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Sandia National Laboratories

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

PRESENTED BY

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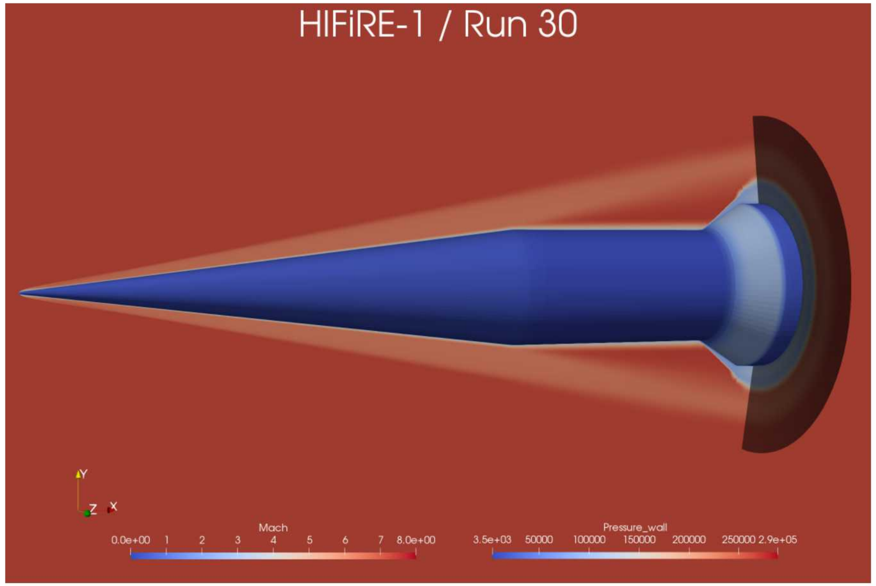
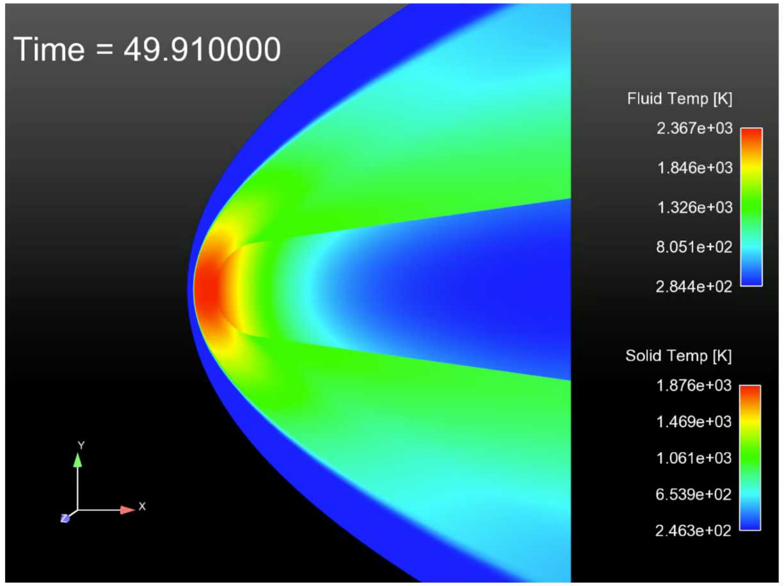
High-Fidelity Simulations are crucial for Hypersonic Vehicle analysis and design

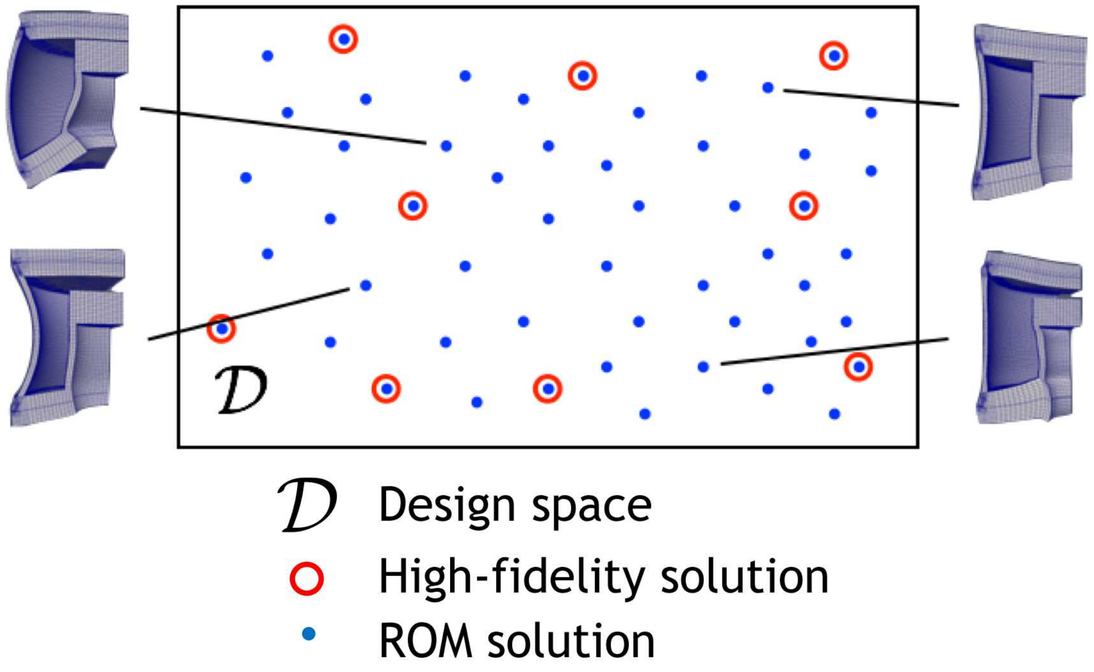




- High-fidelity: extreme-scale, nonlinear dynamical system model.
  - High cost: An unsteady multiphysics simulation can consume **weeks** on a supercomputer.
- Cost poses a "**computational barrier**" to the application of many-query and/or time-critical problems:
  - **Many-Query**: Design Optimization, Model Calibration, Uncertainty Propogation
  - **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 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. ***Structure 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

Previous work on 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]
- ***Structure 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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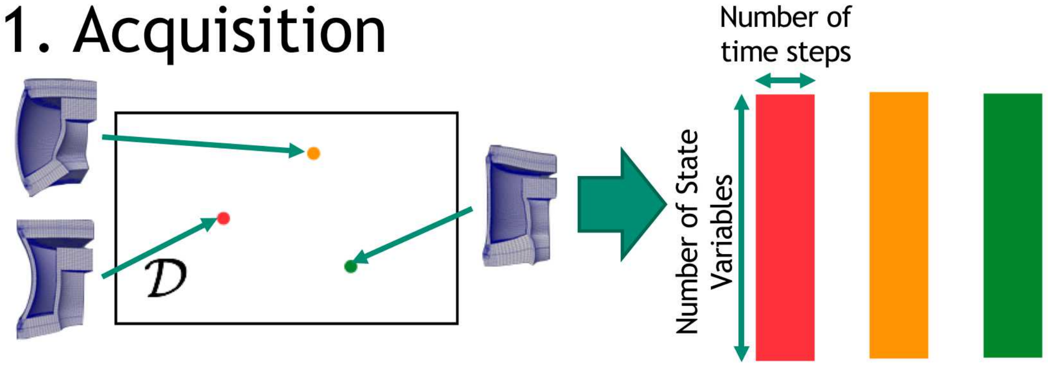
Least Squares Petrov—Galerkin (LSPG) for unsteady systems

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

- High-fidelity simulation = ODE: $\frac{d\mathbf{x}}{dt} = \mathbf{f}(\mathbf{x}; t, \boldsymbol{\mu})$

1. Acquisition

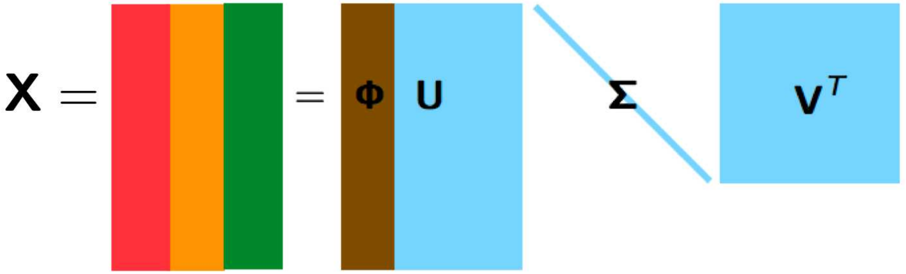


Solve ODE at different design points

Save solution data

2. Learning

Proper Orthogonal Decomposition (POD):



3. Reduction

Choose ODE Temporal Discretization

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

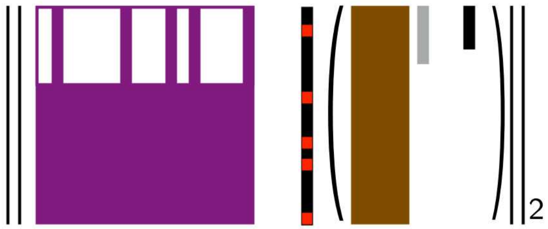
$$\mathbf{r}^n(\mathbf{x}^n; \boldsymbol{\mu}) = \mathbf{0}, \quad n = 1, \ldots, T$$

Reduce the number of unknowns

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

Minimize the Residual

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

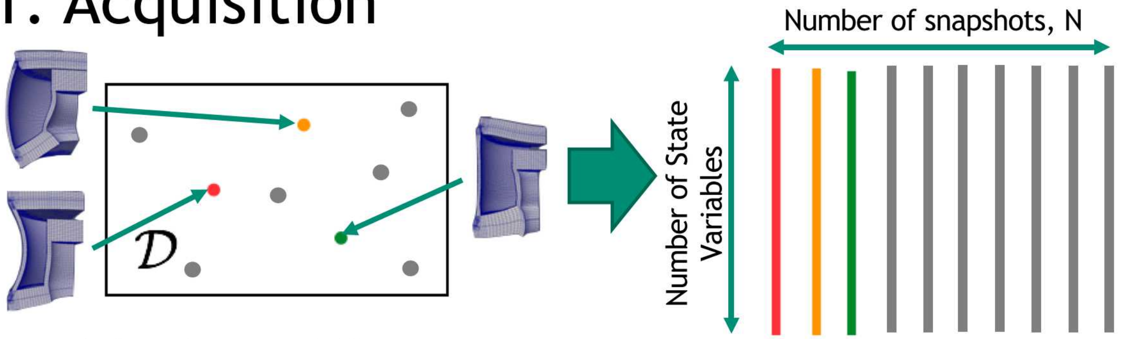


Least Squares Petrov—Galerkin (LSPG) for steady systems

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

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

1. Acquisition

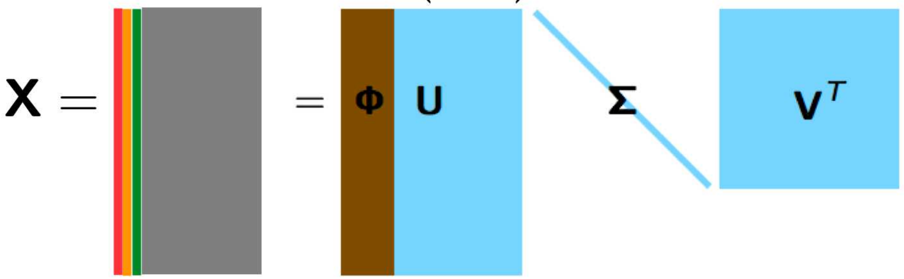


Solve ODE at different design points

Save solution data

2. Learning

Proper Orthogonal Decomposition (POD):



3. Reduction

Reduce the number of unknowns

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

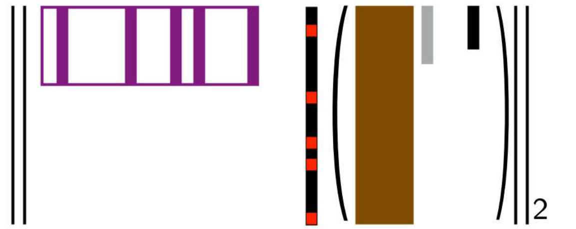
Compute initial guess for $\hat{\mathbf{x}}(\boldsymbol{\mu})$:

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

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

- Collocation:

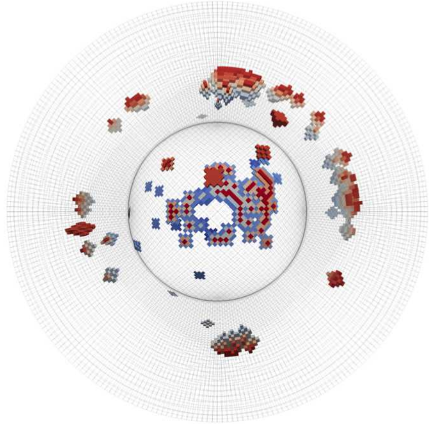
LSPG: $\underset{\hat{\mathbf{v}}}{\text{minimize}} \; \|\mathbf{A}\mathbf{r}(\boldsymbol{\Phi}\hat{\mathbf{v}};\boldsymbol{\mu})\|_2^2$

$\mathbf{A} =$ 

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

$$\begin{pmatrix}1\\0\\0\\0\\\vdots\\0\end{pmatrix}, \begin{pmatrix}0\\0\\1\\0\\\vdots\\0\end{pmatrix}, \begin{pmatrix}0\\\vdots\\0\\1\\0\\0\end{pmatrix}$$

Sample Mesh: cells required to compute residual



- Collocation has been used in past studies of CFD model reduction [Washabaugh, 2016].
- We consider two sample mesh algorithms
  1. Random sampling
  2. Greedy algorithm [Washabaugh, 2016]
     1. Determine reconstruction error $|\mathbf{y} - \Phi(\mathbf{A}\Phi)^{+}\mathbf{A}\mathbf{y}|$
     2. Add cell with largest reconstruction error to **A.**

  ➢ Reconstruction error computed with state vectors, POD basis.

Pressio, a minimally intrusive model reduction library

-Current ROMs require *intrusive* implementations in large-scale codes

-The number of application codes is vast and constantly evolving

-Each newly developed ROM => a separate implementation in each application code

Pressio is a C++ header-only library:

+ Includes the cutting-edge ROM capabilities developed at Sandia

+ Minimally intrusive

+ Aims at easily providing scalable and performant ROMs to any Sandia applications

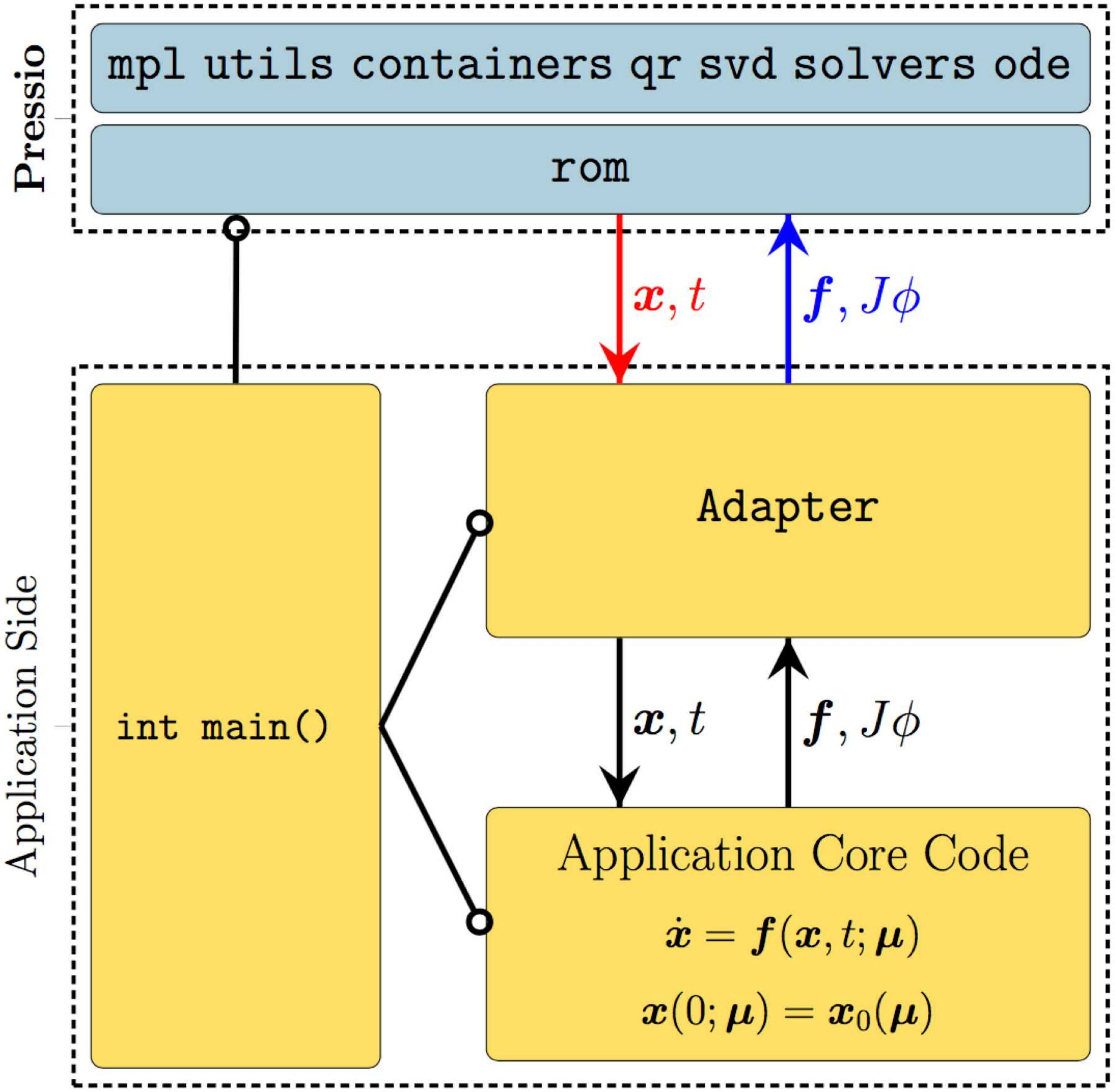
+ New ROMs can be coded only once and seamlessly applied to any application

+ Based on the C++11 standard/features

+ A *simple*, *unique* interface is required from the application to access *any* ROM

+ Can run ROMs on many/multi-core and GPUs

Pressio partitions ROM methods and computational physics application



$x =$ *full-order model (fom) state*

$t =$ *time*

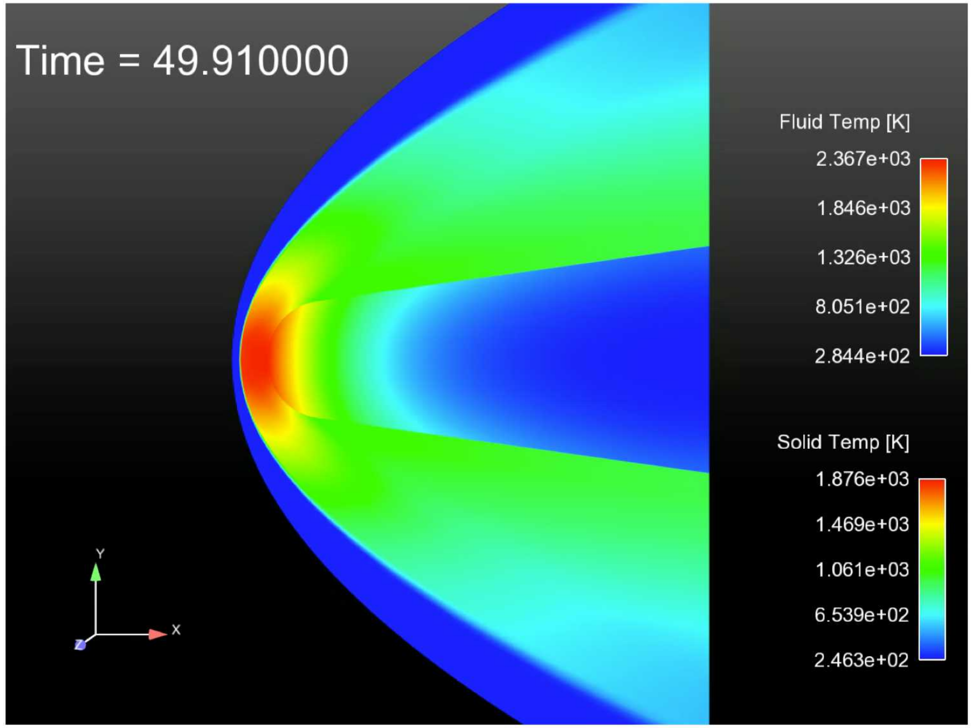
$$J = \frac{\partial f}{\partial x} = full\ order\ model\ jacobian$$

$\Phi =$ *POD Basis*

+ Minimally intrusive
+ Unique interface

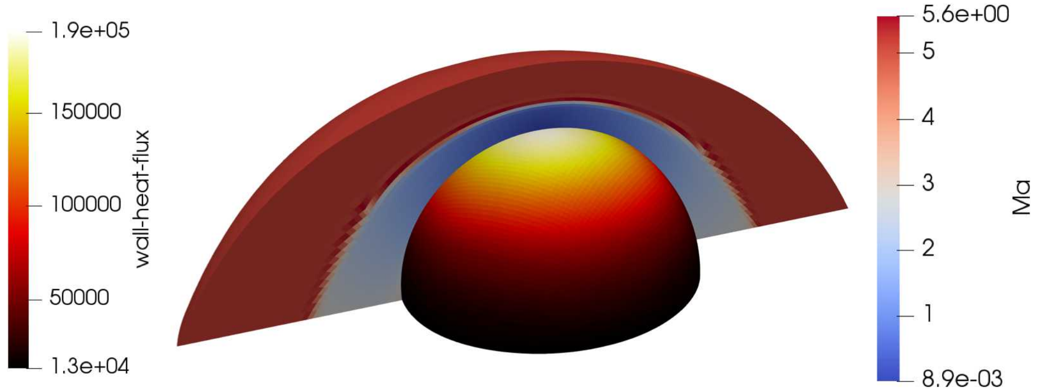
Sandia Parallel Aerodyanmics and Reentry Code (SPARC)

- 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.

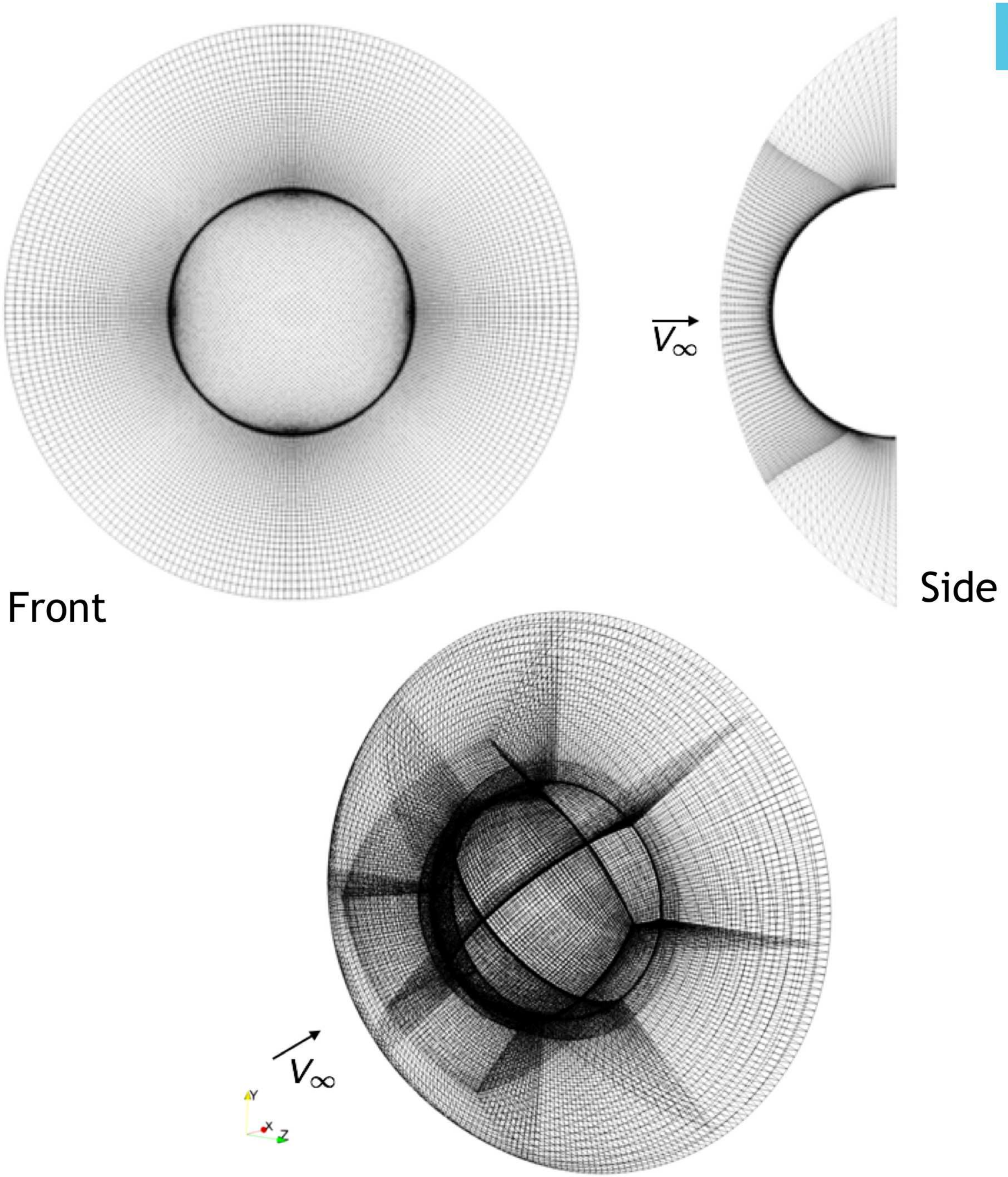


A slender body in hypersonic flow simulated with SPARC

Case 1: The Blottner Sphere



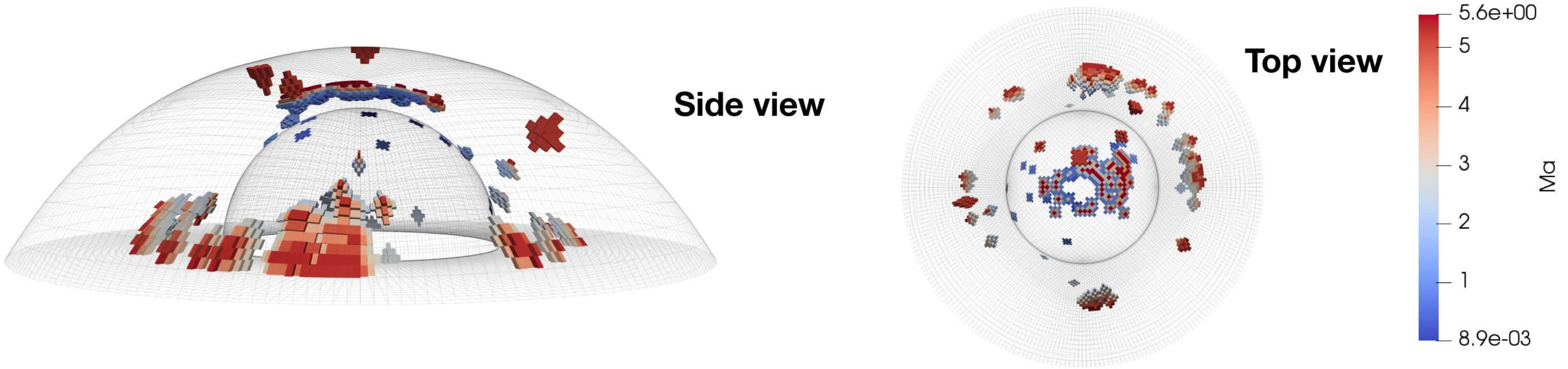
- Flow field:
  - Free stream Mach No. = 5.0
  - Reynolds No. = 1.89 million
  - Laminar flow (no turbulence model)
- Spatial discretization:
  - 2nd-order finite volume
  - 524288 cells



Unsteady reproductive ROM demonstrates cost savings

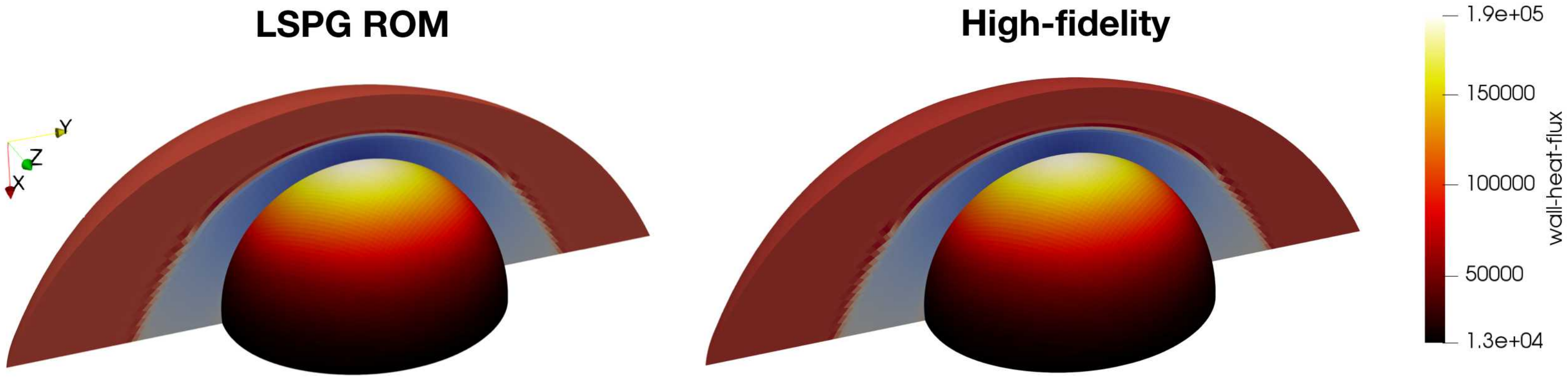
Time discretization: BDF2, time step=0.25μs

Sample mesh
(colored by Mach No.)



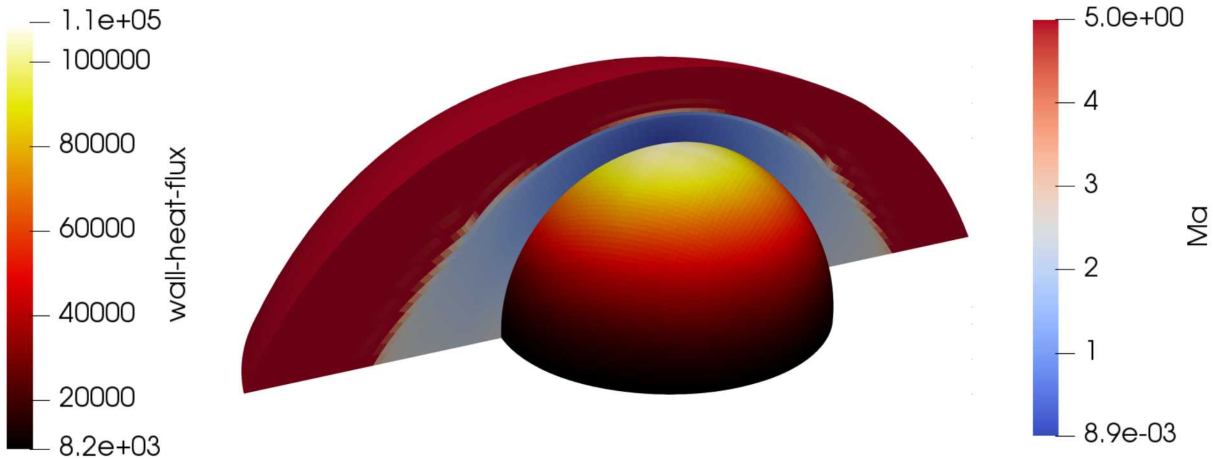
LSPG ROM:
- Sample mesh: 3200 cells, 16,000 dofs (more on next slide)
- 1 MPI rank, ~6 seconds

High-fidelity:
- 524288 cells => 2,621,440 DoFs
- 32 MPI ranks, ~62 seconds



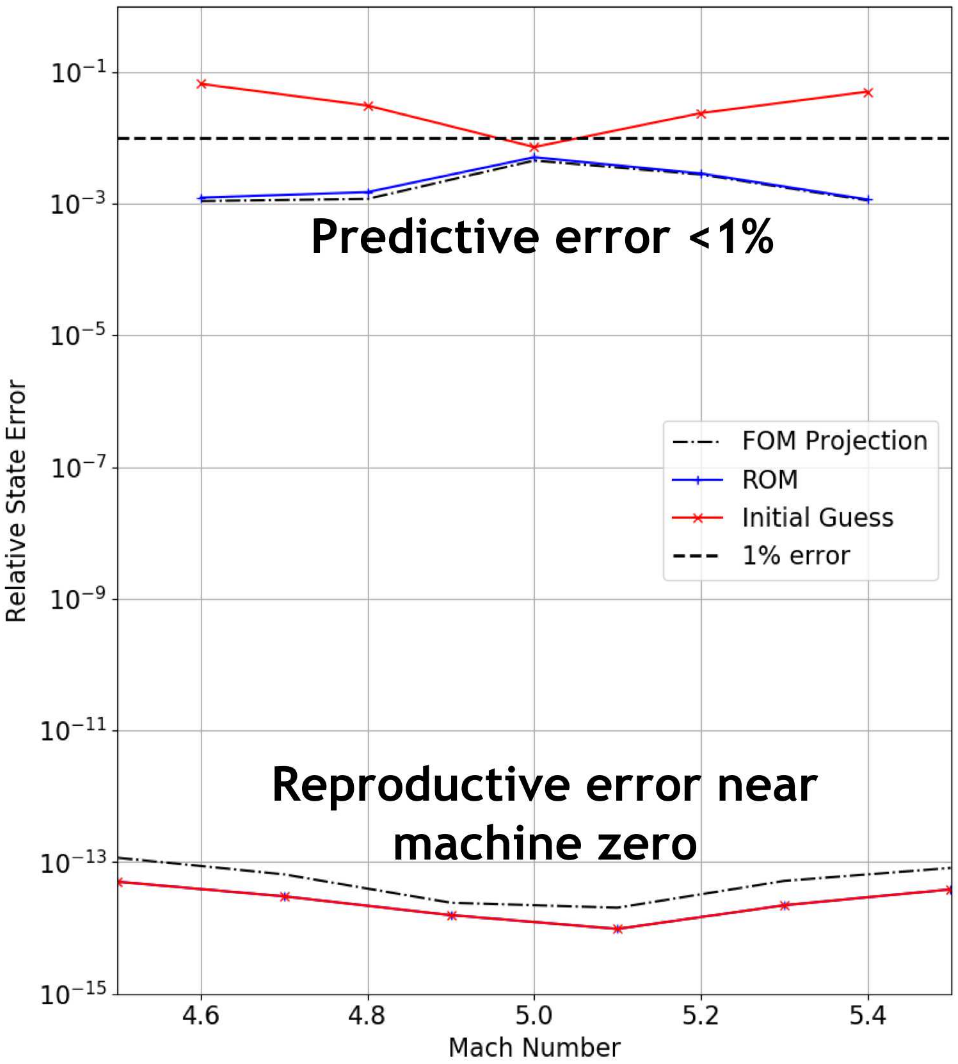
320x savings in core-hours
Reproduced flow field with negligible error

LSPG is accurate for reproductive and predictive steady cases



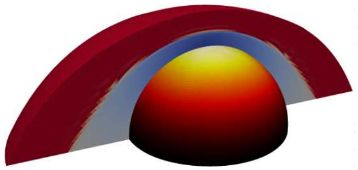
LSPG ROM Predictive Solution, Mach 5.0

- Full Order Model: Blottner Sphere solved with backward Euler pseudo time-stepping, CFL schedule.
- Training set: Mach Numbers [4.5,4.7,4.9,5.1,5.3,5.5]
- Test set: Mach Numbers [4.6,4.8,5.0,5.2,5.4]
- POD basis:
  - columns scaled to be unitary.
  - each conserved quantity scaled by its maximum over all FOM solutions.
- ROM: LSPG solved with Gauss-Newton iteration

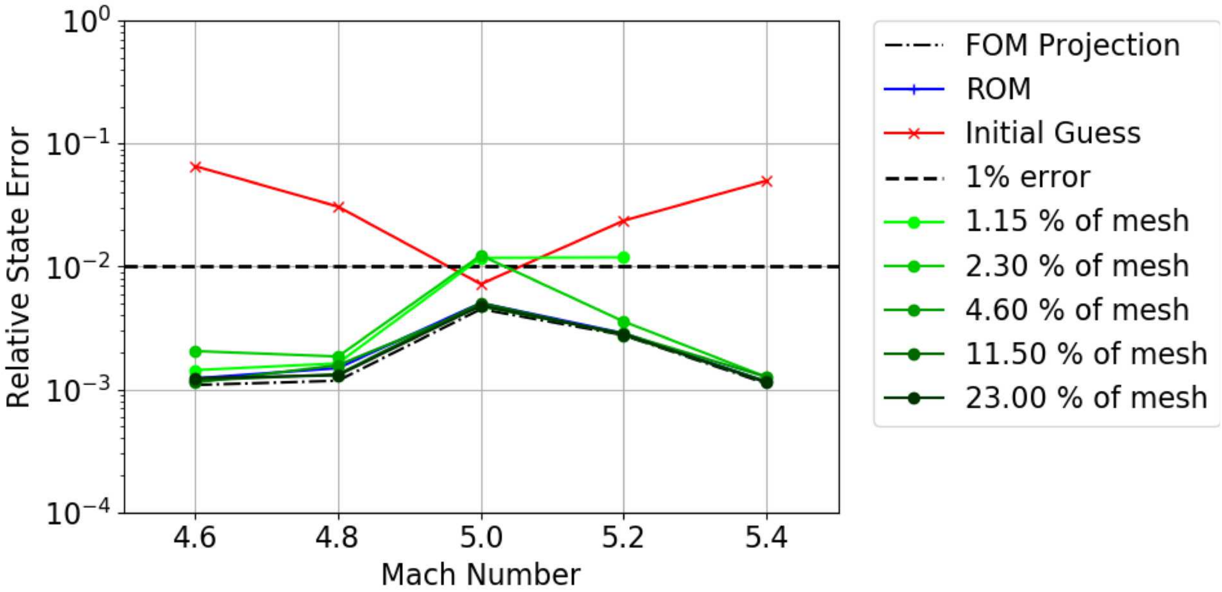


$$\text{Relative State Error} \equiv \frac{\|\mathbf{x} - \tilde{\mathbf{x}}\|_2}{\|\mathbf{x}\|_2}$$

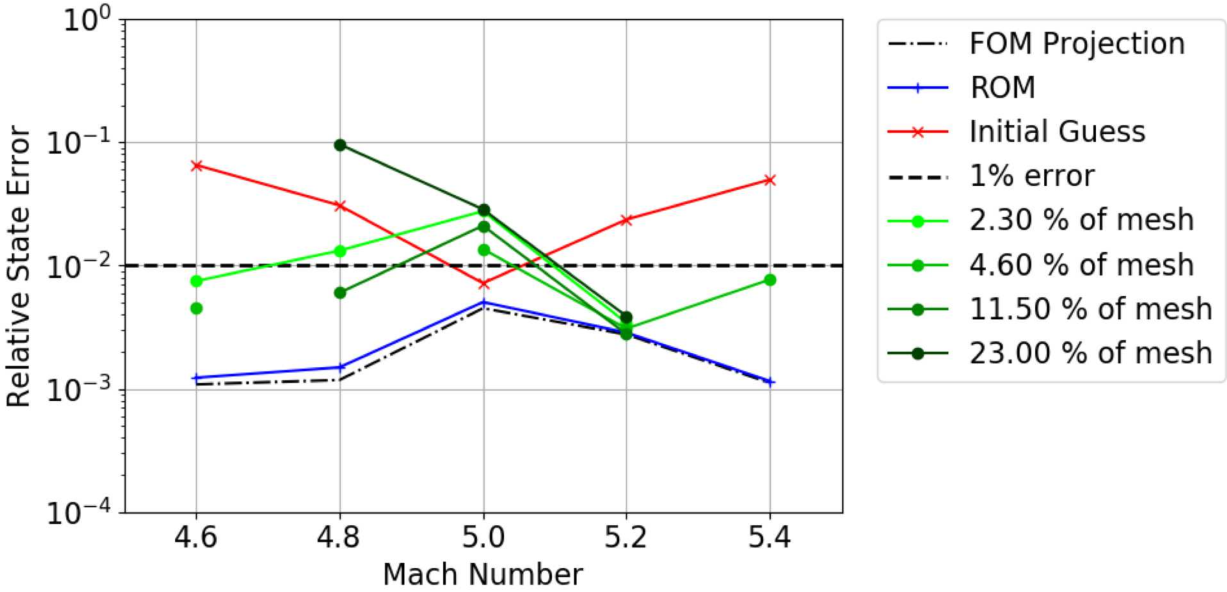
LSPG is still accurate with sample mesh, but greedy algorithm performs poorly relative to random sample mesh



Random Samples



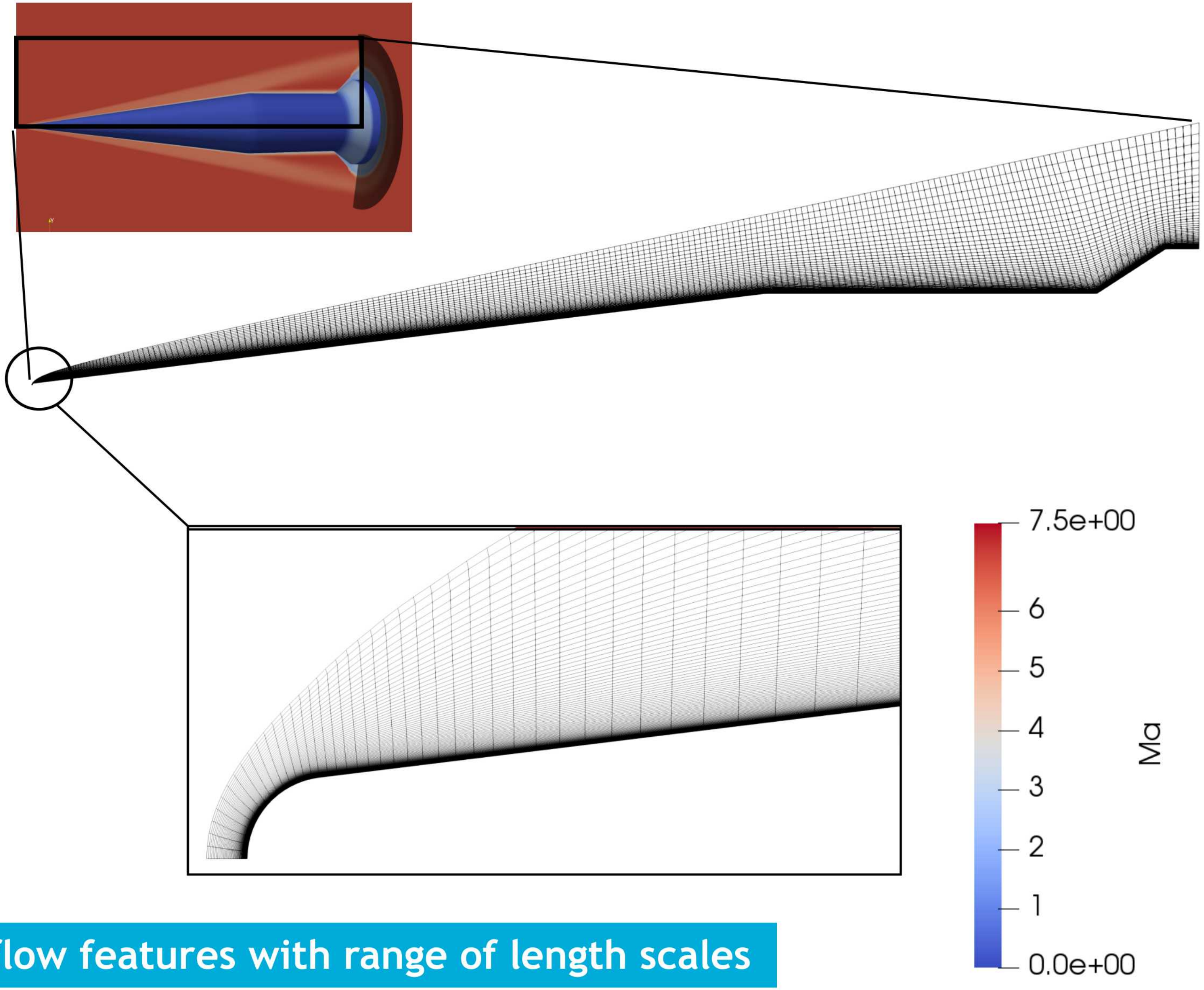
Greedy Algorithm



$$\text{Relative State Error} \equiv \frac{\|\mathbf{x} - \tilde{\mathbf{x}}\|_2}{\|\mathbf{x}\|_2}$$

Case 2: Axis-symetric HIFiRE flight vehicle

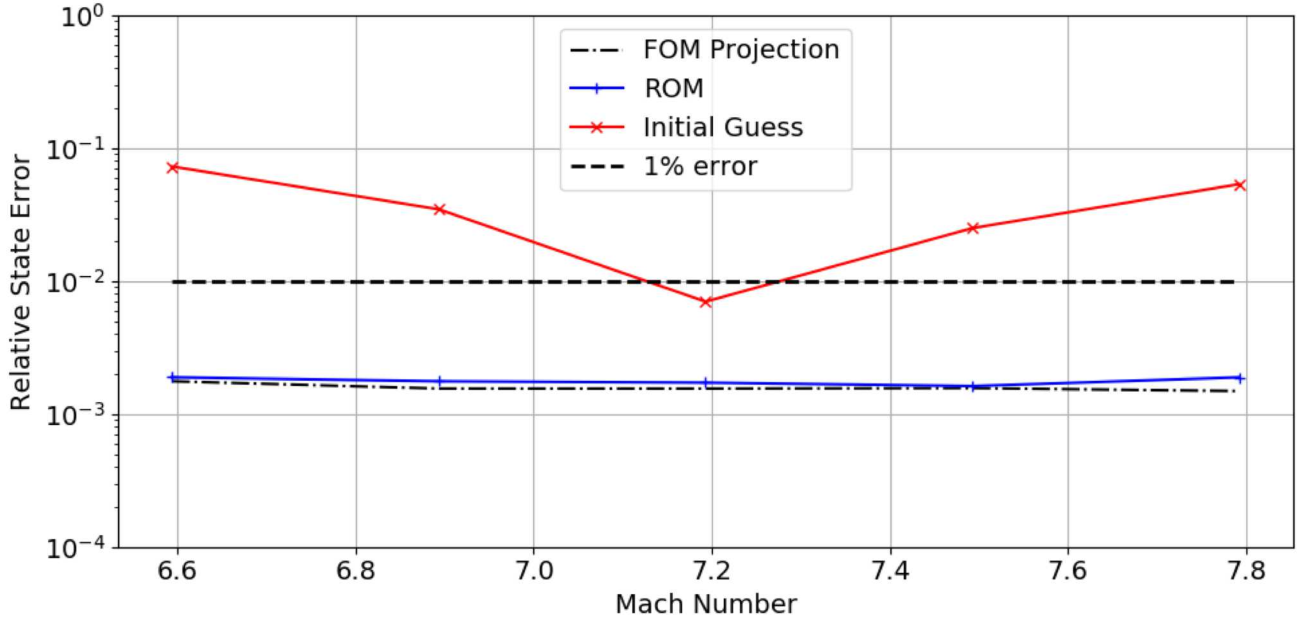
- Flow field:
  - Free stream Mach No. = 7.19
  - Reynolds No. = 41.9 million
  - Boundary layer transitions to turbulence (use Spalart-Allmaras with specified transition location)
- Spatial discretization:
  - 2^{nd}-order finite volume
  - 32768 cells



Numerous flow features with range of length scales

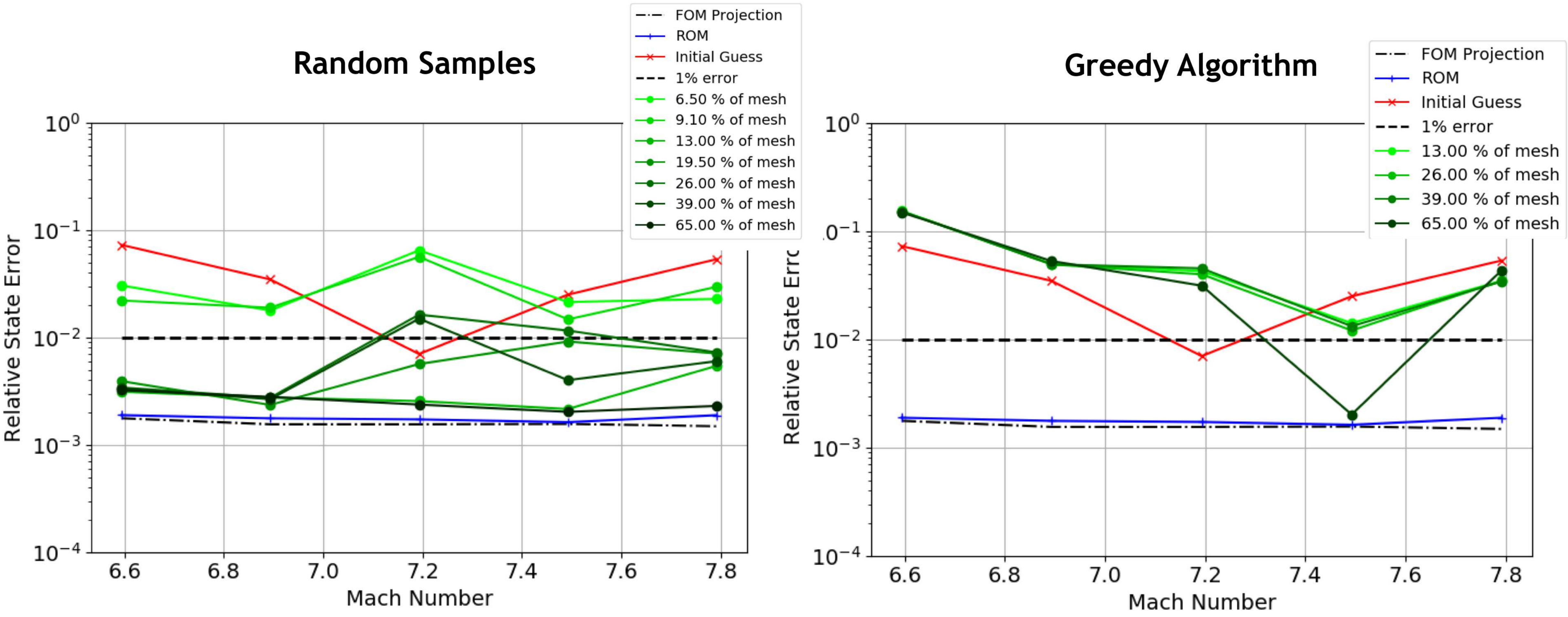
LSPG is accurate for HiFIRE predictive cases

- Full Order Model: 2D HIFiRE solved with backward Euler pseudo time-stepping, CFL schedule.
- Training set: Mach Numbers [6.47, 6.76, 7.04, 7.34, 7.62, 7.91]
- Test set: Mach Numbers [6.59, 6.89, 7.19, 7.49, 7.79]
- POD basis:
  - columns scaled to be unitary.
  - each conserved quantity scaled by its maximum over all FOM solutions.
- ROM: LSPG solved with Gauss-Newton iteration



$$\text{Relative State Error} \equiv \frac{\|\mathbf{x} - \tilde{\mathbf{x}}\|_2}{\|\mathbf{x}\|_2}$$

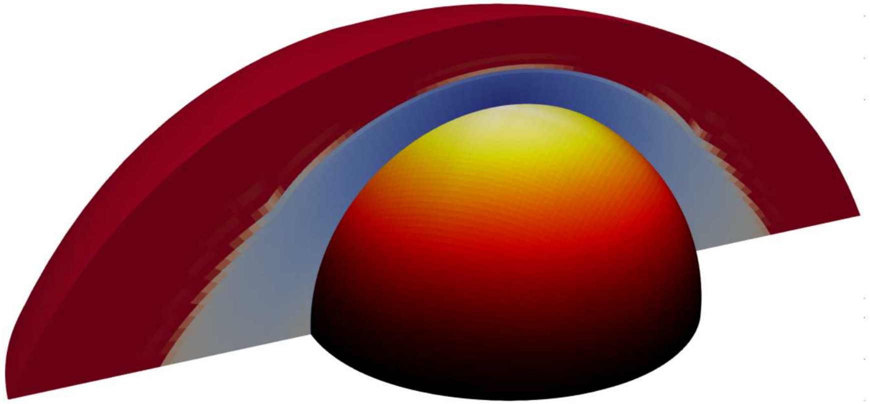
Random hyper-reduction works for HIFiRE predictive cases

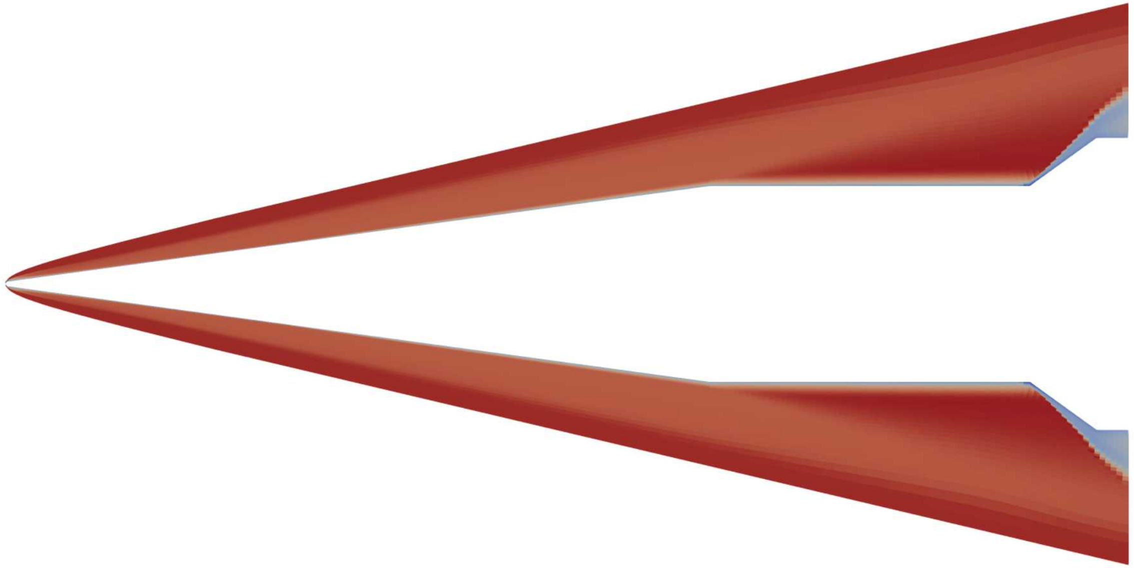


$$\text{Relative State Error} \equiv \frac{\|\mathbf{x} - \tilde{\mathbf{x}}\|_2}{\|\mathbf{x}\|_2}$$

Conclusions

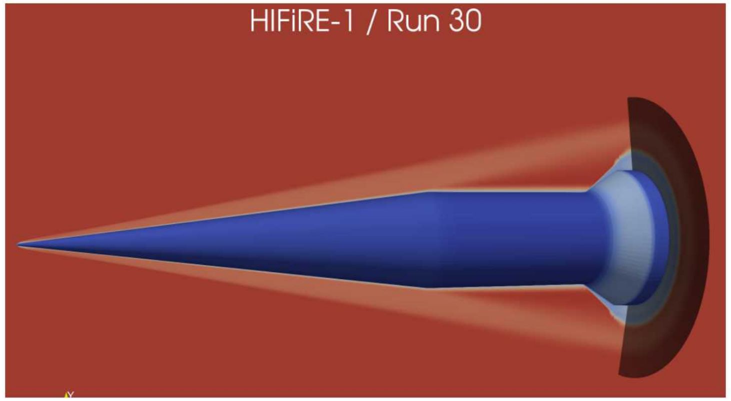
- High-fidelity simulations are crucial, but expensive for hypersonic vehicles
- Model reduction of hypersonic flows with LSPG shows promise:
  - Preliminary results for the Blottner sphere and HIFiRE cases show low cost and accuracy of LSPG.
  - Hyper-reduction works, but the greedy algorithm results in lower accuracy than randomly selecting cells.

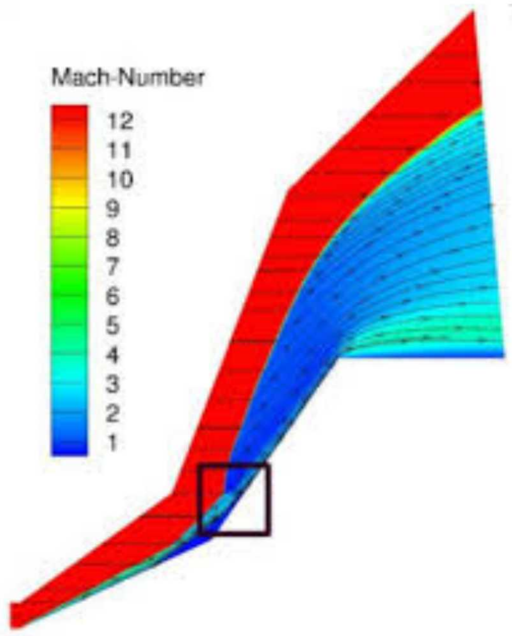




Future Work

- Sample mesh algorithms and implementation for steady problems
- Consider larger parameter variations and multiple parameters
- New cases
  - 3D HIFiRE geometry with asymmetric flow.
  - Double cone with non-equilibrium chemistry.
  - Thermal and Ablation model ROMs
- Different ROM methods
  - LSPG with conservation constraint
  - Manifold-LSPG approach
- **Goal: apply ROM to physically relevant parameter space, such as a range of flight conditions**





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

Backup Slides

Greedy Algorithm [Washabaugh, 2016]

Algorithm 4 Selection of the masks.

Input: Desired number of sampled nodes n_{SN}, and the ROB for the nonlinear terms, $\boldsymbol{\Psi} = [\boldsymbol{\psi}_1, \ldots, \boldsymbol{\psi}_k] \in \mathbb{R}^{n \times k}$

Outputs: $\mathcal{E}$, $\mathcal{E}'$

Find $\xi = \mathrm{nodeWithMax}\left(|\boldsymbol{\psi}_1|\right)$
Identify the degrees of freedom $\{e_{(\xi, i_{\mathrm{DOF}})}\}_{i_{\mathrm{DOF}}=1}^{n_{\mathrm{DOF}}}$ associated with node ξ
Set $\mathcal{E} = \{e_{(\xi,1)}, \cdots, e_{(\xi, n_{\mathrm{DOF}})}\}$
$n_{\mathrm{nodesToAdd}} = \mathrm{ceil}\left(n_{\mathrm{SN}}/k\right)$
for $i_{\mathrm{vec}} = 2, \cdots, k$ **do**
    Set $\mathbf{U} = [\boldsymbol{\psi}_1, \cdots, \boldsymbol{\psi}_{i_{\mathrm{vec}}-1}]$
    for $i_{\mathrm{node}} = 1, \cdots, n_{\mathrm{nodesToAdd}}$ **do**
        Compute masked quantities $\overline{\overline{\boldsymbol{\psi}}}_{i_{\mathrm{vec}}}$ and $\overline{\overline{\mathbf{U}}}$ corresponding to $\mathcal{E}$
        Compute gappy reconstruction $\widetilde{\boldsymbol{\psi}_{i_{\mathrm{vec}}}} = \mathbf{U}\overline{\overline{\mathbf{U}}}^{+}\overline{\overline{\boldsymbol{\psi}}}_{i_{\mathrm{vec}}}$
        Find $\xi = \mathrm{nodeWithMax}\left(|\boldsymbol{\psi}_{i_{\mathrm{vec}}} - \widetilde{\boldsymbol{\psi}_{i_{\mathrm{vec}}}}|\right)$
        $\mathcal{E} \leftarrow \mathcal{E} \cup \{e_{(\xi,1)}, \cdots, e_{(\xi, n_{\mathrm{DOF}})}\}$
    end for
end for
Identify $\mathcal{E}'$, the degrees of freedom necessary to evaluate the residual and Jacobian at $\mathcal{E}$.