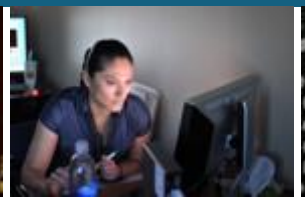
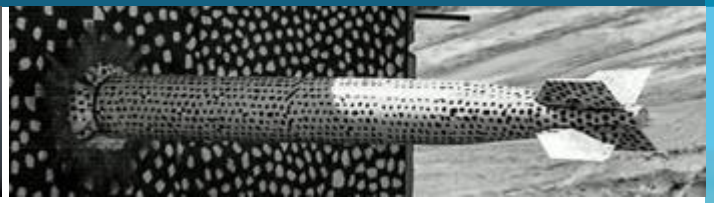
Model Reduction at Sandia National Laboratories


PRESENTED BY

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AIAA SciTech 2021
Jan. 20, 2021
SAND2021-0425C

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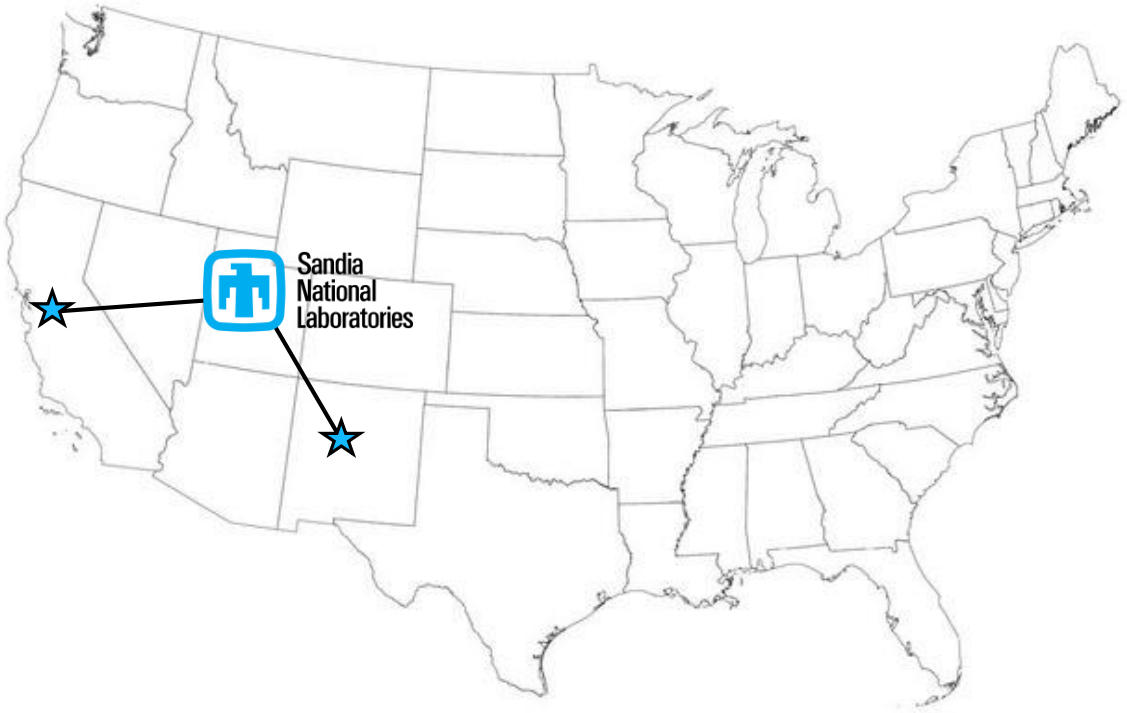
About Sandia National Labs (SNL)

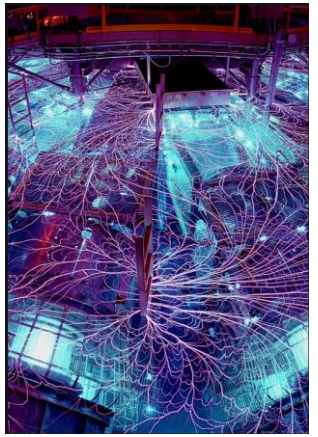


- Sandia is a **multidisciplinary** national lab and Federally Funded Research & Development Center (FFRDC).
- Contractor for the U.S. DOE's National Nuclear Security Administration (**NNSA**).
- **Two main sites**: Albuquerque, NM and Livermore, CA (above).

Sandia's **primary mission** is ensuring the U.S. nuclear arsenal is safe, secure and reliable, and can fully support our nation's deterrence policy.

We have **programs** in the following areas:

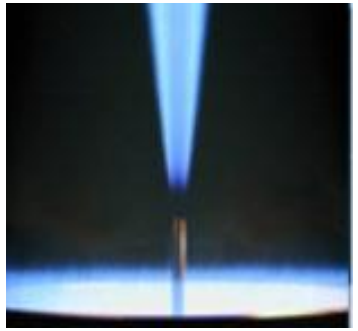
- Nuclear Deterrence
- Defense Nuclear Nonproliferation
- National Security
- Global Security
- Energy & Climate
- Advanced Science & Technology



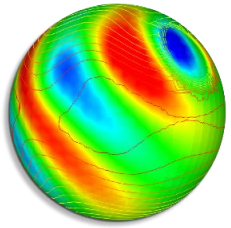
SNL Applications Requiring ROMs

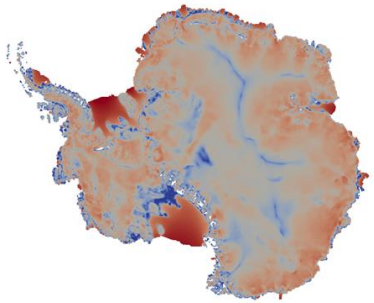
Re-Entry/Captive-Carry Problems

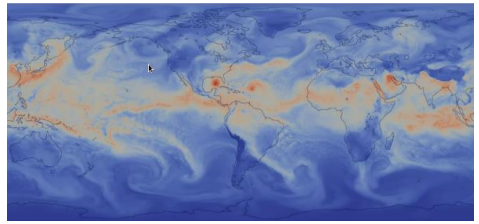
Heat Transfer/Turbulent Combustion



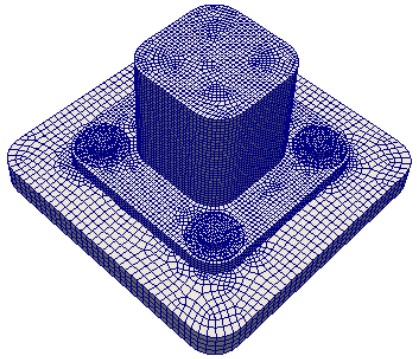
Climate

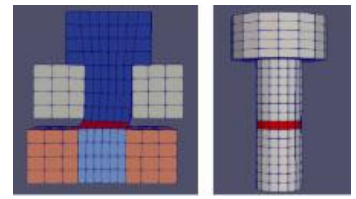




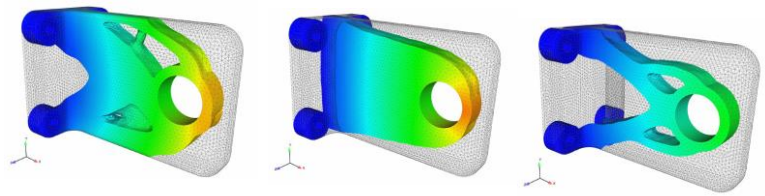


Fastener Modeling





Topology Optimization/ Additive Manufacturing



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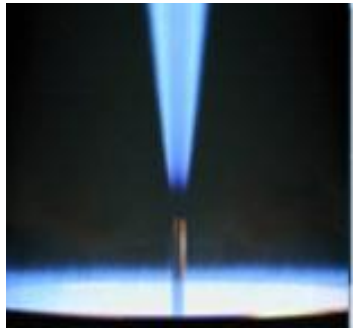
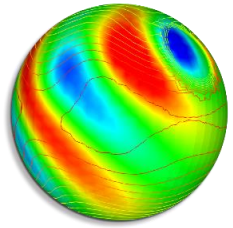
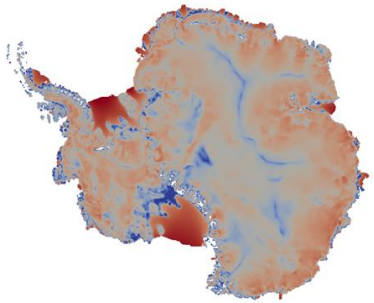
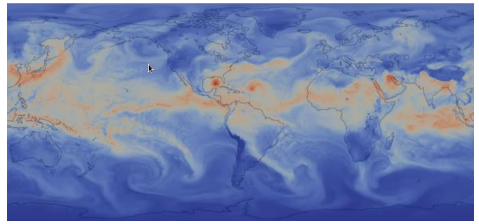


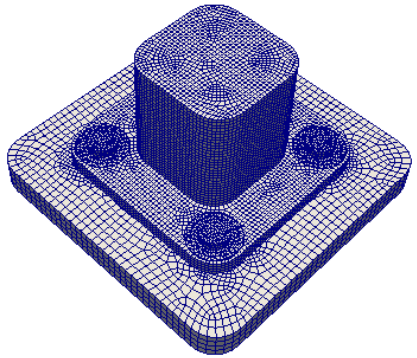
Climate

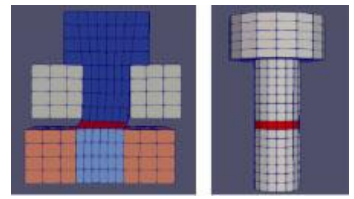




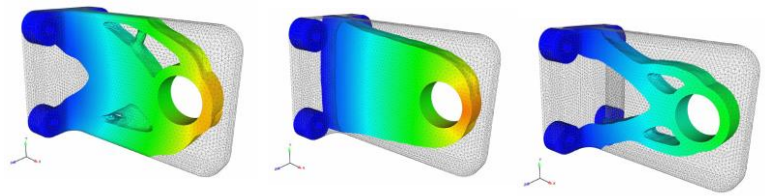


Fastener Modeling





Topology Optimization/ Additive Manufacturing



These are not toy problems that are prevalent in the ROM literature!

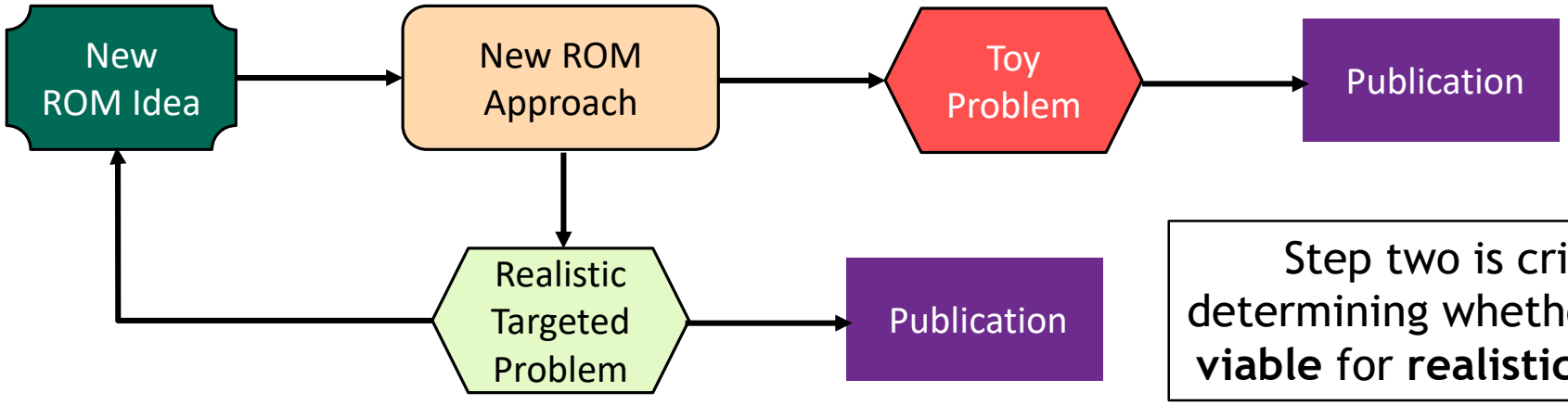
Sandia's ROM Development/Deployment Strategy

Targeted problems present **unique numerical challenges** that you don't run into with toy problems!

(e.g., strong nonlinearities, huge differences scales, turbulence/chaos, multiphysics, multi-D shocks, etc.)

Approach:

- ***Step 1:*** New ideas/methods are first verified/prototyped on **simple benchmarks** (e.g., 1D Burgers).



Step two is critical in determining whether ROMs are **viable** for **realistic problems**!

- ***Step 2:*** Apply methods to targeted **realistic problems** – presents new challenges, requiring new R&D

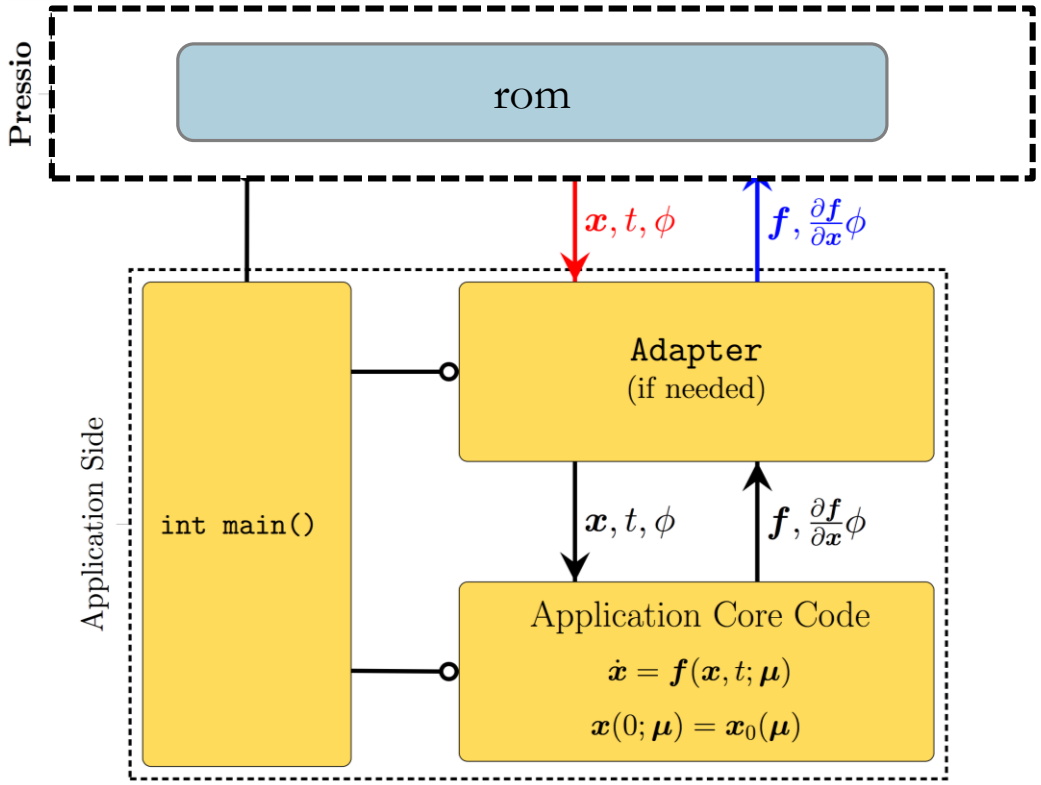
To facilitate step two, we have been developing an **open-source tool** called Pressio

Pressio

An **open-source*** **non-intrusive** computational framework aimed at providing performant projection-based ROMs for generic application codes

Main idea:

- Separate the "application" and the ROM
- ROM methods are contained in the Pressio framework
- Pressio "plugs in" to an application code



Salient features:

- Header-only C++ library
- Supports HPC performance portability via Kokkos
- Supports Python API
- Supports Galerkin, LSPG, and WLS ROMs (with hyper-reduction)
- Pressio's API requires application to expose two main routines: residual and applyJacobian

* https://github.com/Pressio

Advantages:

- Pressio can be used to easily add ROM capabilities to any generic HPC code!
- Methods added to Pressio are at the fingertips of users of HPC codes hooked up to Pressio!

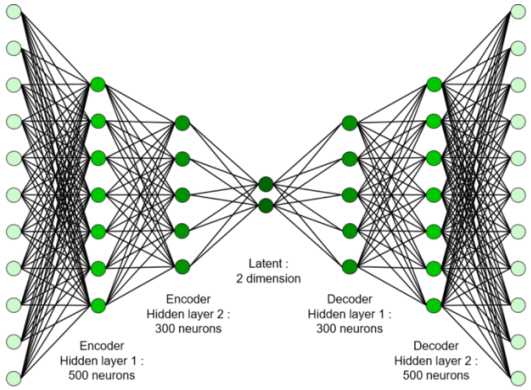
Research Gaps & Directions

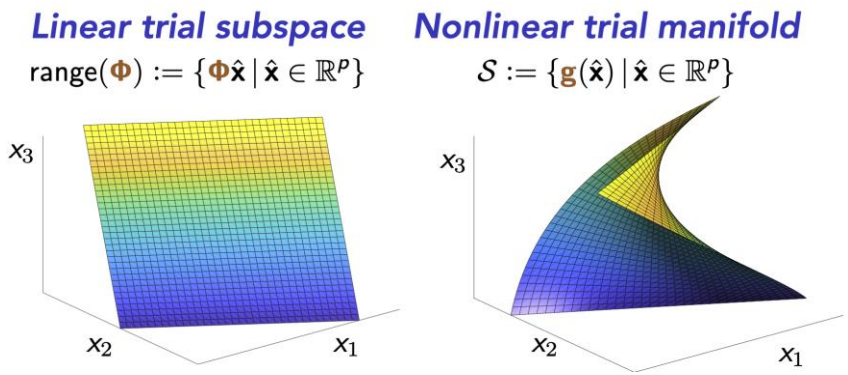
Research Gaps:

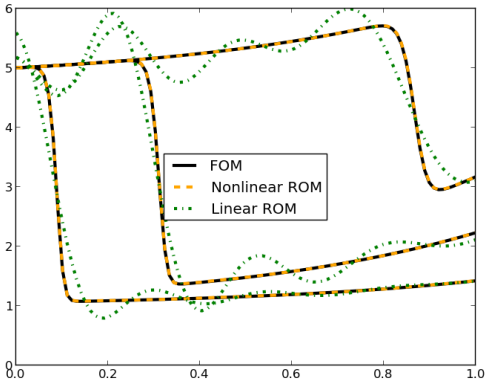
- ROMs with quantified/guaranteed accuracy/robustness in the **predictive regime.**
- ROMs for practical nonlinear multiscale problems exhibiting **shocks**, **chaos**, slow decay of Kolmogorov n-width (**convection-dominated**).
- Relative dearth of ROMs for **compressible flows**.

Current Research Directions at Sandia:

- Windowed least-squares (WLS) ROMs [Parish, Carlberg, 2020; Shimizu, Parish, 2021].
- ROM preconditioners to improve ROM predictability [Fike, Lindsay, Tezaur, Carlberg, 2021].
- Domain decomposed ROMs for networks [Hoang, Choi, Carlberg, 2020].
- Nonlinear manifold ROMs using autoencoders [Lee, Carlberg, 2020].







Suggestions for Benchmarks & ROM Evaluation Strategies

There should be benchmarks that go beyond simple 1D/2D toy problems.

- How to "release"/formulate these is a challenge, as high-fidelity code is likely required.
- Software like Pressio can help bridge the gap between ROM and application developers and give ROM developers access to more realistic problems to test their methods.
- Publishing problem formulations/datasets may help researchers set up more realistic tests in their own codes ("bake-of" problems or "model intercomparison" problems).

It's important to evaluate ROMs in the predictive regime.

- Many researchers/authors never make it past reproductive regime.

In evaluating ROMs, one needs to carefully design relevant QOIs/metrics of success.

- Very application specific – e.g., for compressible flow ROM, analysts care about pressure PSD, not entire solution field.
- While ROMs cannot be expected to reproduce the entire solution field to a specified tolerance for an arbitrarily complex predictive problem, there *is* some hope of a ROM reproducing some relevant QOI.

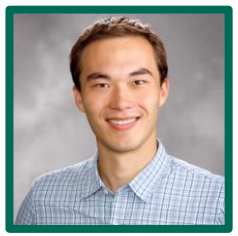
Applying ROM to more **realistic** problems using appropriate **QOIs/metrics** will tell us how **viable** ROMs can be beyond the space of "toy" problems.

Research Team


Marco Arienti


Patrick Blonigan


Victor Brunini


David Ching


Jeff Fike


Chi Hoang


Micah Howard


Kookjin Lee


Samuel Majors


Eric Parish


Flint Pierce


Kevin Potter


Jaideep Ray


Francesco Rizzi


Yuki Shimizu


John Tencer

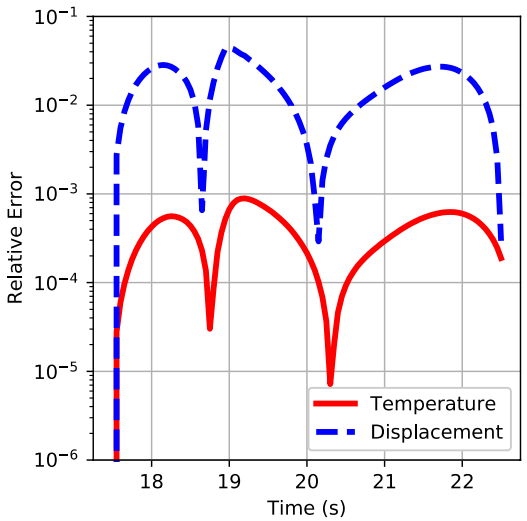

Irina Tezaur

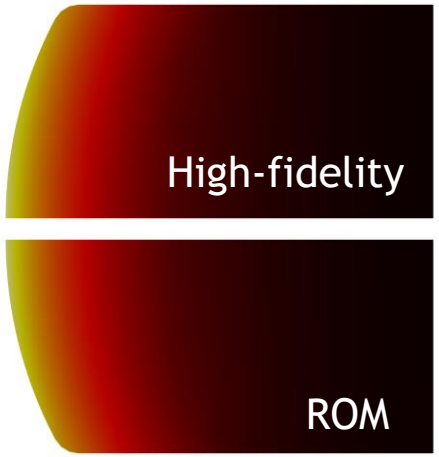

Karen Willcox

Recent ROM Successes at SNL

ROM accelerates **ablation** simulation with SPARC compressible flow solver

- First applications of ROMs to ablation
- Large differences in scales (7 orders of magnitude)
- Iso-q with prescribed axisymmetric heat- and mass-transfer boundary conditions

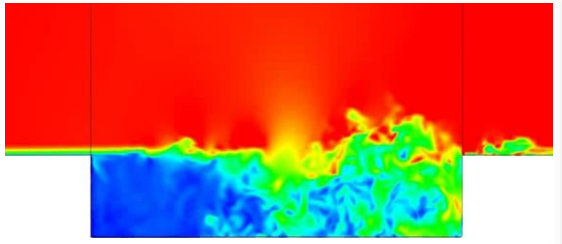


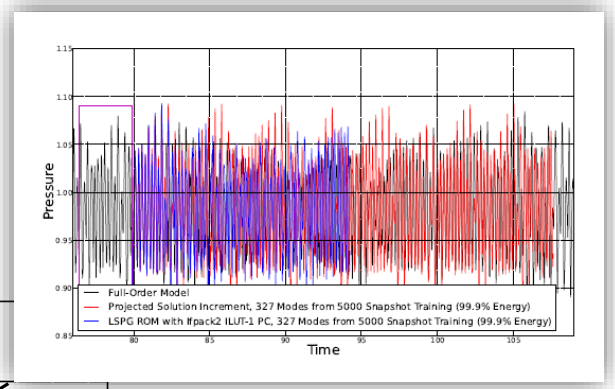


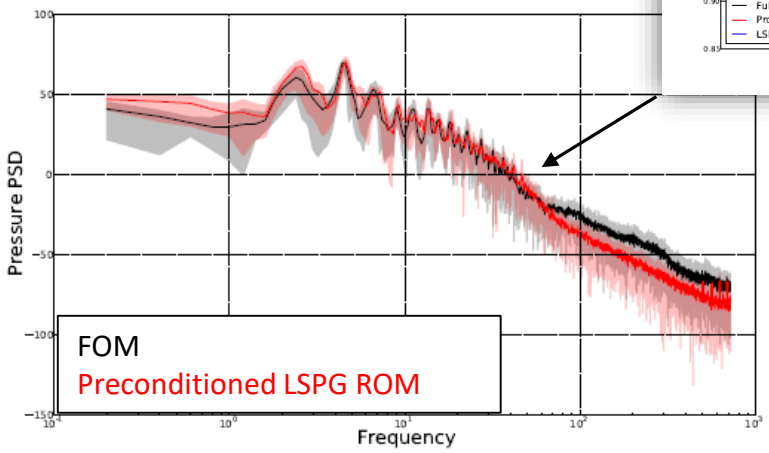
~17x savings in core-hours
<0.1% error in temp, <4% error in disp

Time-predictive preconditioned **captive-carry** ROM in SPARC demonstrated to have sufficiently accurate pressure PSD

- Laminar compressible cavity problem (Ma = 0.6, Re = 3000).
- Primarily interested in prediction in time.



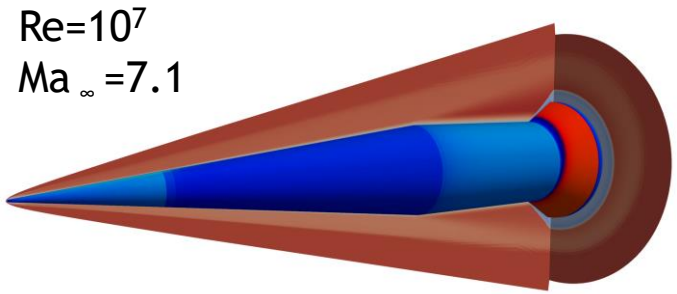




ROM PSD is within FOM PSD range!

Recent ROM Successes at SNL (cont'd)

ROM accelerates **hypersonics** simulation (HiFIRE-1 experiment) using in-house compressible flow solver (SPARC)



- Prediction across param space (Ma, ρ)
- POD-LSPG + Sample Mesh:

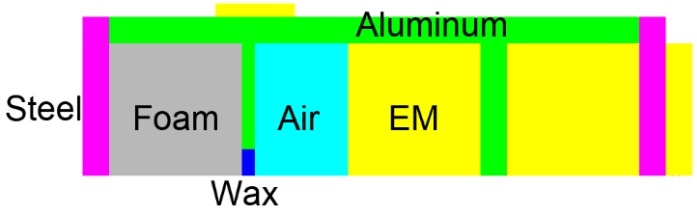
~300-1000x savings in core-hrs
<1% error in density, momentum, energy
~1-2% error in integrated wall heat flux

[Blonigan, Carlberg, Rizzi, Howard, Fike, 2020]

ROM accelerates **transient conduction/thermochemistry** in Aria

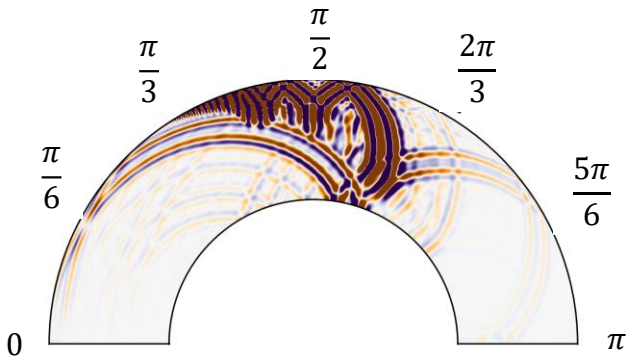
- Transient thermochemistry test
  - Foam decomposition
  - Heat conduction
  - Exothermic chemical reactions

~9000x savings in core-hrs
<1°C error in temp.



ROM accelerates **seismic wave propagation**

- Synthetic seismogram data
- One shot UQ: simultaneous simulation of many trajectories



~950x savings in wall-time
<1% error