This paper describes objective technical results and analysis. Any subjective views or opinions that might be expressed in the paper do not necessarily represent the views of the U.S. Department of Energy or the United States Government.

SAND2019-14459C

Least-Squares Petrov—Galerkin Reduced-Order Models for Hypersonic Flight Vehicles

PRESENTED BY

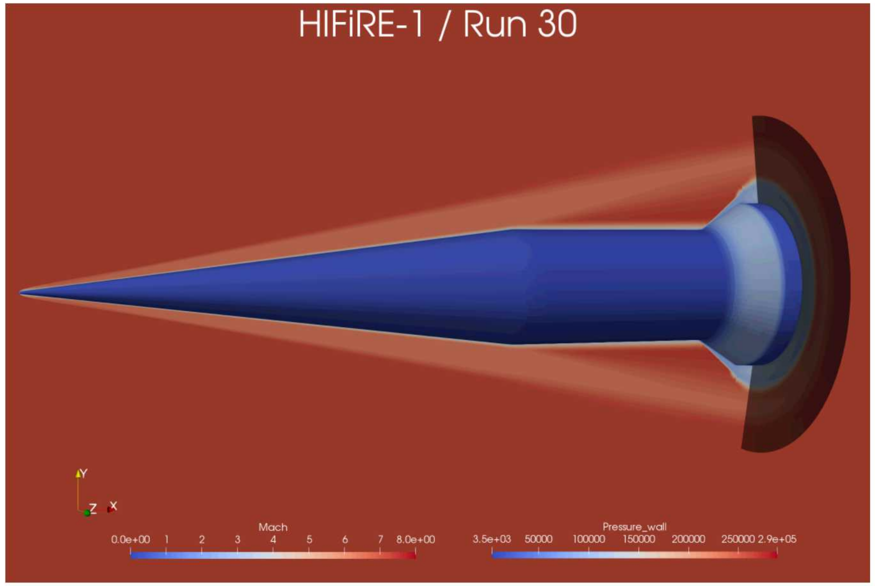
Patrick Blonigan

Collaborators: Francesco Rizzi, Micah Howard, Jeff Fike, and Kevin Carlberg

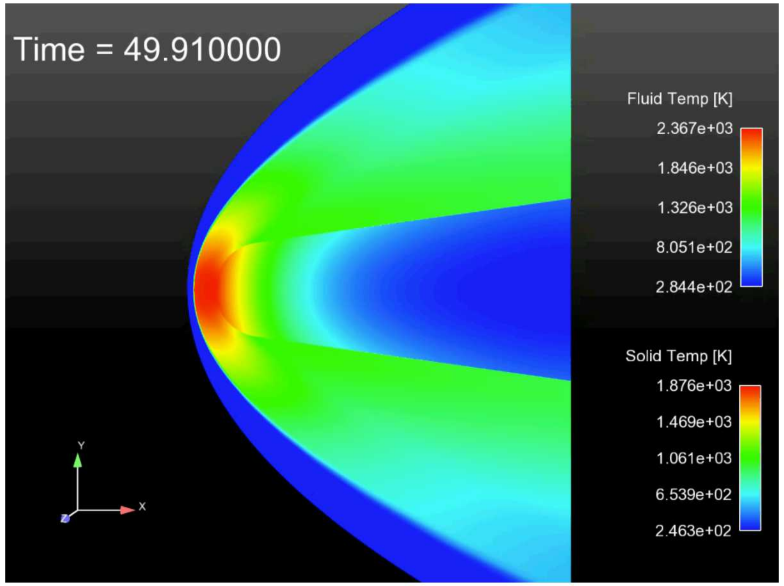
SAND2019-XXXX

Sandia National Laboratories is a multimission laboratory managed and operated by National Technology & 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-NA0003525.

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



Mach # and wall pressure contours for HIFiRE 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

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

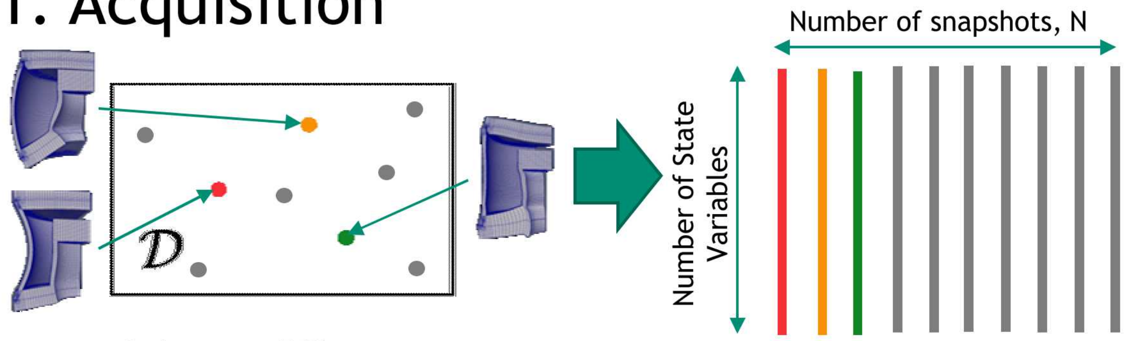
POD-Galerkin ROMs are known to be ineffective for highly nonlinear systems.

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

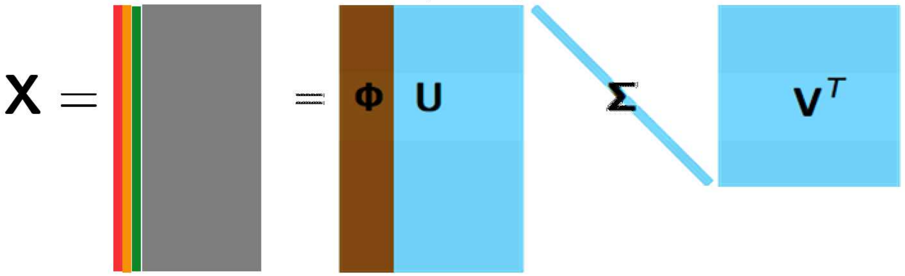


Solve at different design points

Save solution data

2. Learning

Proper Orthogonal Decomposition (POD):



3. Reduction

Reduce the number of unknowns

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

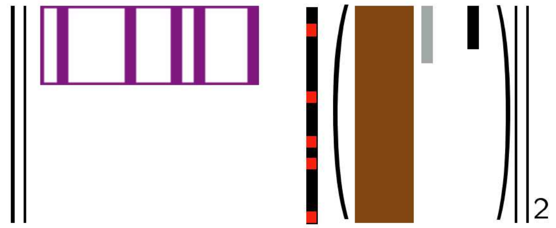
Compute initial guess for $\hat{\mathbf{x}}(\boldsymbol{\mu})$:

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

c = normalization constant

Minimize the Residual

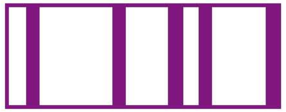
$$\underset{\hat{\mathbf{v}}}{\text{minimize}} \| \mathbf{A}\, \mathbf{r}(\boldsymbol{\Phi}\,\hat{\mathbf{v}};\boldsymbol{\mu}) \|_2$$



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

$\mathbf{A} =$ 

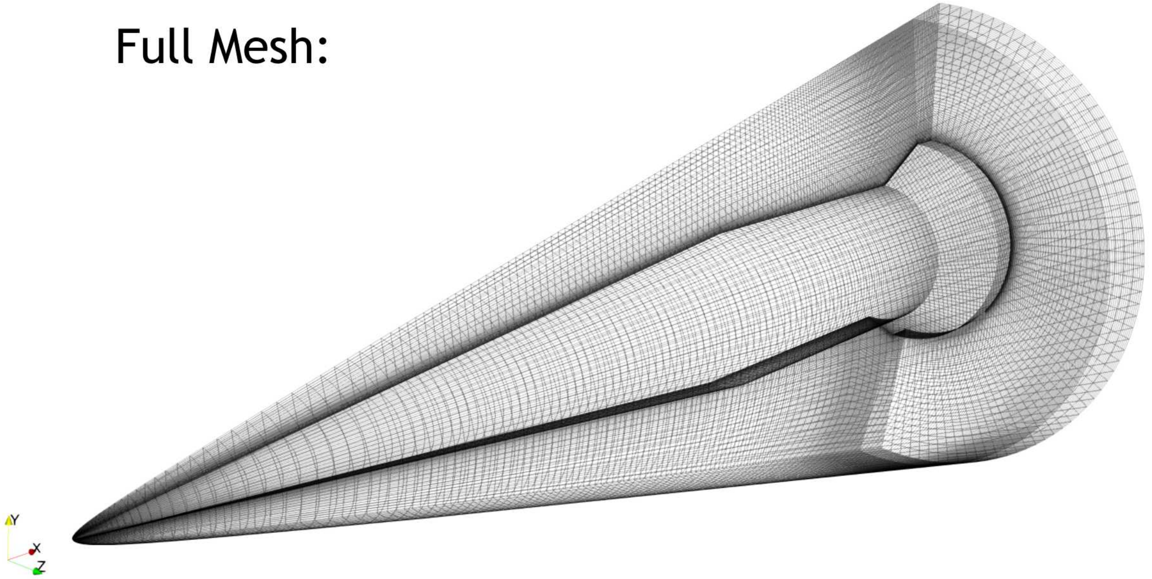
Collocation = choose rows of **A** from identity matrix

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

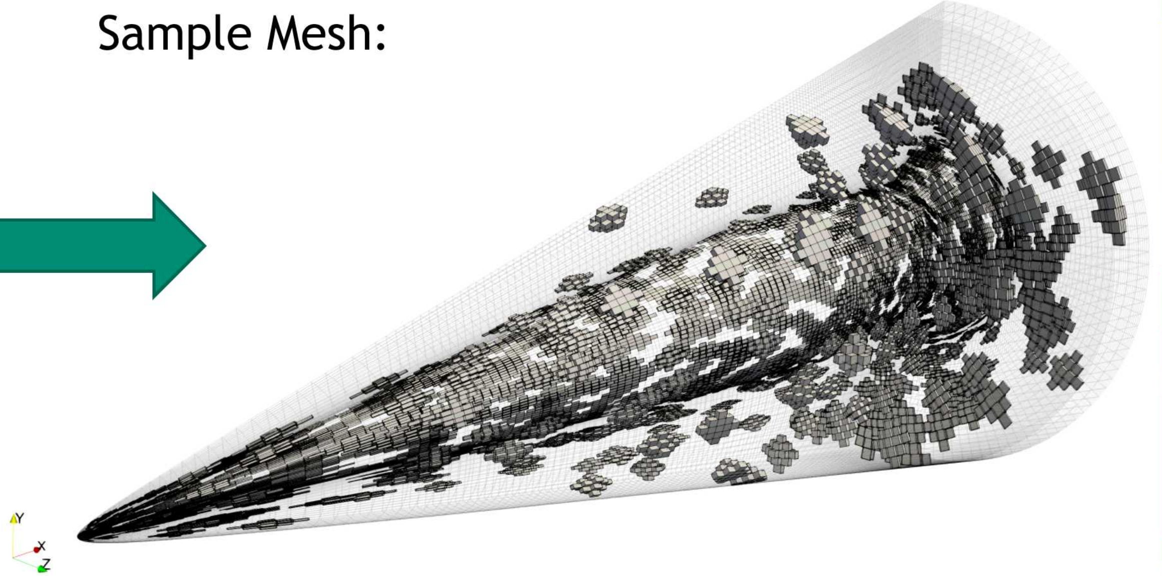
  - Inexpensive compared to DEIM and GNAT.

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

Full Mesh:



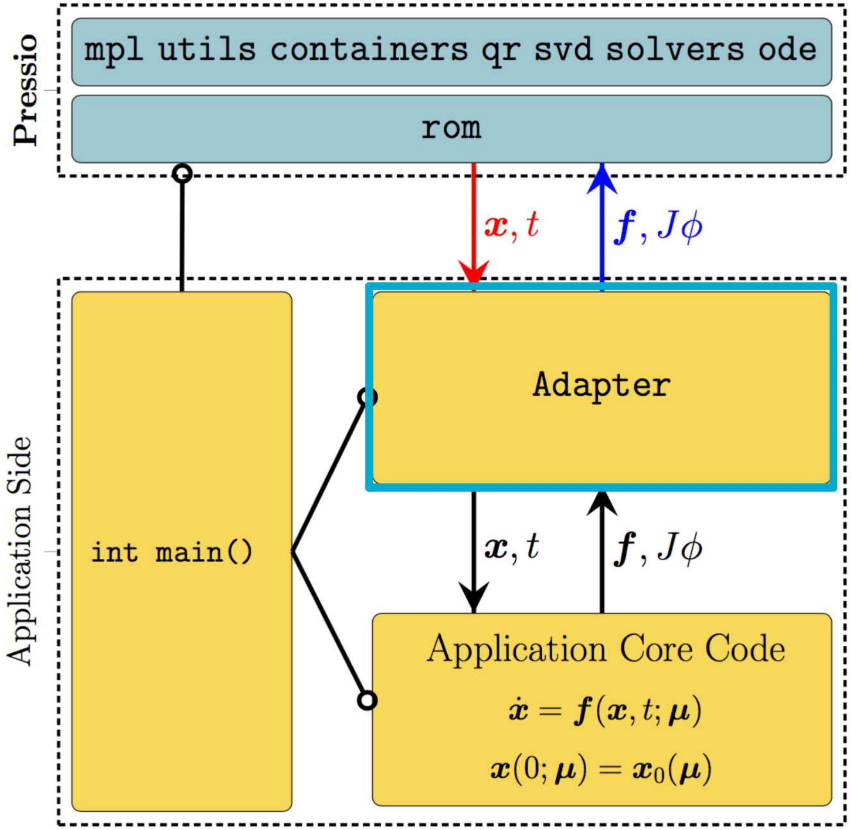
Sample Mesh:



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:
  - ✓ Minimally intrusive 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



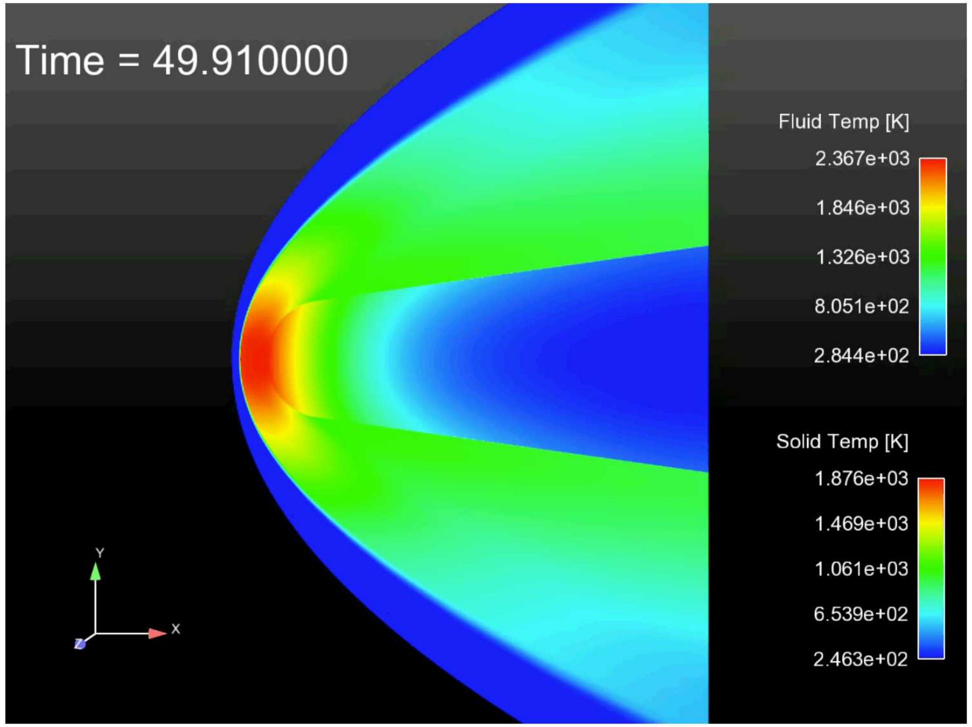
Schematic of Pressio software workflow

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)

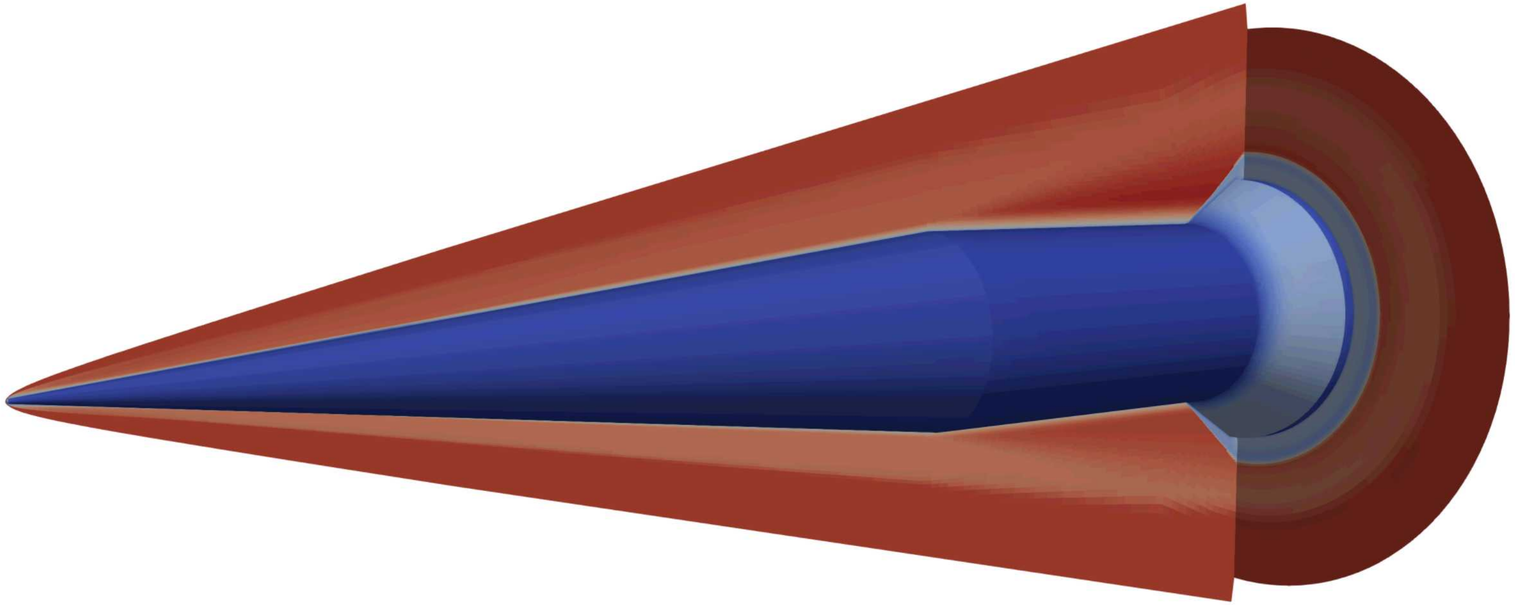
- Physics Capabilities include:
  - **Navier—Stokes, cell-centered finite volume method**
  - **Reynolds-Averaged Navier—Stokes (RANS) , cell-centered finite volume method**
  - Transient Heat Equation, Galerkin finite element method.
  - Decomposing and non-decomposing ablation equations, Galerkin finite element method.
  - One and two-way coupling between ablation, heat equation, RANS.



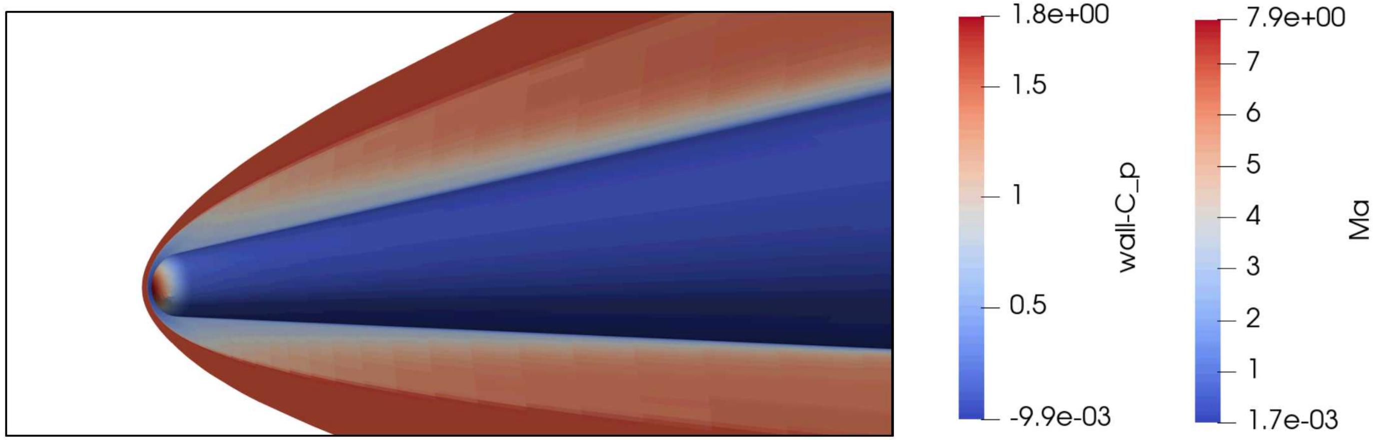
Temperature of a slender body in hypersonic flow simulated with SPARC

Test Case: HIFiRE 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:
  - 2nd-order finite volume
  - 2,031,616 cells
  - $y^+<1$ near wall
- Solver:
  - Pseudo time stepping with backward Euler, CFL schedule.

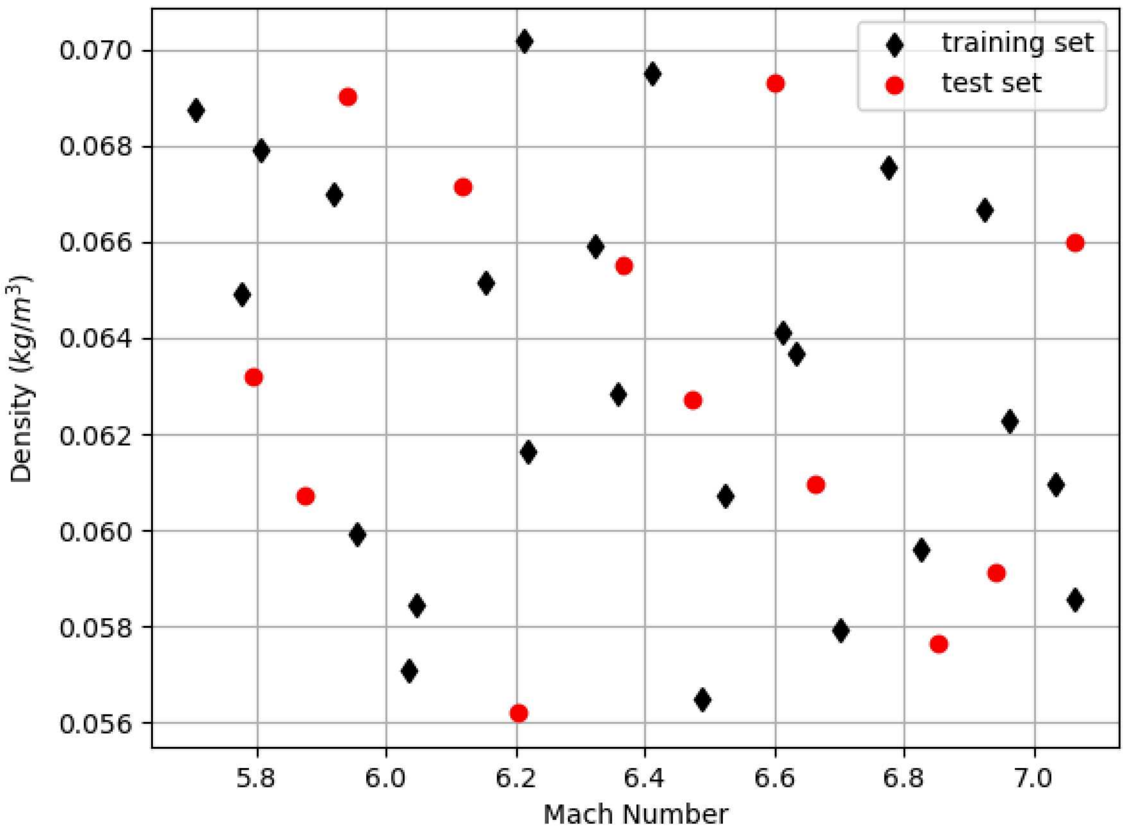


Close up of nose:

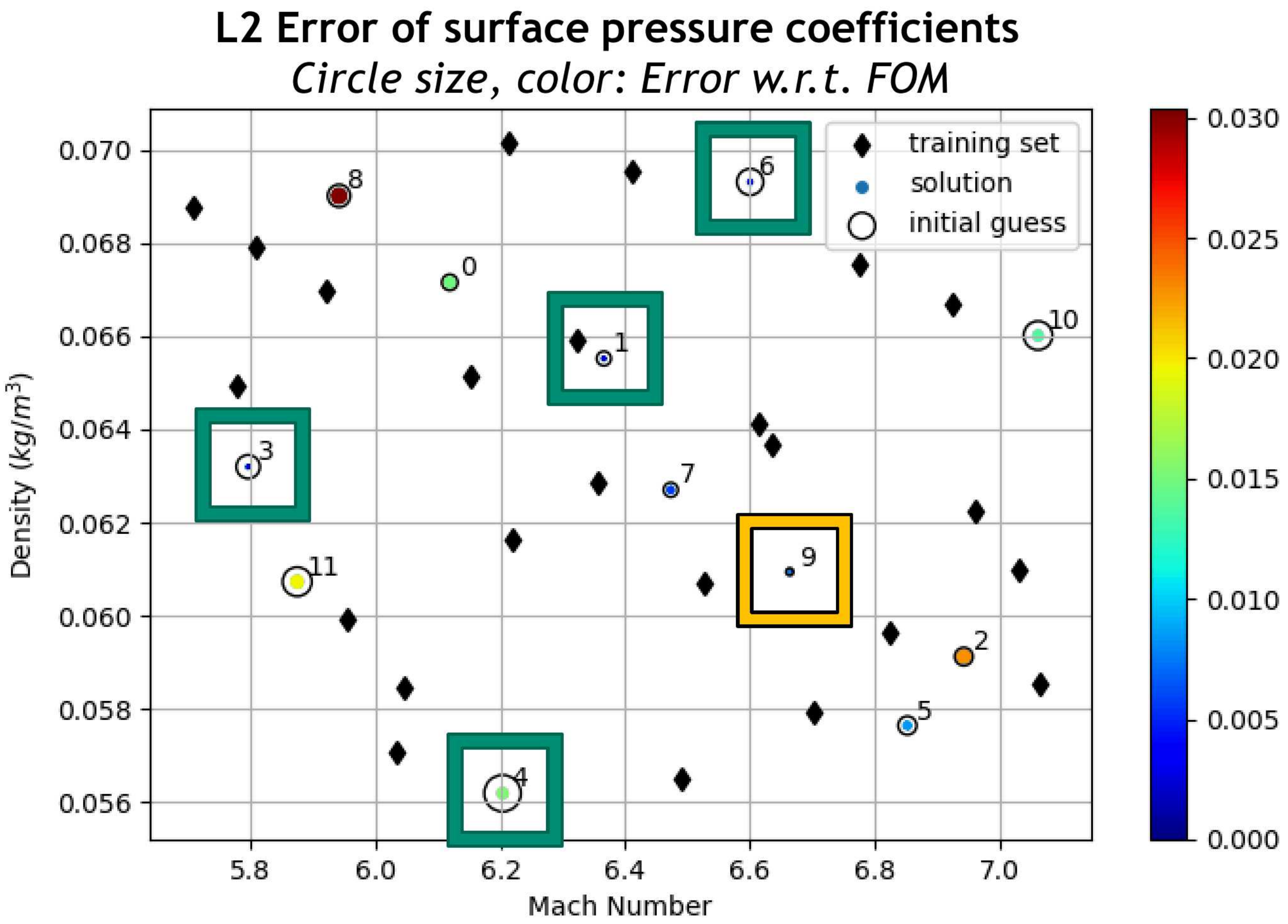


Training Data and Model details

- 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.
  - First 12 modes used for basis.
  - Basis contains over 99.99% of statistical energy.
- ROM: LSPG solved with Gauss-Newton iteration
  - Initial guess obtained via inverse-distance interpolation of POD modes.
  - Sample mesh: 49,467 cells = ~2.5% of mesh



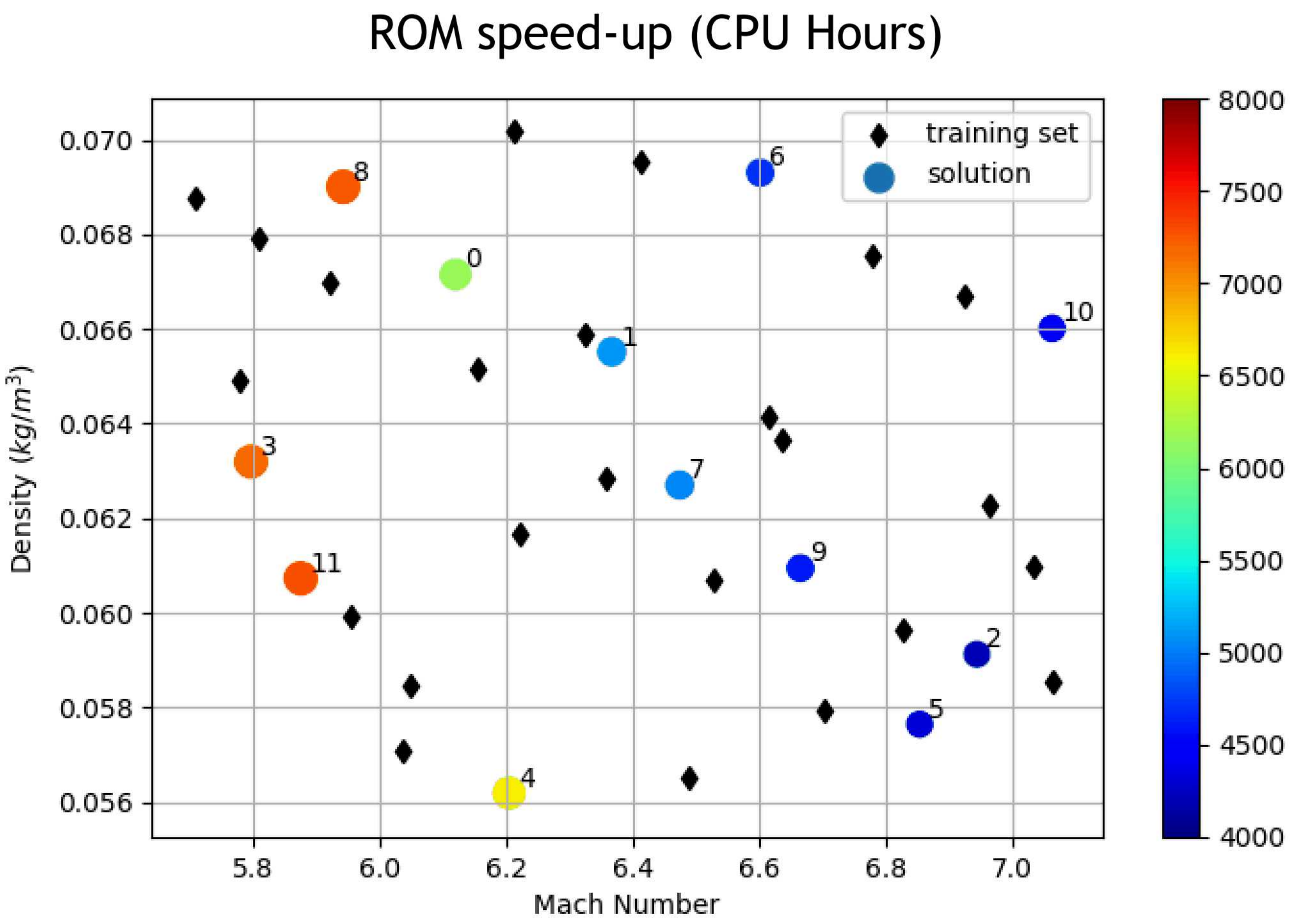
LSPG is accurate for HiFIRE predictive cases



Case	Initial Guess Error w.r.t FOM	ROM Error w.r.t FOM	ROM Error w.r.t. Initial Guess
1	2.96E-02	2.10E-03	7.11E-02
3	8.02E-02	2.00E-03	2.50E-02
4	1.93E-01	1.53E-02	7.96E-02
6	1.00E-01	2.77E-03	2.76E-02
9	7.29E-03	7.61E-03	1.04E+00

- ROM L2 error is under 5% at all cases.
- The ROM solution is much more accurate than the initial guess in several cases: 1,3,4, and 6.
- The ROM solution is just as accurate as the initial guess in case 9.

LSPG is fast for HiFIRE predictive cases

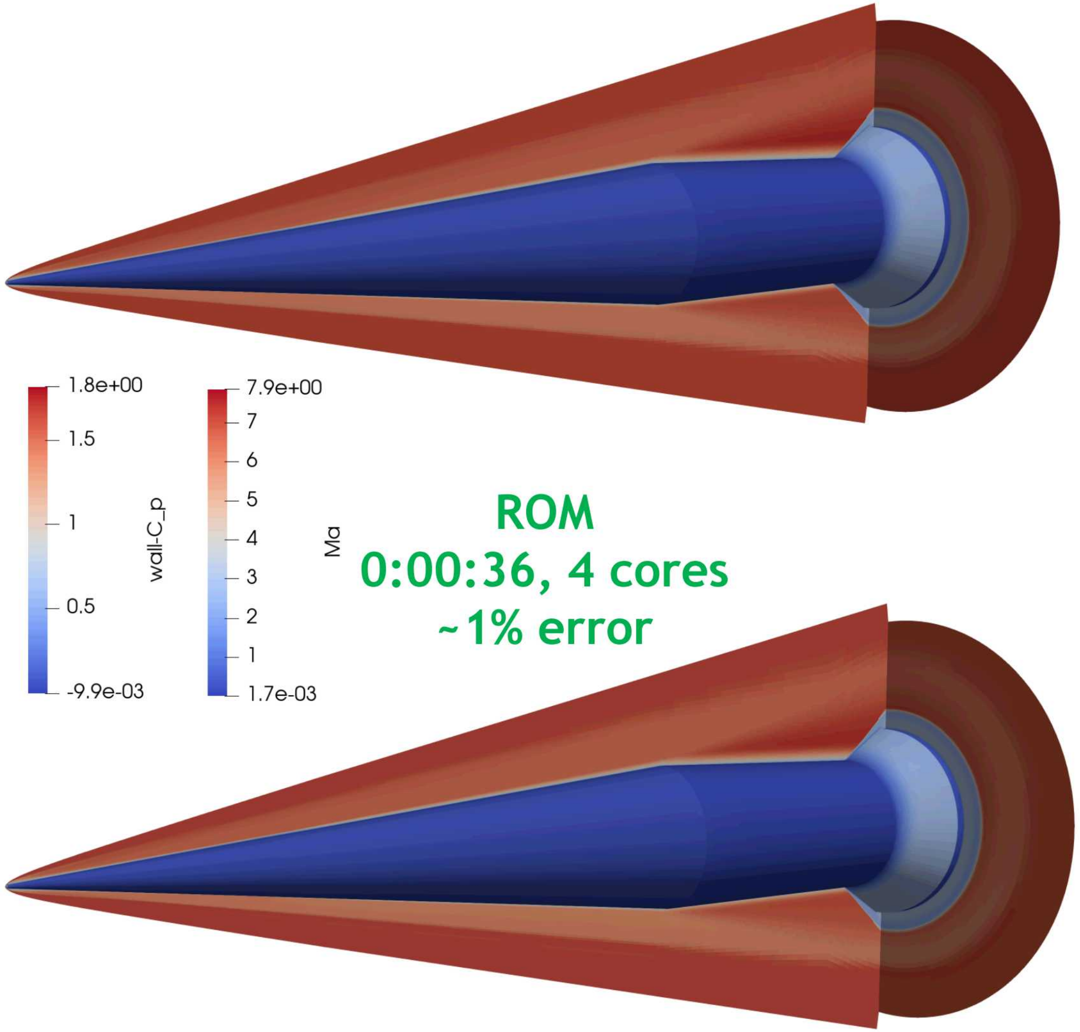


- Could run between ~4000 and ~7000 ROMs with the same CPU hours to compute one FOM solution!
- ROM is between ~100 and ~200 times faster than the FOM in wall time!

Conclusions and Future Work

- 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.
  - ➢ Preliminary results for HIFiRE show low cost and accuracy of LSPG.
- Future Work
  - Larger parameter variations and more parameters
  - Hyper-reduction techniques
  - New cases
    - Double cone with non-equilibrium chemistry
    - Thermal/Ablation models for vehicle
  - Integration with multi-fidelity UQ and/or optimization.
- **Goal: apply ROM to physically relevant parameter space, such as a range of flight conditions**

FOM
1:22:39, 128 cores



ROM
0:00:36, 4 cores
~1% error

https://github.com/Pressio

Backup Slides

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

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

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).

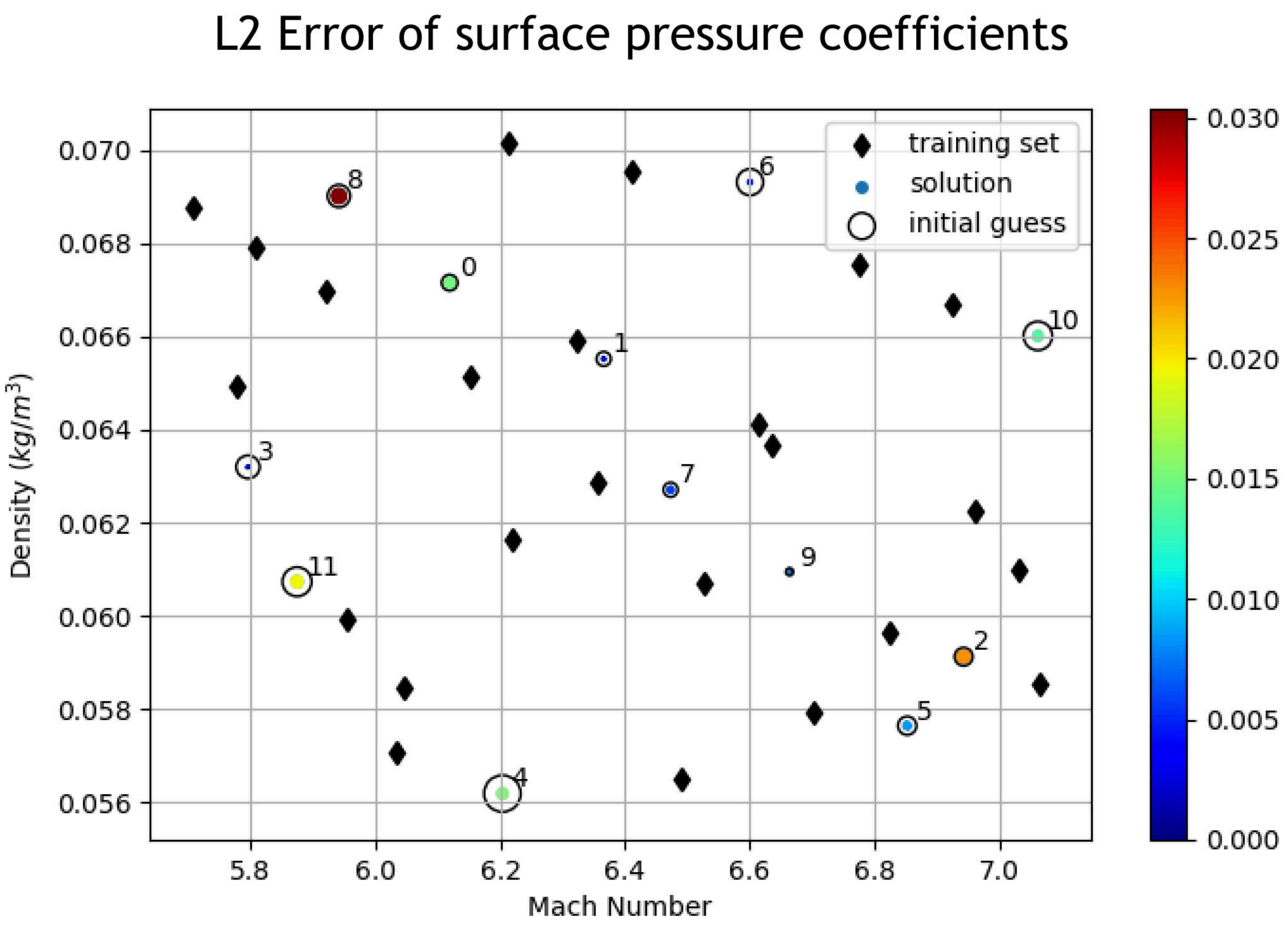
[3] K. Carlberg, C. Farhat, J. Cortial, and D. Amsallam. “The GNAT method for nonlinear model reduction: Effective implementation and application to computational fluid dynamics and turbulent flows,” Journal of Computational Physics, Vol. 242, p. 623–647 (2013).

[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.

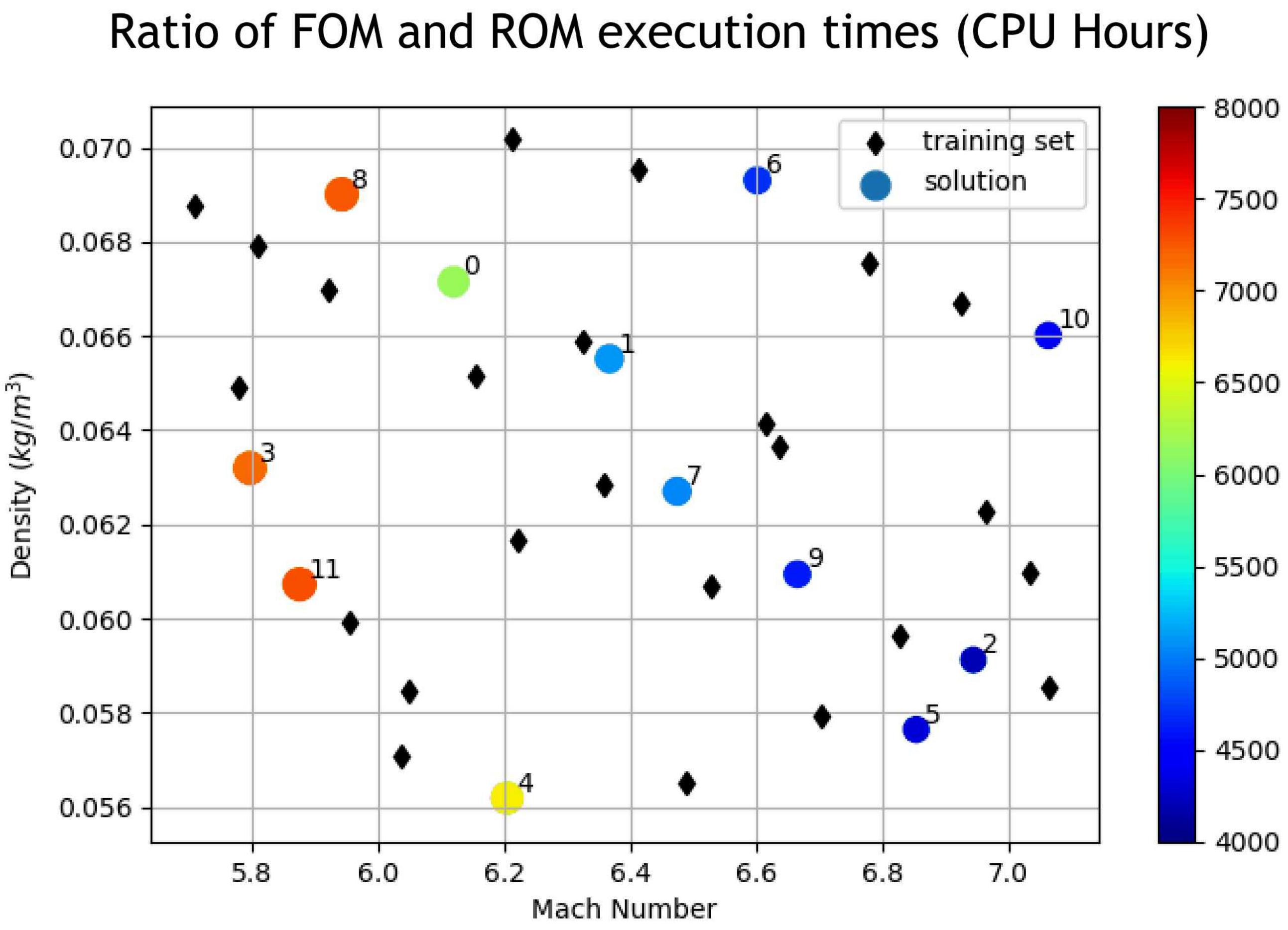
Upcoming: a paper on Pressio (https://github.com/Pressio)

LSPG results for HiFIRE predictive cases



Case	Initial Guess Error w.r.t FOM	ROM Error w.r.t FOM	ROM Error w.r.t. Initial Guess
0	3.66E-02	1.49E-02	4.08E-01
1	2.96E-02	2.10E-03	7.11E-02
2	4.76E-02	2.29E-02	4.82E-01
3	8.02E-02	2.00E-03	2.50E-02
4	1.93E-01	1.53E-02	7.96E-02
5	4.91E-02	8.53E-03	1.74E-01
6	1.00E-01	2.77E-03	2.76E-02
7	3.01E-02	5.49E-03	1.83E-01
8	7.38E-02	3.04E-02	4.11E-01
9	7.29E-03	7.61E-03	1.04E+00
10	1.19E-01	1.39E-02	1.17E-01
11	1.22E-01	1.97E-02	1.61E-01

LSPG results for HiFIRE predictive cases



Case	Wall time (FOM/ ROM)	CPU time (FOM/ ROM)
0	192	6155
1	160	5116
2	132	4233
3	224	7183
4	207	6614
5	135	4321
6	147	4700
7	158	5054
8	226	7246
9	144	4613
10	139	4440
11	228	7286