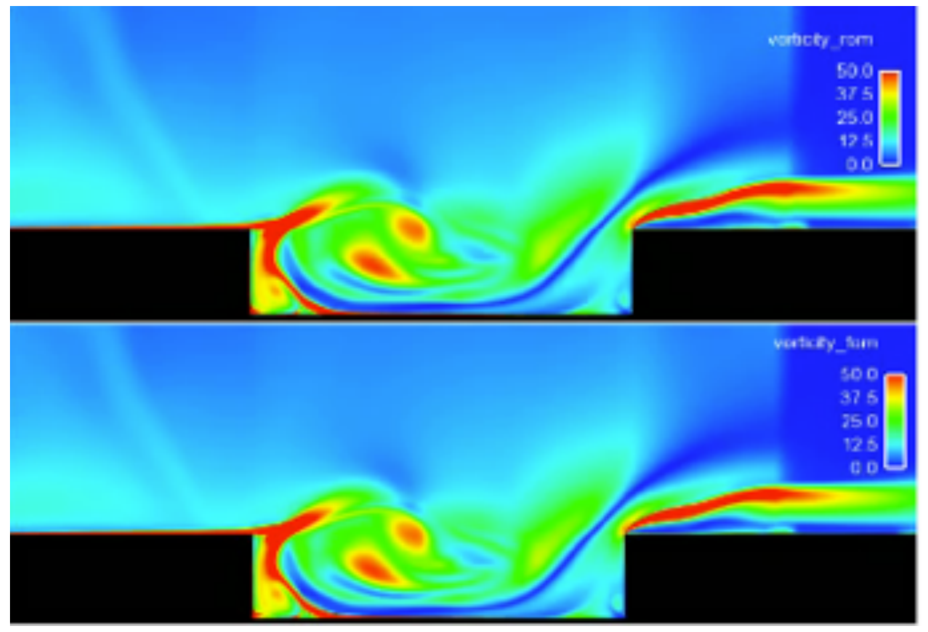
SAND2016-6958C

Nonlinear model reduction in computational fluid dynamics



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References:

- K. Carlberg, C. Bou-Mosleh, and C. Farhat. "Efficient non-linear model reduction via a least-squares Petrov–Galerkin projection and compressive tensor approximations," International Journal for Numerical Methods in Engineering, Vol. 86, No. 2, p. 155–181 (2011).
- K. Carlberg, C. Farhat, J. Cortial, and D. Amsallam. "The GNAT method for nonlinear model reduction: Effective implementation and application to computational fluid dynamics and turbulent flows," Journal of Computational Physics, Vol. 242, p. 623–647 (2013).
- K. Carlberg, M. Barone, and H. Antil. "Galerkin v. least-squares Petrov–Galerkin projection in nonlinear model reduction," arXiv e-Print 1504.03749 (2015).
- K. Carlberg, Y. Choi, and S. Sargsyan, "Structure-preserving nonlinear model reduction for finite-volume models," *in preparation* (2015).

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Goal: break computational barrier

High-fidelity simulation

+ Indispensable for *analysis, design,* and *qualification* of aerospace systems
- *High fidelity*: large-scale nonlinear dynamical-system models

+ *Validated RANS/LES model:* matches experiment to within 5%
- Large scale: 86 million cells, 200,000 time steps
- *High simulation costs*: 6 weeks, 5000 cores

barrier

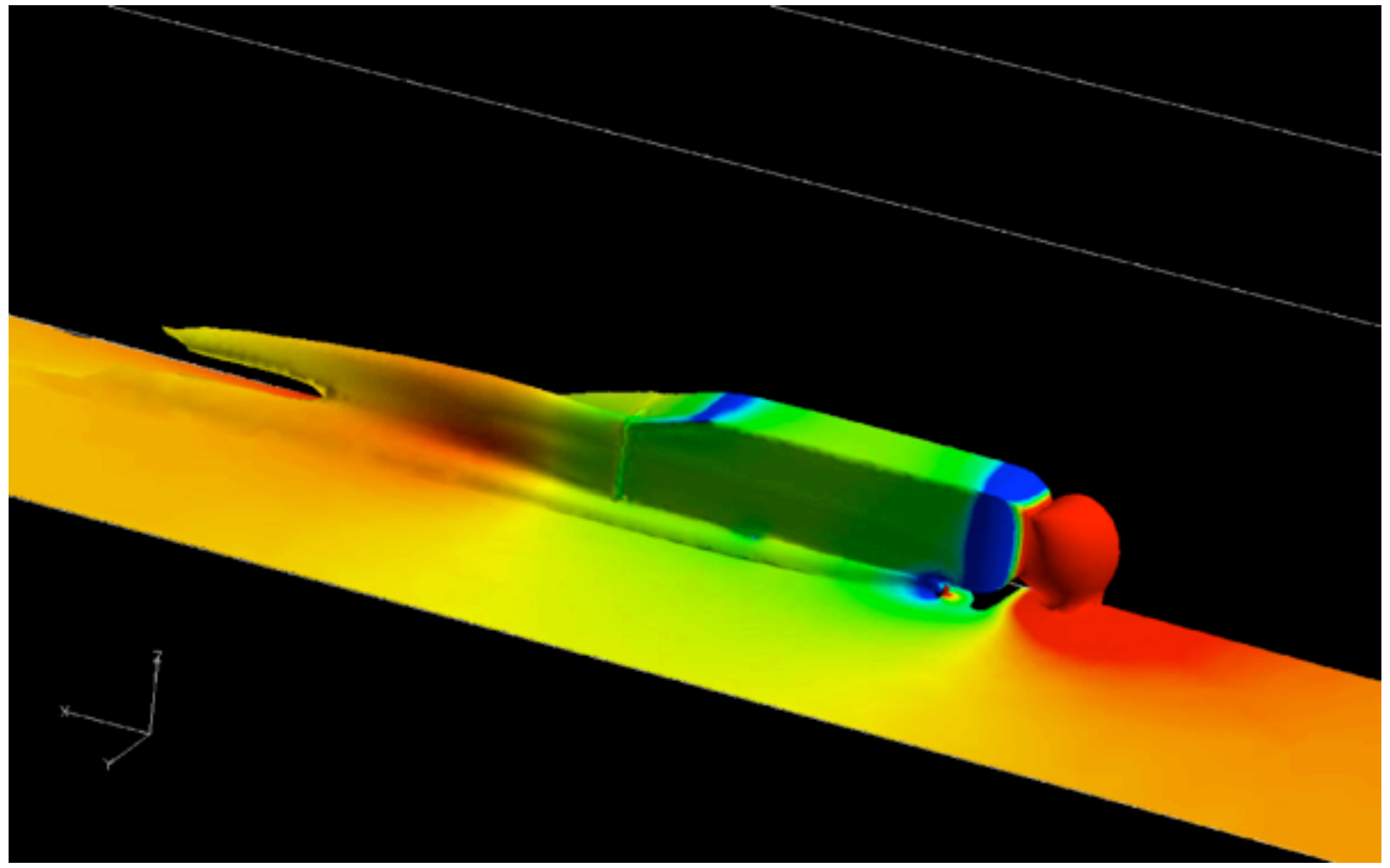
Time-critical aerospace applications

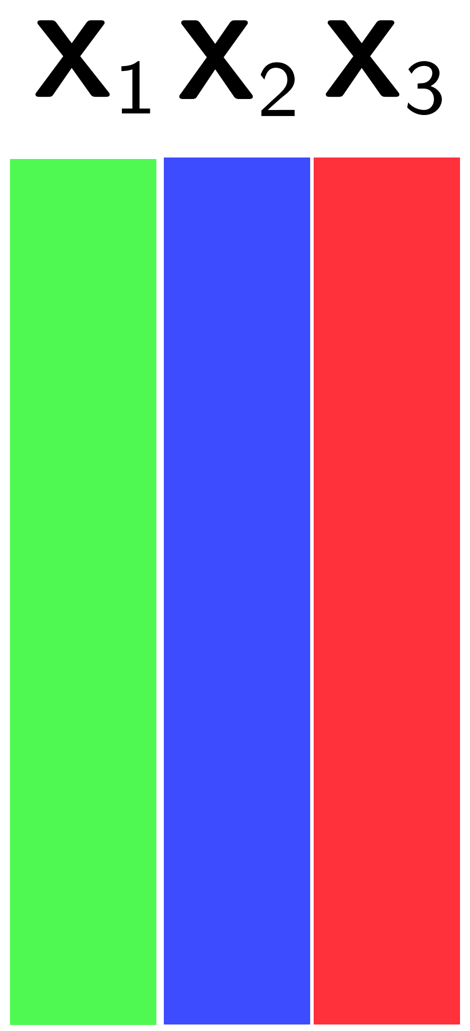
◉ rapid design ◉ UQ ◉ structural health monitoring ◉ model predictive control

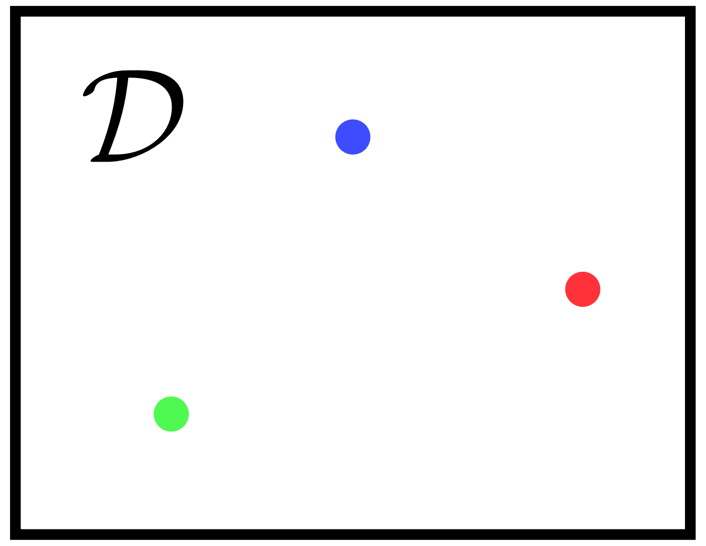
Offline: proper orthogonal decomposition

Full-order model: $\frac{d\mathbf{x}}{dt} = \mathbf{f}(\mathbf{x}; t, \boldsymbol{\mu}); \quad \mathbf{x}(0, \boldsymbol{\mu}) = \mathbf{x}_0(\boldsymbol{\mu}), \quad t \in [0, T], \quad \boldsymbol{\mu} \in \mathcal{D}$

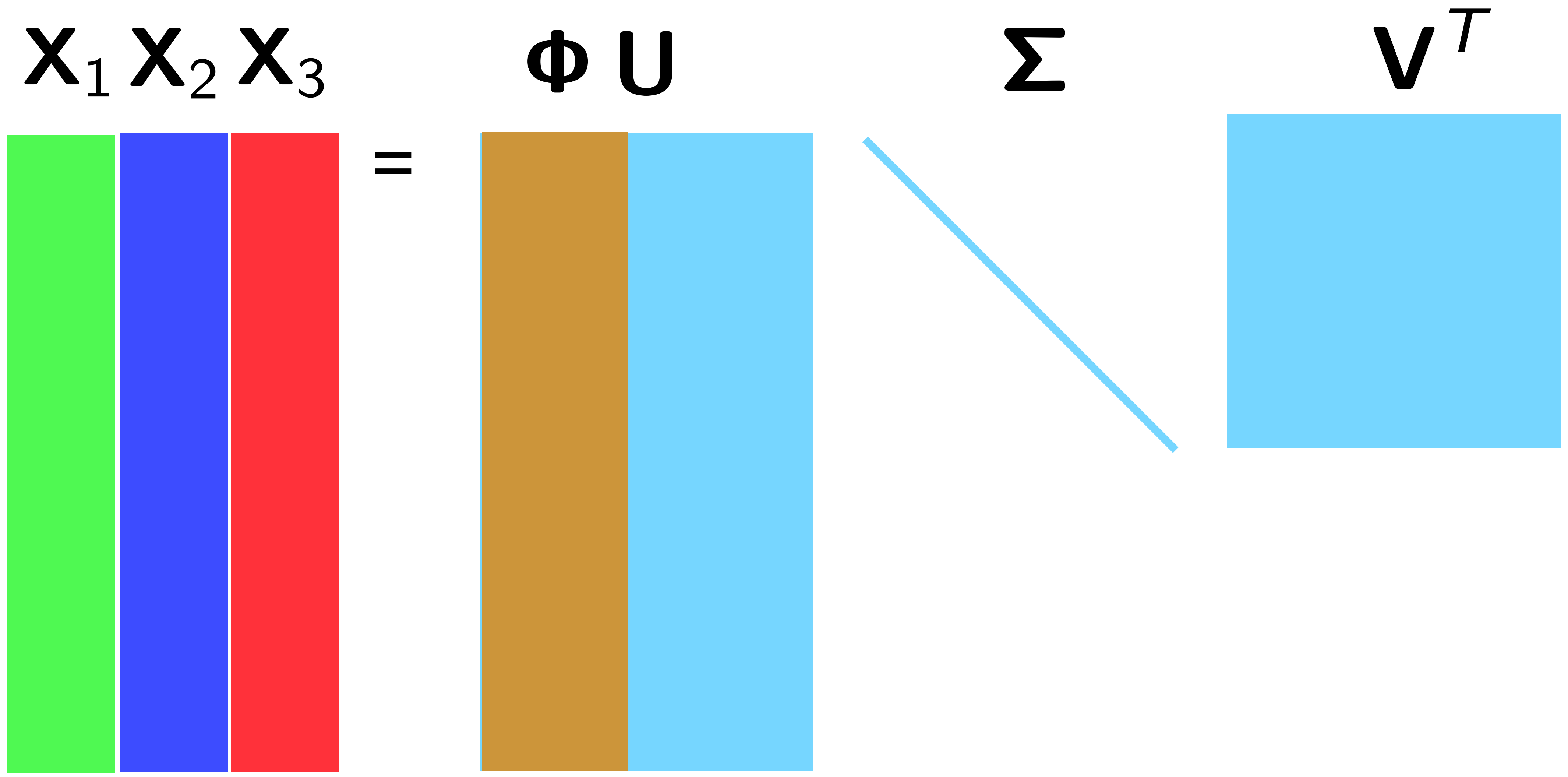
1. Collect state snapshots







2. Compression via SVD:



Online: projection

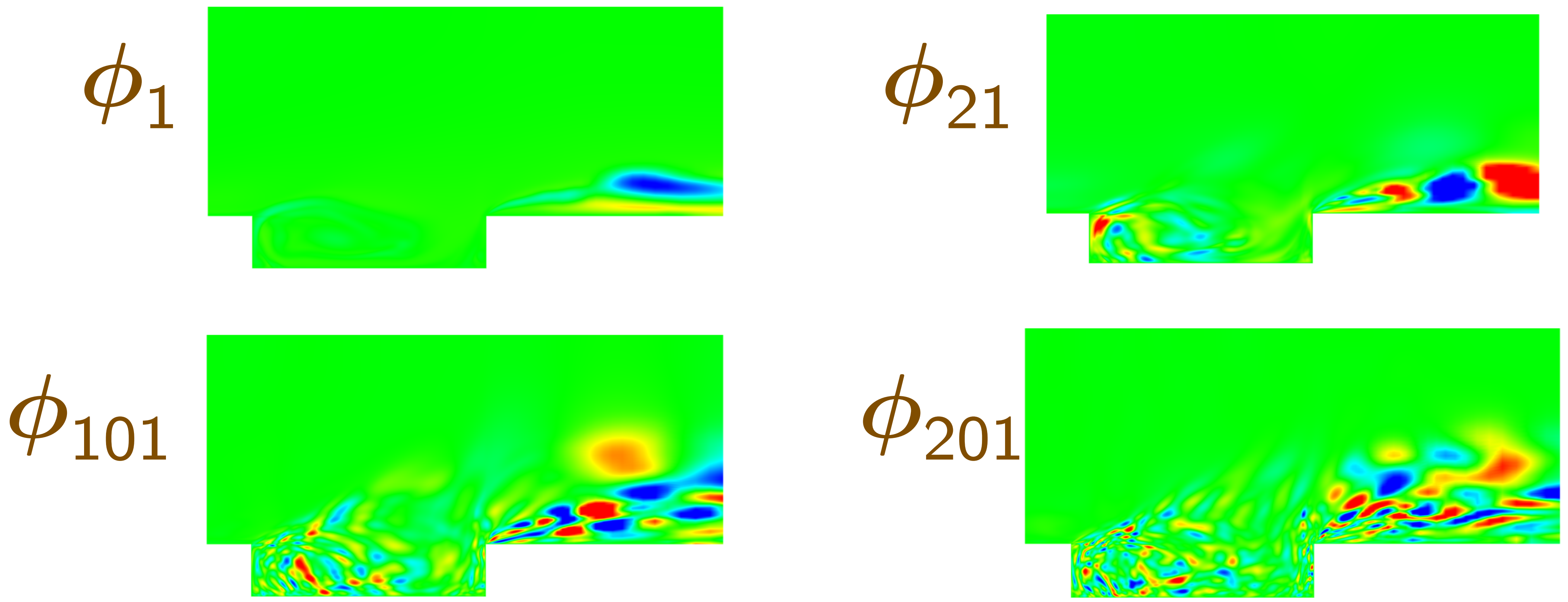
Full-order model: $\frac{d\mathbf{x}}{dt} = \mathbf{f}(\mathbf{x}; t, \boldsymbol{\mu}); \quad \mathbf{x}(0, \boldsymbol{\mu}) = \mathbf{x}_0(\boldsymbol{\mu}), \quad t \in [0, T], \quad \boldsymbol{\mu} \in \mathcal{D}$

1. Reduce number of unknowns

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

2. Reduce number of equations

$$\boldsymbol{\Psi}(\hat{\mathbf{x}}, t)^T \left(\mathbf{f}(\boldsymbol{\Phi}\hat{\mathbf{x}}; t, \mu) - \boldsymbol{\Phi}\frac{d\hat{\mathbf{x}}}{dt}\right) = 0$$



pressure fields for example POD modes

How to select test basis $\boldsymbol{\Psi}(\hat{\mathbf{x}}, t)$*?*

Galerkin v. least-squares Petrov–Galerkin (LSPG)

Key question: *Optimize then discretize* or *discretize then optimize*?

LSPG ROM ODE

$$\boldsymbol{\Psi}(\hat{\mathbf{x}}, t)^T \boldsymbol{\Phi}\dot{\hat{\mathbf{x}}} = \boldsymbol{\Psi}(\hat{\mathbf{x}}, t)^T \mathbf{f}(\boldsymbol{\Phi}\hat{\mathbf{x}}, t)$$

LSPG projection

Full-order model ODE

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

minimize residual

Galerkin ROM ODE

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

time discretization

time discretization

time discretization

LSPG ROM OΔE

$$\hat{\mathbf{x}}^n = \arg\min_{\hat{\mathbf{x}}} \|\mathbf{A}\mathbf{r}^n(\boldsymbol{\Phi}\hat{\mathbf{x}})\|_2^2$$

minimize residual

Full-order model OΔE

$$\mathbf{r}^n(\mathbf{x}) = 0$$

Galerkin projection

Galerkin ROM OΔE

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

$$\boldsymbol{\Psi}(\hat{\mathbf{x}}, t) = \mathbf{A}^T\mathbf{A}\left(\alpha_0 \mathbf{I} - \Delta t \beta_0 \frac{\partial \mathbf{f}}{\partial \mathbf{x}}(\mathbf{x}_0 + \boldsymbol{\Phi}\hat{\mathbf{x}}, t)\right)\boldsymbol{\Phi}$$

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

LSPG and Galerkin are **equivalent**:

- for explicit time integrators,
- in the limit $\Delta t \to 0$, or
- for SPD residual Jacobians.

The **LSPG ROM ODE** exists:

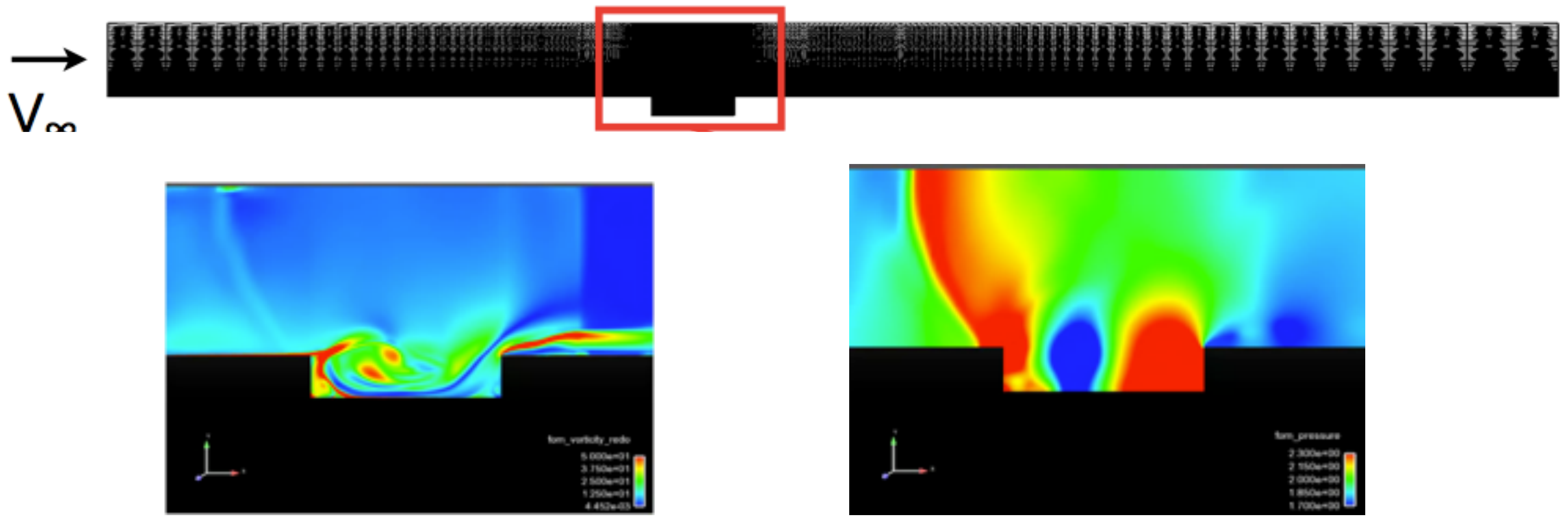
- for explicit time integrators
- for single-step time integrators, or
- if $\mathbf{f}$ is linear in $\mathbf{x}$.

Error analysis (backward Euler):

- LSPG smaller error bound than Galerkin
- LSPG bound minimized for intermediate Δt
- Larger basis dim → smaller optimal Δt

Numerical experiments: cavity flow

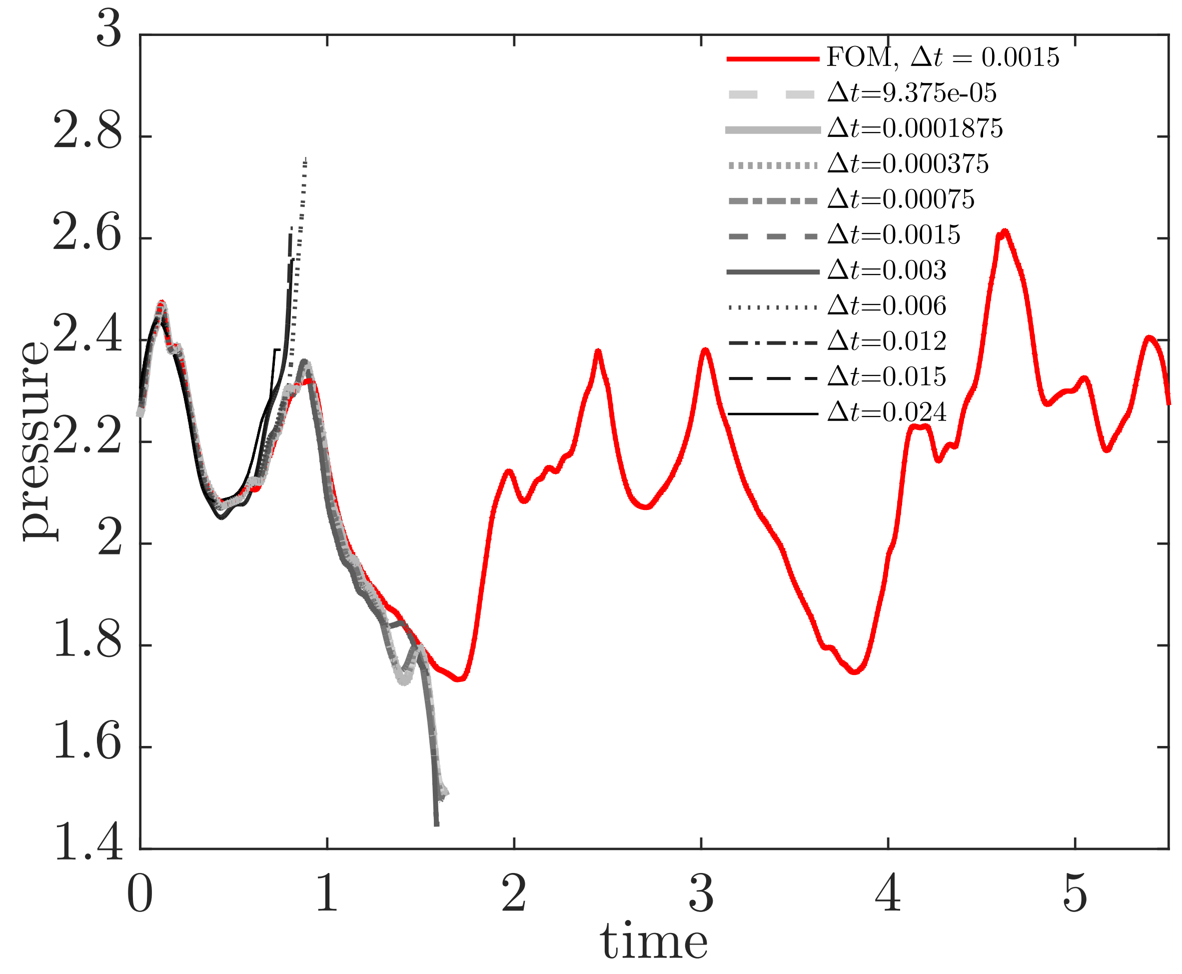
high-fidelity model



- unsteady Navier–Stokes
- DES turbulence model
- 1.2 million dofs

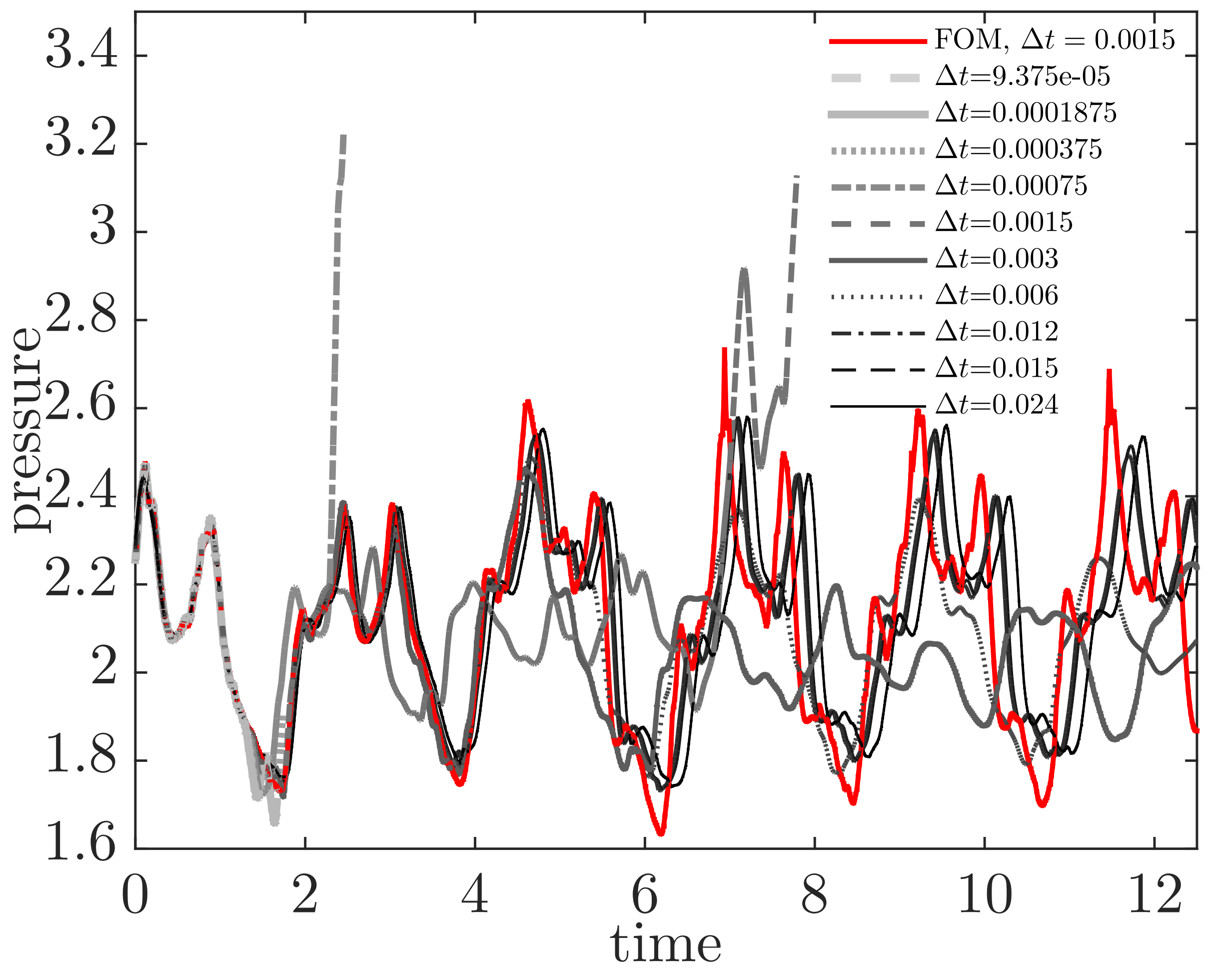
- Re = 6.3 x 10^6
- M_∞ = 0.6
- CFD code: AERO-F

Galerkin ROM



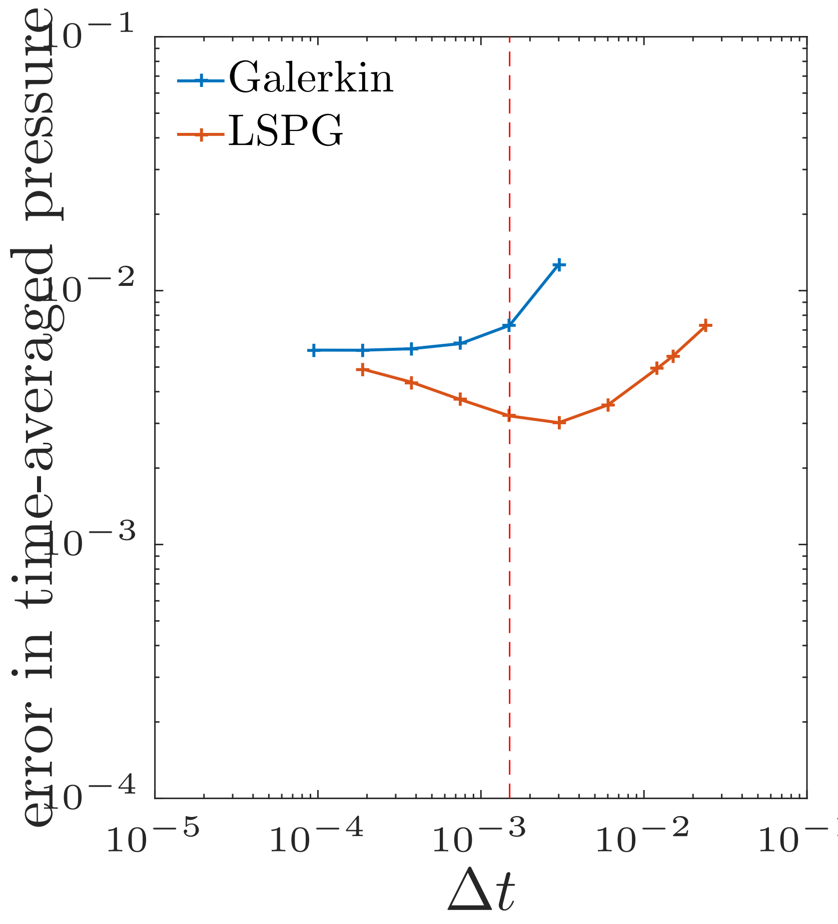
– unstable for long time intervals

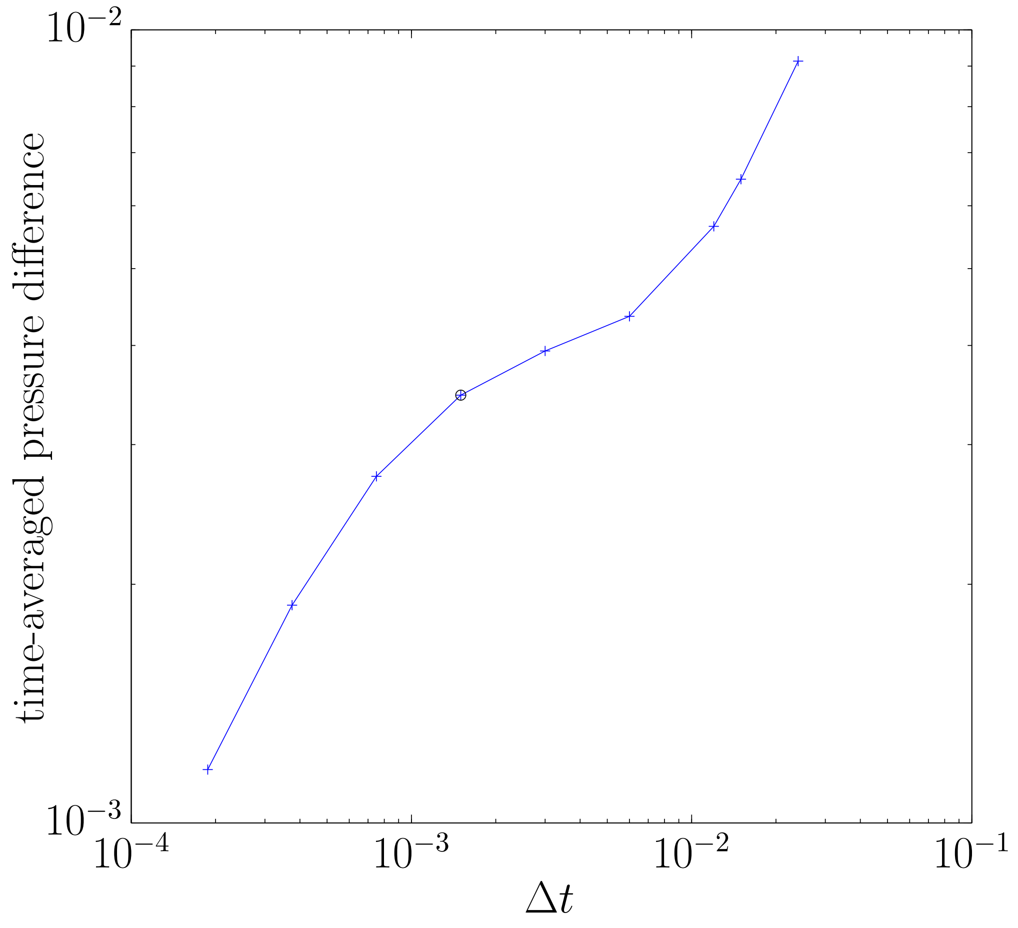
LSPG ROM



+ stable and accurate (most Δt)

$0 \leq t \leq 1.1$

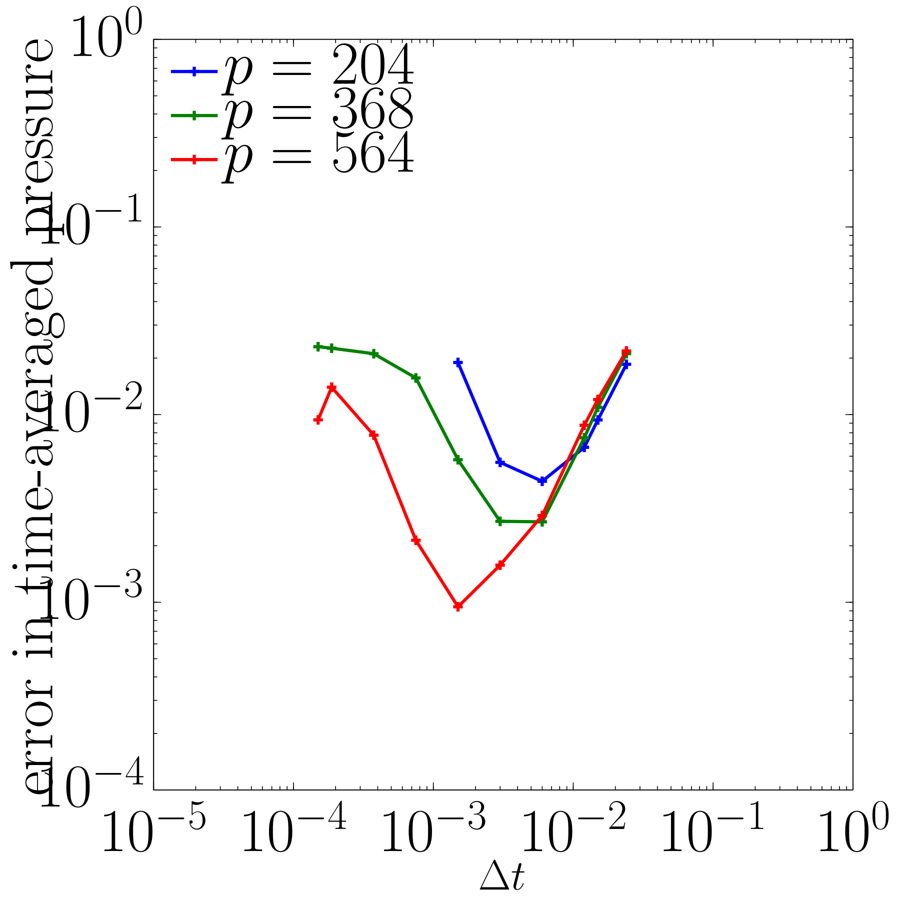


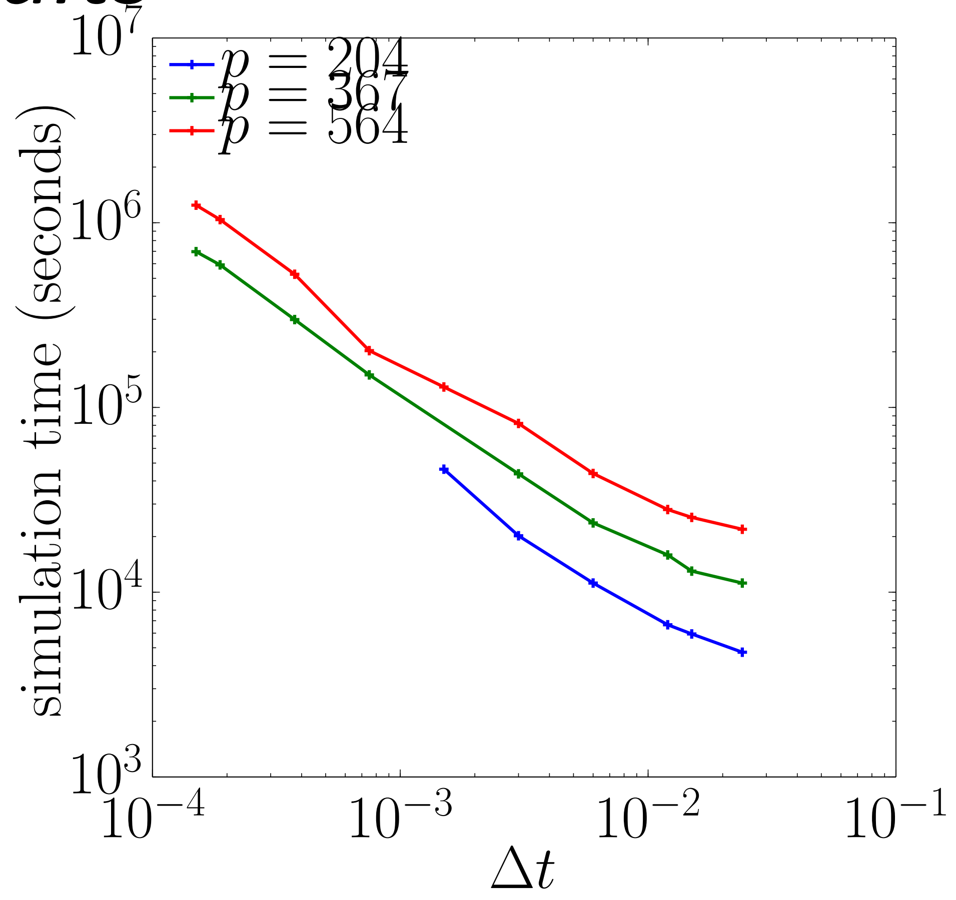


+ LSPG more accurate than Galerkin

✓ Methods equivalent as $\Delta t \to 0$

LSPG ROM results $0 \leq t \leq 2.5$





+ LSPG error minimized for intermediate Δt

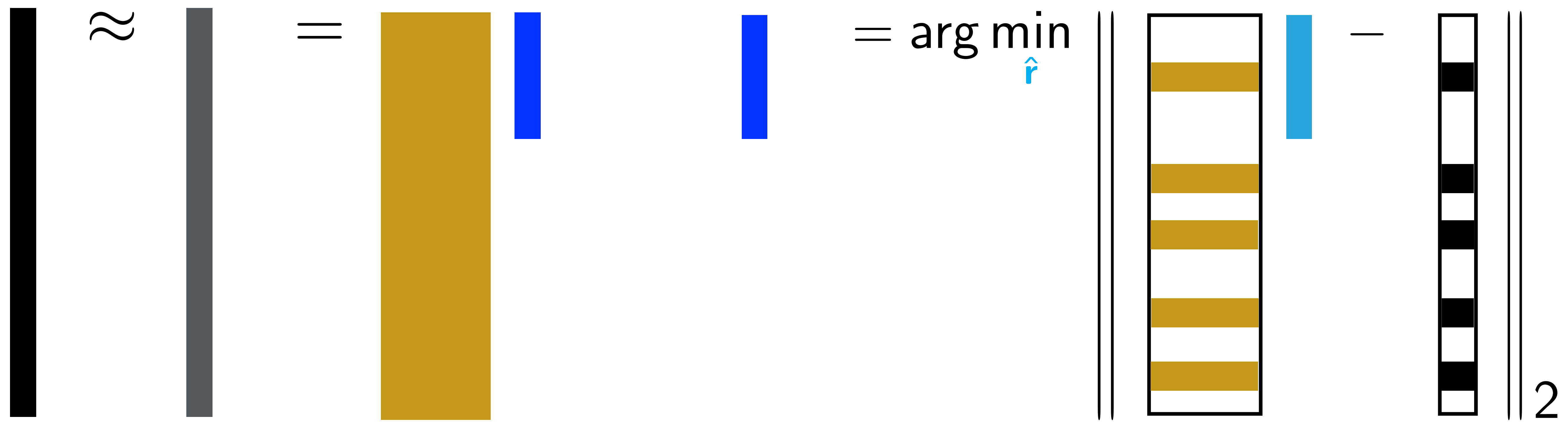
+ LSPG error and wall time reduced by >10x by increasing Δt

Sample mesh

LSPG ROM: $\hat{\mathbf{x}}^n = \arg\min_{\hat{\mathbf{x}}} \|\mathbf{A}\mathbf{r}^n(\mathbf{\Phi}\hat{\mathbf{x}})\|_2^2$

Question: *Can we choose* $\boldsymbol{A}$ *to generate significant speedups?*

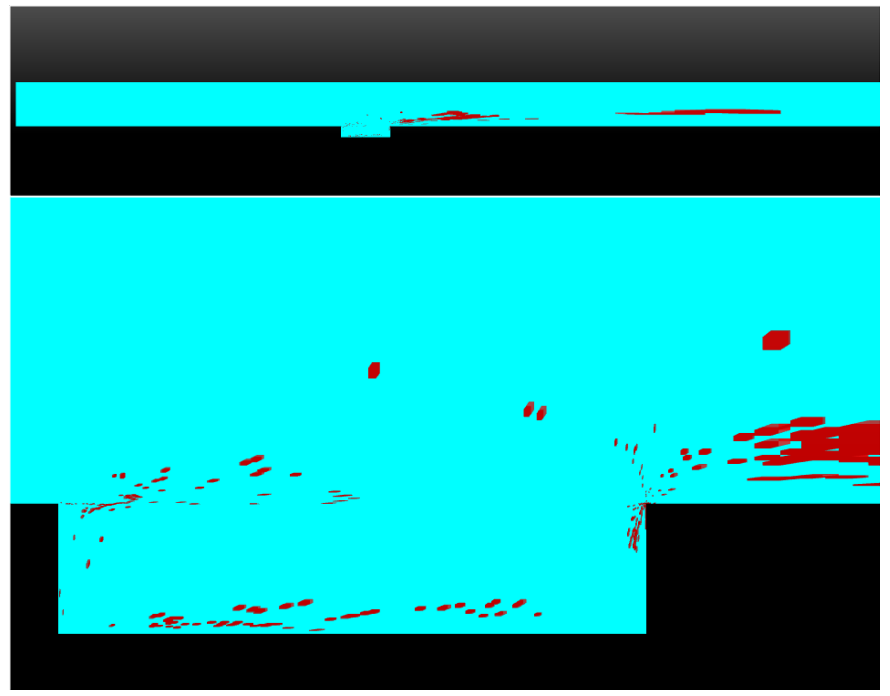
$$\boldsymbol{r}^n(\boldsymbol{x}) \approx \tilde{\boldsymbol{r}}^n(\boldsymbol{x}) = \boldsymbol{\Phi}_R \hat{\boldsymbol{r}}^n(\boldsymbol{x}) \qquad \hat{\boldsymbol{r}}^n(\boldsymbol{x}) = \arg\min_{\hat{\boldsymbol{r}}} \|\boldsymbol{P}\boldsymbol{\Phi}_R\hat{\boldsymbol{r}} - \boldsymbol{P}\boldsymbol{r}^n(\boldsymbol{x})\|_2$$



$$\hat{\boldsymbol{x}}^n = \arg\min_{\hat{\boldsymbol{z}}\in\mathbb{R}^p} \|\tilde{\boldsymbol{r}}^n(\boldsymbol{\Phi}\hat{\boldsymbol{z}})\|_2^2 = \arg\min_{\hat{\boldsymbol{z}}\in\mathbb{R}^p} \|\boldsymbol{\Phi}_R\hat{\boldsymbol{r}}^n(\boldsymbol{\Phi}\hat{\boldsymbol{z}})\|_2^2 = \arg\min_{\hat{\boldsymbol{z}}\in\mathbb{R}^p} \|\hat{\boldsymbol{r}}^n(\boldsymbol{\Phi}\hat{\boldsymbol{z}})\|_2^2$$

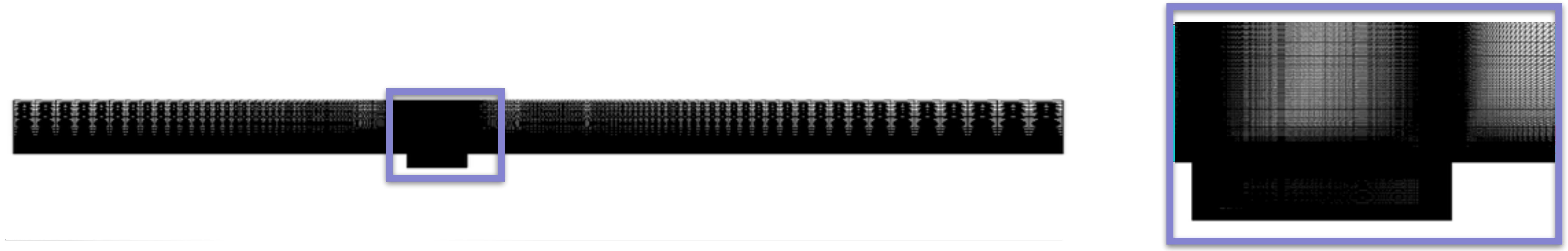
$$= \arg\min_{\hat{\boldsymbol{z}}\in\mathbb{R}^p} \|\underbrace{(\boldsymbol{P}\boldsymbol{\Phi}_R)^+\boldsymbol{P}}_{\boldsymbol{A}}\boldsymbol{r}^n(\boldsymbol{\Phi}\hat{\boldsymbol{z}})\|_2^2.$$

+ **GNAT:** $\boldsymbol{A} = (\boldsymbol{P}\boldsymbol{\Phi}_R)^+\boldsymbol{P}$ leads to low cost
+ HPC implementation: extract sample mesh associated with $\boldsymbol{P}$



GNAT results

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

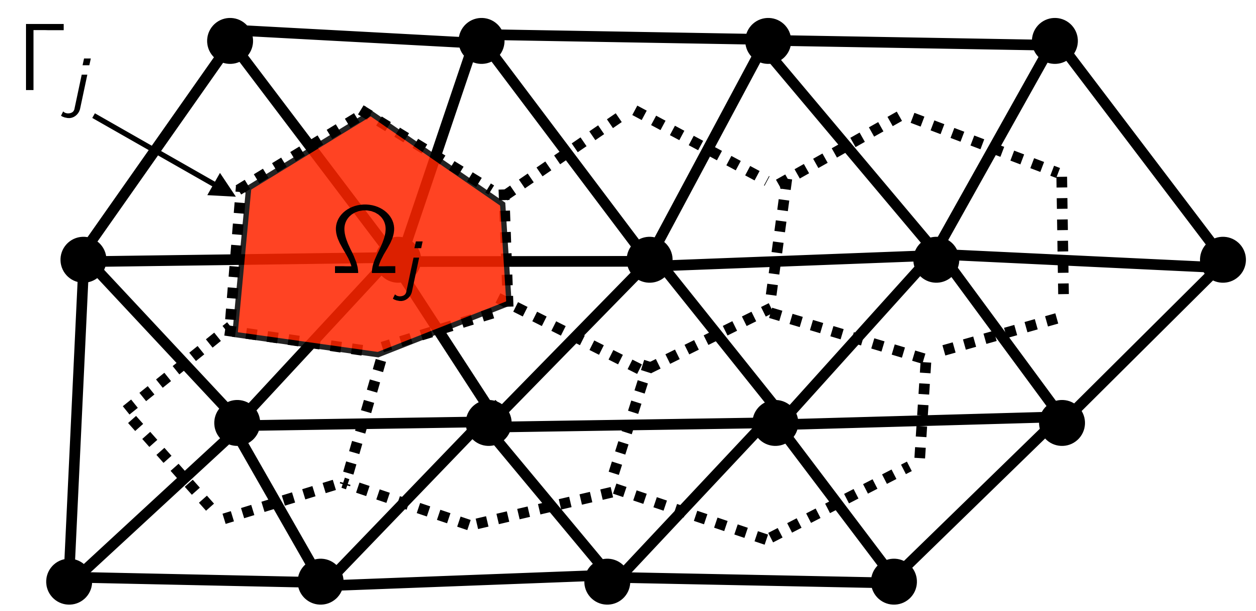
See demo!

Structure preservation for finite-volume methods

Question: *Can we make stronger guarantees of our LSPG ROM solution in CFD?*

Full-order model ODE: $\dfrac{d\mathbf{x}}{dt} = \mathbf{f}(\mathbf{x}; \mathbf{t}, \mu)$

$$x_i = \begin{cases} \int_{\Omega_j} \rho(\vec{x}, t^n) dx \\ \int_{\Omega_j} \rho(\vec{x}, t) v_k(\vec{x}, t) dx \\ \int_{\Omega_j} \rho(\vec{x}, t) E(\vec{x}, t) dx \end{cases} \quad f_i = \begin{cases} -\int_{\Gamma_j} \rho(\vec{x}, t^n) v_\ell(\vec{x}, t) n_\ell(\vec{x}) d\vec{x} \\ -\int_{\Gamma_j} \rho(\vec{x}, t) v_k(\vec{x}, t) v_\ell(\vec{x}, t) n_\ell(\vec{x}) d\vec{x} \\ -\int_{\Gamma_j} \rho(\vec{x}, t) E(\vec{x}, t) v_\ell(\vec{x}, t) n_\ell(\vec{x}) d\vec{x} \end{cases}$$



Full-order model OΔE: $\mathbf{r}^n(\mathbf{x}) = 0$

$$r_i^n(\mathbf{x}) = \begin{cases} \int_{\Omega_j} \rho(\vec{x}, t^{n+1}) - \rho(\vec{x}, t^n) d\vec{x} + \int_{t_n}^{t^{n+1}} \int_{\Gamma_j} \rho(\vec{x}, t) v_\ell(\vec{x}, t) n_\ell(\vec{x}) d\vec{x} dt \\ \int_{\Omega_j} \rho(\vec{x}, t^{n+1}) v_k(\vec{x}, t^{n+1}) - \rho(\vec{x}, t^n) v_k(\vec{x}, t^n) d\vec{x} + \int_{t_n}^{t^{n+1}} \int_{\Gamma_j} \rho(\vec{x}, t) v_k(\vec{x}, t) v_\ell(\vec{x}, t) n_\ell(\vec{x}) d\vec{x} dt \\ \int_{\Omega_j} \rho(\vec{x}, t^{n+1}) E(\vec{x}, t^{n+1}) - \rho(\vec{x}, t^n) E(\vec{x}, t^n) d\vec{x} + \int_{t_n}^{t^{n+1}} \int_{\Gamma_j} \rho(\vec{x}, t) E(\vec{x}, t) v_\ell(\vec{x}, t) n_\ell(\vec{x}) d\vec{x} dt \end{cases}$$

Interpretation of r_i^n**:** Violation of conservation laws over Ω_j

LSPG ROM: $\hat{\mathbf{x}}^n = \arg\min_{\hat{\mathbf{x}}} \|\mathbf{A}\mathbf{r}^n(\mathbf{\Phi}\hat{\mathbf{x}})\|_2^2 \Leftrightarrow$ Min. sum of squares of conservation-law violations

+ Favorable properties over Galerkin projection
- Likely not conservative over any subdomain

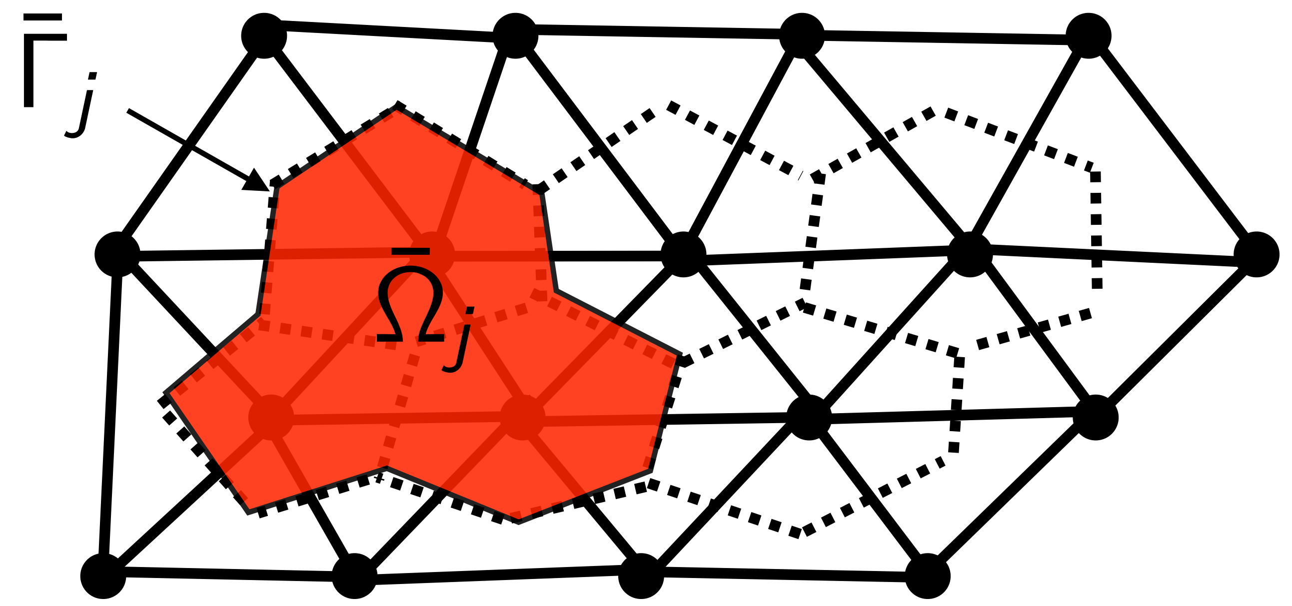
Structure preservation for finite-volume methods

Idea: *Equip LSPG ROM with conservation-law constraints over subdomains*

LSPG ROM: $\underset{\hat{\mathbf{x}}}{\text{minimize}} \ \|\mathbf{A}\mathbf{r}^n(\mathbf{\Phi}\hat{\mathbf{x}})\|_2^2$

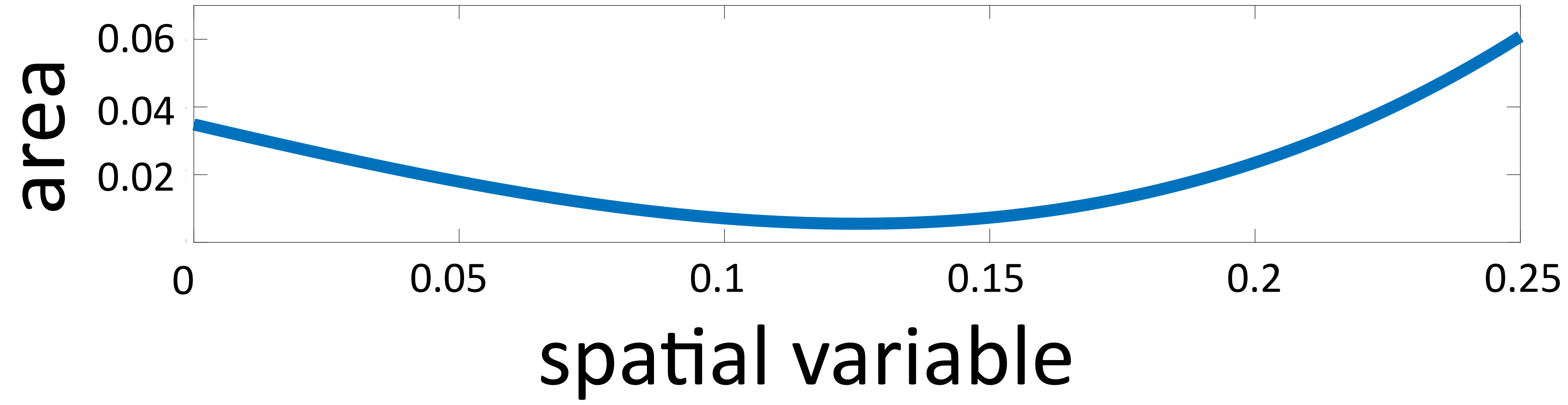
LSPG-FV ROM: $\underset{\hat{\mathbf{x}}}{\text{minimize}} \ \|\mathbf{A}\mathbf{r}^n(\mathbf{\Phi}\hat{\mathbf{x}})\|_2^2$

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

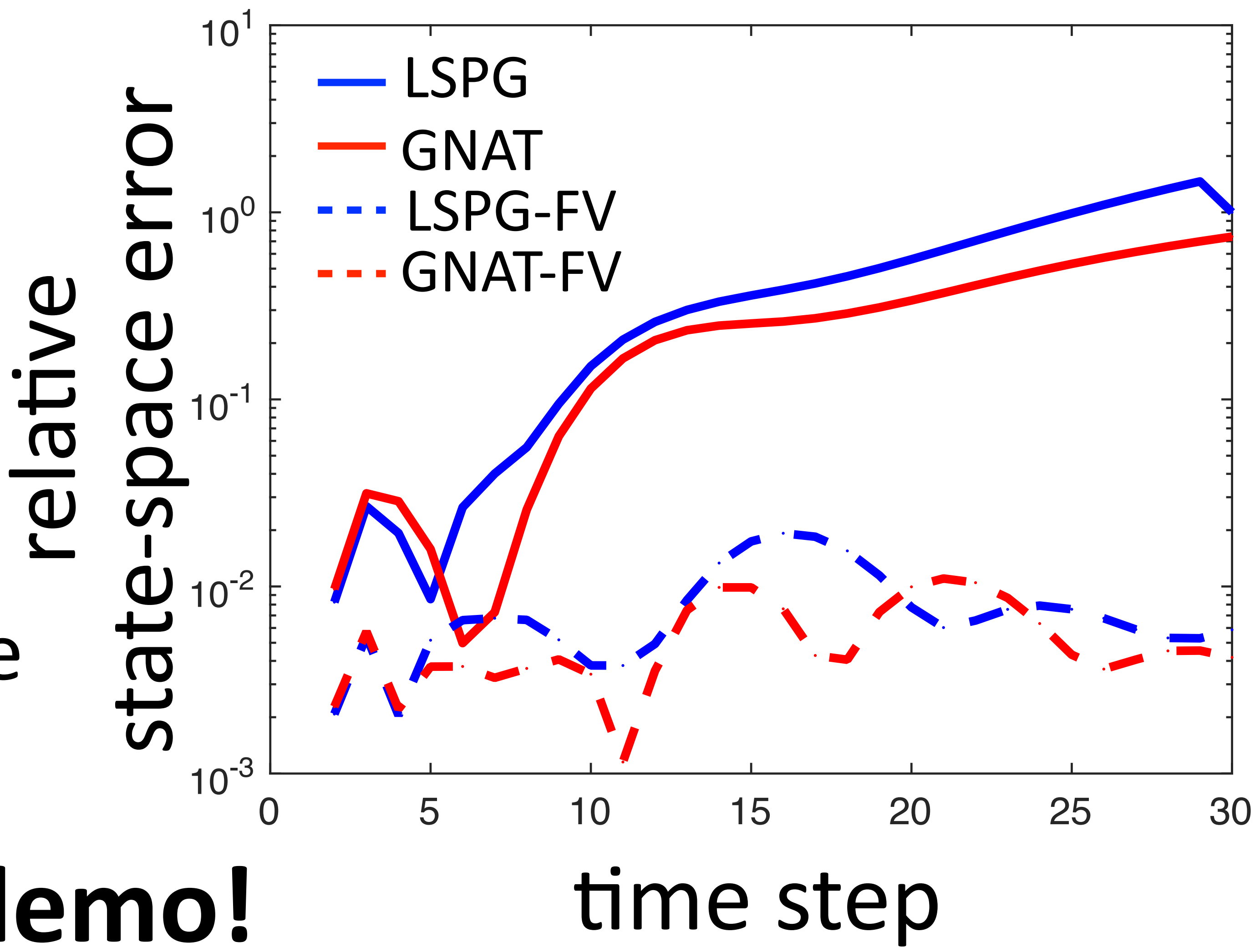


$$\bar{r}_i^n(\mathbf{x}) = \begin{cases} \int_{\bar{\Omega}_j} \rho(\vec{x}, t^{n+1}) - \rho(\vec{x}, t^n) d\vec{x} + \int_{t_n}^{t^{n+1}} \int_{\bar{\Gamma}_j} \rho(\vec{x}, t) v_\ell(\vec{x}, t) n_\ell(\vec{x}) d\vec{x} dt \\ \int_{\bar{\Omega}_j} \rho(\vec{x}, t^{n+1}) v_k(\vec{x}, t^{n+1}) - \rho(\vec{x}, t^n) v_k(\vec{x}, t^n) d\vec{x} + \int_{t_n}^{t^{n+1}} \int_{\bar{\Gamma}_j} \rho(\vec{x}, t) v_k(\vec{x}, t) v_\ell(\vec{x}, t) n_\ell(\vec{x}) d\vec{x} dt \\ \int_{\bar{\Omega}_j} \rho(\vec{x}, t^{n+1}) E(\vec{x}, t^{n+1}) - \rho(\vec{x}, t^n) E(\vec{x}, t^n) d\vec{x} + \int_{t_n}^{t^{n+1}} \int_{\bar{\Gamma}_j} \rho(\vec{x}, t) E(\vec{x}, t) v_\ell(\vec{x}, t) n_\ell(\vec{x}) d\vec{x} dt \end{cases}$$

Example: quasi-1D Euler



- 900 control volumes
- 2700 dofs
- $\boldsymbol{\mu}$: (1) initial M_∞, (2) exit-pressure rate
- constrained ROMs: one subdomain



See demo!

method	speedup
LSPG	0.57
GNAT	4.4
LSPG-FV	0.44
GNAT-FV	5.3

\+ *constraints*: better long-time behavior