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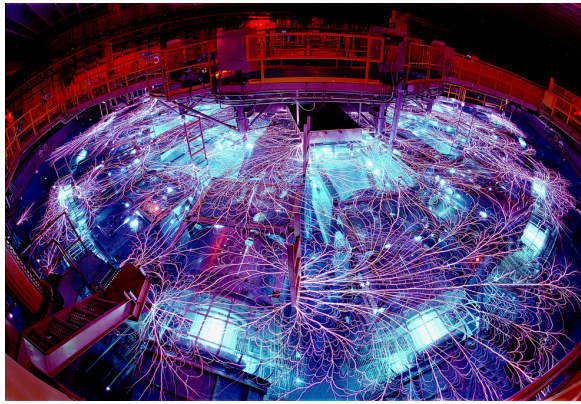

Nonlinear Reduced-Order Models in an Unsteady Compressible CFD Code

J.A. Fike, M.F. Barone, I.K. Tezaur, K.T. Carlberg, M. Howard, and S. Arunajatesan

Sandia National Laboratories

November 19, 2015

U.S. DEPARTMENT OF ENERGY | NNSA National Nuclear Security Administration

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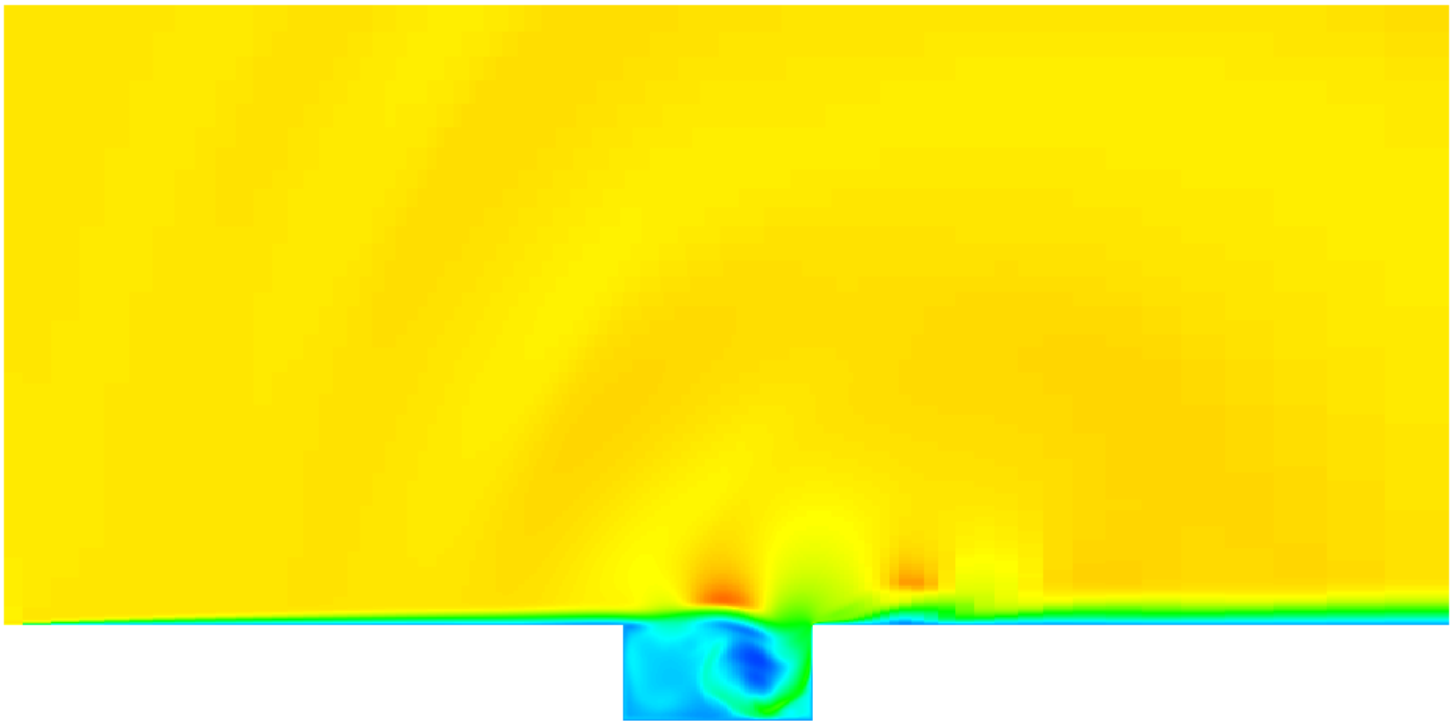
Motivating Example

Perform Uncertainty Quantification (UQ) for complex fluid dynamics problems, such as transonic viscous flow past a cavity



Determine effect of Mach number and Reynolds number on pressure fluctuations inside and outside the cavity.

Challenges

Flow of interest is chaotic in nature

- Interested in statistical output
  - Spectrum of pressure fluctuations at various locations
- Requires simulation over long time intervals
  - High-fidelity simulations may take on the order of weeks using several thousand processors

Interested in performing Uncertainty Quantification

- Quantify effect of uncertainties in Mach number or Reynolds number on the pressure fluctuations at locations inside and outside the cavity
- Sampling based UQ methods require very many simulations
  - Computational cost can be prohibitively high when using high-fidelity simulations

Reduced-Order Modeling

Reduce computational cost of UQ by using a Reduced-Order Model as a surrogate for the high-fidelity simulation, while maintaining a sufficient level of accuracy

Requirements for ROM:

- ROM must accurately replicate the statistical output of the full-order model (FOM), i.e. pressure spectrum
- ROM must have sufficient stability to allow for simulations over long time intervals
- Computational cost of ROM should be sufficiently lower than FOM, i.e. at least a 100x decrease
- ROM should be robust with respect to training data
  - Mach numbers and Reynolds numbers not in training data
  - Time integration beyond training data collection

Reduced-Order Model Implementation

Implement ROMs using discrete projection [GNAT, Carlberg et al. 2013]

- Have also investigated ROMs using continuous projection

  [Kalashnikova et al. 2014]

Currently implementing nonlinear Reduced-Order Modeling capabilities in an in-house Sandia CFD code, SPARC

- Parallel, structured, cell-centered, finite-volume CFD code
- Being developed for Next-Generation Platforms
- Investigate feasibility of ROMs for problems of interest
- Use as a testbed for ROM research

Reduced-Order Model Implementation in SPARC

Create Reduced-Order Models by computing a set of modes and modifying the flow solver to compute the coefficients of these modes.

Reduced-Order Model Implementation in SPARC

Create Reduced-Order Models by computing a set of modes and modifying the flow solver to compute the coefficients of these modes.

- Run the full-order model (FOM) to generate snapshots of the flow field
- Use this snapshot data to compute a set of modes, Φ, using Proper Orthogonal Decomposition (POD)
  - Keep enough modes to capture most of the energy of the flow
- The flow solution can then be approximated as:

$$y \approx \tilde{y} = \bar{y} + \Phi\hat{y}$$

- The flow solver is then used to solve for the values of $\hat{y}$

Reduced-Order Model Implementation in SPARC

ROM implementation in SPARC uses packages from `Trilinos` for parallel scalability

- Tpetra for parallel vector and matrix storage
- Direct or iterative linear solvers using Amesos2 or Belos

Computing POD basis is also done in parallel using Anasazi and RBGen from `Trilinos`

- Can construct a single basis for all flow variables, or separate bases for each variable
- Can choose to subtract a base flow from the snapshots
  - Mean flow field
  - First snapshot
  - Previous snapshot
- Can choose to non-dimensionalize the snapshots

Implicit Time Integration

In an implicit CFD code we solve for the update to the flow solution:

$$\mathbf{A}(y)\Delta y = -\mathbf{b}(y)$$

$$y^k = y^{k-1} + \Delta y$$

The corresponding solution for the ROM would be:

$$\Psi^T \mathbf{A}(\bar{y} + \Phi\hat{y})\Phi\Delta\hat{y} = -\Psi^T \mathbf{b}(\bar{y} + \Phi\hat{y})$$

$$\hat{y}^k = \hat{y}^{k-1} + \Delta\hat{y}$$

- Galerkin Projection: $\Psi = \Phi$
- Petrov-Galerkin Projection: $\Psi = \mathbf{A}\Phi$

Hyper-Reduction

Despite the reduction in the number of unknowns being solved for, the ROM discussed so far does not show a reduction in computational cost

- The residual and Jacobian are evaluated at every cell in the mesh

To reduce the computational cost we use a hyper-reduction technique in which the residual and Jacobian are only evaluated on a subset of the full mesh

- Example sample mesh

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- Example sample mesh

Comparison between FOM and ROM with 100 modes

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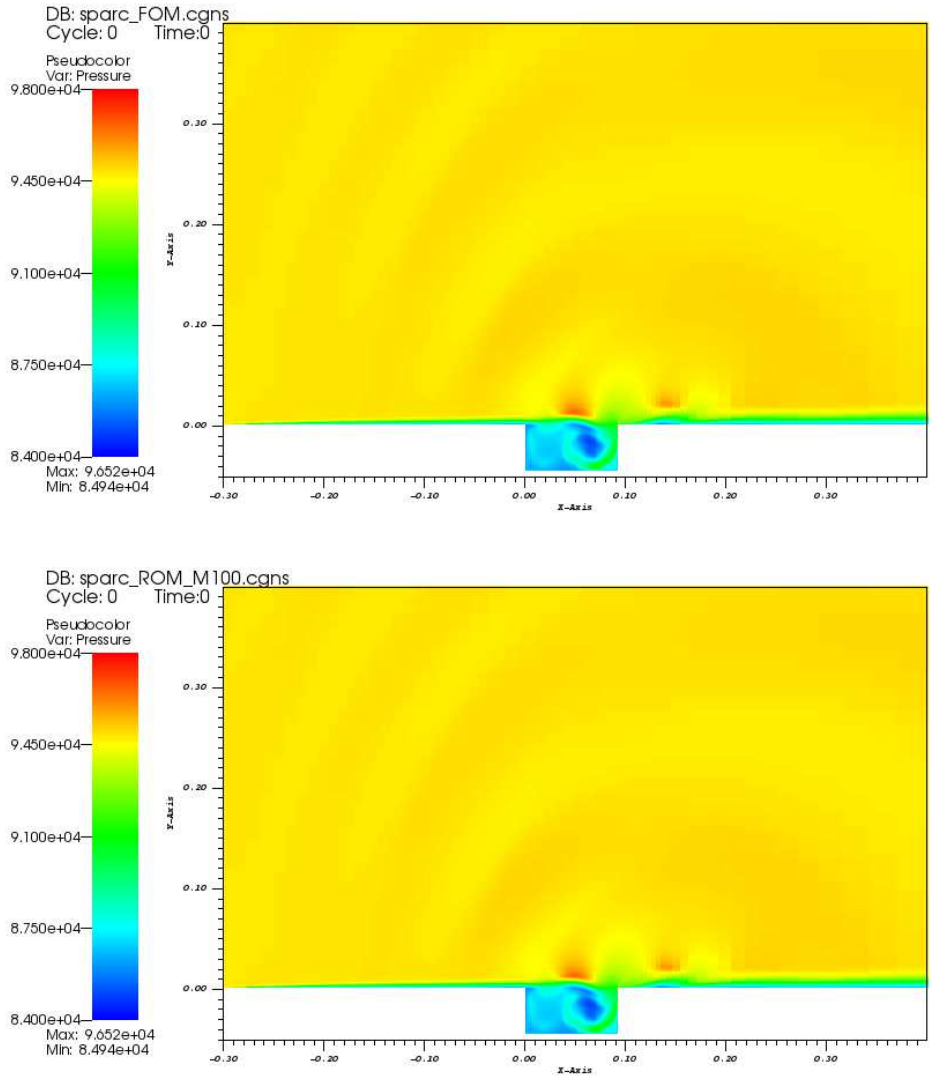

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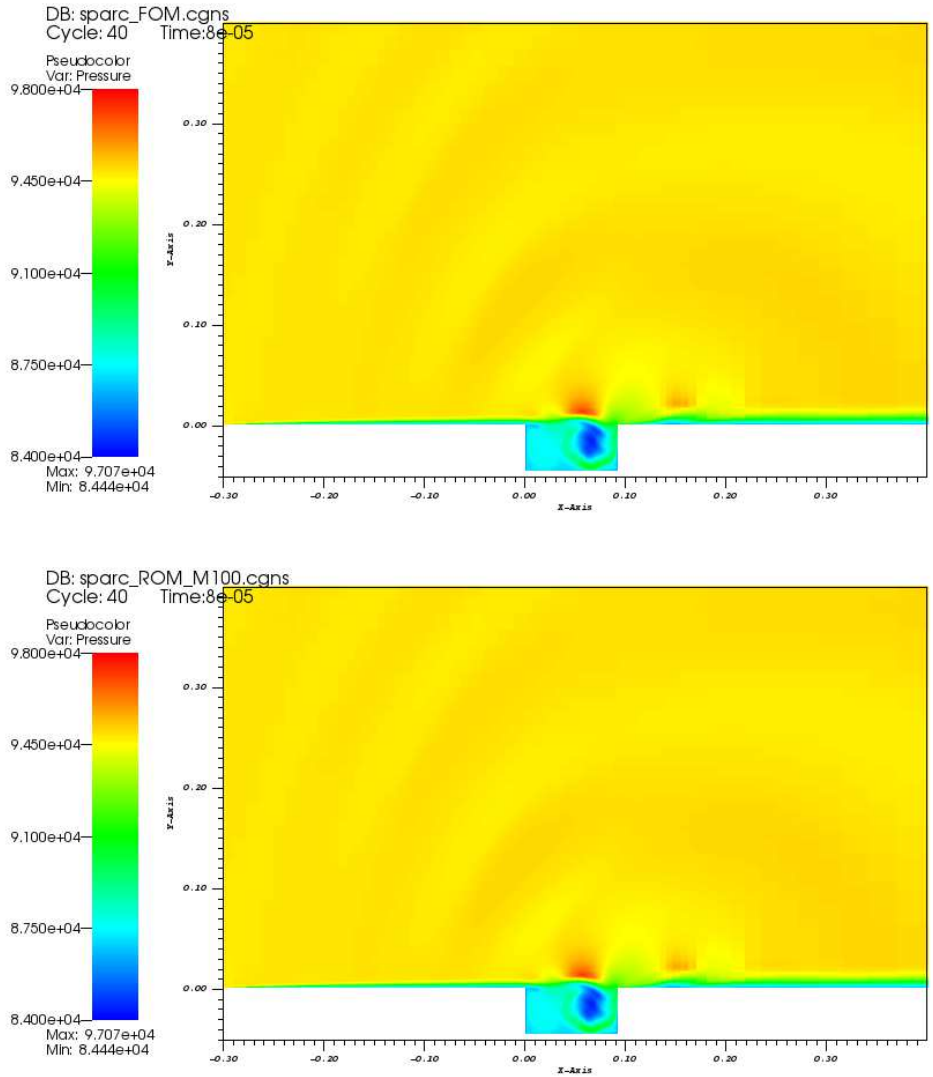

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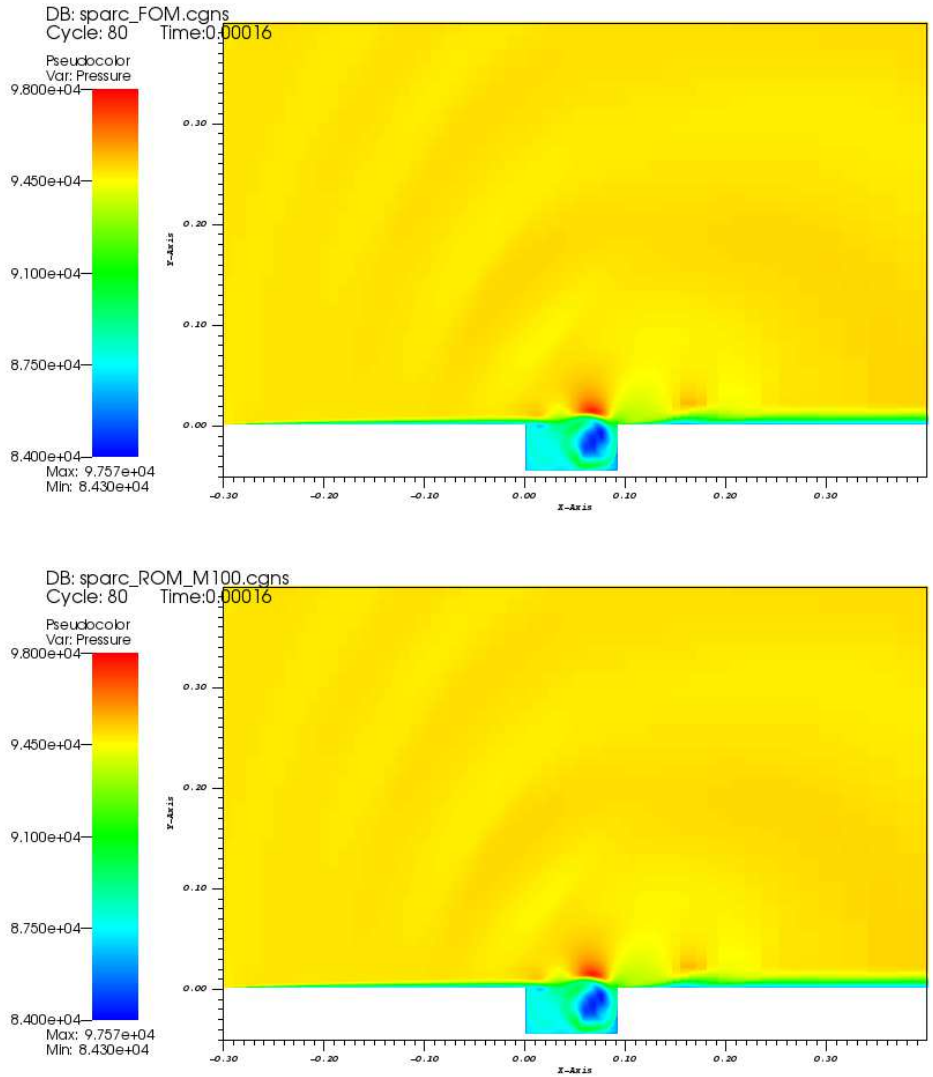

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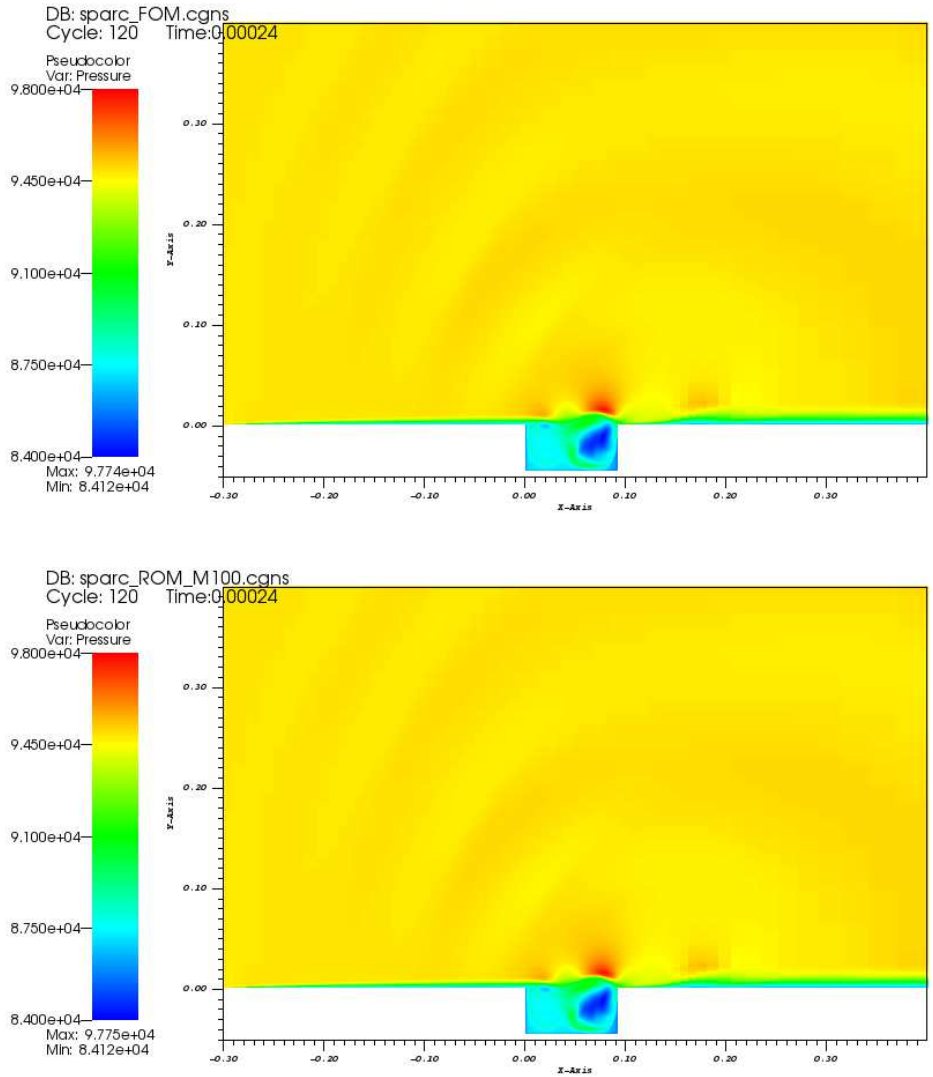

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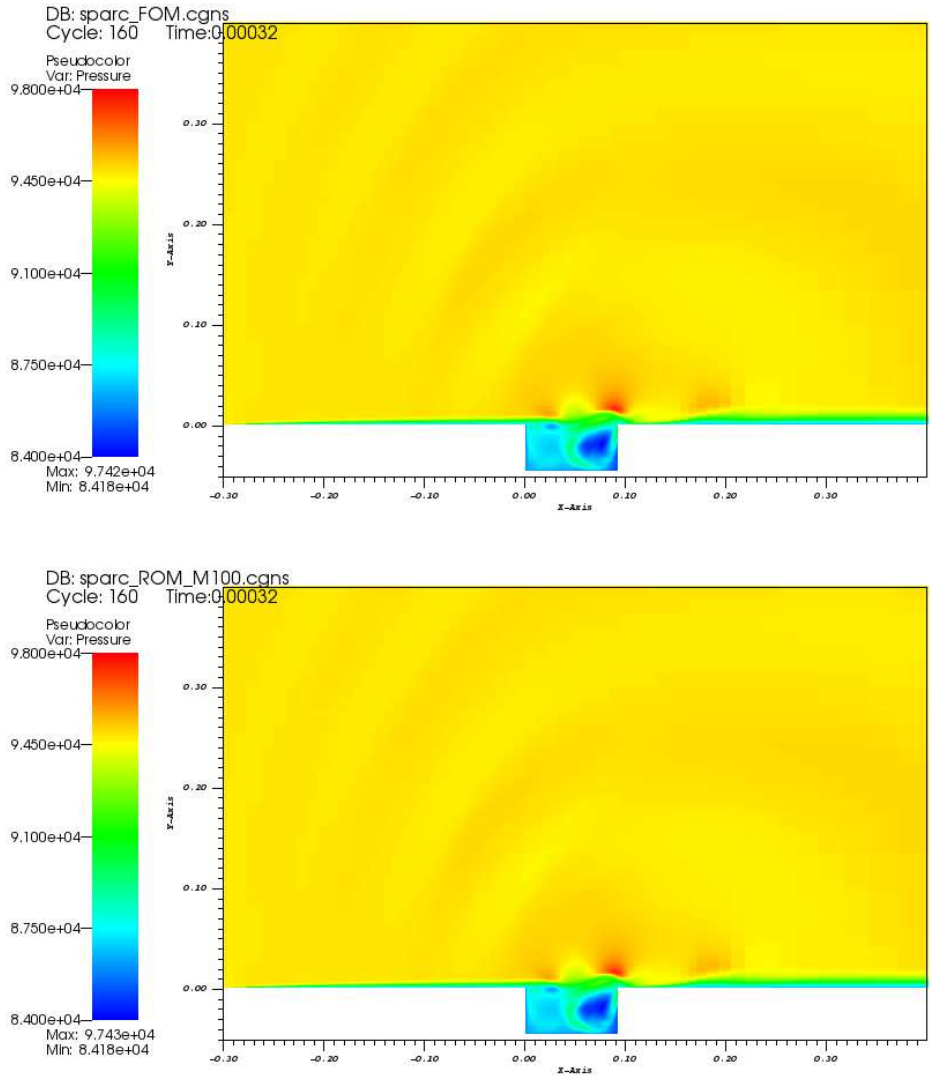

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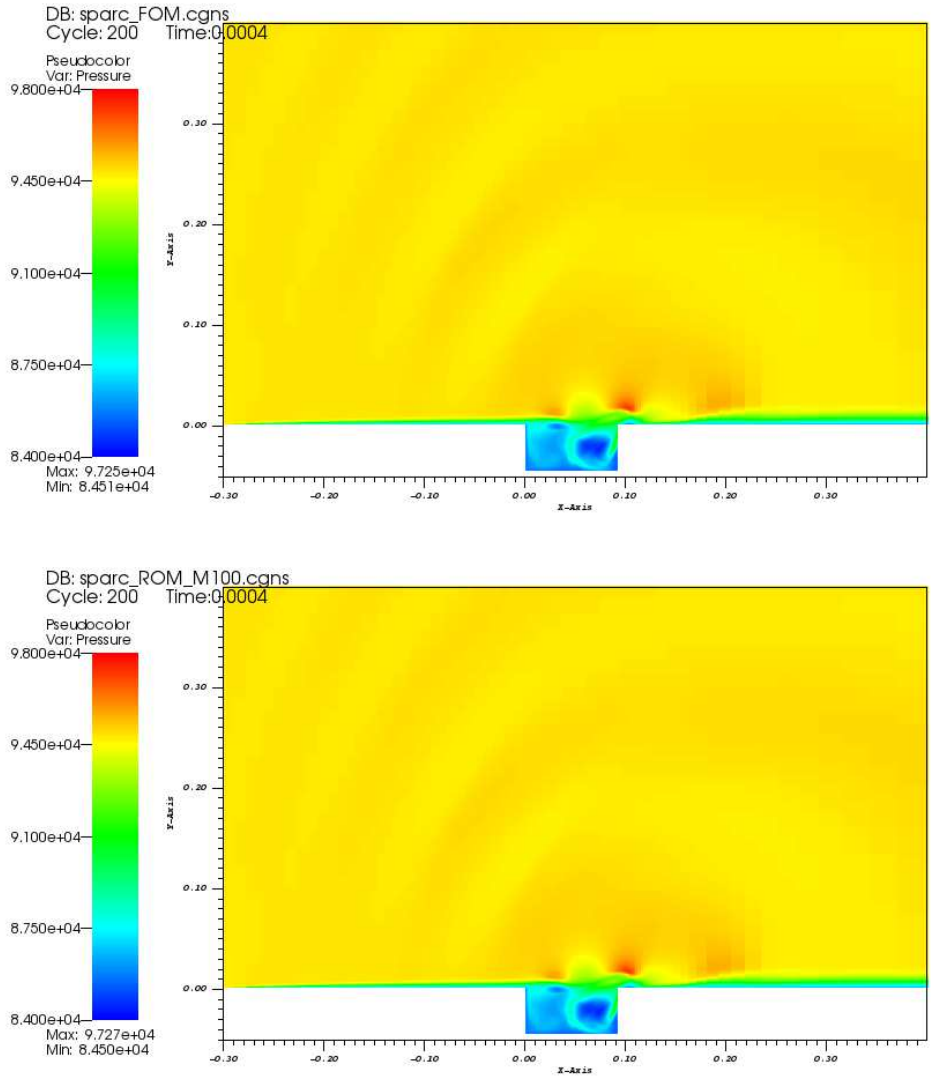

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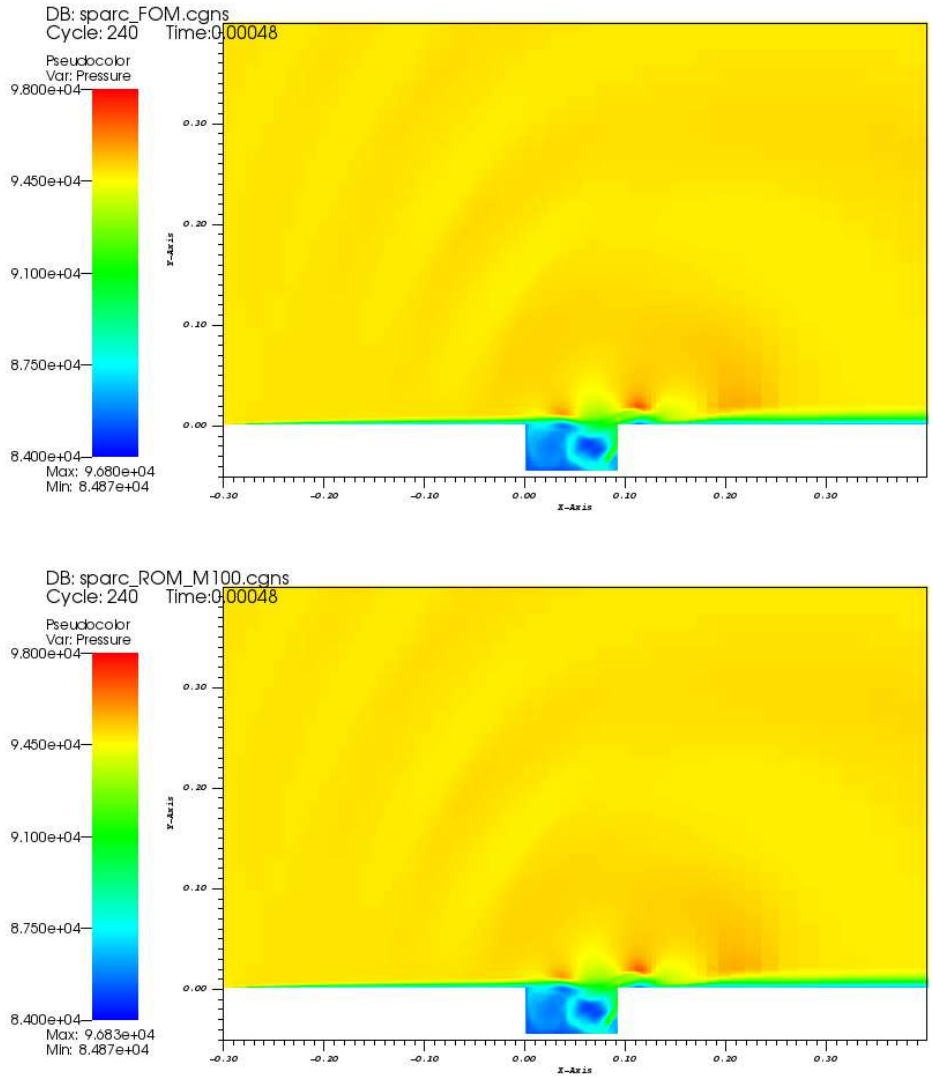

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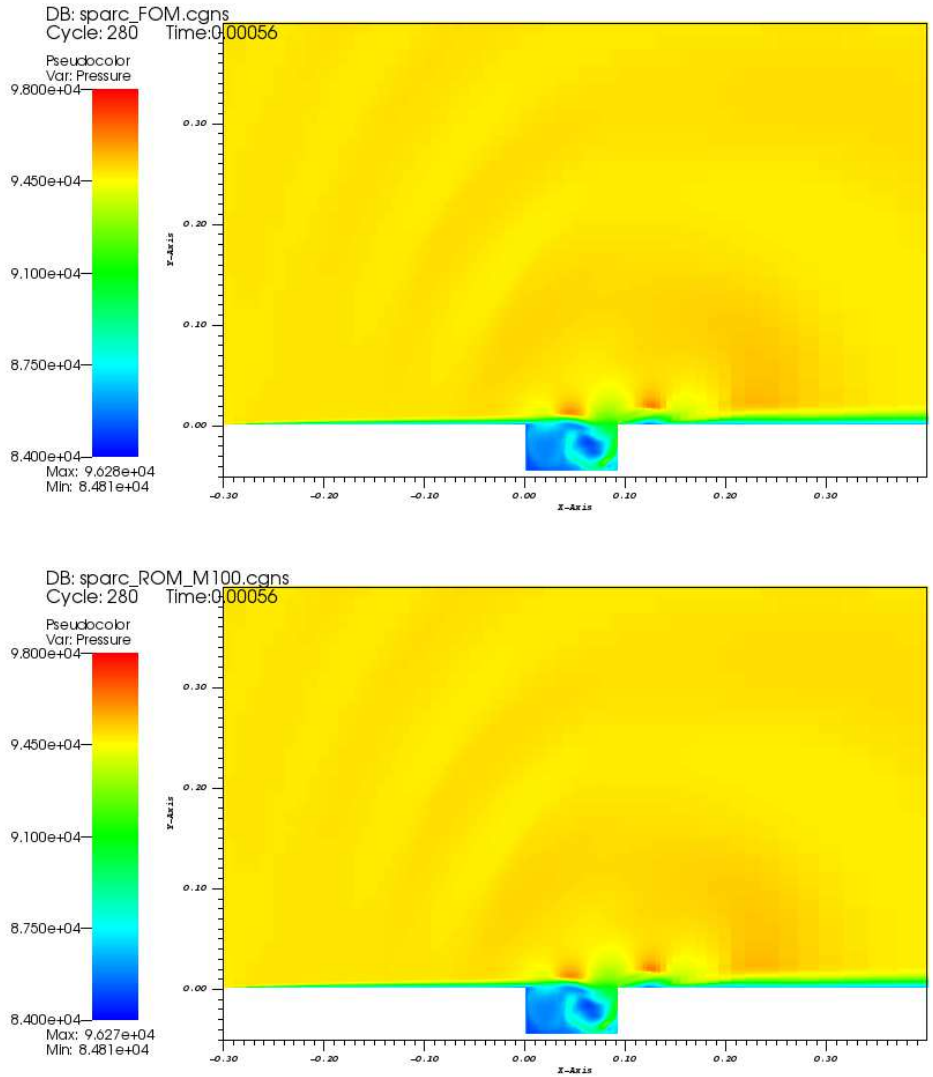

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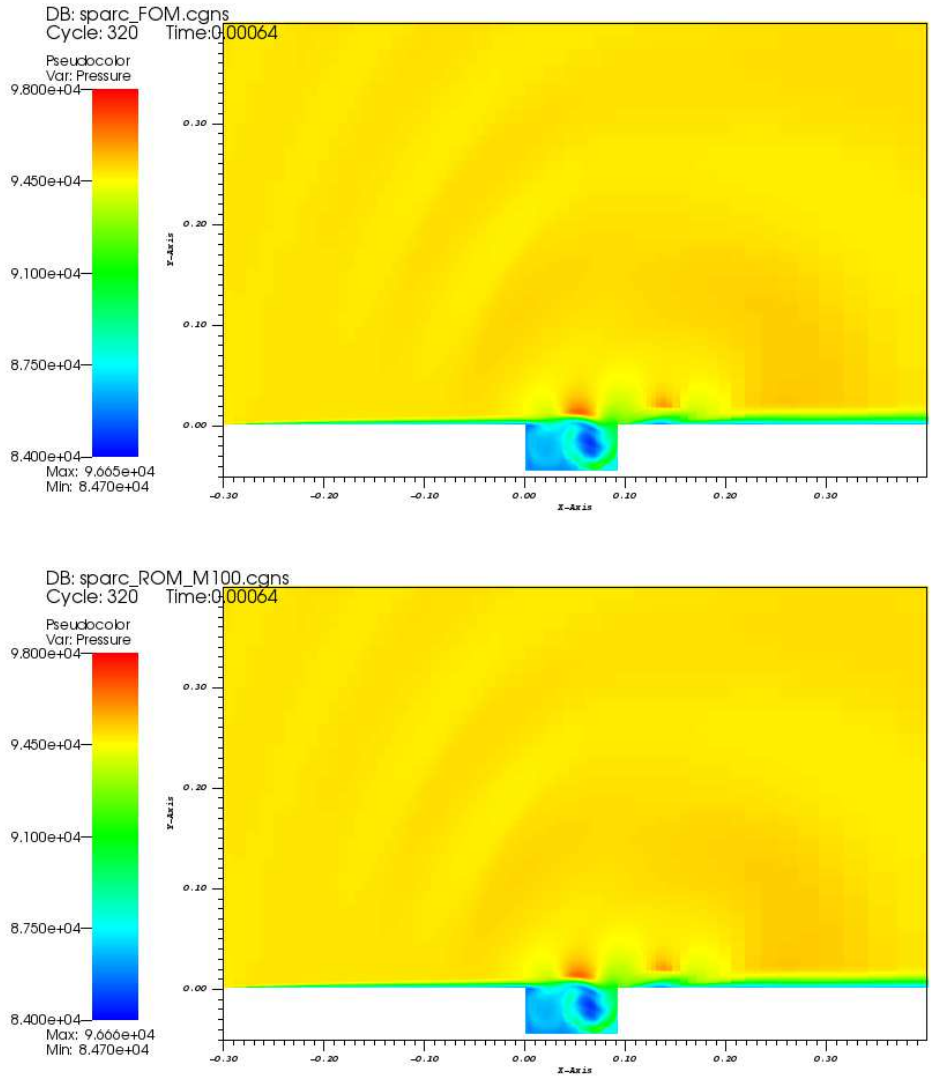

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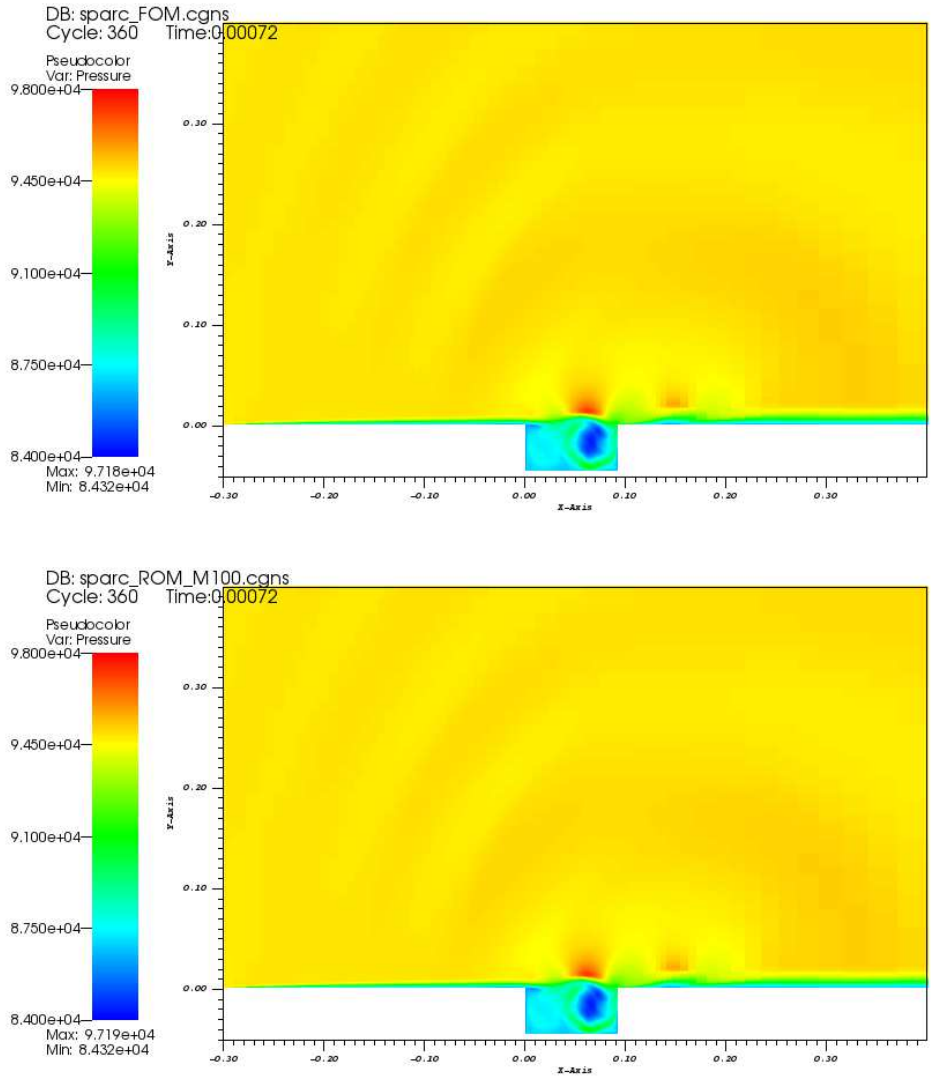

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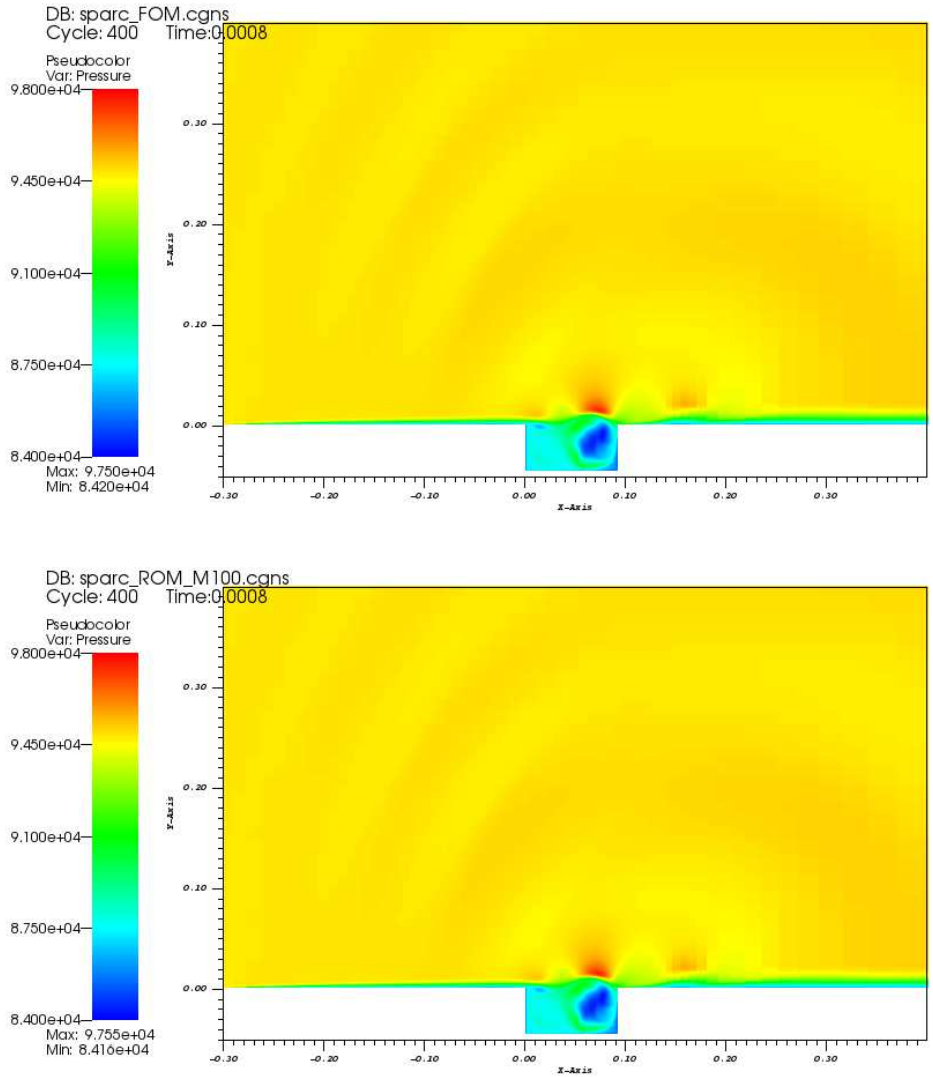

Current Status

ROM implementation in SPARC is currently in progress

- Implemented ROMs for explicit and implicit time integration
  - Currently testing ability to reproduce the snapshots
  - Preliminary results are promising
  - There may be some stability issues to resolve when using a truncated basis and integrating over long time periods
- Current implementation solves the normal equations
  - Investigating use of nonlinear least squares solver
- Preliminary implementation of hyper-reduction using collocation
  - Currently trying to improve computational efficiency of this implementation
  - Investigating other hyper-reduction techniques

Future Work

ROM implementation in SPARC will be used as a testbed for research on improving the stability and accuracy of ROMs for compressible, viscous flows

- Investigating modification of modes for improved stability [Balajewicz and Tezaur]
  - Dissipation of turbulent kinetic energy occurs at the small scales.
  - Truncating the number of modes may lead to unbalanced production of turbulent kinetic energy
  - Modifying the basis to include information from truncated modes may improve stability of the ROM
- Investigating structure preserving constraints [Carlberg]

Other ROM Work at Sandia

Additional ROM work for fluid flows has been done using Spirit

- Continuous projection ROM code that uses `Trilinos`
- Reads in snapshot data from various CFD codes
- Computes POD modes using RBGen
- Projects choice of governing equations onto POD modes using choice of inner product
  - Governing equations include linearized Navier-Stokes, isentropic N-S, and full nonlinear N-S (in several forms)
  - Inner products include standard L^2 inner product and symmetry or energy inner products (depending on governing equations) which may produce ROMs with improved stability
- Outputs resulting ROM ODE system for later time integration

Other ROM Work at Sandia

ROM capabilities have also been implemented in Albany

- Open source finite-element framework built on `Trilinos`
- Variety of physics, ranging from structural mechanics to atmospheric modeling
- ROM capabilities (known as MOR or Razor [Cortial]) can be applied to most physics without any modifications
- Capabilities are similar to those in SPARC:
  - Galerkin or Least-Squares Petrov-Galerkin Projection
  - Hyper-Reduction using collocation on a sample mesh
- Currently exercising and extending these capabilities
- Applications include mechanical and thermo-mechanical simulations

Thermo-Mechanical Test Case using Razor in Albany

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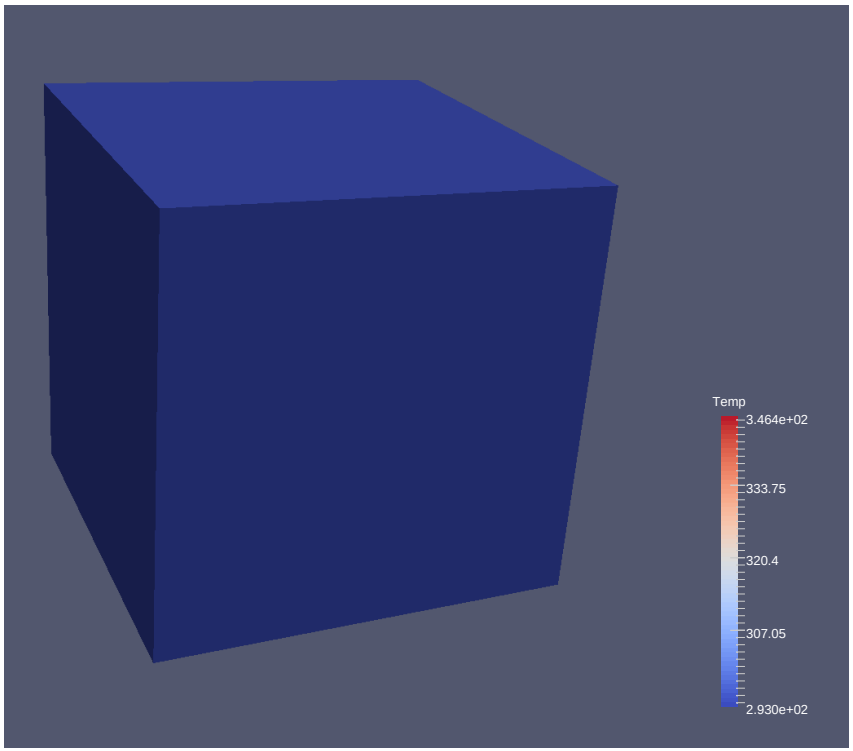
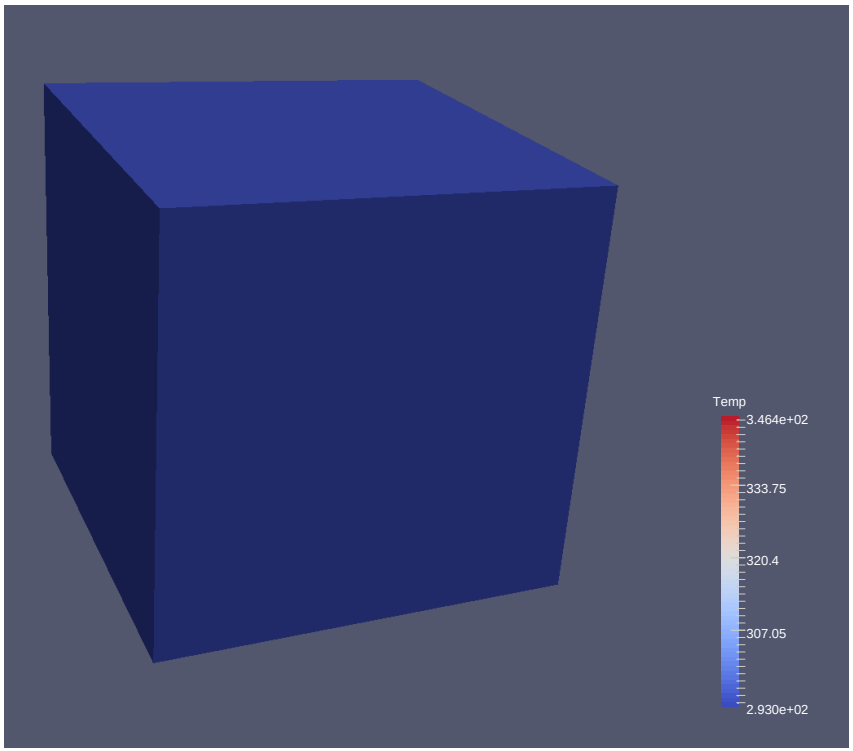
Full-Order Model



Galerkin ROM with 20 modes



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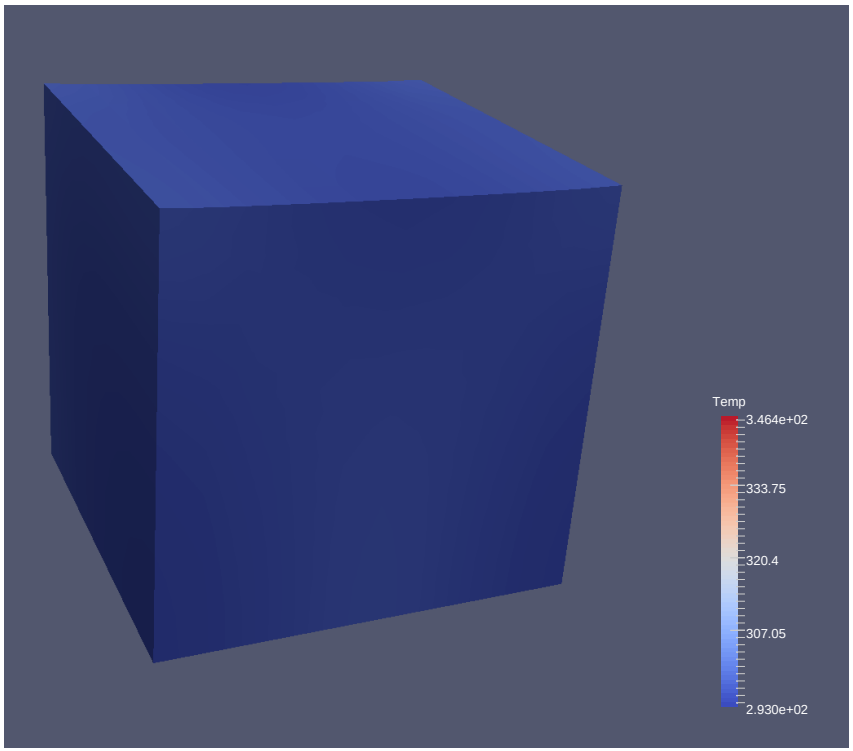

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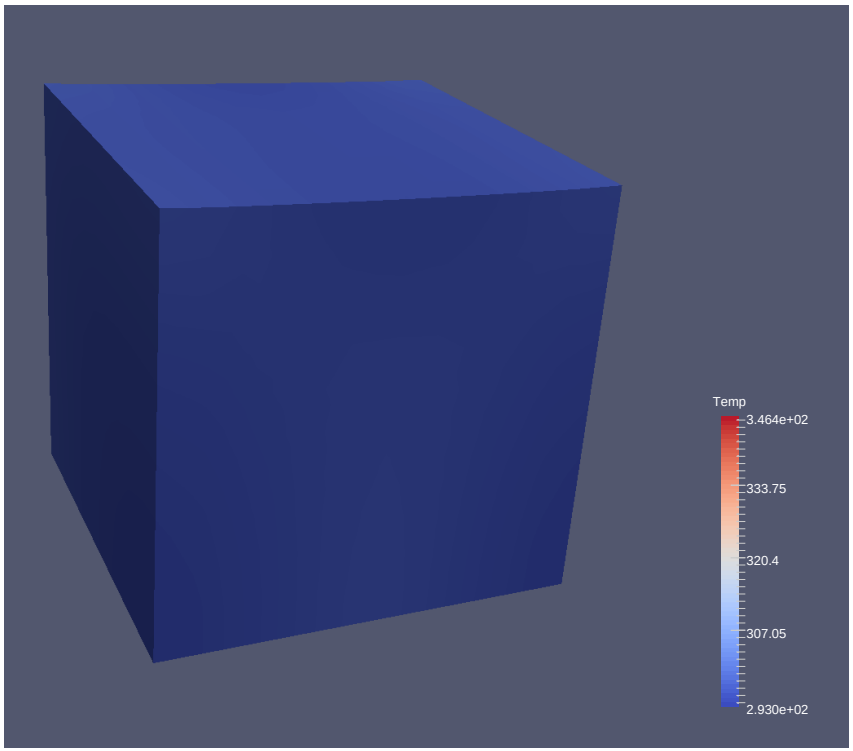

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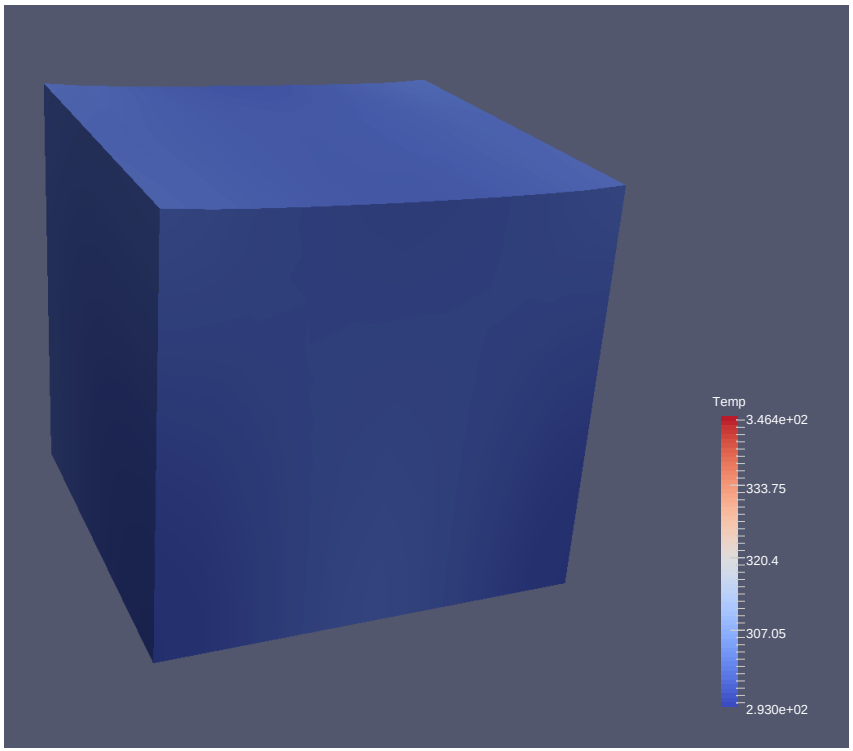

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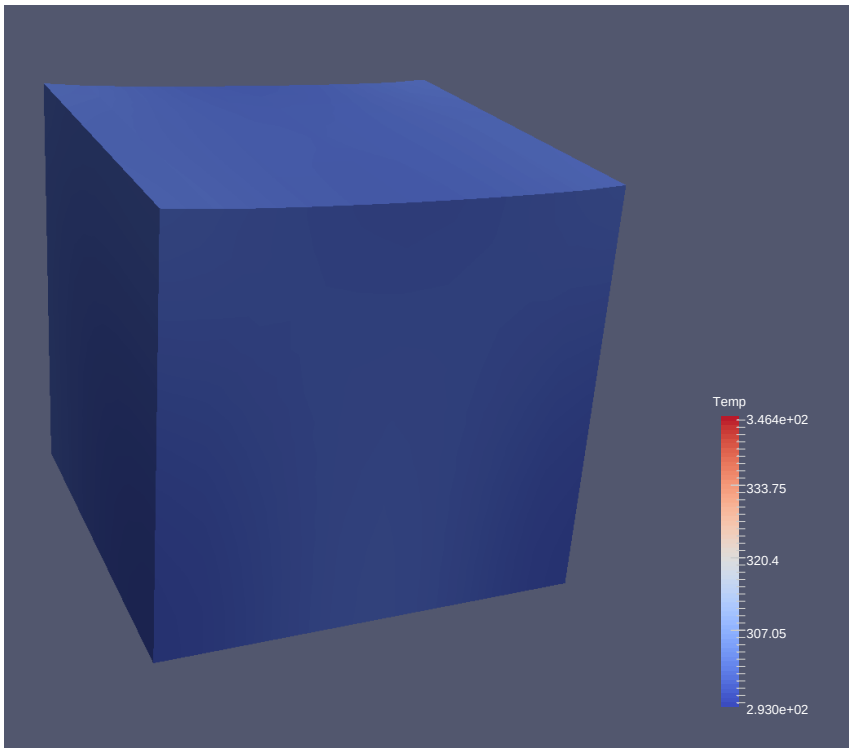

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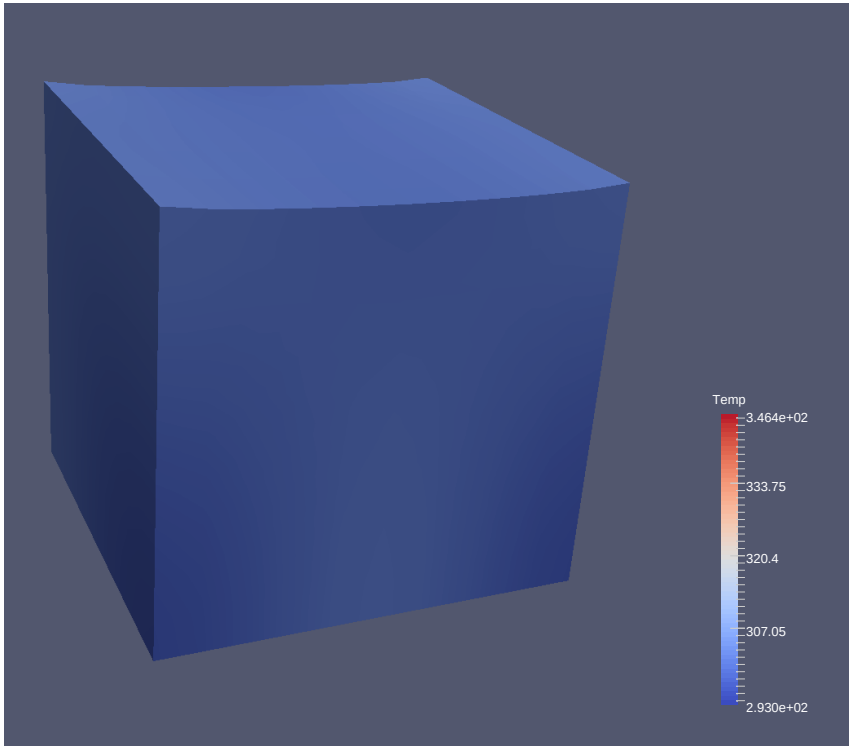

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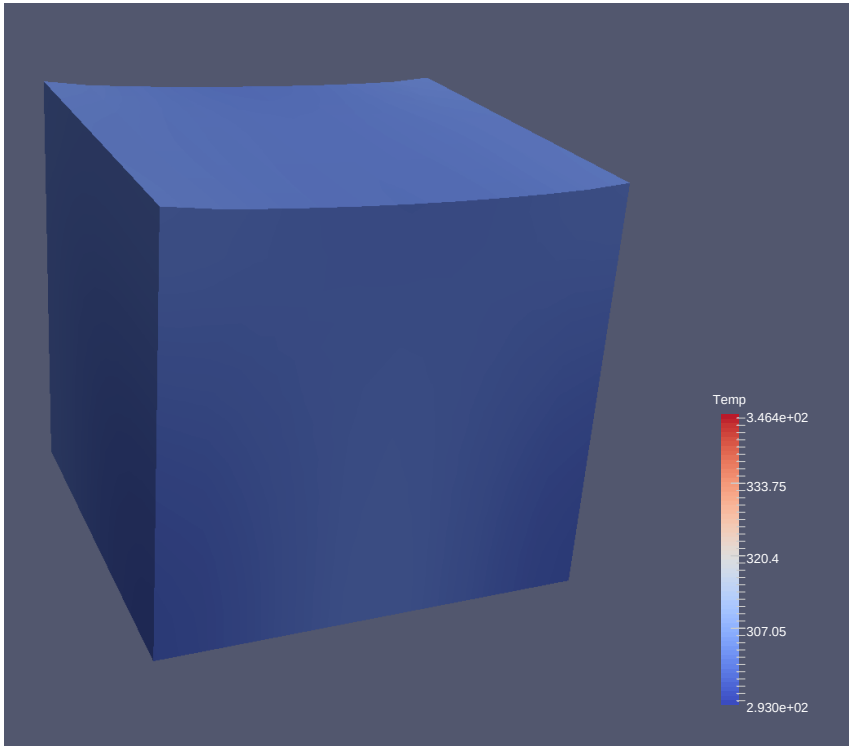

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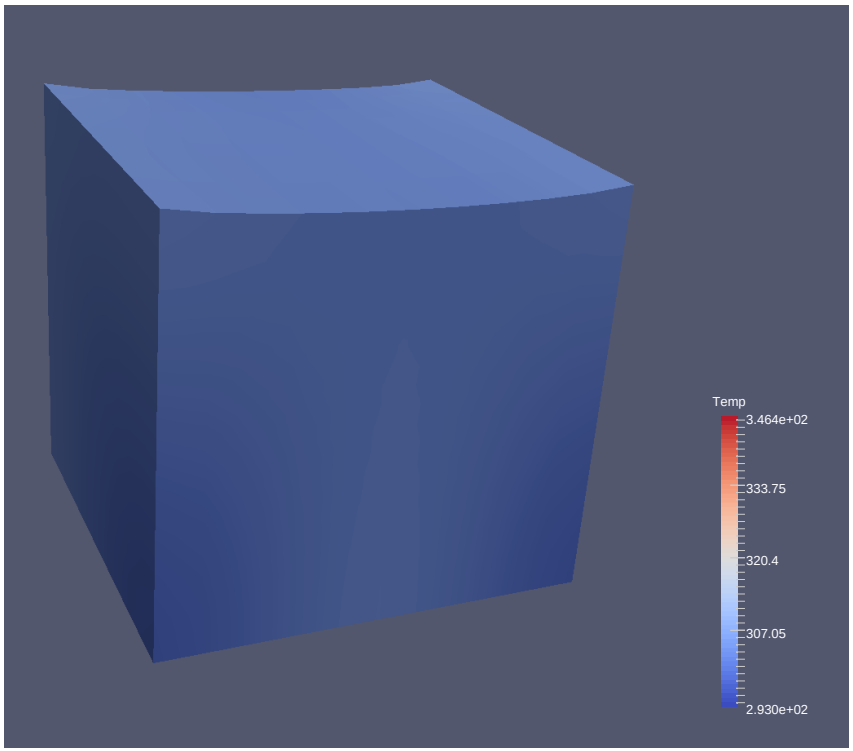

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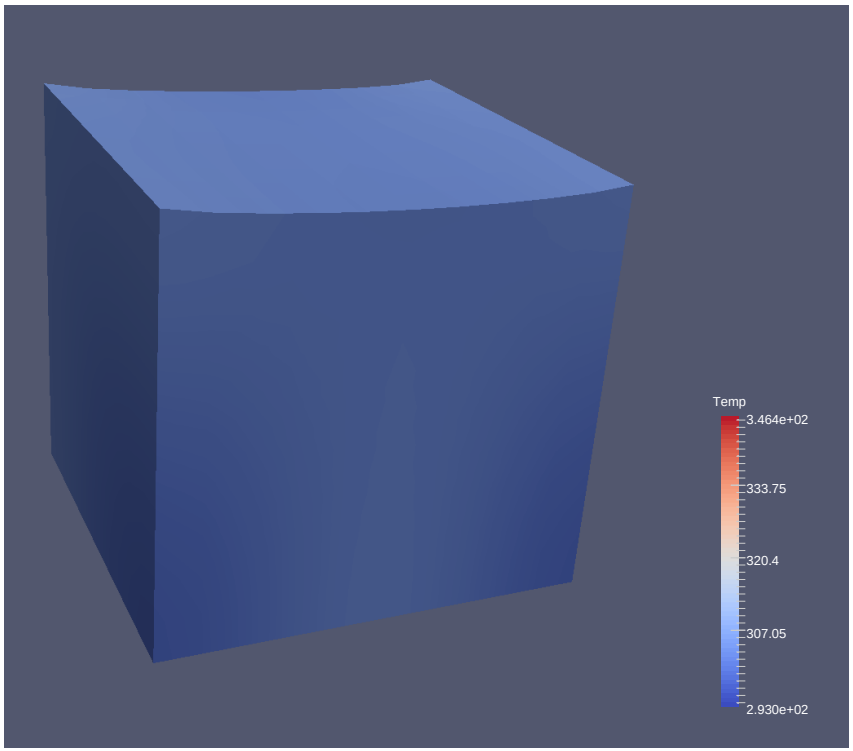

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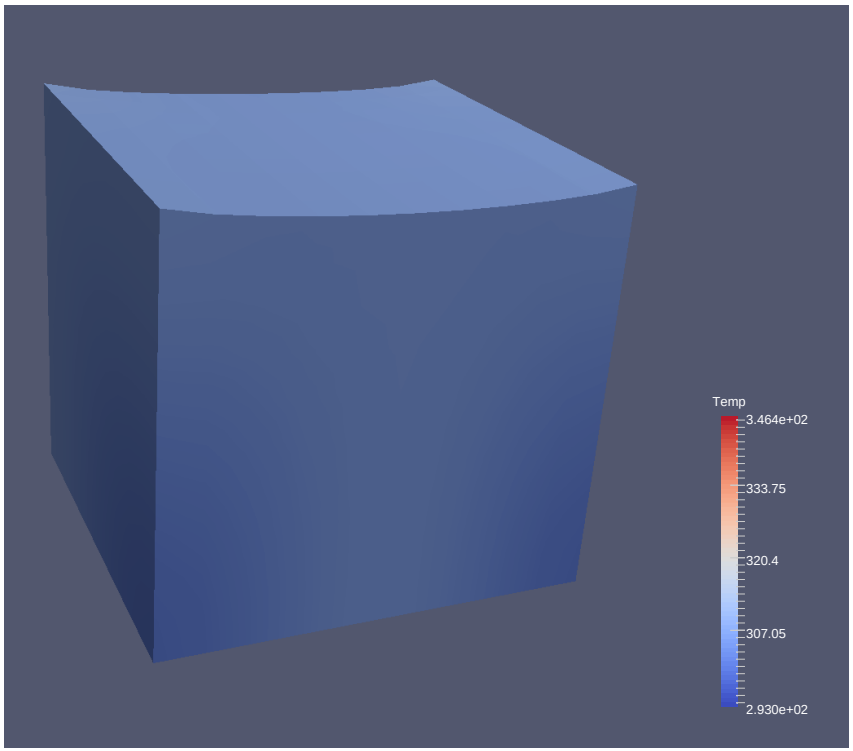

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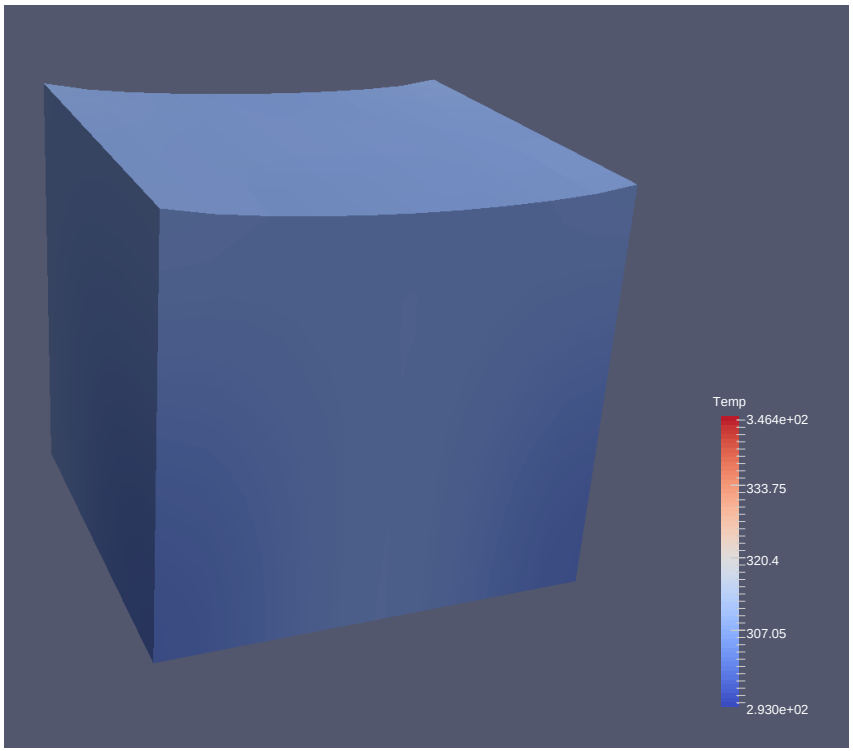

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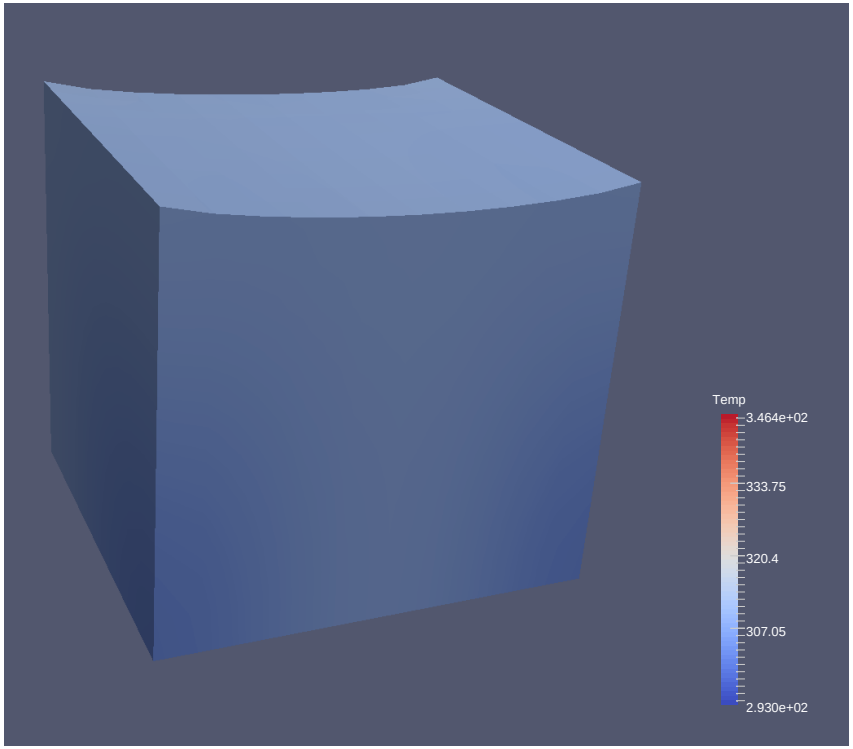

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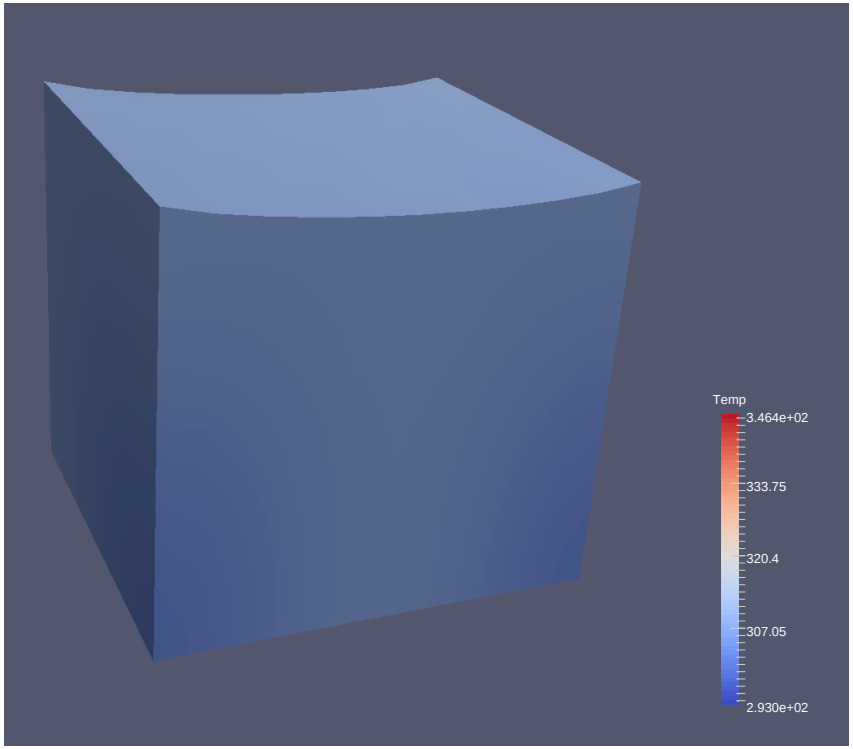

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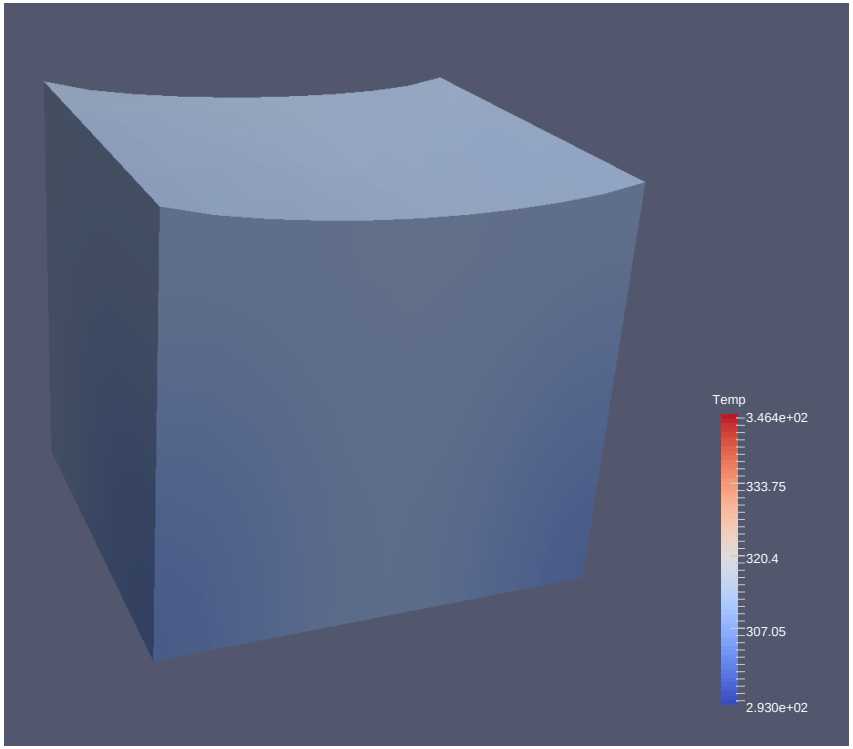

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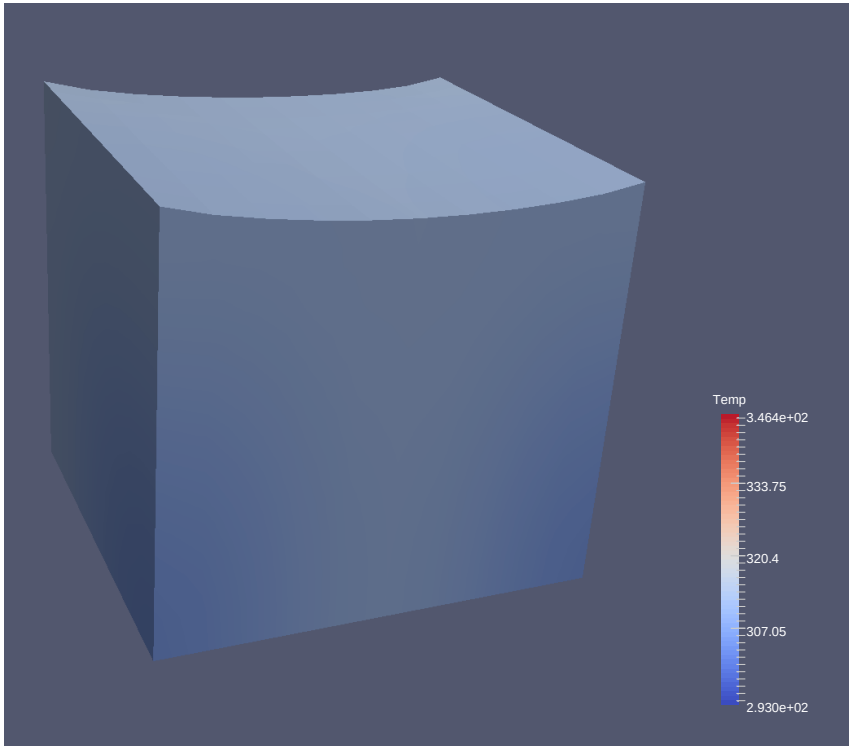

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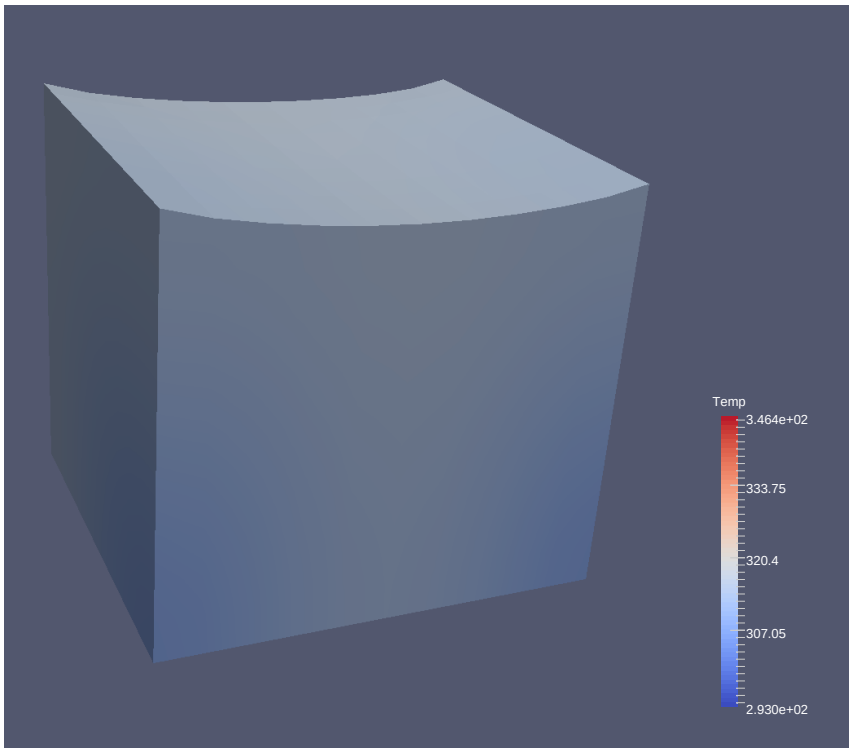

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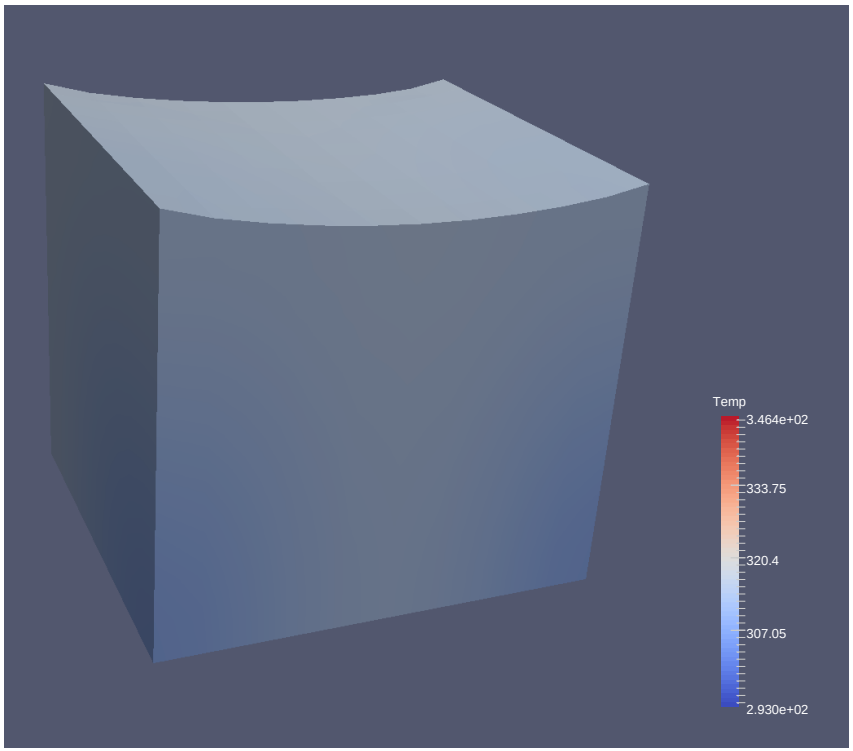

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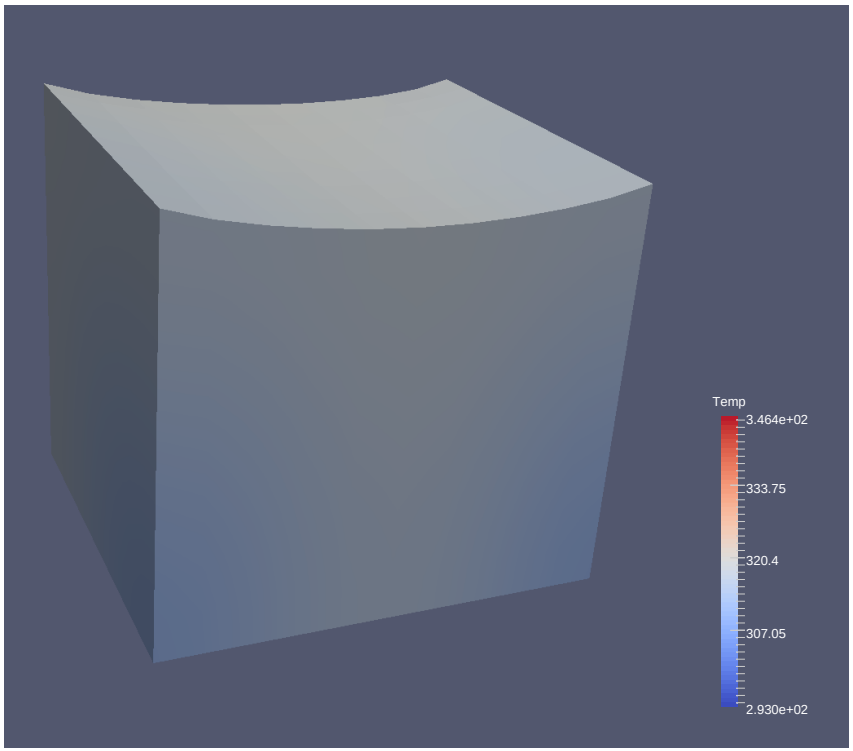

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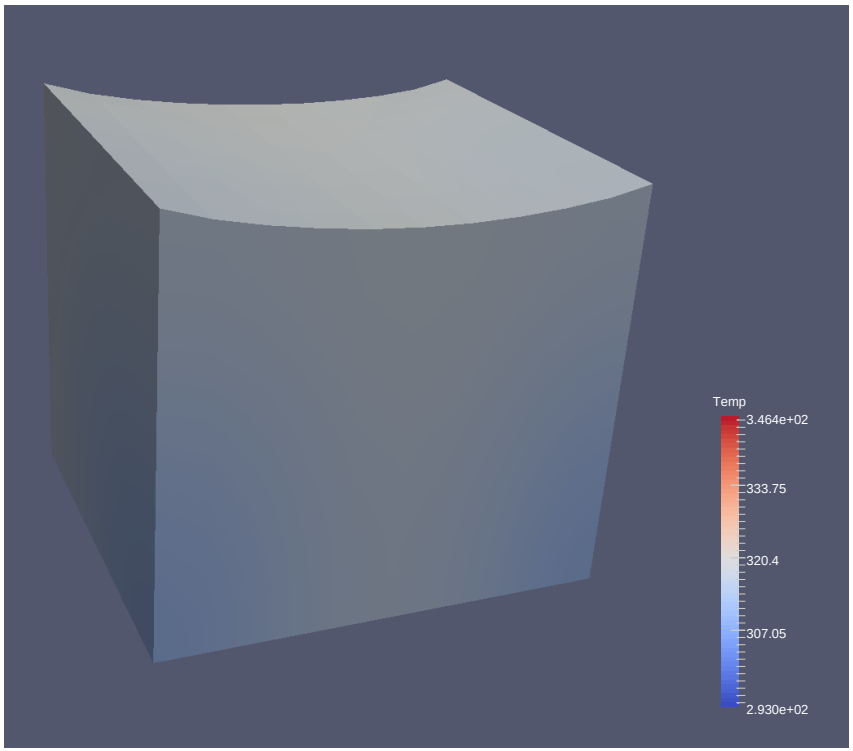

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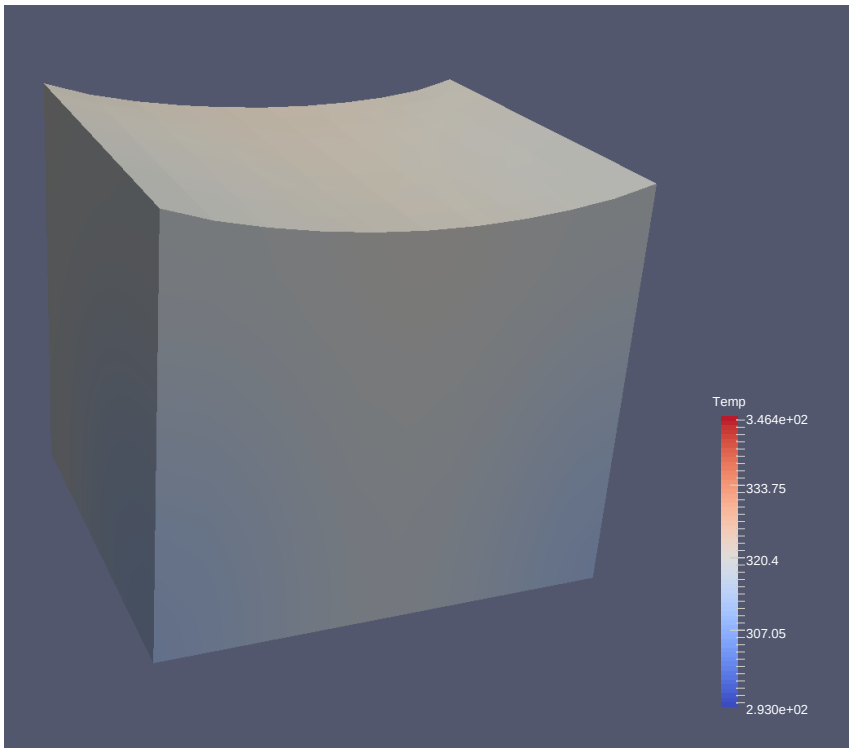

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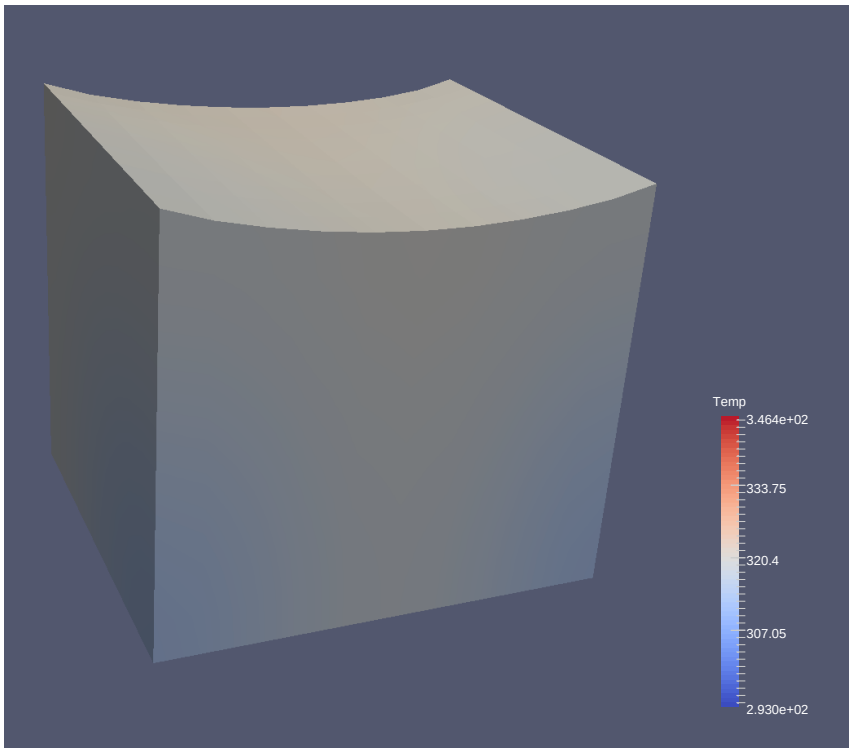

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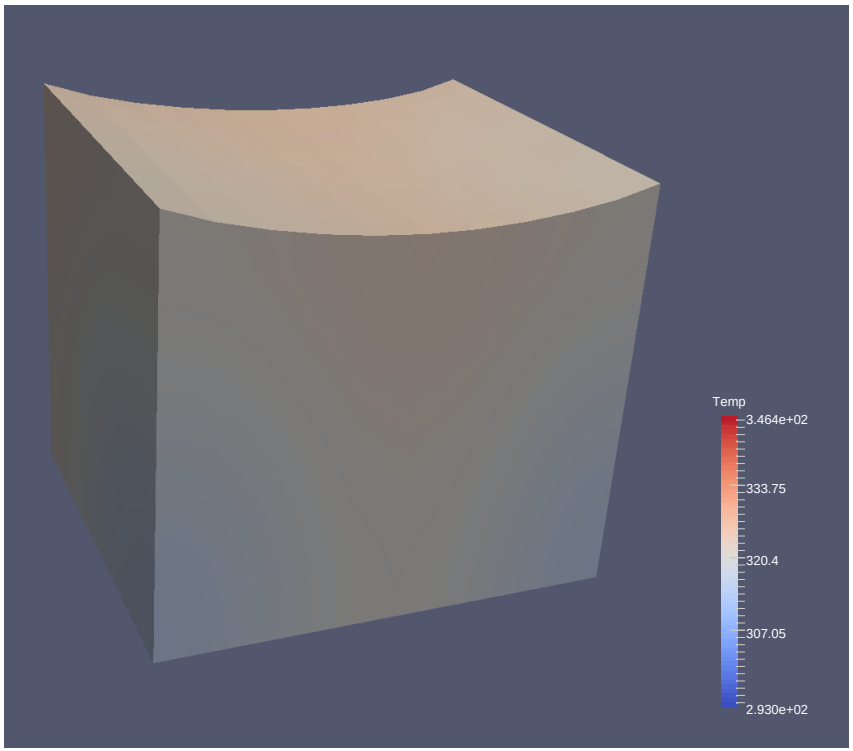

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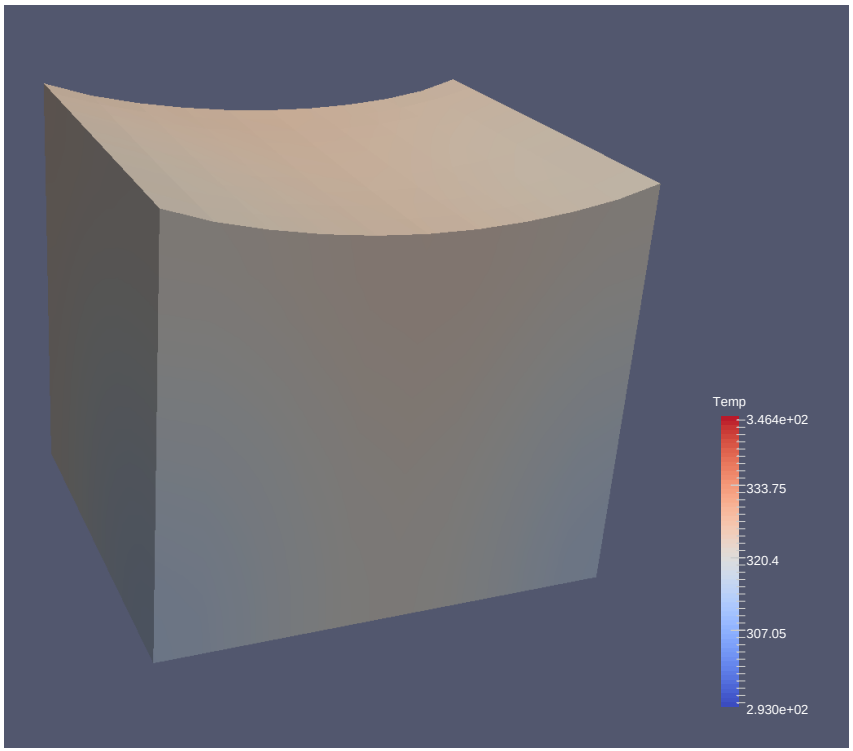

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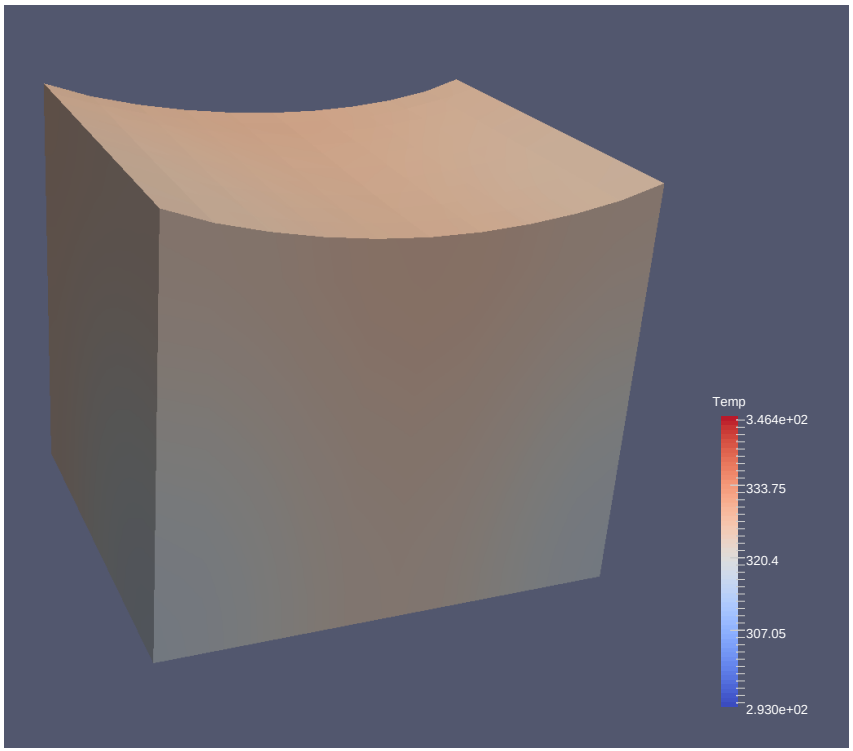

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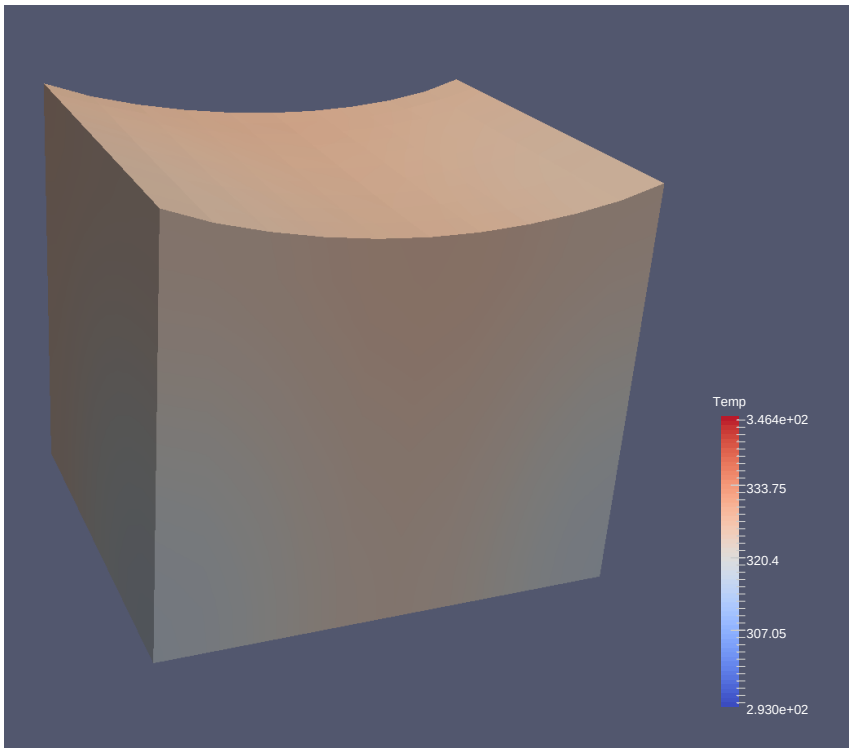

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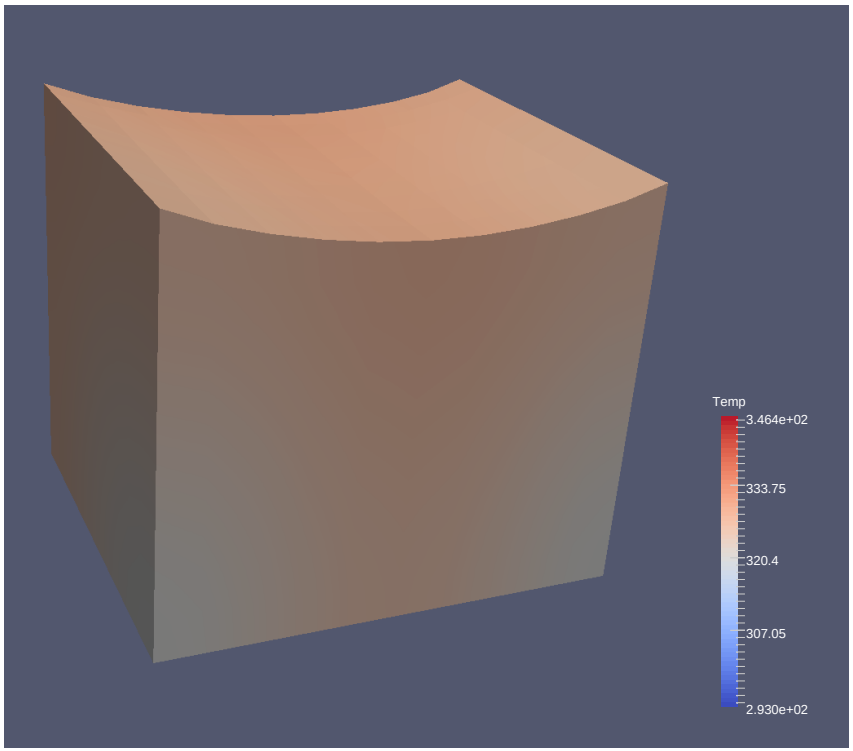

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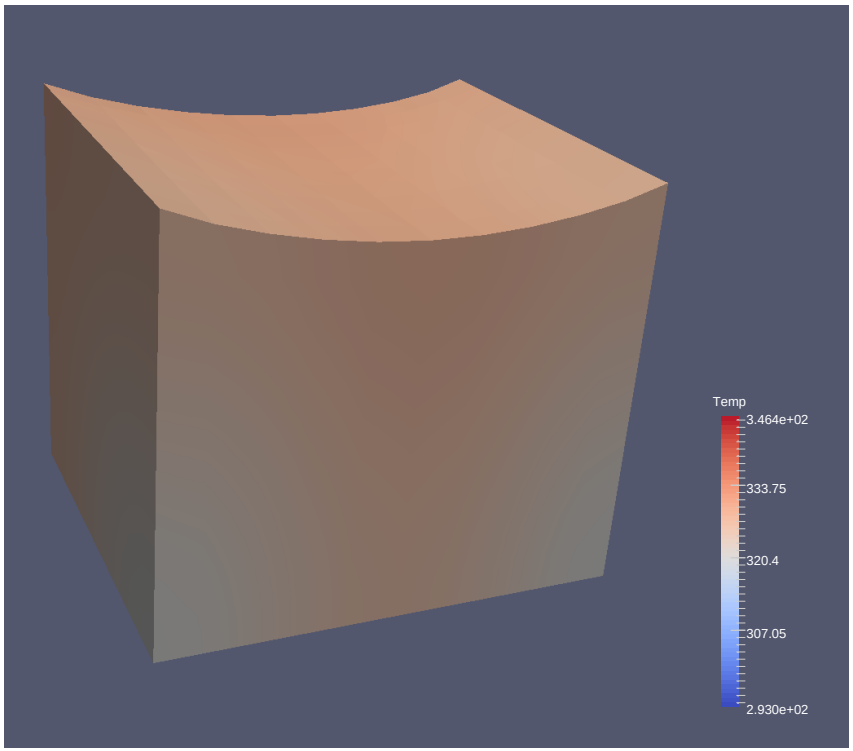

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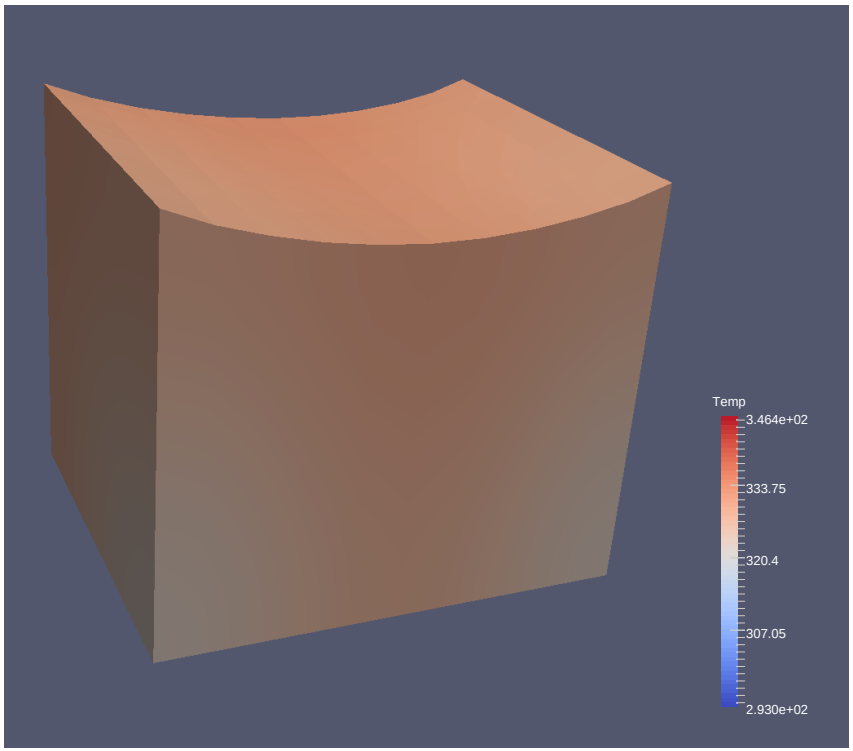

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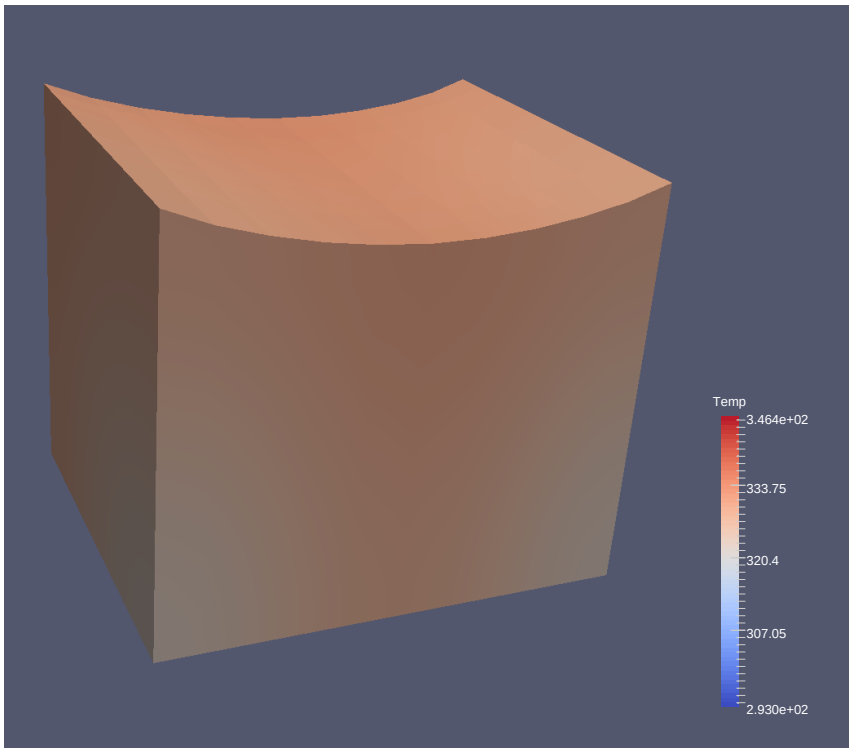

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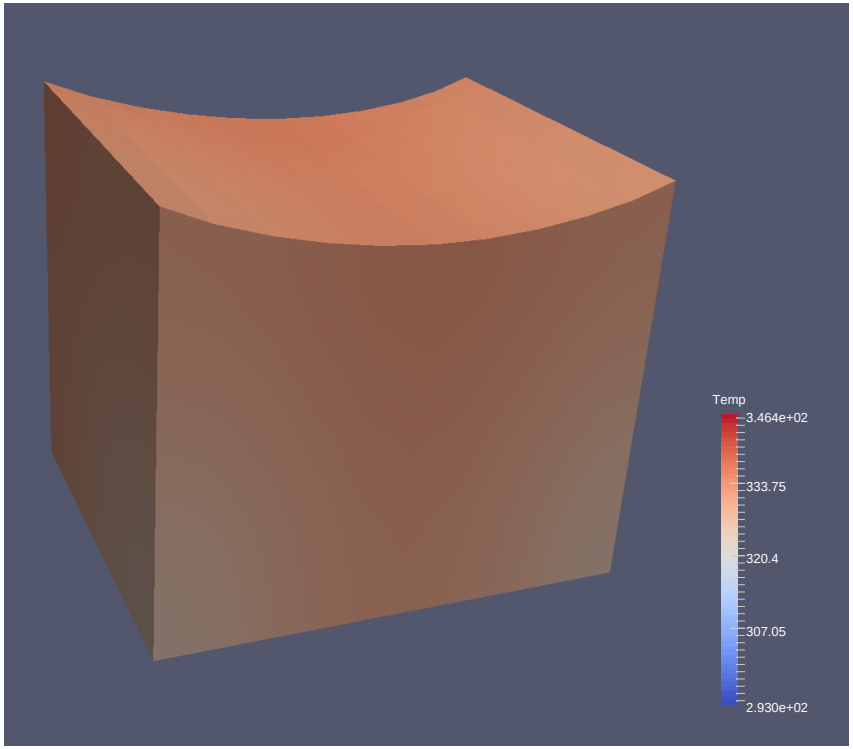
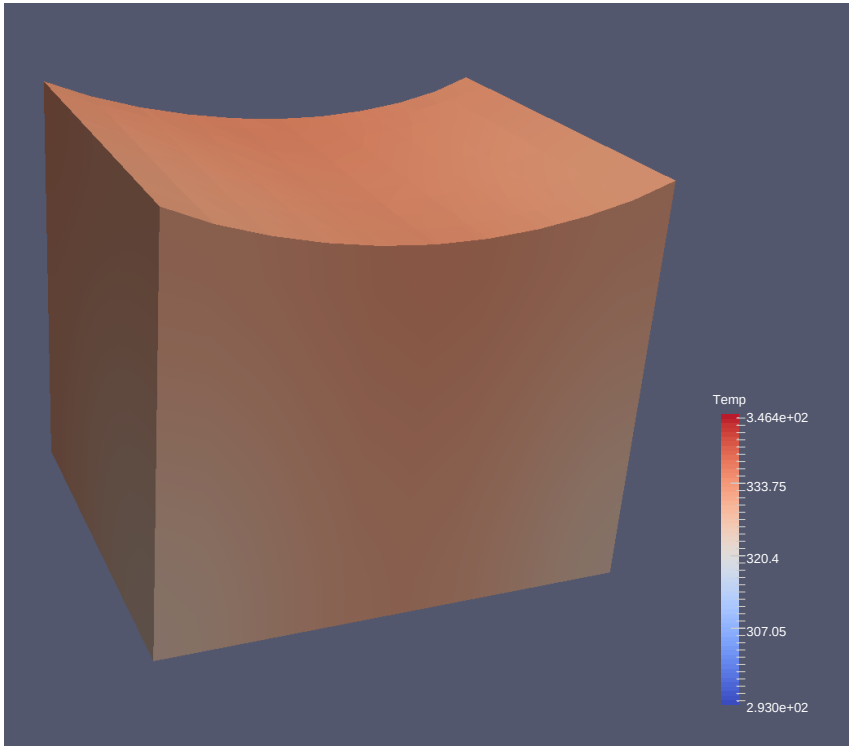
Full-Order Model



Galerkin ROM with 20 modes



Thermo-Mechanical Test Case using Razor in Albany

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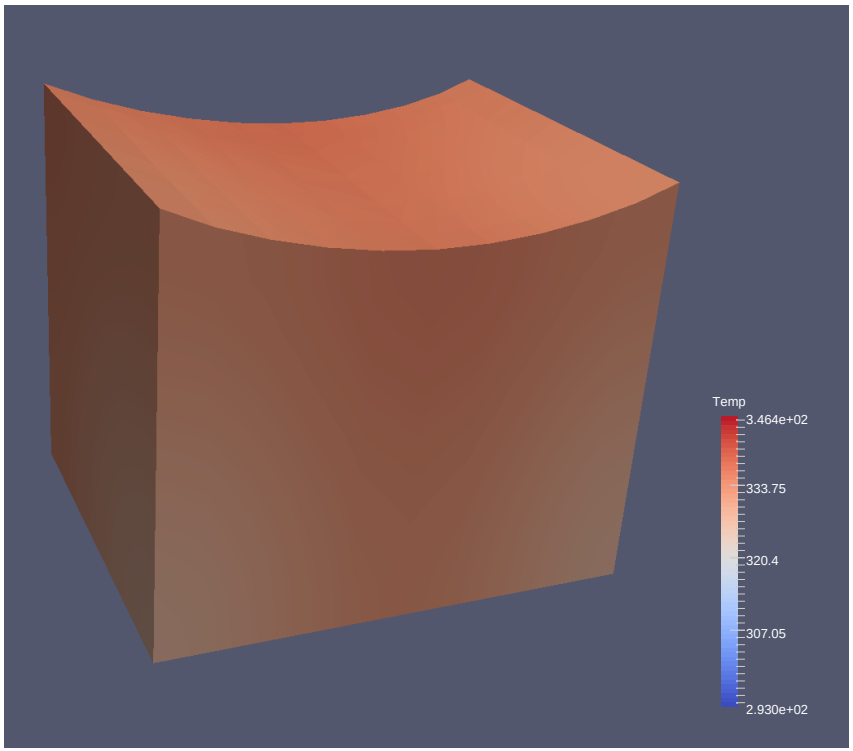
Full-Order Model



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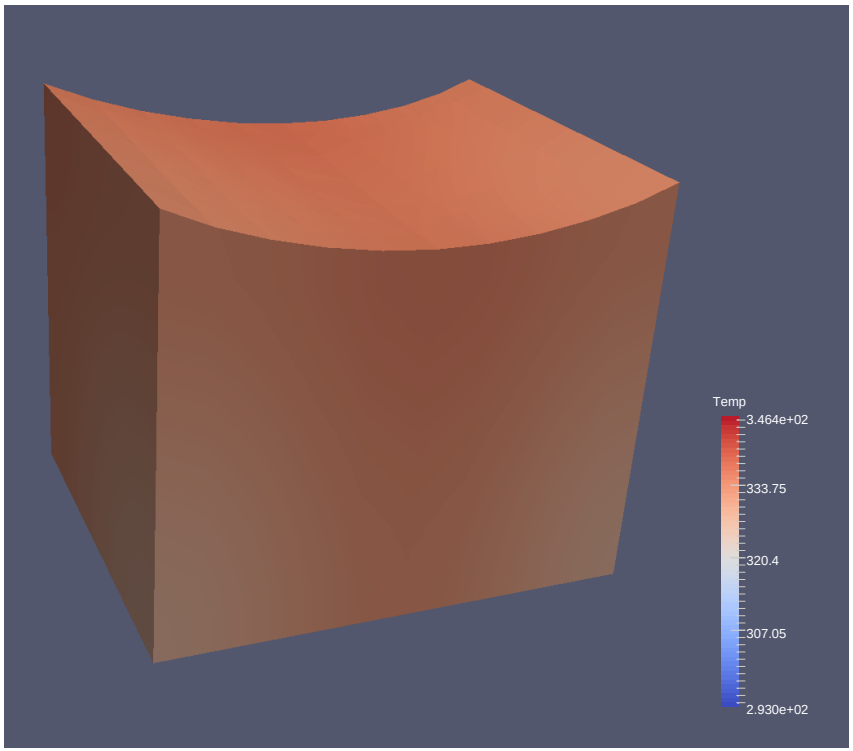

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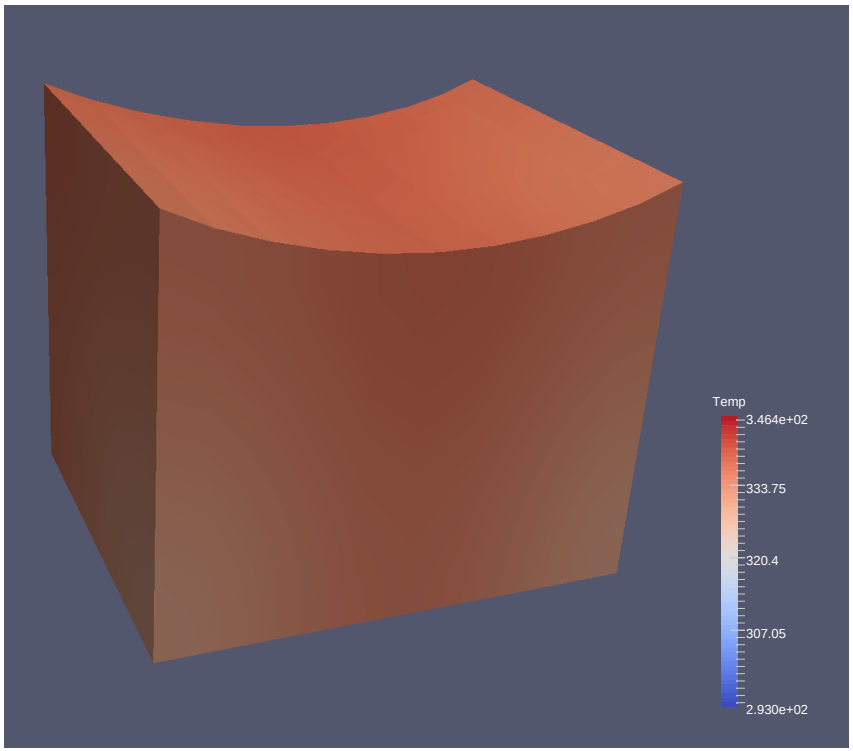
Full-Order Model



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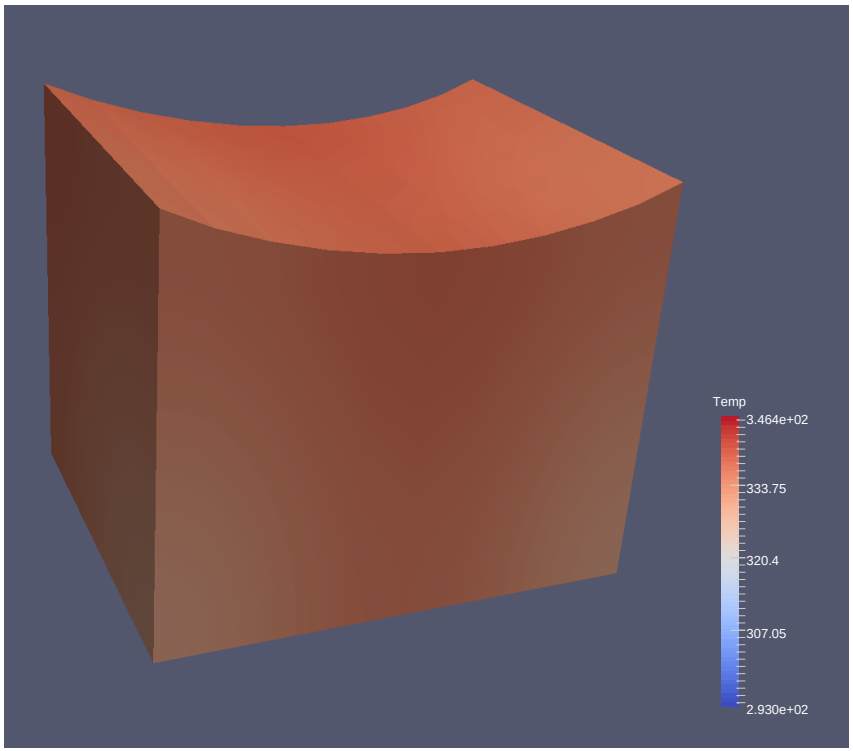

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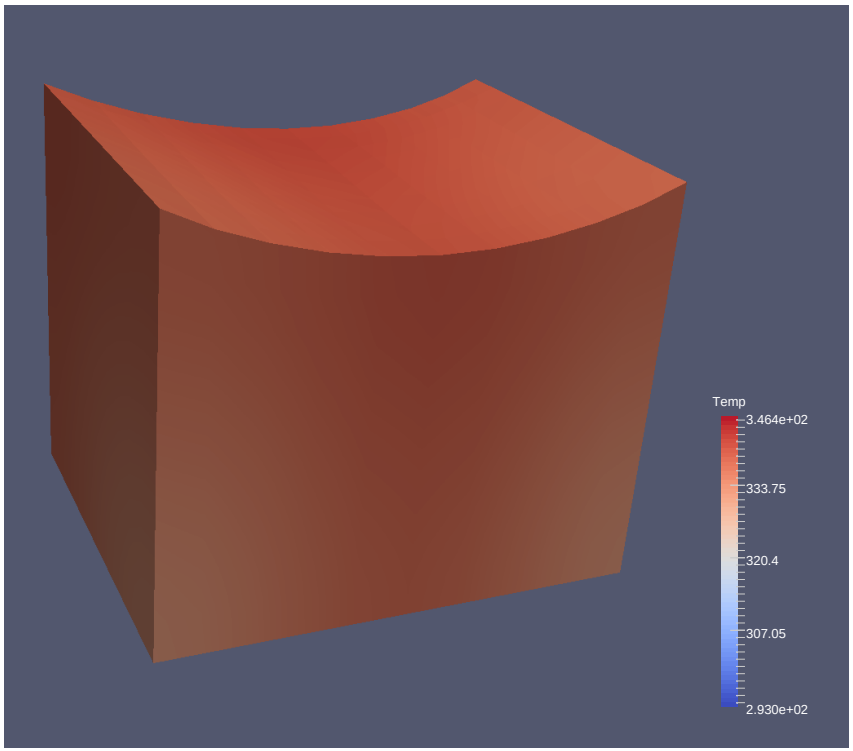
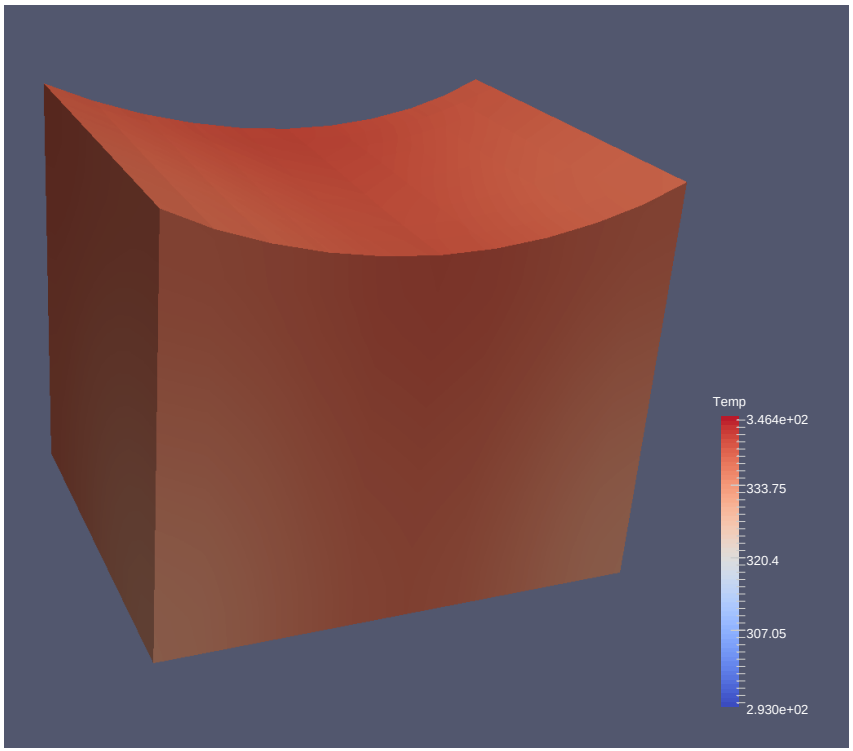


Galerkin ROM with 20 modes



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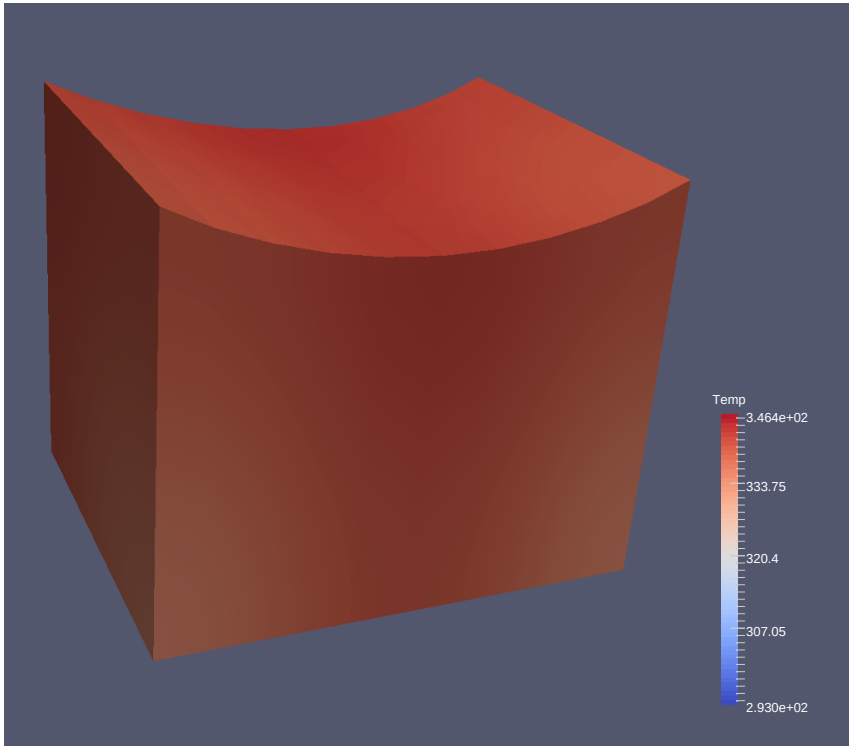
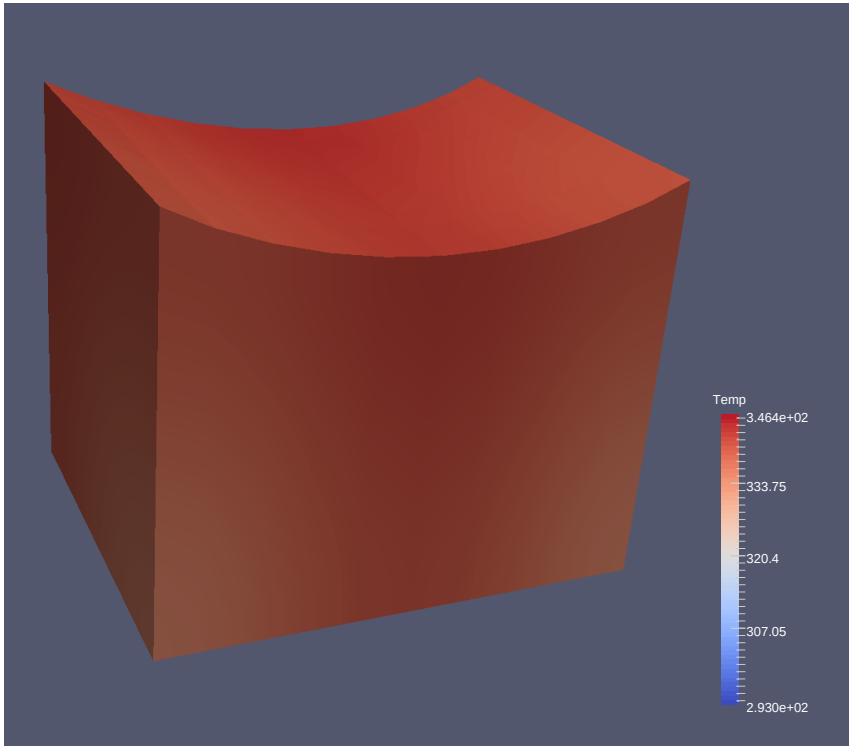
Full-Order Model



Galerkin ROM with 20 modes



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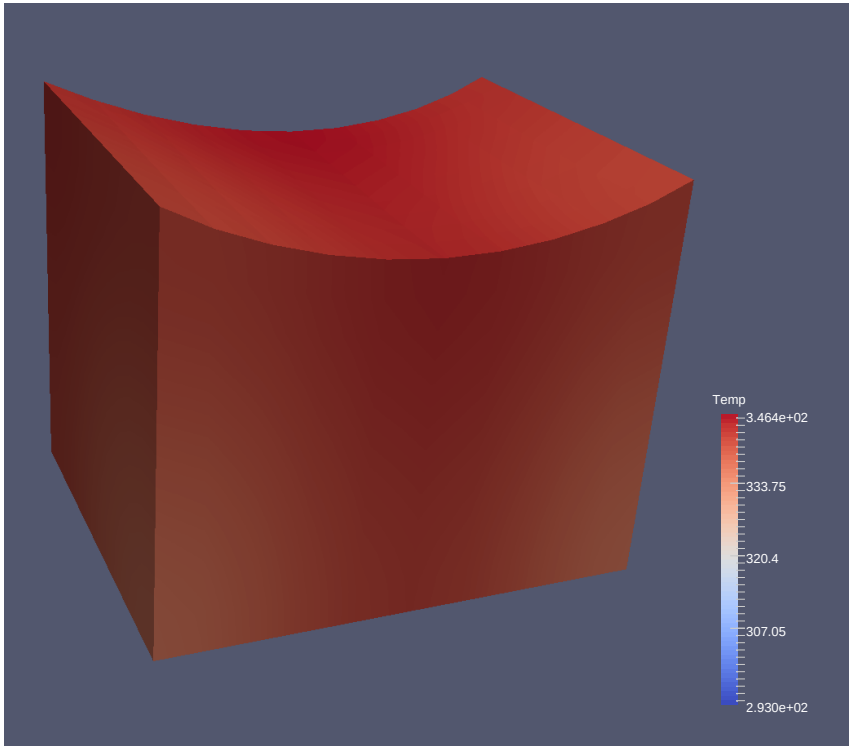
Full-Order Model



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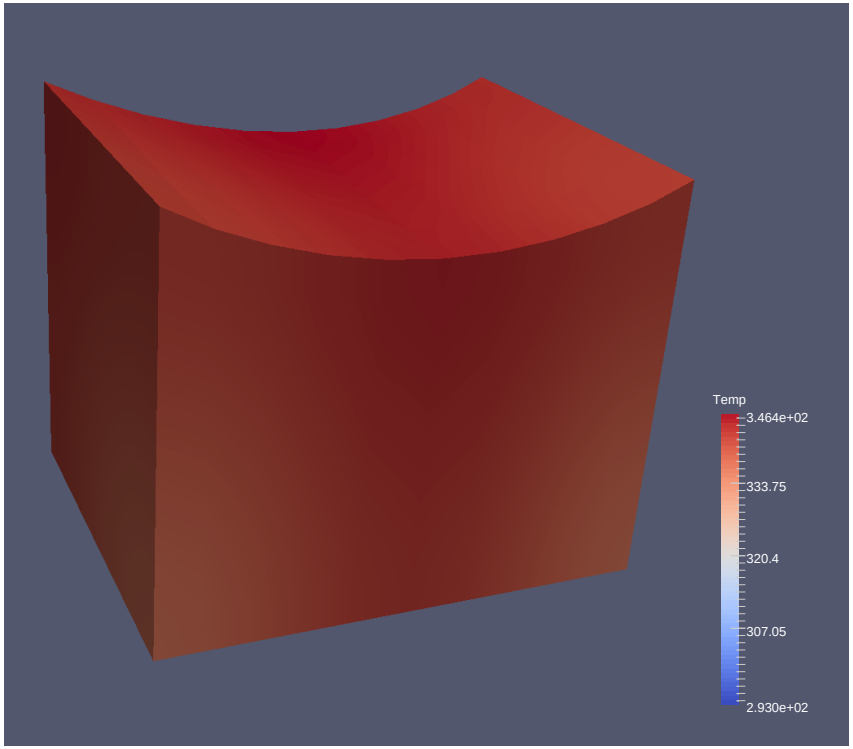

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Questions?