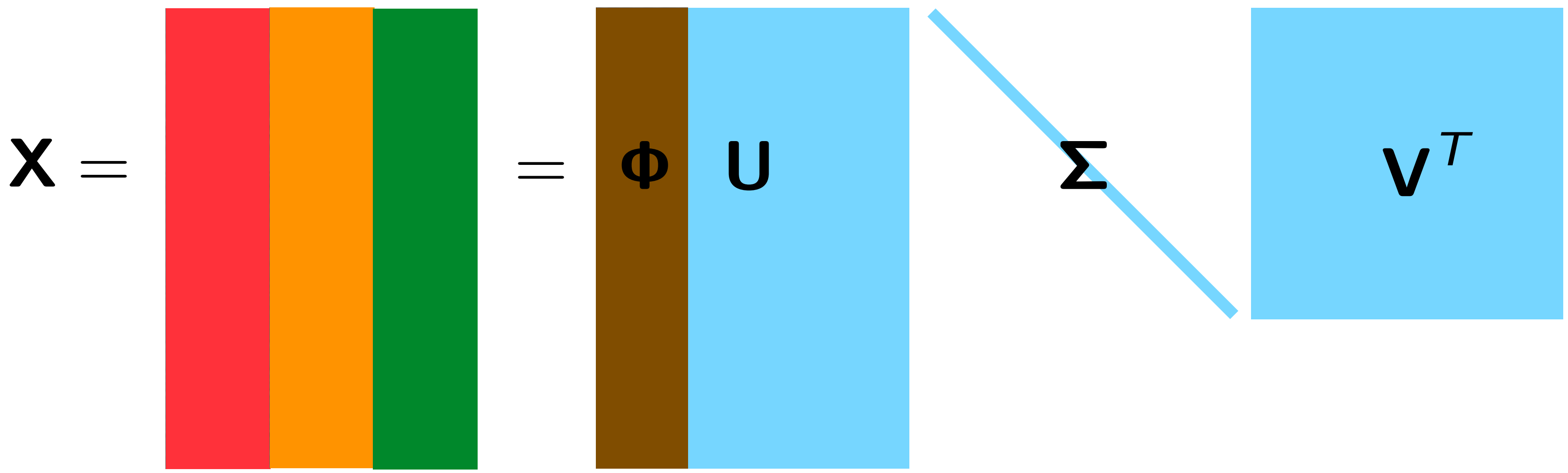

$\mathbf{\Phi}$ *columns are principal components of the spatial simulation data*

1. *Training:* Solve ODE for $\mu \in \mathcal{D}_{\text{training}}$ and collect simulation data
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$$\mathbf{x}(t) \approx \tilde{\mathbf{x}}(t) = \boldsymbol{\Phi}\, \hat{\mathbf{x}}(t)$$

ODE

$$\frac{d\mathbf{x}}{dt} = \mathbf{f}(\mathbf{x}; t)$$

$$\mathbf{r}\left(\frac{d\mathbf{x}}{dt}, \mathbf{x}, t\right) = \mathbf{0}$$

residual minimization →

Galerkin ODE

$$\frac{d\hat{\mathbf{x}}}{dt} = \boldsymbol{\Phi}^T \mathbf{f}(\boldsymbol{\Phi}\hat{\mathbf{x}}, t)$$

$$\boldsymbol{\Phi}\frac{d\hat{\mathbf{x}}}{dt}(\boldsymbol{\Phi}\hat{\mathbf{x}}, t) = \underset{\mathbf{v} \in \text{range}(\boldsymbol{\Phi})}{\arg\min} \|\mathbf{r}(\mathbf{v}, \boldsymbol{\Phi}\hat{\mathbf{x}}, t)\|_2$$

time discretization ↓   *time discretization* ↓

LSPG OΔE

[C., Bou-Mosleh, Farhat, 2011]

$$\boldsymbol{\Phi}\hat{\mathbf{x}}^n = \underset{\mathbf{v} \in \text{range}(\boldsymbol{\Phi})}{\arg\min} \|\mathbf{r}^n(\mathbf{v})\|_2, \quad n = 1, \ldots, T$$

← *residual minimization*

OΔE

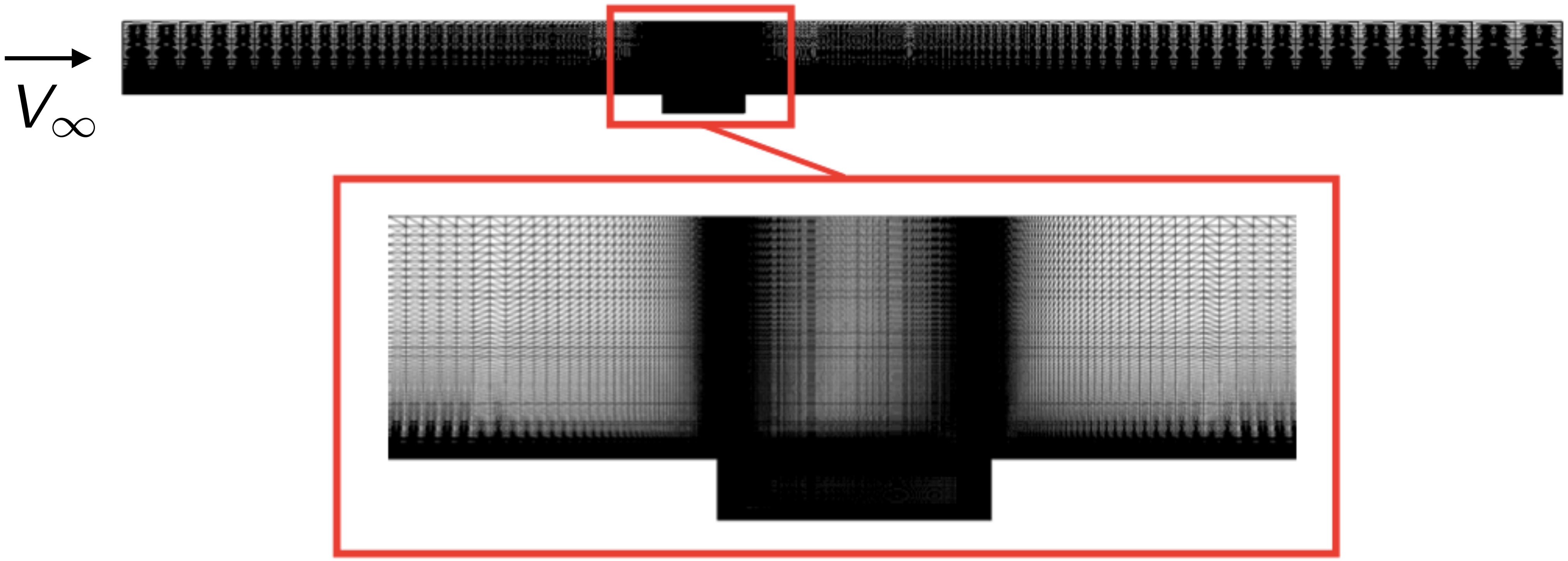
$$\mathbf{r}^n(\mathbf{x}^n) = 0, \quad n = 1, \ldots, T$$

Galerkin OΔE

$$\boldsymbol{\Phi}^T \mathbf{r}^n(\boldsymbol{\Phi}\hat{\mathbf{x}}^n) = 0, \quad n = 1, \ldots, T$$

- ODE residual: $\mathbf{r}(\mathbf{v}, \mathbf{x}, t) := \mathbf{v} - \mathbf{f}(\mathbf{x}, t)$
- OΔE residual: $\mathbf{r}^n(\mathbf{w}) := \alpha_0 \mathbf{w} - \Delta t \beta_0 \mathbf{f}(\mathbf{w}, t^n) + \sum_{j=1}^{k} \alpha_j \mathbf{x}^{n-j} - \Delta t \sum_{j=1}^{k} \beta_j \mathbf{f}(\mathbf{x}^{n-j}, t^{n-j})$
- Other residual-minimizing ROMs [LeGresley and Alonso, 2000; Bui-Thanh et al., 2008; Bui-Thanh et al., 2008; Constantine and Wang, 2012; Choi and C.; 2019; **Parish and C., 2019**]

Captive carry



- Unsteady Navier–Stokes
- Re = 6.3 x 10^6
- $M_\infty = 0.6$

Spatial discretization

- 2nd-order finite volume
- DES turbulence model
- 1.2×10^6 degrees of freedom

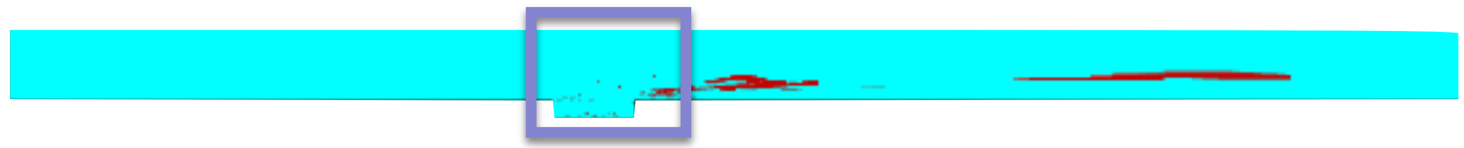
Temporal discretization

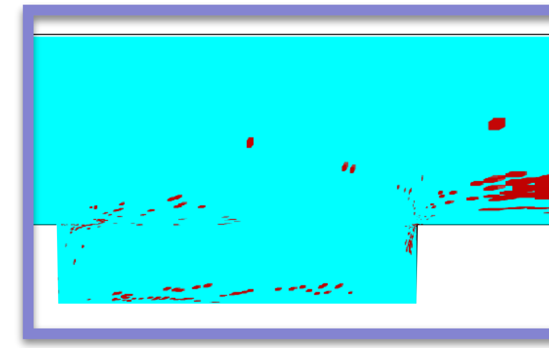
- 2nd-order BDF
- Verified time step $\Delta t = 1.5 \times 10^{-3}$
- 8.3×10^3 time instances

LSPG ROM with sample mesh [C., Farhat, Cortial, Amsallem, 2013]

$$\boldsymbol{\Phi}\hat{\mathbf{x}}^n = \underset{\mathbf{v}\in\mathrm{range}(\boldsymbol{\Phi})}{\arg\min} \left\|\mathbf{r}^n(\mathbf{v})\right\|_{\Theta}$$

sample mesh



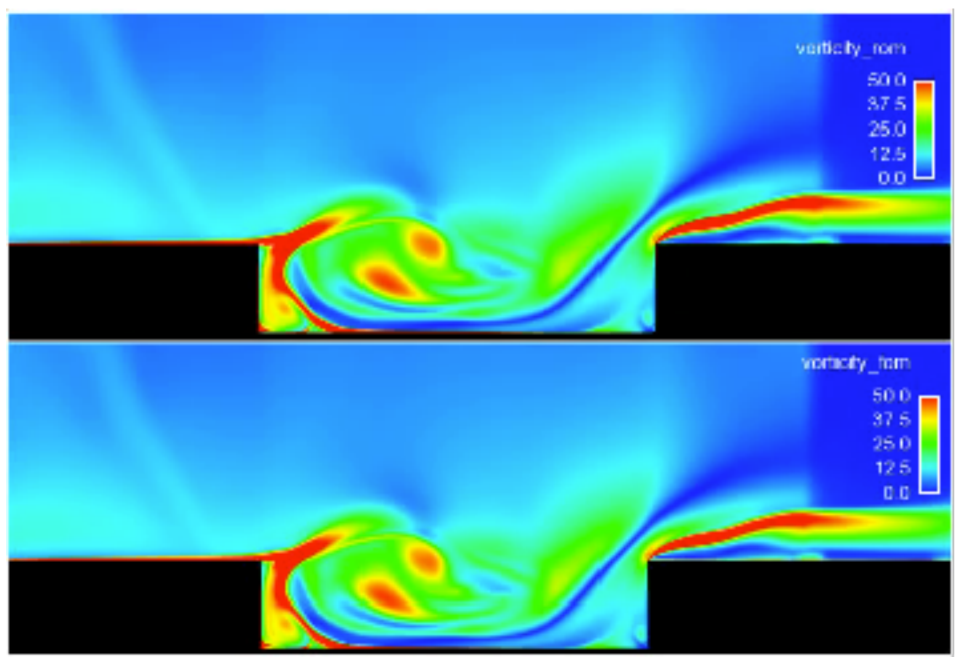


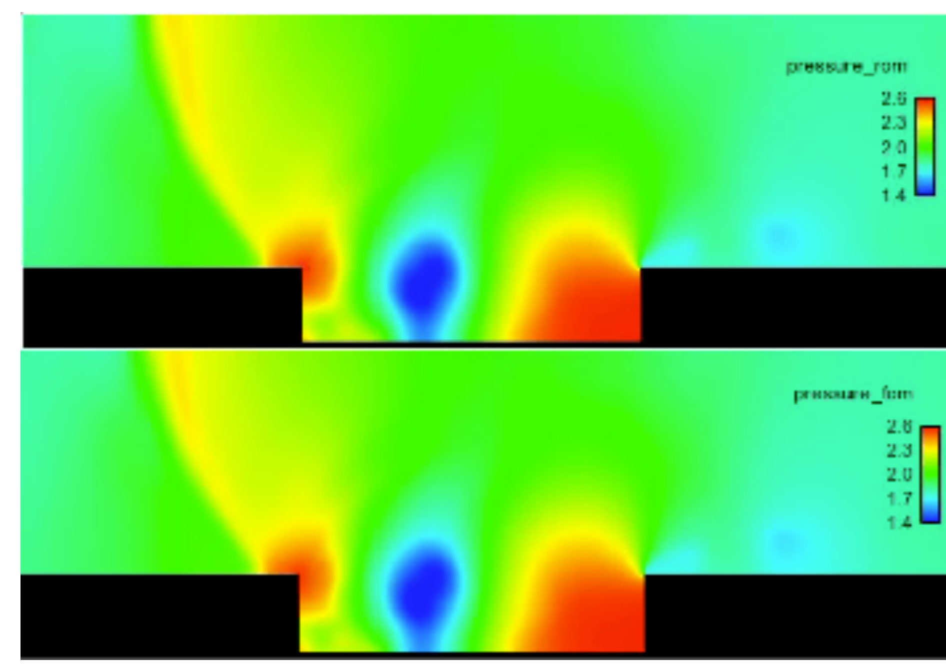
+ *HPC on a laptop*

vorticity field | *pressure field*

LSPG ROM
32 min, 2 cores

high-fidelity
5 hours, 48 cores





+ 229x savings in core–hours
+ < 1% error in time-averaged drag

… so why doesn't everyone use ROMs?

Outstanding challenges in model reduction

1) Linear-subspace assumption is strong

$$\mathbf{x}(t) \approx \tilde{\mathbf{x}}(t) = \boldsymbol{\Phi}\,\hat{\mathbf{x}}(t)$$

- Lee and C. “Model reduction of dynamical systems on nonlinear manifolds using deep convolutional autoencoders.” J Comp Phys, 404:108973, 2020.

2) Important physical properties not satisfied

Galerkin

$$\boldsymbol{\Phi}\frac{d\hat{\mathbf{x}}}{dt}(\mathbf{x}, t) = \underset{\mathbf{v}\in\mathrm{range}(\boldsymbol{\Phi})}{\mathrm{argmin}} \|\mathbf{r}(\mathbf{v}, \mathbf{x}; t)\|_2$$

LSPG

$$\boldsymbol{\Phi}\hat{\mathbf{x}}^n = \underset{\mathbf{v}\in\mathrm{range}(\boldsymbol{\Phi})}{\arg\min} \|\mathbf{r}^n(\mathbf{v})\|_2$$

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3) Error analysis difficult

- Freno and C. “Machine-learning error models for approximate solutions to parameterized systems of nonlinear equations.” CMAME, 348:250–296, 2019.
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Kolmogorov-width limitation of linear subspaces

- $\mathcal{M} := \{\mathbf{x}(t, \boldsymbol{\mu}) \mid t \in [0, T_{\mathsf{final}}],\ \boldsymbol{\mu} \in \mathcal{D}\}$: solution manifold
- $\mathcal{S}_p$: set of all p-dimensional linear subspaces
- $d_p(\mathcal{M}) := \inf_{\mathcal{S} \in \mathcal{S}_p} P_\infty(\mathcal{M}, \mathcal{S})$, $P_\infty(\mathcal{M}, \mathcal{S}) := \sup_{\mathbf{x} \in \mathcal{M}} \inf_{\mathbf{y} \in \mathcal{S}} \|\mathbf{x} - \mathbf{y}\|$

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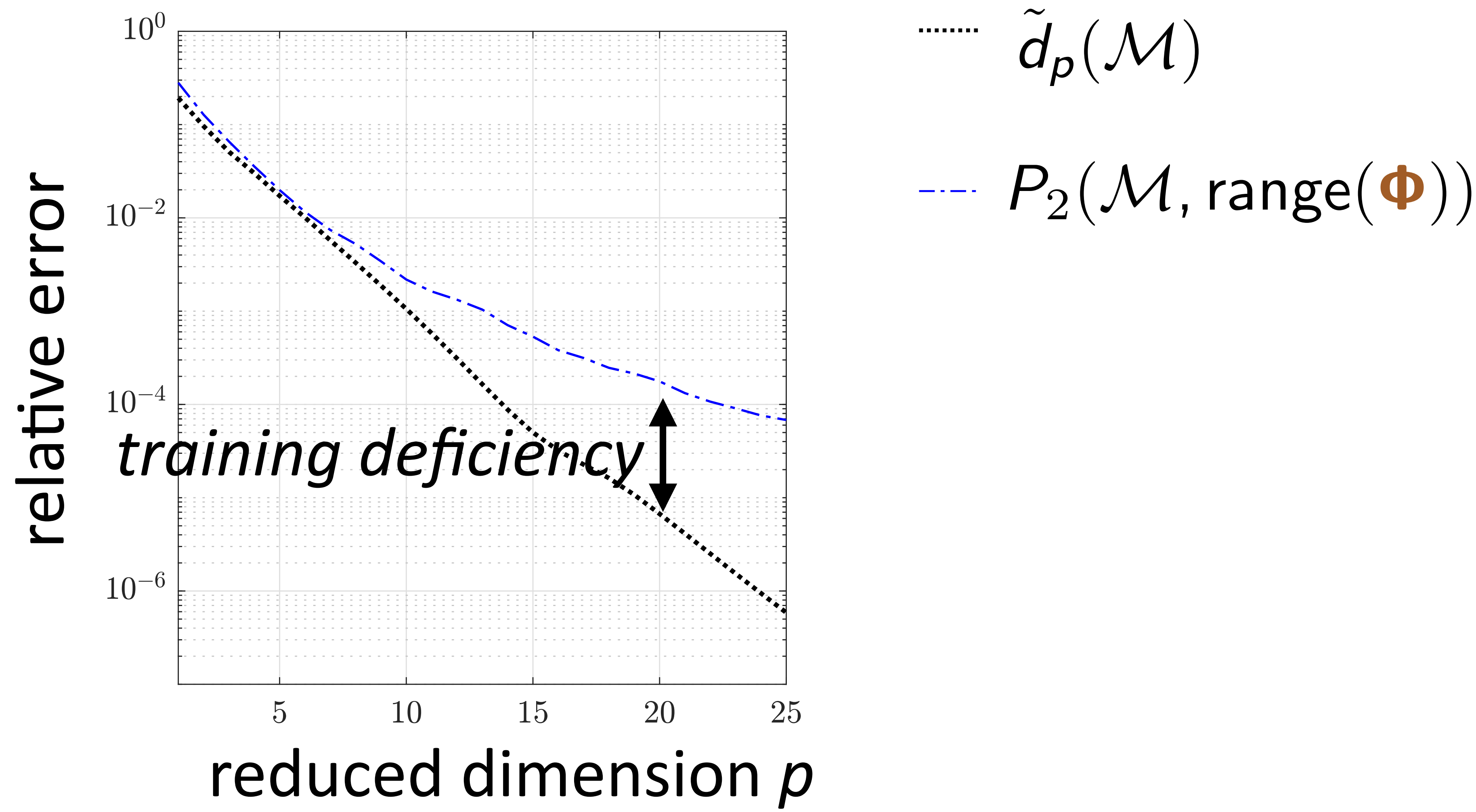

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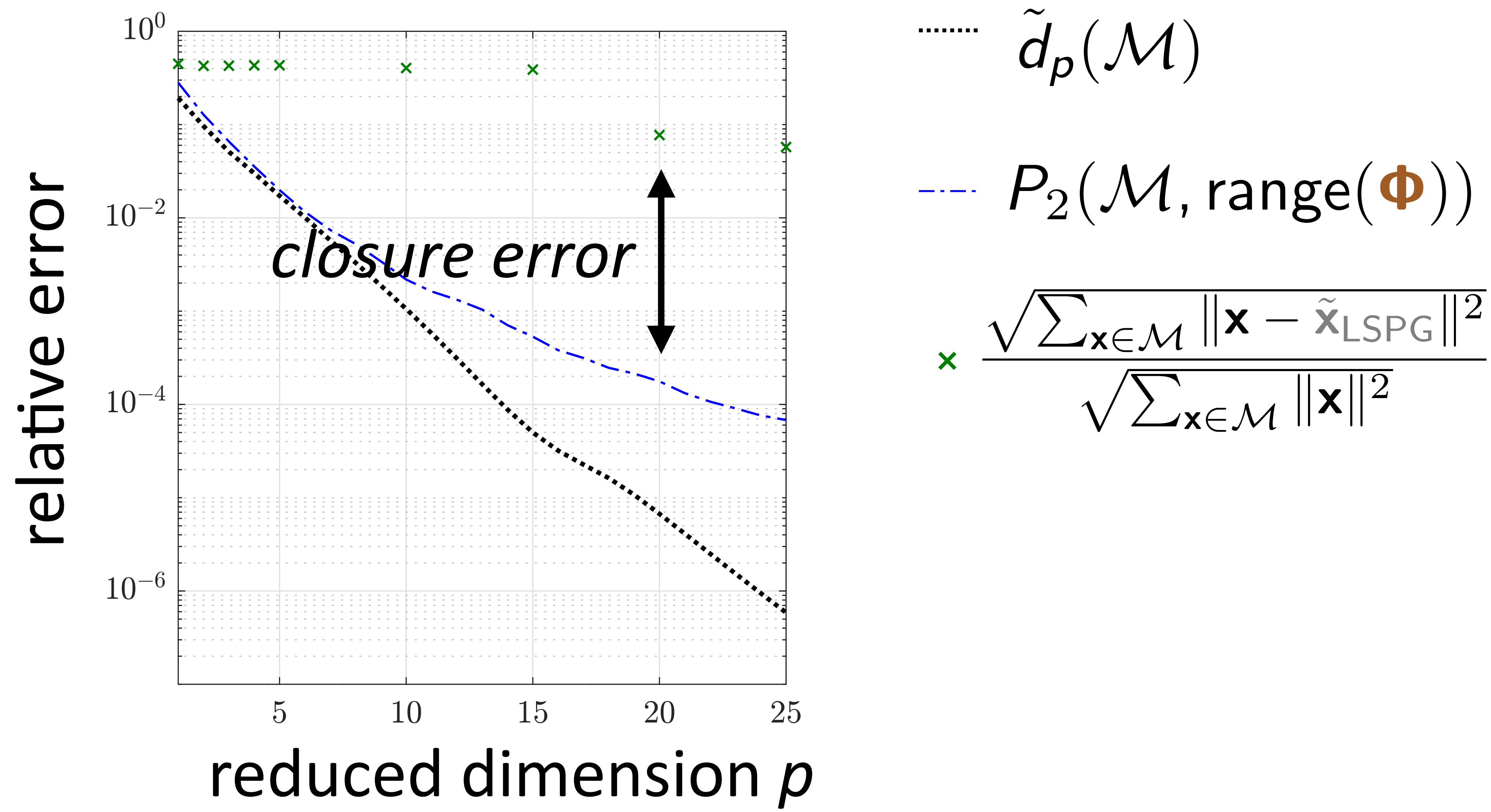

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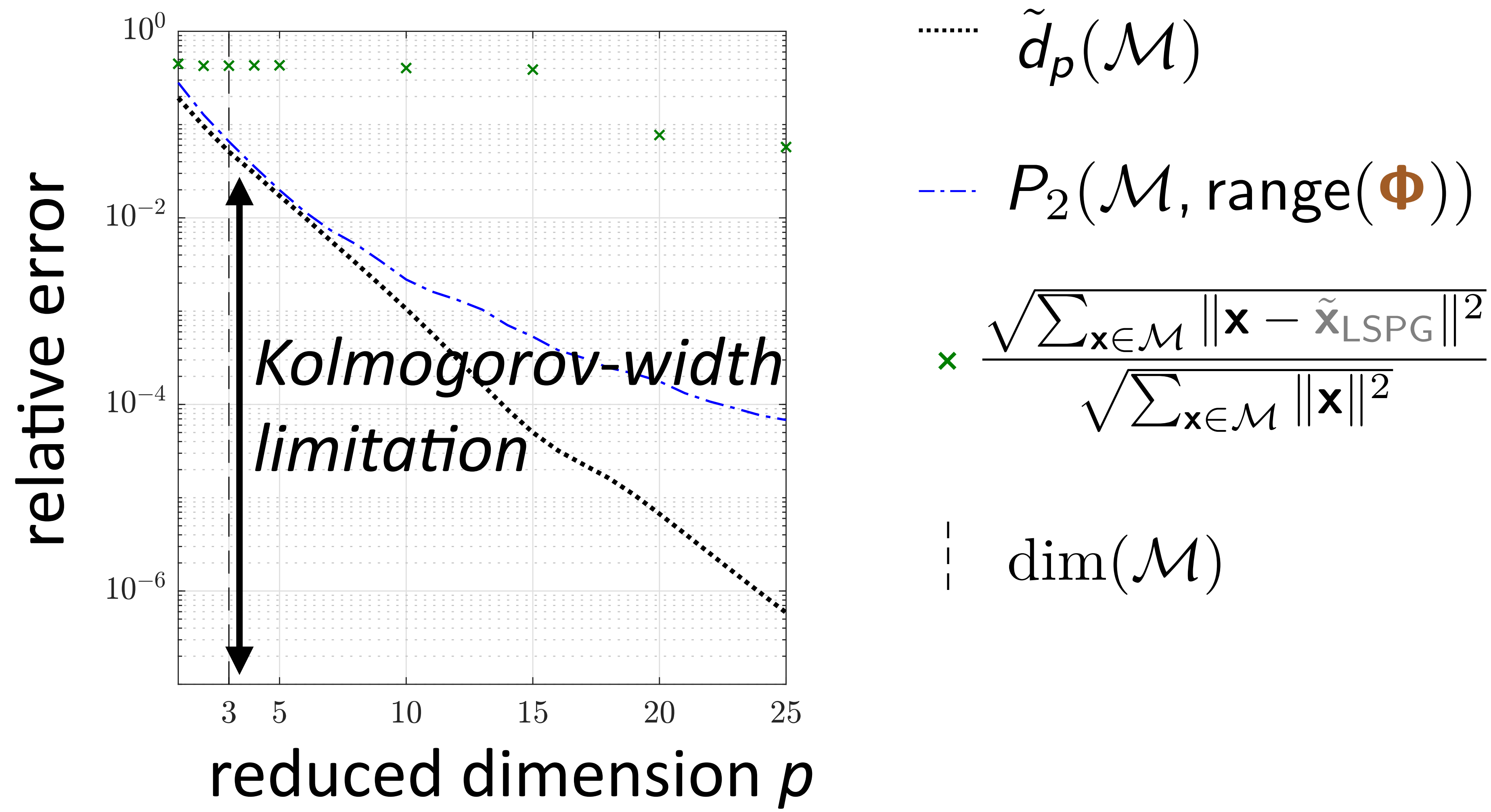

- Kolmogorov-width limitation: significant error for $p = \dim(\mathcal{M})$

***Goal**: overcome limitation via projection onto a nonlinear manifold*

Overcoming Kolmogorov-width limitation

Transform/update the linear subspace

[Ohlberger and Rave, 2013; Iollo and Lombardi, 2014; Gerbeau and Lombardi, 2014; Peherstorfer and Willcox, 2015; Welper, 2017; Mojgani and Balajewicz, 2017; Reiss et al., 2018; Zimmermann et al., 2018; Peherstorfer, 2018; Rim and Mandli, 2018; Rim and Mandli, 2018; Nair and Balajewicz, 2019; Cagniart et al., 2019]

+ Can work much better than a fixed basis
- Some require problem-specific knowledge or characteristics
- Do not consider manifolds of general nonlinear structure

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***A priori* construction of local linear subspaces**

[Dihlmann et al., 2011; Drohmann et al., 2011; Amsallem, Zahr, Farhat, 2012; Peherstorfer et el., 2014; Taddei et al., 2015]

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Model reduction on nonlinear manifolds [Gu, 2011; Kashima, 2016; Hartman and Mestha, 2017]

- Kinematically inconsistent [Kashima, 2016; Hartman and Mestha, 2017]
- Limited to piecewise linear manifolds [Gu, 2011]
- Solutions lack optimality [Gu, 2011; Kashima, 2016; Hartman and Mestha, 2017]

Goals

Overcome shortcomings of existing methods

+ Enable manifolds with general nonlinear structure
+ Kinematically consistent
+ Satisfy optimality property

Manifold Galerkin and LSPG projection

Practical nonlinear-manifold construction

+ No problem-specific knowledge required
+ Use same training data as POD

Deep convolutional autoencoders

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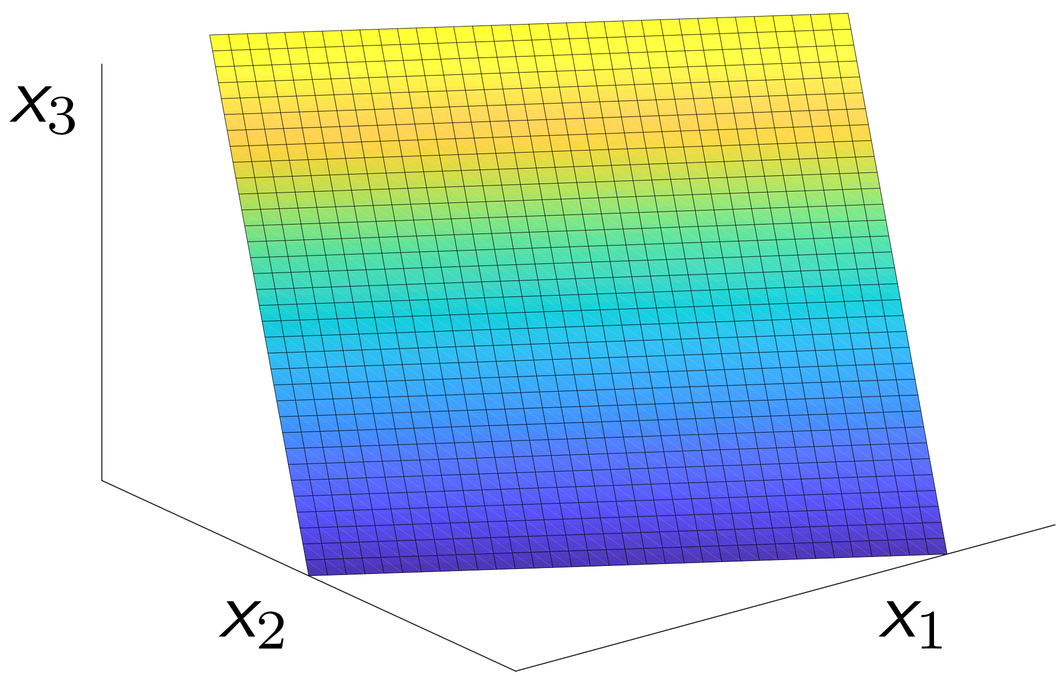
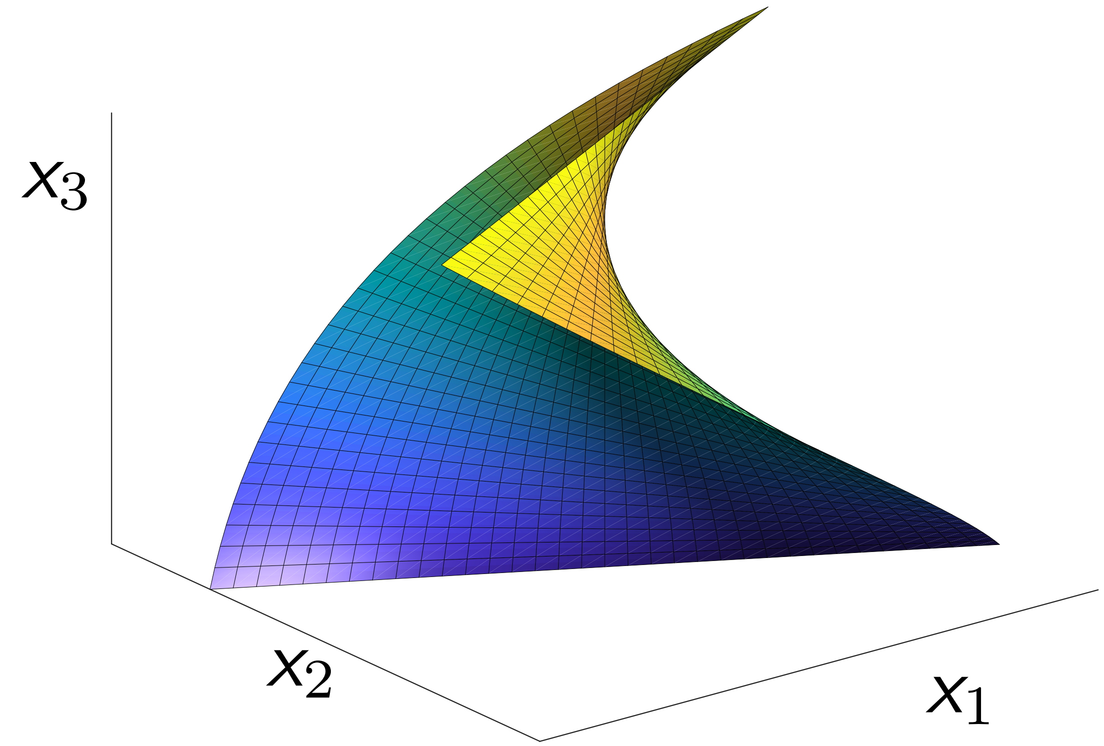
Nonlinear trial manifold

	Linear trial subspace	***Nonlinear trial manifold***
	$\text{range}(\boldsymbol{\Phi}) := \{\boldsymbol{\Phi}\hat{\mathbf{x}} \mid \hat{\mathbf{x}} \in \mathbb{R}^p\}$	$\mathcal{S} := \{\mathbf{g}(\hat{\mathbf{x}}) \mid \hat{\mathbf{x}} \in \mathbb{R}^p\}$
example *N=3* *p=2*		
state	$\mathbf{x}(t) \approx \tilde{\mathbf{x}}(t) = \boldsymbol{\Phi}\,\hat{\mathbf{x}}(t) \in \text{range}(\boldsymbol{\Phi})$	$\mathbf{x}(t) \approx \tilde{\mathbf{x}}(t) = \mathbf{g}(\hat{\mathbf{x}}(t)) \in \mathcal{S}$
		
		+ Manifold has general structure
velocity	$\frac{d\mathbf{x}}{dt} \approx \frac{d\tilde{\mathbf{x}}}{dt} = \boldsymbol{\Phi}\frac{d\hat{\mathbf{x}}}{dt} \in \text{range}(\boldsymbol{\Phi})$	$\frac{d\mathbf{x}}{dt} \approx \frac{d\tilde{\mathbf{x}}}{dt} = \nabla\mathbf{g}(\hat{\mathbf{x}})\frac{d\hat{\mathbf{x}}}{dt} \in T_{\hat{\mathbf{x}}}\mathcal{S}$
		+ Kinematically consistent

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	Linear-subspace ROM	***Nonlinear-manifold ROM***
	Given $\boldsymbol{\Phi}$	Given $\mathbf{g}(\hat{\mathbf{x}})$
Galerkin	$\frac{d\hat{\mathbf{x}}}{dt} = \underset{\hat{\mathbf{v}}\in\mathbb{R}^p}{\operatorname{argmin}} \Vert \mathbf{r}(\boldsymbol{\Phi}\hat{\mathbf{v}}, \boldsymbol{\Phi}\hat{\mathbf{x}}; t)\Vert_2$ $\Updownarrow$ $\frac{d\hat{\mathbf{x}}}{dt} = \boldsymbol{\Phi}^T \mathbf{f}(\boldsymbol{\Phi}\hat{\mathbf{x}}; t)$	$\frac{d\hat{\mathbf{x}}}{dt} = \underset{\hat{\mathbf{v}}\in\mathbb{R}^p}{\operatorname{argmin}} \Vert \mathbf{r}(\nabla\mathbf{g}(\hat{\mathbf{x}})\hat{\mathbf{v}}, \mathbf{g}(\hat{\mathbf{x}}); t)\Vert_2$ $\Updownarrow$ $\frac{d\hat{\mathbf{x}}}{dt} = \nabla\mathbf{g}(\hat{\mathbf{x}})^+ \mathbf{f}(\mathbf{g}(\hat{\mathbf{x}}); t)$
LSPG	$\hat{\mathbf{x}}^n = \underset{\hat{\mathbf{v}}\in\mathbb{R}^p}{\operatorname{argmin}} \Vert \mathbf{r}^n(\boldsymbol{\Phi}\hat{\mathbf{v}})\Vert_2$	$\hat{\mathbf{x}}^n = \underset{\hat{\mathbf{v}}\in\mathbb{R}^p}{\operatorname{argmin}} \Vert \mathbf{r}^n(\mathbf{g}(\hat{\mathbf{v}}))\Vert_2$

\+ Satisfy residual minimization

Theorem [Lee, C., 2020]

Manifold Galerkin and manifold LSPG are equivalent if
1. the nonlinear trial manifold $\mathcal{S}$ is twice continuously differentiable,
2. $\Vert\hat{\mathbf{x}}^{n-j} - \hat{\mathbf{x}}^n\Vert = O(\Delta t)$ for $n = 1, \ldots, T$ and $j = 1, \ldots, k$, and
3. the limit $\Delta t \to 0$ is taken.

Error bound

Theorem [Lee, C., 2020]

If the following conditions hold:

1. $\mathbf{f}(\cdot; t)$ is Lipschitz continuous with Lipschitz constant κ
2. Δt is small enough such that $0 < h := |\alpha_0| - |\beta_0|\kappa\Delta t$, then

$$\|\mathbf{x}^n - \mathbf{g}(\hat{\mathbf{x}}_{\mathrm{G}}^n)\|_2 \leq \frac{1}{h}\|\mathbf{r}_{\mathrm{G}}^n(\mathbf{g}(\hat{\mathbf{x}}_{\mathrm{G}}))\|_2 + \frac{1}{h}\sum_{\ell=1}^{k}|\gamma_\ell|\|\mathbf{x}^{n-\ell} - \mathbf{g}(\hat{\mathbf{x}}_{\mathrm{G}})\|_2$$

$$\|\mathbf{x}^n - \mathbf{g}(\hat{\mathbf{x}}_{\mathrm{LSPG}}^n)\|_2 \leq \frac{1}{h}\min_{\hat{\mathbf{v}}}\|\mathbf{r}_{\mathrm{LSPG}}^n(\mathbf{g}(\hat{\mathbf{v}}))\|_2 + \frac{1}{h}\sum_{\ell=1}^{k}|\gamma_\ell|\|\mathbf{x}^{n-\ell} - \mathbf{g}(\hat{\mathbf{x}}_{\mathrm{LSPG}})\|_2$$

\+ Manifold LSPG sequentially minimizes the error bound

How to construct manifold $\mathcal{S} := \{\mathbf{g}(\hat{\mathbf{x}}) \mid \hat{\mathbf{x}} \in \mathbb{R}^p\}$ ***from training data?***

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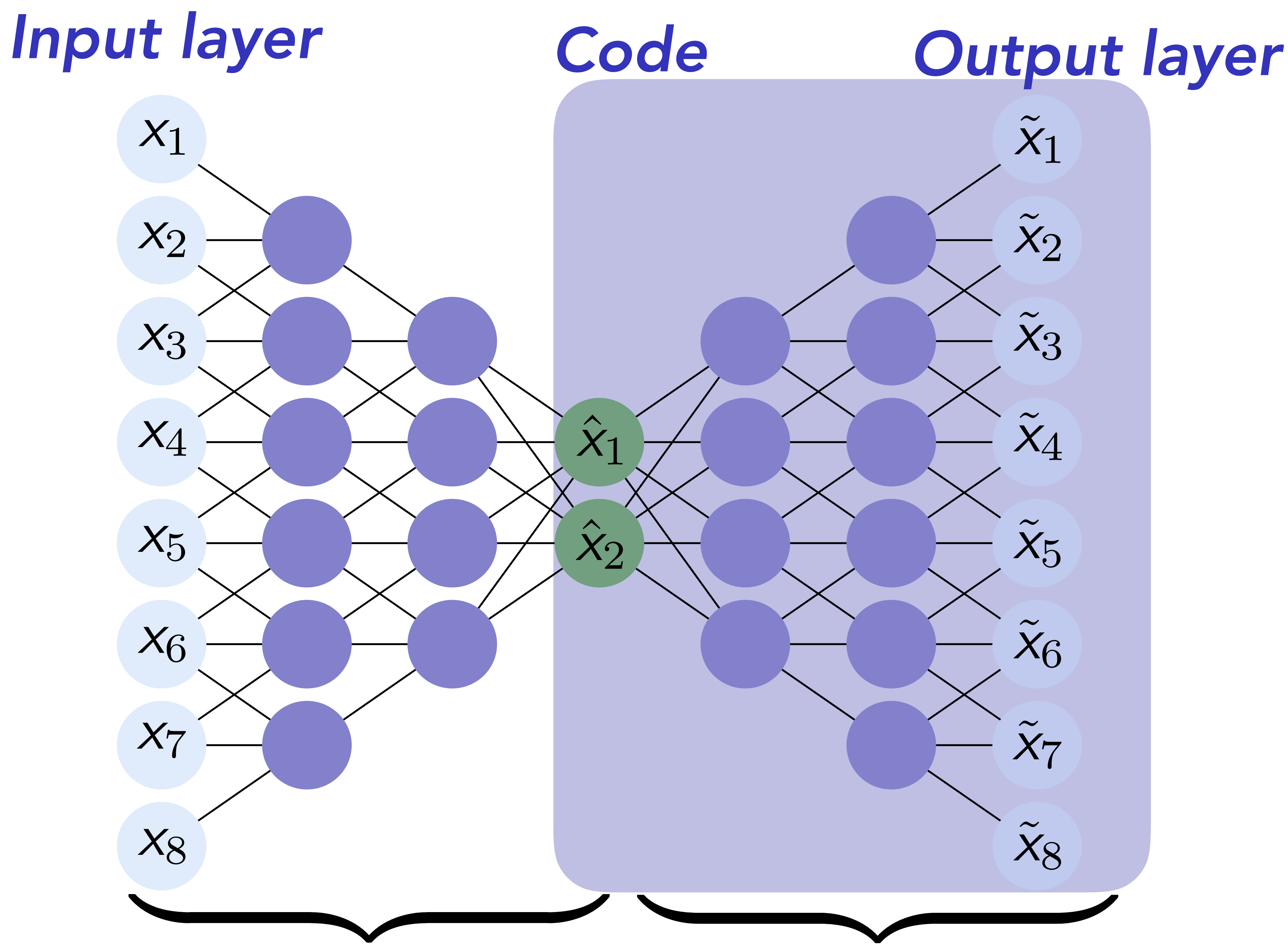
Practical nonlinear-manifold construction

+ No problem-specific knowledge required
+ Use same training data as POD

Deep convolutional autoencoders

$$\mathcal{S} := \{\mathbf{g}(\hat{\mathbf{x}}) \mid \hat{\mathbf{x}} \in \mathbb{R}^p\}$$

Deep autoencoders

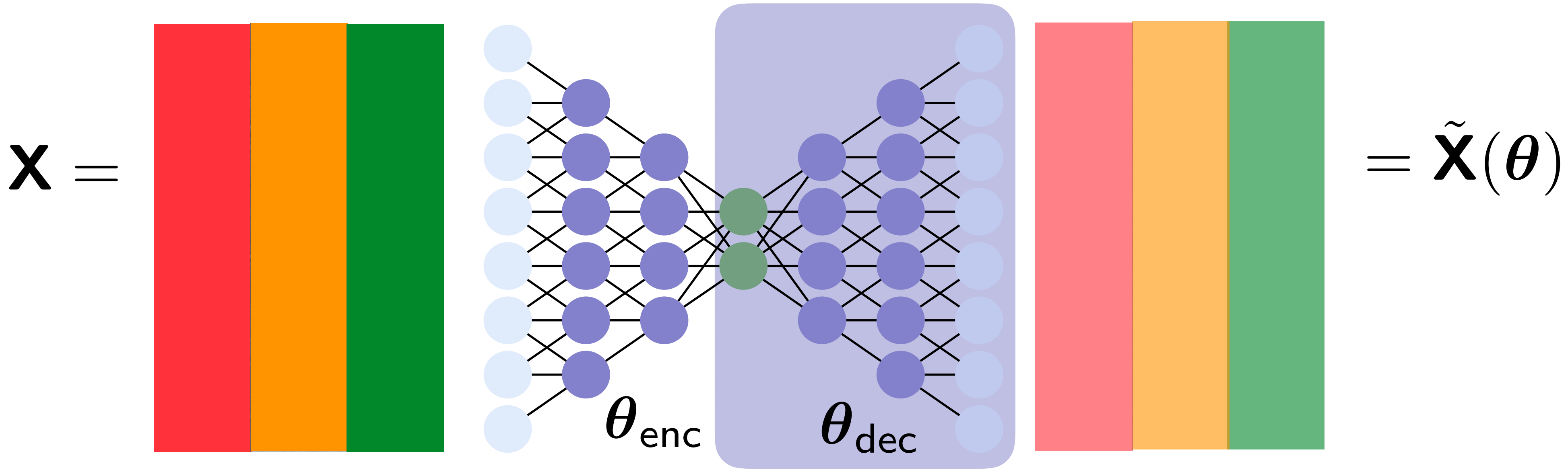


Encoder $\mathbf{h}_{\text{enc}}(\cdot;\boldsymbol{\theta}_{\text{enc}})$ ***Decoder*** $\mathbf{h}_{\text{dec}}(\cdot;\boldsymbol{\theta}_{\text{dec}})$

$$\tilde{\mathbf{x}} = \mathbf{h}_{\text{dec}}(\cdot;\boldsymbol{\theta}_{\text{dec}}) \circ \mathbf{h}_{\text{enc}}(\mathbf{x};\boldsymbol{\theta}_{\text{enc}})$$

+ If $\tilde{\mathbf{x}} \approx \mathbf{x}$ for $\boldsymbol{\theta}^\star_{\text{dec}}$, then $\mathbf{g} = \mathbf{h}_{\text{dec}}(\cdot;\boldsymbol{\theta}^\star_{\text{dec}})$ is accurate manifold parameterization

1. *Training:* Solve ODE for $\mu \in \mathcal{D}_{\text{training}}$ and collect simulation data
2. *Machine learning:* Identify structure in data
3. *Reduction:* Reduce the cost of solving ODE for $\mu \in \mathcal{D}_{\text{query}} \setminus \mathcal{D}_{\text{training}}$



- Compute $\boldsymbol{\theta}^\star$ by approximately solving $\underset{\boldsymbol{\theta}}{\text{minimize}} \|\mathbf{X} - \tilde{\mathbf{X}}(\boldsymbol{\theta})\|_F$
- Define nonlinear trial manifold by setting $\mathbf{g} = \mathbf{h}_{\text{dec}}(\cdot; \boldsymbol{\theta}^\star_{\text{dec}})$

\+ Same snapshot data, no specialized problem knowledge

1. *Training:* Solve ODE for $\mu \in \mathcal{D}_{\text{training}}$ and collect simulation data
2. *Machine learning:* Identify structure in data
3. *Reduction:* Reduce the cost of solving ODE for $\boldsymbol{\mu} \in \mathcal{D}_{\text{query}} \setminus \mathcal{D}_{\text{training}}$

Subspace ROM | *Manifold ROM*

Given $\boldsymbol{\Phi}$ | Given $\mathbf{g}(\hat{\mathbf{x}})$

Galerkin

$$\frac{d\hat{\mathbf{x}}}{dt} = \underset{\hat{\mathbf{v}} \in \mathbb{R}^p}{\operatorname{argmin}} \|\mathbf{r}(\boldsymbol{\Phi}\hat{\mathbf{v}}, \boldsymbol{\Phi}\hat{\mathbf{x}}; t)\|_2 \quad\quad \frac{d\hat{\mathbf{x}}}{dt} = \underset{\hat{\mathbf{v}} \in \mathbb{R}^p}{\operatorname{argmin}} \|\mathbf{r}(\nabla \mathbf{g}(\hat{\mathbf{x}})\hat{\mathbf{v}}, \mathbf{g}(\hat{\mathbf{x}}); t)\|_2$$

$$\Updownarrow \quad\quad \Updownarrow$$

$$\frac{d\hat{\mathbf{x}}}{dt} = \boldsymbol{\Phi}^T \mathbf{f}(\boldsymbol{\Phi}\hat{\mathbf{x}}; t) \quad\quad \frac{d\hat{\mathbf{x}}}{dt} = \nabla \mathbf{g}(\hat{\mathbf{x}})^+ \mathbf{f}(\mathbf{g}(\hat{\mathbf{x}}); t)$$

LSPG

$$\hat{\mathbf{x}}^n = \underset{\hat{\mathbf{v}} \in \mathbb{R}^p}{\operatorname{argmin}} \|\mathbf{r}^n(\boldsymbol{\Phi}\hat{\mathbf{v}})\|_2 \quad\quad \hat{\mathbf{x}}^n = \underset{\hat{\mathbf{v}} \in \mathbb{R}^p}{\operatorname{argmin}} \|\mathbf{r}^n(\mathbf{g}(\hat{\mathbf{v}}))\|_2$$

+ Satisfy residual minimization
+ Predictions directly integrate deep learning with computational physics

Numerical results

1D Burgers' equation

$$\frac{\partial w(x,t;\boldsymbol{\mu})}{\partial t} + \frac{\partial f(w(x,t;\boldsymbol{\mu}))}{\partial x} = 0.02e^{\alpha x}$$

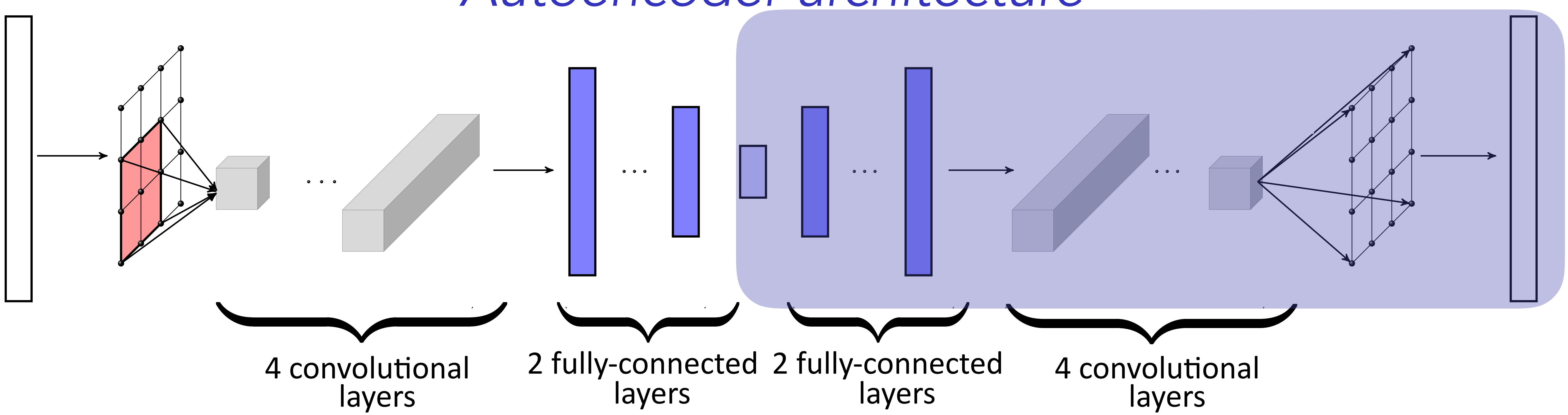
- $\boldsymbol{\mu}$: α, inlet boundary condition
- *Spatial discretization*: finite volume
- *Time integrator:* backward Euler

2D reacting flow

$$\frac{\partial \mathbf{w}(\vec{x},t;\boldsymbol{\mu})}{\partial t} = \nabla\cdot(\kappa\nabla\mathbf{w}(\vec{x},t;\boldsymbol{\mu})) - \mathbf{v}\cdot\nabla\mathbf{w}(\vec{x},t;\boldsymbol{\mu}) + \mathbf{q}(\mathbf{w}(\vec{x},t;\boldsymbol{\mu});\boldsymbol{\mu})$$

- $\boldsymbol{\mu}$: two terms in reaction
- *Spatial discretization*: finite difference
- *Time integrator*: BDF2

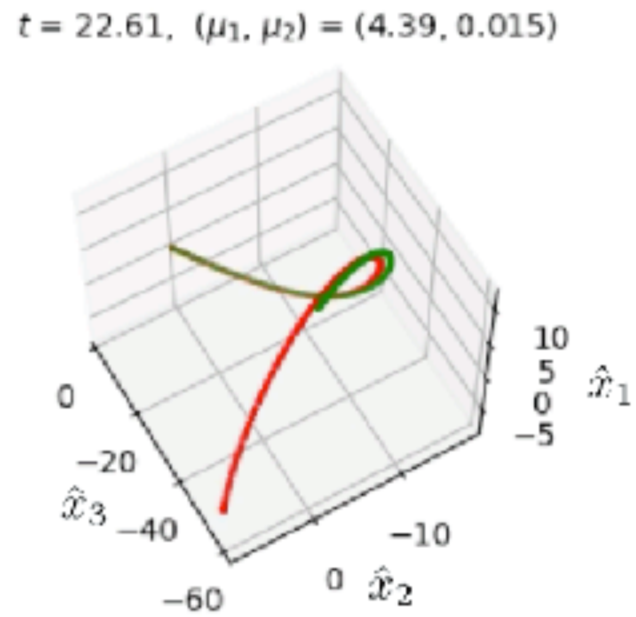
Autoencoder architecture



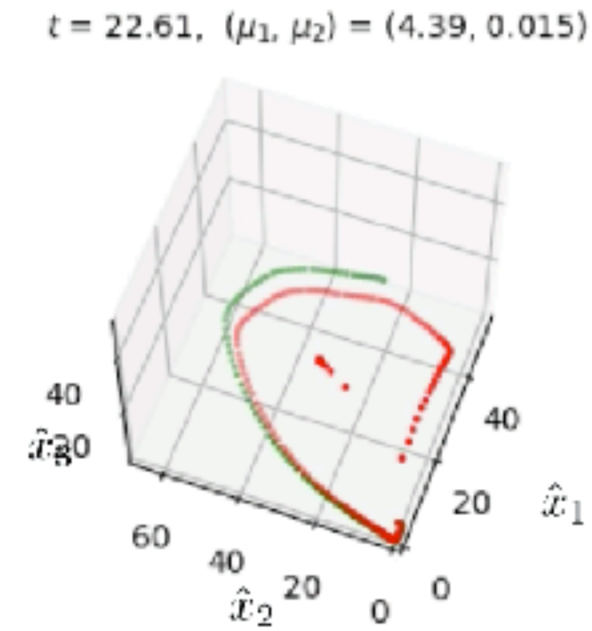
Manifold interpretation: Burgers' equation

FOM

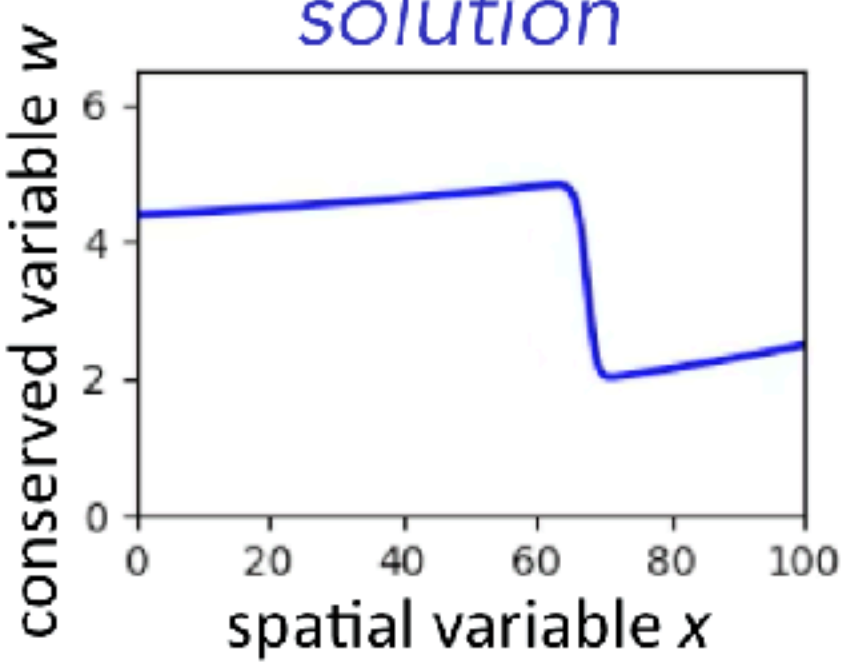
POD, p=3
projection



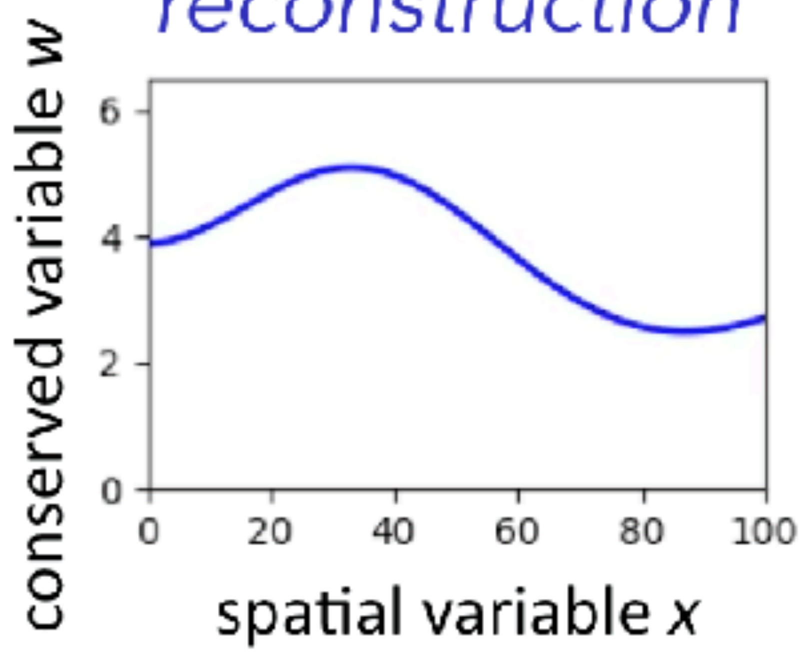
Autoencoder, p=3
projection



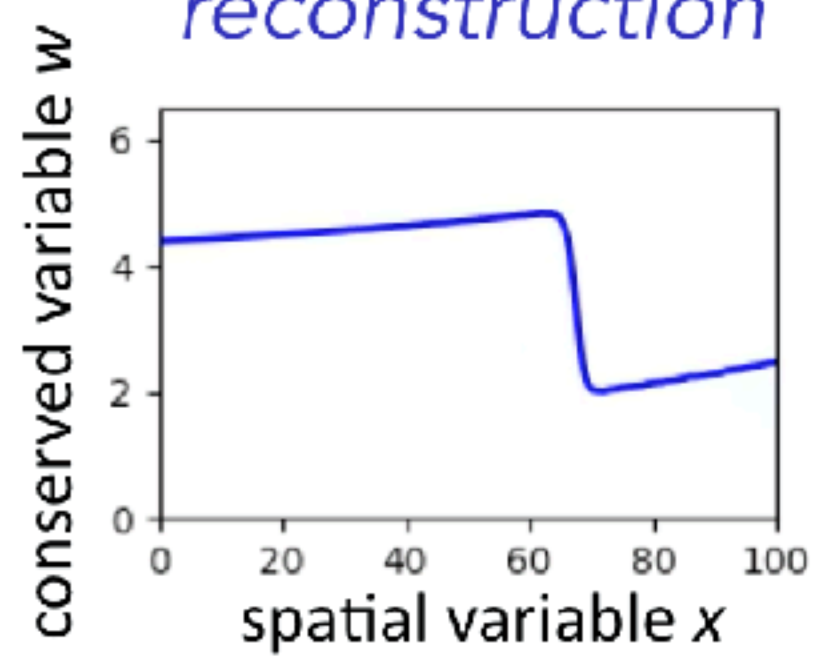
solution



reconstruction



reconstruction



+ Projection error onto 3-dimensional manifold nearly perfect

Manifold LSPG outperforms optimal linear subspace

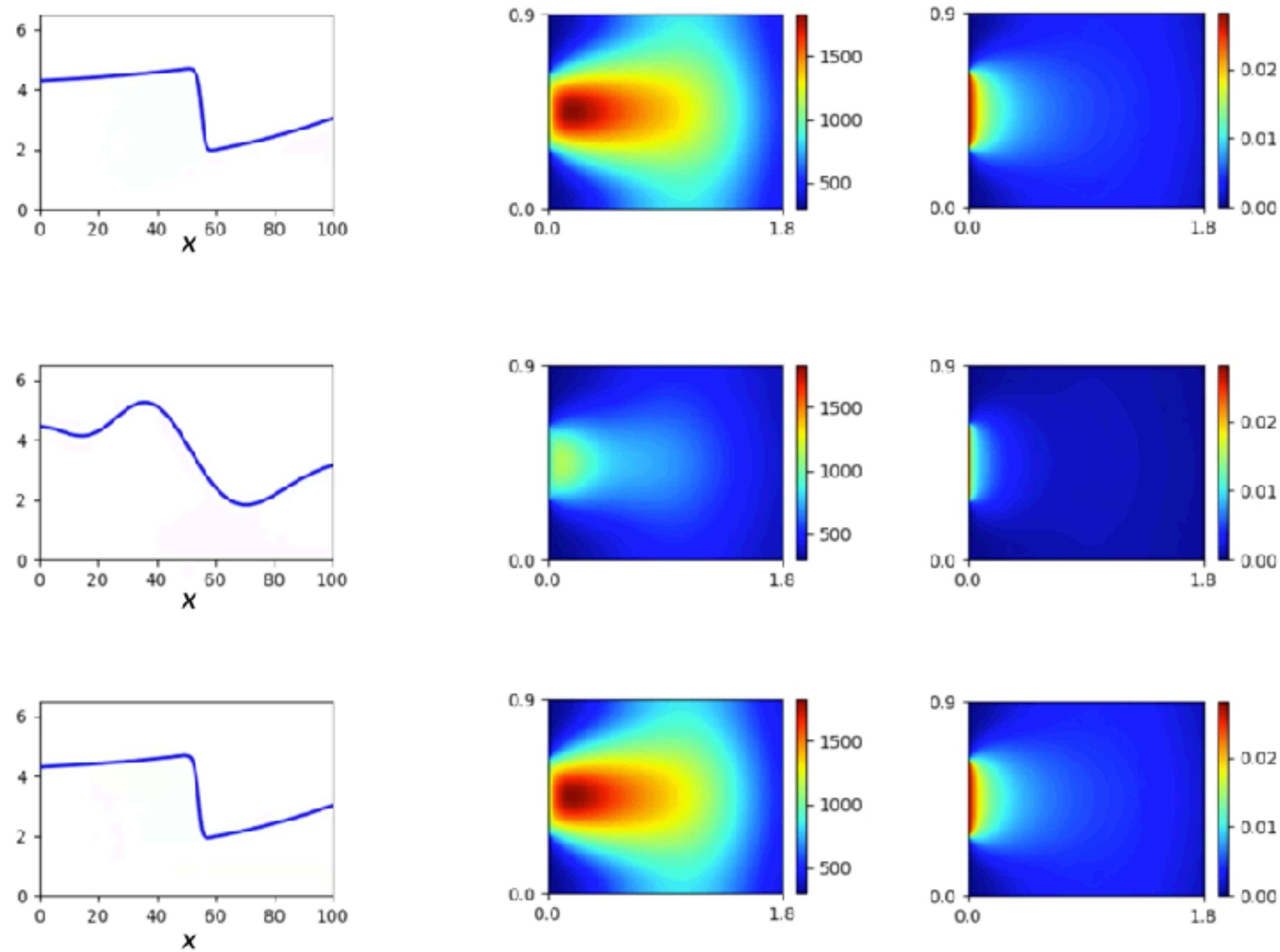
1D Burgers' equation — conserved variable

2D reacting flow — temperature, H_2 fraction

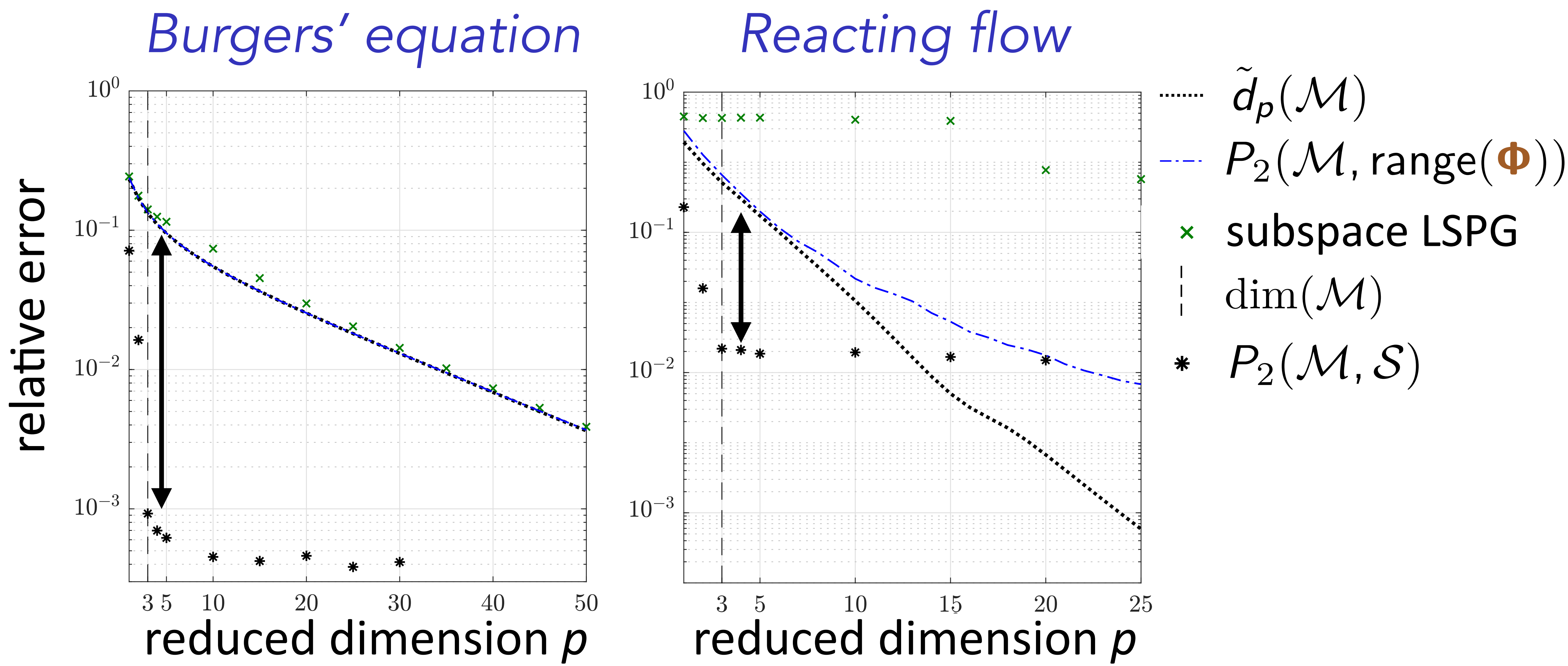
high-fidelity model

POD-LSPG p=5

Manifold LSPG p=5

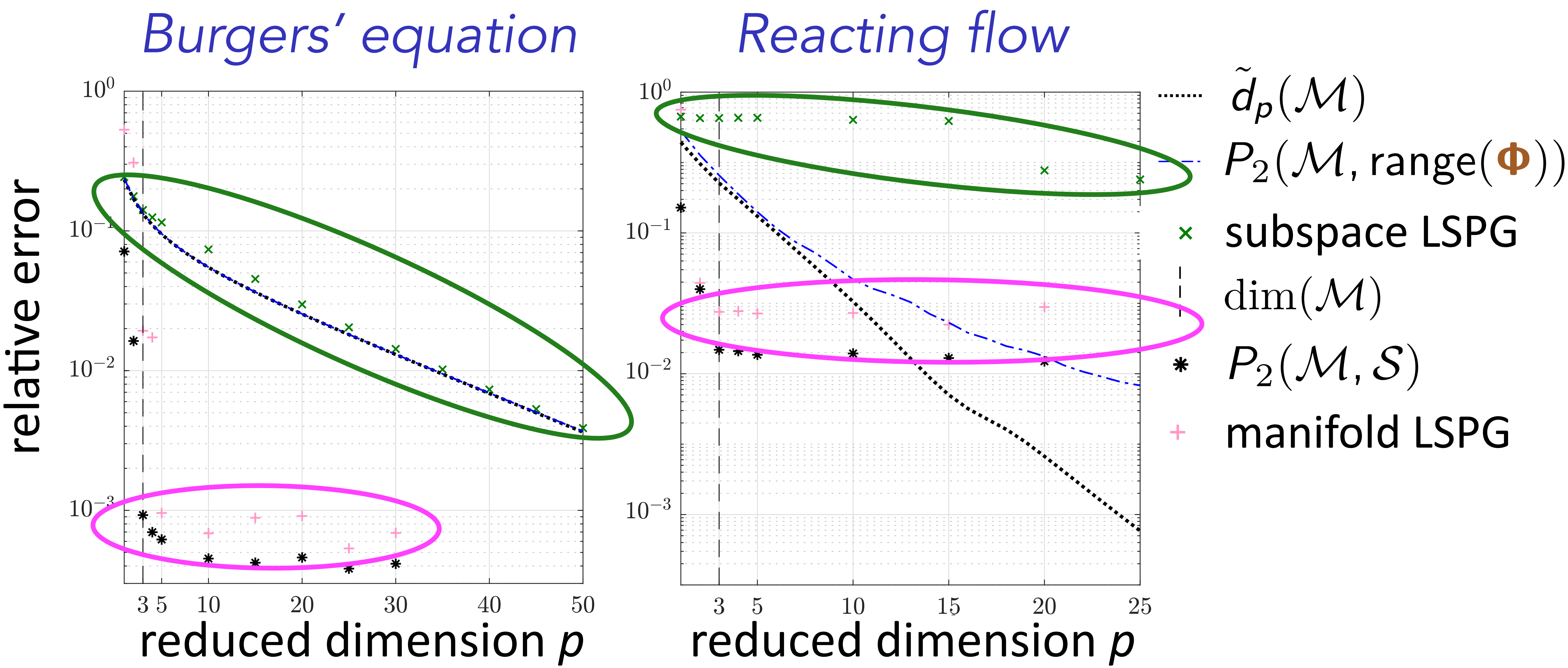


Method improves generalization performance



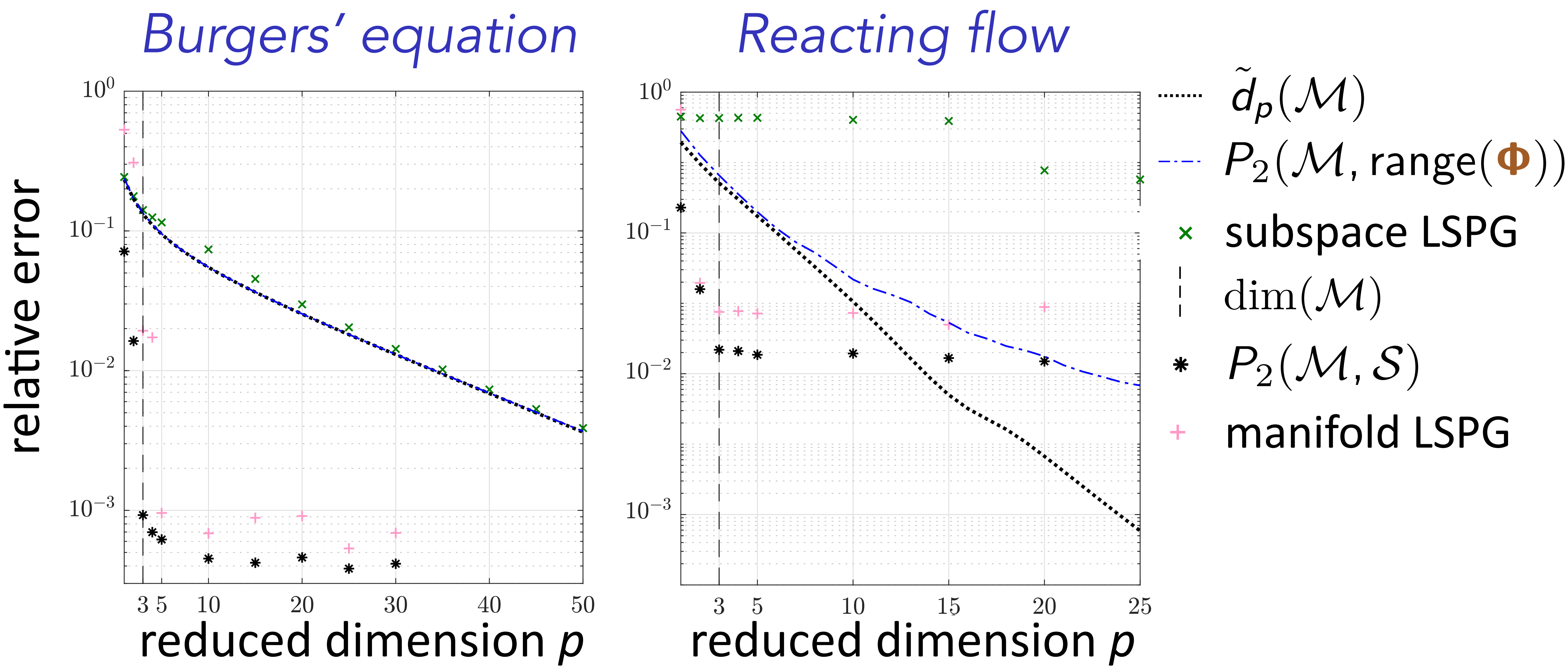
+ Autoencoder manifold significantly better than optimal linear subspace

Method improves generalization performance



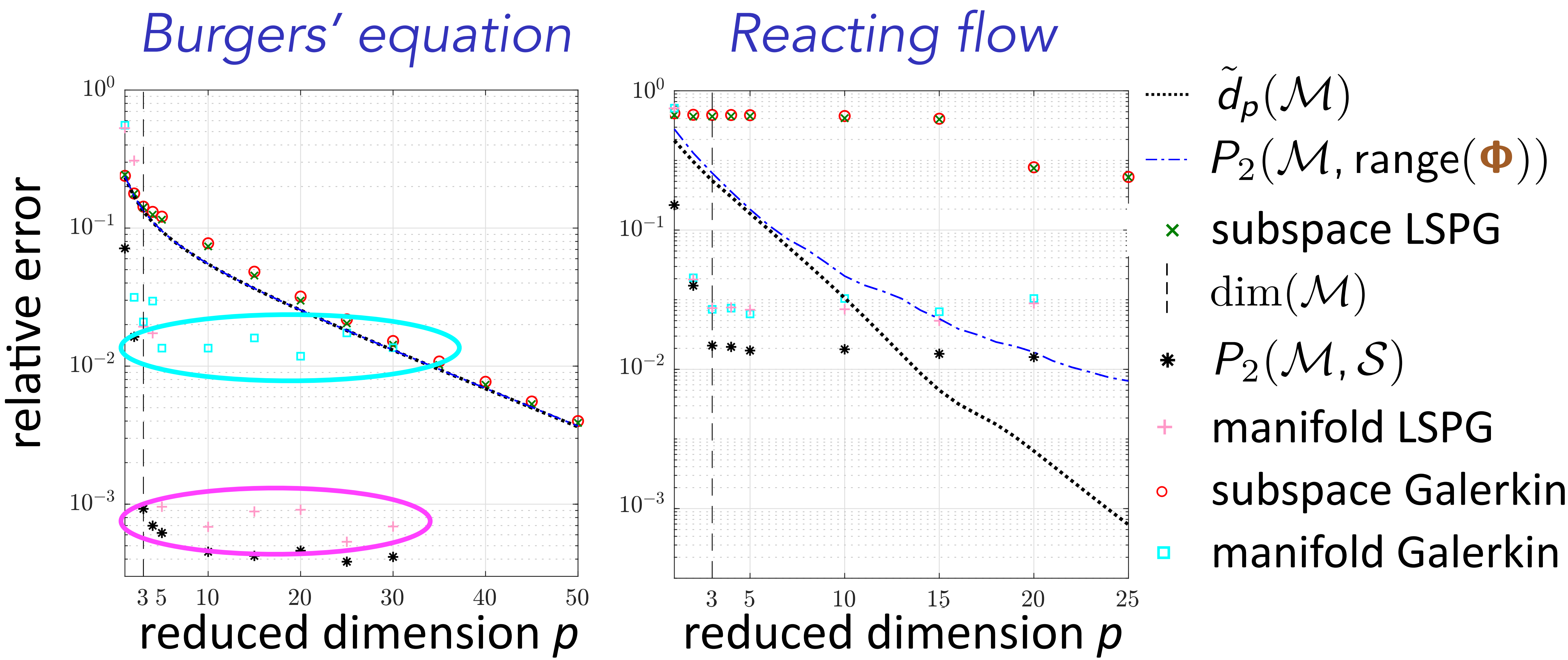
+ Autoencoder manifold significantly better than optimal linear subspace
+ Manifold LSPG orders-of-magnitude more accurate than subspace LSPG

Method improves generalization performance



- Autoencoder manifold significantly better than optimal linear subspace
- Manifold LSPG orders-of-magnitude more accurate than subspace LSPG
- Method breaks Kolmogorov-width barrier

Method improves generalization performance



+ Autoencoder manifold significantly better than optimal linear subspace
+ Manifold LSPG orders-of-magnitude more accurate than subspace LSPG
+ Method breaks Kolmogorov-width barrier
+ Manifold LSPG outperforms manifold Galerkin on 1D Burgers' equation

Outstanding challenges in model reduction

1) Linear-subspace assumption is strong

$$\mathbf{x}(t) \approx \tilde{\mathbf{x}}(t) = \boldsymbol{\Phi}\,\hat{\mathbf{x}}(t)$$

- Lee and C. "Model reduction of dynamical systems on nonlinear manifolds using deep convolutional autoencoders." J Comp Phys, 404:108973, 2020.

2) Important physical properties not satisfied

Galerkin

$$\boldsymbol{\Phi}\frac{d\hat{\mathbf{x}}}{dt}(\mathbf{x}, t) = \underset{\mathbf{v}\in\mathrm{range}(\boldsymbol{\Phi})}{\mathrm{argmin}}\ \|\mathbf{r}(\mathbf{v}, \mathbf{x}; t)\|_2$$

LSPG

$$\boldsymbol{\Phi}\hat{\mathbf{x}}^n = \underset{\mathbf{v}\in\mathrm{range}(\boldsymbol{\Phi})}{\arg\min}\ \|\mathbf{r}^n(\mathbf{v})\|_2$$

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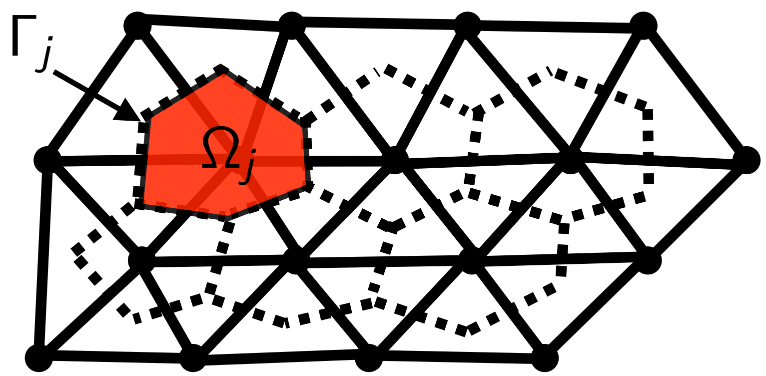
- Lee and C. "Deep conservation: A latent dynamics model for exact satisfaction of physical conservation laws ." arXiv e-print 1909.09754, 2019.

3) Error analysis difficult

- Freno and C. "Machine-learning error models for approximate solutions to parameterized systems of nonlinear equations." CMAME, 348:250–296, 2019.
- Parish and C. "Time-series machine-learning error models for approximate solutions to parameterized dynamical systems." arXiv e-print, (1907.11822).

Finite-volume method

$$\boxed{\text{ODE:}\quad \frac{d\mathbf{x}}{dt} = \mathbf{f}(\mathbf{x};t)}$$



$$x_{\mathcal{I}(i,j)}(t) = \frac{1}{|\Omega_j|}\int_{\Omega_j} u_i(\vec{x},t)\,\mathrm{d}\vec{x}$$

- average value of conserved variable i over control volume j

$$f_{\mathcal{I}(i,j)}(\mathbf{x},t) = -\frac{1}{|\Omega_j|}\int_{\Gamma_j} \underbrace{\mathbf{g}_i(\mathbf{x};\vec{x},t)}_{\text{flux}}\cdot\mathbf{n}_j(\vec{x})\,\mathrm{d}\vec{s}(\vec{x}) + \frac{1}{|\Omega_j|}\int_{\Omega_j}\underbrace{s_i(\mathbf{x};\vec{x},t)}_{\text{source}}\,\mathrm{d}\vec{x}$$

- flux and source of conserved variable i within control volume j

$$r_{\mathcal{I}(i,j)} = \frac{dx_{\mathcal{I}(i,j)}}{dt}(t) - f_{\mathcal{I}(i,j)}(\mathbf{x},t)$$

- **rate of conservation violation** of variable i in control volume j

$$\boxed{\text{O}\Delta\text{E:}\quad \mathbf{r}^n(\mathbf{x}^n) = 0,\ \ n = 1,\ldots,N}$$

$$r^n_{\mathcal{I}(i,j)} = x_{\mathcal{I}(i,j)}(t^{n+1}) - x_{\mathcal{I}(i,j)}(t^n) + \int_{t^n}^{t^{n+1}} f_{\mathcal{I}(i,j)}(\mathbf{x},t)dt$$

- **conservation violation** of variable i in control volume j over time step n

Conservation is the intrinsic structure enforced by finite-volume methods

Conservative manifold model reduction

Manifold Galerkin

$$\underset{\hat{\mathbf{v}}\in\mathbb{R}^p}{\text{minimize}}\ \|\mathbf{r}(\nabla\mathbf{g}(\hat{\mathbf{x}})\hat{\mathbf{v}};\mathbf{g}(\hat{\mathbf{x}});t)\|_2$$

- Minimize conservation-violation rates

Manifold LSPG

$$\hat{\mathbf{x}}^n = \underset{\hat{\mathbf{v}}\in\mathbb{R}^p}{\text{argmin}}\|\mathbf{r}^n(\mathbf{g}(\hat{\mathbf{v}}))\|_2$$

- Minimize conservation violations over time step *n*

- Neither enforces conservation!

Conservative manifold Galerkin

$$\underset{\hat{\mathbf{v}}\in\mathbb{R}^p}{\text{minimize}}\ \|\mathbf{r}(\nabla\mathbf{g}(\hat{\mathbf{x}})\hat{\mathbf{v}};\mathbf{g}(\hat{\mathbf{x}});t)\|_2$$

$$\text{subject to }\mathbf{C}\mathbf{r}(\nabla\mathbf{g}(\hat{\mathbf{x}})\hat{\mathbf{v}};\mathbf{g}(\hat{\mathbf{x}});t) = \mathbf{0}$$

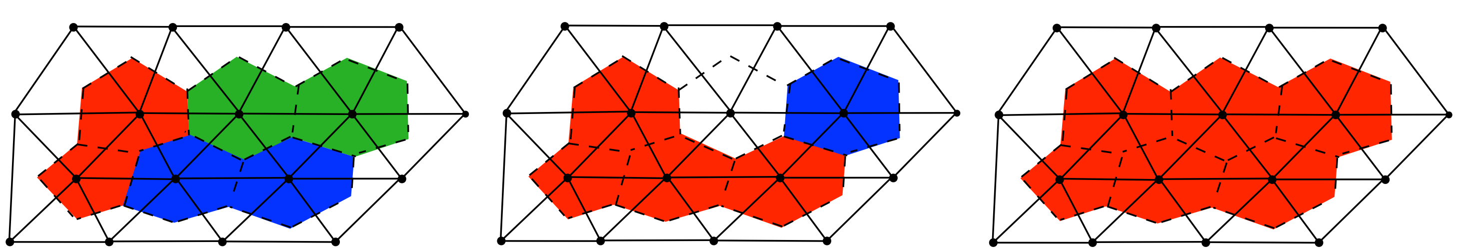
- Minimize conservation-violation rates subject to zero conservation-violation rates **over subdomains**

Conservative manifold LSPG

$$\underset{\hat{\mathbf{v}}\in\mathbb{R}^p}{\text{minimize}}\ \|\mathbf{r}^n(\mathbf{g}(\hat{\mathbf{v}}))\|_2$$

$$\text{subject to }\mathbf{C}\mathbf{r}^n(\mathbf{g}(\hat{\mathbf{v}})) = \mathbf{0}$$

- Minimize conservation violations over time step *n* subject to zero conservation violations over time step ***n* over subdomains**



+ Conservation enforced over prescribed subdomains

Discrete-time error bound (linear subspaces)

Lemma: local conserved-quantity error bounds [C., Choi, Sargsyan, 2018]

The error in the conserved quantities computed with either conservative Galerkin or conservative LSPG can be bounded as:

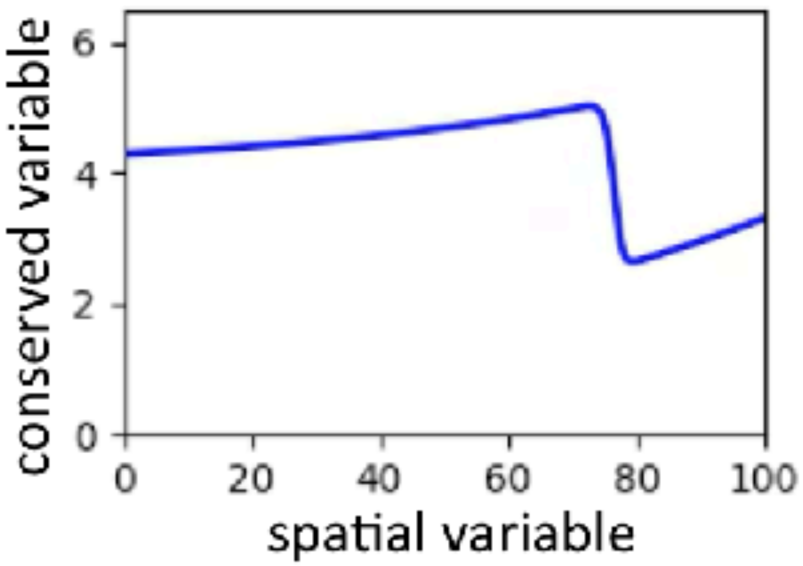
$$\|\bar{\mathbf{C}}(\mathbf{x}^n - \mathbf{\Phi}\hat{\mathbf{x}}^n)\|_2 \leq \sum_{\ell=0}^{k} \frac{|\beta_\ell^n|\Delta t}{|\alpha_0^n|} \|\bar{\mathbf{C}}\mathbf{f}(\mathbf{x}^{n-\ell}) - \bar{\mathbf{C}}\mathbf{f}(\mathbf{\Phi}\hat{\mathbf{x}}^{n-\ell})\|_2$$

$$+ \sum_{\ell=1}^{k} \frac{|\alpha_\ell^n|}{|\alpha_0^n|} \|\bar{\mathbf{C}}(\mathbf{x}^{n-\ell} - \mathbf{\Phi}\hat{\mathbf{x}}^{n-\ell})\|_2$$

- Error depends only on velocity error on *decomposed mesh*

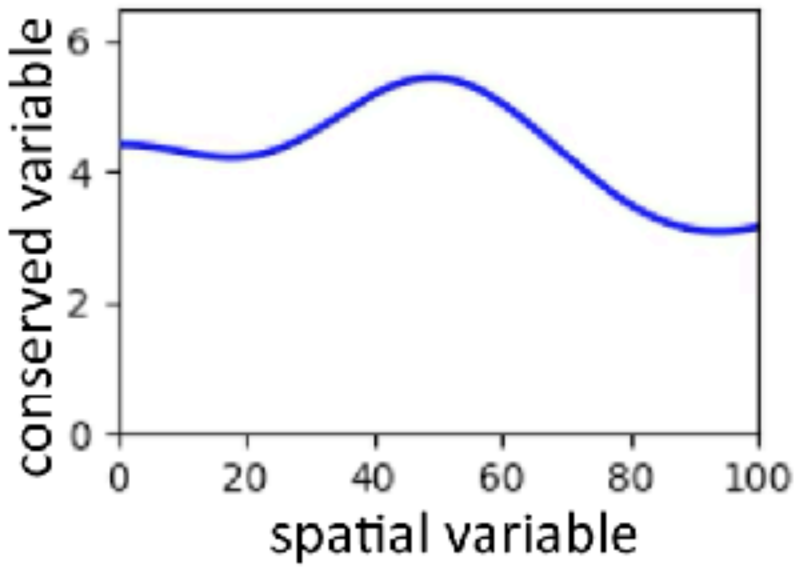
\+ No source, global conservation: error due to flux error along boundary!

High-fidelity model



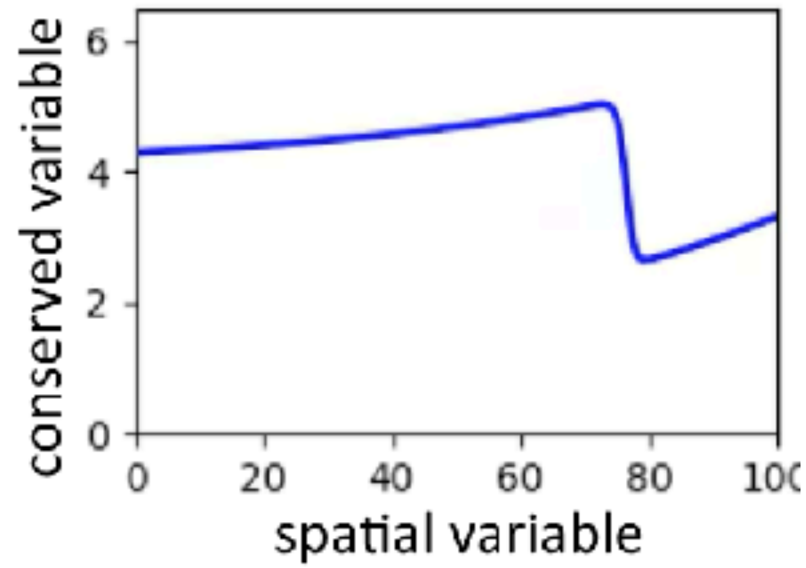
Reduced-order models

POD subspace



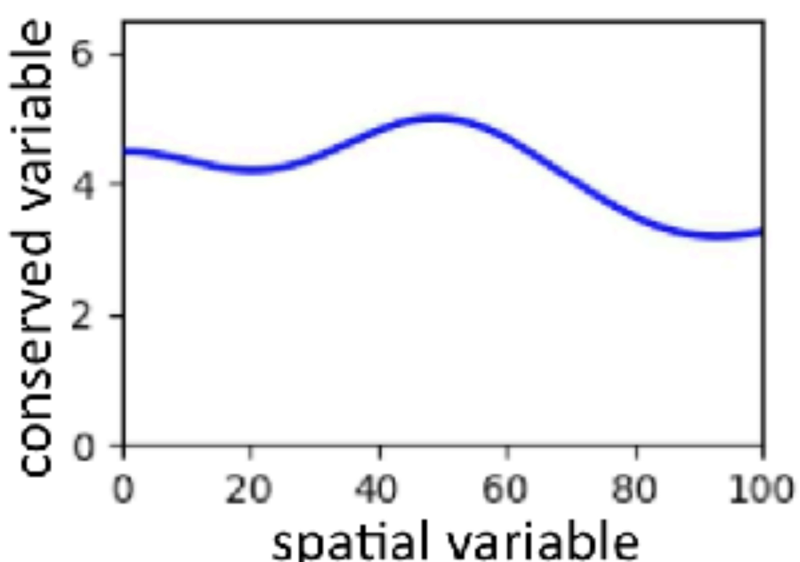
Solution error: 13%
Conservation violation: 16%

Autoencoder manifold



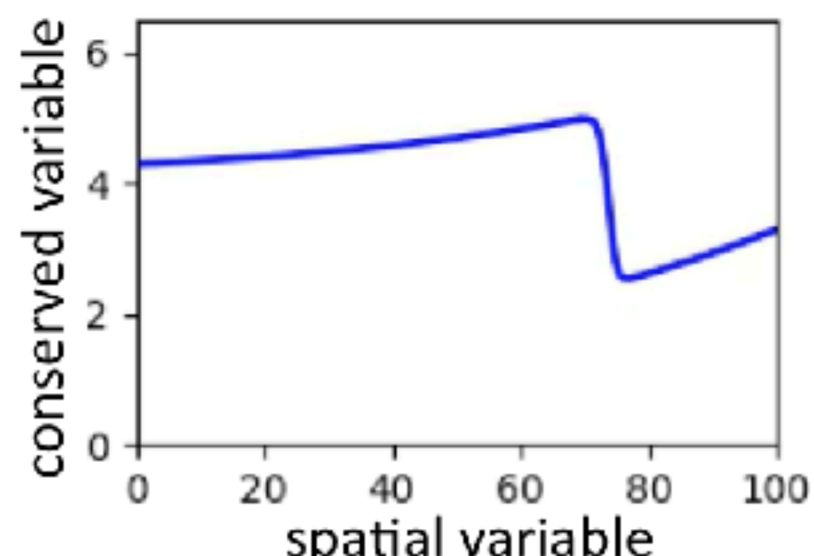
Solution error: 0.5%
Conservation violation: 1%

POD subspace with conservation constraints



Solution error: 12%
Conservation violation: <0.001%

Autoencoder manifold with conservation constraints



Solution error: 0.2%
Conservation violation: <0.001%

Outlook

Conservative manifold Galerkin

$$\underset{\hat{\mathbf{v}}\in\mathbb{R}^p}{\text{minimize}} \|\mathbf{r}(\nabla\mathbf{g}(\hat{\mathbf{x}})\hat{\mathbf{v}};\mathbf{g}(\hat{\mathbf{x}});t)\|_2$$

$$\text{subject to } \mathbf{C}\mathbf{r}(\nabla\mathbf{g}(\hat{\mathbf{x}})\hat{\mathbf{v}};\mathbf{g}(\hat{\mathbf{x}});t) = \mathbf{0}$$

Conservative manifold LSPG

$$\underset{\hat{\mathbf{v}}\in\mathbb{R}^p}{\text{minimize}} \|\mathbf{r}^n(\mathbf{g}(\hat{\mathbf{v}}))\|_2$$

$$\text{subject to } \mathbf{C}\mathbf{r}^n(\mathbf{g}(\hat{\mathbf{v}})) = \mathbf{0}$$

Interpretation

- Integrates computational physics with deep learning
- *Projection-based latent dynamics model* that enforces conservation
- Nearly all existing methods are *data-driven latent dynamics models*

[Böhmer et al., 2015; Goroshin et al., 2015; Watter et al., 2015; Karl et al., 2017; Takeishi et al., 2017; Banijamali et al., 2018; Lesort et al., 2018; Lusch et al., 2018; Morton et al., 2018 Otto and Rowley, 2019]

Gradient computation

- Backpropagation used to compute decoder Jacobian $\nabla\mathbf{g}(\hat{\mathbf{x}})$
- Quasi-Newton solvers directly call TensorFlow

Ongoing work

- *Hyper-reduction*: “easy” because convolutional layers preserve sparsity
- Integration in large-scale code underway in Pressio

Shortcomings of state-of-the-art ROMs

1) Linear-subspace assumption is strong

$$\mathbf{x}(t) \approx \tilde{\mathbf{x}}(t) = \boldsymbol{\Phi}\, \hat{\mathbf{x}}(t)$$

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2) Important physical properties not guaranteed

Galerkin

$$\boldsymbol{\Phi} \frac{d\hat{\mathbf{x}}}{dt}(\mathbf{x}, t) = \underset{\mathbf{v}\in \text{range}(\boldsymbol{\Phi})}{\text{argmin}} \|\mathbf{r}(\mathbf{v}, \mathbf{x}; t)\|_2$$

LSPG

$$\boldsymbol{\Phi}\hat{\mathbf{x}}^n = \underset{\mathbf{v}\in \text{range}(\boldsymbol{\Phi})}{\arg\min} \|\mathbf{r}^n(\mathbf{v})\|_2$$

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Discrete-time error bound

Theorem: error bound for BDF integrators [C., Barone, Antil, 2017]

If the following conditions hold:

1. $\mathbf{f}(\cdot;t)$ is Lipschitz continuous with Lipschitz constant κ
2. The time step Δt is small enough such that $0 < h := |\alpha_0| - |\beta_0|\kappa\Delta t$,

$$\|\mathbf{x}^n - \mathbf{g}(\hat{\mathbf{x}}_{\mathrm{G}}^n)\|_2 \leq \frac{1}{h}\|\mathbf{r}_{\mathrm{G}}^n(\mathbf{g}(\hat{\mathbf{x}}_{\mathrm{G}}))\|_2 + \frac{1}{h}\sum_{\ell=1}^{k}|\gamma_\ell|\|\mathbf{x}^{n-\ell} - \mathbf{g}(\hat{\mathbf{x}}_{\mathrm{G}})\|_2$$

$$\|\mathbf{x}^n - \mathbf{g}(\hat{\mathbf{x}}_{\mathrm{LSPG}}^n)\|_2 \leq \frac{1}{h}\min_{\hat{\mathbf{v}}}\|\mathbf{r}_{\mathrm{LSPG}}^n(\mathbf{g}(\hat{\mathbf{v}}))\|_2 + \frac{1}{h}\sum_{\ell=1}^{k}|\gamma_\ell|\|\mathbf{x}^{n-\ell} - \mathbf{g}(\hat{\mathbf{x}}_{\mathrm{LSPG}})\|_2$$

Can we use these error bounds for error estimation?

Discrete-time error bound

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$$\|\mathbf{x}^n - \mathbf{g}(\hat{\mathbf{x}}_G^n)\|_2 \leq \frac{\gamma_1(\gamma_2)^n \exp(\gamma_3 t^n)}{\gamma_4 + \gamma_5 \Delta t} \max_{j \in \{1,\ldots,N\}} \|\mathbf{r}_{\mathrm{LSPG}}^j(\mathbf{g}(\hat{\mathbf{x}}_G^j))\|_2$$

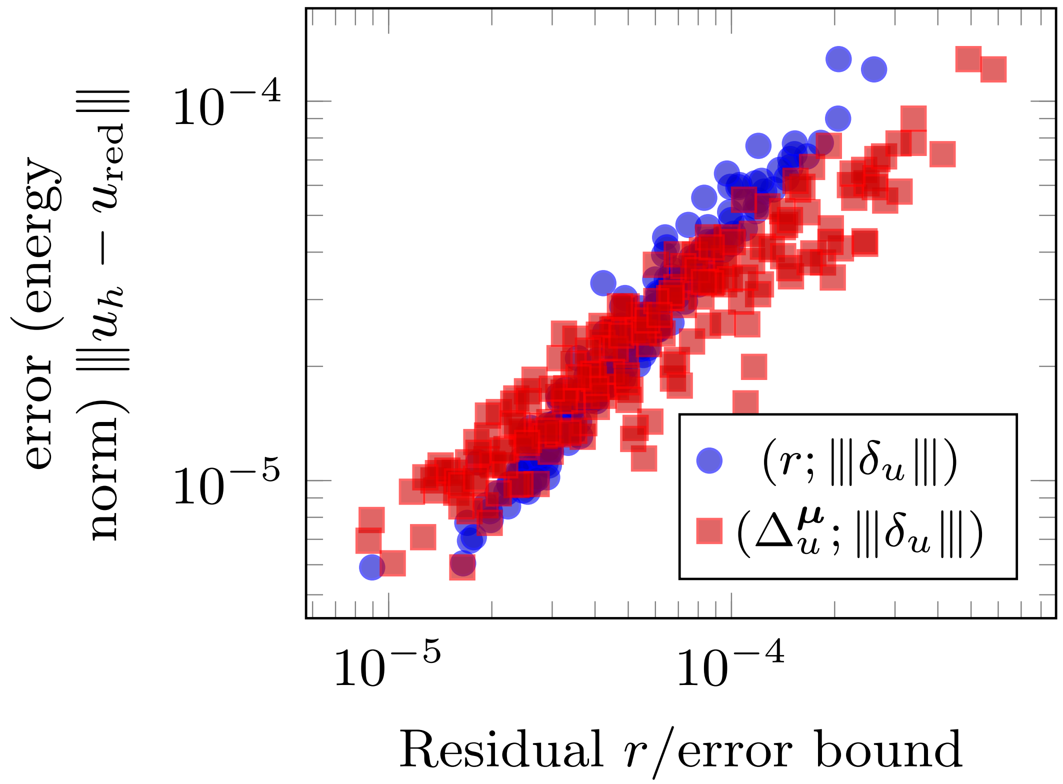
$$\|\mathbf{x}^n - \mathbf{g}(\hat{\mathbf{x}}_{\mathrm{LSPG}}^n)\|_2 \leq \frac{\gamma_1(\gamma_2)^n \exp(\gamma_3 t^n)}{\gamma_4 + \gamma_5 \Delta t} \max_{j \in \{1,\ldots,N\}} \min_{\hat{\mathbf{v}}} \|\mathbf{r}_{\mathrm{LSPG}}^j(\mathbf{g}(\hat{\mathbf{v}}))\|_2$$

Can we use these error bounds for error estimation?

- grow exponentially in time
- deterministic: not amenable to uncertainty quantification

Main idea

- **Observation**: ROMs generate quantities that are informative of the error



- **ML perspective**: these are good features for predicting the error

Idea: *Apply **machine learning regression** to generate a mapping from residual-based quantities to a random variable for the error*

Machine-learning error models [Freno and C., 2019; Parish and C., 2019]

Machine-learning error models: formulation

What attributes does the ROM error have?

$$\|\mathbf{x}^n - \mathbf{g}(\hat{\mathbf{x}}^n_{\mathrm{LSPG}})\|_2 \leq \frac{\gamma_1(\gamma_2)^n \exp(\gamma_3 t^n)}{\gamma_4 + \gamma_5 \Delta t} \max_{j\in\{1,\ldots,T\}} \min_{\hat{\mathbf{v}}} \|\mathbf{r}^j_{\mathrm{LSPG}}(\mathbf{g}(\hat{\mathbf{v}}))\|_2$$

1. Dependence on non-local quantities in time
2. Dependence on the residual

Regression model

$$\boxed{\hat{\delta}^n(\boldsymbol{\mu}) = \underbrace{\hat{\delta}^n_f(\boldsymbol{\mu})}_{\text{deterministic}} + \underbrace{\hat{\delta}^n_\epsilon(\boldsymbol{\mu})}_{\text{stochastic}}}$$

- regression function: $\hat{\delta}^n_f(\boldsymbol{\mu}) = \hat{f}(\boldsymbol{\rho}^n(\boldsymbol{\mu}), \boldsymbol{h}^{n-1}(\boldsymbol{\mu}), \hat{\delta}^{n-1}_f(\boldsymbol{\mu}))$

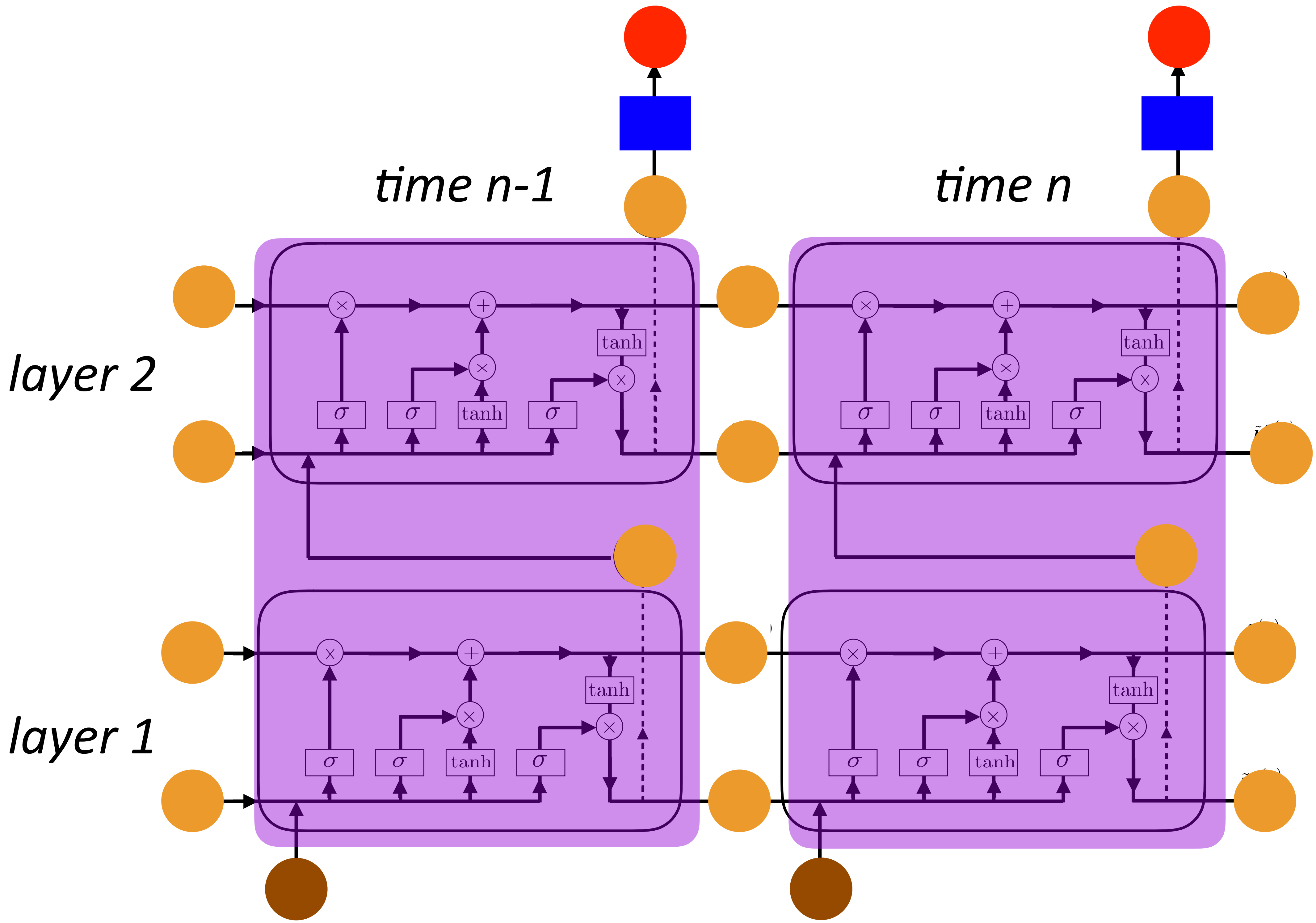
$$\boldsymbol{h}^n(\boldsymbol{\mu}) = \mathrm{g}(\boldsymbol{\rho}^n(\boldsymbol{\mu}), \boldsymbol{h}^{n-1}(\boldsymbol{\mu}), \hat{\delta}^{n-1}_f(\boldsymbol{\mu}))$$

  + latent variables $\boldsymbol{h}^n(\boldsymbol{\mu})$: enable capturing non-local dependencies
  + features $\boldsymbol{\rho}^n(\boldsymbol{\mu})$: residual-based (and cheaply computable)
  + general formulation encompasses ARX, LARX, RNN, LSTM, GRU

Example: long short-term memory (LSTM)

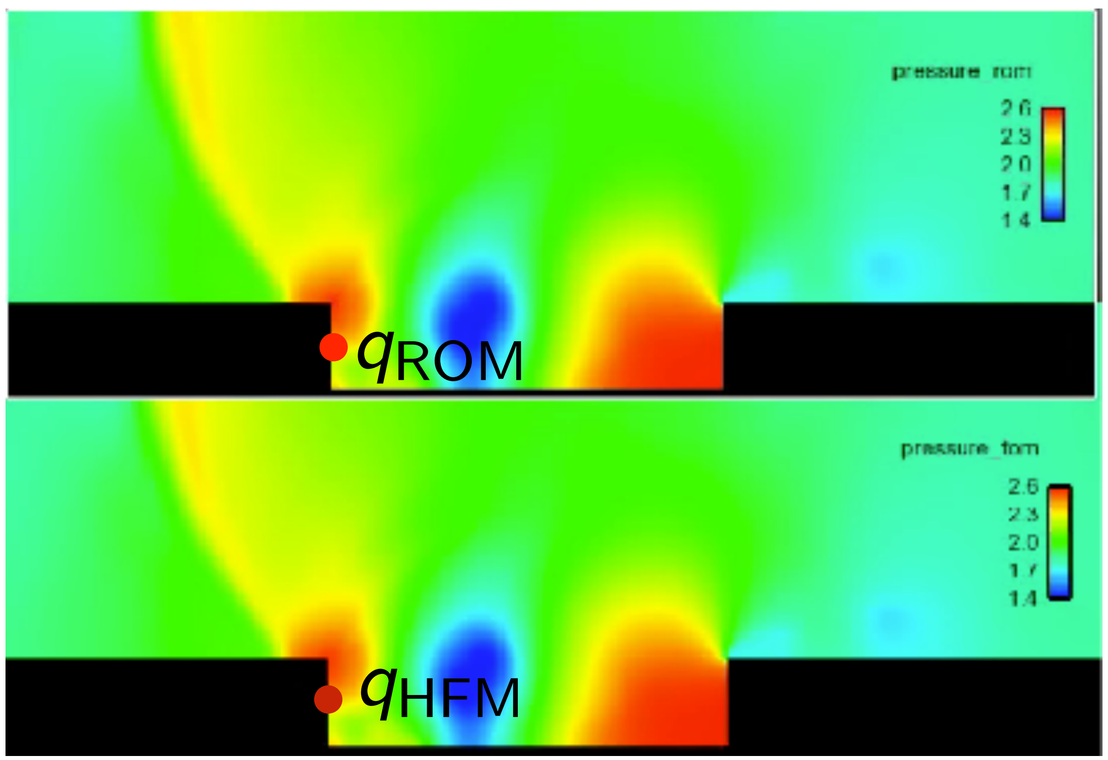
$$\hat{\delta}_f^n(\boldsymbol{\mu}) = \hat{f}(\rho^n(\boldsymbol{\mu}), \boldsymbol{h}^{n-1}(\boldsymbol{\mu}))$$

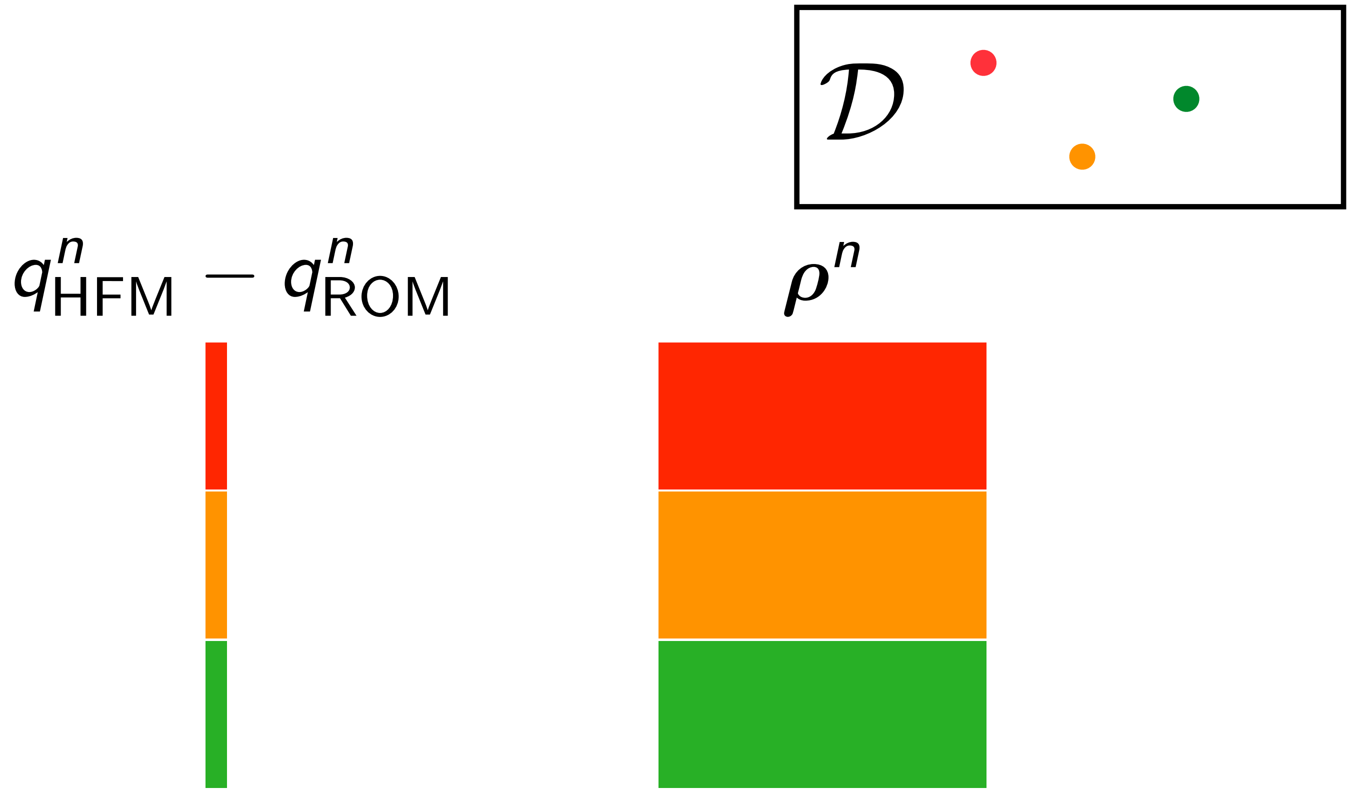
$$\boldsymbol{h}^n(\boldsymbol{\mu}) = \mathbf{g}(\rho^n(\boldsymbol{\mu}), \boldsymbol{h}^{n-1}(\boldsymbol{\mu}))$$



Training and machine learning: error modeling

1. *Training:* Solve high-fidelity and reduced-order models for $\boldsymbol{\mu} \in \mathcal{D}_{\text{training}}$
2. *Machine learning:* Construct regression model
3. *Reduction:* predict reduced-order-model error for $\boldsymbol{\mu} \in \mathcal{D}_{\text{query}} \setminus \mathcal{D}_{\text{training}}$



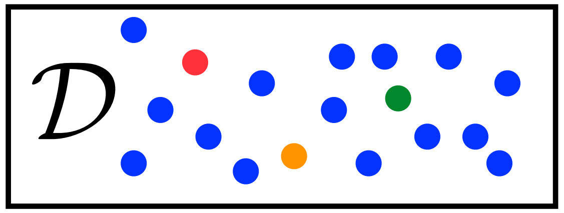


- randomly divide data into (1) training data and (2) testing data
- construct regression function $\hat{\delta}^n_f$ via cross validation on **training data**
- construct noise model $\hat{\delta}^n_\epsilon$ from sample variance on **test data**

Reduction

1. *Training:* Solve high-fidelity and reduced-order models for $\boldsymbol{\mu} \in \mathcal{D}_{\text{training}}$
2. *Machine learning:* Construct regression model
3. *Reduction:* predict reduced-order-model error for $\boldsymbol{\mu} \in \mathcal{D}_{\text{query}} \setminus \mathcal{D}_{\text{training}}$

inputs $\boldsymbol{\mu}$ → *reduced-order model* → *outputs* q^n_{ROM}, $n = 1, \ldots, T$



↓

features $\boldsymbol{\rho}^n$, $n = 1, \ldots, T$

↓

regression model

$$\hat{\delta}^n(\boldsymbol{\mu}) = \hat{\delta}^n_f(\boldsymbol{\mu}) + \hat{\delta}^n_\epsilon(\boldsymbol{\mu})$$

→ *machine learning error model* $\hat{\delta}^n$ $n = 1, \ldots, T$

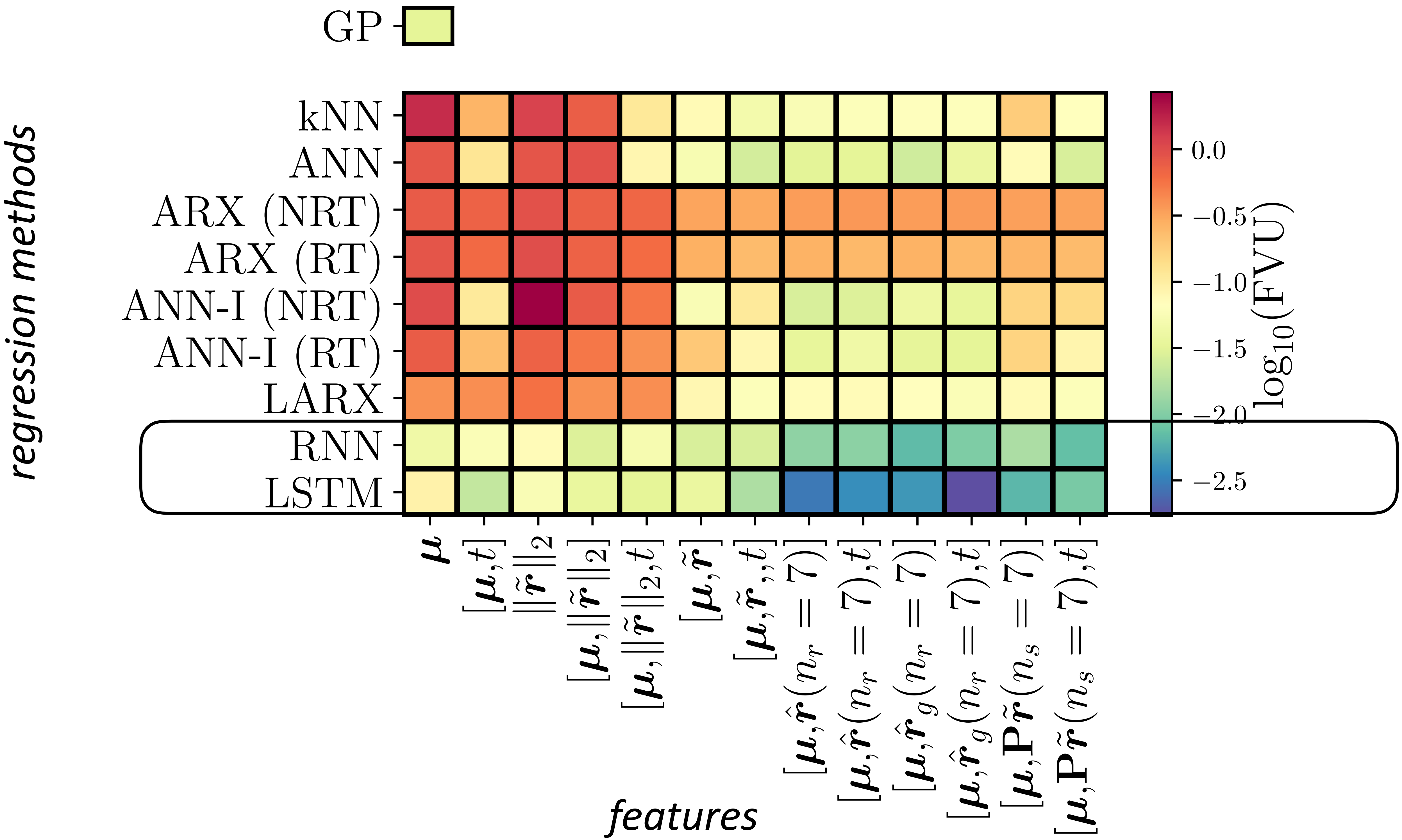
$$\boldsymbol{h}^n(\boldsymbol{\mu}) = \mathbf{g}(\boldsymbol{\rho}^n(\boldsymbol{\mu}), \boldsymbol{h}^{n-1}(\boldsymbol{\mu}), \hat{\delta}^{n-1}_f(\boldsymbol{\mu}))$$

- *Latent dynamics learning*

$$\hat{\delta}^n_f(\boldsymbol{\mu}) = \hat{f}(\boldsymbol{\rho}^n(\boldsymbol{\mu}), \boldsymbol{h}^{n-1}(\boldsymbol{\mu}), \hat{\delta}^{n-1}_f(\boldsymbol{\mu}))$$

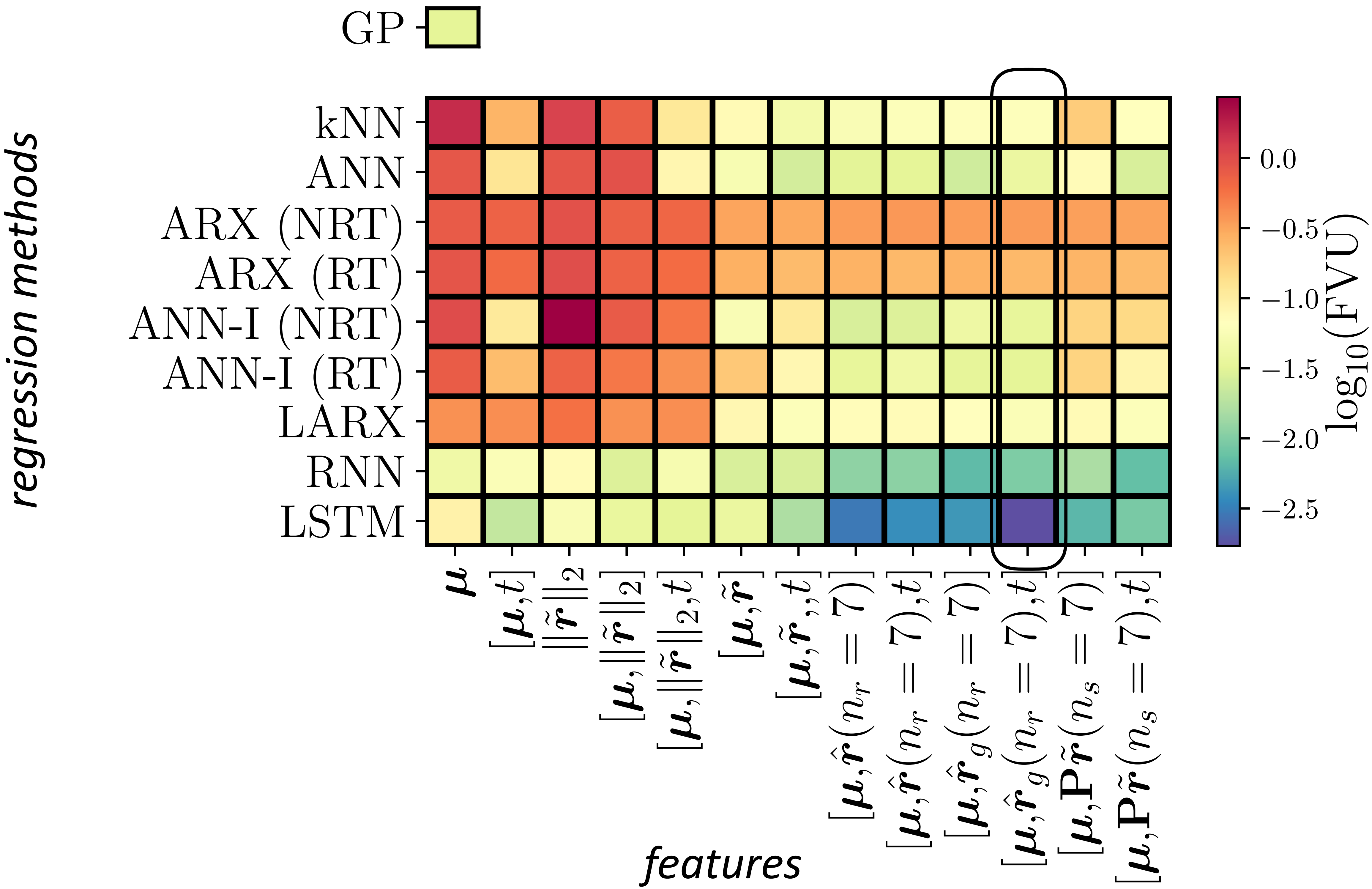
$$\underbrace{\tilde{q}^n_{HFM}(\boldsymbol{\mu})}_{\text{stochastic}} = \underbrace{q^n_{\text{ROM}}(\boldsymbol{\mu})}_{\text{deterministic}} + \underbrace{\hat{\delta}^n(\boldsymbol{\mu})}_{\text{stochastic}}$$

Application: Advection–diffusion equation



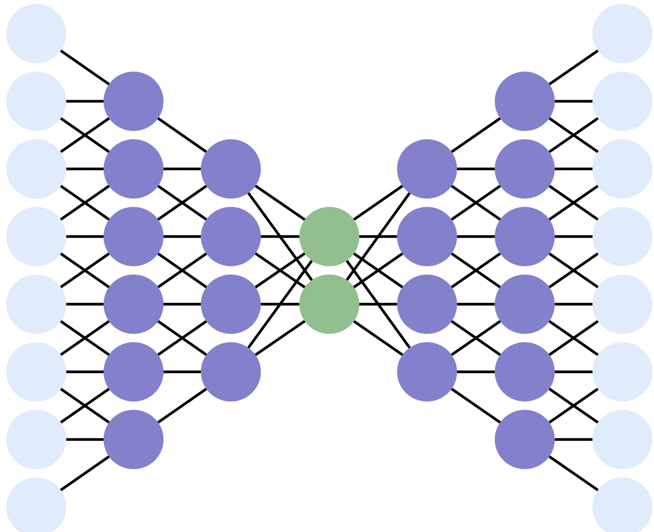
+ *regression methods:* classical RNN and LSTM most accurate

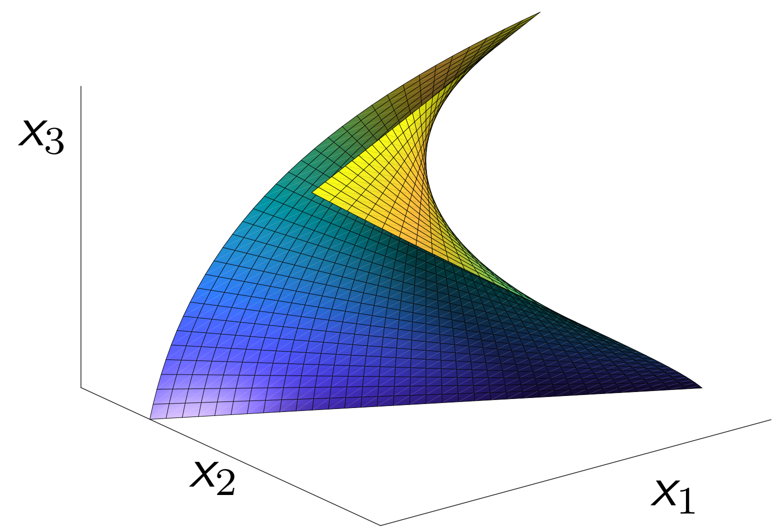
Application: Advection–diffusion equation

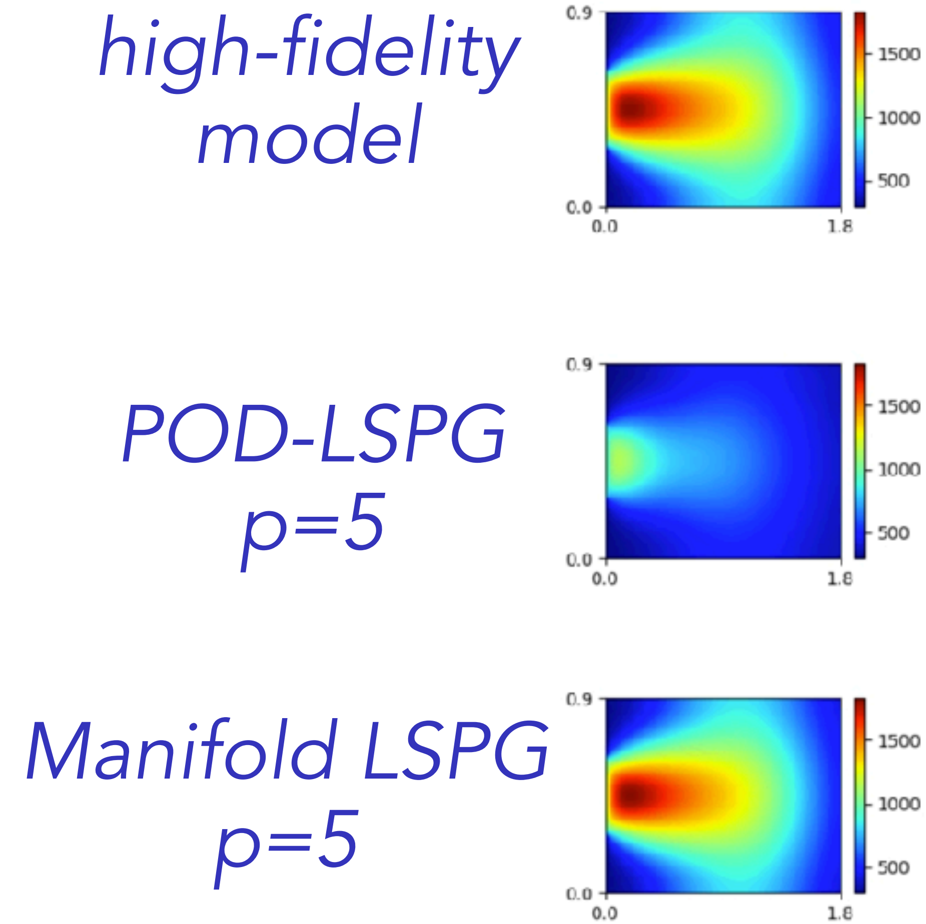


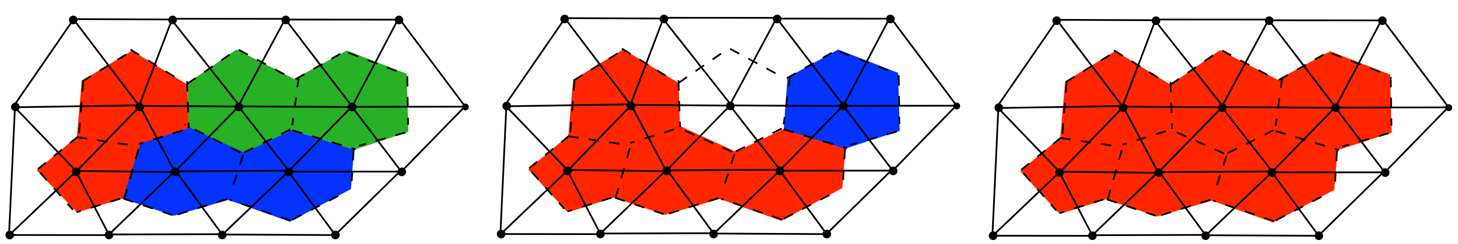
- *regression methods:* classical RNN and LSTM most accurate
- *features:* only 7 residual samples needed for good accuracy

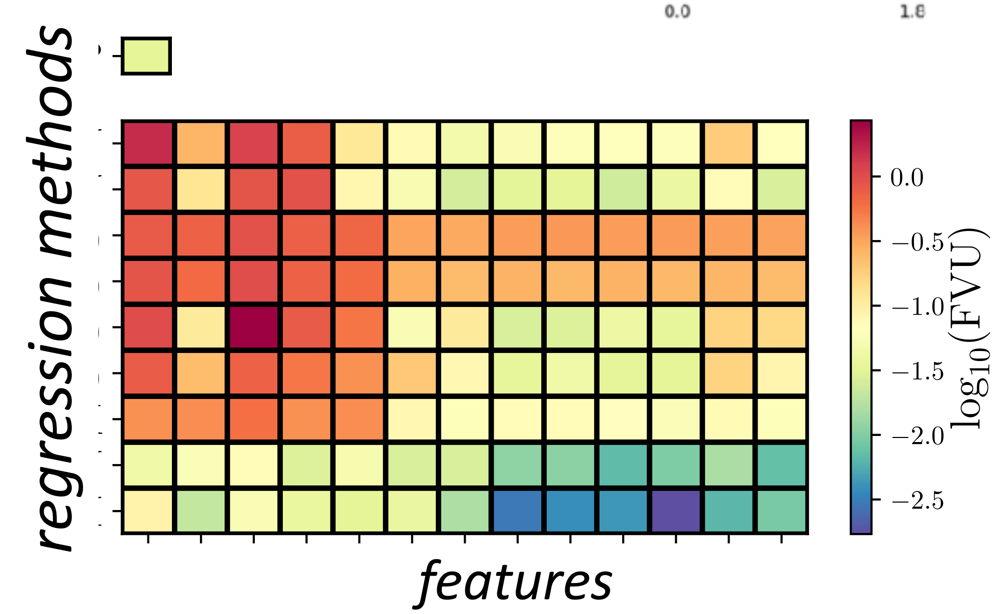
Questions?











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