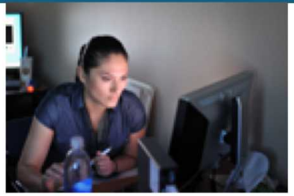
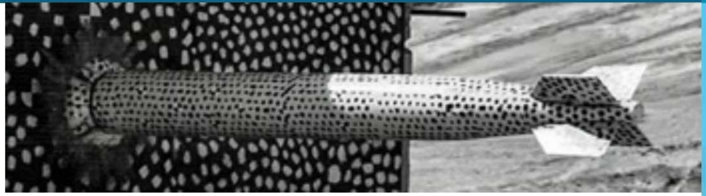
SAND2019-9726PE

Machine-learned reduced-order modeling





PRESENTED BY

Patrick Blonigan

Collaborators: Kevin Carlberg, Brian Freno, Francesco Rizzi, Chi Hoang, Kookjin Lee, Eric Parish, Jaideep Ray, Yukiko Shimizu, John Tencer, Irina Tezaur

CIS External Review, August 26-29, 2019

SAND 2019XXX-XX

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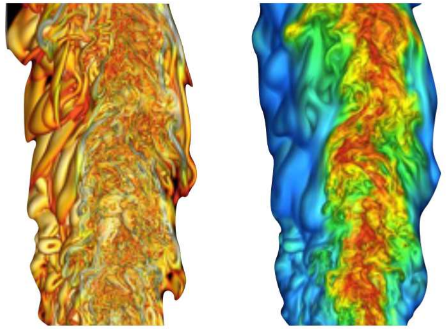
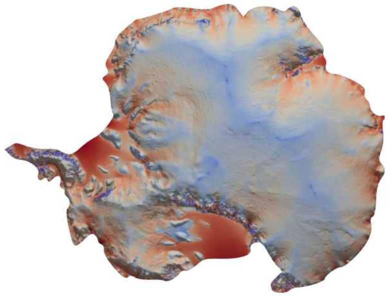
High-fidelity simulations are crucial, but often too costly for rigorous use within Sandia's mission

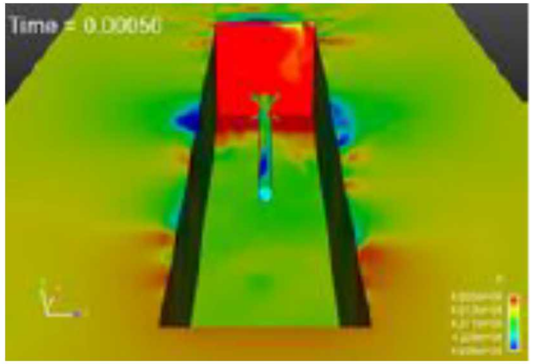
- **High-fidelity simulation:**
  - Extreme-scale nonlinear computational models,
  - Indispensable for a wide range of engineering and scientific applications.
  - Example: captive carry aerodynamics simulation
    - Extreme-scale: 100 million cells, 200,000 time steps.
    - High cost: 6 weeks on 5000 cores.
- **Mission problems:**
  - **Time-critical:**
    - Model predictive control
    - Health monitoring
  - **Many-query:**
    - Uncertainty quantification
    - Design optimization



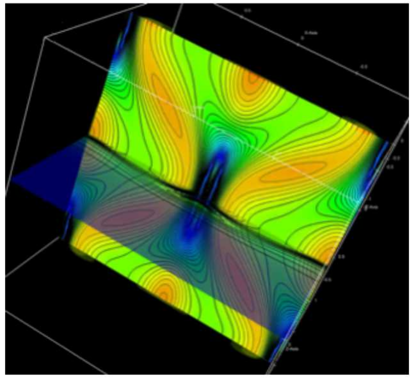
Turbulent reacting flows
courtesy J. Chen



Antarctic ice sheet modeling
courtesy R. Tuminaro



Captive carry aerodynamics
courtesy M. Barone



Magnetohydrodynamics
courtesy J. Shadid

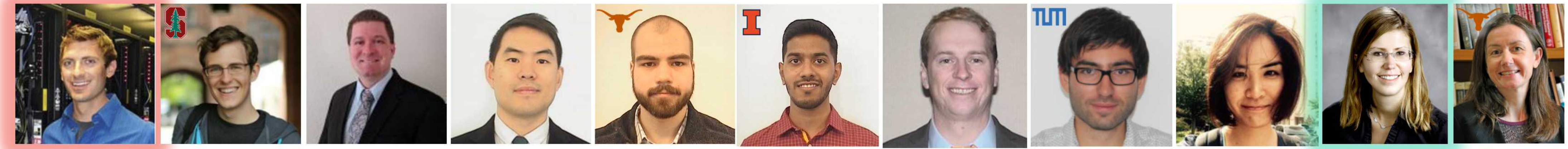
We use model reduction to exploit high-fidelity simulation data for use within many-query and time-critical mission applications

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
5. ***Certification:*** accurately quantify the reduced order model (ROM) error
6. ***Extensibility:*** should work for many application codes

Model reduction at Sandia is a large multidisciplinary effort supported by researchers spanning centers and institutions

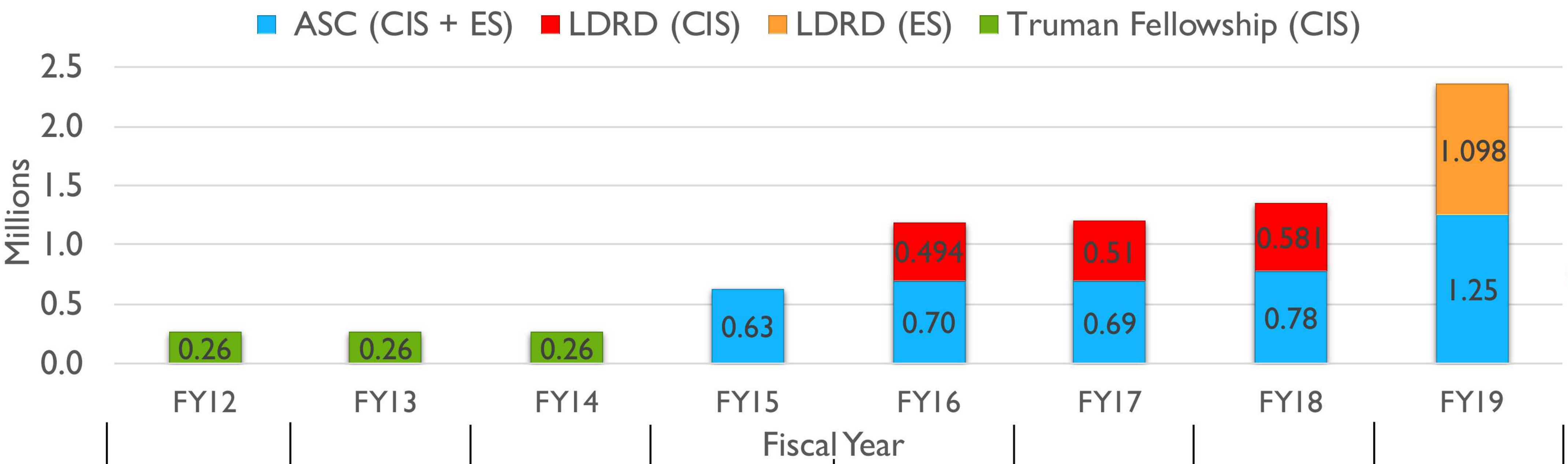
- **Started by Kevin Carlberg with 3 people in FY12, focused on applied math research**
- **Grown to 21 in FY19, with a leadership team spanning the Computing and Information Sciences (CIS) and Engineering Science (ES) research foundations and institutions**
- **Applied Math (CIS+ES)**: method development and analysis



- **Computer Science (CIS)**: generalized, minimally intrusive model reduction implementation

- **Engineering science (ES)**: deployment of model reduction in engineering applications and analysis

The funding scope and technology readiness level of our work are growing



	FY12–FY17	FY18–FY19
Applied Math	*Method development and analysis* **(TRL 1-2)**	*Method development and analysis* **(TRL 1-2)**
Computer Science		*Extensible implementation* **(TRL 4-5)**
Engineering Science	*Deployment: direct implementation within specific simulation codes* **(TRL 3-4)**	*Deployment: extensible software* **(TRL 4-5)**

[Software-specific Technology Readiness Level (TRL) https://trl.sandia.gov](https://trl.sandia.gov)

1 2 3 4 5 6 7 8 9

Historical model reduction approaches are ineffective for nonlinear dynamical systems, which arise often in Sandia's mission applications

Historical model reduction work external to Sandia

- **Linear time-invariant systems**: **mature** [Antoulas, 2005]
  - Balanced truncation [Moore, 1981; Willcox and Peraire, 2002; Rowley, 2005]
  - Transfer-function interpolation [Bai, 2002; Freund, 2003; Gallivan et al, 2004; Baur et al., 2011]
  - ✓ ***Accurate, generalizes, certified***: sharp *a priori* error bounds
  - ✓ ***Inexpensive***: pre-assemble operators
  - ✓ ***Property preservation***: guaranteed stability
- **Elliptic/parabolic PDEs**: **mature** [Prud'Homme et al., 2002; Barrault et al., 2004; Rozza et al., 2007]
  - Reduced-basis method
  - ✓ ***Accurate, generalizes, certified***: sharp *a priori* error bounds
  - ✓ ***Inexpensive***: pre-assemble operators
  - ✓ ***Property preservation***: preserve operator properties
- **Nonlinear dynamical systems**: **ineffective**
  - Proper orthogonal decomposition (POD)–Galerkin [Sirovich, 1987; Colonius, 2004]
  - ✗ ***Inaccurate, doesn't generalize***: often unstable
  - ✗ ***Not certified***: error bounds grow exponentially in time
  - ✗ ***Expensive***: projection insufficient for speedup
  - ✗ ***Structure not preserved***: physical properties ignored
  - ✗ ***Not extensible***: highly intrusive implementation required

Model Reduction Criteria

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5. ***Certification:*** accurately quantify the ROM error
6. ***Extensibility:*** should work for many application codes

Our research is focused on satisfying model reduction criteria for nonlinear dynamical systems

Our model reduction research at Sandia

- ***Accuracy***
  - **Least-Squares Petrov—Galerkin (LSPG) projection**: *our baseline approach* [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]
- ***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; Parish and Carlberg, 2019]
- ***Extensibility***
  - Pressio software: *deploy methods for many application codes*

Model Reduction Criteria

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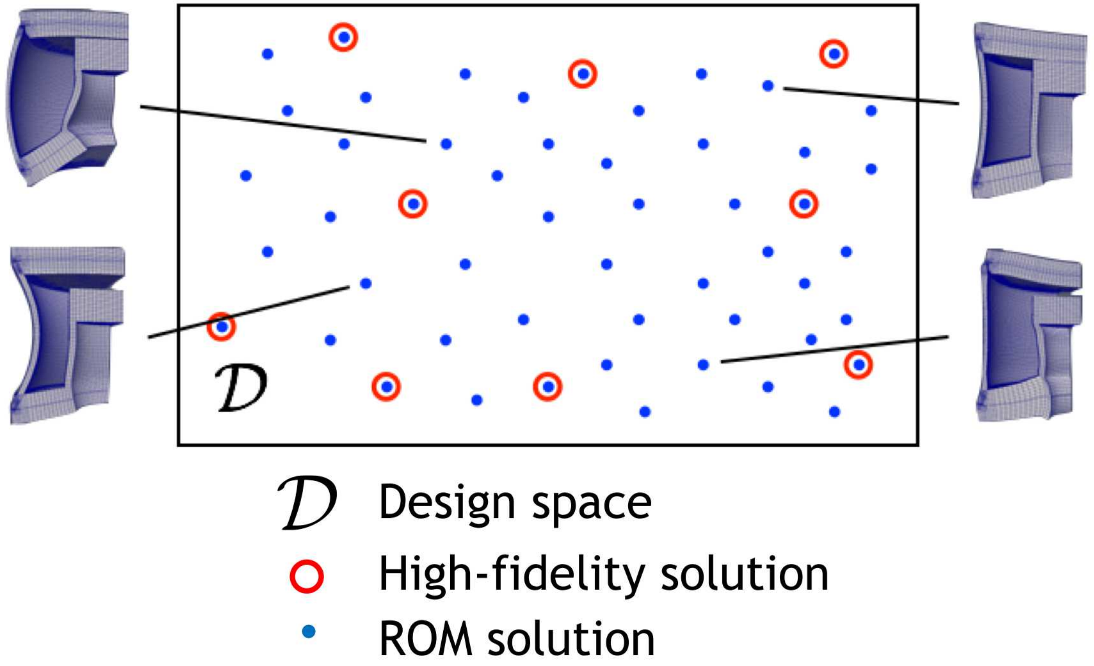
We employ a machine-learned model reduction approach that has four stages

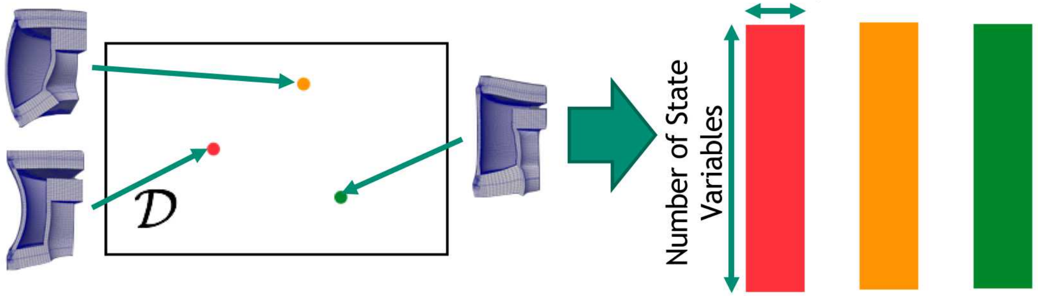
1. **Acquisition**: Run high-fidelity simulation at a few design points, save simulation data
2. **Learning**: Use machine learning techniques to identify low-dimensional structure in the high-fidelity simulation data
3. **Reduction**: Build a reduced-order model (ROM) with extracted data structures,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



Our baseline approach* leverages a linear basis computed with unsupervised learning

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

1. Acquisition

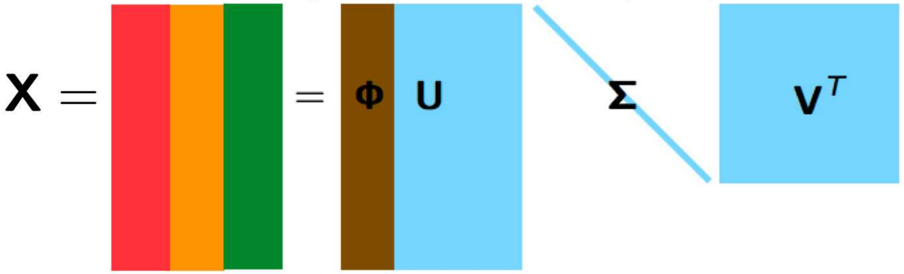


Solve ODE at different design points

Save solution data

2. Learning

Unsupervised Learning with Principal Component Analysis (PCA):



3. Reduction

Choose ODE Temporal Discretization

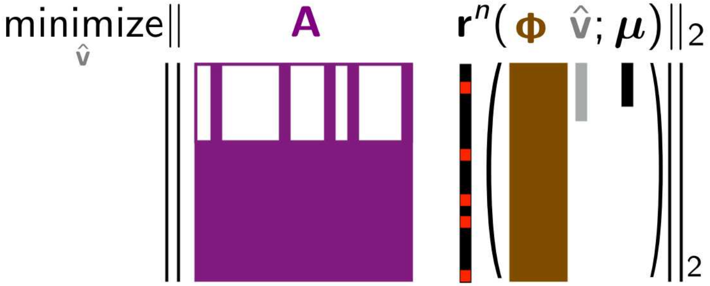
$$\frac{d\mathbf{x}}{dt} = \mathbf{f}(\mathbf{x}; t, \boldsymbol{\mu})$$

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

Reduce the number of unknowns

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

Minimize the Residual

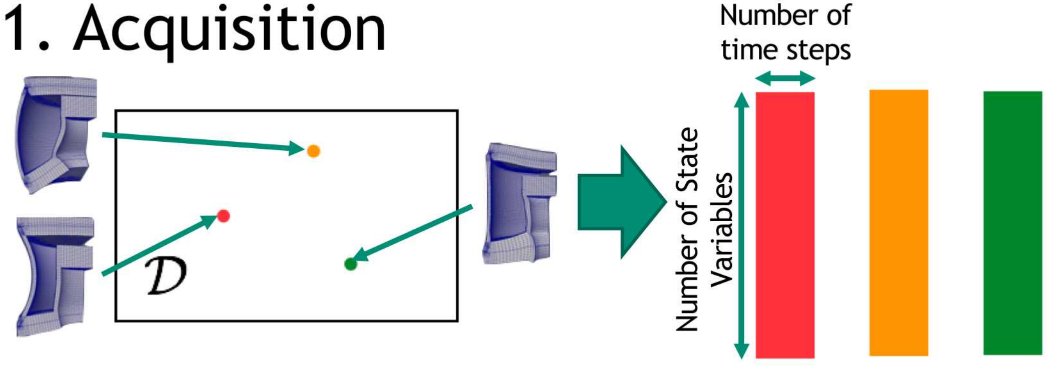


*Least-Squares Petrov–Galerkin (LSPG) Projection [Carlberg, Bou-Mosleh, Farhat, 2011; Carlberg, Barone, Antil, 2017]

Property preservation is enforced with additional constraints

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

1. Acquisition



Solve ODE at different design points

Save solution data

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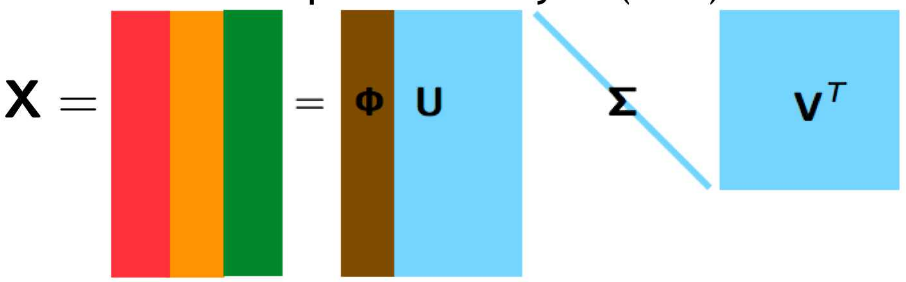
Unsupervised Learning with Principal Component Analysis (PCA):



3. Reduction

Choose ODE Temporal Discretization

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

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Reduce the number of unknowns

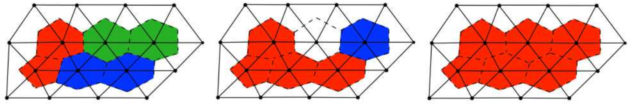
$$\mathbf{x}(t) \approx \tilde{\mathbf{x}}(t) = \boldsymbol{\Phi}\,\hat{\mathbf{x}}(t)$$

Minimize the Residual

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

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

Enforce conservation over subdomains:

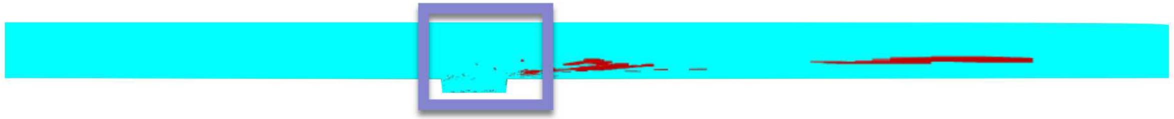


[Carlberg, Choi, Sargsyan, 2018]

Our baseline approach achieves high accuracy at a low cost for captive carry application

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

Sample mesh

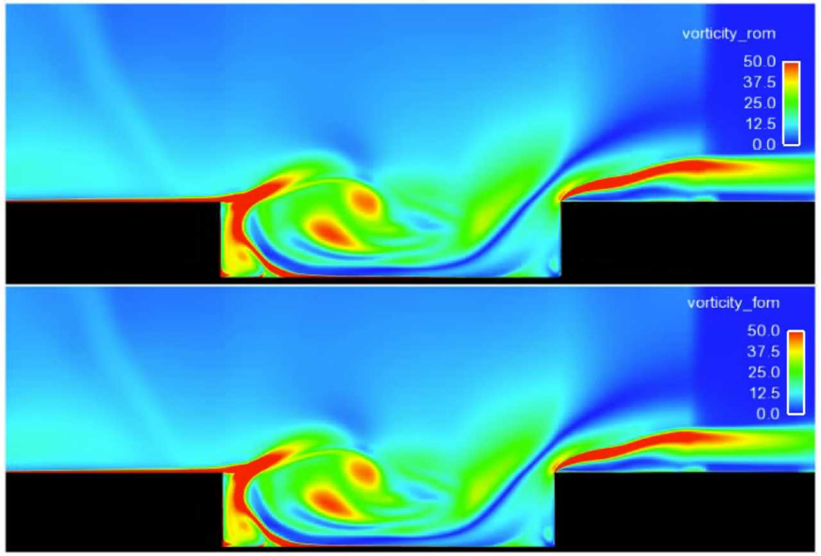


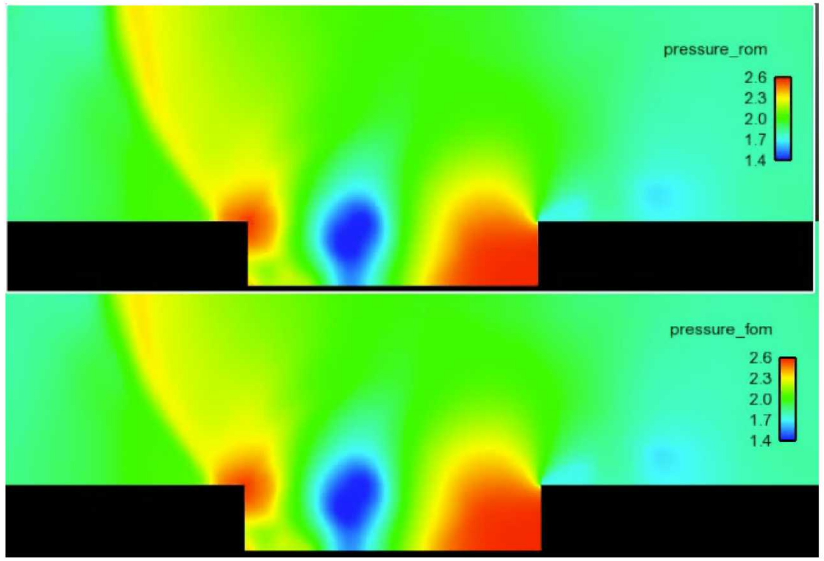
Vorticity Field

Pressure Field

LSPG ROM
- 32 min, 2 cores

High-fidelity
- 5 hours, 48 cores





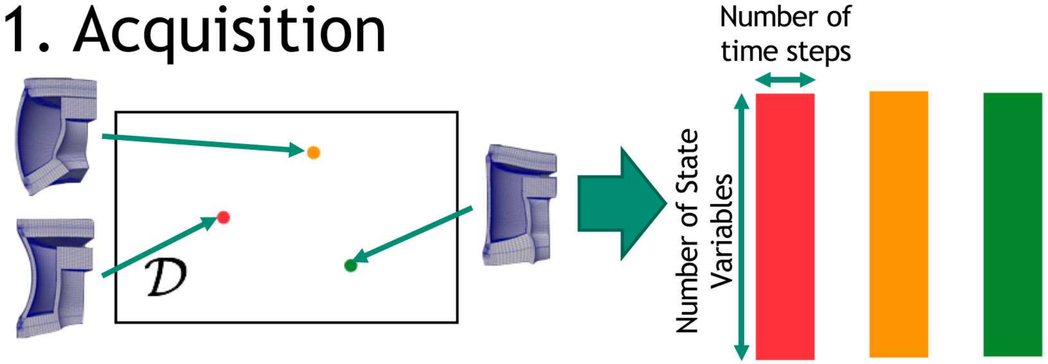
229x savings in core-hours
< 1% error in time-averaged drag

[Carlberg, Barone, Antil, 2017]

Manifold model reduction uses a nonlinear function instead of a linear basis

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

1. Acquisition

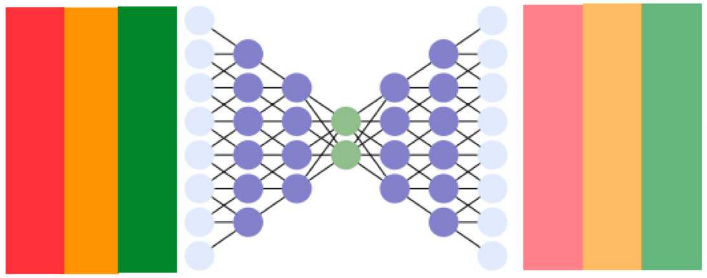


Solve ODE at different design points

Save solution data

2. Learning

Unsupervised Learning with non-linear manifold approach (e.g. deep autoencoder):

$\mathbf{X} =$  $= \tilde{\mathbf{X}}(\boldsymbol{\theta})$

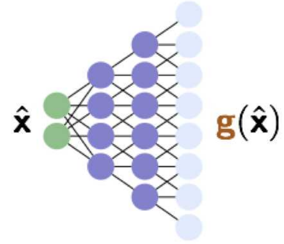
3. Reduction

Choose ODE Temporal Discretization

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

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

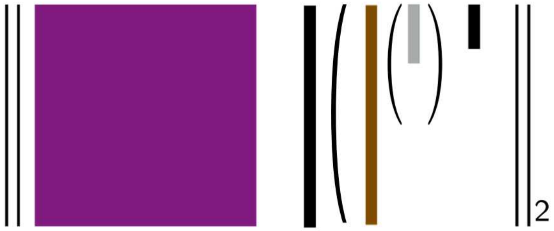
Reduce the number of unknowns



$$\mathbf{x}(t) \approx \tilde{\mathbf{x}}(t) = \mathbf{g}(\hat{\mathbf{x}}(t)) \in \mathcal{S}$$

Minimize the Residual

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



Manifold LSPG Projection [Lee & Carlberg, 2019]

We achieve large improvements in the generalization criteria with manifold model reduction

2D Chemically reacting flow

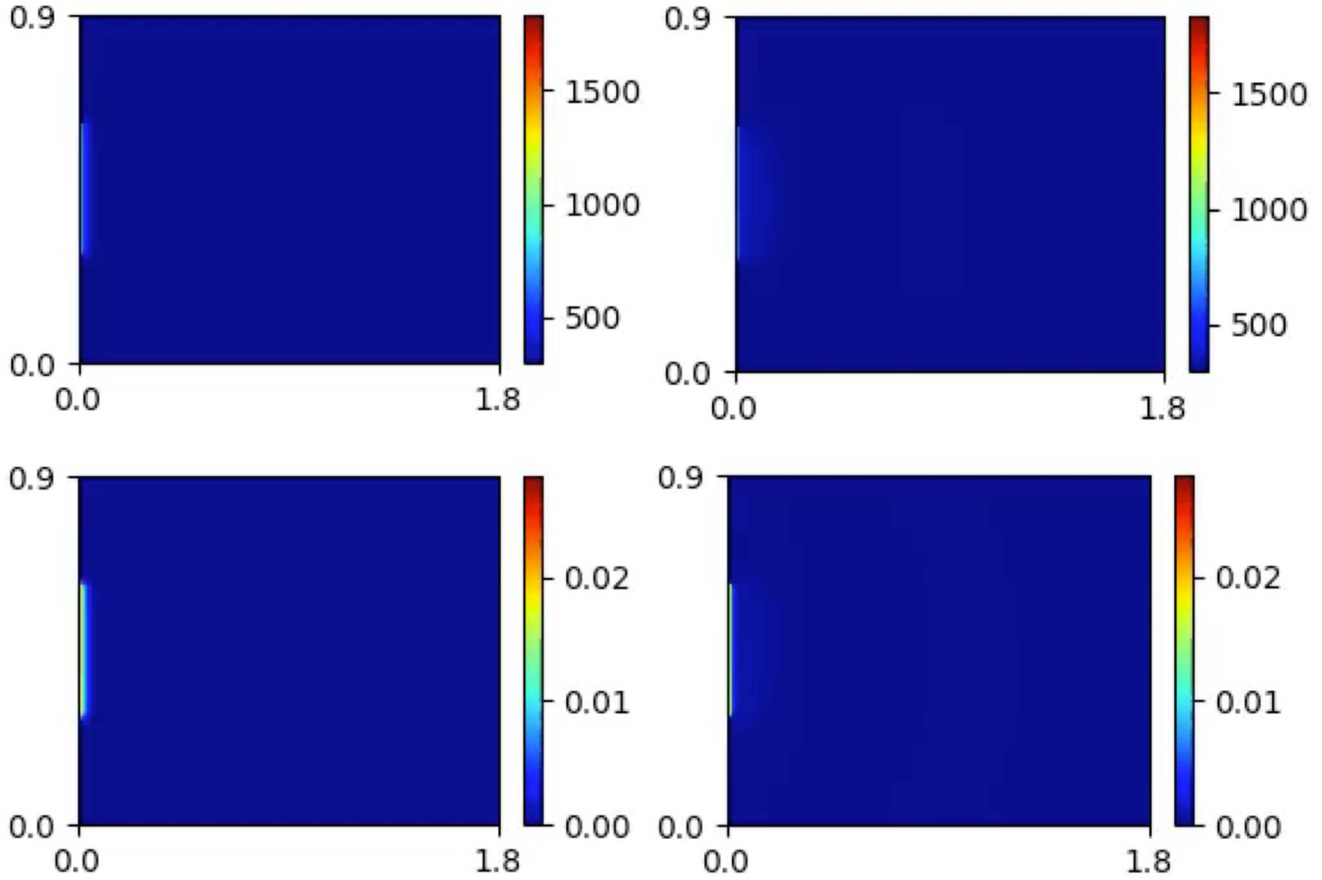
$$\frac{\partial \mathbf{w}(\vec{x}, t; \boldsymbol{\mu})}{\partial t} = \nabla \cdot (\kappa \nabla \mathbf{w}(\vec{x}, t; \boldsymbol{\mu})) - \mathbf{v} \cdot \nabla \mathbf{w}(\vec{x}, t; \boldsymbol{\mu}) + \mathbf{q}(\mathbf{w}(\vec{x}, t; \boldsymbol{\mu}); \boldsymbol{\mu})$$

high-fidelity model

LSPG w/ PCA ROM dimension=5

temperature

H2 fraction



[Lee & Carlberg, 2019]

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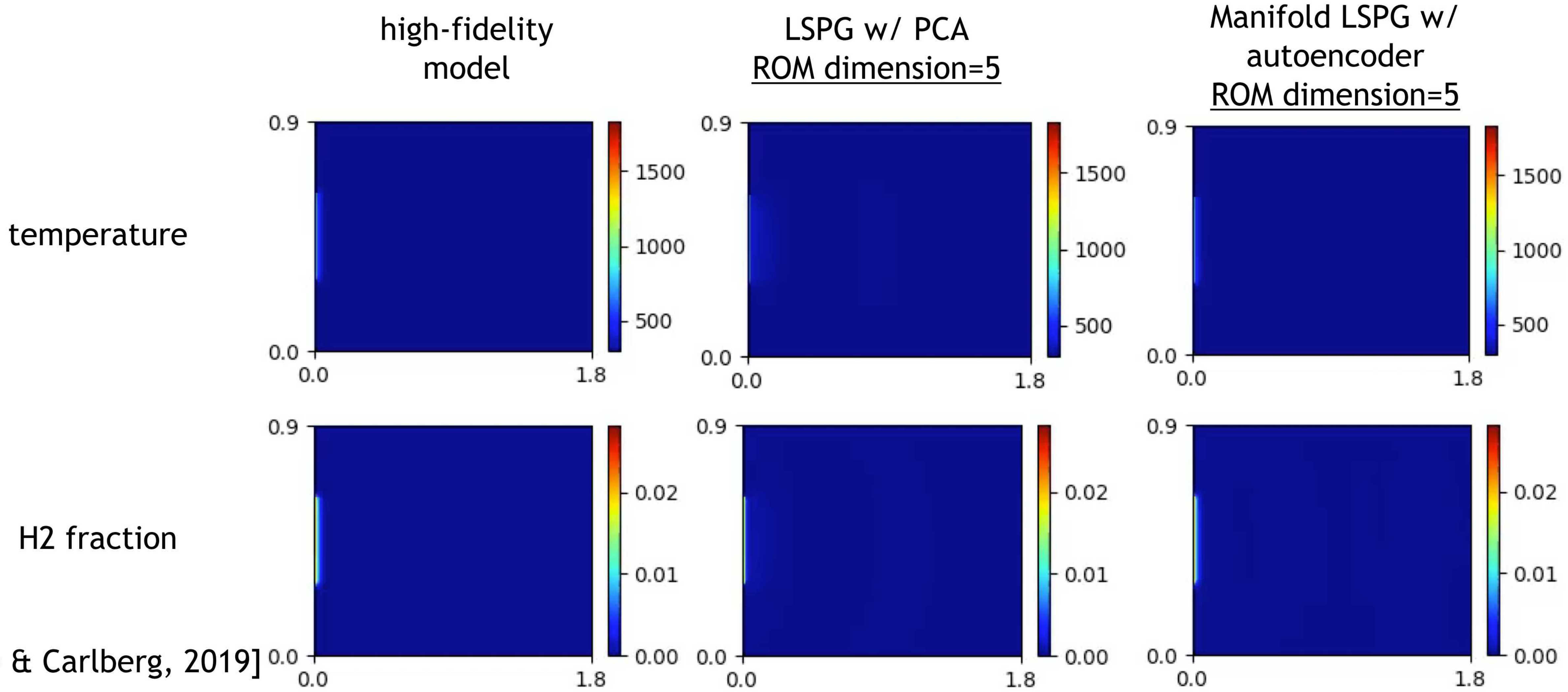
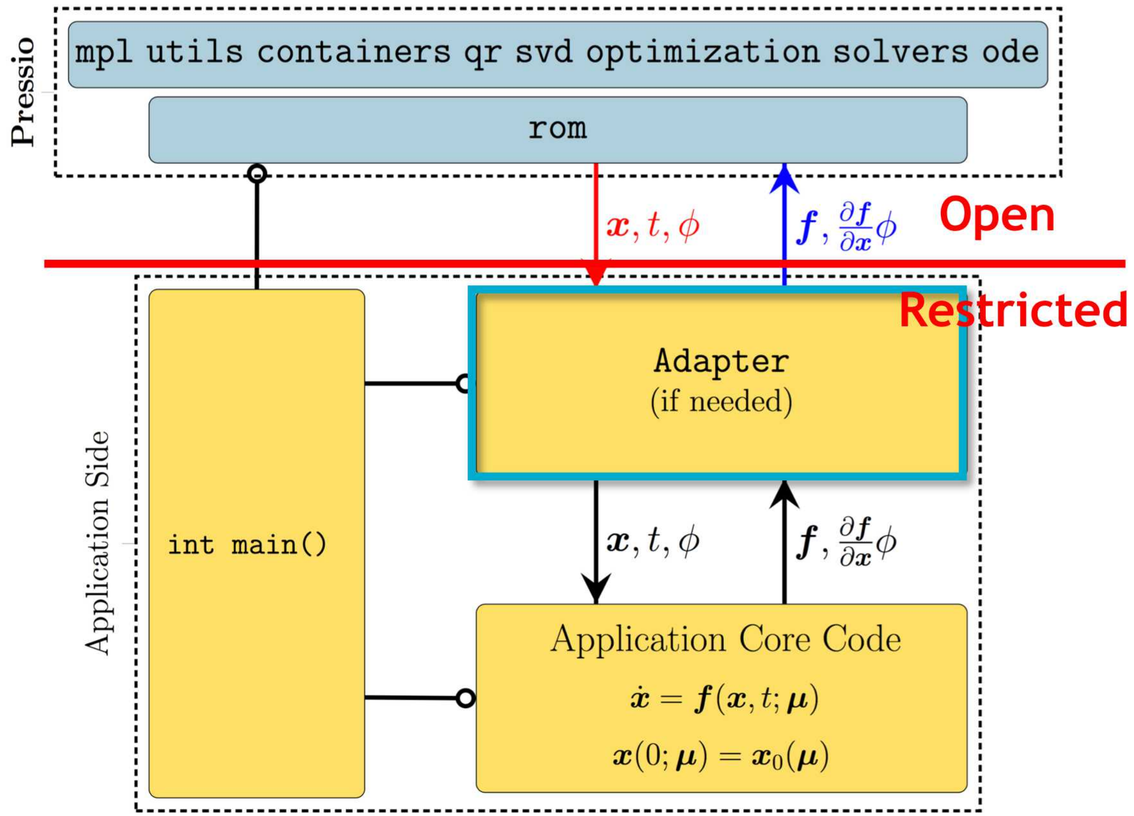


[Lee & Carlberg, 2019]

Pressio enables deployment of model reduction methods to a range of simulation codes

- Previous ROM methods were implemented directly in multiple application codes
  - ✗ **Highly intrusive**: major changes to application code
  - ✗ **Not extensible**: 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)
    - ➢ Portable implementation that works on different architectures, including GPUs
    - ➢ Restricted to practices used by mission application partners
  - ✓ Facilitates contributions from external partners
    - ➢ Undergoing open source copyright assertion
  - ✓ Clear separation between methods and application
    - ➢ Enables methods work without access to restricted applications (ITAR,Classified, etc.)



Schematic of Pressio software workflow (F. Rizzi)

We are building Pressio adapters for three simulation codes

SPARC

Hypersonic Aerothermodynamics

- Key Personnel: P. Blonigan, M. Howard, J. Fike, F. Rizzi
- Progress: creating and running ROMs for aerodynamics

LDRD
Laboratory Directed Research and Development

ARIA

Heat Transfer

- Key Personnel: J. Tencer, F. Pierce, F. Rizzi
- Progress: interface complete, setting up basis computation

LDRD
Laboratory Directed Research and Development

Sierra Aero

Compressible Aerodynamics

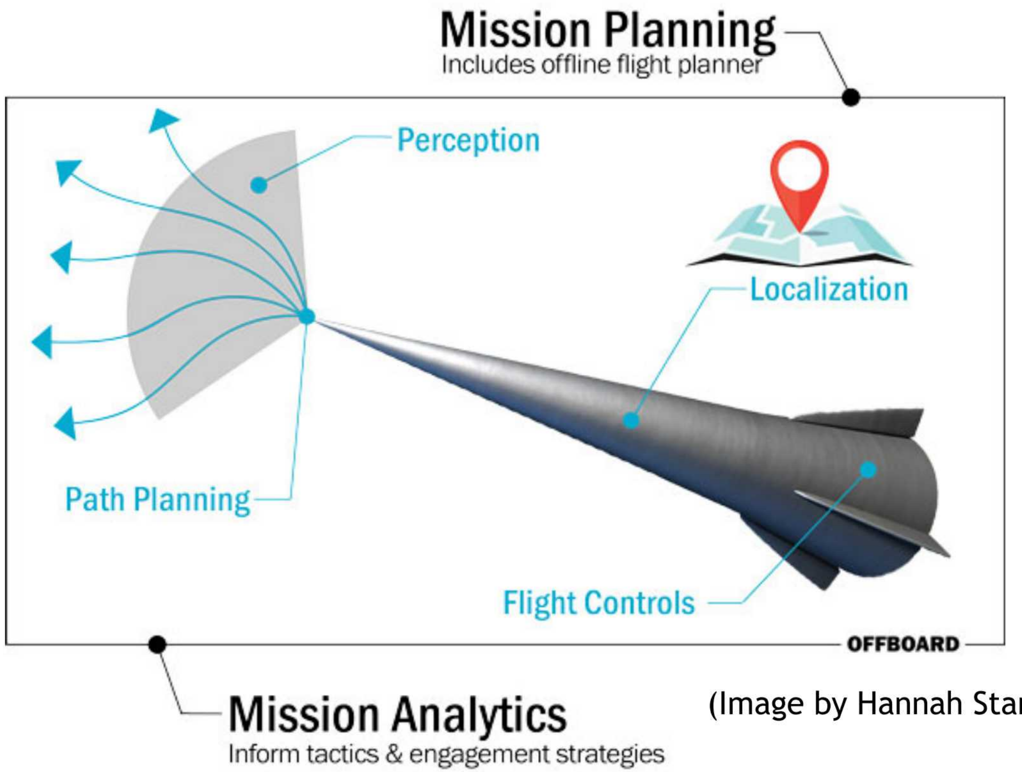
- Key Personnel: J. Tencer, C. Proctor, M. McWherter-Payne, P. Blonigan
- Progress: creating high fidelity models

LDRD
Laboratory Directed Research and Development

We are integrating our model reduction tools with many-query and time-critical applications

- Multi-fidelity Uncertainty Quantification
  - P. Blonigan, G. Geraci, and M. Eldred
- Network Uncertainty Quantification with ROMs for system-component design:
  - J. Tencer, K. Carlberg, C. Proctor, M. McWherter-Payne, and P. Blonigan
- Optimization under uncertainty
  - External collaboration, key personnel: M. Zahr, K. Carlberg, and D. Kouri
  - [Zahr, Carlberg and Kouri, 2019].
- Autonomy for hypersonics: path planning and adaptive control
  - P. Blonigan, K. Carlberg, M. Howard, J. Fike, and F. Rizzi

The Autonomy For Hypersonics (A4H) mission campaign focuses on time-critical problems for hypersonic vehicles



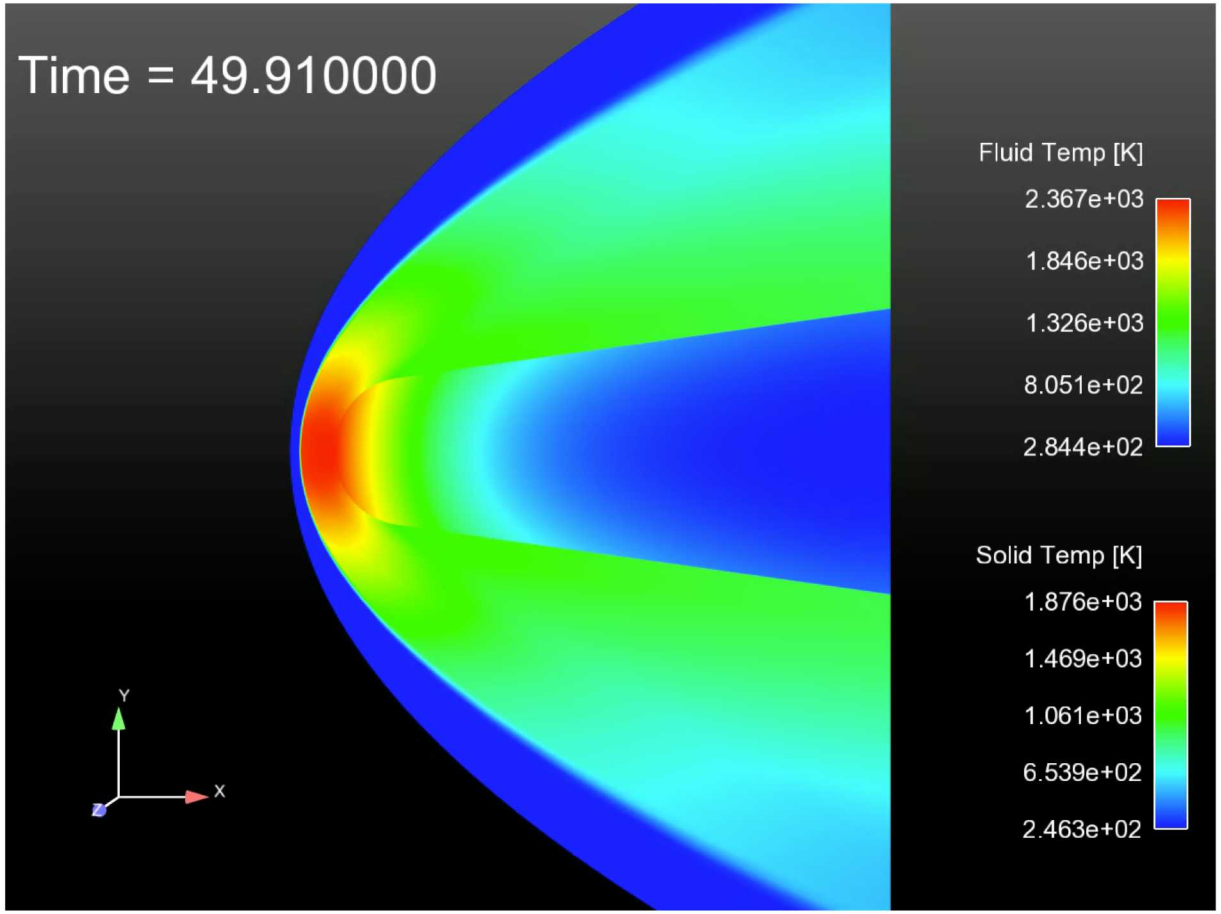
(Image by Hannah Stangebye)

Sandia's A4H Mission Campaign seeks to:

- Significantly decrease the time required for hypersonic missile flight planning using artificial intelligence.
- Enable semi-autonomous hypersonic missiles to self-correct in flight to compensate for unexpected flight conditions or a change in the target's location.
  - http://www.sandia.gov/news/publications/labnews/articles/2019/04-26/hypersonics.html

Our A4H project* will use our model reduction tool chain to accelerate path planning, design, and control of hypersonic vehicles

- Our project uses model reduction to:
    1. Generate large databases with quantified uncertainties for path planning.
    2. Enable rapid interactive simulation for vehicle design and control.
- We use Pressio (F. Rizzi) and SPARC (M. Howard) to create ROMs for hypersonic aerodynamics
- Joint work with aerosciences team (M. Howard, J. Fike) and UT Austin (K. Willcox, S. Majors)



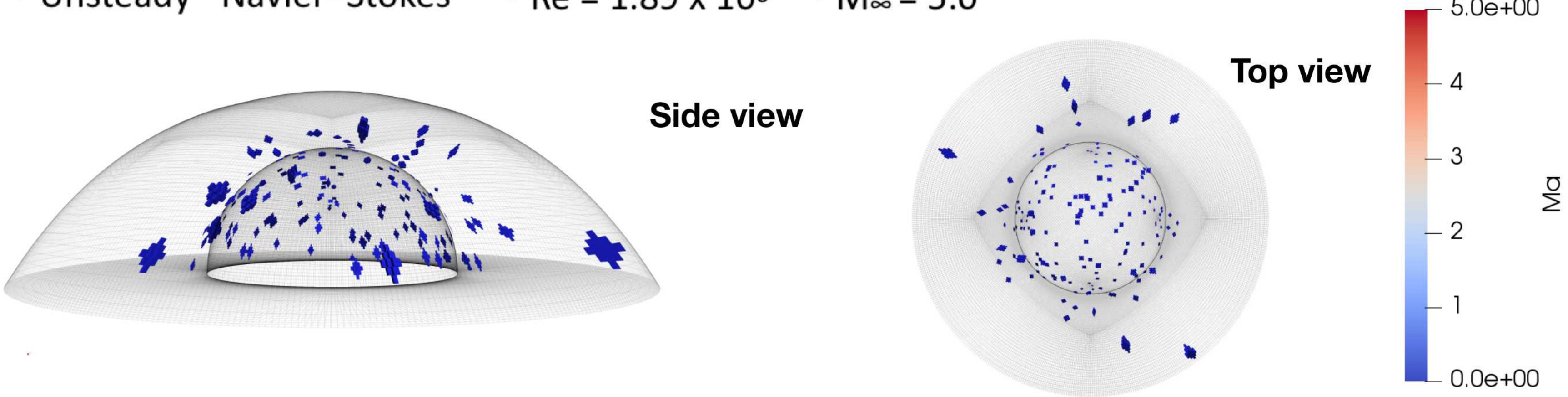
A slender body in hypersonic flow simulated with SPARC (courtesy M. Howard)

*Rapid high-fidelity aerothermal responses with quantified uncertainties via reduced-order modeling

Preliminary results show that our model reduction tool chain will be effective for this application space

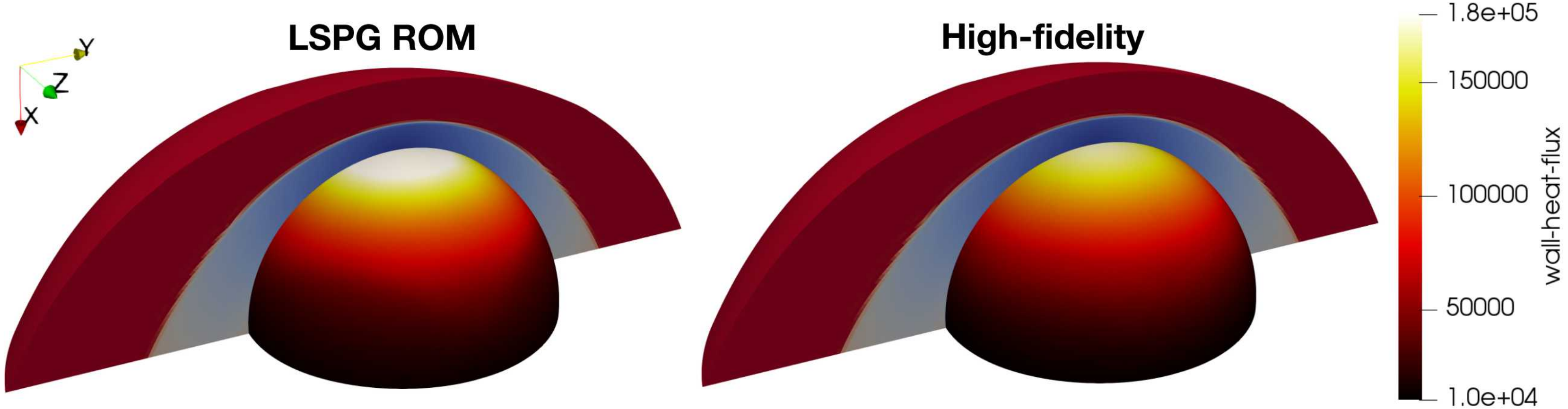
Blottner Sphere: ‣ Unsteady* Navier–Stokes ‣ Re = 1.89 x 10^6 ‣ $M_\infty = 5.0$

Sample mesh



LSPG ROM:
- Sample mesh: 4,150 cells= 20,750 DoFs
- 1 MPI rank, ~18 seconds

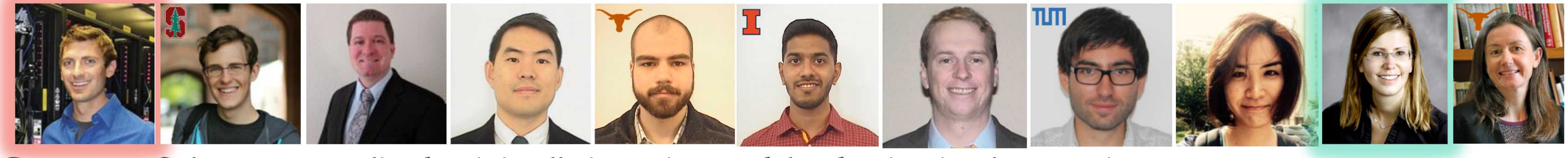
High-fidelity:
- 4,194,304 cells=20,971,520 DoFs
- 128 MPI ranks, ~147 seconds



1060x savings in core-hours
< 1% error in density, Mach number, and temperature fields
< 1% error in axial force, heat flux

Model reduction at Sandia is a large multidisciplinary effort supported by researchers spanning centers and institutions

- **Applied Math**: method development and analysis

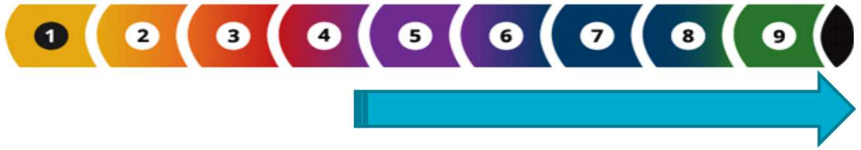


- **Computer Science**: generalized, minimally intrusive model reduction implementation

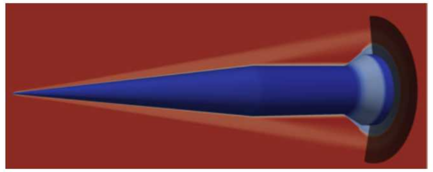
- **Engineering science**: deployment of model reduction in engineering applications and analysis

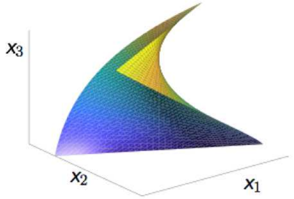
Future work will continue to span computer science, engineering science, and applied math research and development

- Computer Science R&D:
  - Adding existing methods to Pressio
  - Pathway to production for Pressio

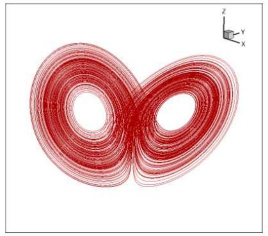


- Engineering Science R&D:
  - Apply Pressio to increasingly complex physical systems
  - New Pressio adaptors for additional simulation capabilities
  - Integration of model reduction techniques with time-critical/many-query methods/frameworks:
    - Network UQ
    - Multi-fidelity UQ
    - Verification and Validation, Other UQ/Optimization approaches





- Applied Math R&D:
  - Nonlinear manifold model reduction methods
  - Develop methods for chaotic dynamical systems



- Maintain current projects and create new projects with internal and external collaborators.

Massachusetts Institute of Technology · ILLINOIS University of Illinois at Urbana-Champaign · University of Michigan · University of Notre Dame · Stanford University · Technische Universität München · TEXAS The University of Texas at Austin · University of Washington

Summary of accomplishments and key references

Team grew from **3** in FY12 to **21** in FY19

2 keynote presentations
34 conference presentations
32 invited talks

23 Journal publications (7 in review)
6 Conference publications

#1 most-cited paper, 2011, IJNME
#1 most-cited paper, 2013, JCP
Featured article, 2015, SIAM JSC
Top 5 most-cited paper, 2017, JCP

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- Contact information:

  - Patrick Blonigan
  - pblonig@sandia.gov / 925-294-6707
  - https://www.sandia.gov/~pblonig
  - ROM group email: wg-rom-group@sandia.gov

Backup slides

More Information

- Other References

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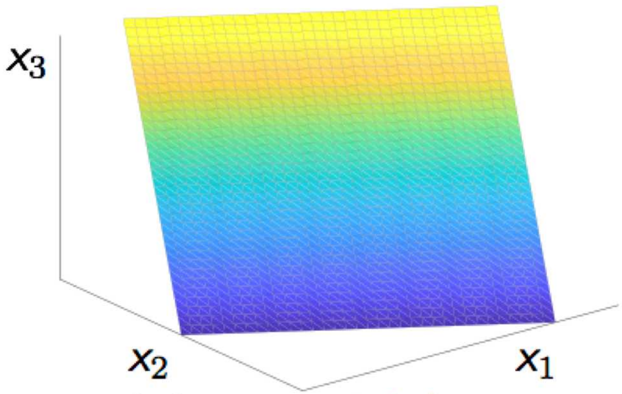
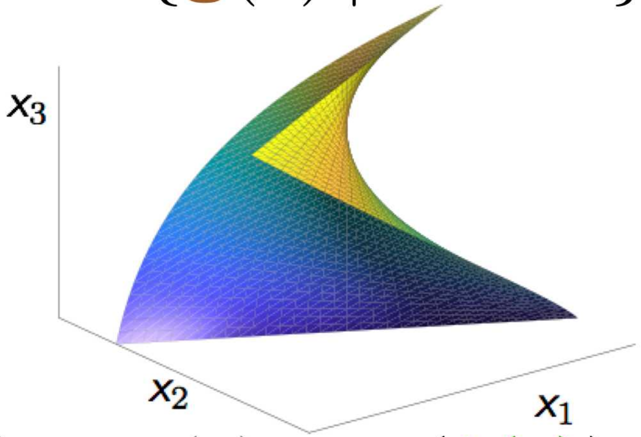
Manifold LSPG projection uses a nonlinear function instead of a linear basis, resulting in more capacity [Lee & Carlberg, 2019]

$$\text{range}(\boldsymbol{\Phi}) := \{\boldsymbol{\Phi}\hat{\mathbf{x}} \mid \hat{\mathbf{x}} \in \mathbb{R}^p\}$$

$$\mathcal{S} := \{\mathbf{g}(\hat{\mathbf{x}}) \mid \hat{\mathbf{x}} \in \mathbb{R}^p\}$$

Example:
N=3
P=2

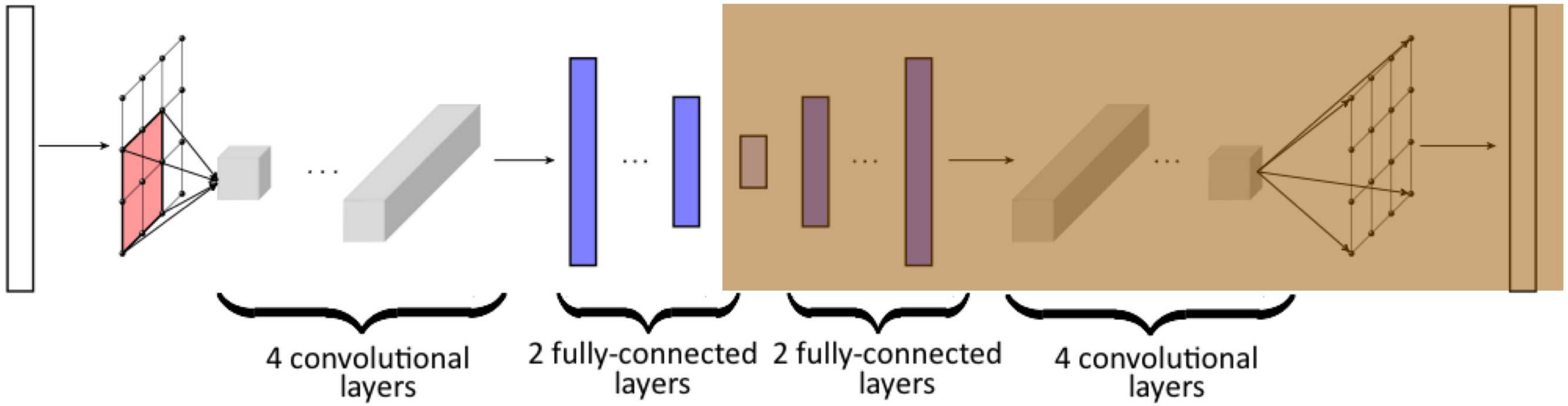




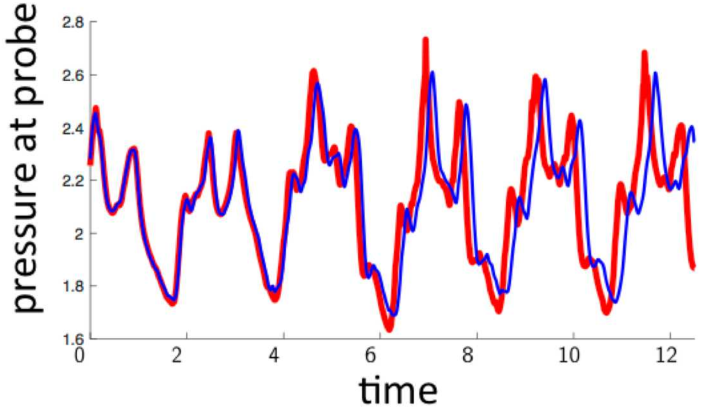
$$\mathbf{x}(t) \approx \tilde{\mathbf{x}}(t) = \boldsymbol{\Phi}\,\hat{\mathbf{x}}(t) \in \text{range}(\boldsymbol{\Phi})$$

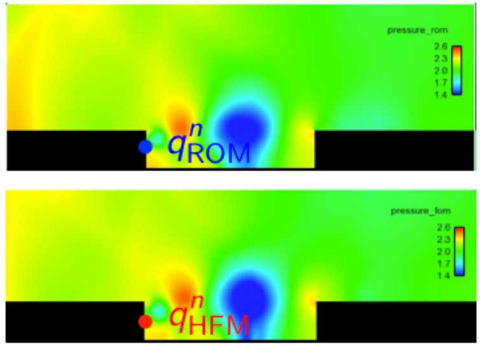
$$\mathbf{x}(t) \approx \tilde{\mathbf{x}}(t) = \mathbf{g}(\hat{\mathbf{x}}(t)) \in \mathcal{S}$$

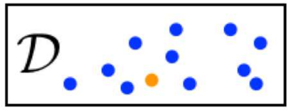
Decoder:
One choice of nonlinear function



Machine Learning Error Models [Carlberg & Freno, 2018]







inputs $\boldsymbol{\mu}$ → *reduced-order model* → *outputs* q^n_{ROM}, $n = 1, \dots, T$

↓

features ρ^n, $n = 1, \dots, N$

↓

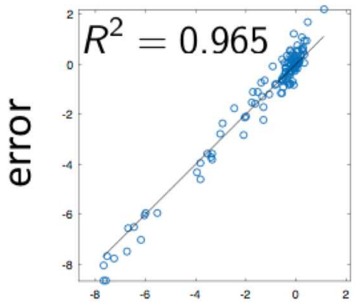
regression model → *stochastic error prediction* $\hat{\delta}^n \approx q^n_{\mathrm{HFM}} - q^n_{\mathrm{ROM}}$, $n = 1, \dots, T$

$$q^n_{\mathrm{HFM}} \approx q^n_{\mathrm{ROM}} + \hat{\delta}^n$$

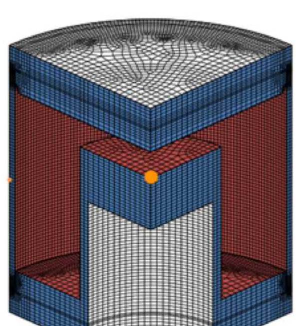
+ *Statistical model of high-fidelity-model output*

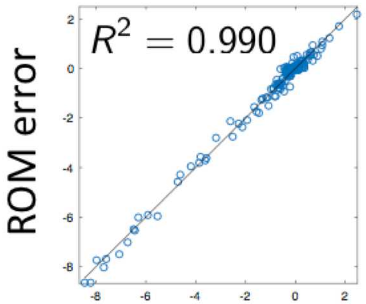
Physics-based feature engineering to determine ρ^n

Example: Component Structural Model

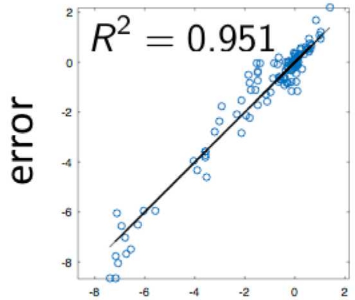


random forest
error prediction





support vector machine
error prediction



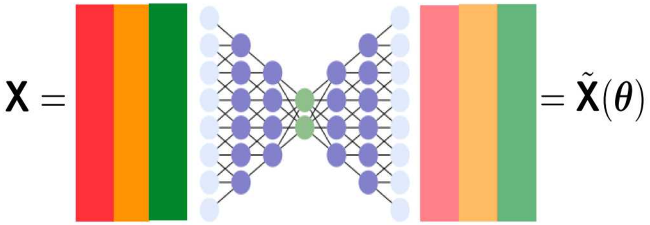
k-NN
error prediction

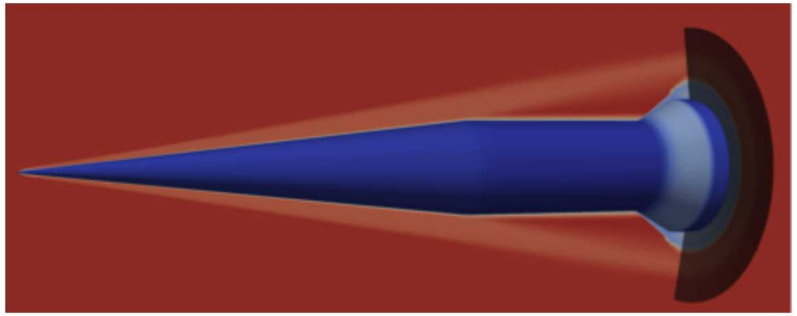
ML methods yield low-variance error predictions

Our vision statement informs our current and future research

Establish a research-to-production capability, based on projection-based reduced-order models (ROMs), that enables deployment of high-fidelity physics & engineering simulations in time-critical (e.g., control, rapid analysis) and many-query applications (e.g., uncertainty quantification, design optimization, parameter-space exploration), in support of the Department of Energy mission.

Software-specific Technology Readiness Level (TRL) https://trl.sandia.gov

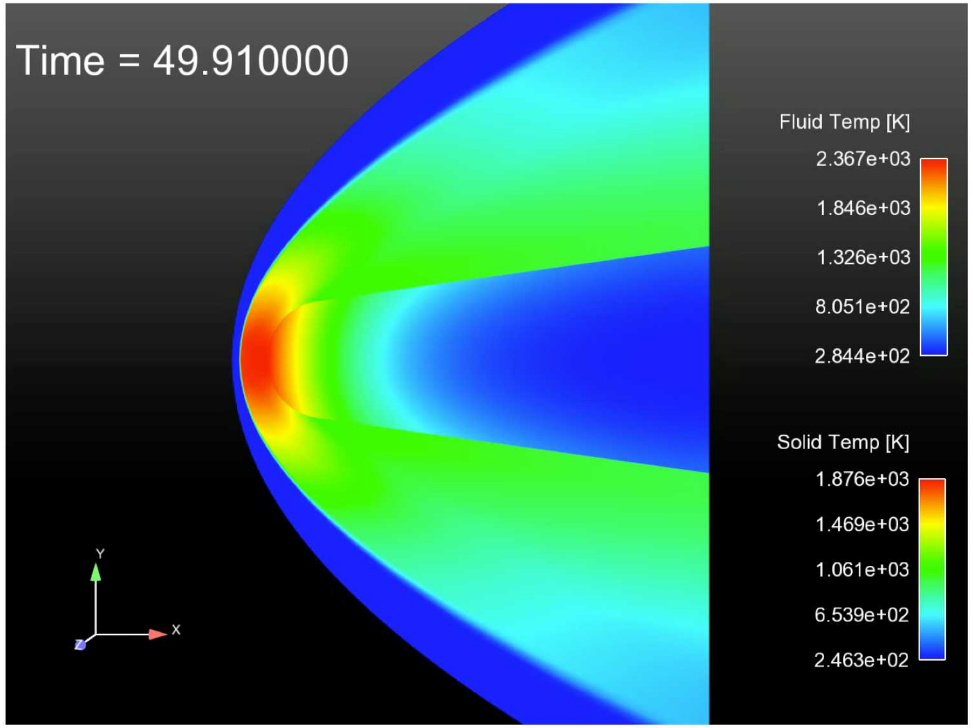




U.S. DEPARTMENT OF ENERGY

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