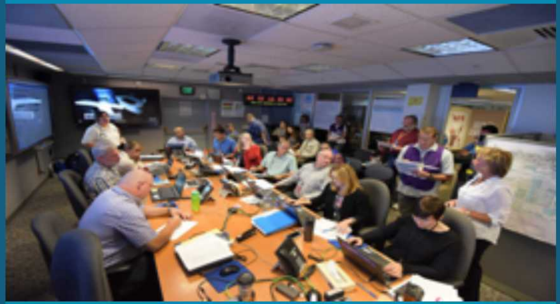
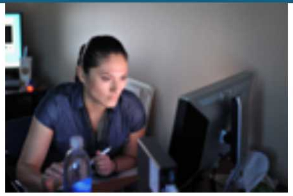
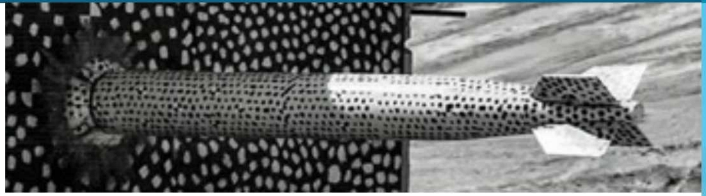
SAND2020-9915PE

Projection-based ROMs at SNL: Where/When?







PRESENTED BY

John Tencer

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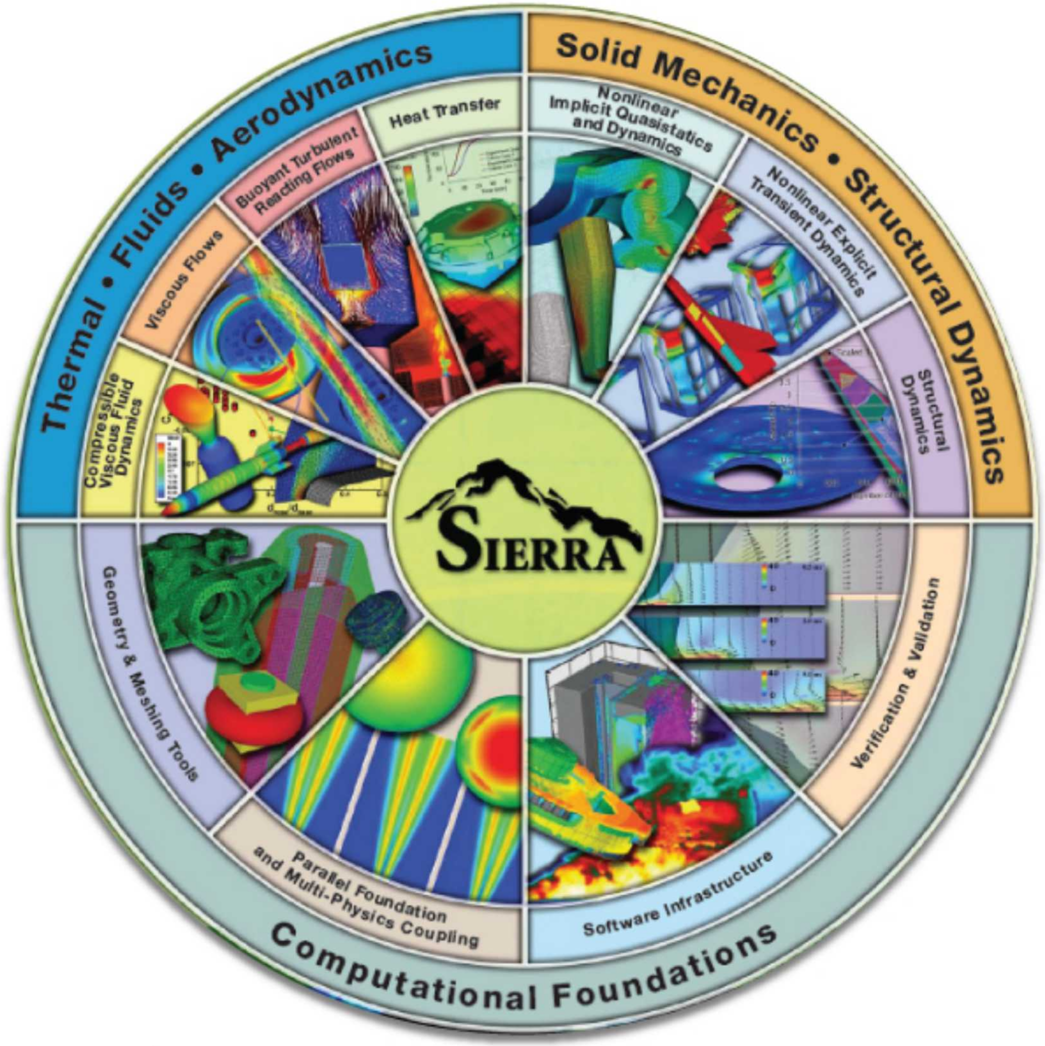
Why would one want to use pROMs?

- Directly tied to a "full-order model"
  - Allows us to **leverage Sandia's suite** of application codes
- pROMs are "physics-based" surrogates
  - Results are **explainable**
  - Evaluating **known dynamics** rather than *learning* unknown dynamics
- Compatible with *a priori* and *a posteriori* error bounds
  - **Quantifying the uncertainty of the pROM is critical** for Sandia's missions
- Enables full-field predictions
  - Useful for engineering design and analysis



RAMSES

ITS SCEPTRE NuGET EIGER EMPHASIS Xyce Charon
CHEETAH Gemma EMPIRE

When are pROMs appropriate?

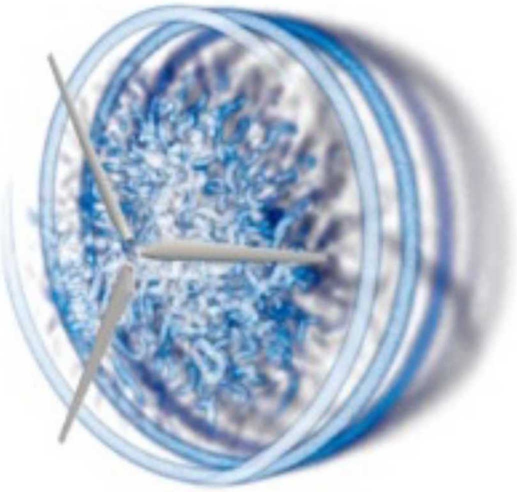
1. Well understood physics
   - The FOM exists, is robust, and is capable of generating training data
2. The full-order model (FOM) is too computationally expensive (but not intractable)
   - Complex, high-fidelity, multiphysics simulations
   - Time critical applications (control)
   - Many-query applications (optimization, uncertainty quantification)
3. FOM is reducible
   - Solution evolves on a low-dimensional manifold

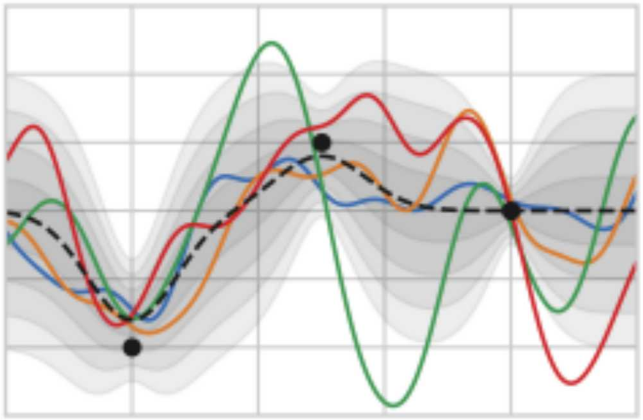
AND either

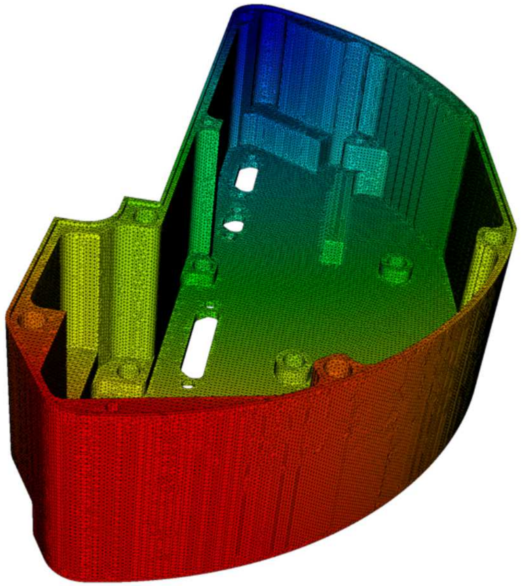
➢ Explainability/Credibility is required

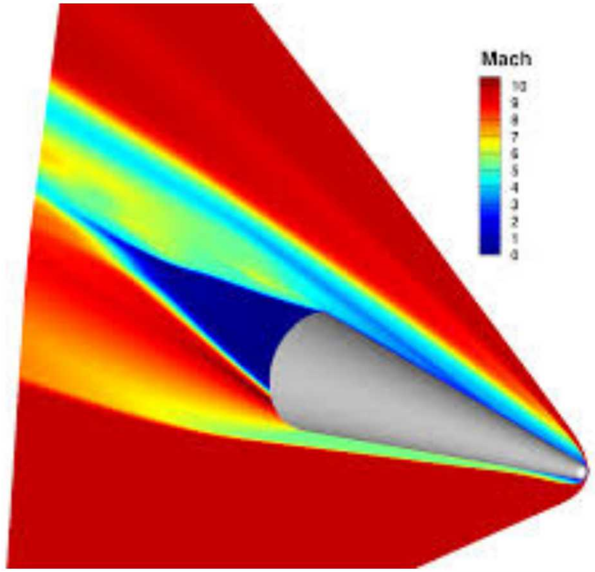
OR

➢ Traditional surrogates fail to achieve accuracy requirements



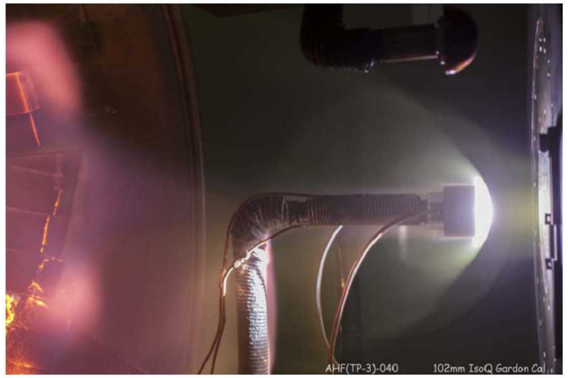


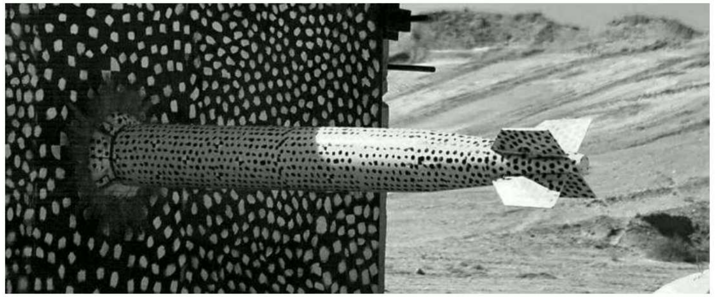


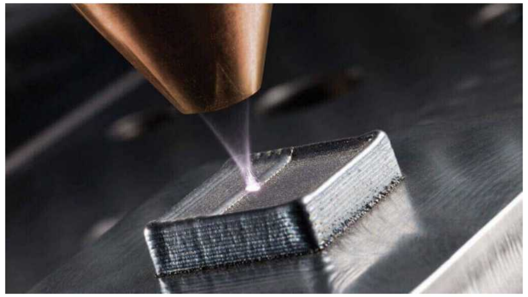


Application Use Cases – current state

- Interfaces implemented for SPARC and ARIA.
- Use cases supported:
  1. conduction/heat transfer (both)
  2. re-entry problems (SPARC)
  3. non-decomposing ablation (SPARC)
  4. Domain decomposed ROMS as applied to network of components (ARIA)
  5. Machine Learning Error Models (SPARC)
- Planned use cases:
  1. Trajectory planning, rapid vehicle design for A4H (SPARC)
  2. Organic matter decomposition, crash and burn scenarios, carbon-phenolic ablators (ARIA/SPARC)
- Areas for growth
  - SD&SM
    - Vibration environments during reentry
    - Buckling and crushing of thin-walled shells
  - Construction of additively manufactured components
  - Rad effects (RAMSES)
  - Hydrodynamics



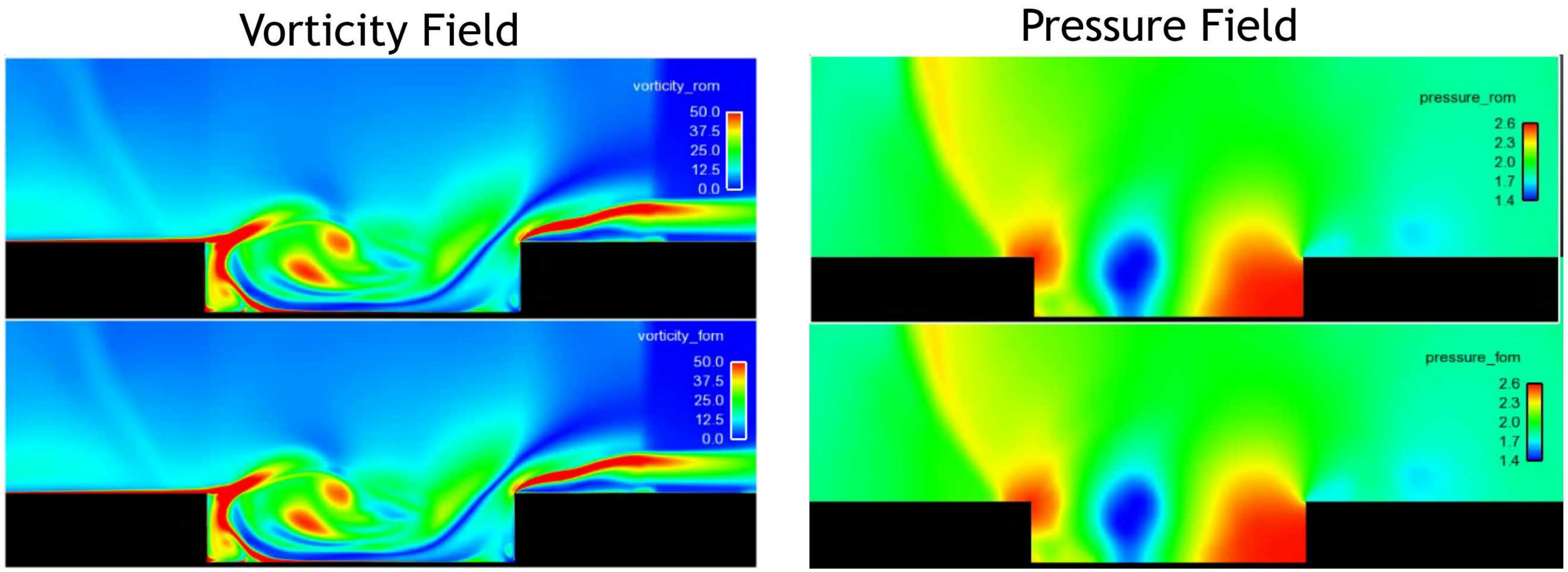




Our baseline approach achieves high accuracy at a low cost for captive carry application

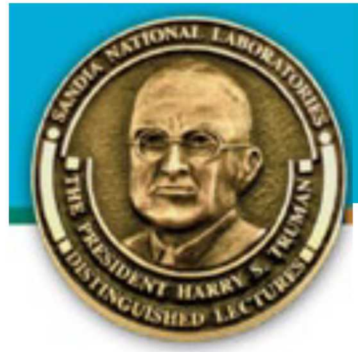
pROM
- 32 min, 2 cores

High-fidelity
- 5 hours, 48 cores



229x savings in core-hours

< 1% error in time-averaged drag



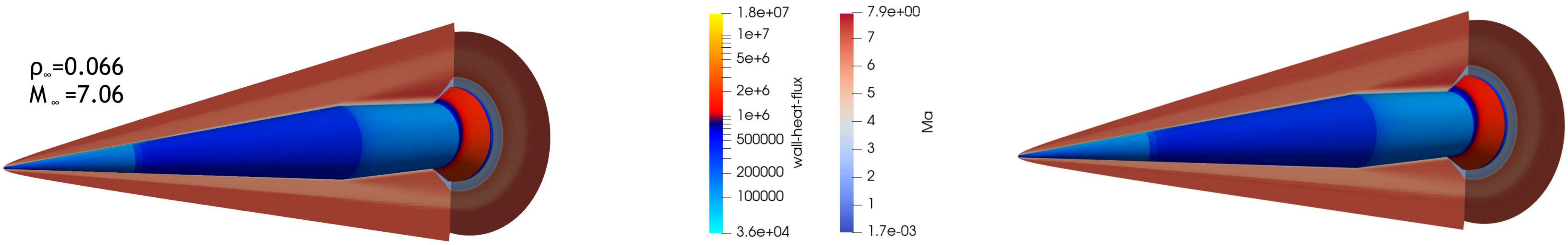
[Carlberg, Barone, Antil, 2017]

pROM accelerates hypersonics simulation with SPARC

- HiFIRE-1 experiment. Baseline case: Re=10^7, Ma=7.1, AoA=2° .
- Training data set: 24 simulation results sampled over a range of freestream conditions:
  - Density: 0.056 to 0.070 kg/m^3
  - Mach number: 5.7 to 7.1
- Initial guess computed by inverse distance interpolation.

High-fidelity: 128 MPI ranks, ~2,500-5,000 seconds

pROM: 16 MPI ranks, ~30-55 seconds



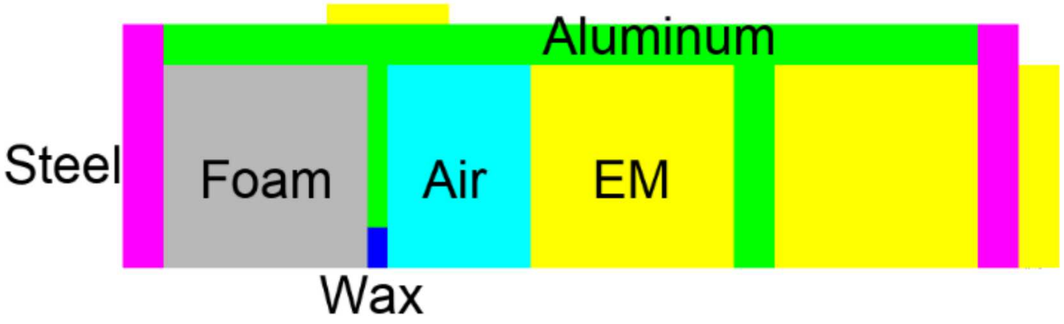
~300-1,000x savings in core–hours
< 1% error in density, momentum, and energy fields
~ 1-2% error in integrated wall heat flux

LDRD
Laboratory Directed Research and Development

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

pROM accelerates transient conduction/thermochemistry with Aria

- Aria transient thermochemistry test
  - Foam decomposition
  - Heat conduction
  - Exothermic chemical reactions



High-fidelity: 144 MPI ranks, ~450 seconds

pROM: 1 MPI rank, ~7 seconds

LDRD
Laboratory Directed Research and Development

ASC

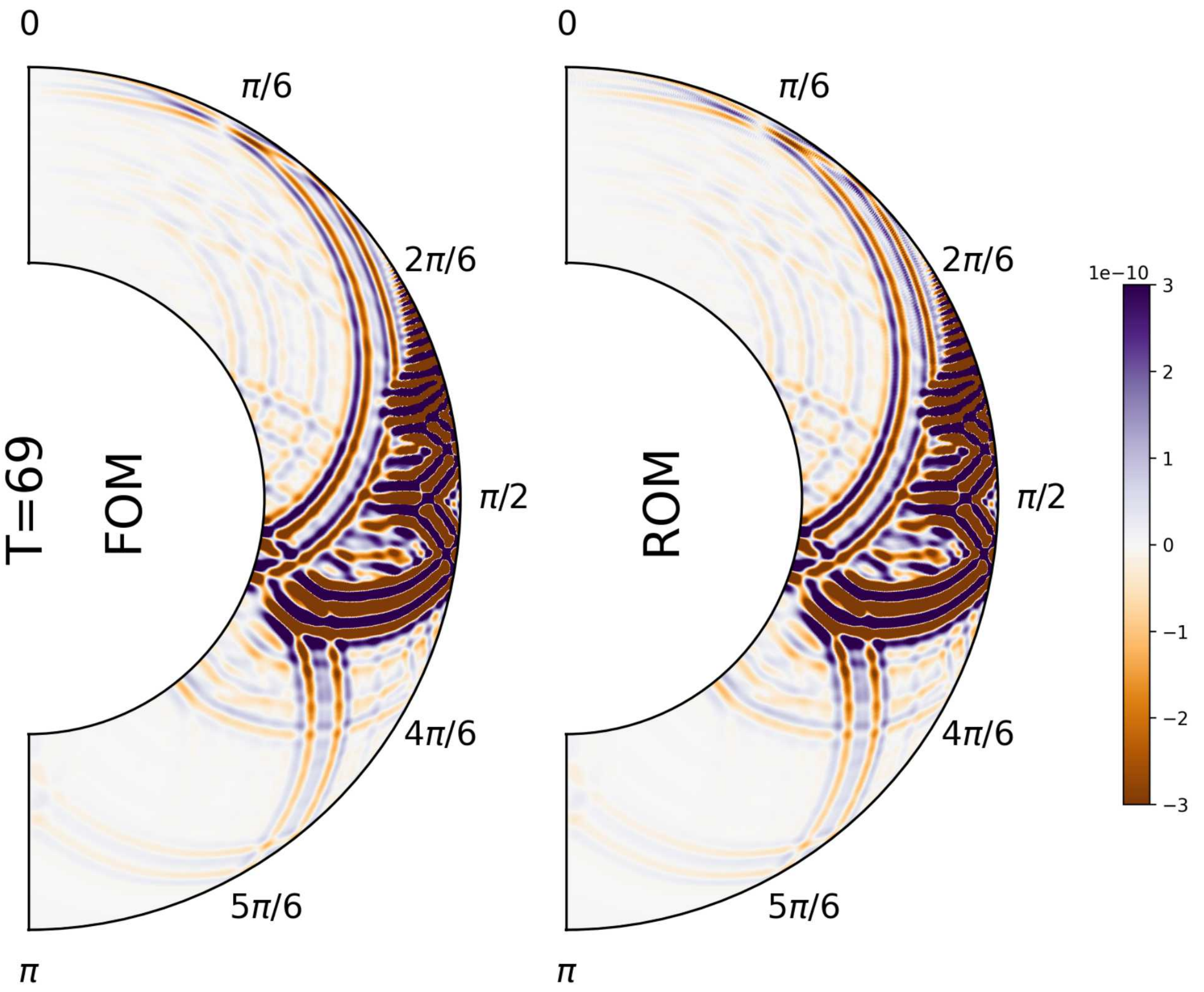
~9,000x savings in core–hours
< 1°C error in temperature anywhere in domain

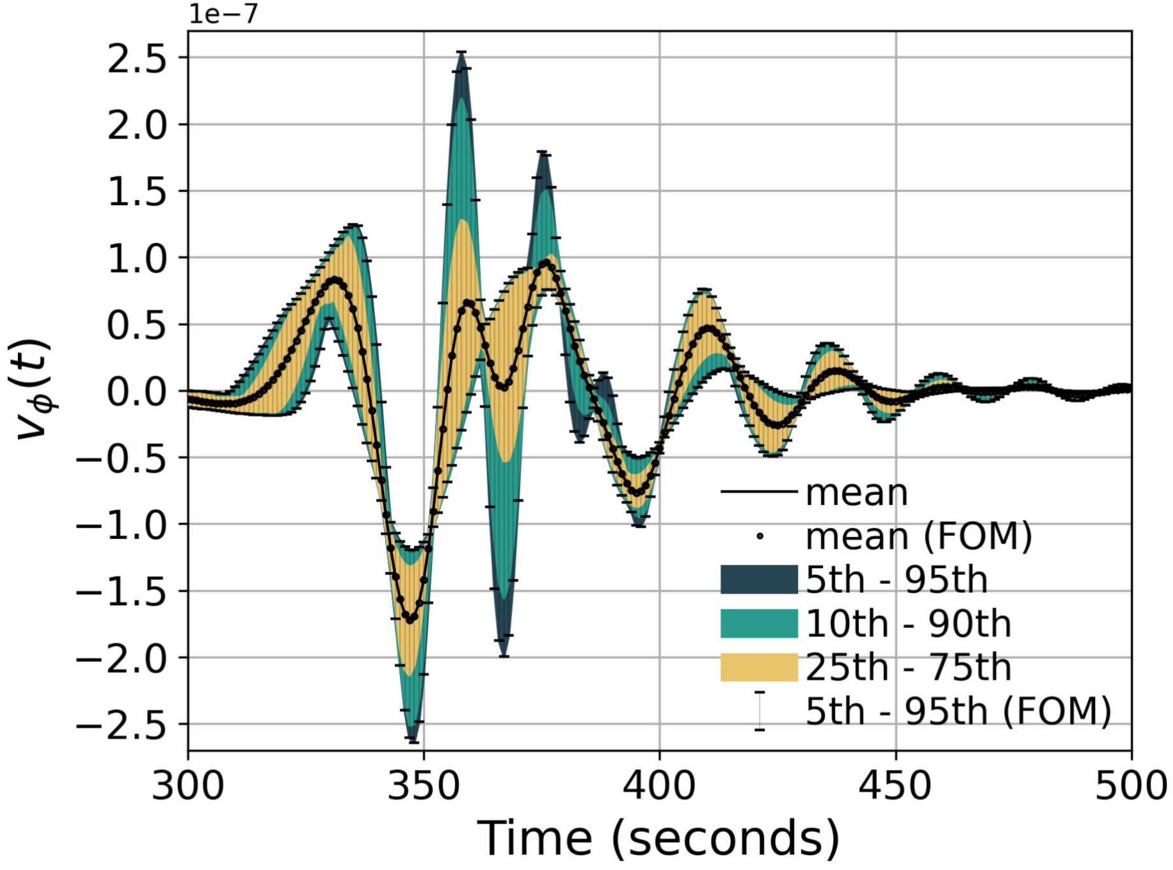
pROM accelerates seismic wave propagation

- Synthetic seismogram data
- Simultaneous simulation of many trajectories

~950x savings in wall time

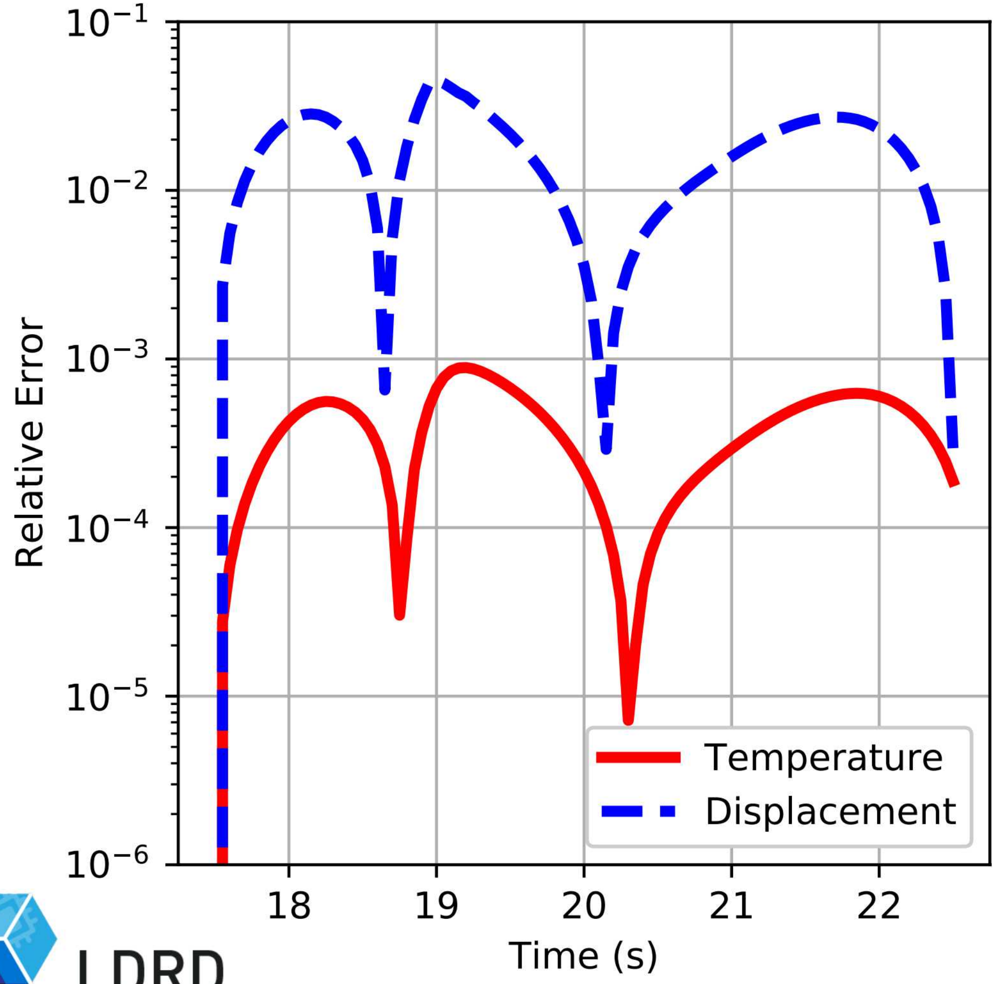
< 1% error in state prediction



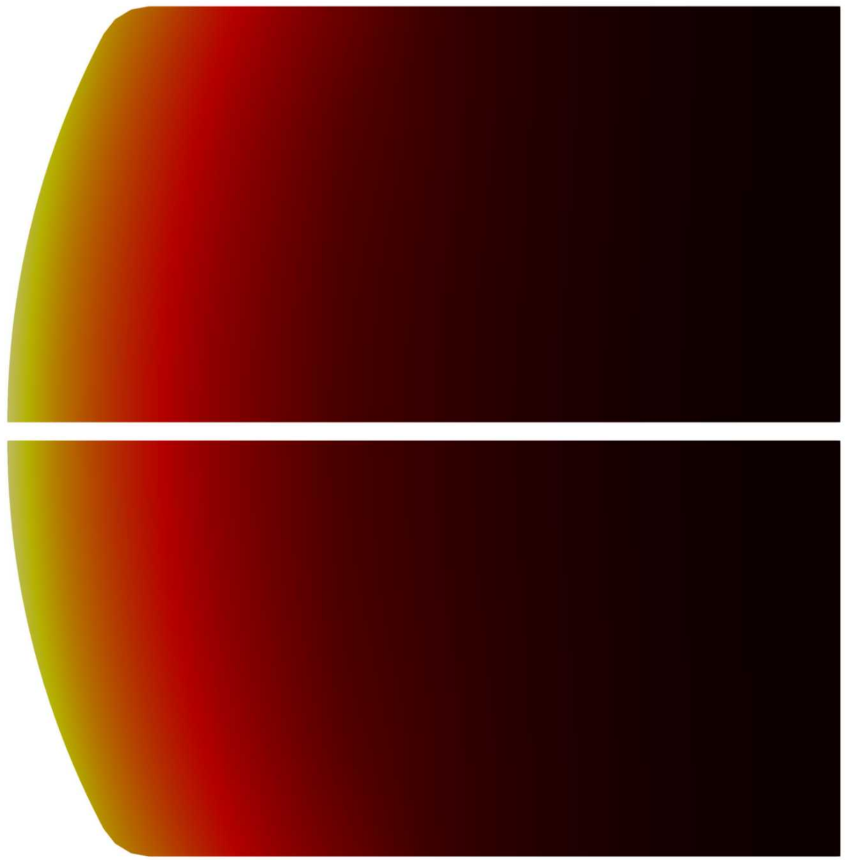


pROM accelerates ablation simulation with SPARC

- iso-q with prescribed axisymmetric heat- and mass-transfer boundary conditions



High-fidelity
52.6 s



pROM
3.1 s

~17x savings in core–hours
< 0.1% relative error in temperature
< 4% relative error in displacement

Transition to Patrick

pROMs are *intrusive*. That comes with benefits (accuracy, credibility) but also drawbacks (can't treat application code as a black box).

- Potentially requires modifications to the application to expose necessary data structures and functions
- Need buy-in and support from application developers

Previously, this has involved adding ROM capabilities to each application code

- Not sustainable
- Inefficient use of code development efforts

Pressio development has enabled rapid roll out of pROM capabilities to new applications (<1 year from start to results)

Patrick will explain