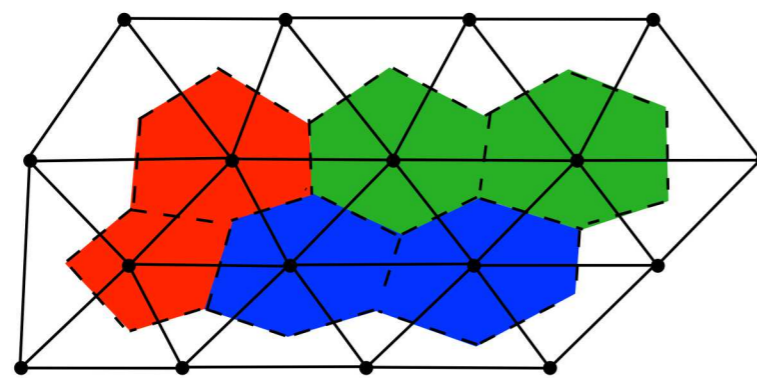
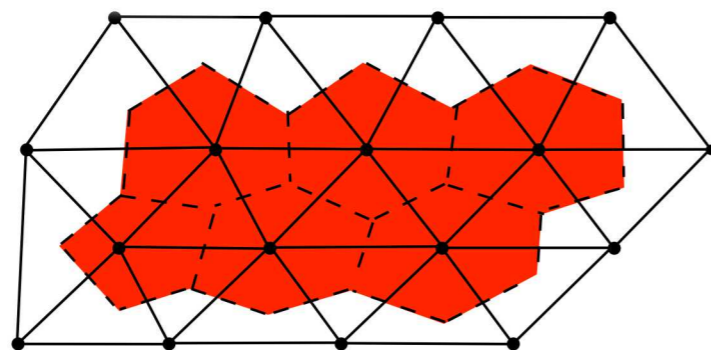


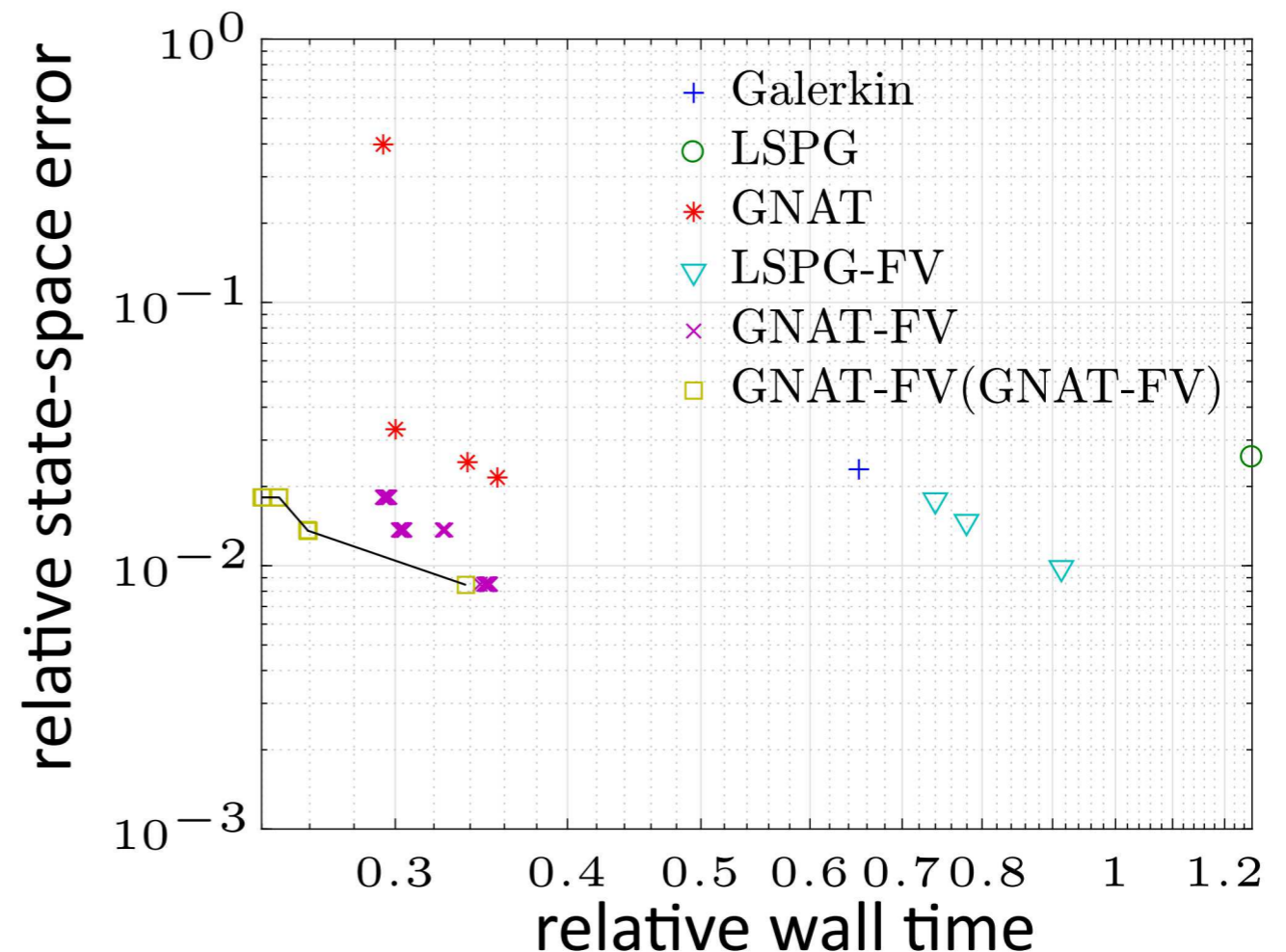
Conservative model reduction for finite-volume models in CFD



3 subdomains



1 (global) subdomain



Kevin Carlberg, Youngsoo Choi, Syuzanna Sargsyan

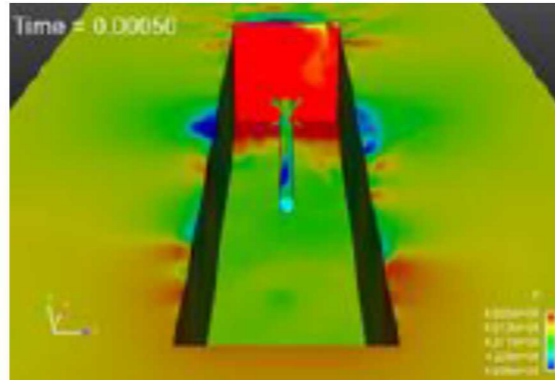
Sandia National Laboratories

WCCM 2018

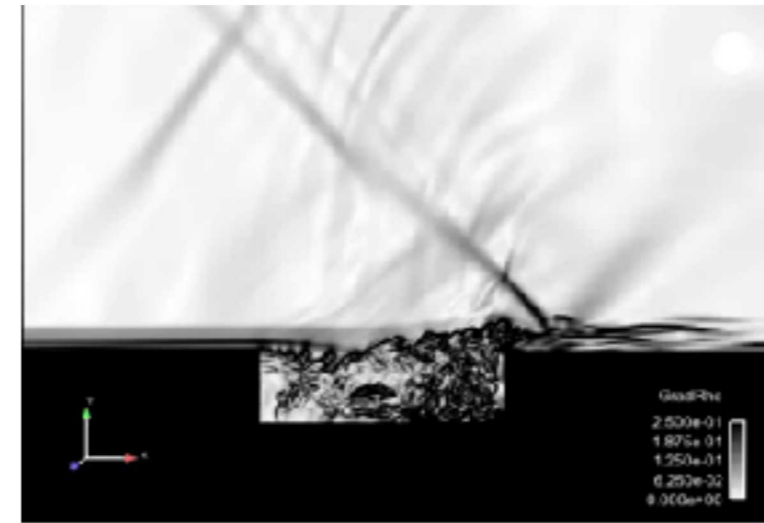
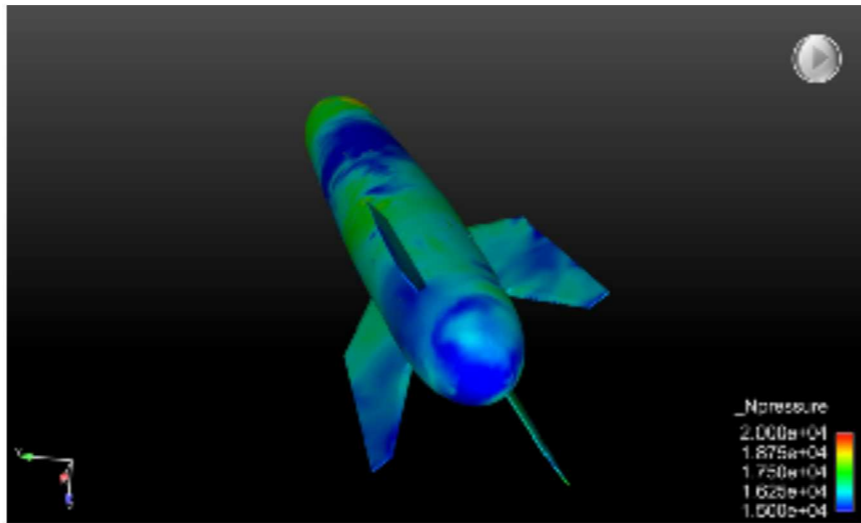
New York, New York

July 26, 2018

High-fidelity simulation: captive carry



High-fidelity simulation: captive carry



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

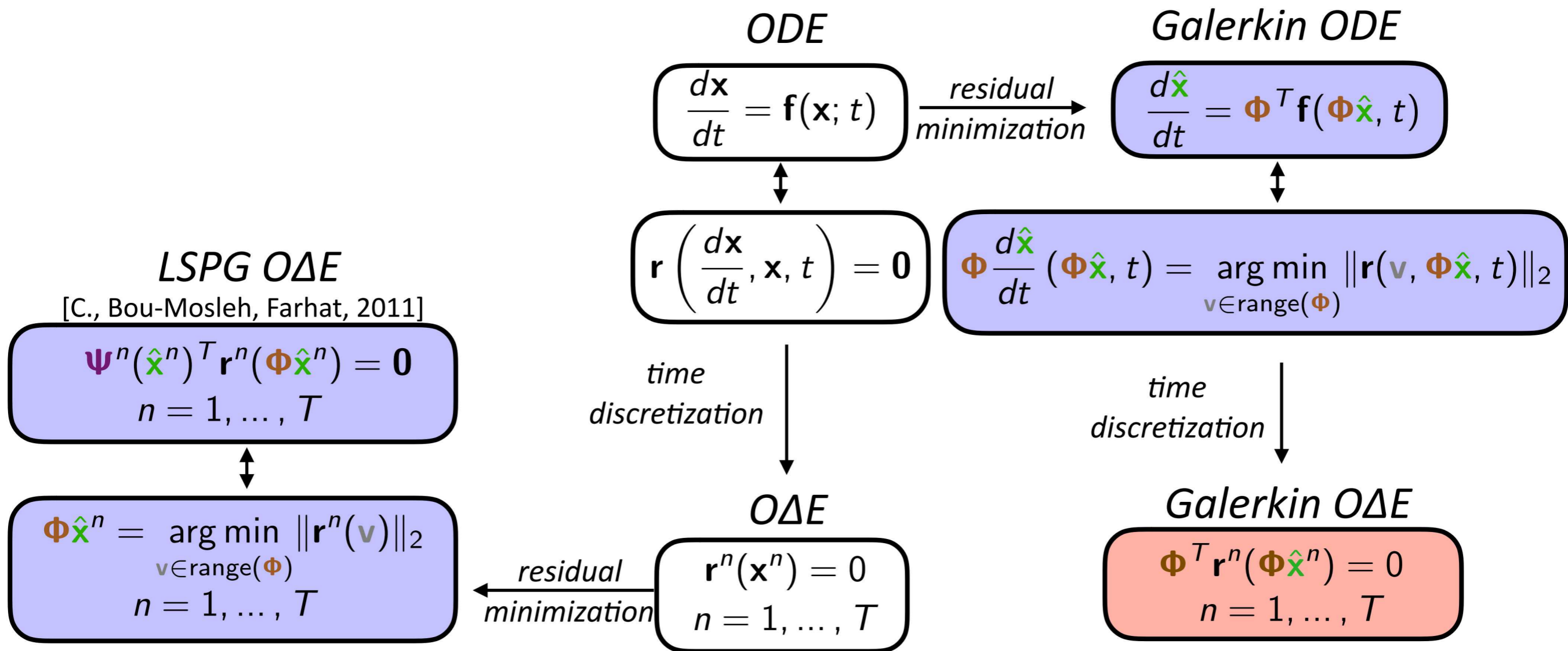
computational barrier

Many-query problems

- explore flight envelope
- quantify effects of uncertainties on store load
- robust design of store and cavity

Goal: break computational barrier

How to construct a ROM given a basis Φ ?



- FOM ODE residual: $\mathbf{r}(\mathbf{v}, \mathbf{x}, t) := \mathbf{v} - \mathbf{f}(\mathbf{x}, t)$
- FOM O\Delta E residual: $\mathbf{r}^n(\mathbf{w}) := \alpha_0 \mathbf{w} - \Delta t \beta_0 \mathbf{f}(\mathbf{w}, t^n) + \sum_{j=1}^k \alpha_j \mathbf{x}^{n-j}(\nu) - \Delta t \sum_{j=1}^k \beta_j \mathbf{f}(\mathbf{x}^{n-j}, t^{n-j})$
- LSPG test basis: $\Psi^n(\hat{\mathbf{w}}) := \left(\alpha_0 \mathbf{I} + \beta_0 \Delta t \frac{\partial \mathbf{f}}{\partial \mathbf{x}}(\Phi \hat{\mathbf{w}}, t^n) \right) \Phi$
- Detailed comparative analysis: C, Barone, Antil, *J Comp Phys*, 2017.

Discrete-time error bound

Theorem [C., Barone, Antil, 2017]

If the following conditions hold:

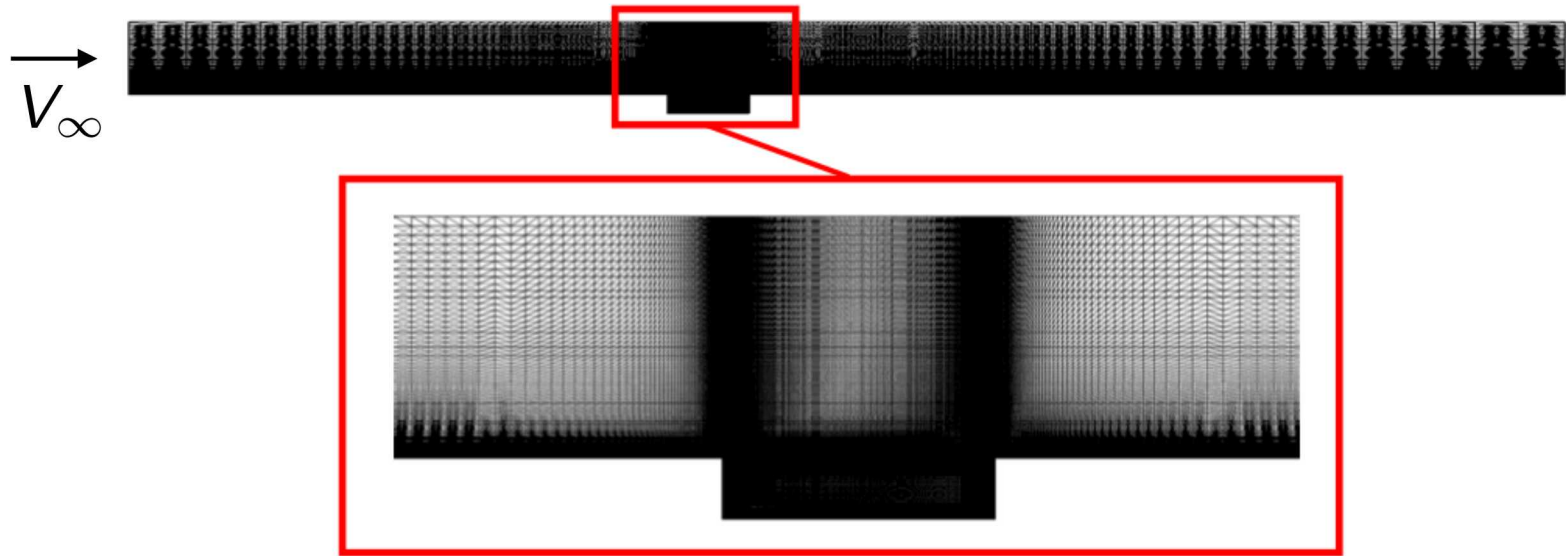
1. $\mathbf{f}(\cdot; t)$ is Lipschitz continuous with Lipschitz constant κ
2. The time step Δt is small enough such that $0 < h := |\alpha_0| - |\beta_0|\kappa\Delta t$,
3. A backward differentiation formula (BDF) time integrator is used,

$$\|\mathbf{x}^n - \Phi \hat{\mathbf{x}}_G^n\|_2 \leq \frac{1}{h} \|\mathbf{r}_G^n(\Phi \hat{\mathbf{x}}_G^n)\|_2 + \frac{1}{h} \sum_{\ell=1}^k |\alpha_\ell| \|\mathbf{x}^{n-\ell} - \Phi \hat{\mathbf{x}}_G^{n-\ell}\|_2$$

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

+ LSPG sequentially minimizes the error bound

Captive carry



- Unsteady Navier–Stokes
- $\text{Re} = 6.3 \times 10^6$
- $M_\infty = 0.6$

Spatial discretization

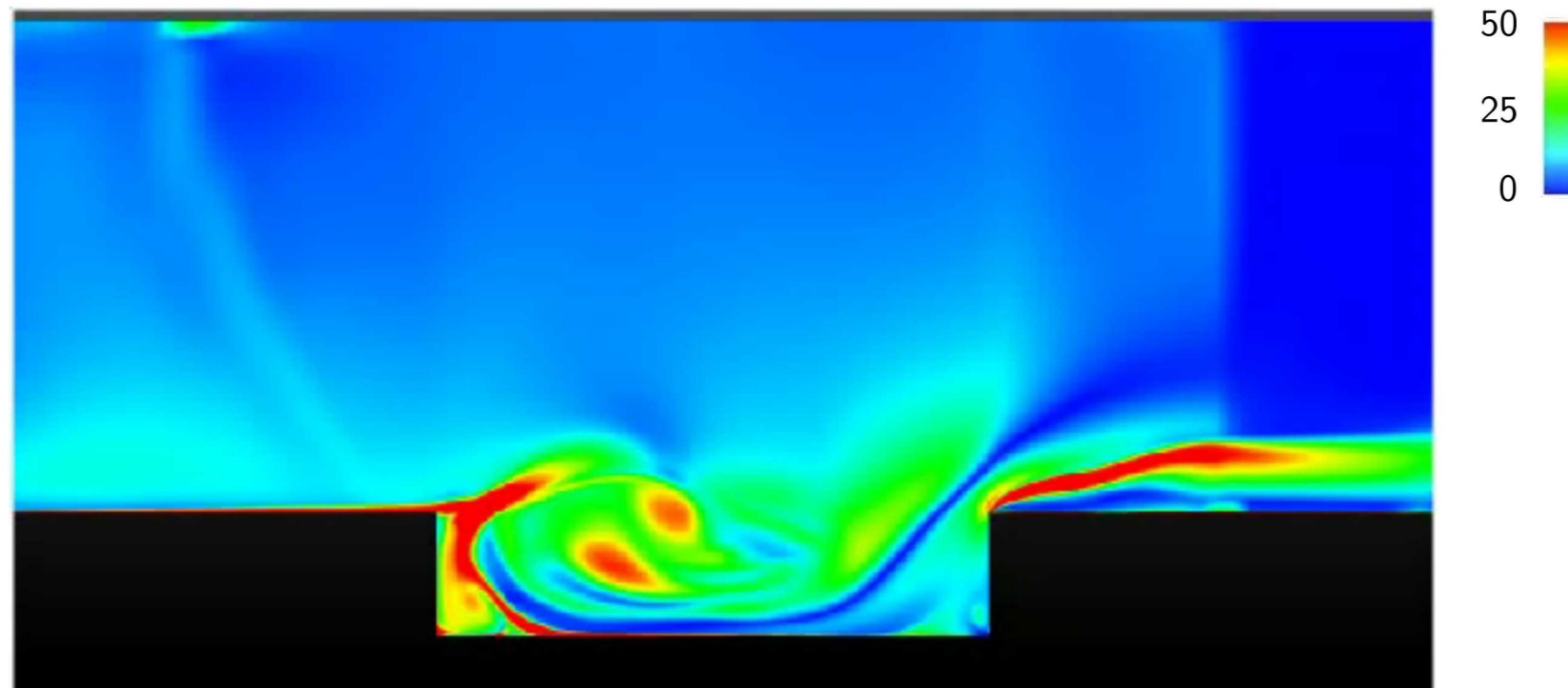
- 2nd-order finite volume
- DES turbulence model
- 1.2×10^6 degrees of freedom

Temporal discretization

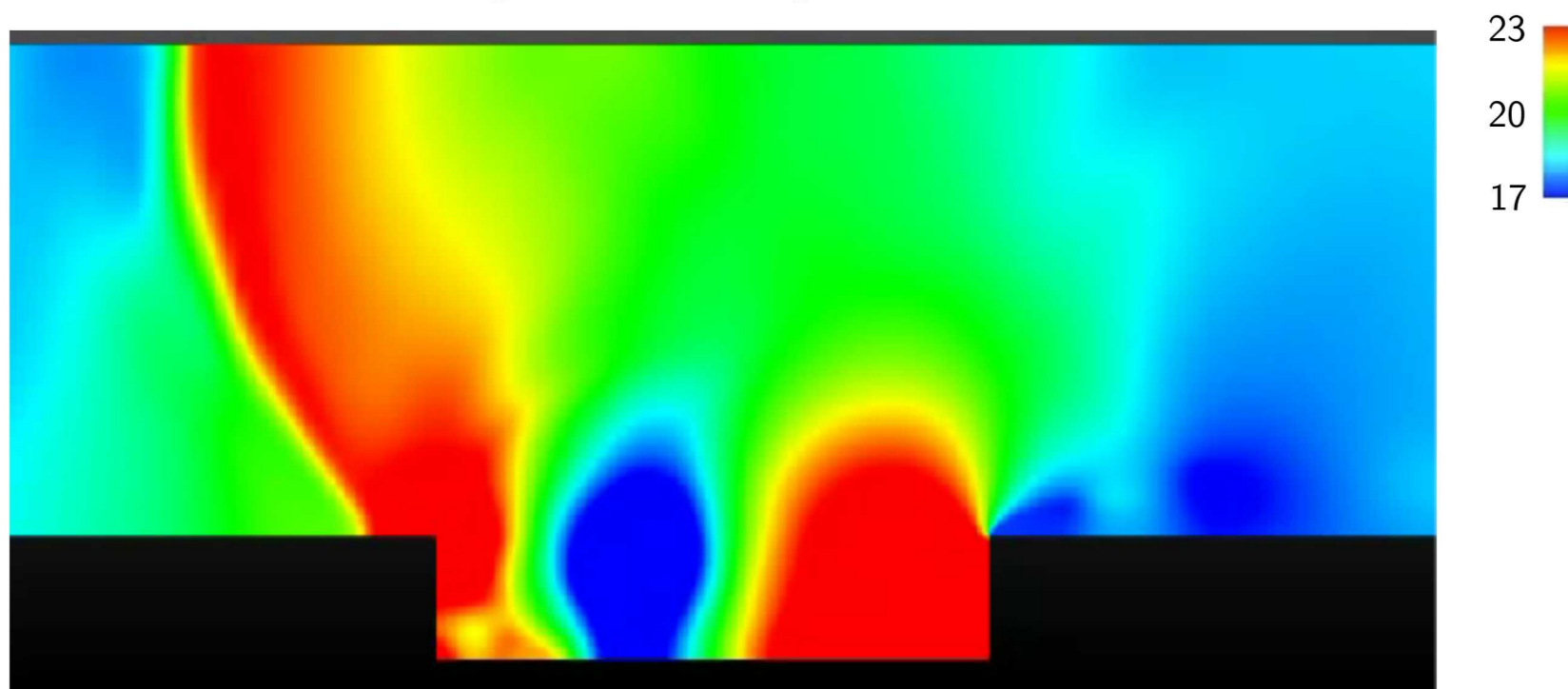
- 2nd-order BDF
- Verified time step $\Delta t = 1.5 \times 10^{-3}$
- 8.3×10^3 time instances

High-fidelity model solution

vorticity field

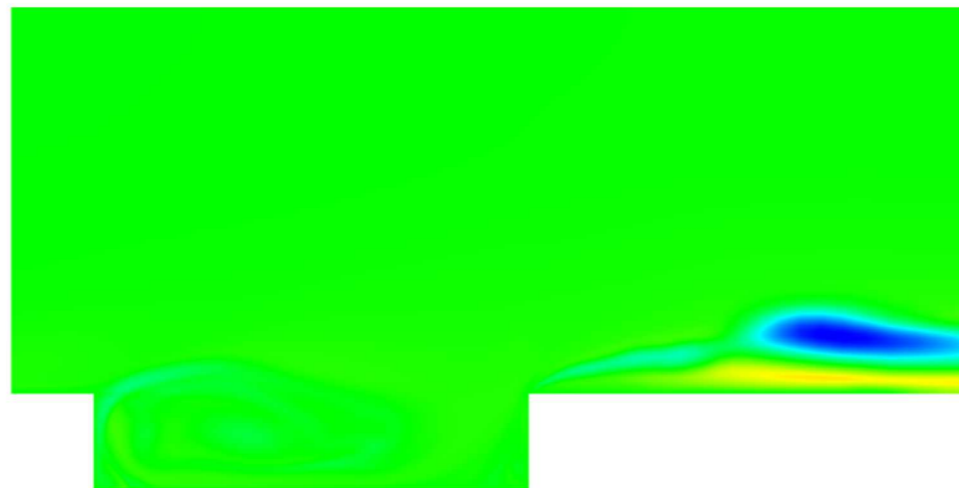
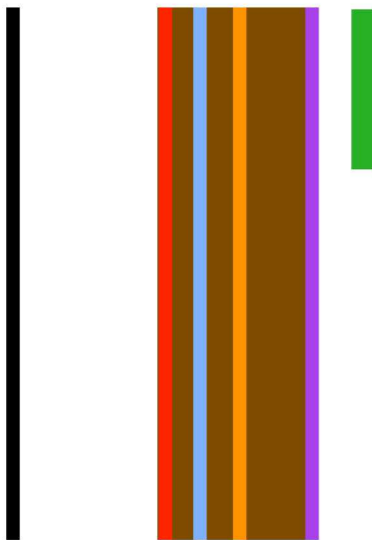


pressure field

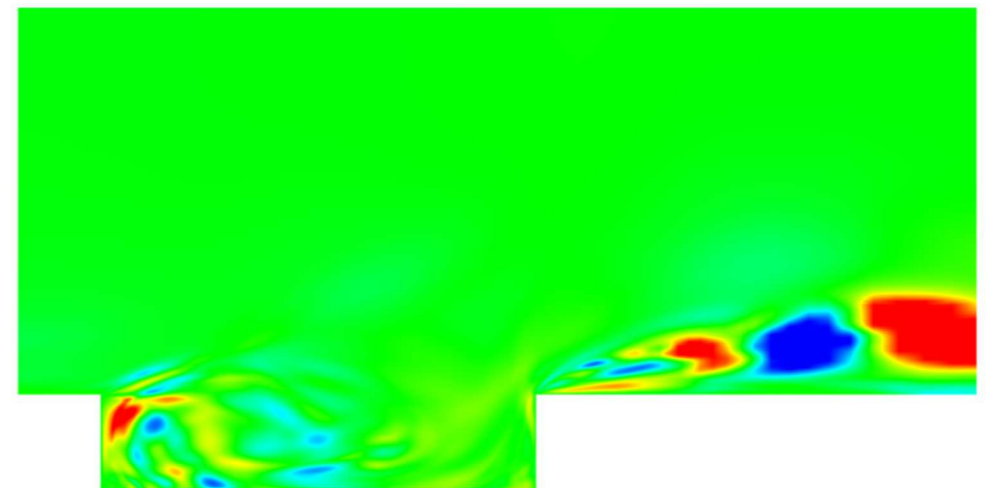


Principal components

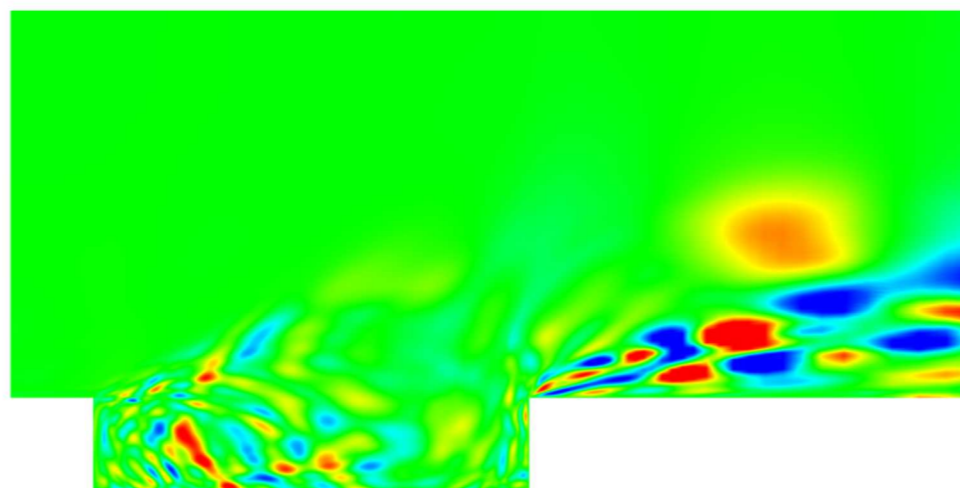
$$\mathbf{x}(t) \approx \mathbf{\Phi} \hat{\mathbf{x}}(t)$$



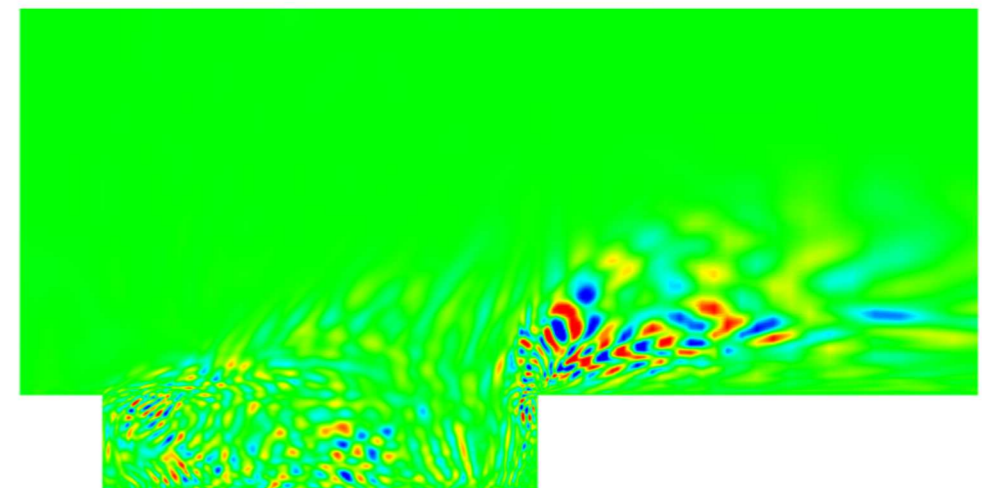
ϕ_1



ϕ_{21}

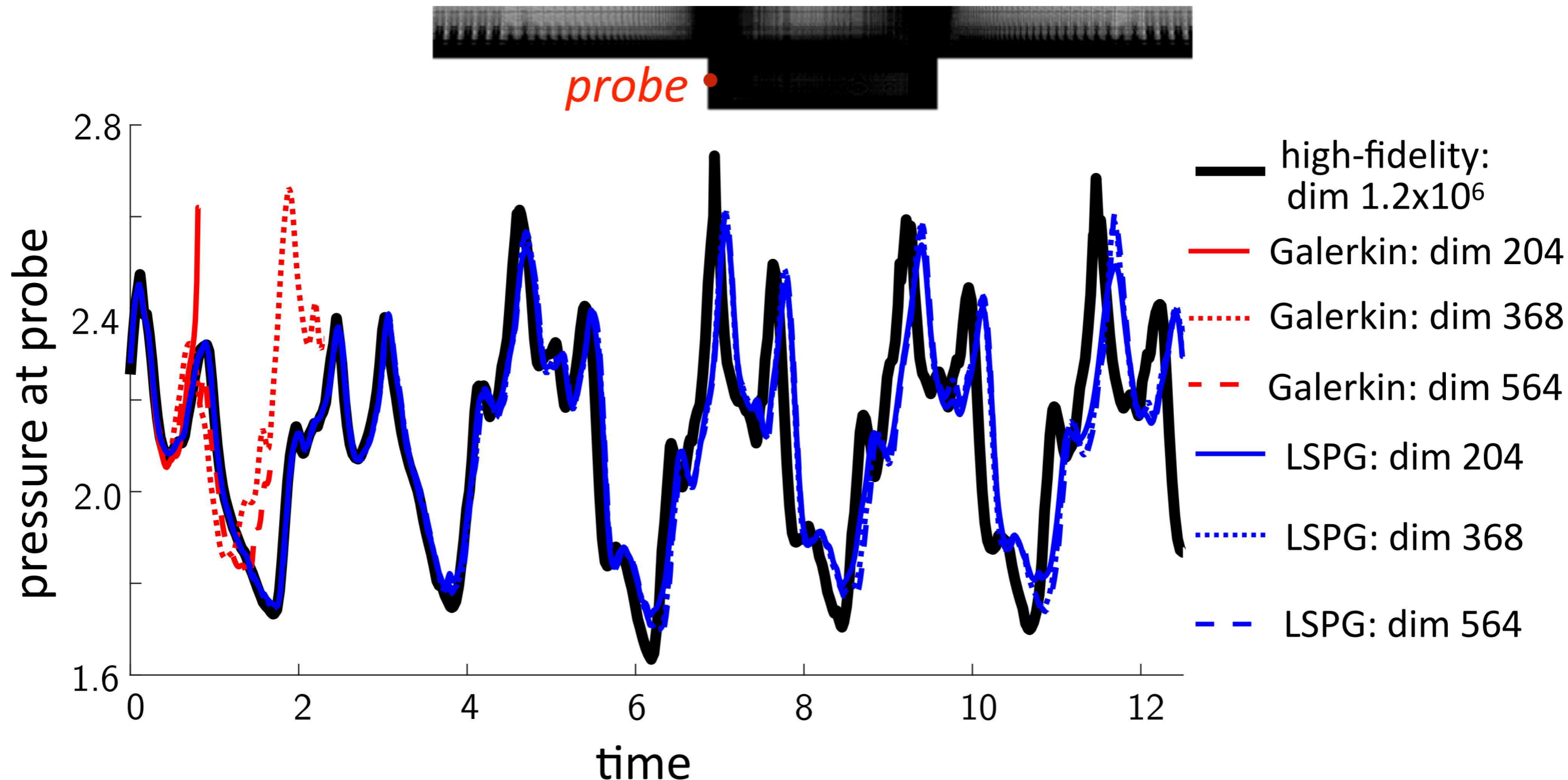


ϕ_{101}



ϕ_{401}

Galerkin and LSPG performance

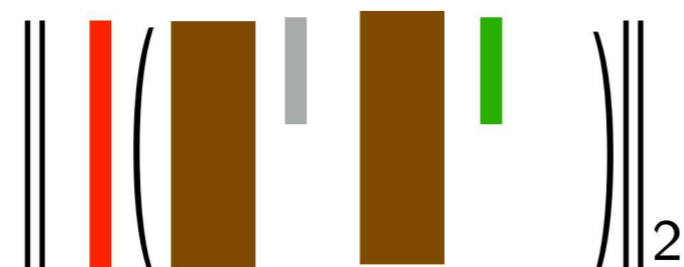


- Galerkin projection fails regardless of basis dimension
- + LSPG is far more accurate than Galerkin
- However, both ROMs are slower than the high-fidelity model

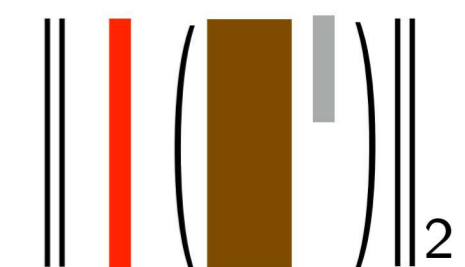
Why does this occur, and can we fix it?

Hyper-reduction

Galerkin: minimize _{$\hat{\mathbf{v}}$} $\| \mathbf{r}(\Phi \hat{\mathbf{v}}, \Phi \hat{\mathbf{x}}, t) \|_2$



LSPG: minimize _{$\hat{\mathbf{v}}$} $\| \mathbf{r}^n(\Phi \hat{\mathbf{v}}) \|_2$

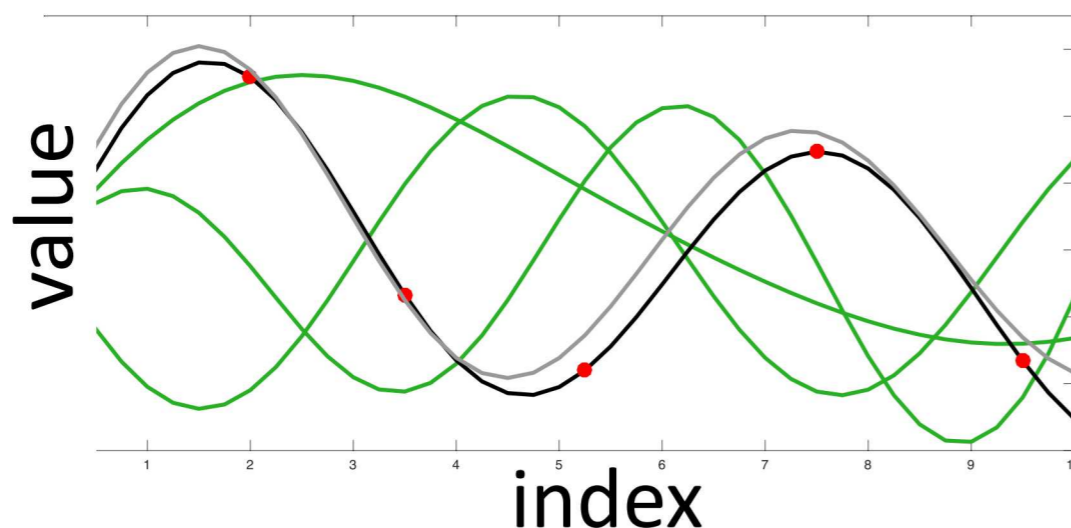


- **Costly:** minimizing **large-scale** high-fidelity model residual

Hyper-reduction: minimize **sampling-based** residual approximations

HR-Galerkin: minimize _{$\hat{\mathbf{v}}$} $\| \tilde{\mathbf{r}}(\Phi \hat{\mathbf{v}}, \Phi \hat{\mathbf{x}}, t) \|_2$ **HR-LSPG:** minimize _{$\hat{\mathbf{v}}$} $\| \tilde{\mathbf{r}}^n(\Phi \hat{\mathbf{v}}) \|_2$

1. Residual gappy POD: $\tilde{\mathbf{r}} = \Phi_r(\mathbf{P}_r \Phi_r)^+ \mathbf{P}_r \mathbf{r}$, $\tilde{\mathbf{r}}^n = \Phi_r(\mathbf{P}_r \Phi_r)^+ \mathbf{P}_r \mathbf{r}^n$



— Φ_r
— \mathbf{r}^n
• $\mathbf{P}_r \mathbf{r}^n$
— $\tilde{\mathbf{r}}^n$

+ Cost independent of
high-fidelity model
dimension

▸ GNAT [C., Bou-Mosleh, Farhat, 2011] = LSPG + residual gappy POD

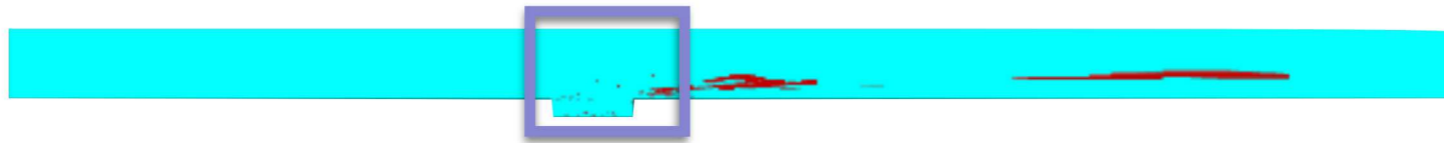
2. Velocity gappy POD: $\tilde{\mathbf{r}}$ and $\tilde{\mathbf{r}}^n$ computed from $\tilde{\mathbf{f}} = \Phi_f(\mathbf{P}_f \Phi_f)^+ \mathbf{P}_f \mathbf{f}$

▸ POD-DEIM [Chaturantabut and Sorensen, 2011] = Galerkin + velocity gappy POD

Sample mesh [C., Farhat, Cortial, Amsallem, 2013]

$$\underset{\hat{\mathbf{v}}}{\text{minimize}} \left\| (\mathbf{P}\Phi_r)^+ \underbrace{\mathbf{P}\mathbf{r}^n}_{\text{}} (\Phi\hat{\mathbf{v}}) \right\|_2$$

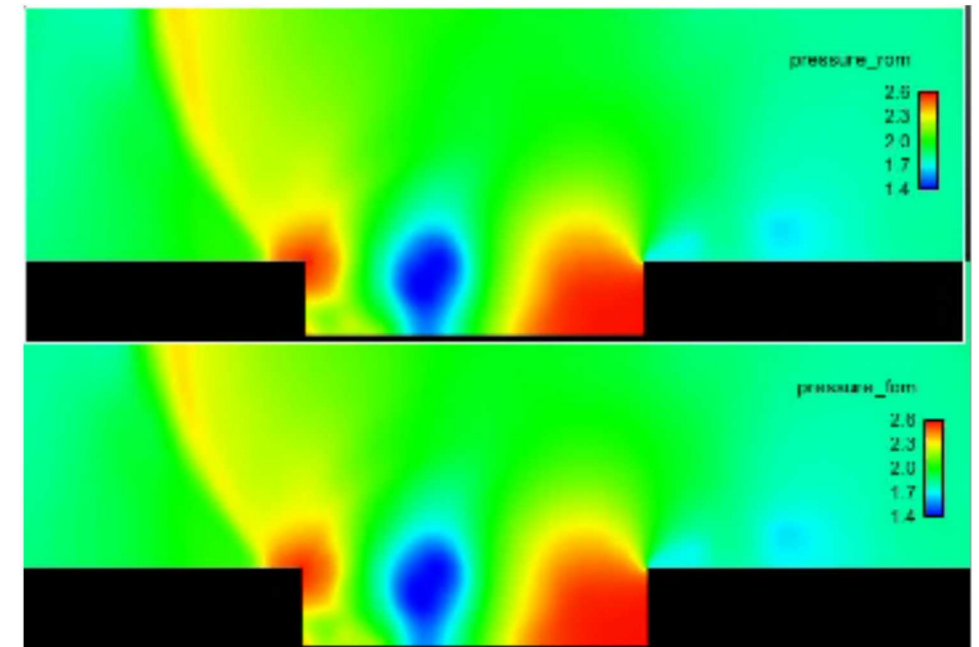
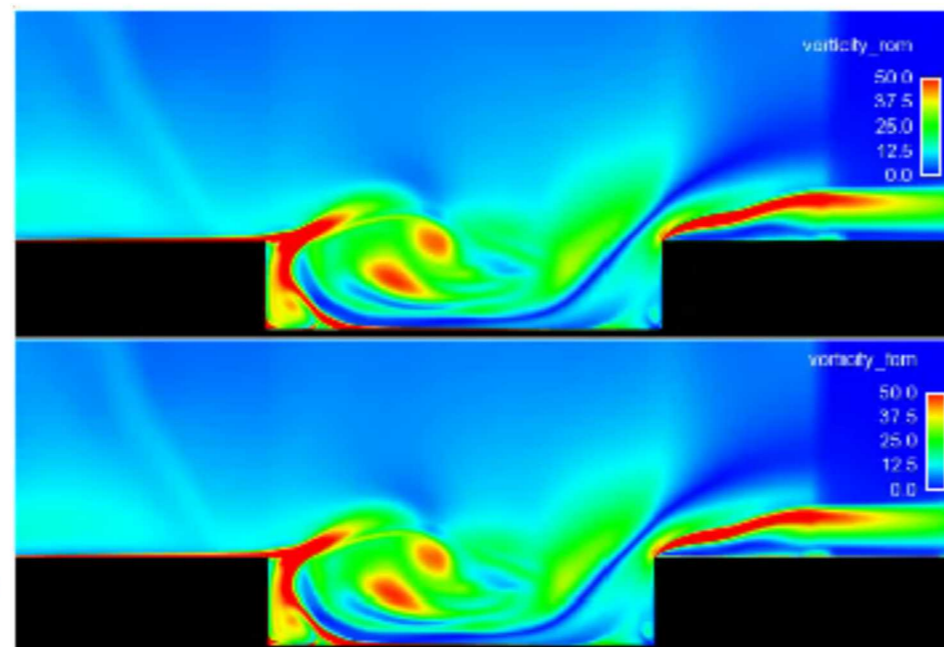
sample
mesh



+ *HPC on a laptop*

vorticity field

pressure field



GNAT ROM

32 min, 2 cores

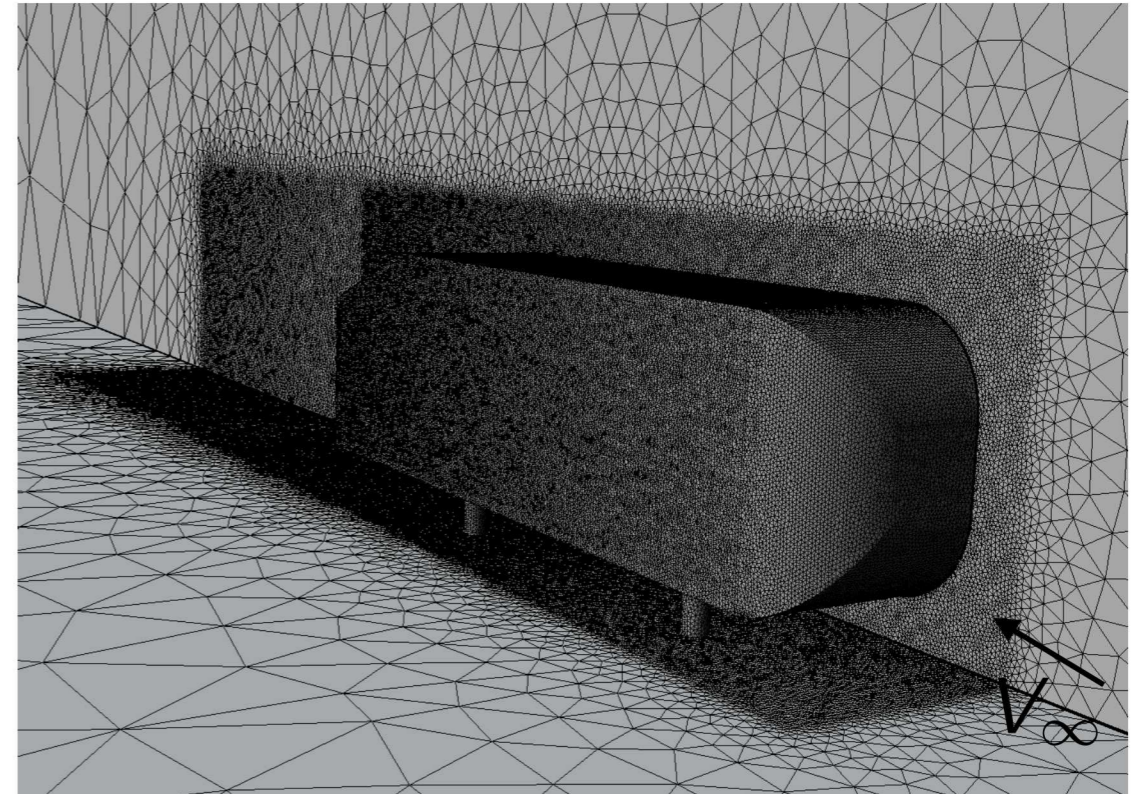
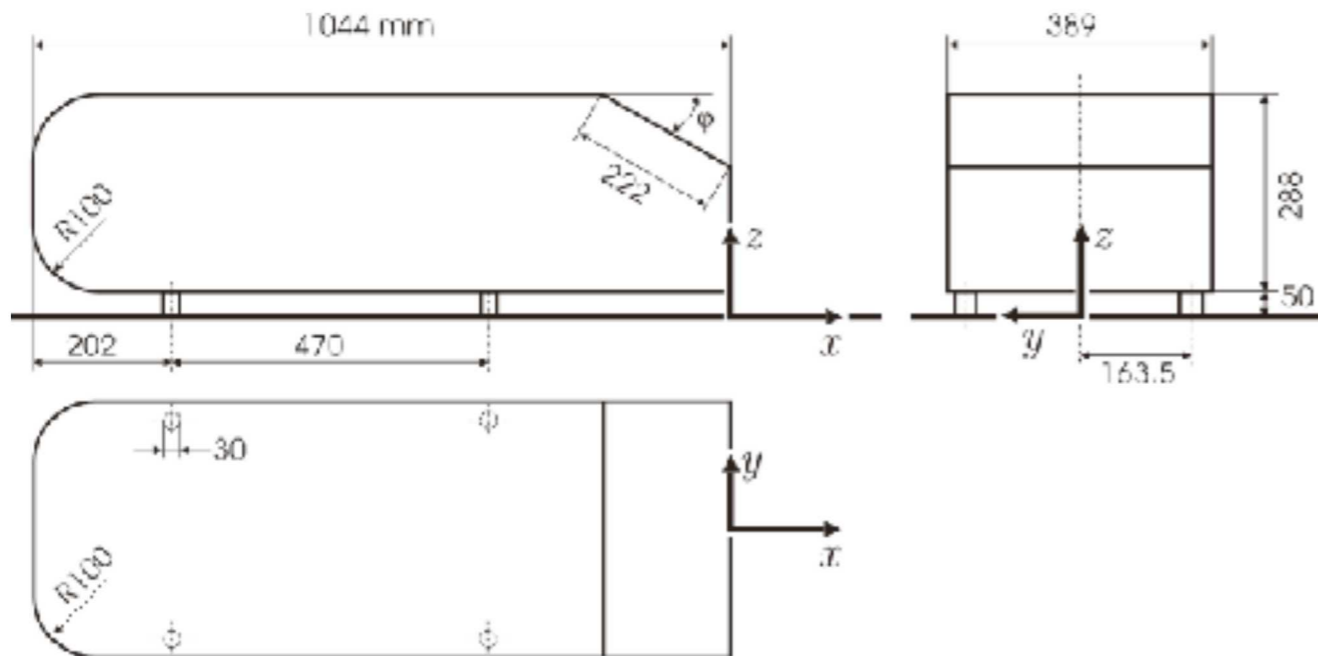
high-fidelity

5 hours, 48 cores

+ *229x savings in core-hours*

+ *< 1% error in time-averaged drag*

Ahmed body [Ahmed, Ramm, Faitin, 1984]



- Unsteady Navier–Stokes
- $Re = 4.3 \times 10^6$
- $M_\infty = 0.175$

Spatial discretization

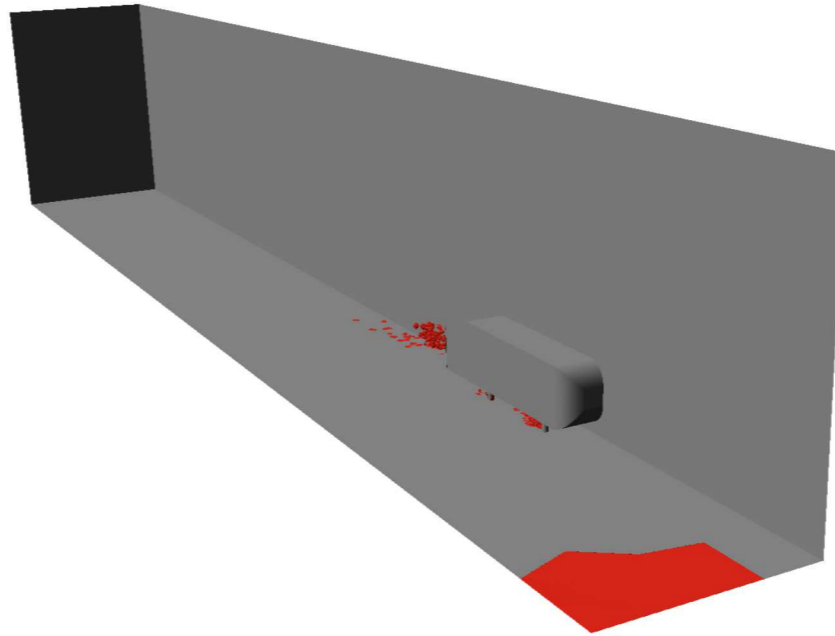
- 2nd-order finite volume
- DES turbulence model
- 1.7×10^7 degrees of freedom

Temporal discretization

- 2nd-order BDF
- Time step $\Delta t = 8 \times 10^{-5} s$
- 1.3×10^3 time instances

Ahmed body results [C., Farhat, Cortial, Amsallem, 2013]

sample
mesh



+ *HPC on a laptop*

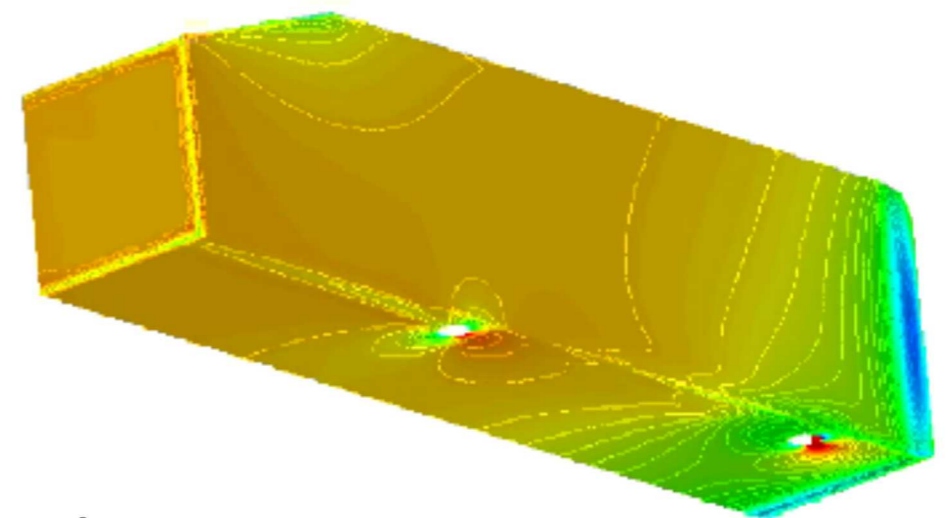
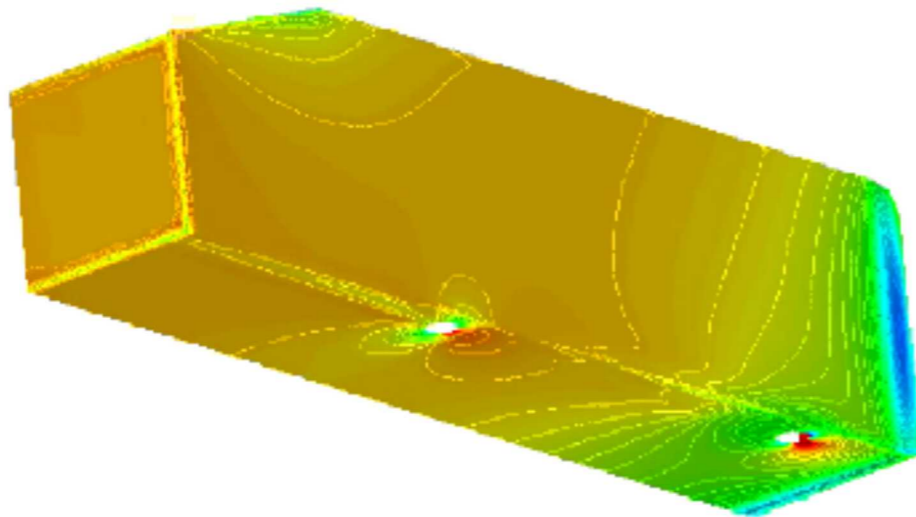
GNAT ROM

4 hours, 4 cores

high-fidelity model

13 hours, 512 cores

*pressure
field*



+ *438x savings in core-hours*

Can we equip the ROM with stronger a priori guarantees?

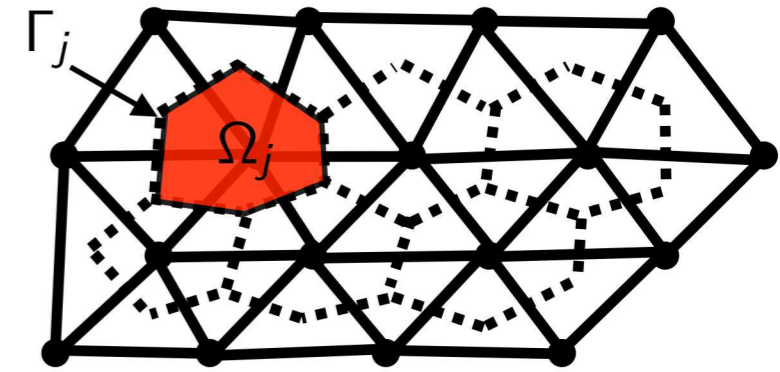
Structure preservation in model reduction

- **Stability** [Moore, 1981; Bond and Daniel, 20018; Amsallem and Farhat, 2012; Kalashnikova et al., 2014]
- **Second-order structure** [Freund 2005; Salimbahrami, 2005; Chahlaoui, 2015]
- **Delay** [Beattie and Gugercin, 2008; Michiels et al., 2011; Schulze and Unger, 2015]
- **Bilinear** [Zhang and Lam, 2002; Benner and Damm, 2011; Benner and Breiten, 2012; Flagg and Gugercin, 2015]
- **Inf–sup stability** [Rozza and Veroy, 2007; Gerner and Veroy, 2012; Rozza et al., 2013; Ballarin et al., 2014]
- **Passivity** [Phillips et al., 2003; Sorensen 2005; Wolf et al., 2010]
- **Energy conservation** [Farhat et al., 2014; Farhat et al., 2015]
- **(Port-)Hamiltonian** [Polyuga and van der Schaft, 2008; Beattie and Gugercin, 2011; Arkham and Hesthaven, 2016; Chaturantabut et al., 2016; Peng and Mohseni, 2016]

What structure should we preserve in finite-volume models?

Finite-volume method

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



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

- average value of conserved variable i over control volume j

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

- 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

$$\text{ODE: } \mathbf{r}^n(\mathbf{x}^n) = 0, \quad n = 1, \dots, N$$

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

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

Conservation is the intrinsic structure enforced by finite-volume methods

Galerkin and LSPG violate conservation

Galerkin

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

- Minimize sum of squared **conservation-violation rates** over all conserved variables and control volumes

LSPG

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

- Minimize sum of squared **conservation violations** **over time step n** over all conserved variables and control volumes

- Neither Galerkin nor LSPG enforces conservation!

Objectives

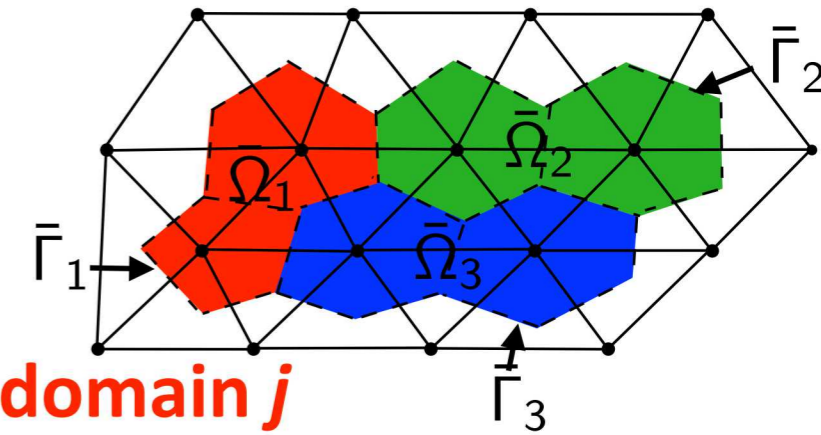
- + Reduced-order models that **enforce conservation**
- + Conditions that determine **when conservation enforcement is ensured**
- + **Hyper-reduction** to ensure low cost if nonlinear flux and source
- + *A posteriori* **error bounds**

Approach: leverage optimization structure of Galerkin and LSPG

Reference: C., Choi, and Sargsyan. Conservative model reduction for finite-volume models. *Journal of Computational Physics*, 371:280–314, 2018.

Finite-volume method over subdomains

$$\text{ODE: } \bar{\mathbf{C}} \frac{d\mathbf{x}}{dt} = \bar{\mathbf{C}} \mathbf{f}(\mathbf{x}, t)$$



$$\bar{c}_{\bar{\mathcal{I}}(i,j), \mathcal{I}(\ell,k)} = |\Omega_k| / |\bar{\Omega}_j| \delta_{i\ell} I(\Omega_k \subseteq \bar{\Omega}_j)$$

- performs summation over control volumes within **subdomain j**

$$[\bar{\mathbf{C}}\mathbf{x}(t)]_{\bar{\mathcal{I}}(i,j)}(\mathbf{x}, t; \mu) = \frac{1}{|\bar{\Omega}_j|} \int_{\bar{\Omega}_j} u_i(\vec{x}, t; \mu) d\vec{x}$$

- average value of **conserved variable i** over **subdomain j**

$$[\bar{\mathbf{C}}\mathbf{f}(\mathbf{x}, t)]_{\bar{\mathcal{I}}(i,j)} = -\frac{1}{|\bar{\Omega}_j|} \int_{\bar{\Gamma}_j} \underbrace{\mathbf{g}_i(\mathbf{x}; \vec{x}, t) \cdot \bar{\mathbf{n}}_j(\vec{x})}_{\text{flux}} d\vec{s}(\vec{x}) + \frac{1}{|\bar{\Omega}_j|} \int_{\bar{\Omega}_j} \underbrace{s_i(\mathbf{x}; \vec{x}, t)}_{\text{source}} d\vec{x}$$

- flux and source of **conserved variable i** within **subdomain j**

$$[\bar{\mathbf{C}}\mathbf{r}]_{\bar{\mathcal{I}}(i,j)} = d[\bar{\mathbf{C}}\mathbf{x}(t)]_{\bar{\mathcal{I}}(i,j)} / dt - [\bar{\mathbf{C}}\mathbf{f}(\mathbf{x}, t)]_{\bar{\mathcal{I}}(i,j)}$$

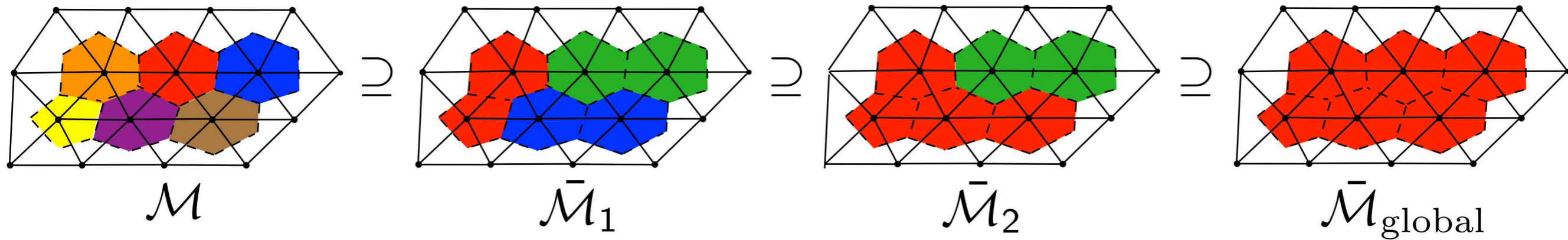
- rate of conservation violation** of **conserved variable i** in **subdomain j**

$$\text{O}\Delta\text{E: } \bar{\mathbf{C}}\mathbf{r}^n(\mathbf{x}^n) = \mathbf{0}, \quad n = 1, \dots, T$$

$$[\bar{\mathbf{C}}\mathbf{r}^n]_{\bar{\mathcal{I}}(i,j)} = [\bar{\mathbf{C}}\mathbf{x}(t^{n+1})]_{\bar{\mathcal{I}}(i,j)} - [\bar{\mathbf{C}}\mathbf{x}(t^n)]_{\bar{\mathcal{I}}(i,j)} + \int_{t^n}^{t^{n+1}} [\bar{\mathbf{C}}\mathbf{f}(\mathbf{x}, t)]_{\bar{\mathcal{I}}(i,j)} dt$$

- conservation violation** of **conserved variable i** in **subdomain j** over **time step n**

Nested conservation



Theorem: Nested conservation [C., Choi, Sargsyan, 2018]

- If a decomposed mesh $\bar{\bar{\mathcal{M}}}$ is nested in another decomposed mesh $\bar{\mathcal{M}}$ such that $\bar{\bar{\Omega}}_i = \cup_{j \in \bar{\bar{K}} \subseteq \{1, \dots, N_{\bar{\Omega}}\}} \bar{\Omega}_j$, $i = 1, \dots, N_{\bar{\bar{\Omega}}}$, then we say $\bar{\bar{\mathcal{M}}} \subseteq \bar{\mathcal{M}}$.
- If $\bar{\bar{\mathcal{M}}} \subseteq \bar{\mathcal{M}}$ and $\bar{\mathcal{M}}$ is non-overlapping, then satisfaction of conservation on $\bar{\mathcal{M}}$ implies satisfaction of conservation on $\bar{\bar{\mathcal{M}}}$, i.e.,

$$\bar{\mathbf{C}}\mathbf{r}\left(\frac{d\mathbf{x}}{dt}, \mathbf{x}, t\right) = \mathbf{0} \Rightarrow \bar{\bar{\mathbf{C}}}\mathbf{r}\left(\frac{d\mathbf{x}}{dt}, \mathbf{x}, t\right) = \mathbf{0}, \quad \bar{\mathbf{C}}\mathbf{r}^n(\mathbf{x}^n) = 0 \Rightarrow \bar{\bar{\mathbf{C}}}\mathbf{r}^n(\mathbf{x}^n) = 0$$

Corollary: Global conservation [C., Choi, Sargsyan, 2018]

If the decomposed mesh $\bar{\mathcal{M}}$ satisfies $\cup_{i=1}^{N_{\bar{\Omega}}} \bar{\Omega}_i = \Omega$ and is non-overlapping, then it is globally conservative.

Conservative model reduction

Conservative Galerkin

$$\underset{\hat{\mathbf{v}} \in \mathbb{R}^p}{\text{minimize}} \quad \|\mathbf{r}(\Phi \hat{\mathbf{v}}, \Phi \hat{\mathbf{x}}, t)\|_2$$

$$\text{subject to } \bar{\mathbf{C}}\mathbf{r}(\Phi \hat{\mathbf{v}}, \Phi \hat{\mathbf{x}}, t) = \mathbf{0}$$

- Minimize sum of squared **conservation-violation rates** over all conserved variables and control volumes **subject to zero conservation-violation rates** over subdomains

Conservative LSPG

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

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

- Minimize sum of squared **conservation violations** **over time step n** over all conserved variables and control volumes **subject to zero conservation violations over time step n** over subdomains

+ If feasible, ROMs enforce conservation over subdomains

Questions

Conservative Galerkin

$$\underset{\hat{\mathbf{v}} \in \mathbb{R}^p}{\text{minimize}} \quad \|\mathbf{r}(\Phi \hat{\mathbf{v}}, \Phi \hat{\mathbf{x}}, t)\|_2$$

$$\text{subject to } \bar{\mathbf{C}}\mathbf{r}(\Phi \hat{\mathbf{v}}, \Phi \hat{\mathbf{x}}, t) = \mathbf{0}$$

Conservative LSPG

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

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

- What are conditions for feasibility?
- How to handle infeasibility?
- How to solve?
- Are the two methods ever equivalent?
- How to apply hyper-reduction in a structure-preserving way?
- How do *a posteriori* error bounds compare with standard ROMs?

Questions

Conservative Galerkin

$$\underset{\hat{\mathbf{v}} \in \mathbb{R}^p}{\text{minimize}} \quad \|\mathbf{r}(\Phi \hat{\mathbf{v}}, \Phi \hat{\mathbf{x}}, t)\|_2$$

$$\text{subject to } \bar{\mathbf{C}}\mathbf{r}(\Phi \hat{\mathbf{v}}, \Phi \hat{\mathbf{x}}, t) = \mathbf{0}$$

Conservative LSPG

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

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

- **What are conditions for feasibility?**
- How to handle infeasibility?
- How to solve?
- Are the two methods ever equivalent?
- How to apply hyper-reduction in a structure-preserving way?
- How do *a posteriori* error bounds compare with standard ROMs?

Conservative Galerkin feasibility

Conservative Galerkin

$$\underset{\hat{\mathbf{v}} \in \mathbb{R}^p}{\text{minimize}} \quad \|\mathbf{r}(\Phi \hat{\mathbf{v}}, \Phi \hat{\mathbf{x}}, t)\|_2$$

$$\text{subject to } \bar{\mathbf{C}}\mathbf{r}(\Phi \hat{\mathbf{v}}, \Phi \hat{\mathbf{x}}, t) = \mathbf{0}$$

Definition: conservative Galerkin feasibility

The conservative Galerkin model is feasible if the Galerkin feasible set

$$\mathcal{F}_G(\Phi \hat{\mathbf{x}}, t) := \{\hat{\mathbf{v}} \in \mathbb{R}^p \mid \bar{\mathbf{C}}\mathbf{r}(\Phi \hat{\mathbf{v}}, \Phi \hat{\mathbf{x}}, t) = \mathbf{0}\}$$

is non-empty.

Proposition: sufficient conditions for conservative Galerkin feasibility

The conservative Galerkin model is feasible, i.e., $\mathcal{F}_G(\Phi \hat{\mathbf{x}}, t) \neq \emptyset$ if $\bar{\mathbf{C}}\Phi$ has full row rank (i.e., inf-sup stability). This in turn requires fewer constraints (i.e., rows in $\bar{\mathbf{C}}$) than unknowns (i.e., columns in Φ).

Constraint equations should be underdetermined.

Conservative LSPG feasibility

Conservative LSPG

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

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

Definition: conservative LSPG feasibility

The conservative LSPG model is feasible if the LSPG feasible set

$$\mathcal{F}_P^n := \{\hat{\mathbf{v}} \in \mathbb{R}^p \mid \bar{\mathbf{C}}\mathbf{r}^n(\Phi \hat{\mathbf{v}}) = \mathbf{0}\}$$

is non-empty.

Proposition: sufficient conditions for conservative LSPG feasibility

The conservative LSPG model is feasible, i.e., $\mathcal{F}_P^n \neq \emptyset$ if

1. an explicit time integrator is used and $\bar{\mathbf{C}}\Phi$ has full row rank
2. the limit $\Delta t \rightarrow 0$ is taken, or
3. The velocity \mathbf{f} is linear in the state and $\bar{\mathbf{C}}[\alpha_0 \mathbf{I} - \Delta t \beta_0 \partial \mathbf{f} / \partial \mathbf{x}(\cdot, t^n)]\Phi$ has full row rank.

Constraint equations should be underdetermined.

Questions

Conservative Galerkin

$$\underset{\hat{\mathbf{v}} \in \mathbb{R}^p}{\text{minimize}} \quad \|\mathbf{r}(\Phi \hat{\mathbf{v}}, \Phi \hat{\mathbf{x}}, t)\|_2$$

$$\text{subject to } \bar{\mathbf{C}}\mathbf{r}(\Phi \hat{\mathbf{v}}, \Phi \hat{\mathbf{x}}, t) = \mathbf{0}$$

Conservative LSPG

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

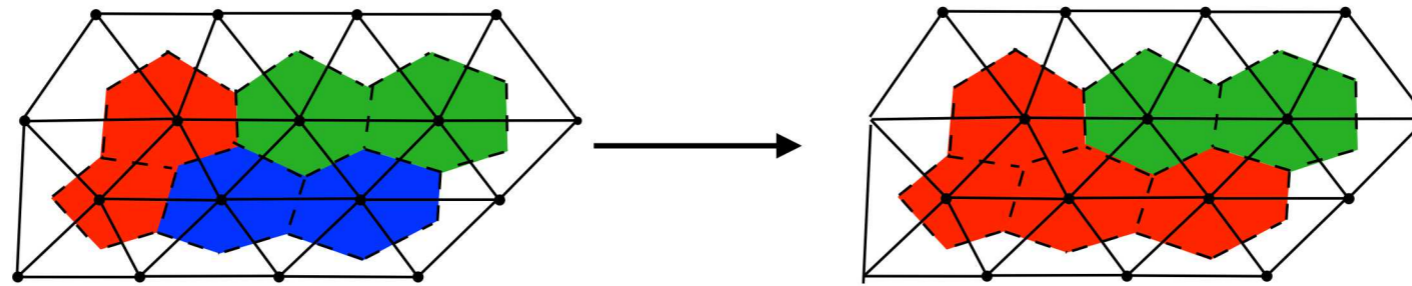
$$\text{subject to } \bar{\mathbf{C}}\mathbf{r}^n(\Phi \hat{\mathbf{v}}) = \mathbf{0}$$

- What are conditions for feasibility?
- **How to handle infeasibility?**
- How to solve?
- Are the two methods ever equivalent?
- How to apply hyper-reduction in a structure-preserving way?
- How do *a posteriori* error bounds compare with standard ROMs?

Handling infeasibility

What if infeasibility is detected?

1. Reduce number of subdomains



- + Fewer constraints, so **likelihood of feasibility increases**
- + Nested: solutions at previous time steps are **feasible on new mesh**
- **No guarantee of feasibility** (global conservation may be infeasible)

2. Penalty formulation

- Penalized Galerkin: minimize $\|\mathbf{r}(\Phi \hat{\mathbf{v}}, \Phi \hat{\mathbf{x}}, t)\|_2^2 + \rho \|\bar{\mathbf{C}}\mathbf{r}(\Phi \hat{\mathbf{v}}, \Phi \hat{\mathbf{x}}, t)\|_2^2$
 $\hat{\mathbf{v}} \in \mathbb{R}^p$
- Penalized LSPG: minimize $\|\mathbf{r}^n(\Phi \hat{\mathbf{v}})\|_2^2 + \rho \|\bar{\mathbf{C}}\mathbf{r}^n(\mathbf{x}^0(\mu) + \Phi \hat{\mathbf{v}})\|_2^2$
 $\hat{\mathbf{v}} \in \mathbb{R}^p$

+ **Always solvable**

- **No longer strictly conservative**

Questions

Conservative Galerkin

$$\underset{\hat{\mathbf{v}} \in \mathbb{R}^p}{\text{minimize}} \quad \|\mathbf{r}(\Phi \hat{\mathbf{v}}, \Phi \hat{\mathbf{x}}, t)\|_2$$

$$\text{subject to } \bar{\mathbf{C}}\mathbf{r}(\Phi \hat{\mathbf{v}}, \Phi \hat{\mathbf{x}}, t) = \mathbf{0}$$

Conservative LSPG

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

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

- What are conditions for feasibility?
- How to handle infeasibility?
- **How to solve?**
- Are the two methods ever equivalent?
- How to apply hyper-reduction in a structure-preserving way?
- How do *a posteriori* error bounds compare with standard ROMs?

Conservative Galerkin

$$\underset{\hat{\mathbf{v}} \in \mathbb{R}^p}{\text{minimize}} \quad \|\mathbf{r}(\Phi \hat{\mathbf{v}}, \Phi \hat{\mathbf{x}}, t)\|_2$$

$$\text{subject to } \bar{\mathbf{C}}\mathbf{r}(\Phi \hat{\mathbf{v}}, \Phi \hat{\mathbf{x}}, t) = \mathbf{0}$$

Convex linear least-squares problem with linear equality constraints

Theorem

If the conservative Galerkin model is feasible, i.e., $\mathcal{F}_G(\Phi \hat{\mathbf{x}}, t) \neq \emptyset$ then its solution exists, is unique, and satisfies the following:

1. a time-dependent saddle point problem

$$\begin{bmatrix} \mathbf{I} & \Phi^T \bar{\mathbf{C}}^T \\ \bar{\mathbf{C}}\Phi & \mathbf{0} \end{bmatrix} \begin{bmatrix} \frac{d\hat{\mathbf{x}}}{dt} \\ \frac{d\lambda_G}{dt} \end{bmatrix} = \begin{bmatrix} \Phi^T \mathbf{f}(\Phi \hat{\mathbf{x}}, t) \\ \bar{\mathbf{C}}\mathbf{f}(\Phi \hat{\mathbf{x}}, t; \mu) \end{bmatrix}$$

2. a modified Galerkin projection

$$\frac{d\hat{\mathbf{x}}}{dt} = \Phi^T \mathbf{f}(\Phi \hat{\mathbf{x}}, t) + \underbrace{(\bar{\mathbf{C}}\Phi)^+ [\bar{\mathbf{C}}\mathbf{f}(\mathbf{x}, t; \nu) - \bar{\mathbf{C}}\Phi\Phi^T \mathbf{f}(\mathbf{x}, t)]}_{\text{modification from Galerkin velocity}}$$

3. orthogonal projection of the Galerkin velocity onto the feasible set

$$\frac{d\hat{\mathbf{x}}}{dt}(\Phi \hat{\mathbf{x}}, t) = \arg \min_{\mathbf{v} \in \mathcal{F}_G(\Phi \hat{\mathbf{x}}, t)} \|\mathbf{v} - \Phi^T \mathbf{f}(\Phi \hat{\mathbf{x}}, t)\|_2$$

► **Solver:** any time integrator applied to these systems of ODEs

Conservative LSPG

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

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

Non-convex nonlinear least-squares problem with nonlinear equality constraints

Theorem

If the conservative LSPG model is feasible, i.e., $\mathcal{F}_p^n \neq \emptyset$, then its solution exists and satisfies the nonlinear saddle-point problem

$$\begin{aligned} \Psi^n(\hat{\mathbf{x}}^n)^T \left[\mathbf{r}^n(\Phi \hat{\mathbf{x}}^n) + \bar{\mathbf{C}}^T \lambda_p^n \right] &= \mathbf{0} \\ \bar{\mathbf{C}} \mathbf{r}^n(\Phi \hat{\mathbf{x}}^n) &= \mathbf{0} \end{aligned}$$

► **Solver:** SQP with Gauss–Newton Hessian approximation

$$\begin{aligned} & \begin{bmatrix} \Psi^n(\hat{\mathbf{x}}^{n(k)})^T \Psi^n(\hat{\mathbf{x}}^{n(k)}) & \Psi^n(\hat{\mathbf{x}}^{n(k)})^T \bar{\mathbf{C}}^T \\ \bar{\mathbf{C}} \Psi^n(\hat{\mathbf{x}}^{n(k)}) & \mathbf{0} \end{bmatrix} \begin{bmatrix} \delta \hat{\mathbf{x}}^{n(k)} \\ \delta \lambda_p^{n(k)} \end{bmatrix} \\ &= - \begin{bmatrix} \Psi^n(\hat{\mathbf{x}}^{n(k)})^T \left(\mathbf{r}^n(\mathbf{x}^0(\mu) + \Phi \hat{\mathbf{x}}^{n(k)}) + \bar{\mathbf{C}}^T \lambda_p^{n(k)} \right) \\ \bar{\mathbf{C}} \mathbf{r}^n(\mathbf{x}^0(\mu) + \Phi \hat{\mathbf{x}}^{n(k)}) \end{bmatrix} \end{aligned}$$

Questions

Conservative Galerkin

$$\underset{\hat{\mathbf{v}} \in \mathbb{R}^p}{\text{minimize}} \quad \|\mathbf{r}(\Phi \hat{\mathbf{v}}, \Phi \hat{\mathbf{x}}, t)\|_2$$

$$\text{subject to } \bar{\mathbf{C}}\mathbf{r}(\Phi \hat{\mathbf{v}}, \Phi \hat{\mathbf{x}}, t) = \mathbf{0}$$

Conservative LSPG

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

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

- What are conditions for feasibility?
- How to handle infeasibility?
- How to solve?
- **Are the two methods ever equivalent?**
- How to apply hyper-reduction in a structure-preserving way?
- How do *a posteriori* error bounds compare with standard ROMs?

Are the two approaches ever equivalent?

Conservative Galerkin OΔE

$$\Phi^T [\mathbf{r}^n(\Phi \hat{\mathbf{x}}_G^n) + \sum_{j=0}^k \alpha_j \bar{\mathbf{C}}^T \lambda_G^{n-j}] = 0$$

$$\bar{\mathbf{C}} \mathbf{r}^n(\Phi \hat{\mathbf{x}}_G^n) = 0$$

Conservative LSPG OΔE

$$\Psi^n(\hat{\mathbf{x}}_P^n)^T [\mathbf{r}^n(\Phi \hat{\mathbf{x}}_P^n) + \bar{\mathbf{C}}^T \lambda_P^n] = 0$$

$$\bar{\mathbf{C}} \mathbf{r}^n(\Phi \hat{\mathbf{x}}_P^n) = 0$$

These are equivalent if, for some constant a ,

$$\Psi^n(\hat{\mathbf{x}}^n) = a\Phi \quad \text{and} \quad \Psi^n(\hat{\mathbf{x}}^n)^T \bar{\mathbf{C}}^T \lambda_P^n = a \sum_{j=0}^k \alpha_j \Phi^T \bar{\mathbf{C}}^T \lambda_G^{n-j}.$$

Recall $\Psi^n(\hat{\mathbf{x}}^n) := (\alpha_0 \mathbf{I} - \Delta t \beta_0 \frac{\partial \mathbf{f}}{\partial \mathbf{x}}(\Phi \hat{\mathbf{x}}^n; t)) \Phi$

Theorem: equivalence

The two approaches are equivalent (with $a = \alpha_0$)

1. in the limit of $\Delta t \rightarrow 0$, or
2. if the scheme is explicit ($\beta_0 = 0$).

Further, the Lagrange multipliers are related as $\lambda_P^n = \sum_{j=0}^k \alpha_j \lambda_G^{n-j}$

Questions

Conservative Galerkin

$$\underset{\hat{\mathbf{v}} \in \mathbb{R}^p}{\text{minimize}} \quad \|\mathbf{r}(\Phi \hat{\mathbf{v}}, \Phi \hat{\mathbf{x}}, t)\|_2$$

$$\text{subject to } \bar{\mathbf{C}}\mathbf{r}(\Phi \hat{\mathbf{v}}, \Phi \hat{\mathbf{x}}, t) = \mathbf{0}$$

Conservative LSPG

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

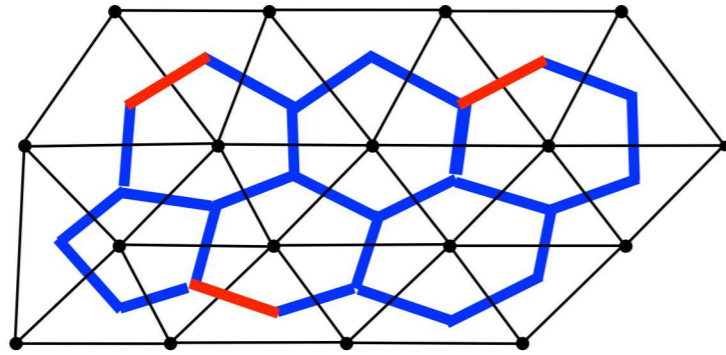
$$\text{subject to } \bar{\mathbf{C}}\mathbf{r}^n(\Phi \hat{\mathbf{v}}) = \mathbf{0}$$

- What are conditions for feasibility?
- How to handle infeasibility?
- How to solve?
- Are the two methods ever equivalent?
- **How to apply hyper-reduction in a structure-preserving way?**
- How do *a posteriori* error bounds compare with standard ROMs?

Hyper-reduction for finite-volume models

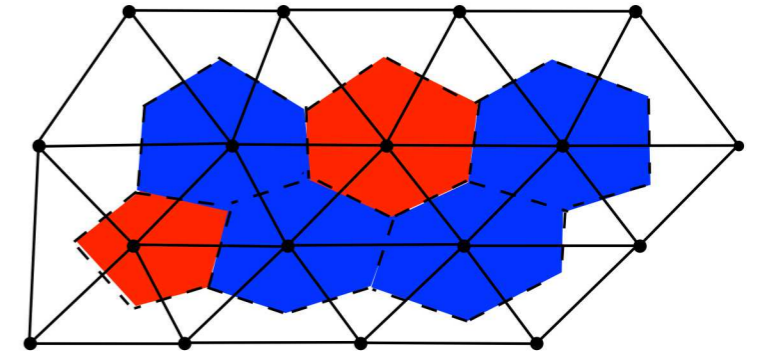
1. Residual gappy POD: $\tilde{\mathbf{r}} = \Phi_r(\mathbf{P}_r\Phi_r)^+ \mathbf{P}_r \mathbf{r}$, $\tilde{\mathbf{r}}^n = \Phi_r(\mathbf{P}_r\Phi_r)^+ \mathbf{P}_r \mathbf{r}^n$
2. Velocity gappy POD: $\tilde{\mathbf{r}}$ and $\tilde{\mathbf{r}}^n$ computed from $\tilde{\mathbf{f}} = \Phi_f(\mathbf{P}_f\Phi_f)^+ \mathbf{P}_f \mathbf{f}$
3. Flux and source gappy POD

*flux
gappy POD*



$$\tilde{\mathbf{h}} = \Phi_h(\mathbf{P}_h\Phi_h)^+ \mathbf{P}_h \mathbf{h}$$

*source
gappy POD*



$$\tilde{\mathbf{f}}^s = \Phi_s(\mathbf{P}_s\Phi_s)^+ \mathbf{P}_s \mathbf{f}^s$$

▸ $\tilde{\mathbf{r}}$ and $\tilde{\mathbf{r}}^n$ computed from $\tilde{\mathbf{f}} = \tilde{\mathbf{f}}^g + \tilde{\mathbf{f}}^s$ where $\tilde{\mathbf{f}}^g = \mathbf{B}\tilde{\mathbf{h}}$

+ **Structure preserving**: approximated velocity is sum of flux and source

+ **Less expensive**: no need to compute all fluxes for a control volume

$$\underset{\hat{\mathbf{v}} \in \mathbb{R}^p}{\text{minimize}} \quad \|\tilde{\mathbf{r}}(\Phi\hat{\mathbf{v}}, \Phi\hat{\mathbf{x}}, t)\|_2$$

$$\text{subject to } \bar{\mathbf{C}}\tilde{\mathbf{r}}(\Phi\hat{\mathbf{v}}, \Phi\hat{\mathbf{x}}, t) = \mathbf{0}$$

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

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

+ Can apply **different hyper-reduction** to the objective $\tilde{\mathbf{r}}$ and constraints $\tilde{\mathbf{r}}$

- Constraint hyper-reduction: **no longer strictly conservative**

+ Constraint hyper-reduction: **unneeded** if no source and few subdomains

Questions

Conservative Galerkin

$$\underset{\hat{\mathbf{v}} \in \mathbb{R}^p}{\text{minimize}} \quad \|\mathbf{r}(\Phi \hat{\mathbf{v}}, \Phi \hat{\mathbf{x}}, t)\|_2$$

$$\text{subject to } \bar{\mathbf{C}}\mathbf{r}(\Phi \hat{\mathbf{v}}, \Phi \hat{\mathbf{x}}, t) = \mathbf{0}$$

Conservative LSPG

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

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

- What are conditions for feasibility?
- How to handle infeasibility?
- How to solve?
- Are the two methods ever equivalent?
- How to apply hyper-reduction in a structure-preserving way?
- **How do *a posteriori* error bounds compare with standard ROMs?**

Discrete-time error bound: previous results

Theorem: state-space error bounds [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 $0 < h := |\alpha_0| - |\beta_0|\kappa\Delta t$,
3. A backward differentiation formula (BDF) time integrator is used,

$$\|\mathbf{x}^n - \Phi \hat{\mathbf{x}}_G^n\|_2 \leq \frac{1}{h} \|\mathbf{r}_G^n(\Phi \hat{\mathbf{x}}_G^n)\|_2 + \frac{1}{h} \sum_{\ell=1}^k |\alpha_\ell| \|\mathbf{x}^{n-\ell} - \Phi \hat{\mathbf{x}}_G^{n-\ell}\|_2$$

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

+ LSPG sequentially minimizes the error bound

Discrete-time error bound: new results

Theorem: local state-space error bounds

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 $0 < h := |\alpha_0| - |\beta_0|\kappa\Delta t$,
3. A backward differentiation formula (BDF) time integrator is used,

$$\|\mathbf{x}^n - \Phi \hat{\mathbf{x}}_G^n\|_2 \leq (1 + \zeta_G) \frac{1}{h} \|\mathbf{r}_G^n(\Phi \hat{\mathbf{x}}_G^n)\|_2 + \frac{1}{h} \sum_{\ell=1}^k |\alpha_\ell| \|\mathbf{x}^{n-\ell} - \Phi \hat{\mathbf{x}}_G^{n-\ell}\|_2$$

$$\|\mathbf{x}^n - \Phi \hat{\mathbf{x}}_{\text{LSPG}}^n\|_2 \leq \frac{1}{h} \|\mathbf{r}_{\text{LSPG}}^n(\Phi \hat{\mathbf{x}}_{\text{LSPG}}^n)\|_2 + \frac{1}{h} \sum_{\ell=1}^k |\alpha_\ell| \|\mathbf{x}^{n-\ell} - \Phi \hat{\mathbf{x}}_{\text{LSPG}}^{n-\ell}\|_2$$

$$+ \frac{\zeta_{\text{LSPG}}^n \Delta t}{h} \|(\mathbf{I} - [\mathbb{P}^n]^T \mathbb{P}^n) \mathbf{f}(\Phi \hat{\mathbf{x}}_{\text{LSPG}}^n)\|_2 + \frac{\zeta_{\text{LSPG}}^n \|\Delta^n\|_2}{h^n} \sum_{\ell=0}^k |\alpha_\ell^n| \|\hat{\mathbf{x}}_{\text{LSPG}}^{n-\ell}\|_2$$

$$\triangleright \zeta_G := \|\Sigma_G^{-1} \mathbf{U}_G^T \bar{\mathbf{C}}\|_2, \zeta_{\text{LSPG}} := \|[\Sigma_{\text{LSPG}}^n]^{-1} [\mathbf{U}_{\text{LSPG}}^n]^T \bar{\mathbf{C}}\|_2, \Delta^n := \Psi^n (\Phi^T \Psi^n)^{-1} - \Phi$$

$$\triangleright \bar{\mathbf{C}} \Phi = \mathbf{U}_G \Sigma_G \mathbf{V}_G^T, \bar{\mathbf{C}} \Psi^n (\Phi^T \Psi^n)^{-1} = \mathbf{U}_{\text{LSPG}}^n \Sigma_{\text{LSPG}}^n [\mathbf{V}_{\text{LSPG}}^n]^T$$

- State-space **error bound is larger** for both models
- LSPG **no longer strictly minimizes the residual**

Discrete-time error bound: new results

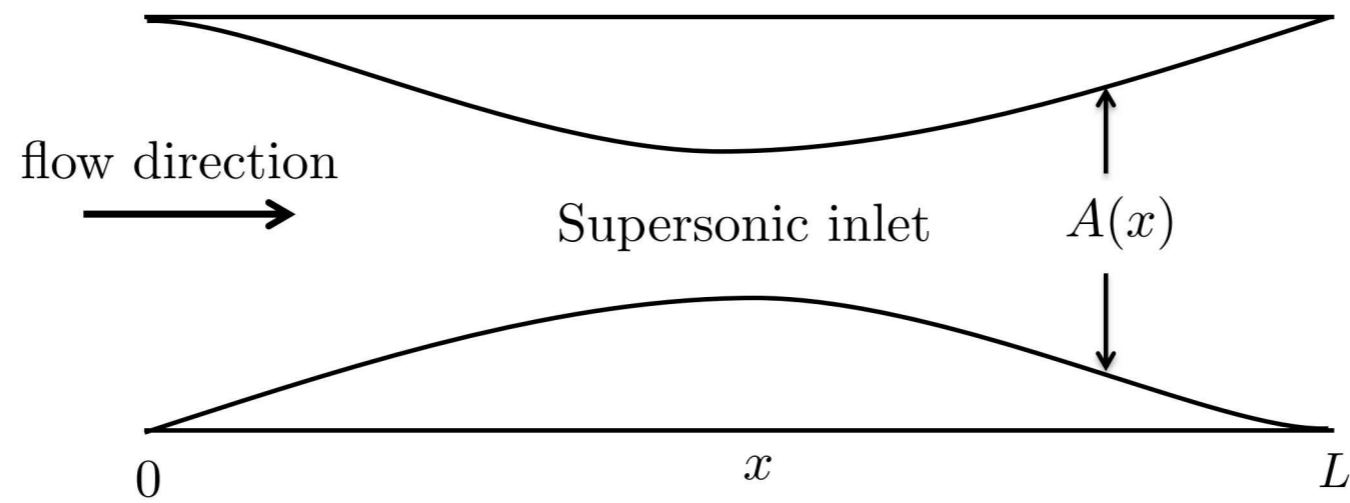
Lemma: local conserved-quantity error bounds

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

$$\begin{aligned} \|\bar{\mathbf{C}}(\mathbf{x}^n - \Phi \hat{\mathbf{x}}^n)\|_2 &\leq \sum_{\ell=0}^k \frac{|\beta_{\ell}^n| \Delta t}{|\alpha_0^n|} \|\bar{\mathbf{C}}\mathbf{f}(\mathbf{x}^{n-\ell}) - \bar{\mathbf{C}}\mathbf{f}(\Phi \hat{\mathbf{x}}^{n-\ell})\|_2 \\ &\quad + \sum_{\ell=1}^k \frac{|\alpha_{\ell}^n|}{|\alpha_0^n|} \|\bar{\mathbf{C}}(\mathbf{x}^{n-\ell} - \Phi \hat{\mathbf{x}}^{n-\ell})\|_2 \end{aligned}$$

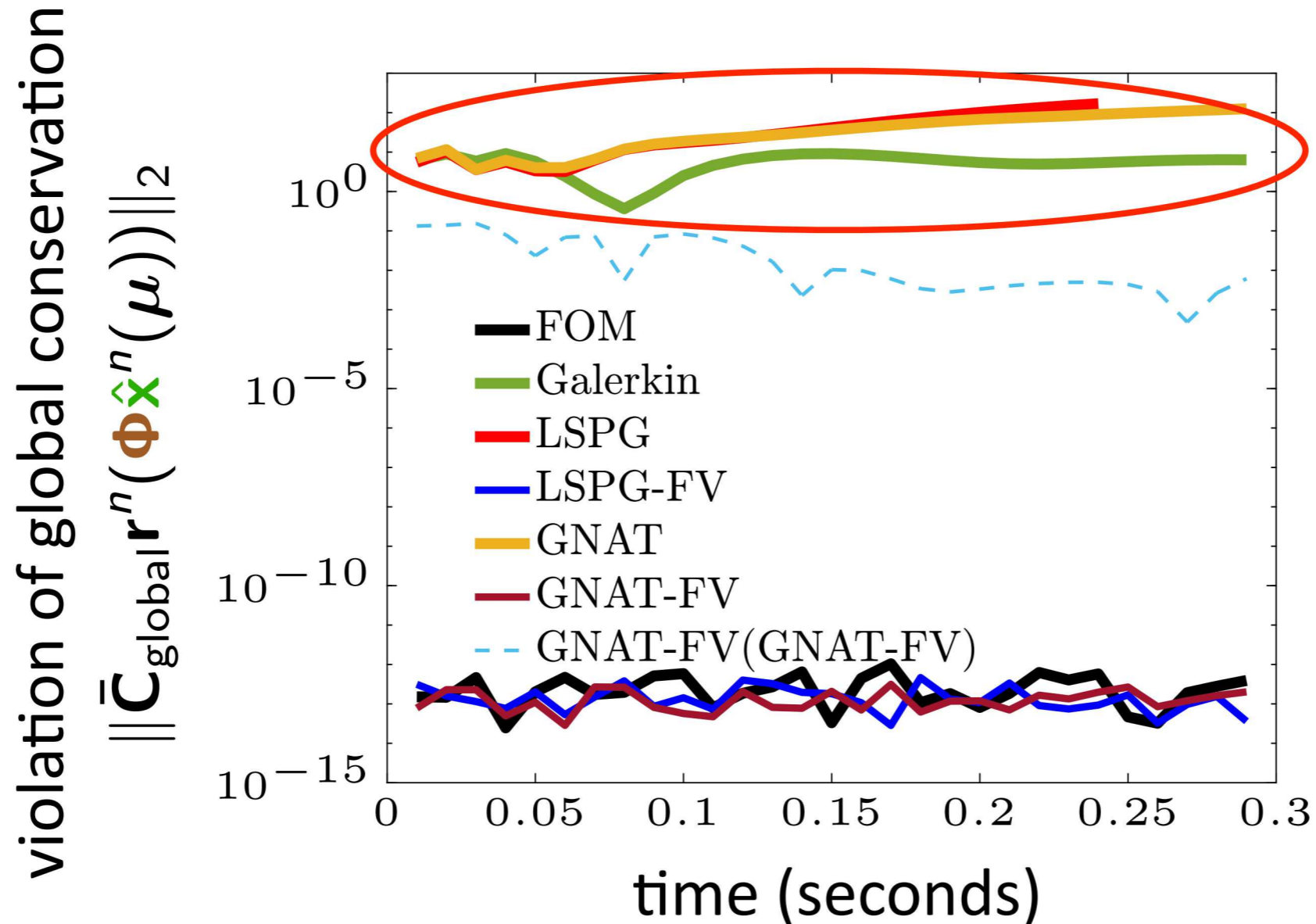
- Error depends only on velocity error on *decomposed mesh*
- + No source, global conservation: error due to **flux error along boundary!**

Quasi-1D Euler equation



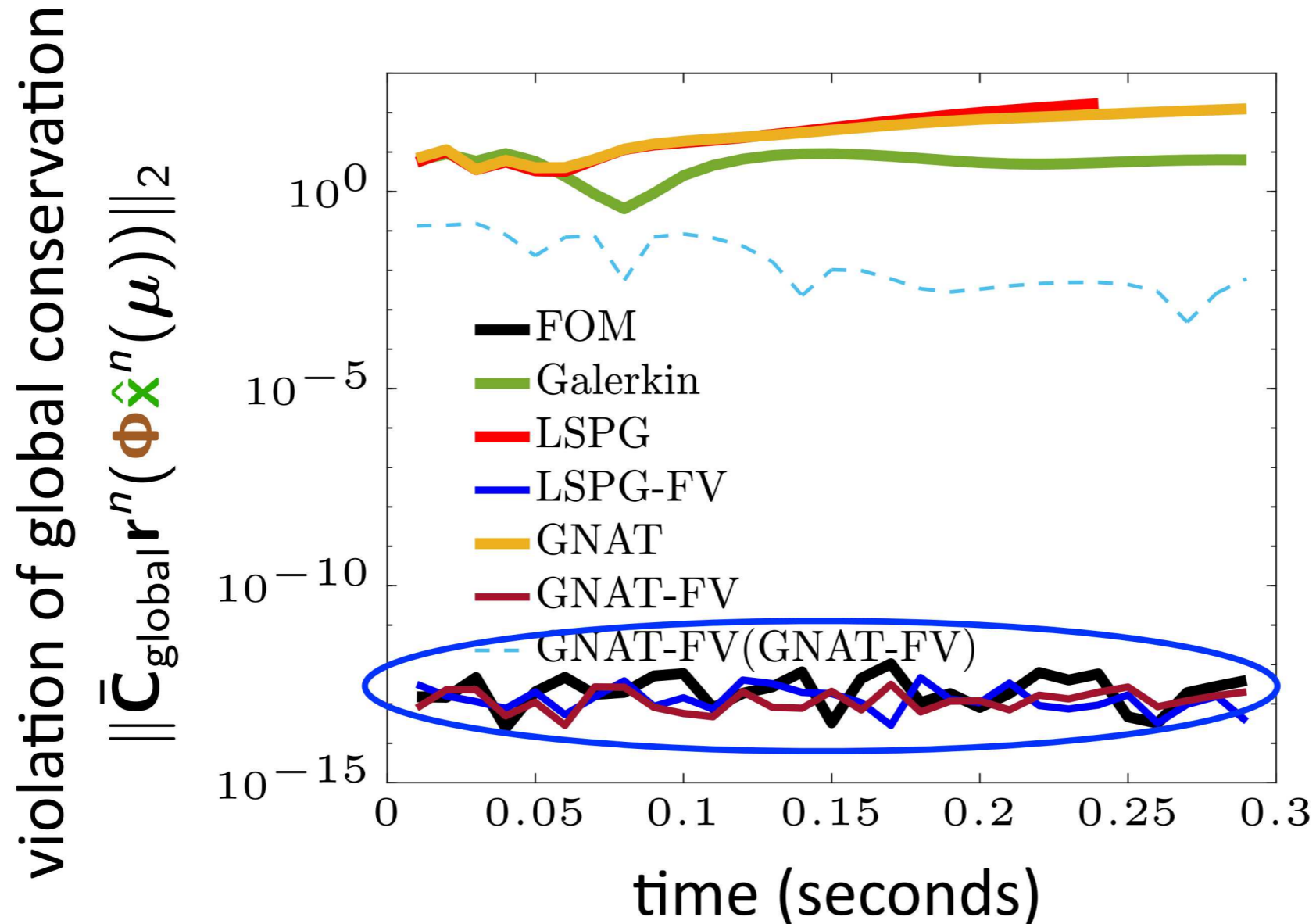
- 3 conserved variables: $u_1 = A\rho$, $u_2 = A\rho u$, $u_3 = Ae$
- Flux: $g_1 = A\rho u$, $g_2 = A(\rho u^2 + p)$, $g_3 = A(e + p)u$
- Source: $s_1 = s_3 = 0$, $s_2 = p \frac{\partial A}{\partial x}$
- Domain length: $L=0.25$ m
- Time domain: $t \in [0, 0.29$ s]
- Time integration: backward Euler with $\Delta t = 0.01$ s
- Parameter: the initial Mach number at the domain center
- Considered ROMs:
 - Galerkin
 - GNAT: hyper-reduced objective
 - LSPG
 - GNAT-FV: hyper-reduced objective
 - LSPG-FV
 - GNAT-FV(GNAT-FV): hyper-reduced objective & constraints

Global conservation ($\bar{\mathcal{M}} = \bar{\mathcal{M}}_{\text{global}}$)



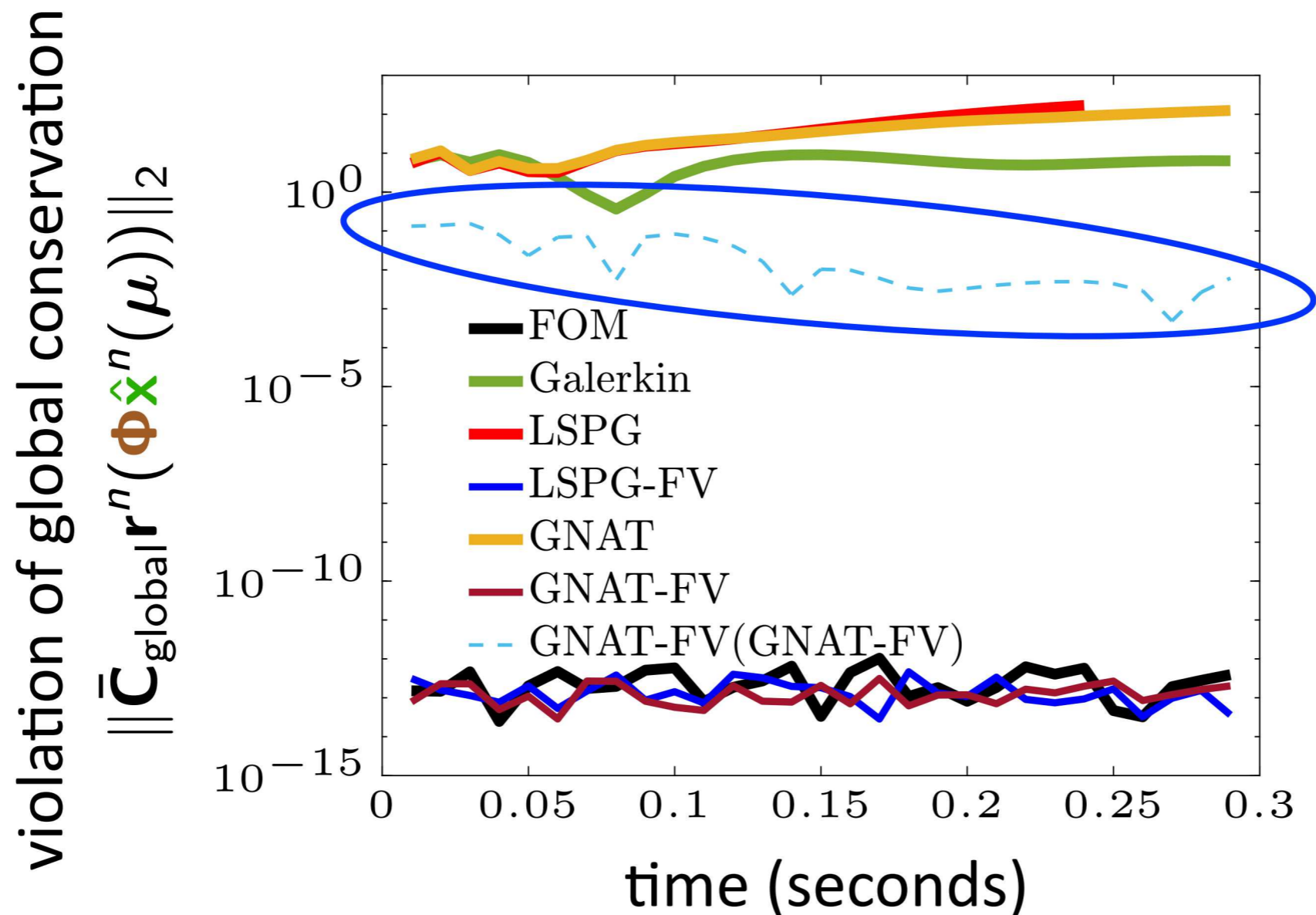
- Standard ROMs: significant **global-conservation violation**

Global conservation ($\bar{\mathcal{M}} = \bar{\mathcal{M}}_{\text{global}}$)



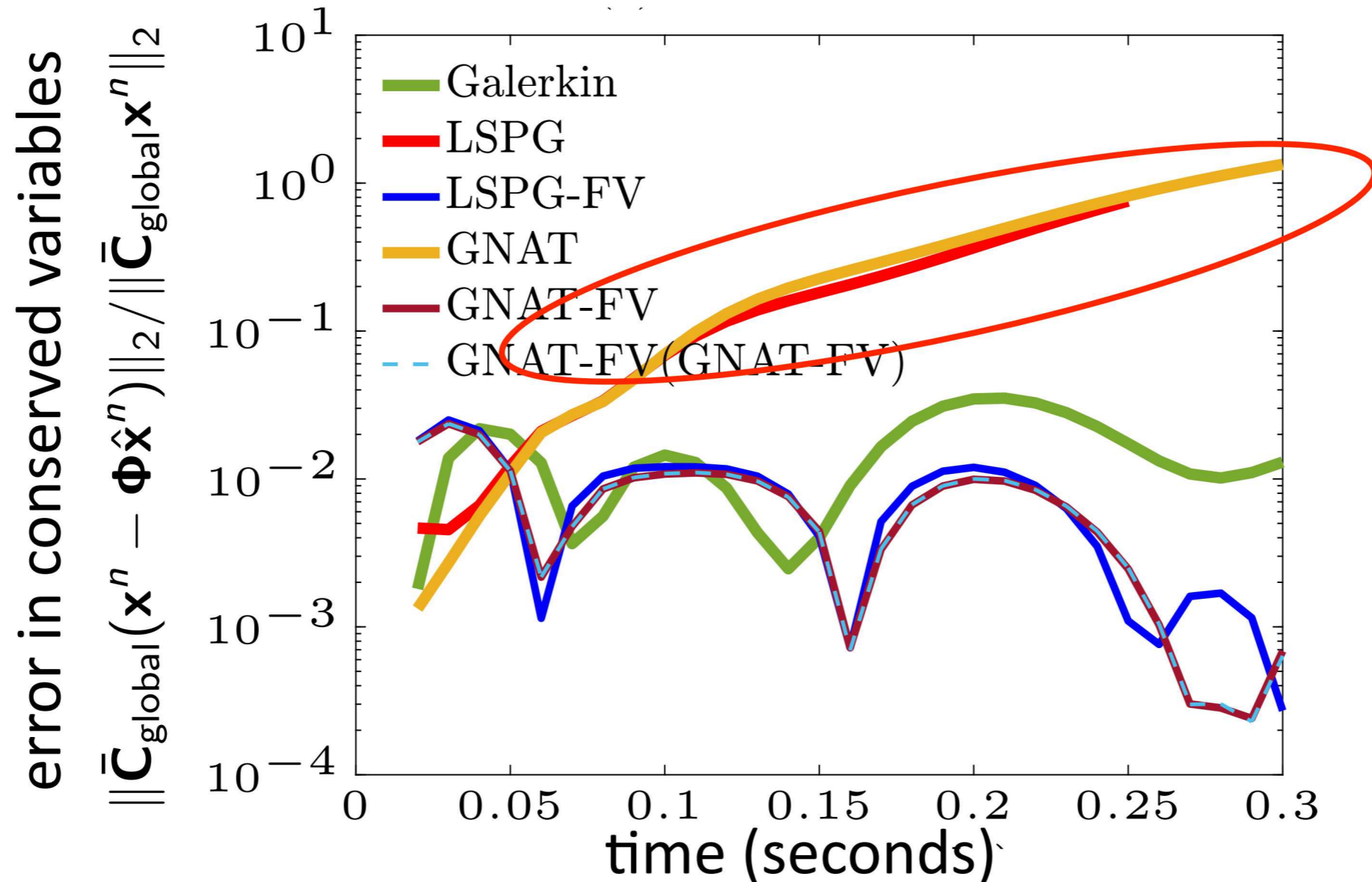
- Standard ROMs: significant **global-conservation violation**
- + Conservative ROMs: **global conservation satisfied (always feasible)**

Global conservation ($\bar{\mathcal{M}} = \bar{\mathcal{M}}_{\text{global}}$)



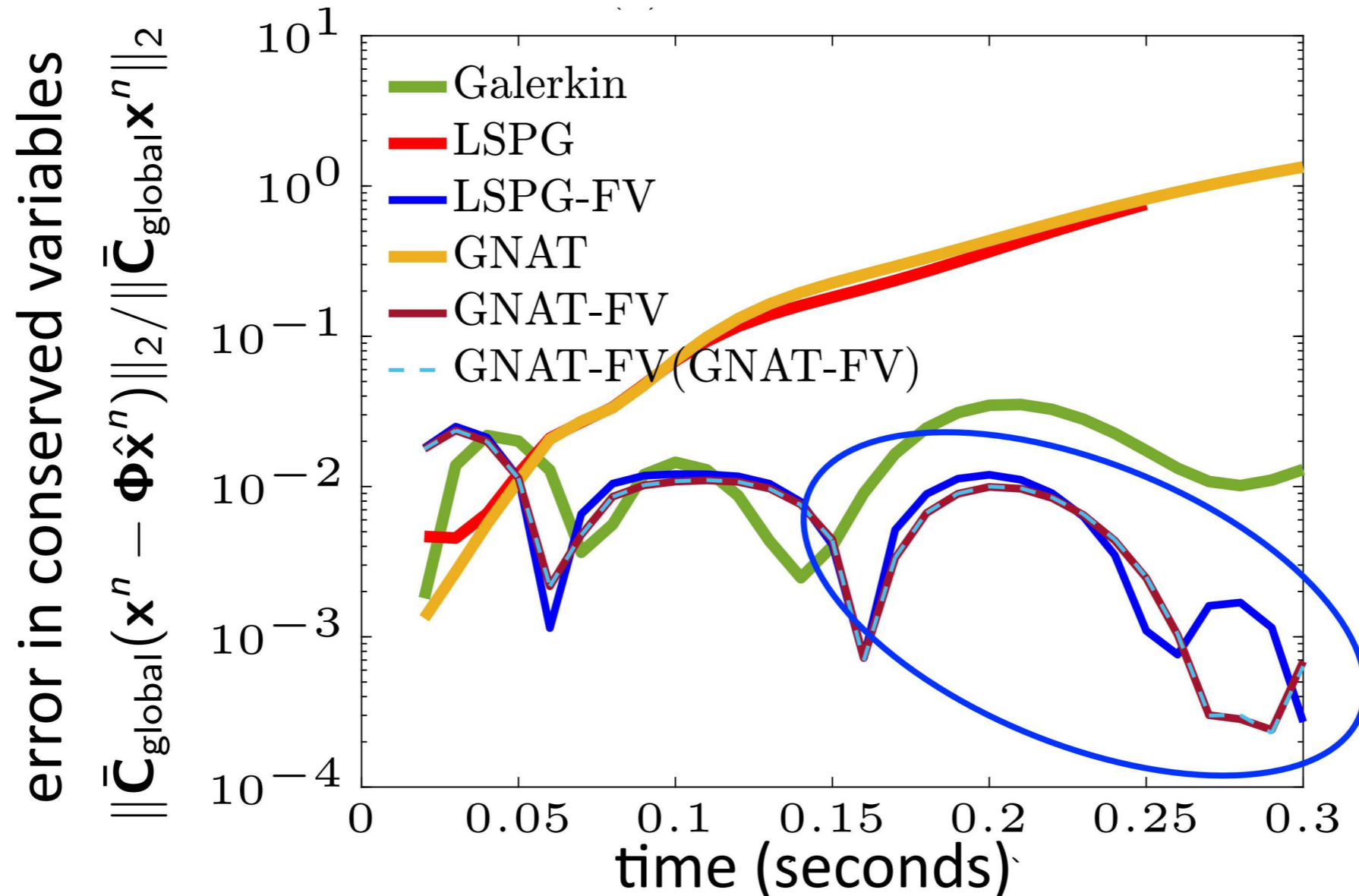
- Standard ROMs: significant **global-conservation violation**
- + Conservative ROMs: **global conservation satisfied (always feasible)**
- + Hyper-reduced constraints: **relatively small global-conservation violation**

Error in conserved variables ($\bar{\mathcal{M}} = \bar{\mathcal{M}}_{\text{global}}$)



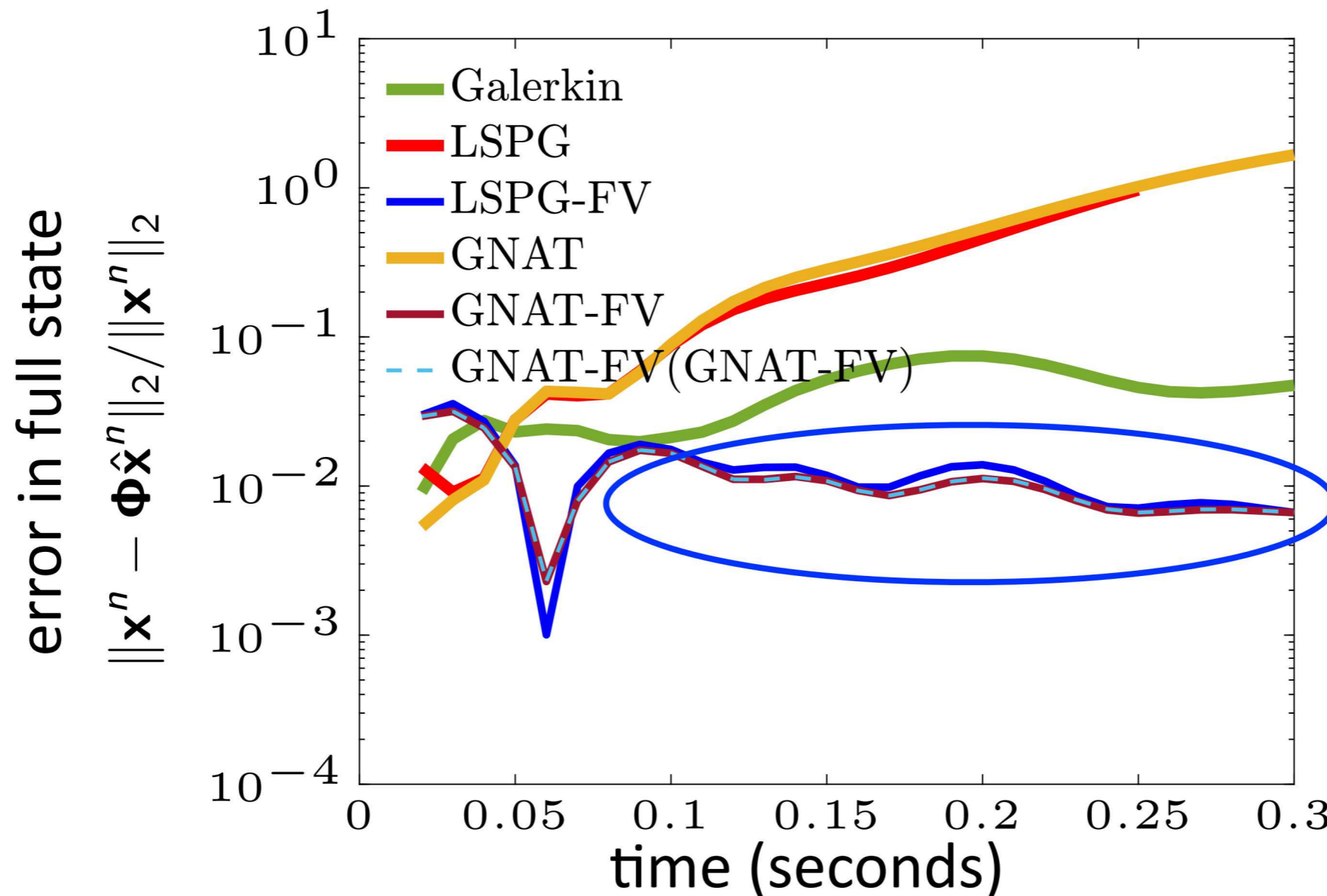
- Standard ROMs: can produce large errors in conserved quantities

Error in conserved variables ($\bar{\mathcal{M}} = \bar{\mathcal{M}}_{\text{global}}$)



- Standard ROMs: can produce large errors in conserved quantities
- + Conservative ROMs: **small** (but **nonzero**) errors in conserved quantities

Error in conserved variables ($\bar{\mathcal{M}} = \bar{\mathcal{M}}_{\text{global}}$)

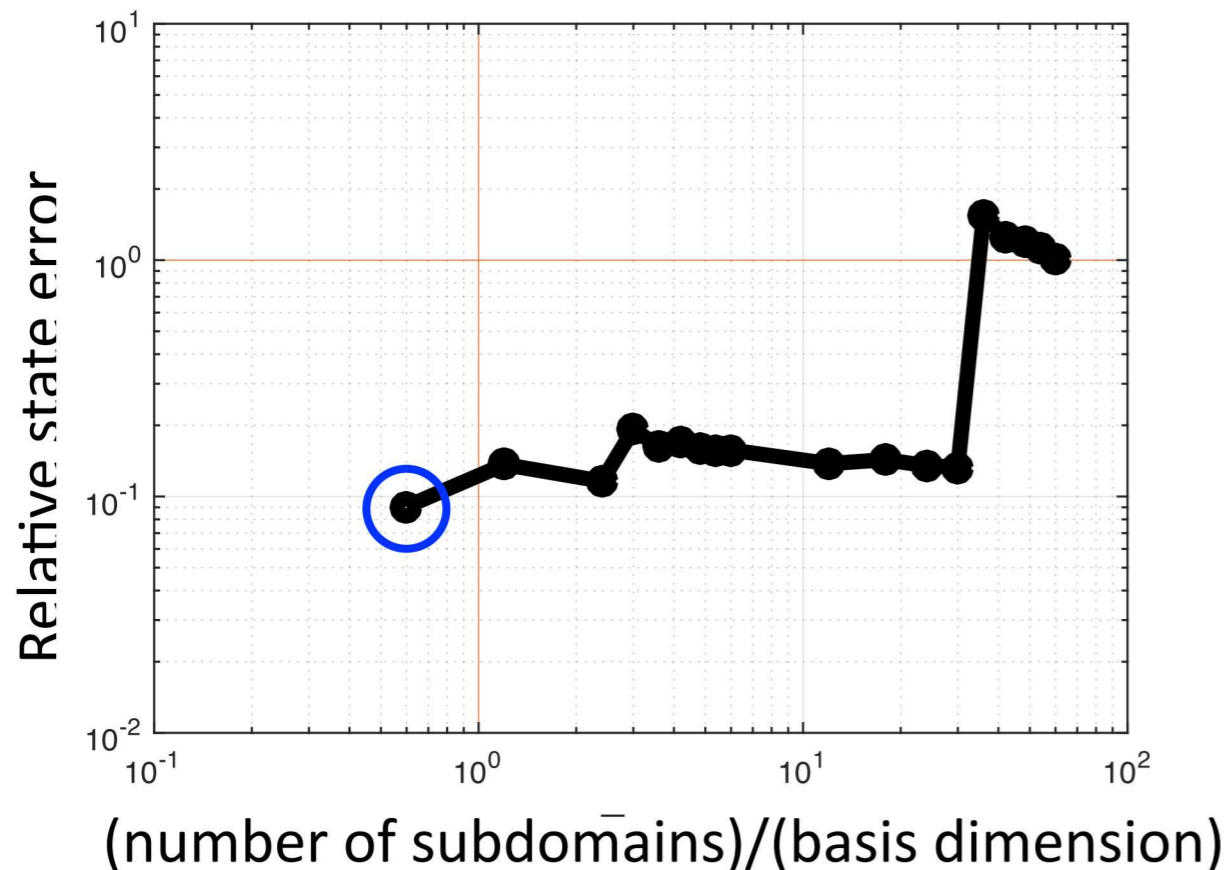


- + Conservative ROMs: **smaller state-space errors**
- Similar behavior of full-state error and globally-conserved quantity error!
- + Implies satisfying global conservation **can improve overall accuracy**

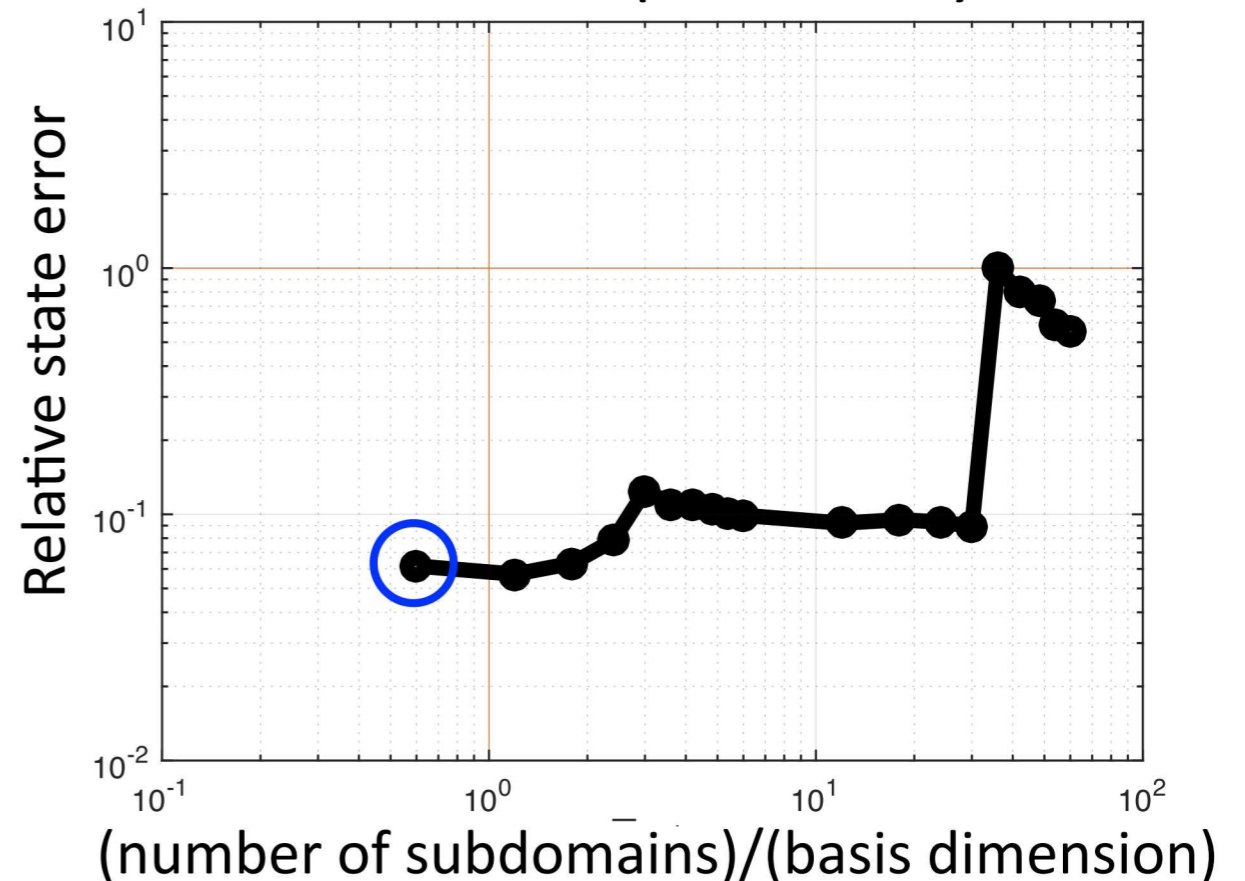
Varying number of subdomains

- If infeasible, adopt penalty formulation with $\rho = 10^3$

LSPG-FV

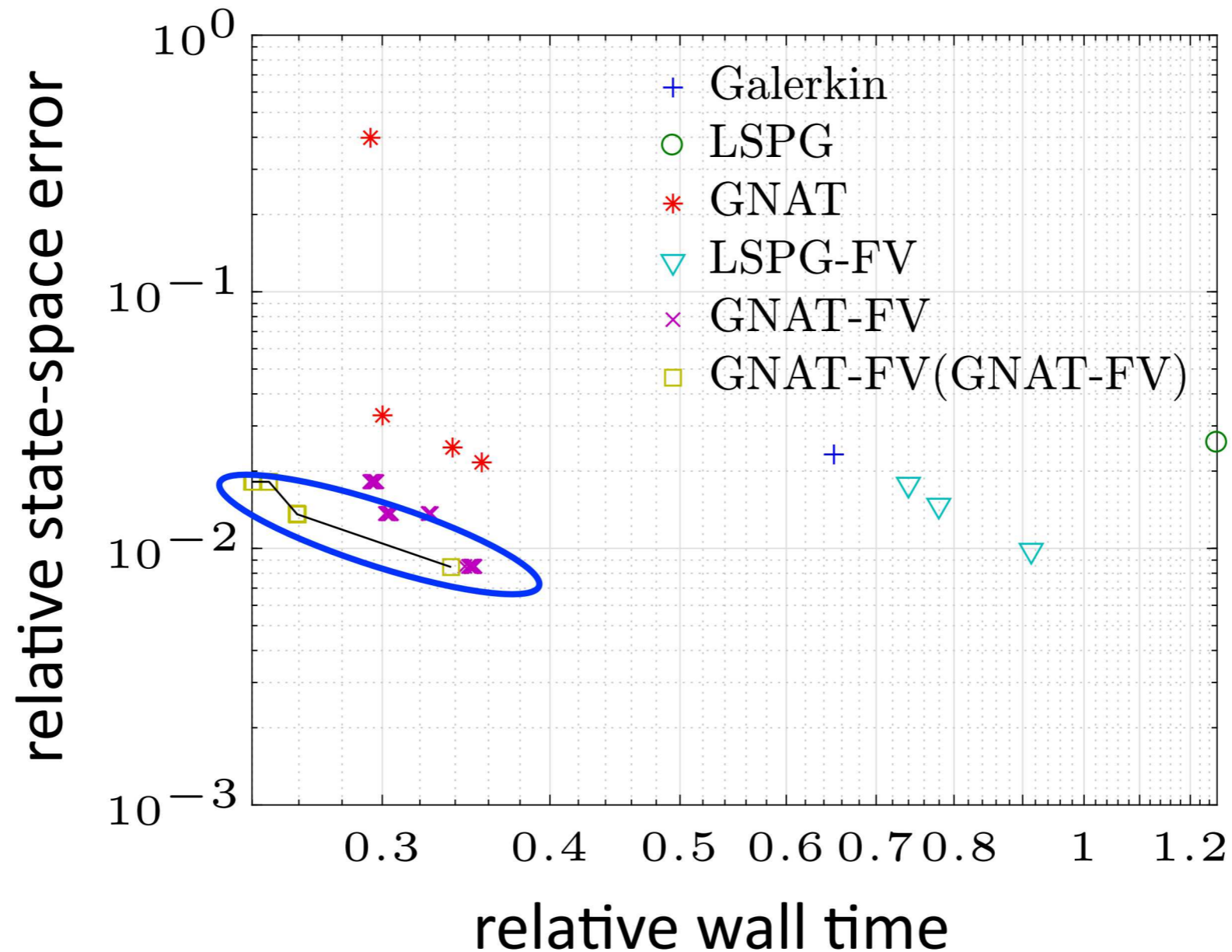


GNAT-FV(GNAT-FV)



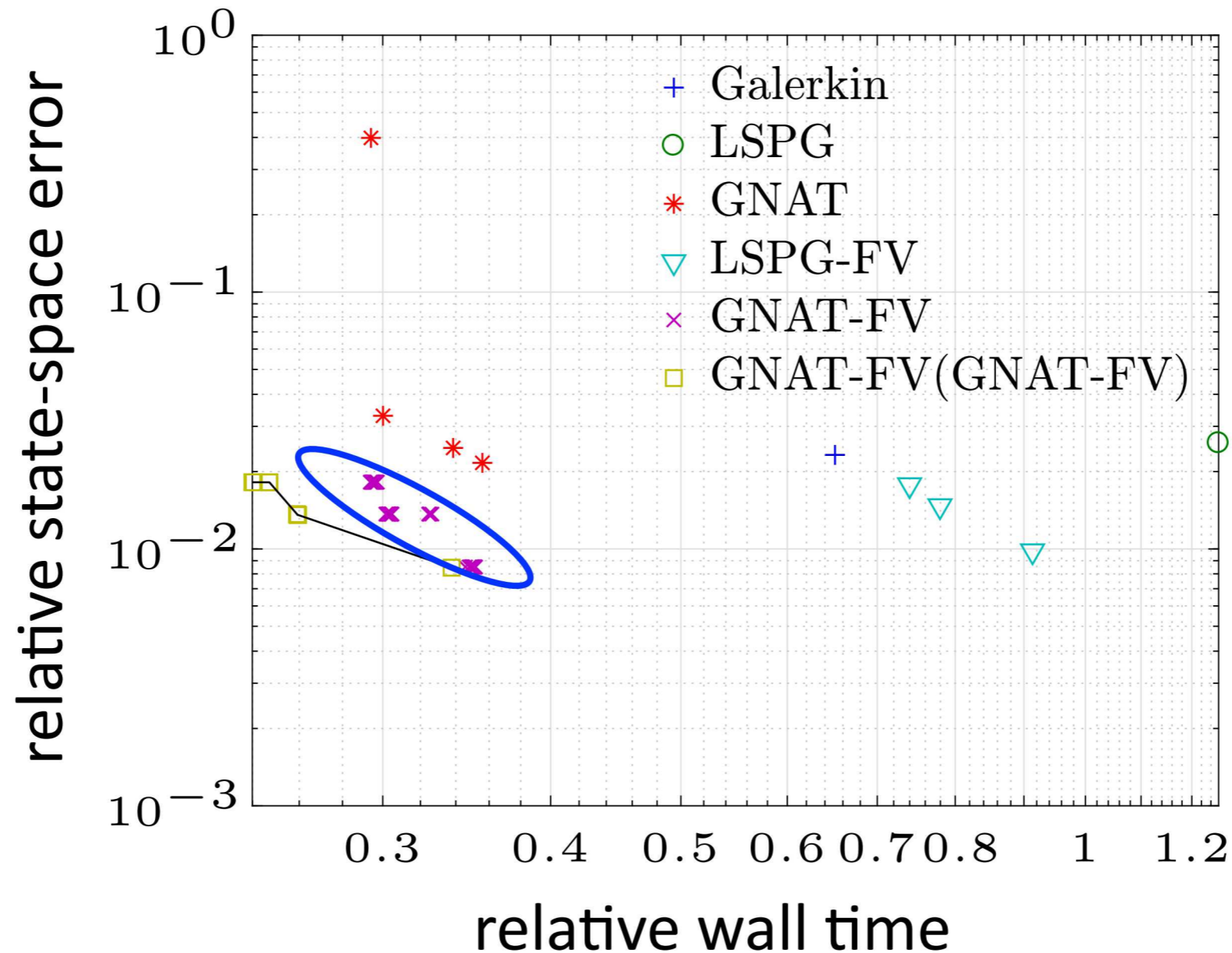
- + Global conservation yields the best performance
- + Global conservation reduces errors by 10X from the unconstrained case

Pareto optimality



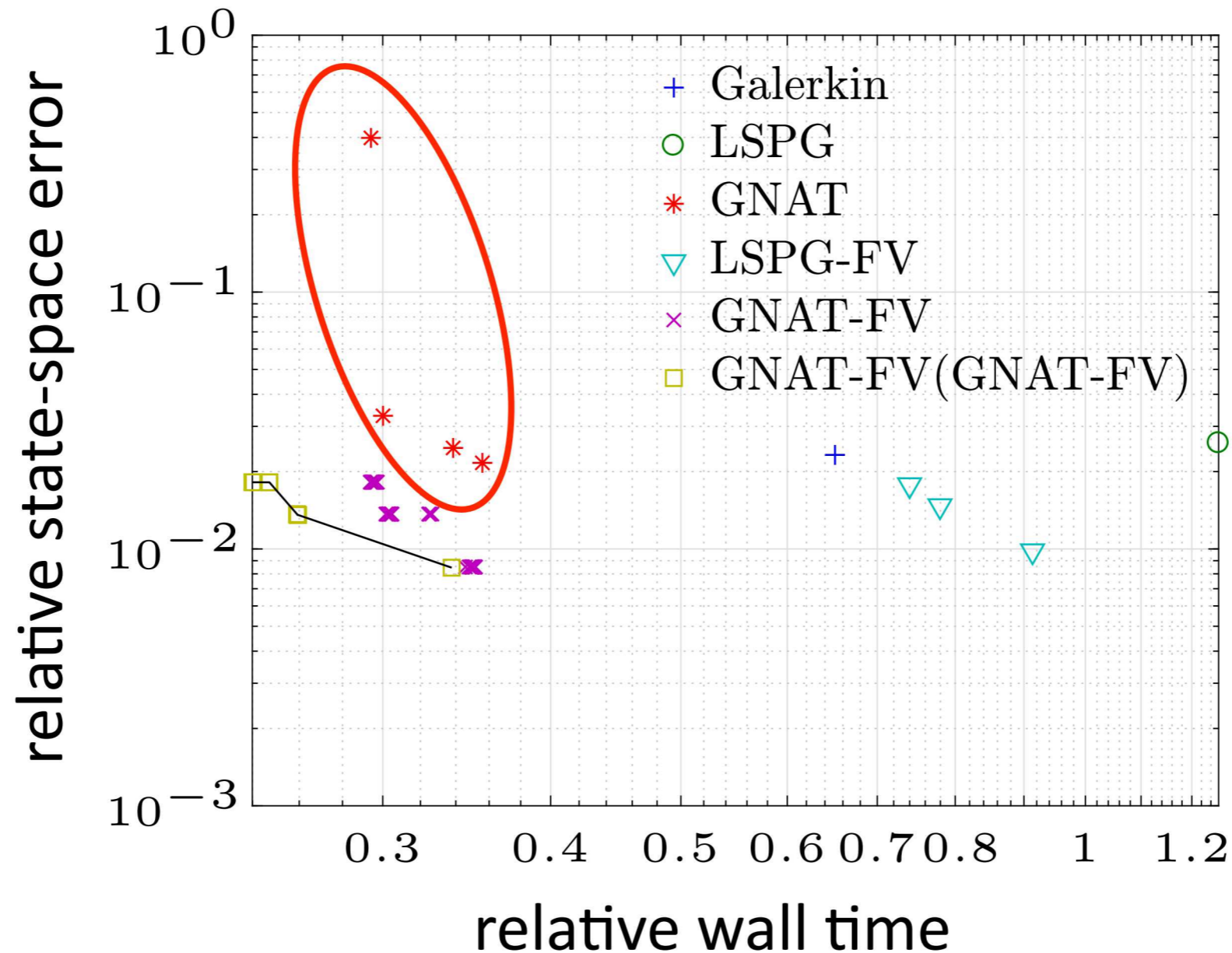
+ GNAT-FV(GNAT-FV) (hyper-reduced objective/constraints): Pareto optimal

Pareto optimality



- + GNAT-FV(GNAT-FV) (hyper-reduced objective/constraints): Pareto optimal
- + GNAT-FV (hyper-reduced objective, exact constraints): second-best

Pareto optimality



- + GNAT-FV(GNAT-FV) (hyper-reduced objective/constraints): Pareto optimal
- + GNAT-FV (hyper-reduced objective, exact constraints): second-best
- GNAT (hyper-reduced objective, no constraints): dominated

Conclusions

- + Reduced-order models that enforce conservation
- + Conditions that determine when conservation enforcement is ensured
- + Ways to handle infeasibility
- + Structure-preserving hyper-reduction that respects the velocity structure
- + *A posteriori* error bounds
- Numerical experiments:
 - + global conservation can reduce errors by 10X
 - + hyper-reduced constraints nearly as accurate as strict constraints

Questions?

Reference: C., Choi, and Sargsyan. Conservative model reduction for finite-volume models. *Journal of Computational Physics*, 371:280–314, 2018.

Conservative Galerkin

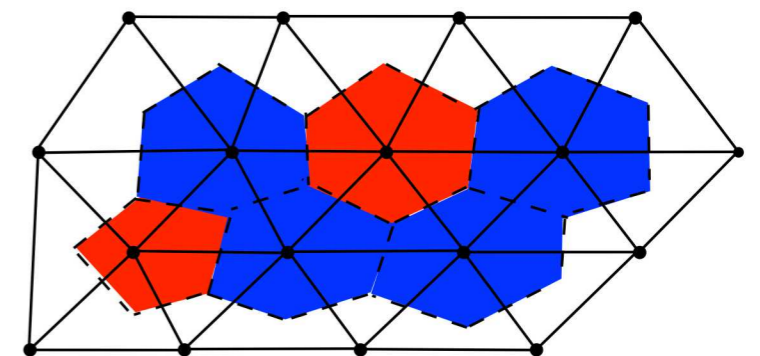
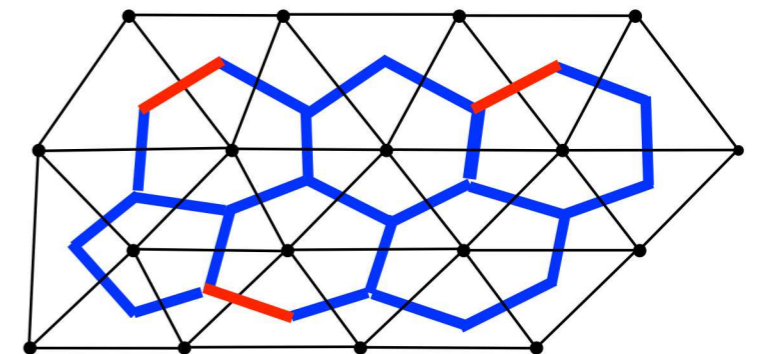
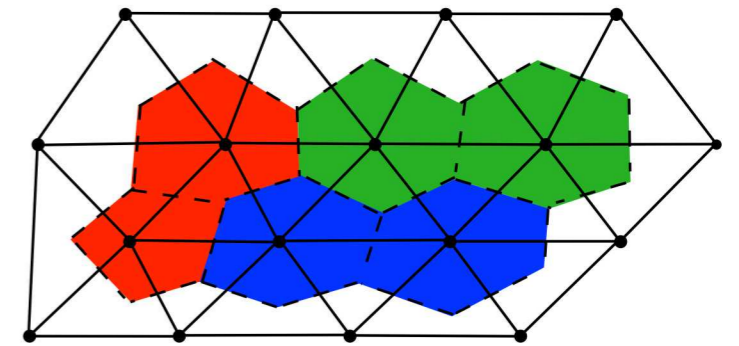
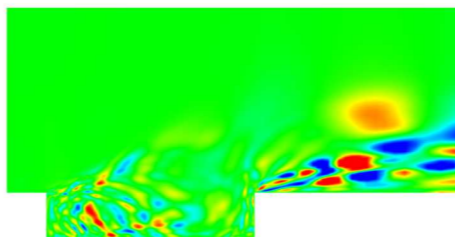
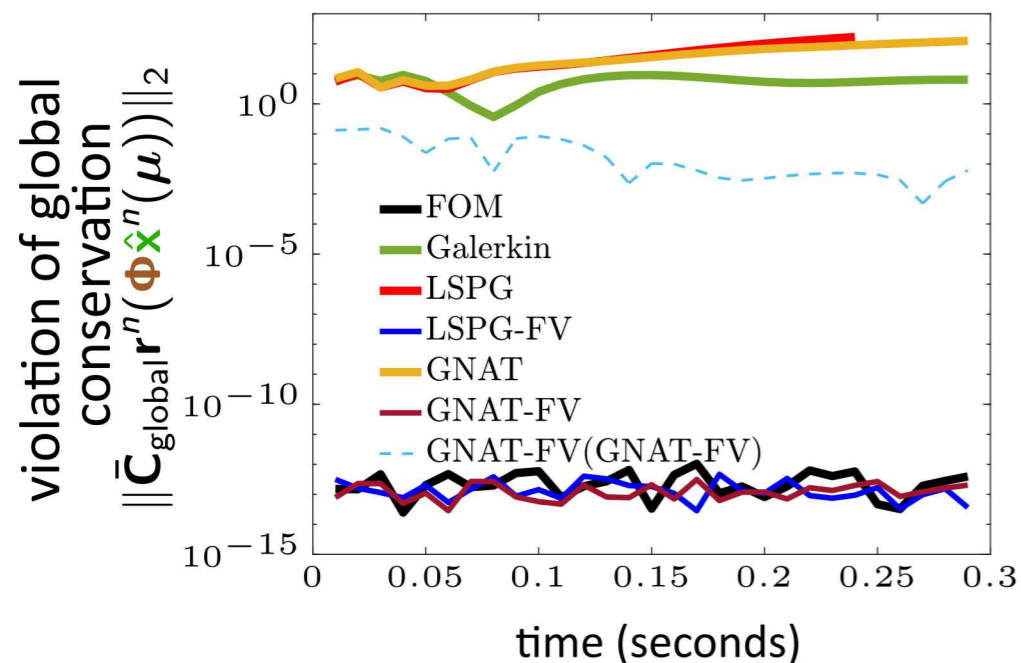
$$\text{minimize}_{\hat{\mathbf{v}} \in \mathbb{R}^p} \|\mathbf{r}(\Phi \hat{\mathbf{v}}, \Phi \hat{\mathbf{x}}, t)\|_2$$

$$\text{subject to } \bar{\mathbf{C}}\mathbf{r}(\Phi \hat{\mathbf{v}}, \Phi \hat{\mathbf{x}}, t) = \mathbf{0}$$

Conservative LSPG

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

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



Sandia National Laboratories is a multimission laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC., a wholly owned subsidiary of Honeywell International, Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA-0003525. Lawrence Livermore National Laboratory is operated by Lawrence Livermore National Security, LLC, for the U.S. Department of Energy, National Nuclear Security Administration under Contract DE-AC52-07NA27344.