SAND2019-15477C

Model reduction for hypersonic aerodynamics via conservative LSPG projection and hyper-reduction

PRESENTED BY

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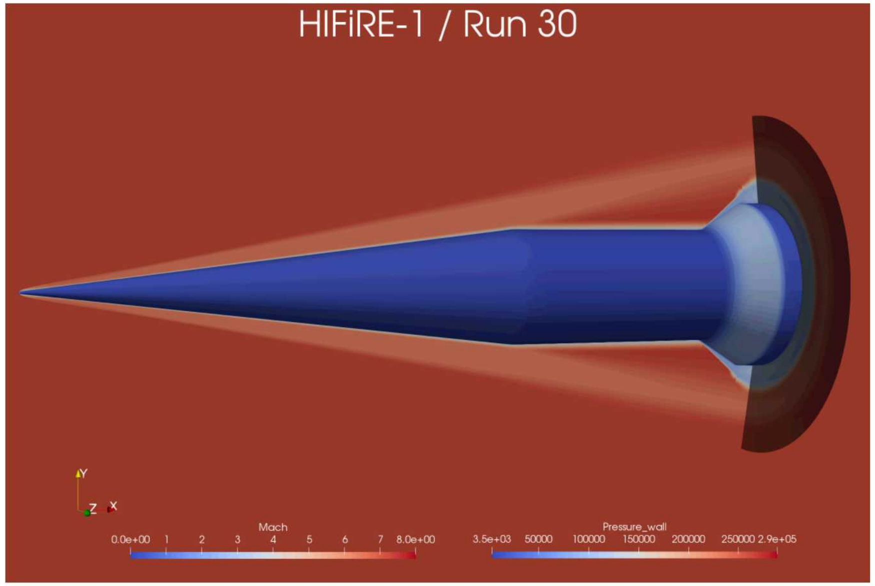
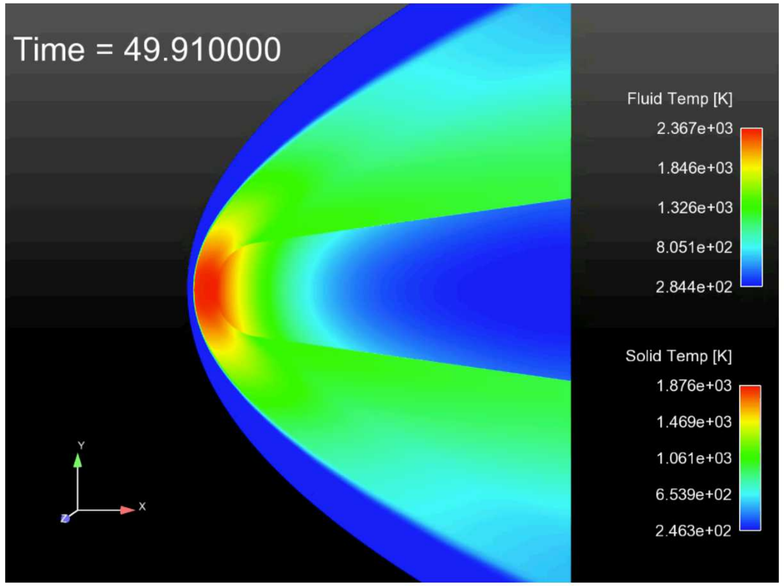
High-fidelity simulations are crucial for hypersonic vehicle analysis and design



Mach # and wall pressure contours for HIFiRE-1 obtained from the SPARC CFD solver

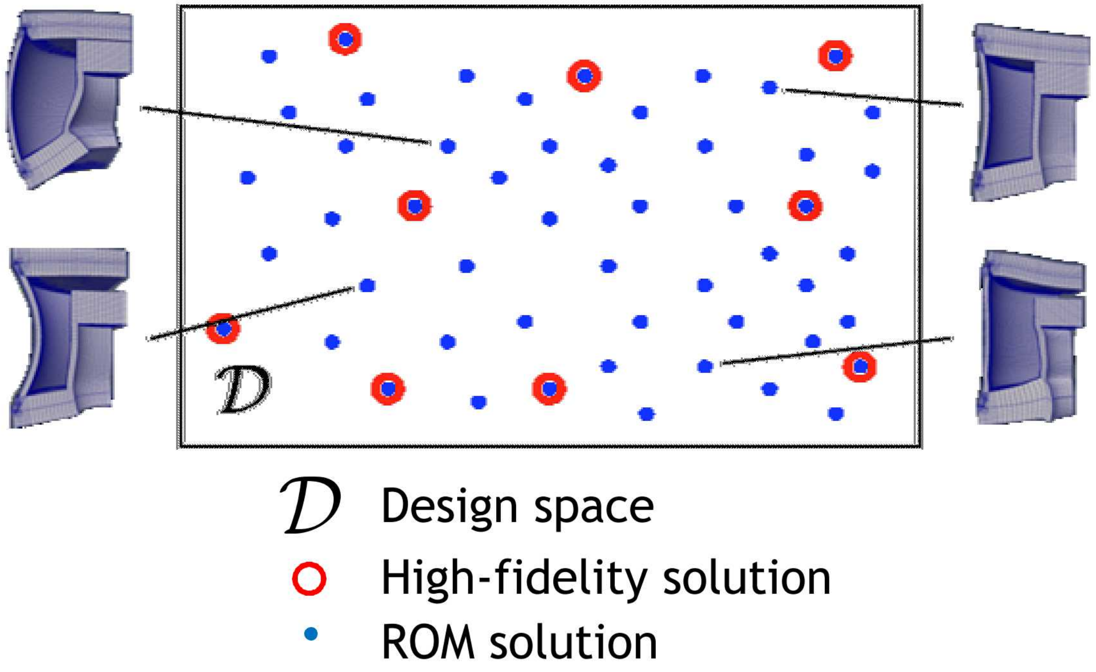


Temperature of a slender body in hypersonic flow obtained from the SPARC CFD solver

- High-fidelity: extreme-scale, nonlinear dynamical system model.
  - High cost: An unsteady multi-physics simulation can consume **weeks** on a supercomputer.
- High cost creates a "**computational barrier**" to the application of many-query and/or time-critical problems:
  - **Many-Query**: Design Optimization, Model Calibration, Uncertainty Propagation
  - **Time-Critical**: Path Planning, Model Predictive Control, Health Monitoring

We use model reduction to break the computational barrier by exploiting high-fidelity simulation data

1. **Acquisition**: Run high-fidelity simulation at a few design points, save simulation data
2. **Learning**: Use machine learning techniques to identify low-dimensional structure in the high-fidelity simulation data
3. **Reduction**: Build a reduced order model (ROM) with extracted data structures, high-fidelity governing equations
4. **Deployment**: Use ROM at remaining design points



Model Reduction Criteria

1. ***Accuracy:*** achieves less than 1% error
2. ***Low cost:*** achieves at least 100x computational savings
3. ***Property preservation:*** preserves important physical properties
4. ***Generalization:*** should work even in difficult cases and for many application codes
5. ***Certification:*** accurately quantify the ROM error

There is very little previous work on projection-based model reduction for Hypersonic Vehicles

- No projection-based ROMs for hypersonic aerodynamics!
- [Dalle et al. 2010]: simplified aerodynamics and propulsion model for scramjet.
- [Falkiewicz and Cesnik 2011]: linear POD-Galerkin projection ROM for unsteady heat transfer finite-element model.
- [Falkiewicz et al. 2011]: Multi-physics Hypersonic vehicle ROM: coupled heat transfer ROM to piston-theory aerodynamics model, kriging surrogate for aerodynamic heat loads, and modal response structural model.
- [Crowell and McNamara, 2012]: kriging-based surrogate model approaches for vehicle surface pressures and temperatures.
- [Klock and Cesnik, 2017]: nonlinear POD-Galerkin projection ROM for unsteady heat transfer finite-element model

POD-Galerkin ROMs are known to be ineffective for highly nonlinear systems.

Our research satisfies model reduction criteria for nonlinear dynamical systems

Our model reduction research at Sandia

- ***Accuracy***
  - **LSPG projection**: *our baseline approach, has been applied to a compressible solver* [Carlberg, Bou-Mosleh, Farhat, 2011; Carlberg, Barone, Antil, 2017]
- ***Low cost***
  - **Sample mesh**: *use a fraction of the data for evalutaing nonlinear functions* [Carlberg, Farhat, Cortial, Amsallem, 2013]
  - Space–time LSPG projection: *learn and exploit structure in spatial and temporal data* [Carlberg, Ray, van Bloemen Waanders, 2015; Carlberg, Brencher, Haasdonk, Barth, 2017; Choi and Carlberg, 2019]
- ***Property preservation***
  - *Impose additional physical constraints (e.g. conservation)* [Carlberg, Tuminaro, Boggs, 2015; Peng and Carlberg, 2017; Carlberg, Choi, Sargsyan, 2018]
- ***Generalization***
  - Projection onto nonlinear manifolds: *high capacity nonlinear approximation* [Lee, Carlberg, 2018]
  - *h*-adaptivity: *trade cost for accuracy* [Carlberg, 2015; Etter and Carlberg, 2019]
  - Pressio software: *deploy methods for many application codes*
- ***Certification***
  - Machine learning error model: *quantify reduced model uncertainties* [Drohmann and Carlberg, 2015; Trehan, Carlberg, Durlofsky, 2017; Freno and Carlberg, 2019; Pagani, Manzoni, Carlberg, 2019]

Model Reduction Criteria

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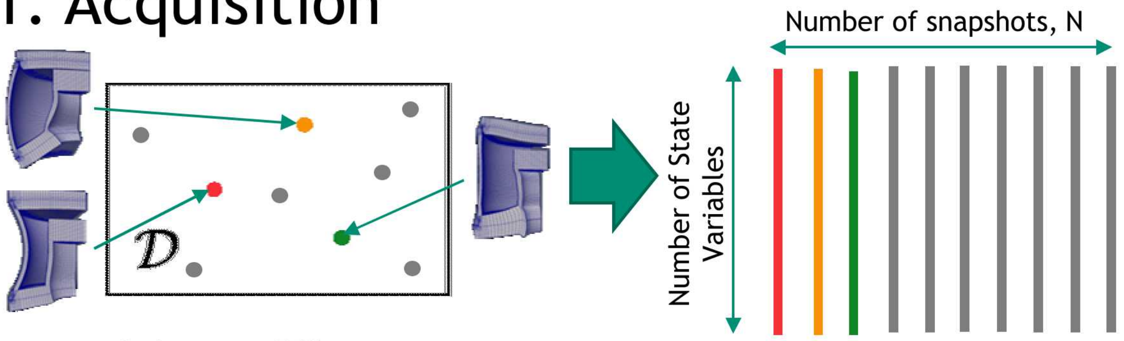
Least Squares Petrov—Galerkin (LSPG) for steady systems

[Carlberg, Bou-Mosleh, Farhat, 2011; Carlberg, Barone, Antil, 2017]

- High-fidelity simulation = $\mathbf{r}(\mathbf{x};\boldsymbol{\mu}) = \mathbf{0}$

1. Acquisition

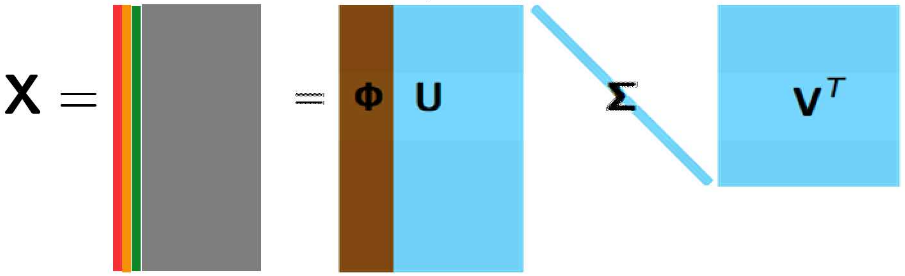


Solve at different design points

Save solution data

2. Learning

Proper Orthogonal Decomposition (POD):



3. Reduction

Reduce the number of unknowns

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

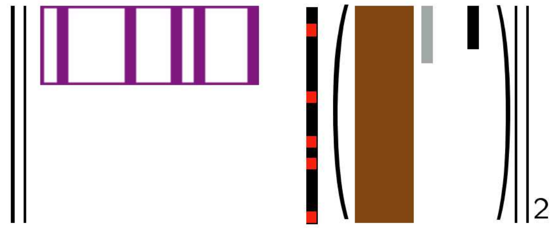
Compute initial guess for $\hat{\mathbf{x}}(\boldsymbol{\mu})$:

$$\hat{\mathbf{x}}^{IG}(\boldsymbol{\mu}) = \sum_{i=0}^{N} \frac{c}{\boldsymbol{\mu} - \boldsymbol{\mu}_i}\hat{\mathbf{x}}^{IG}(\boldsymbol{\mu}_i),$$

c = normalization constant

Minimize the Residual

$$\underset{\hat{\mathbf{v}}}{\text{minimize}} \| \mathbf{A}\, \mathbf{r}(\mathbf{\Phi}\,\hat{\mathbf{v}};\boldsymbol{\mu}) \|_2$$

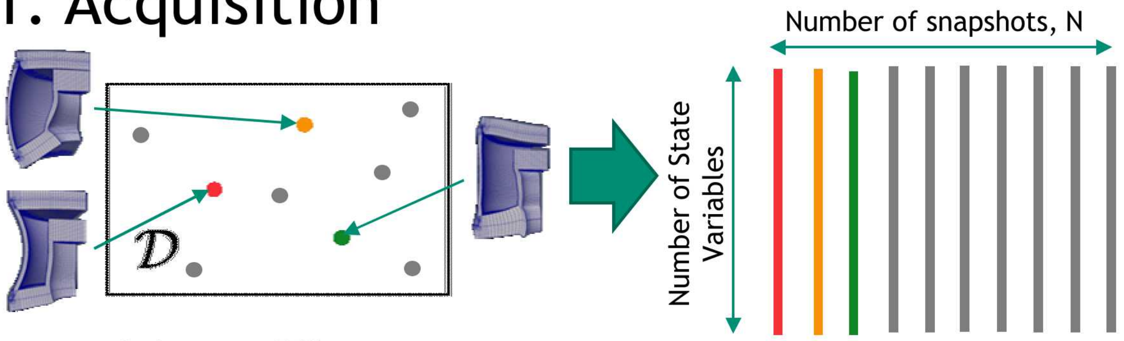


Conservation can be enforced with additional constraints

[Carlberg, Choi, Sargsyan, 2018]

- High-fidelity simulation = $\mathbf{r}(\mathbf{x};\boldsymbol{\mu}) = \mathbf{0}$

1. Acquisition

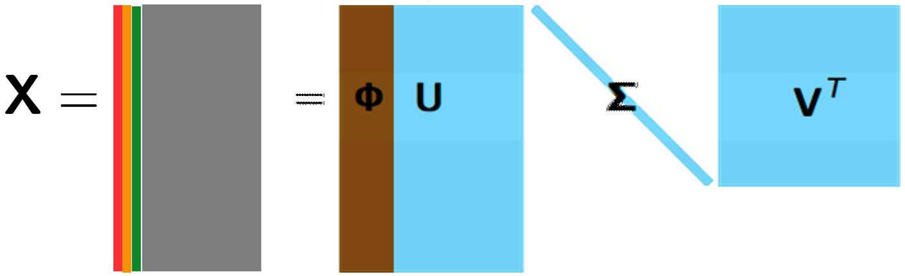


Solve at different design points

Save solution data

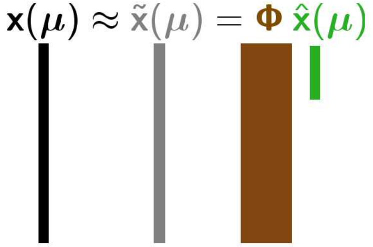
2. Learning

Proper Orthogonal Decomposition (POD):



3. Reduction

Reduce the number of unknowns



Compute initial guess for $\hat{\mathbf{x}}(\boldsymbol{\mu})$:

$$\hat{\mathbf{x}}^{IG}(\boldsymbol{\mu}) = \sum_{i=0}^{N} \frac{c}{\boldsymbol{\mu} - \boldsymbol{\mu}_i} \hat{\mathbf{x}}^{IG}(\boldsymbol{\mu}_i),$$

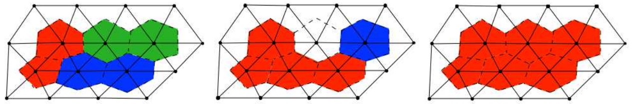
c = normalization constant

Minimize the Residual

$$\underset{\hat{\mathbf{v}}}{\text{minimize}}\ \|\mathbf{A}\mathbf{r}(\boldsymbol{\Phi}\hat{\mathbf{v}};\boldsymbol{\mu})\|_2^2$$

$$\text{s.t. } \mathbf{C}\mathbf{r}(\boldsymbol{\Phi}\hat{\mathbf{v}};\boldsymbol{\mu}) = \mathbf{0}$$

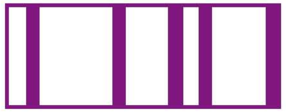
Enforce conservation over subdomains:



We do hyper-reduction with collocation to keep offline costs down

- Collocation has been used in past studies of CFD model reduction [Washabaugh, 2016]:

LSPG: $\underset{\hat{\mathbf{v}}}{\text{minimize}} \ \|\mathbf{A}\mathbf{r}(\mathbf{\Phi}\hat{\mathbf{v}};\boldsymbol{\mu})\|_2^2$

$\mathbf{A} =$ 

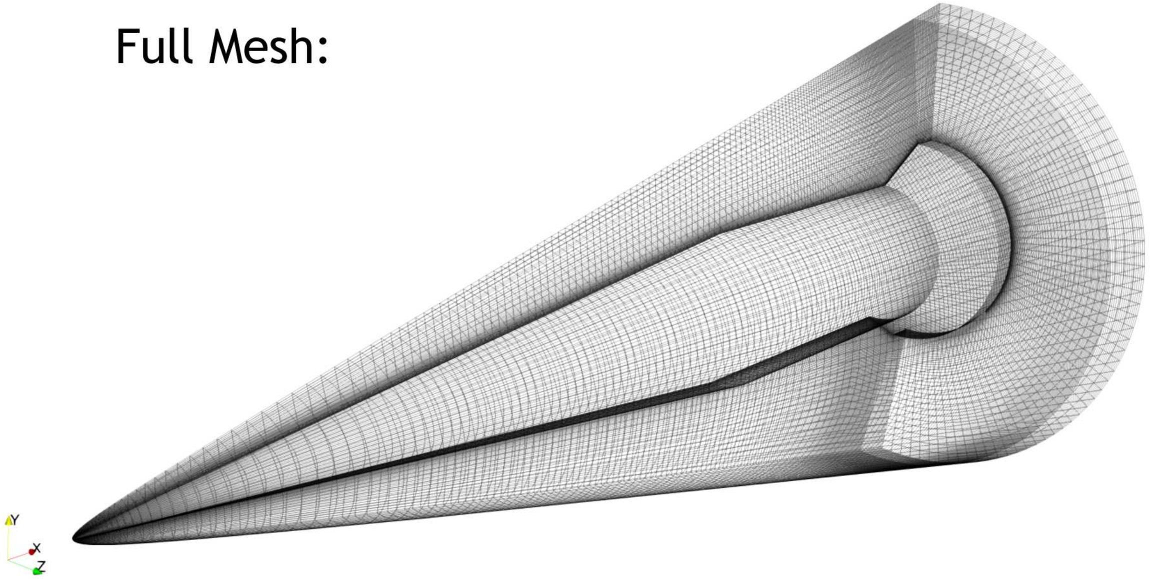
Collocation
=
choose rows of **A**
from identity matrix

$$\begin{matrix} (1 & 0 & 0 & 0 & \dots & 0) \\ (0 & 0 & 1 & 0 & \dots & 0) \\ (0 & \dots & 0 & 1 & 0 & 0) \end{matrix}$$

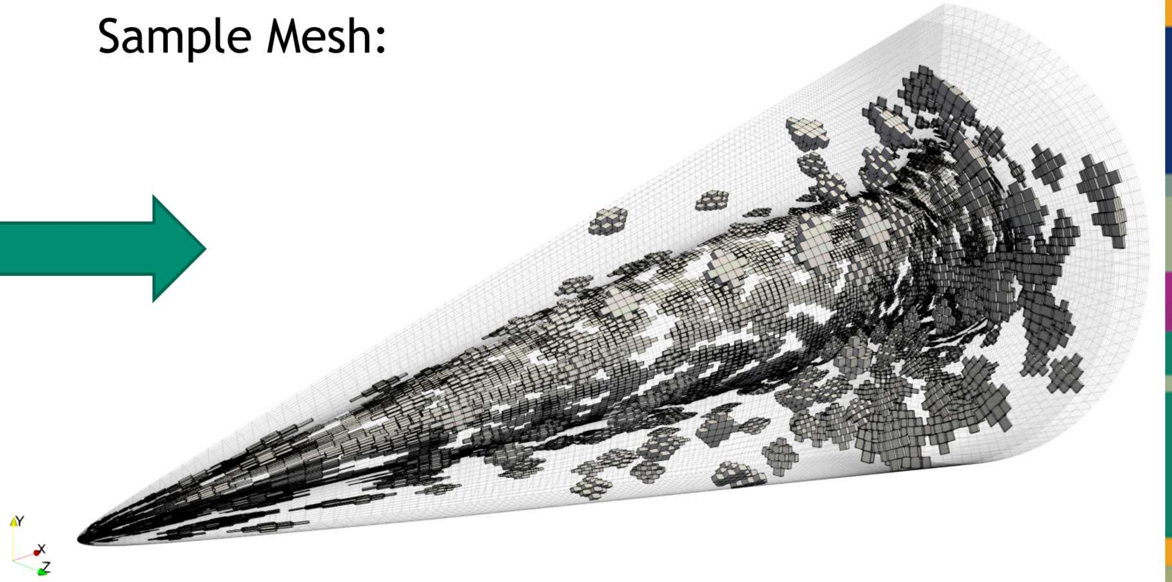
  - ➢ Inexpensive compared to DEIM and GNAT.

- Sample mesh: subset of cells required to compute residual
- We consider random sampling of cells in this study.

Full Mesh:

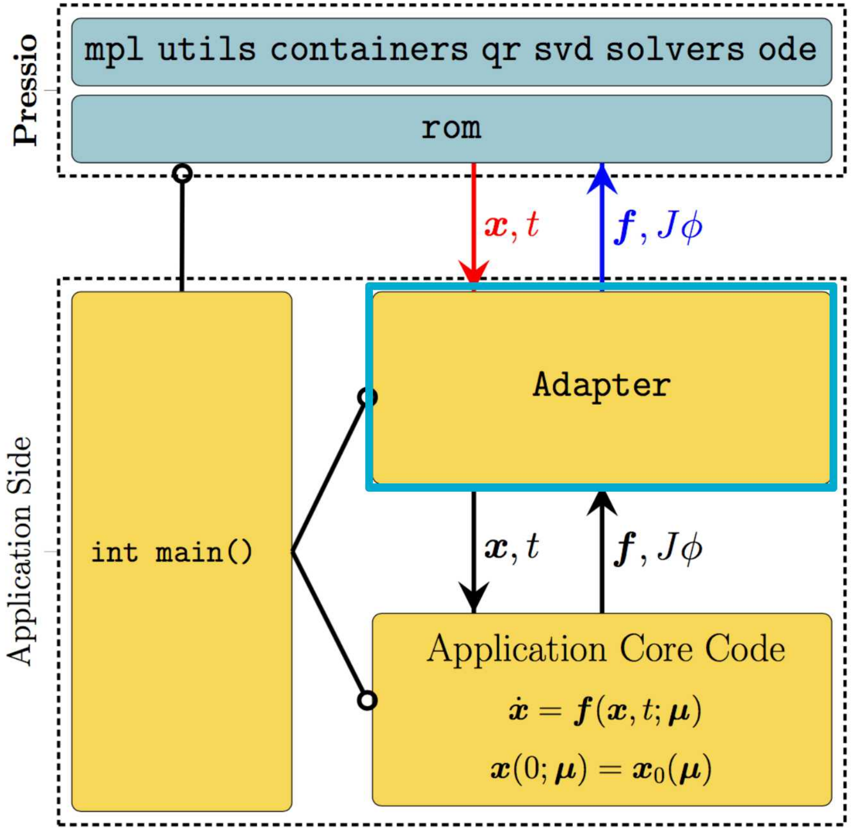


Sample Mesh:



Pressio enables deployment of ROM methods to a range of applications

- Previous ROM methods were implemented directly in multiple application codes
  - ✗ **Highly intrusive**: major changes to application code
  - ✗ **Not generalizable**: individual ROM implementation for each application
  - ✗ **Access requirements**: developers need direct access to application
- Pressio, a software package that addresses all three of these issues:
  - ✓ Minimal API method implementation.
  - ✓ Leverages modern software engineering practices (e.g. C++ template-metaprogramming)
    - ➢ Restricted to practices used by mission application partners
  - ✓ Facilitates contributions from external partners
    - ➢ Open source
  - ✓ Clear separation between methods and application

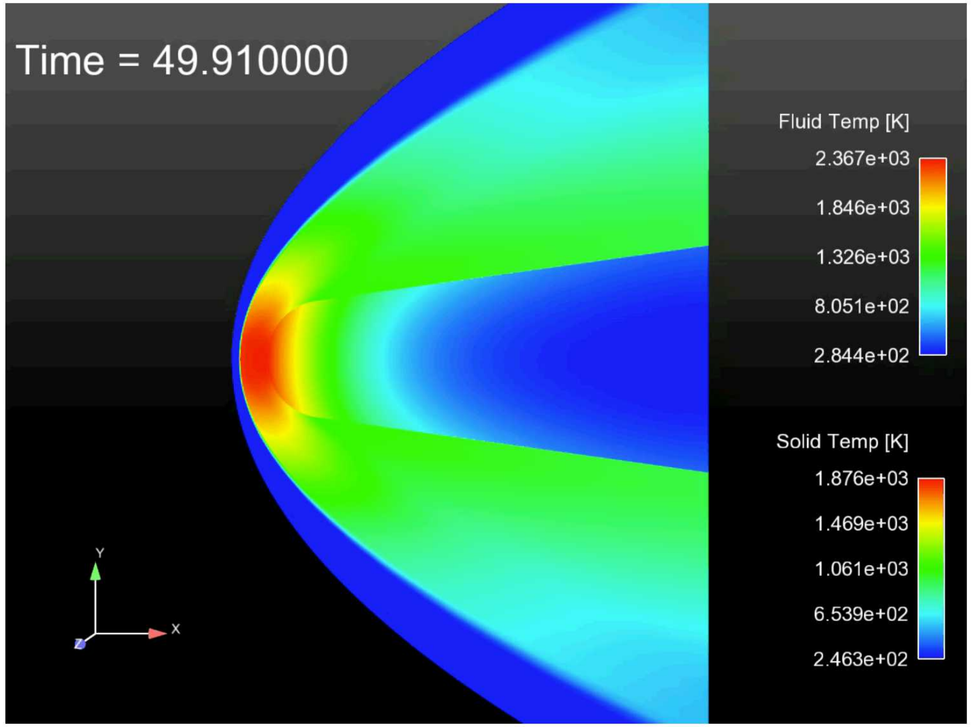


Schematic of Pressio software workflow

https://github.com/Pressio

Sandia Parallel Aerodyanmics and Reentry Code (SPARC)

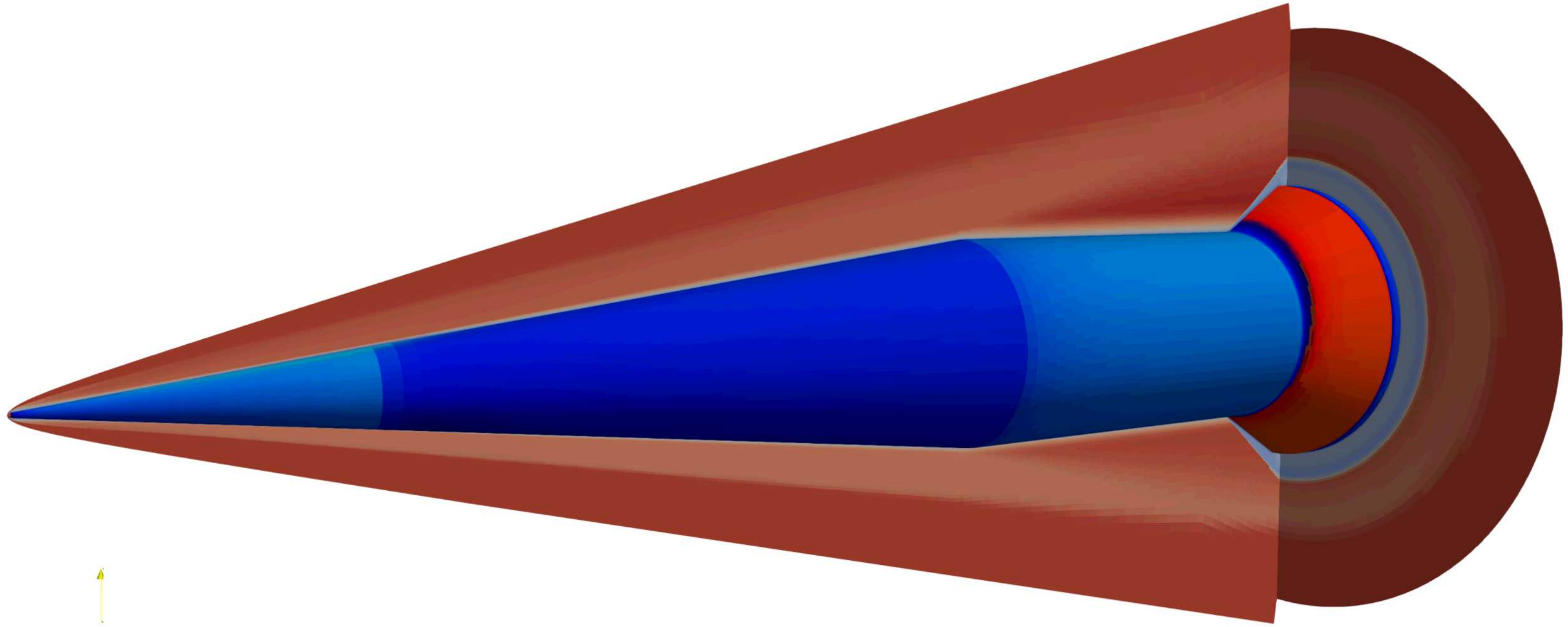
- Compressible CFD code focused on aerodynamics and aerothermodynamics in the Transonic and Hypersonic regimes
  - Being developed to run on today's leadership-class supercomputers and exascale machines.
  - Performance portability: SPARC leverages Kokkos to run on multiple machines with different architectures (e.g. CPU vs. CPU/GPU)
- Physics Capabilities include:
  - Navier—Stokes, cell-centered finite volume method
  - **Reynolds-Averaged Navier—Stokes (RANS) , cell-centered finite volume method**
  - Transient Heat Equation, Galerkin finite element method.
  - Decomposing and non-decomposing ablation equations, Galerkin finite element method.
  - One and two-way coupling between ablation, heat equation, RANS.



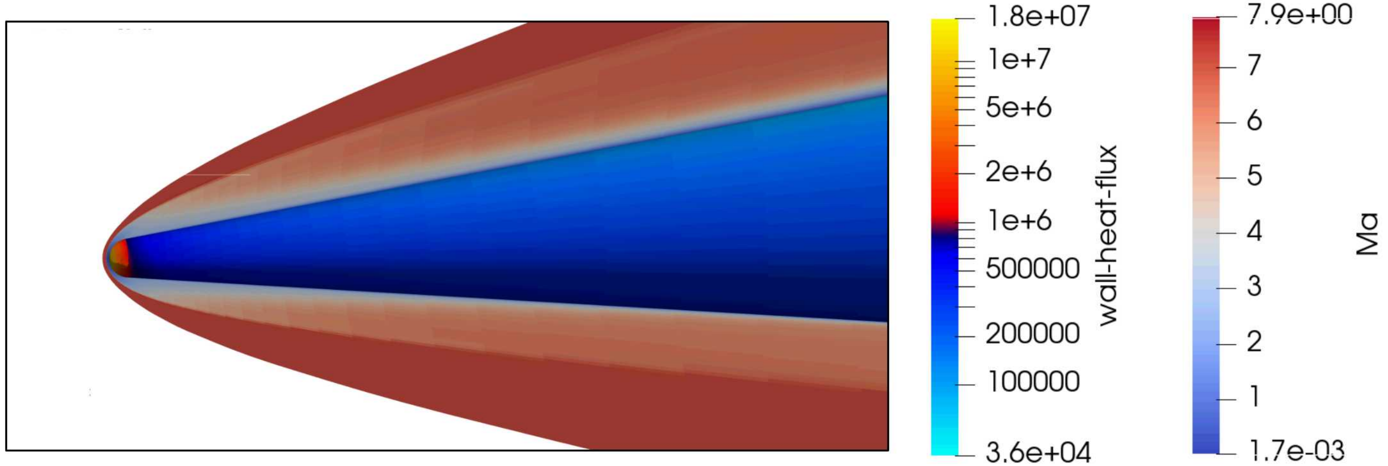
Temperature of a slender body in hypersonic flow simulated with SPARC

Test Case: HIFiRE-1 flight vehicle

- Flow field:
  - Free stream Mach No. = 7.1
  - Reynolds No. = 10.0 million/meter
  - Angle of Attack = 2 degrees
  - Boundary layer transitions to turbulence (use Spalart-Allmaras with specified transition location)
- Spatial discretization:
  - 2^{nd}-order finite volume
  - 2,031,616 cells
  - $y^+<1$ near wall
- Solver:
  - Pseudo time stepping with backward Euler, CFL schedule.

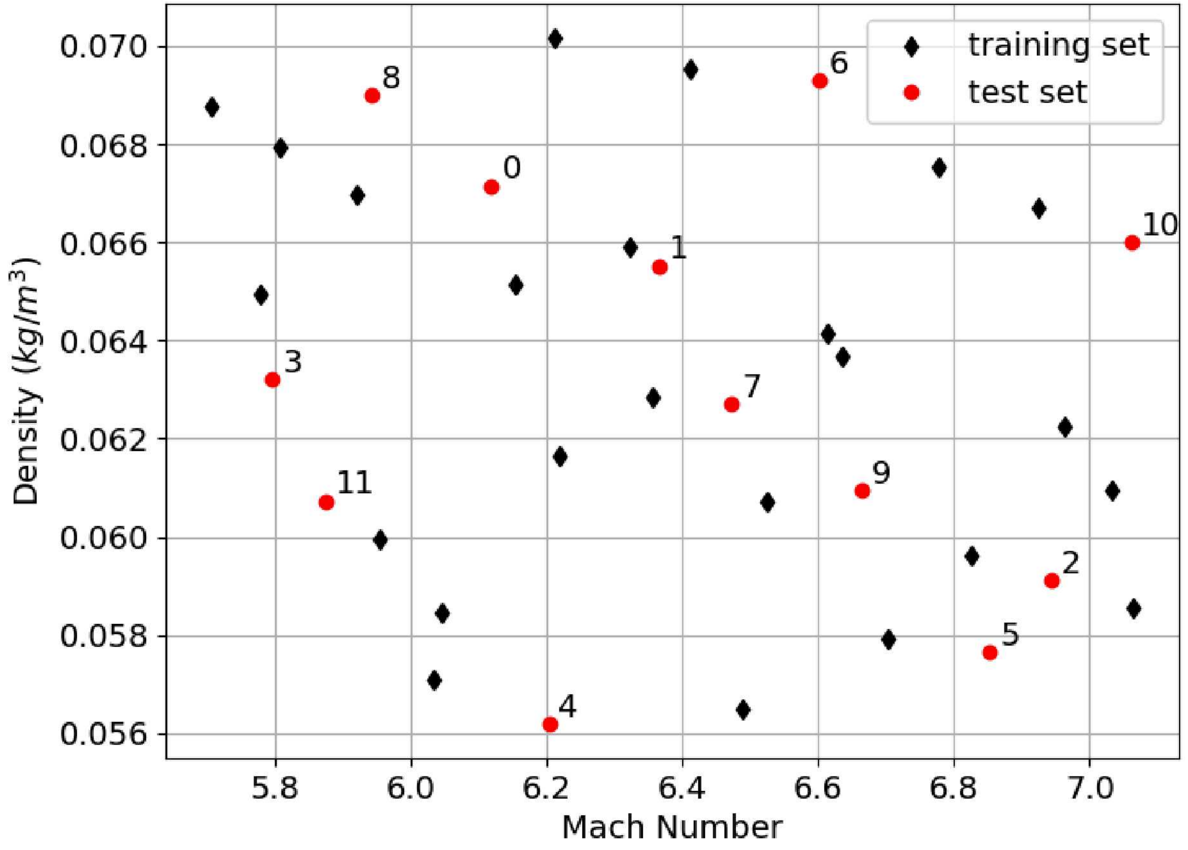


Close up of nose:



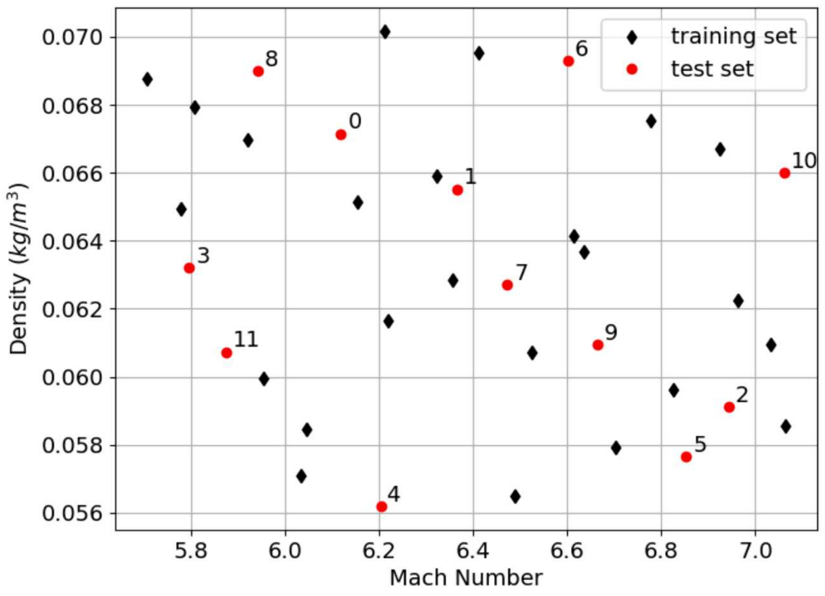
Training Data and Model details

- Samples:
  - Varied freestream density and velocity
  - Training set: 24 sample Latin hypercube
  - Test set: 12 sample Latin hypercube
- POD basis:
  - Mean flow subtracted from each snapshot.
  - Each conserved quantity scaled by its maximum over all FOM solutions.
  - 2,4, and 8 mode basis were considered.
- ROM: LSPG solved with Gauss-Newton iteration
  - Initial guess obtained via inverse-distance interpolation of POD modes.
  - Full mesh, two sample meshes considered



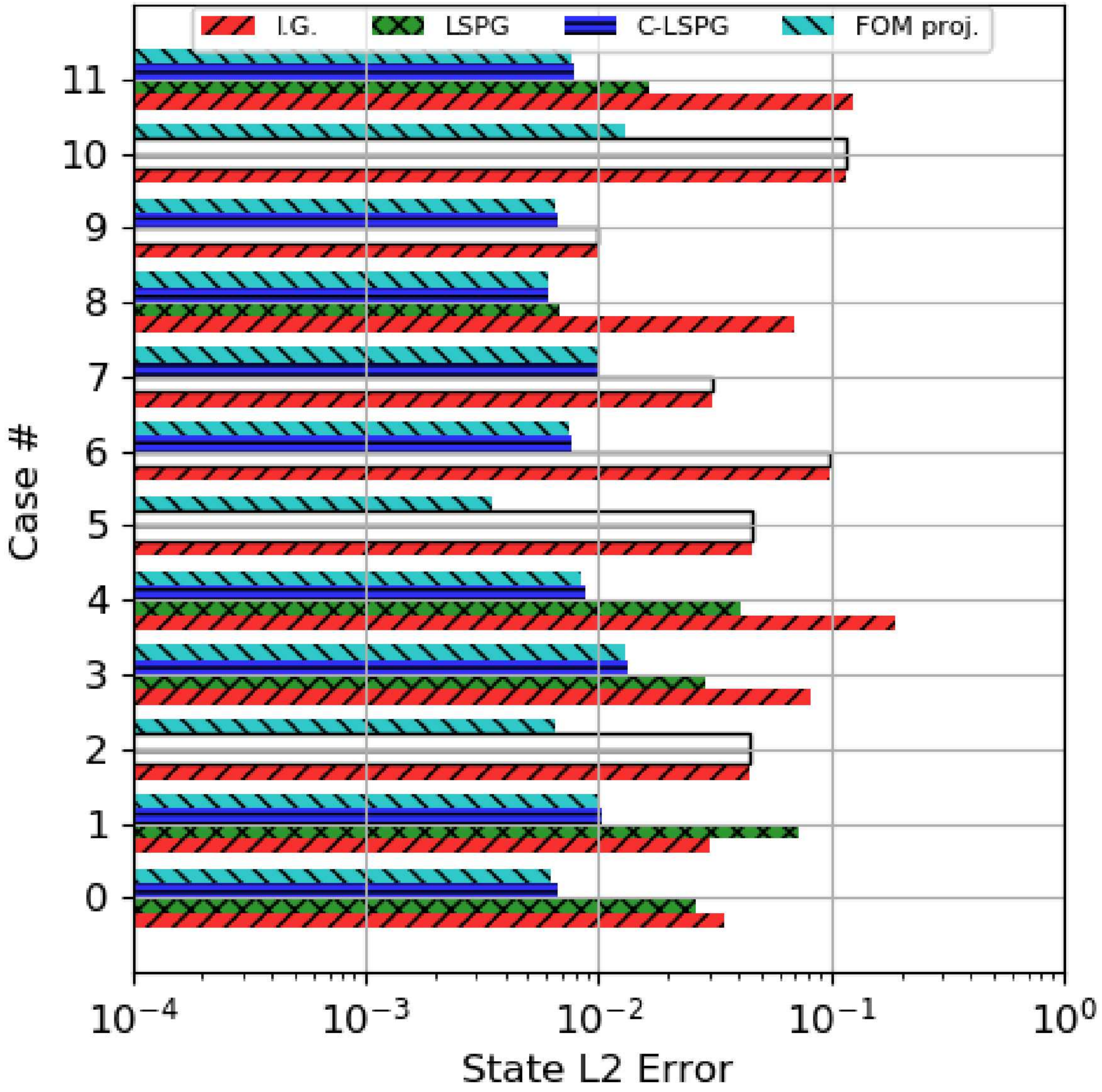
Full Mesh ROM L2 State Error

Parameter Space:



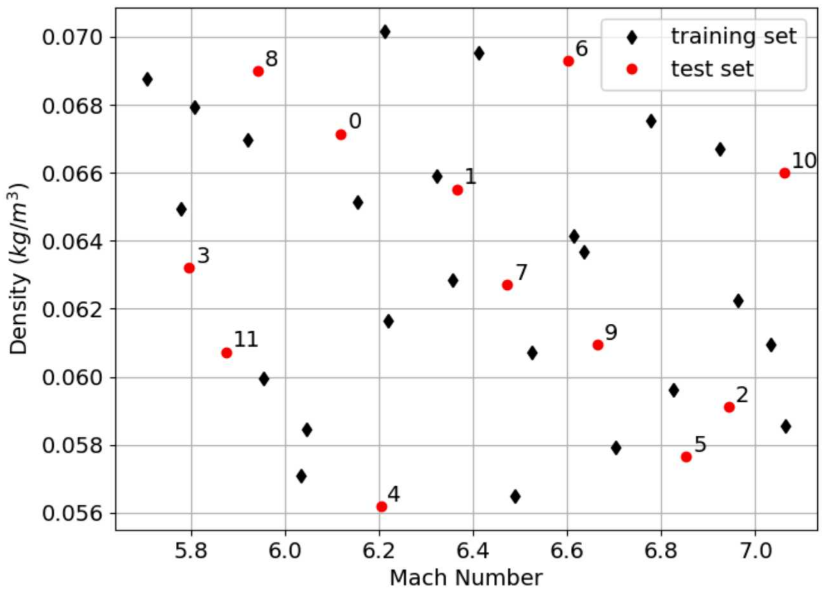
- State error around 1% or less
- Interpolated state error up to 20%
- Conservation constraint improves accuracy
- Accuracy increases with number of modes

2 Modes



Full Mesh ROM L2 State Error

Parameter Space:



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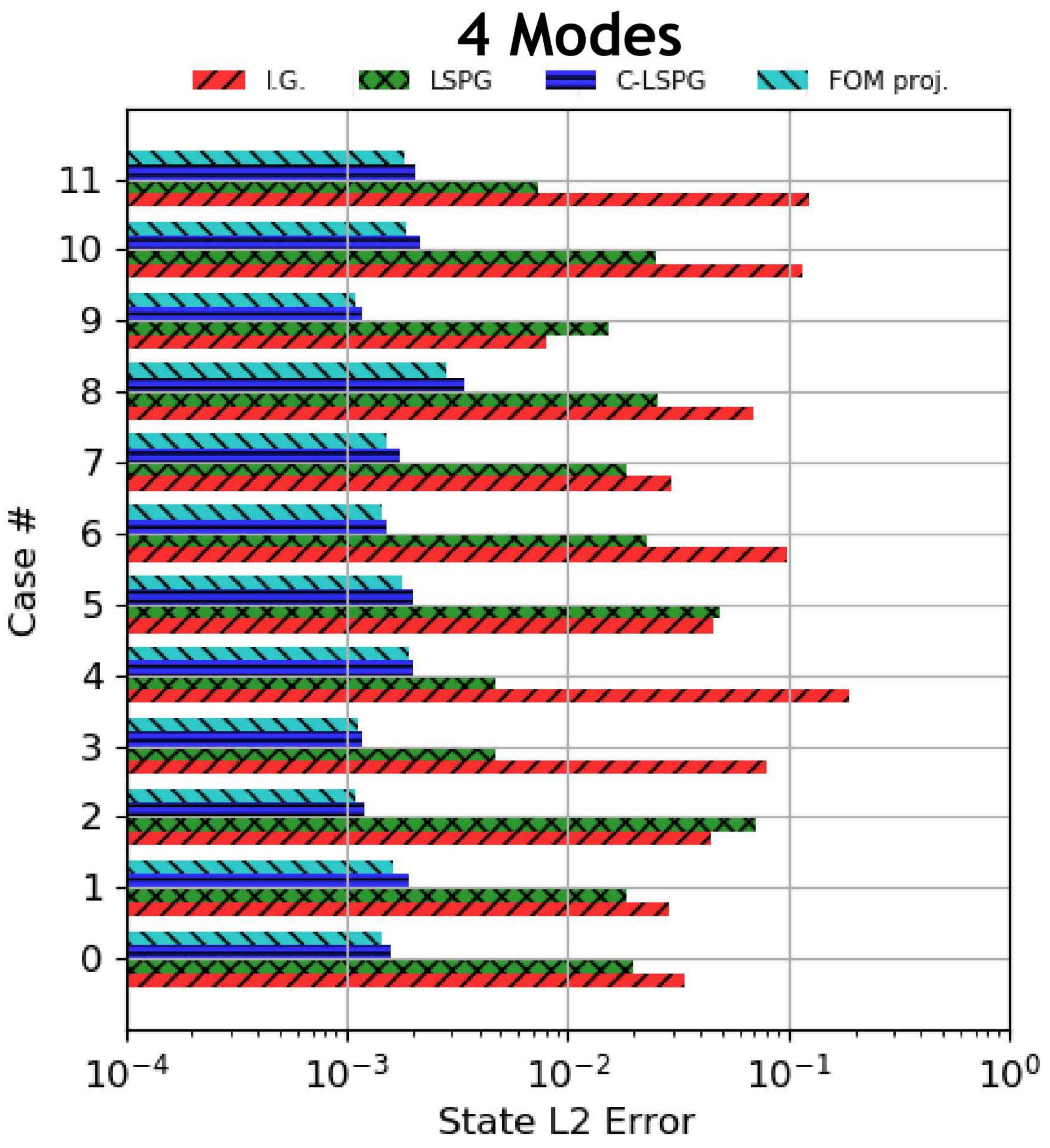
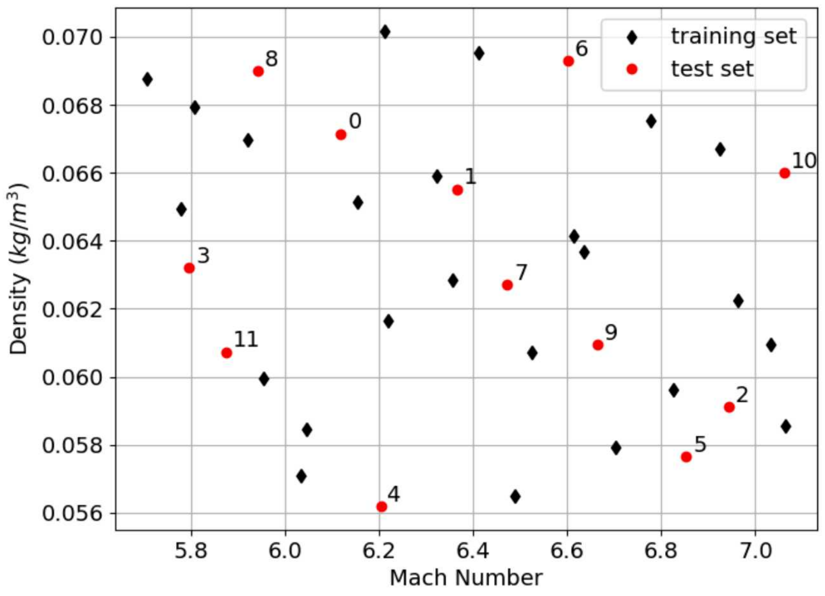


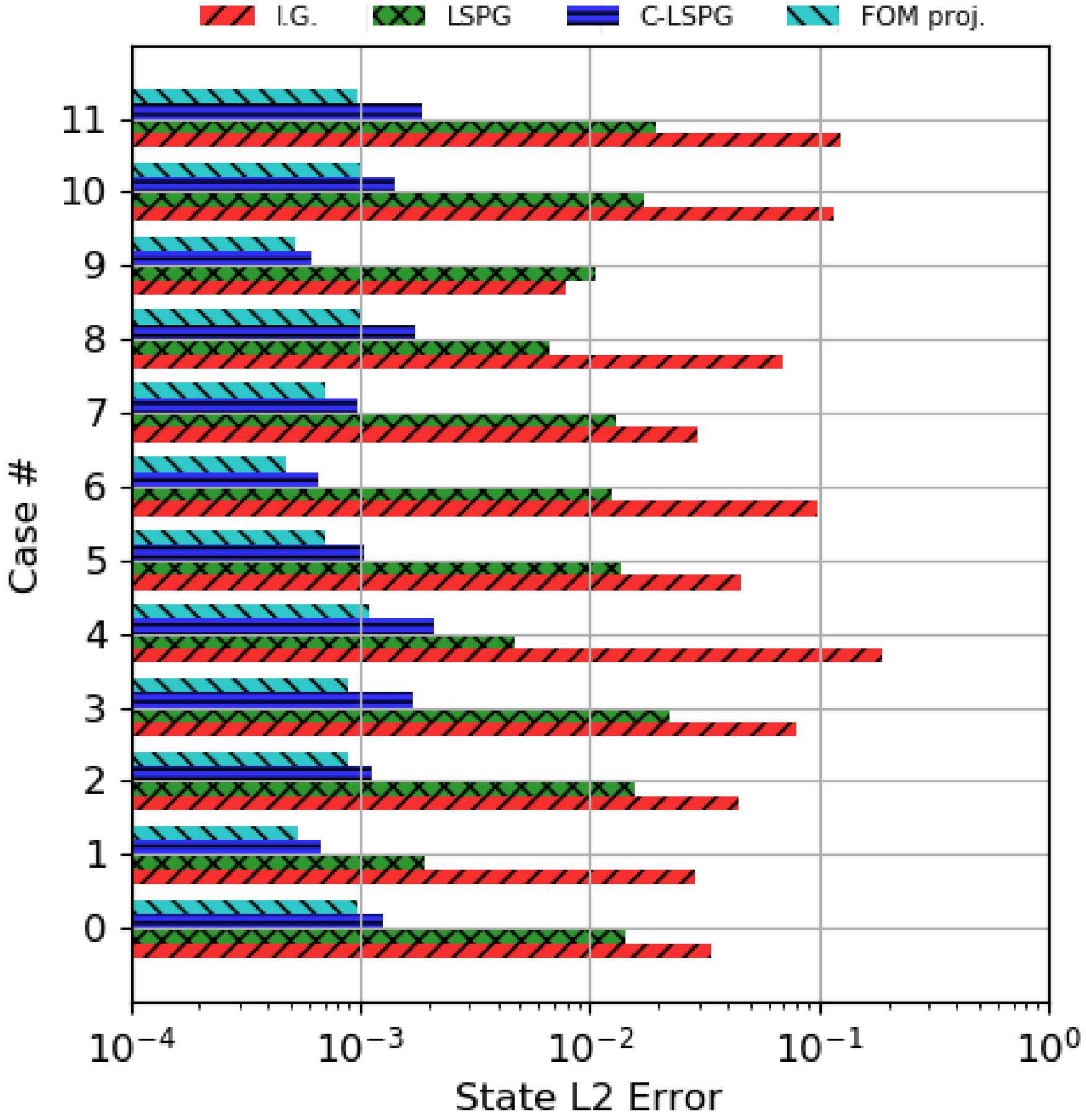
Full Mesh ROM L2 State Error

Parameter Space:



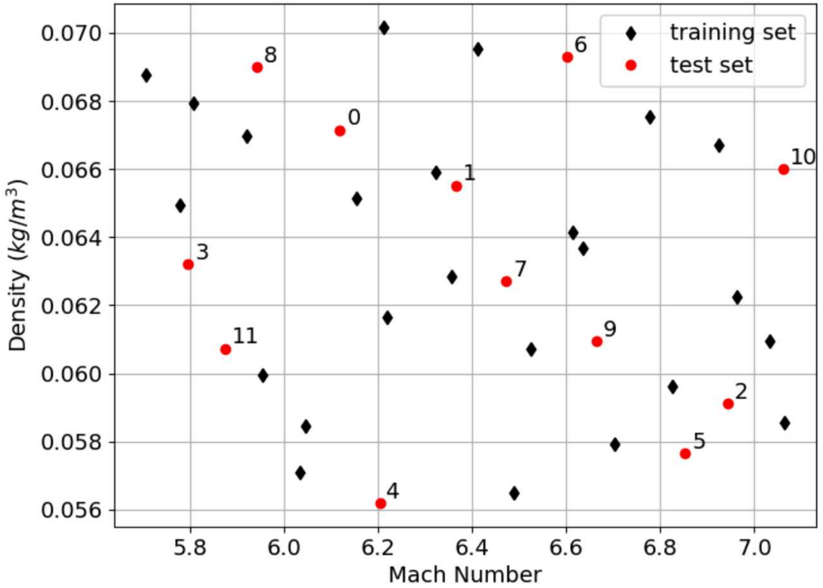
- State error around 1% or less
- Interpolated state error up to 20%
- Conservation constraint improves accuracy
- Accuracy increases with number of modes

8 Modes

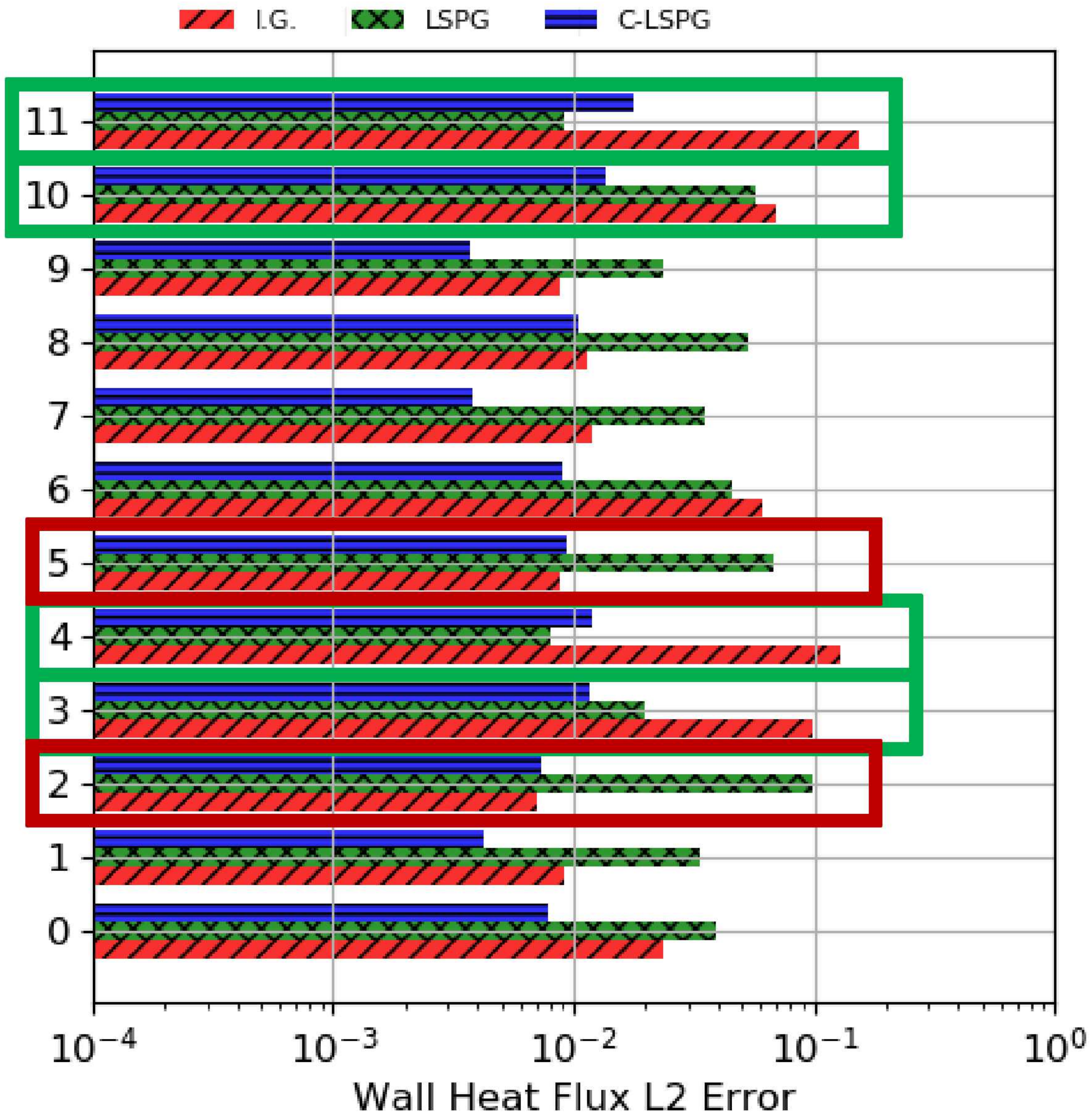


Full Mesh ROM Wall Heat Flux Error

Parameter Space:



4 Modes



- Wall heat flux error around 1-3%
- Wall heat flux from initial guess varies widely
- Conservation constraint improves accuracy
- Accuracy increases with number of modes

Sample Meshes

Sample Mesh A

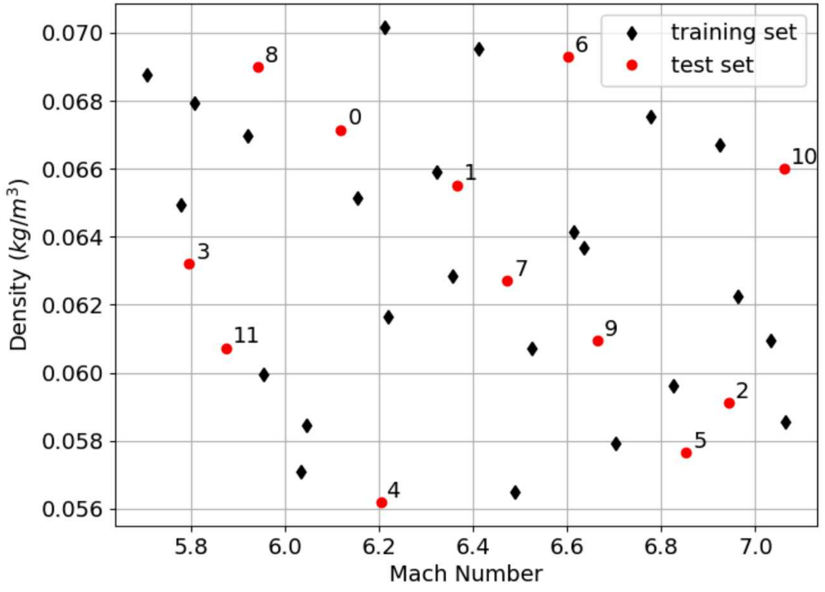
- 2032 Random cells (0.1% of full mesh)
- 49467 cells (2.4% of full mesh)

Sample Mesh B

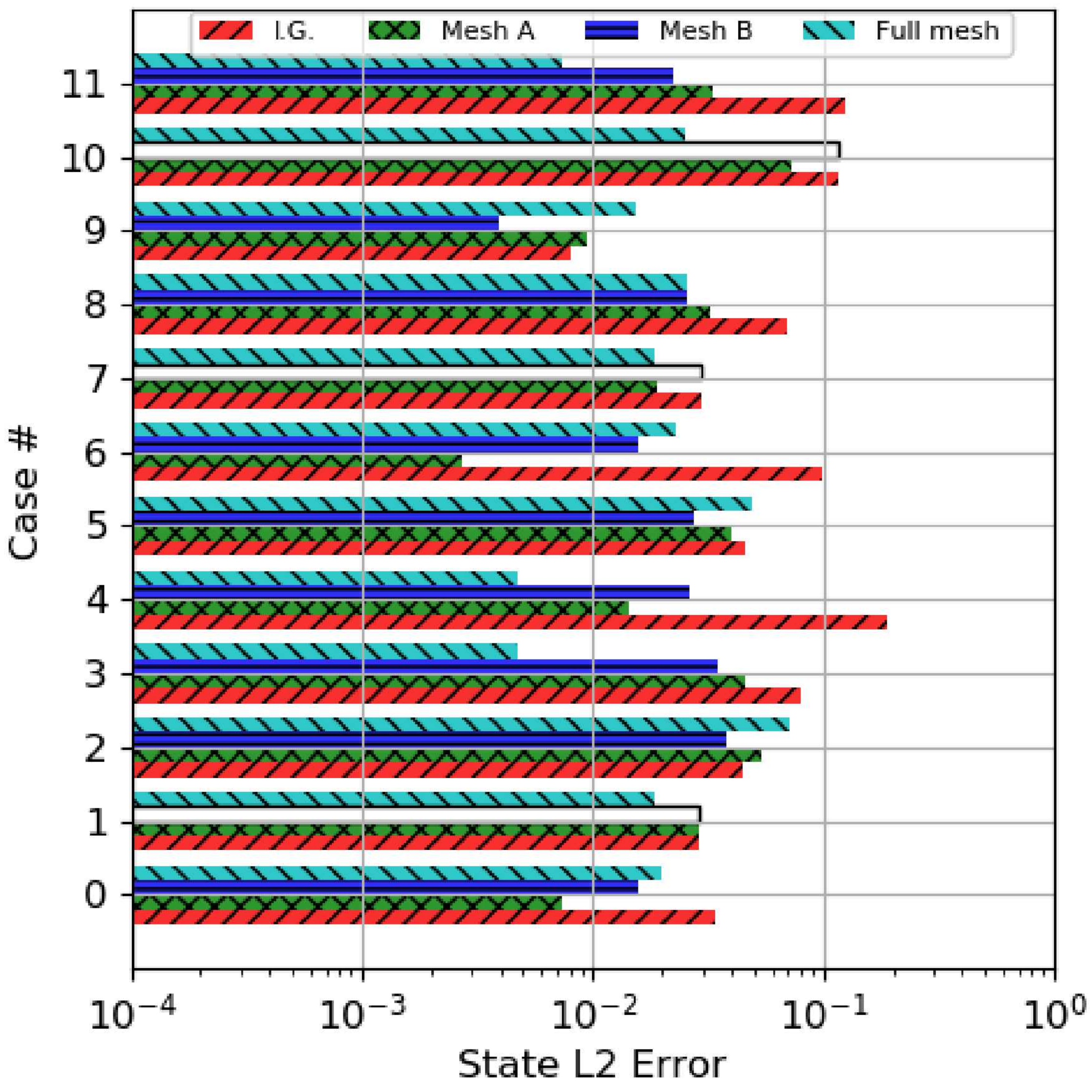
- 813 Random cells (0.04% of full mesh)
- 19901 cells (0.98% of full mesh)

Sample Mesh ROM L2 State Error

Parameter Space:



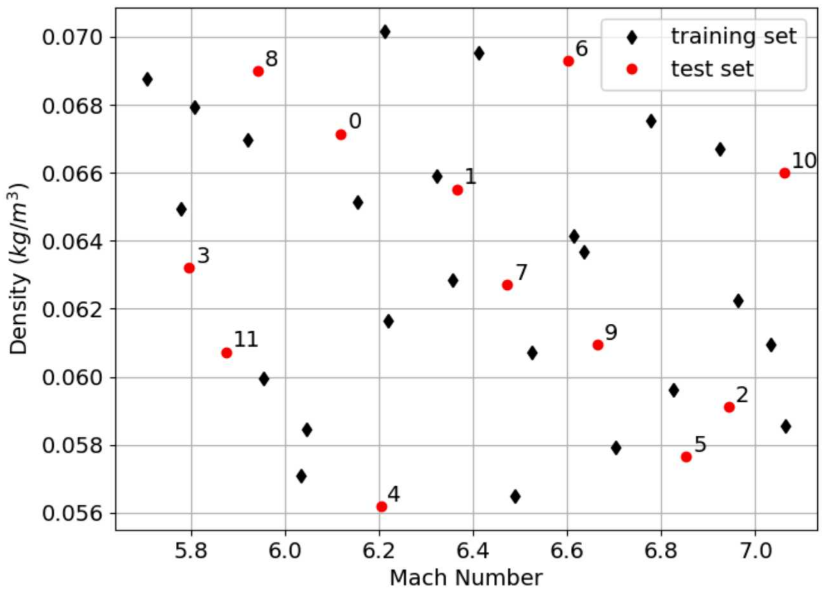
LSPG



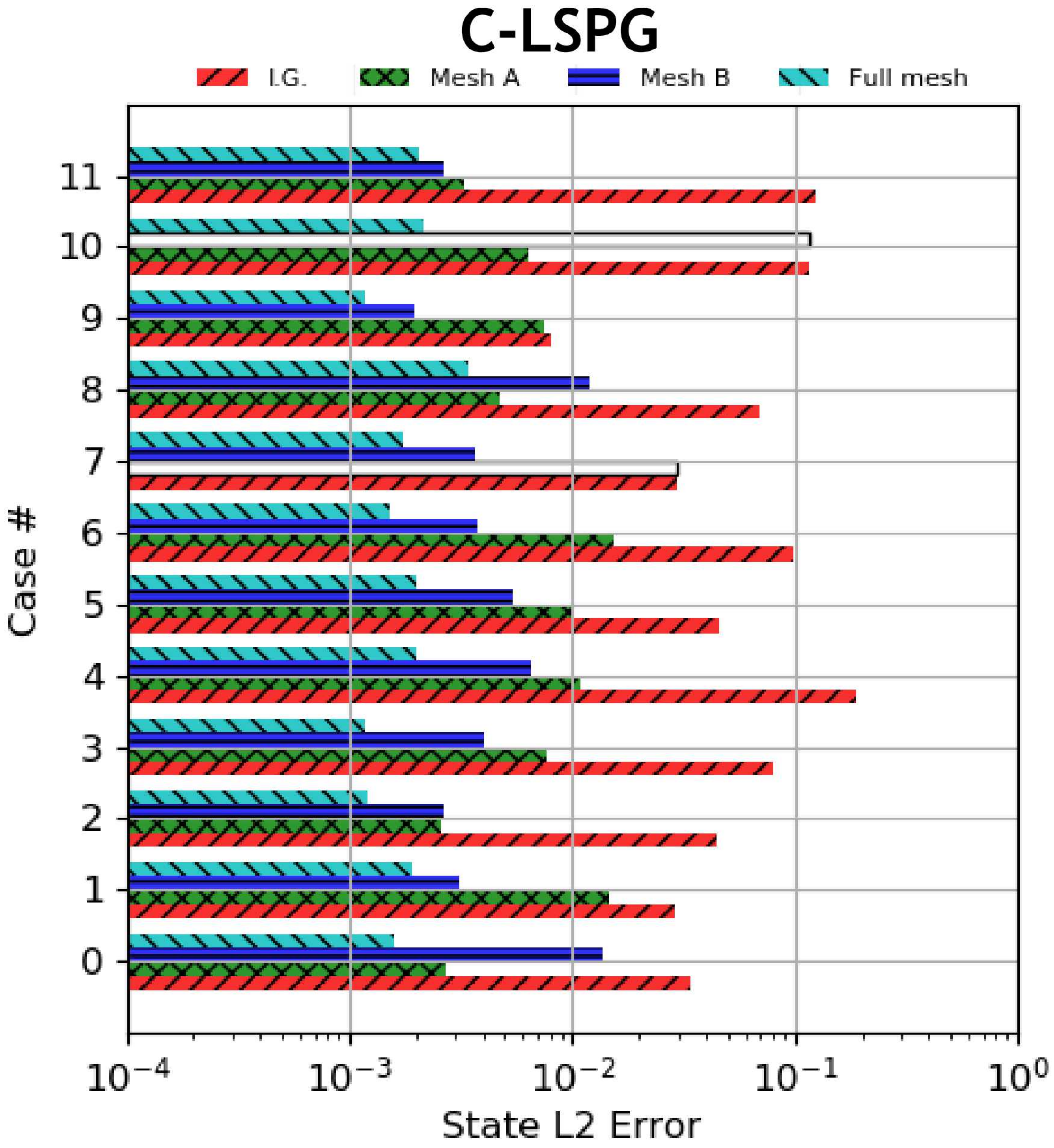
- State error around 1% or less
- Interpolated state error up to 20%
- Conservation constraint improves accuracy

Sample Mesh ROM L2 State Error

Parameter Space:

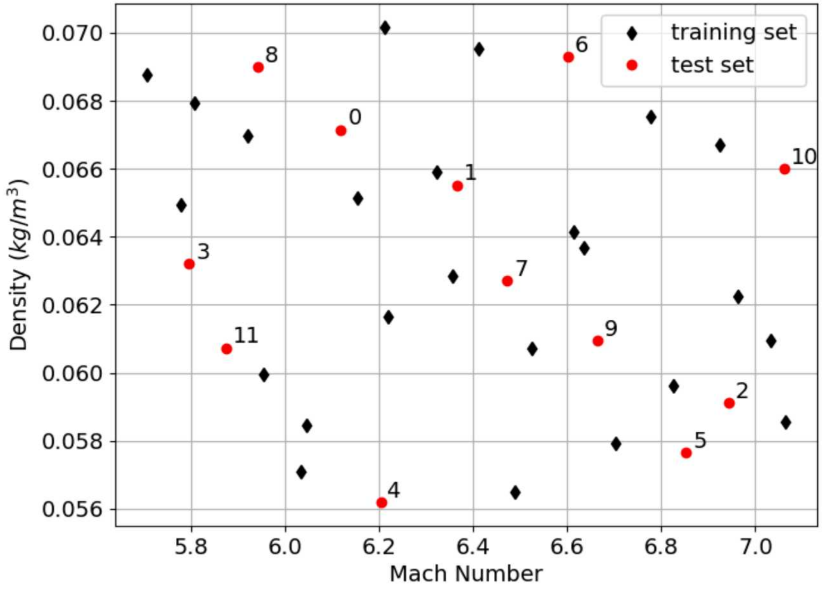


- State error around 1% or less
- Interpolated state error up to 20%
- Conservation constraint improves accuracy



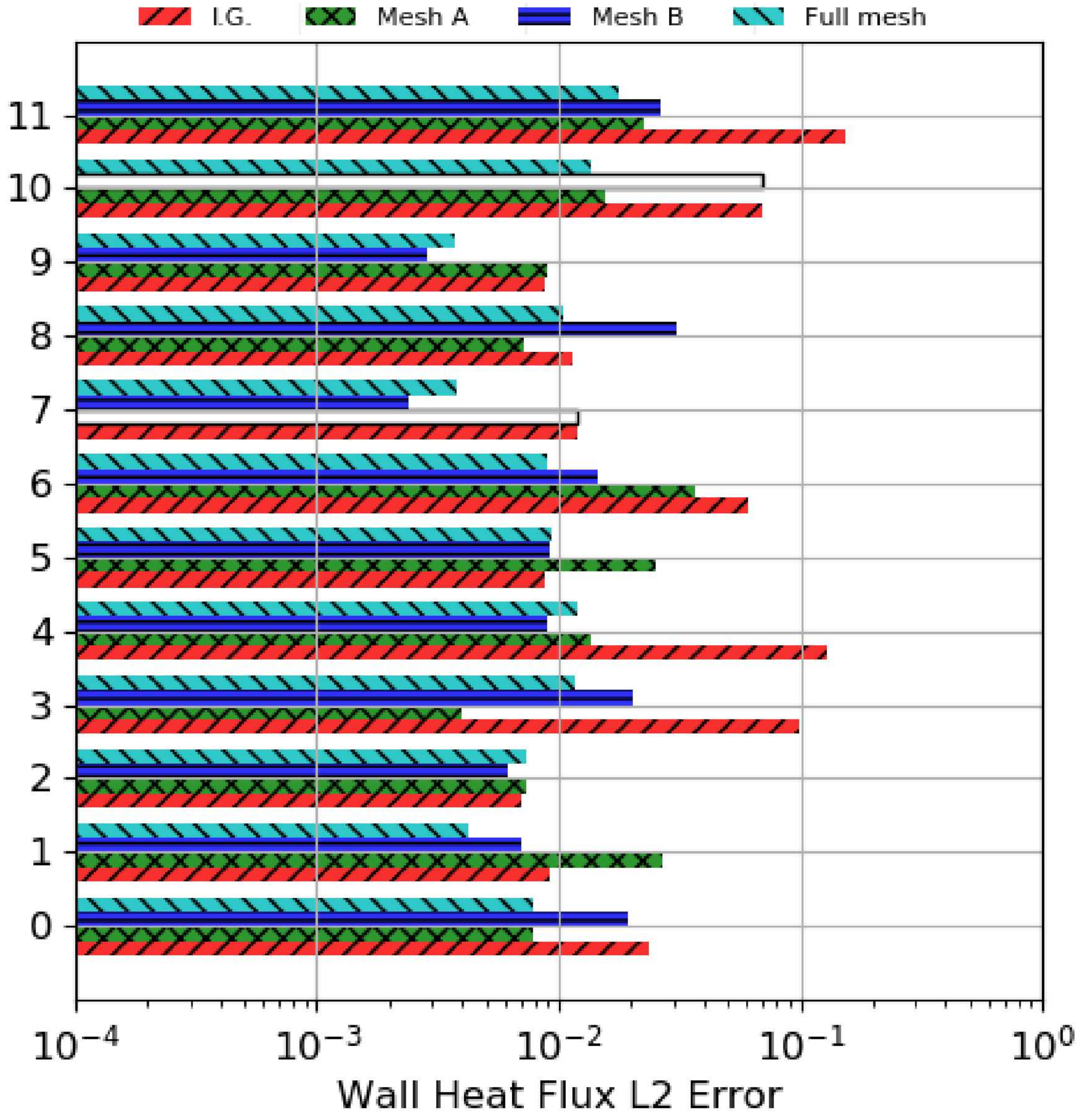
Sample Mesh ROM Heat Flux Error

Parameter Space:



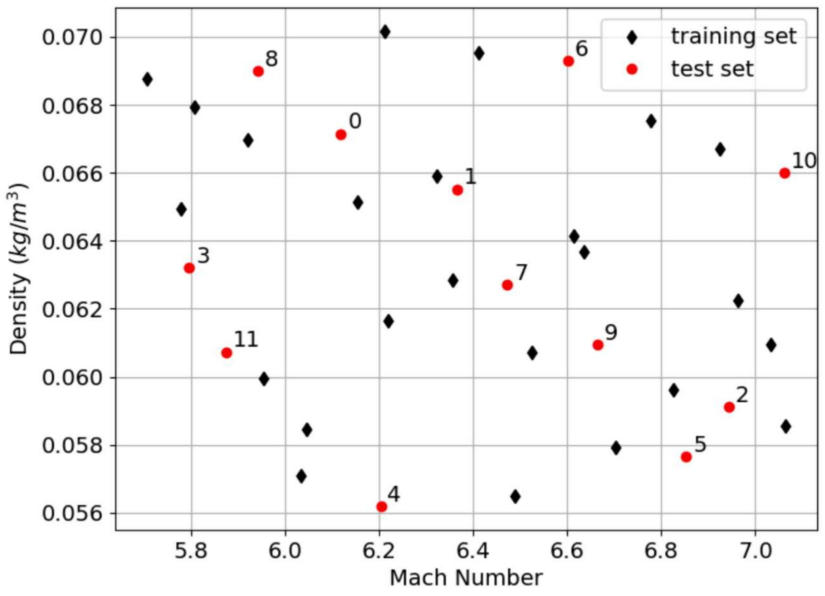
- Wall heat flux error around 1-3%
- Conservation constraint improves accuracy
- Sample mesh can be more accurate than full mesh!

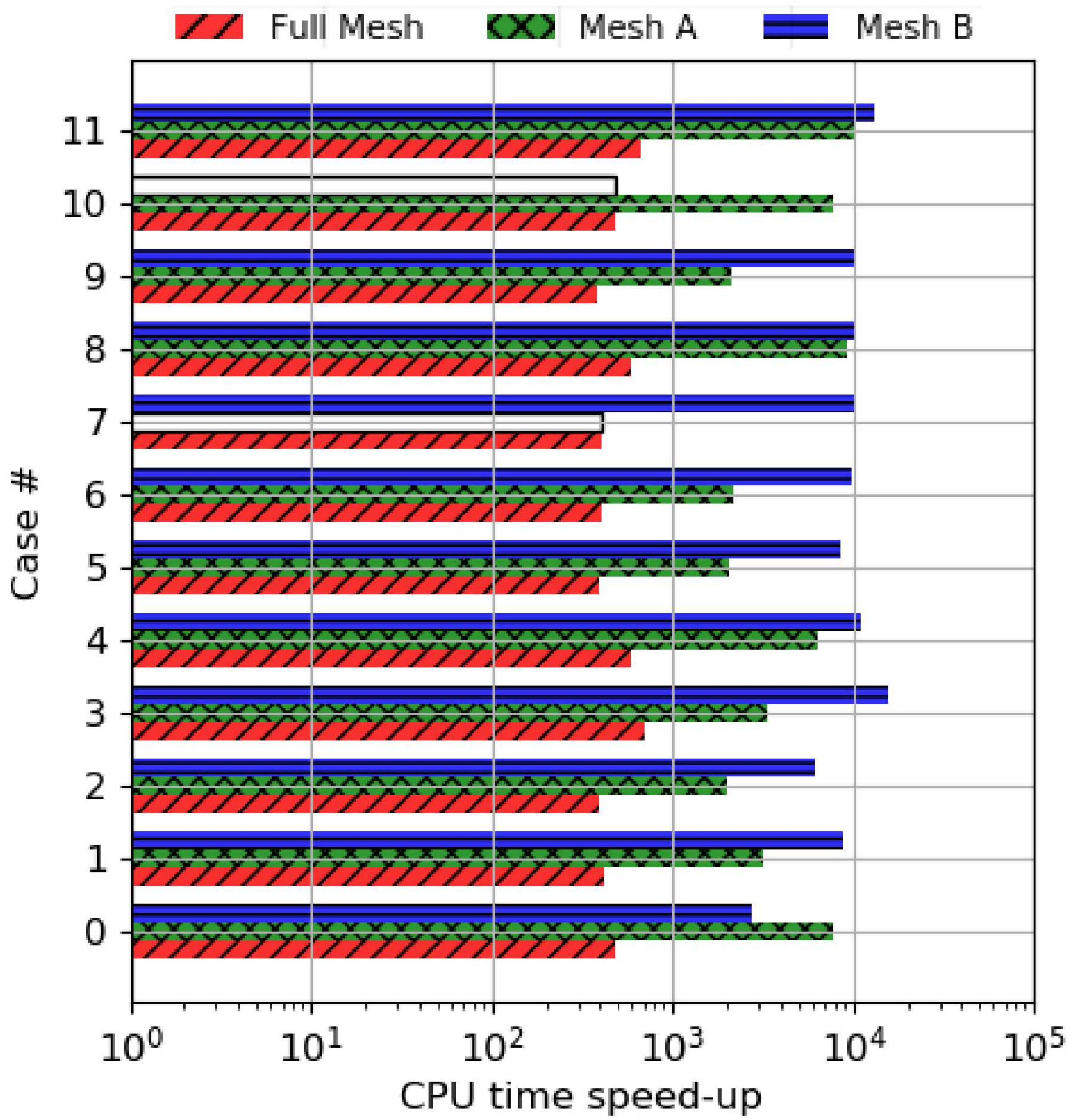
C-LSPG



Performance of ROM with conservation constraint

Parameter Space:





- Could run hundreds or thousands of ROMs in the same CPU time as one FOM!
- Full mesh ROM is at least 400X faster than the corresponding FOM run.
- Hyper-reduced ROMs are 2,000-10,000X faster than the corresponding FOM run.

Increasing ROM robustness with nonlinear mapping of POD basis

- Failed cases shown earlier are due to small regions of negative temperature.
- States with non-physical features are encountered by ROM solver more often as basis is made smaller and/or parameter space is increased in size.
- **Solution**: nonlinear mapping of POD modes to remove non-physical features from approx. state vector:

$$\underset{\hat{\mathbf{v}}}{\text{minimize}} \ \|\mathbf{A}\mathbf{r}(\mathbf{\Phi}\hat{\mathbf{v}};\boldsymbol{\mu})\|_2^2 \ \longrightarrow \ \underset{\hat{\mathbf{v}}}{\text{minimize}} \ \|\mathbf{A}\mathbf{r}(\mathbf{g}(\mathbf{\Phi}\hat{\mathbf{v}});\boldsymbol{\mu})\|_2^2$$

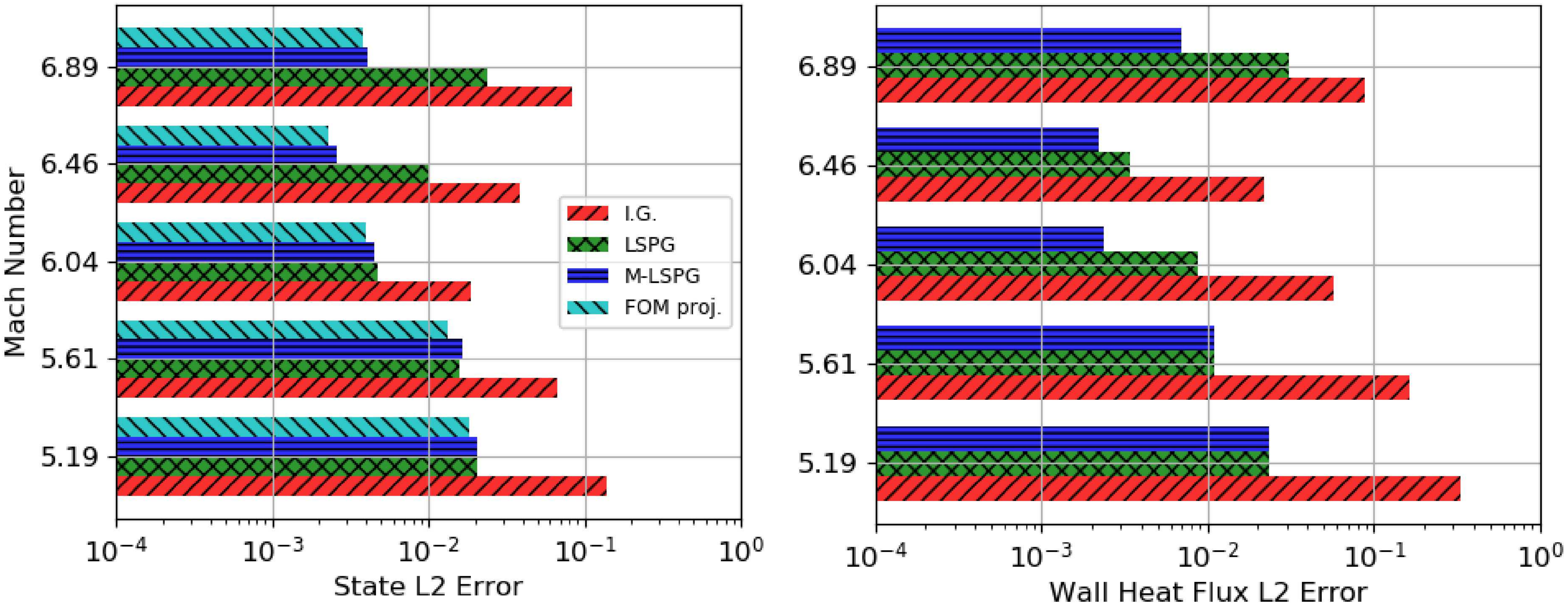
Where **g** transforms the conserved quantities in each cell as follows:

$$\begin{aligned}
\tilde{\tilde{u}}_1 &= \max(\epsilon_1, \tilde{u}_1) \\
\tilde{\tilde{u}}_2 &= \tilde{u}_2 \\
\tilde{\tilde{u}}_3 &= \tilde{u}_3 \\
\tilde{\tilde{u}}_4 &= \tilde{u}_4 \\
\tilde{\tilde{u}}_5 &= \max\left(\epsilon_5 + \frac{1}{2\tilde{\tilde{u}}_1}\left[\tilde{u}_2^2 + \tilde{u}_3^2 + \tilde{u}_4^2\right]\ ,\ \tilde{u}_5\right)
\end{aligned}$$

Training Data and Model details

- Samples:
  - Varied freestream density and velocity
  - Training set: Mach Numbers [4.97, 5.40, 5.83, 6.25, 6.68, 7.10]
  - Test set: Mach Numbers [5.19, 5.61, 6.04, 6.46, 6.89]
- POD basis:
  - Mean flow subtracted from each snapshot.
  - Each conserved quantity scaled by its maximum over all FOM solutions.
  - Basis truncated to 4 modes, capturing 99.98% of statistical energy.
- ROM: LSPG solved with Gauss-Newton iteration
  - Initial guess obtained via inverse-distance interpolation of POD modes.
  - Simple Armijo rule line search OR nonlinear mapping used to avoid non-physical solutions
  - Hyper-reduction not tested for this case.

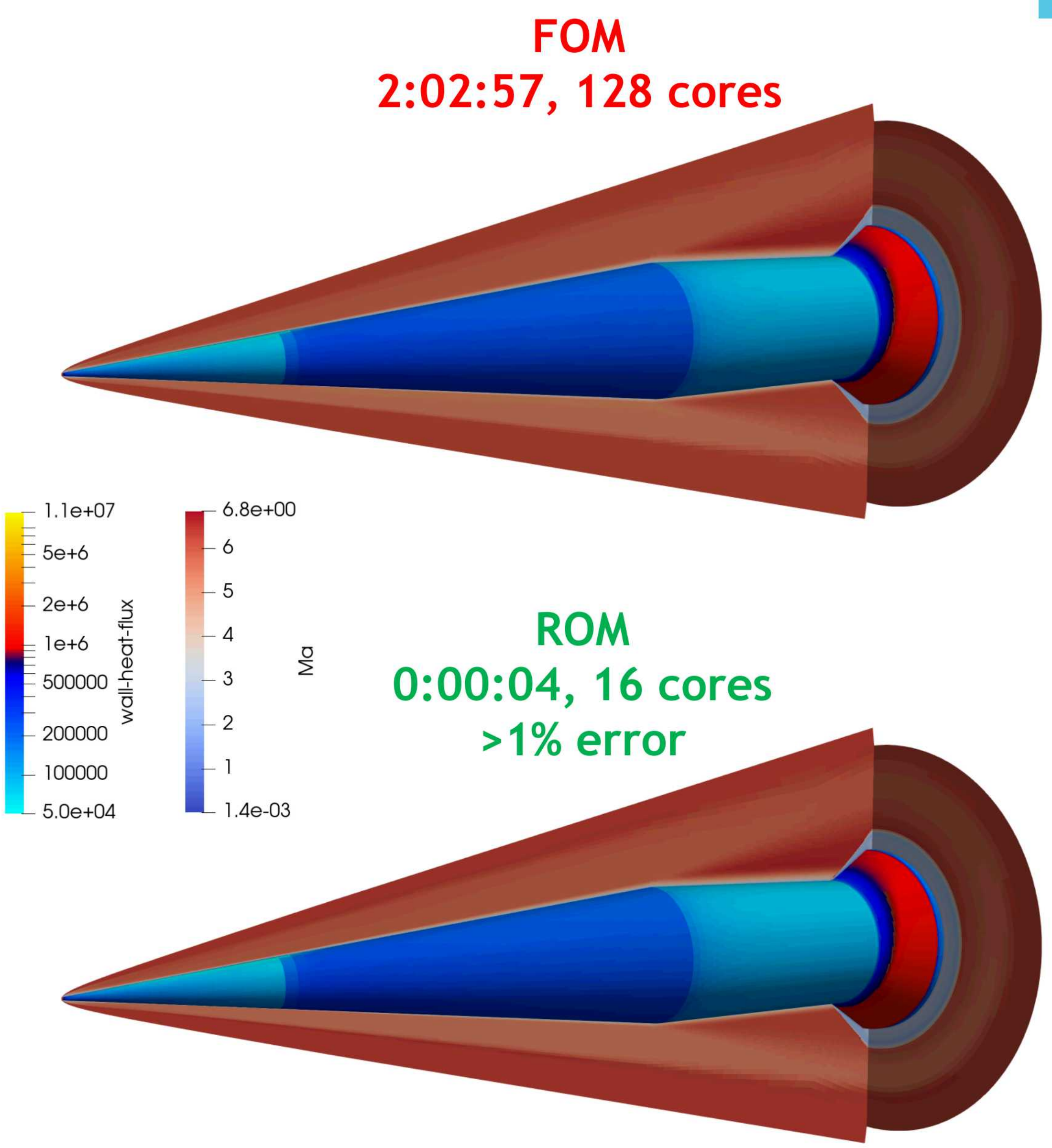
Nonlinear mapping vastly improves robustness and accuracy of ROM



- Without nonlinear mapping or line search, only the Ma=5.19 case converges.
- Nonlinear mapping is more accurate than line search for higher Mach numbers

Conclusions

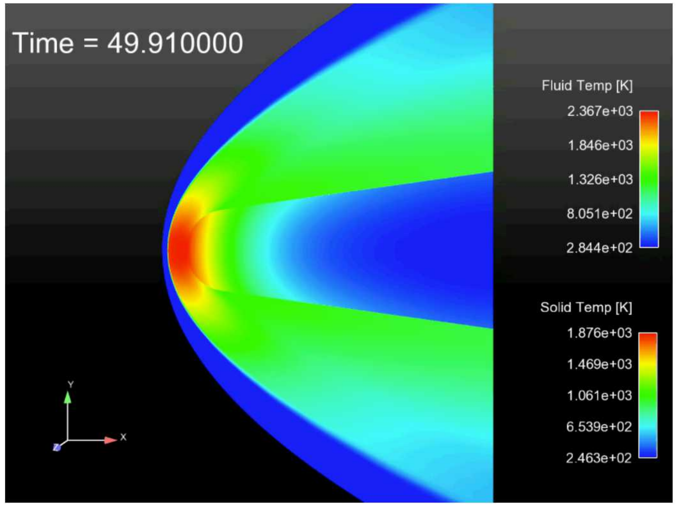
- High-fidelity simulations are crucial, but expensive for hypersonic vehicles
- Model reduction of hypersonic flows with LSPG shows promise:
  - ➢Pressio-SPARC adapter enables minimally intrusive ROM implementation.
  - ➢Results for HIFiRE show low cost and accuracy of LSPG.
  - ➢Global conservation constraint improves ROM accuracy considerably
  - ➢Nonlinear mapping of POD modes improves ROM robustness, allows for less snapshots and/or larger parameter range.



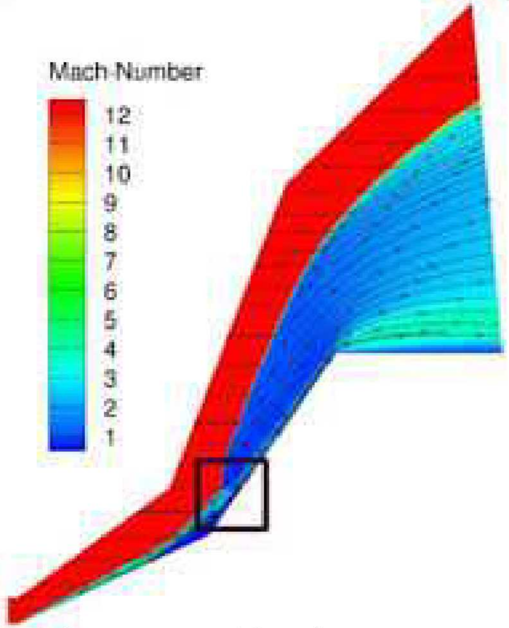
https://github.com/Pressio

Future Work

- Sample mesh/hyper-reduction algorithms
- Consider larger parameter variations and multiple parameters
- Efficient M-ROM implementation, extension to non-equilibrium chemistry
- New cases
  - Double cone with non-equilibrium chemistry.
  - Thermal and Ablation model ROMs
- **Goal: apply ROM to physically relevant parameter space, such as a range of flight conditions**



Temperature of a slender body in hypersonic flow simulated with SPARC



Double cone Mach contours courtesy J. Ray, Sandia

Relevant Publications

[1] 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).

[2] K. Carlberg, Y. Choi, and S. Sargsyan. "Conservative model reduction for finite-volume models," Journal of Computational Physics, Vol. 371, p. 280–314 (2018).

[3] 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).

[4] K. Carlberg, M. Barone, and H. Antil. "Galerkin v. least-squares Petrov–Galerkin projection in nonlinear model reduction," Journal of Computational Physics, Vol. 330, p. 693–734 (2017).

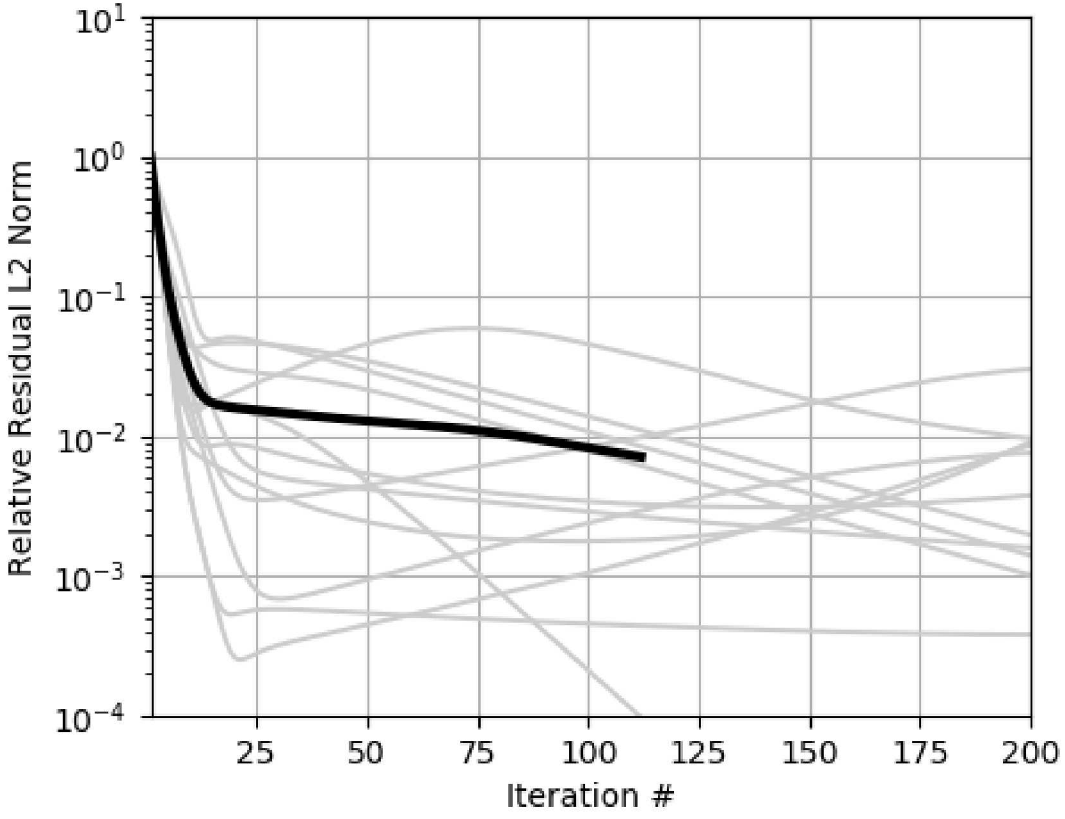
[5] K. M. Washabaugh, "Fast Fidelity for Better Design: A Scalable Model Order Reduction Framework for Steady Aerodynamic Design Applications", PhD Thesis, Department of Aeronautics and Astronautics, Stanford University, August 2016.

Upcoming: a paper on Pressio (https://github.com/Pressio)

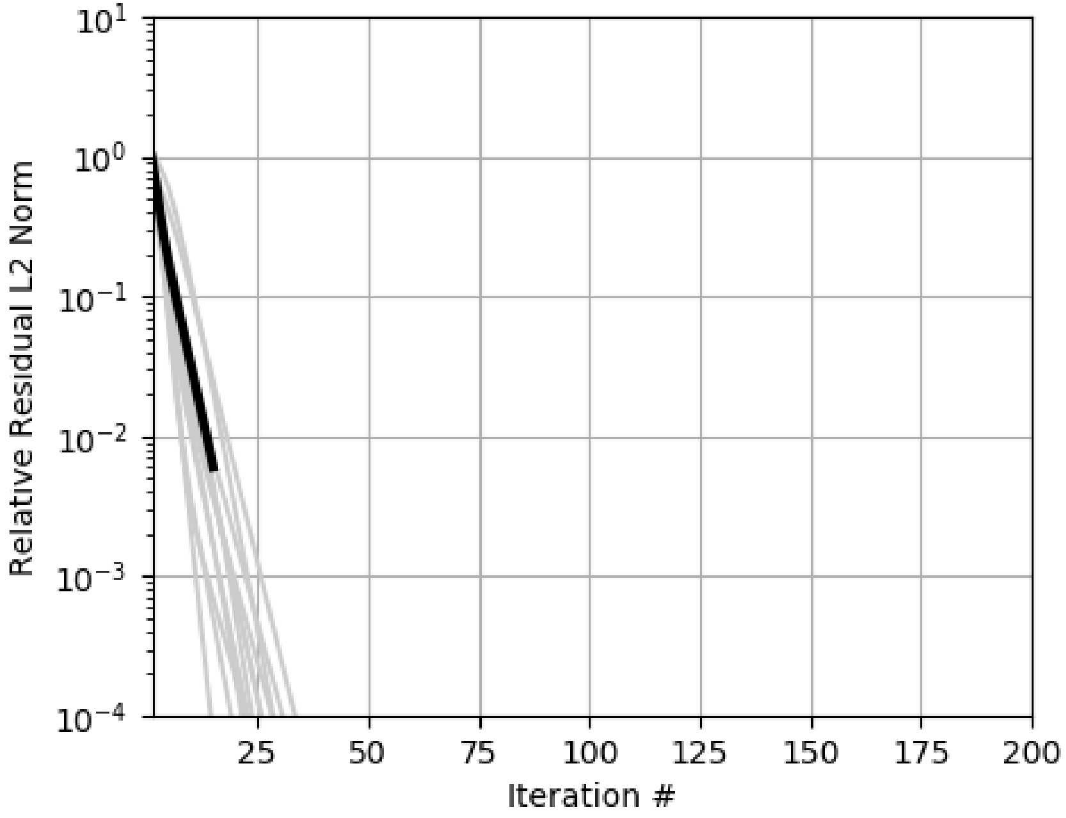
Backup Slides

Convergence for Full Mesh ROMs

LSPG, 4 Modes

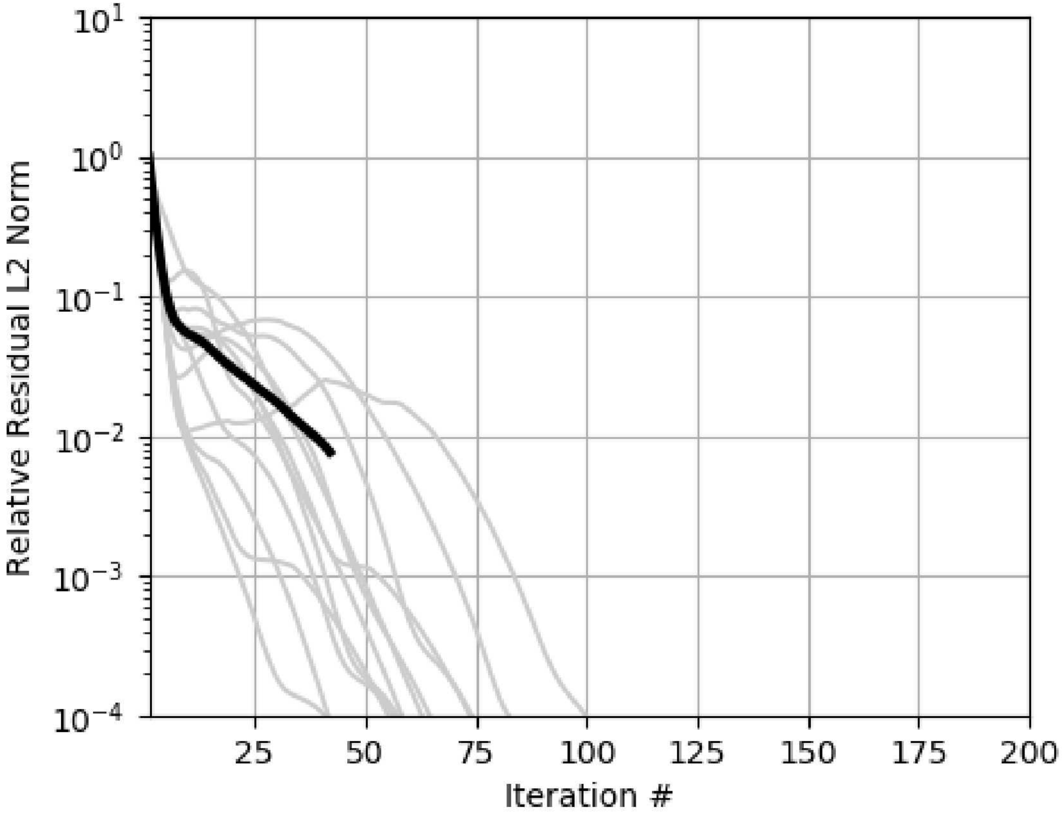


C-LSPG 4 Modes

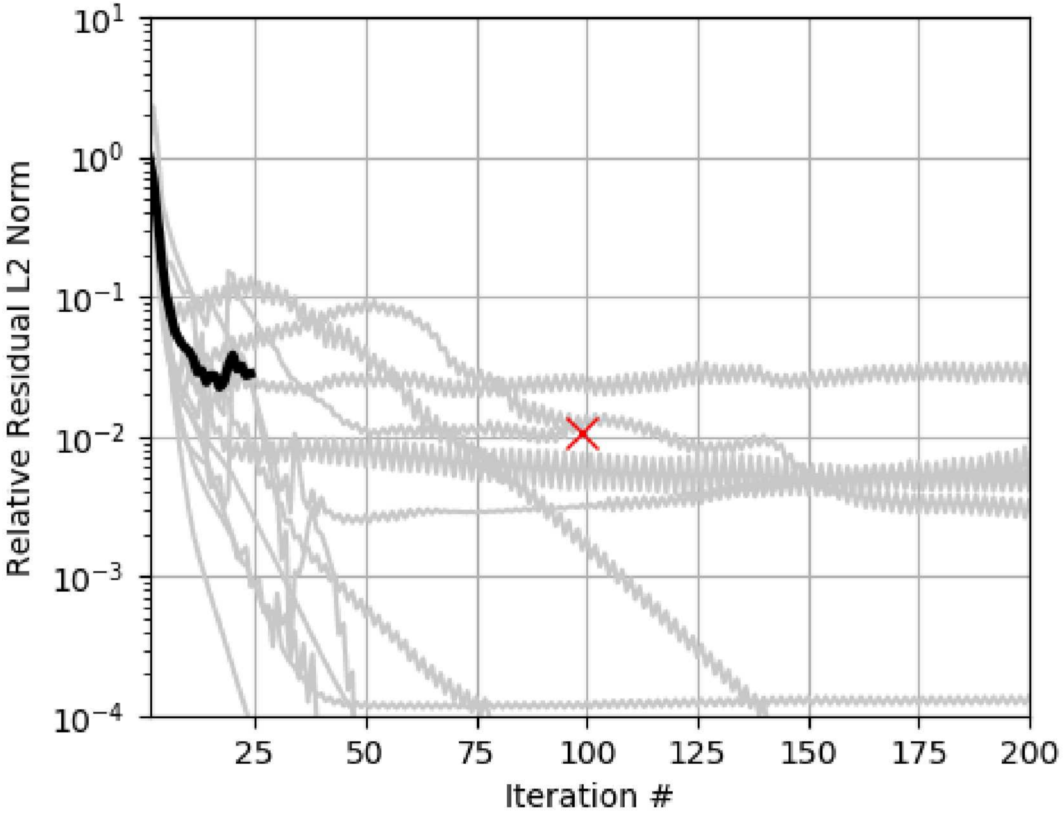


Convergence for HROM, Sample Mesh A

LSPG, 4 Modes

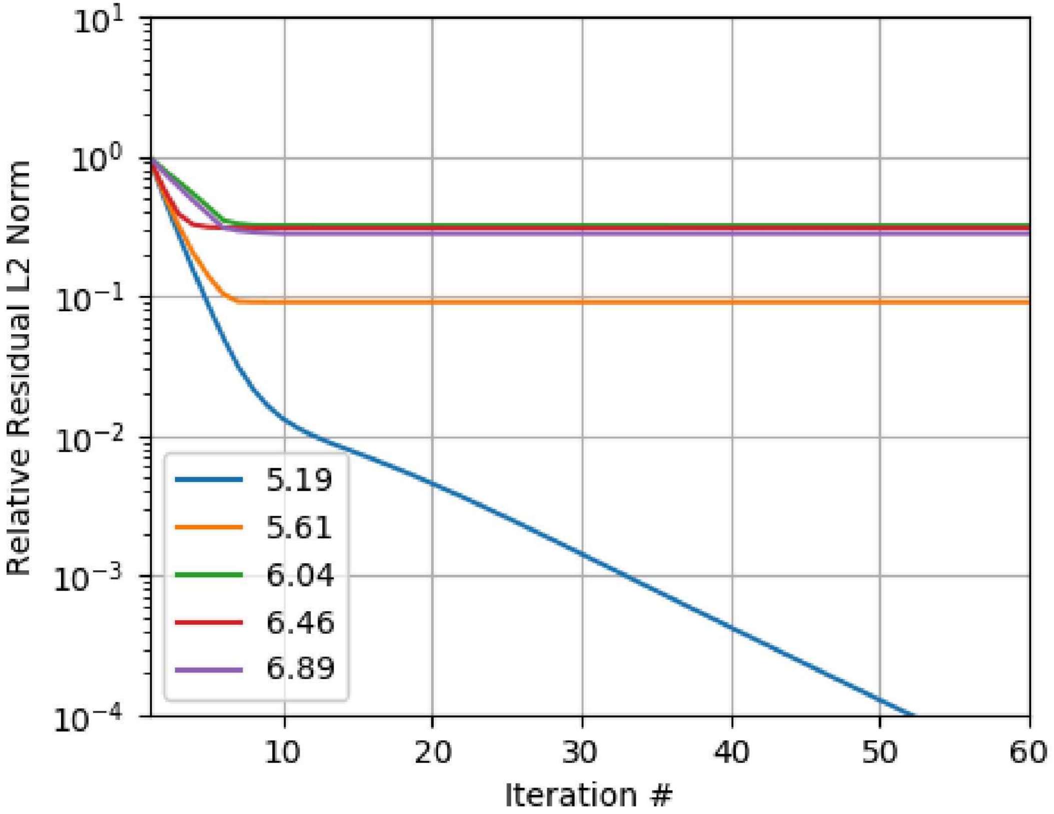


C-LSPG 4 Modes



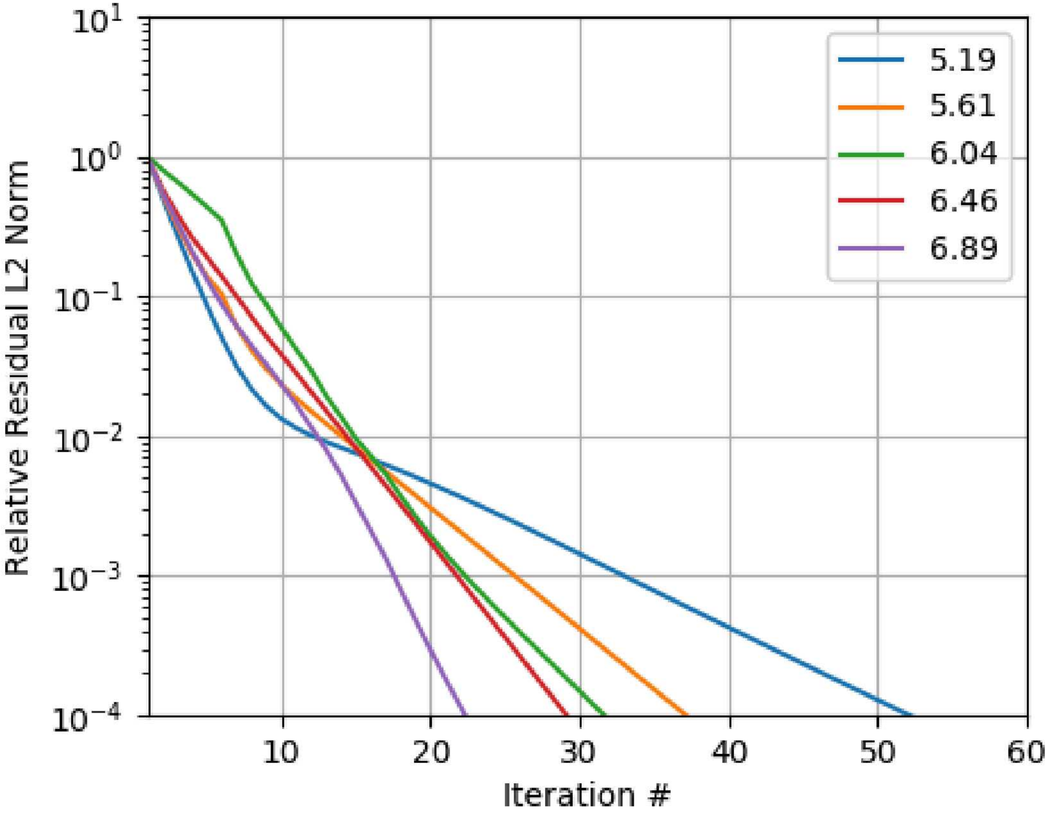
Convergence for line search and nonlinear mapping ROMs

LSPG with line search



$$\underset{\hat{\mathbf{v}}}{\text{minimize}} \; \|\mathbf{A}\mathbf{r}(\mathbf{\Phi}\hat{\mathbf{v}};\boldsymbol{\mu})\|_2^2$$

LSPG with nonlinear mapping



$$\underset{\hat{\mathbf{v}}}{\text{minimize}} \; \|\mathbf{A}\mathbf{r}(\mathbf{g}(\mathbf{\Phi}\hat{\mathbf{v}});\boldsymbol{\mu})\|_2^2$$