SAND2016-11361C

Structure-preserving model finite-volume discretizations of conservation laws

Kevin Carlberg[1], Youngsoo Choi[1], Syuzanna Sargsyan[2]

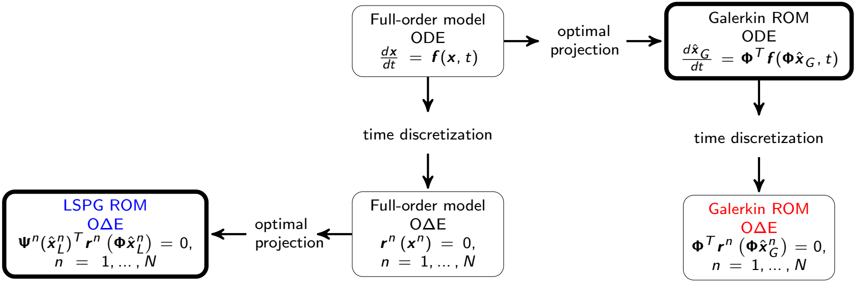
[1]Sandia National Laboratories

[2]University of Washington

Recent developments in numerical methods for model reduction
Institut Henri Poincaré
Paris, France
November 10, 2016

Optimize then discretize, or discretize then optimize?

[Carlberg et al., 2016]



Full-order model
ODE
$\frac{d\boldsymbol{x}}{dt} = \boldsymbol{f}(\boldsymbol{x}, t)$

optimal projection

Galerkin ROM
ODE
$\frac{d\hat{\boldsymbol{x}}_G}{dt} = \boldsymbol{\Phi}^T \boldsymbol{f}(\boldsymbol{\Phi}\hat{\boldsymbol{x}}_G, t)$

time discretization

time discretization

LSPG ROM
OΔE
$\boldsymbol{\Psi}^n(\hat{\boldsymbol{x}}_L^n)^T \boldsymbol{r}^n\left(\boldsymbol{\Phi}\hat{\boldsymbol{x}}_L^n\right) = 0,$
$n = 1, \ldots, N$

optimal projection

Full-order model
OΔE
$\boldsymbol{r}^n\left(\boldsymbol{x}^n\right) = 0,$
$n = 1, \ldots, N$

Galerkin ROM
OΔE
$\boldsymbol{\Phi}^T \boldsymbol{r}^n\left(\boldsymbol{\Phi}\hat{\boldsymbol{x}}_G^n\right) = 0,$
$n = 1, \ldots, N$

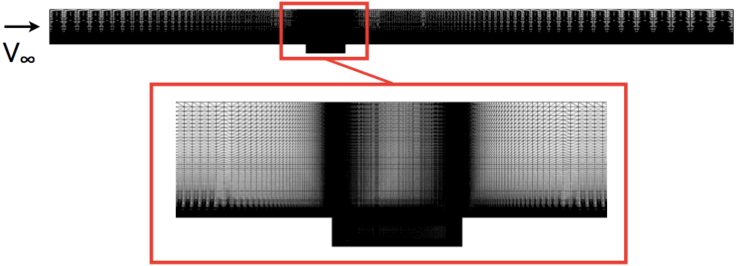
- Galerkin: continuous-residual minimization

$$\frac{d\hat{\boldsymbol{x}}_G}{dt}(\boldsymbol{x}, t) = \arg\min_{\boldsymbol{z}} \left\| \boldsymbol{\Phi}\boldsymbol{z} - \boldsymbol{f}(\boldsymbol{x}, t) \right\|_2^2$$

- LSPG: discrete-residual minimization

$$\hat{\boldsymbol{x}}_L^n = \arg\min_{\boldsymbol{z}} \left\| \boldsymbol{A}\boldsymbol{r}^n\left(\boldsymbol{\Phi}\boldsymbol{z}\right) \right\|_2^2, \quad n = 1, \ldots, N$$

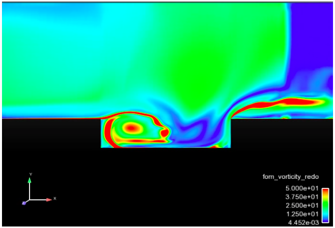
Cavity-flow problem. Collaborator: M. Barone (SNL)



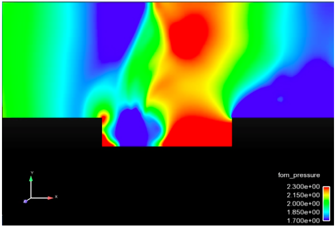
- Unsteady Navier–Stokes
- DES turbulence model
- 1.2 million degrees of freedom

- $\mathrm{Re} = 6.3 \times 10^6$
- $M_\infty = 0.6$
- CFD code: AERO-F [?]

Full-order model responses

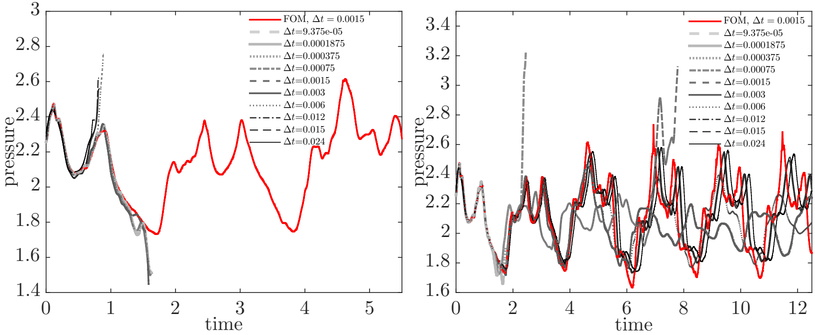


vorticity field



pressure field

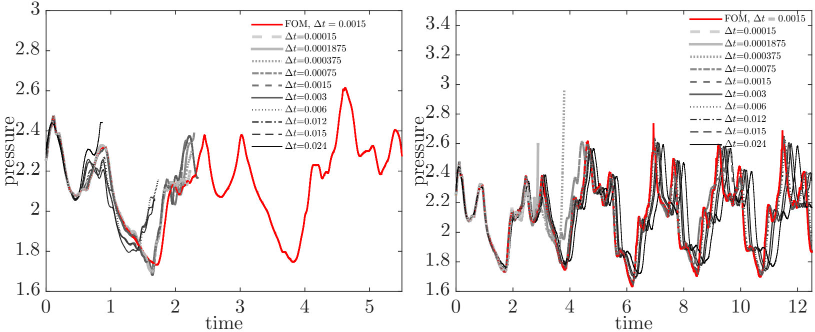
Galerkin and LSPG responses for basis dimension $p = 204$



(a) Galerkin (b) LSPG

- Galerkin ROMs unstable for long time intervals
+ LSPG ROMs accurate and stable (most time steps)

Galerkin and LSPG responses for basis dimension $p = 564$



(c) Galerkin (d) LSPG

- – Galerkin ROMs remain unstable
- LSPG ROMs
  - + accuracy improves as basis dimension increases
  - – more expensive than the FOM (1.3 hours>1 hour, 48 CPU)

Sample mesh [?]: HPC implementation

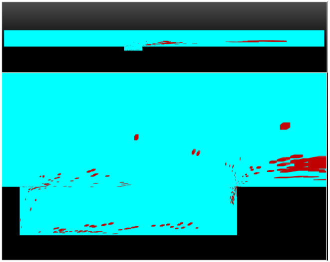
$$\hat{\boldsymbol{x}}^n = \arg\min_{\hat{\boldsymbol{z}}\in\mathbb{R}^p} \| \underbrace{(\boldsymbol{P}\boldsymbol{\Phi}_R)^+ \boldsymbol{P}}_{\boldsymbol{A}} \boldsymbol{r}^n(\boldsymbol{\Phi}\hat{\boldsymbol{z}}) \|_2^2$$

- *Key*: GNAT samples only a few entries of the residual $\boldsymbol{P}\boldsymbol{r}^n$
- *Idea*: Extract minimal subset of the mesh

Sample mesh [?]: HPC implementation

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

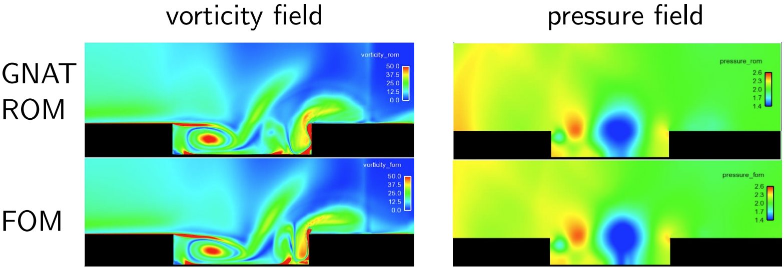
- *Key*: GNAT samples only a few entries of the residual $\boldsymbol{P}\boldsymbol{r}^n$
- *Idea*: Extract minimal subset of the mesh



- Sample mesh: 4.1% nodes, 3.0% cells

\+ Small problem size: can run on many fewer cores

GNAT performance ($t \leq 12.5$ sec)



- $+$ $< 1\%$ error in time-averaged drag
- $+$ 229x CPU-hour savings
  - FOM: 5 hour x 48 CPU
  - GNAT ROM: 32 min x 2 CPU

Why is LSPG more accurate than Galerkin?

Theorem (Local *a posteriori* state-space error bounds)

If the following conditions hold:

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

then

$$\|\delta \boldsymbol{x}_G^n\| \leq \frac{\Delta t}{h}\sum_{\ell=0}^{k}|\beta_\ell|\|\left(\boldsymbol{I} - \mathbb{V}\right)\boldsymbol{f}\left(\boldsymbol{x}^0 + \boldsymbol{\Phi}\hat{\boldsymbol{x}}_G^{n-\ell}\right)\| + \frac{1}{h}\sum_{\ell=1}^{k}\left(|\beta_\ell|\kappa\Delta t + |\alpha_\ell|\right)\|\delta \boldsymbol{x}_G^{n-\ell}\|$$

$$\|\delta \boldsymbol{x}_L^n\| \leq \frac{\Delta t}{h}\sum_{\ell=0}^{k}|\beta_\ell|\|\left(\boldsymbol{I} - \mathbb{P}^n\right)\boldsymbol{f}\left(\boldsymbol{x}^0 + \boldsymbol{\Phi}\hat{\boldsymbol{x}}_L^{n-\ell}\right)\| + \frac{1}{h}\sum_{\ell=1}^{k}\left(|\beta_\ell|\kappa\Delta t + |\alpha_\ell|\right)\|\delta \boldsymbol{x}_L^{n-\ell}\|,$$

with

- $\delta \boldsymbol{x}_G^n := \boldsymbol{x}_\star^n - \boldsymbol{\Phi}\hat{\boldsymbol{x}}_G^n.$
- $\delta \boldsymbol{x}_L^n := \boldsymbol{x}_\star^n - \boldsymbol{\Phi}\hat{\boldsymbol{x}}_L^n$
- $\mathbb{V} := \boldsymbol{\Phi}\boldsymbol{\Phi}^T$
- $\mathbb{P}^n := \boldsymbol{\Phi}\left(\left(\boldsymbol{\Psi}^n\right)^T\boldsymbol{\Phi}\right)^{-1}\left(\boldsymbol{\Psi}^n\right)^T$

LSPG can minimize a term in the error bound

$$\|\delta \boldsymbol{x}_G^n\| \leq \frac{\Delta t}{h}\sum_{\ell=0}^{k}|\beta_\ell|\|\left(\boldsymbol{I}-\mathbb{V}\right)\boldsymbol{f}\left(\boldsymbol{x}^0+\boldsymbol{\Phi}\hat{\boldsymbol{x}}_G^{n-\ell}\right)\|+\frac{1}{h}\sum_{\ell=1}^{k}\left(|\beta_\ell|\kappa\Delta t+|\alpha_\ell|\right)\|\delta \boldsymbol{x}_G^{n-\ell}\|$$

$$\|\delta \boldsymbol{x}_L^n\| \leq \frac{\Delta t}{h}\sum_{\ell=0}^{k}|\beta_\ell|\|\left(\boldsymbol{I}-\mathbb{P}^n\right)\boldsymbol{f}\left(\boldsymbol{x}^0+\boldsymbol{\Phi}\hat{\boldsymbol{x}}_L^{n-\ell}\right)\|+\frac{1}{h}\sum_{\ell=1}^{k}\left(|\beta_\ell|\kappa\Delta t+|\alpha_\ell|\right)\|\delta \boldsymbol{x}_L^{n-\ell}\|,$$

Lemma (Oblique projection as discrete-residual minimization)

If $\beta_j^n = 0$, $j \geq 1$ (e.g., backward differentiation formulas), then

$$|\beta_0^n|\Delta t\|(\boldsymbol{I}-\mathbb{V})\boldsymbol{f}\left(\boldsymbol{x}^0+\boldsymbol{\Phi}\hat{\boldsymbol{x}}_G^n, t^n\right)\|_2 = \|\boldsymbol{r}_G^n(\boldsymbol{\Phi}\hat{\boldsymbol{x}}_G^n)\|_2$$

$$|\beta_0^n|\Delta t\|(\boldsymbol{I}-\mathbb{P}^n)\boldsymbol{f}\left(\boldsymbol{x}^0+\boldsymbol{\Phi}\hat{\boldsymbol{x}}_L^n, t^n\right)\|_2 = \|\boldsymbol{r}_P^n(\boldsymbol{\Phi}\hat{\boldsymbol{x}}_L^n)\|_2.$$

If additionally the LSPG ROM employs $\boldsymbol{A} = \boldsymbol{I}$, then

$$\|\boldsymbol{r}_P^n(\boldsymbol{\Phi}\hat{\boldsymbol{x}}_L^n)\|_2 = \min_{\boldsymbol{y}\in\mathrm{Ran}(\boldsymbol{\Phi})}\|\boldsymbol{r}_P^n(\boldsymbol{y})\|_2.$$

LSPG can produce a smaller *a posteriori* error bound

$$\|\delta \boldsymbol{x}_G^n\| \leq \frac{\Delta t}{h}\sum_{\ell=0}^{k}|\beta_\ell|\| (\boldsymbol{I}-\mathbb{V})\,\boldsymbol{f}\left(\boldsymbol{x}^0+\boldsymbol{\Phi}\hat{\boldsymbol{x}}_G^{n-\ell}\right)\| + \frac{1}{h}\sum_{\ell=1}^{k}\left(|\beta_\ell|\kappa\Delta t+|\alpha_\ell|\right)\|\delta\boldsymbol{x}_G^{n-\ell}\|$$

$$\|\delta \boldsymbol{x}_L^n\| \leq \frac{\Delta t}{h}\sum_{\ell=0}^{k}|\beta_\ell|\| (\boldsymbol{I}-\mathbb{P}^n)\,\boldsymbol{f}\left(\boldsymbol{x}^0+\boldsymbol{\Phi}\hat{\boldsymbol{x}}_L^{n-\ell}\right)\| + \frac{1}{h}\sum_{\ell=1}^{k}\left(|\beta_\ell|\kappa\Delta t+|\alpha_\ell|\right)\|\delta\boldsymbol{x}_L^{n-\ell}\|,$$

Corollary (Discrete v. continuous residual minimization)

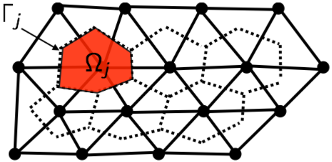
If $\beta_j^n = 0$, $j \geq 1$ *(e.g., backward differentiation formulas), the LSPG ROM employs* $\boldsymbol{A} = \boldsymbol{I}$, *and* $\hat{\boldsymbol{x}}_L^{n-\ell} = \hat{\boldsymbol{x}}_G^{n-\ell}$, $\ell = 1, \ldots, k$, *then*

$$\begin{aligned}&\min_{\boldsymbol{y}\in\mathrm{Ran}(\boldsymbol{\Phi})}\|\boldsymbol{r}_P^n(\boldsymbol{y})\|_2 = |\beta_0^n|\Delta t\|(\boldsymbol{I}-\mathbb{P}^n)\boldsymbol{f}\left(\boldsymbol{x}^0+\boldsymbol{\Phi}\hat{\boldsymbol{x}}_L^n, t^n\right)\|_2\\ &\leq |\beta_0^n|\Delta t\|(\boldsymbol{I}-\mathbb{V})\boldsymbol{f}\left(\boldsymbol{x}^0+\boldsymbol{\Phi}\hat{\boldsymbol{x}}_G^n, t^n\right)\|_2 = |\beta_0^n|\Delta t\min_{\boldsymbol{y}\in\mathrm{Ran}(\boldsymbol{\Phi})}\|\boldsymbol{y}-\boldsymbol{f}\left(\boldsymbol{x}^0+\boldsymbol{\Phi}\hat{\boldsymbol{x}}_G^n, t^n\right)\|_2.\end{aligned}$$

Thus, the LSPG error bound is smaller than the Galerkin error bound.

However, still no guarantee of special properties in practice.

Finite-volume model: full-order model formulation



- Full-order model ODE: $\frac{d\boldsymbol{x}}{dt} = \boldsymbol{f}(\boldsymbol{x}, t)$

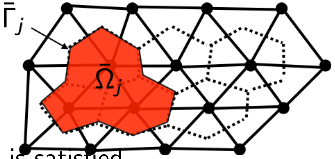
$$x_i = \begin{cases} \int_{\Omega_j} \rho(\vec{x}, t^n) dx \\ \int_{\Omega_j} \rho(\vec{x}, t) v_k(\vec{x}, t) dx \\ \int_{\Omega_j} \rho(\vec{x}, t) E(\vec{x}, t) dx \end{cases} \qquad f_i = \begin{cases} -\int_{\Gamma_j} \rho(\vec{x}, t^n) v_\ell(\vec{x}, t) n_\ell(\vec{x}) d\vec{x} \\ -\int_{\Gamma_j}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

- Full-order model OΔE: $\boldsymbol{r}^n(\boldsymbol{x}^n) = 0, \; n = 1, \ldots, N$

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

Interpretation of r_i^n: Conservation-law violation over Ω_j and $[t^n, t^{n+1}]$.

Equip LSPG ROM with conservation-law constraints over subdomains



- LSPG ROM: $\underset{\boldsymbol{z}}{\text{minimize}} \; \left\| \boldsymbol{A}\boldsymbol{r}^n\left(\boldsymbol{\Phi}\boldsymbol{z}\right)\right\|_2^2$
  - \+ Minimizes sum of squares of conservation-law violations
  - \- Does not ensure any conservation law is satisfied
- LSPG-FV ROM:

$$\underset{\boldsymbol{z}}{\text{minimize}} \; \left\| \boldsymbol{A}\boldsymbol{r}^n\left(\boldsymbol{\Phi}\boldsymbol{z}\right)\right\|_2^2$$

$$\text{subject to } \bar{\boldsymbol{r}}^n(\boldsymbol{\Phi}\boldsymbol{z}) = \boldsymbol{0}$$

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

  - \+ Minimizes sum of squares of conservation-law violations
  - \+ Ensure conservation laws are satisfied over n_Ω subdomains

LSPG-FV: three conditions

- $\boldsymbol{r}^n : \mathbb{R}^p \to \mathbb{R}^p$
- $\boldsymbol{\Phi} \in \mathbb{R}^{N \times p}$
- $\bar{\boldsymbol{r}}^n : \mathbb{R}^p \to \mathbb{R}^{n_C}$

- # of subdomains n_Ω
- # of conservation laws n_ℓ
- # of constraints $n_C = n_\Omega n_\ell$

Conditions:

1. Underdetermined constraint problem $(p > n_C)$

$$\underset{\boldsymbol{z}}{\text{minimize}} \ \|\boldsymbol{A}\boldsymbol{r}^n(\boldsymbol{\Phi}\boldsymbol{z})\|_2^2$$
$$\text{subject to } \bar{\boldsymbol{r}}^n(\boldsymbol{\Phi}\boldsymbol{z}) = \boldsymbol{0}$$

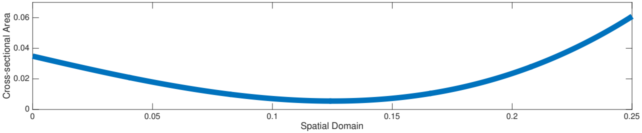
2. Well-posed constraint problem $(p = n_C)$

$$\bar{\boldsymbol{r}}^n(\boldsymbol{\Phi}\boldsymbol{z}) = \boldsymbol{0}$$

3. Overdetermined constraint problem $(p < n_C)$

$$\underset{\boldsymbol{z}}{\text{minimize}} \ \|\boldsymbol{A}\bar{\boldsymbol{r}}^n(\boldsymbol{\Phi}\boldsymbol{z})\|_2^2$$

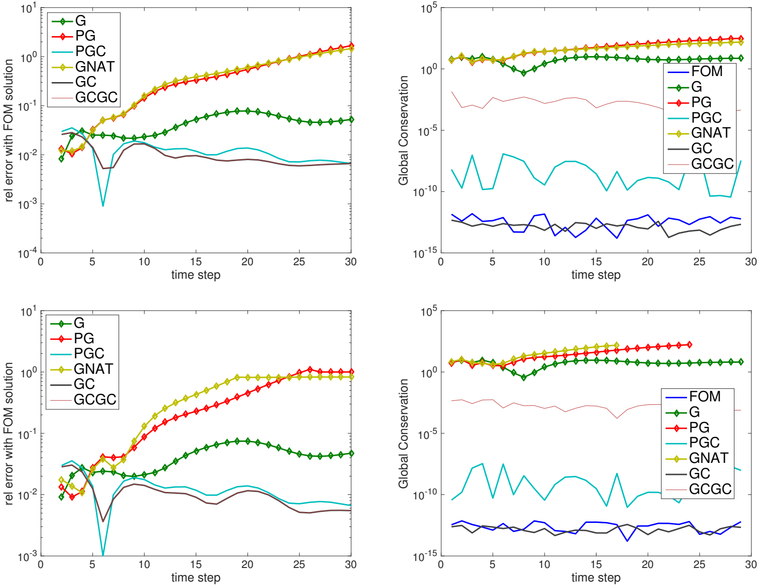
Example: Quasi-1D Euler equation



- The length of the nozzle is 0.25 m
- The specific heat ratio (γ) is 1.3
- The gas constant (R) is 355.4
- The total temperature is 2800 K

- Number of control volumes : varies throughout this section
- Number of time steps : 29
- The time step size : 0.01

Proposed methods produce low long-time errors



Conclusions

- New LSPG ROM method guarantees conservation-law constraints satisfied.
- Equipped with hyper-reduction
- Superior long-time behavior observed
- Best results obtained for $n_C = 1$: satisfying global conservation

Acknowledgments

- This research was supported in part by an appointment to the Sandia National Laboratories Truman Fellowship in National Security Science and Engineering, sponsored by Sandia Corporation (a wholly owned subsidiary of Lockheed Martin Corporation) as Operator of Sandia National Laboratories under its U.S. Department of Energy Contract No. DE-AC04-94AL85000.

Carlberg, K., Barone, M., and Antil, H. (2016).
Galerkin v. least-squares Petrov–Galerkin projection in nonlinear model reduction.
Journal of Computational Physics, accepted.

Carlberg, K., Farhat, C., Cortial, J., and Amsallem, D. (2013).
The GNAT method for nonlinear model reduction: effective implementation and application to computational fluid dynamics and turbulent flows.
Journal of Computational Physics, 242:623–647.

Farhat, C., Geuzaine, P., and Brown, G. (2003).
Application of a three-field nonlinear fluid-structure formulation to the prediction of the aeroelastic parameters of an F-16 fighter.
Computers & Fluids, 32(1):3–29.