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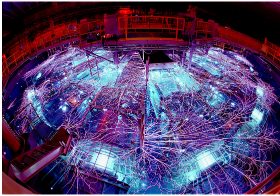

Model Reduction Capabilities in Albany

Albany User Meeting, January 2017

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Sandia National Laboratories

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Acknowledgement

The majority of the capabilities described here were originally implemented in Albany by Julian Cortial.

Outline

Motivation and Introduction

Model Reduction Implementation in Albany

Reduced-Order Model Workflow

Current and Future Work

Motivation

High-fidelity computational analysis is often accurate but very computationally expensive

- In some cases, a single analysis run can take several weeks using thousands of processors on modern supercomputers

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Reduced-order models (ROMs) can be used as surrogates for the high-fidelity analysis

- Need to retain a sufficient level of accuracy
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Reduced-order models (ROMs) can be used as surrogates for the high-fidelity analysis

- Need to retain a sufficient level of accuracy
- Need to have a significantly lower computational cost

ROMs can then be used for:

- Real-time analysis
- Uncertainty Quantification (UQ) methods, which often require very many analysis runs

Offline/Online Separation

Offline Training Stage:

- Generate and store information to be used during online stage
- Involves one (or more) high-fidelity analysis run(s)
- Computuationally expensive, but performed once

Online Evaluation Stage:

- Many evaluations of the reduced-order model
- Computationally inexpensive

Nomenclature

The following terms are used throughout this presentation, often interchangeably:

- High-fidelity analysis, full-order model, FOM
- Model reduction, MOR, reduced-order model, ROM
- Reduced basis, modal basis, POD basis, basis
- Galerkin projection, Galerkin ROM
- Least-squares Petrov-Galerkin projection, LSPG ROM, minimum-residual ROM
- Generalized coordinates, modal coefficients, ROM coefficients

Projection-Based Model Reduction

During the offline training stage, we construct a modal basis, Φ

Unlimited Release

Projection-Based Model Reduction

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The state of the system, x, can then be approximated as

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

- $\bar{x}$ is some reference state
- $\hat{x}$ are the modal coefficients that are determined during the online evaluation stage

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The system of equations for the ROM coefficients is constructed by projecting the governing equations onto a test basis, Ψ

Continuous vs. Discrete Projection

Continuous Projection

- The continuous governing equations (PDEs) are projected onto the test basis in offline stage
- For polynomial nonlinearites, this results in a set of ODEs for the modal coefficients
- For other nonlinearities, techniques such as Gappy POD or Empirical Interpolation are required

Discrete Projection

- The discretized governing equations (discrete residual and Jacobian) are projected onto the test basis
- For nonlinear equations this requires embedding the projection operation in the analysis code

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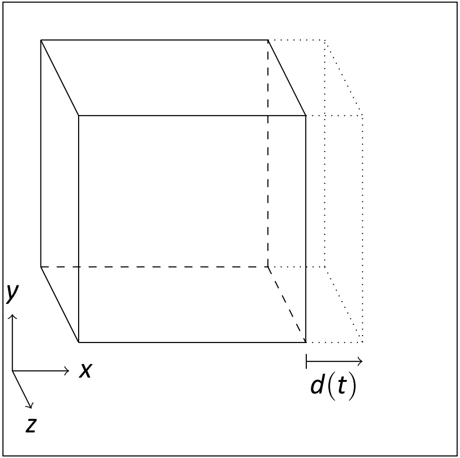
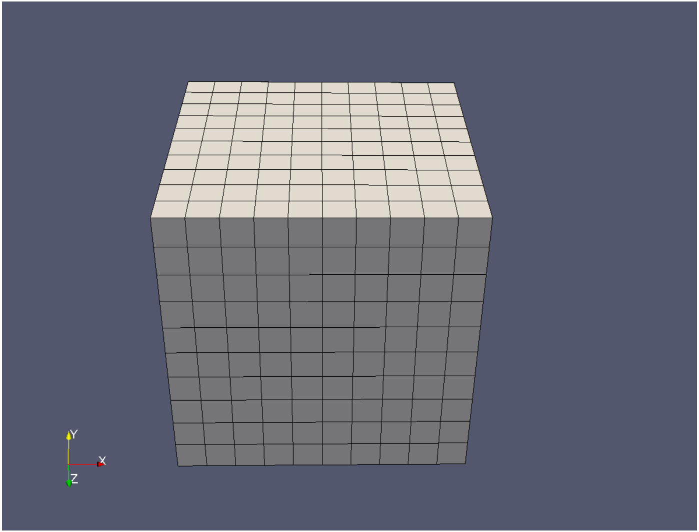


- Steel cube
- Time-varying displacement applied to one side
- Fixed displacement on other end
- Quasistatic problem using LOCA

Solid Mechanics Example in Albany



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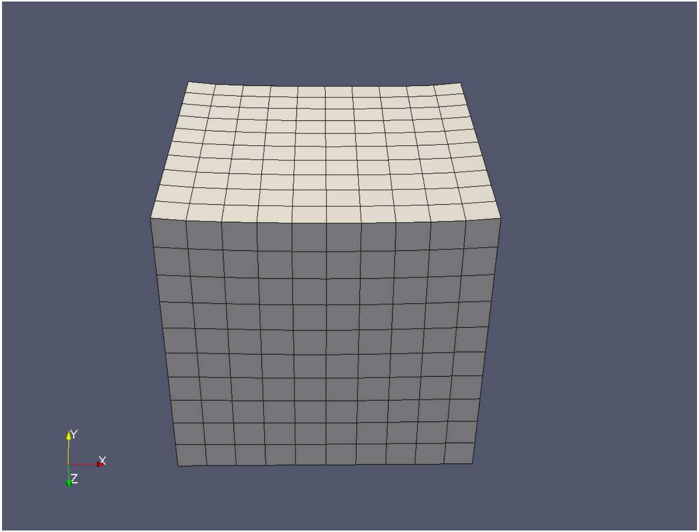

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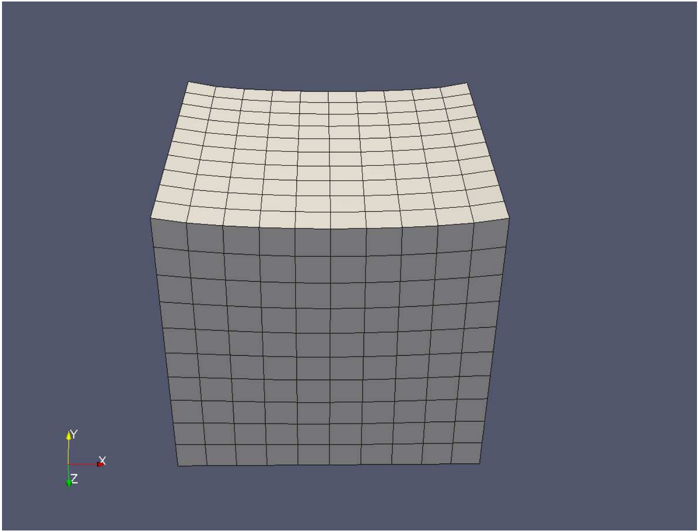

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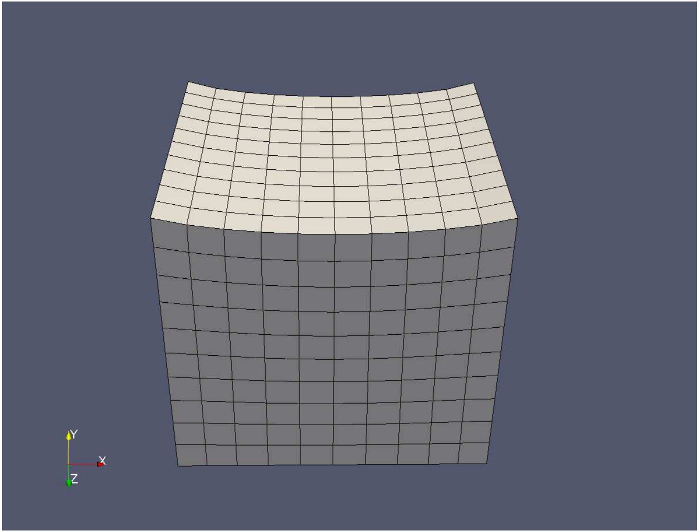

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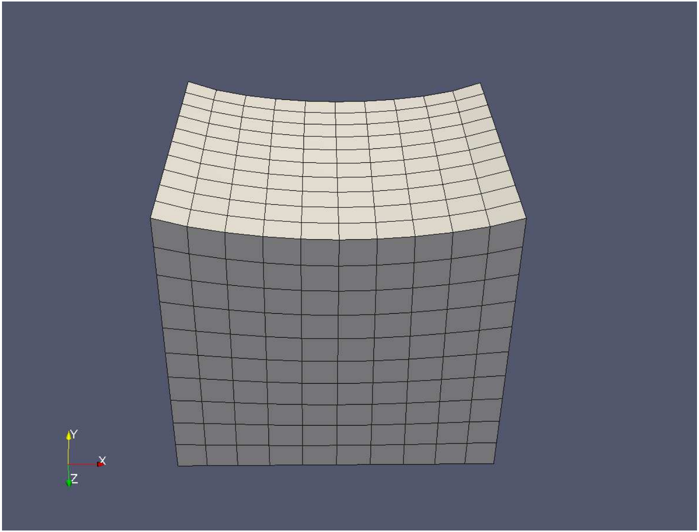

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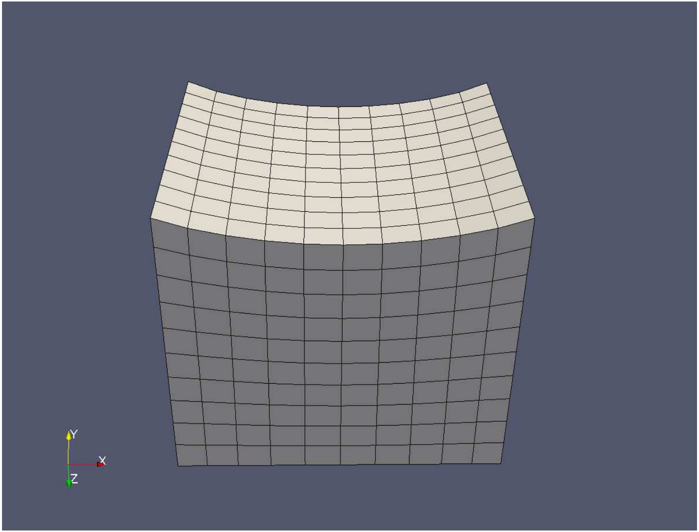

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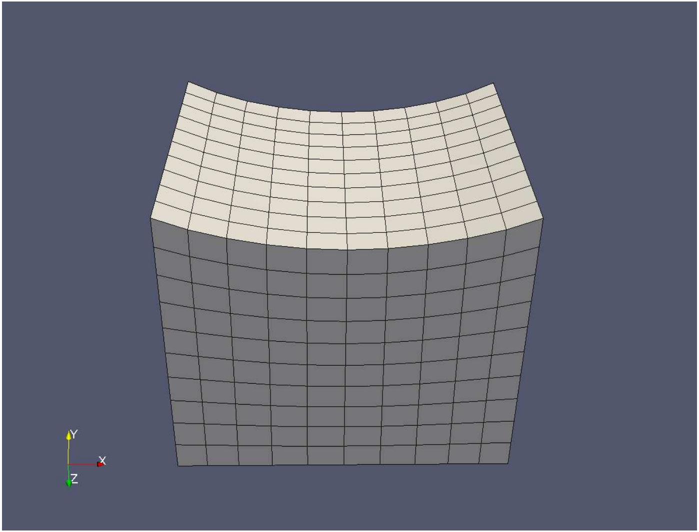

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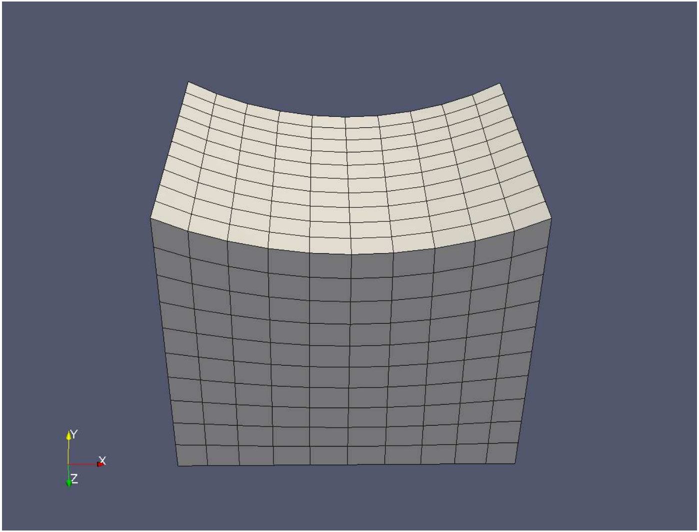
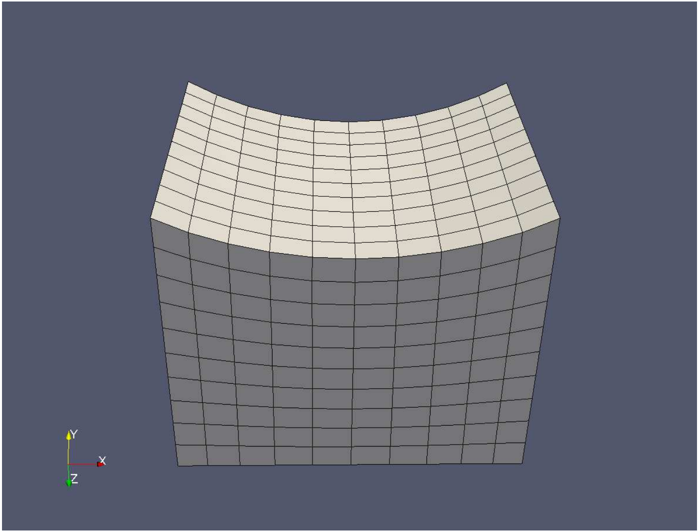


Solid Mechanics Example in Albany



Quasistatic Problem Solved Using Continuation (LOCA)

During each continuation step:

- Increment time, i.e. $t = t + \Delta t$
- Applied displacement boundary condition increases linearly with time
- Solve for change in state of the system (i.e. deformation) using Newton iterations (NOX)

$$W(x)\Delta x = -f(x)$$

Albany_ModelEvaluator provides residual, f, and Jacobian, W

Reduced-Order Model Solution

During each continuation step:

- Increment time, i.e. $t = t + \Delta t$
- Approximate the state of the system $x \approx \tilde{x} = \bar{x} + \Phi\hat{x}$
- Applied displacement boundary condition increases linearly with time
- Solve for change in modal coefficients, $\Delta\hat{x}$, using Newton iterations (NOX)

$$W_r(\tilde{x})\Delta\hat{x} = -f_r(\tilde{x})$$

MOR_ReducedOrderModelEvaluator provides reduced residual, f_r, and reduced Jacobian, W_r

- Calls Albany_ModelEvaluator to get full residual, f, and full Jacobian, W

MOR Implementation in Albany

The MOR_ReducedOrderModelEvaluator can be thought of as a wrapper around the Albany_ModelEvaluator

- Sometimes referred to as the MOR facade
- Only activated when reduced-order model options are enabled in the input file

Implementation generic enough to create ROMs for various solvers and physics sets enabled in Albany

- Current projects focus on using LOCA for LCM problems

However, the current MOR capabilities are built on the EpetraExt_ModelEvaluator

- Will not work for packages that are built only on the Thyra_ModelEvaluator, such as Aeras
- Future work may convert implementation to Thyra

Reduced-Order Model Details

Full-Order Model involves solving

$$W(x)\Delta x = -f(x)$$

Reduced-Order Model involves solving

$$W_r(\tilde{x})\Delta\hat{x} = -f_r(\tilde{x})$$

where

$$W_r(\tilde{x}) = \Psi^T W(\tilde{x})\Phi$$

$$f_r(\tilde{x}) = \Psi^T f(\tilde{x})$$

and the choice of the test basis, Ψ, depends on the type of reduced-order model chosen

Reduced-Order Model Types in Albany

There are currently two options implemented in Albany for the type of reduced-order model

- Galerkin Projection
- Minimum Residual (aka Least-Squares Petrov-Galerkin)

In Galerkin projection, the test basis, Ψ, is the trial basis, Φ and we have

$$W_r(\tilde{x}) = \Phi^T W(\tilde{x})\Phi$$

$$f_r(\tilde{x}) = \Phi^T f(\tilde{x})$$

Minimum Residual ROM

The minimum residual or least-squares Pretrov-Galerkin ROM involves finding the solution to the nonlinear least-squares problem

$$\hat{x} = \arg\min_{y} \|f(\bar{x} + \Phi y)\|_2^2$$

Using the Gauss-Newton approach, this involves solving a sequence of linear least-squares problems

$$\Delta\hat{x} = \arg\min_{y} \|W(\tilde{x})\Phi y + f(\tilde{x})\|_2^2$$

The normal equation form is

$$\Phi^T W^T(\tilde{x}) W(\tilde{x}) \Phi \Delta\hat{x} = -\Phi^T W^T(\tilde{x}) f(\tilde{x})$$

which corresponds to choosing $\Psi = W(\tilde{x})\Phi$, and giving

$$W_r(\tilde{x}) = \Phi^T W^T(\tilde{x}) W(\tilde{x}) \Phi$$

$$f_r(\tilde{x}) = \Phi^T W^T(\tilde{x}) f(\tilde{x})$$

Dimension Reduction

Full-Order Model involves solving

$$W(x)\Delta x = -f(x)$$

- Typically $\mathcal{O}(10^6)$ degrees of freedom

Reduced-Order Model involves solving

$$W_r(\tilde{x})\Delta \hat{x} = -f_r(\tilde{x})$$

- Typically $\mathcal{O}(100)$ modal coefficients

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$$W_r(\tilde{x})\Delta\hat{x} = -f_r(\tilde{x})$$

- Typically $\mathcal{O}(100)$ modal coefficients

Despite the reduction in the dimension of the problem, there is not typically a reduction in computational cost

- Constructing reduced residual and Jacobian requires evaluating full residual and Jacobian for every DOF

Hyper-Reduction

Introduce a sampling operation to select a small subset of the total DOFs where the residual and Jacobian are computed

- $Zf(\tilde{x})$ and $ZW(\tilde{x})$ are the selected residual and Jacobian entries
- Z denotes the concept of a sampling matrix
- In practice there is no actual multiplication, the selected entries are simply evaluated without explicitly forming Z, f, or W

For the LSPG ROM, this gives

$$W_r(\tilde{x}) = \Phi^T W^T(\tilde{x}) Z^T Z W(\tilde{x}) \Phi$$

$$f_r(\tilde{x}) = \Phi^T W^T(\tilde{x}) Z^T Z f(\tilde{x})$$

- Provides reduction in computational cost

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Configure and Build Albany and Trilinos

Configure Trilinos and build:

- -D Trilinos_ENABLE_Anasazi:BOOL=ON
- -D Anasazi_ENABLE_RBGen:BOOL=ON
- -D CMAKE_CXX_FLAGS:STRING=”-DEPETRA_LAPACK3”

Configure and Build Albany and Trilinos

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Configure Albany:

- -D ENABLE_MOR=ON

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- -D Trilinos_ENABLE_Anasazi:BOOL=ON
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Configure Albany:

- -D ENABLE_MOR=ON

Building Albany should produce the standard executables, plus some ROM specific utilities

- AlbanyRBGen - used to generate modal basis
- AlbanyMeshSample - used to generate sample mesh
- AlbanyRomPostProcess - used to recreate full solution after running ROM with sample mesh

Reduced-Order Model Workflow

Offline Stage:

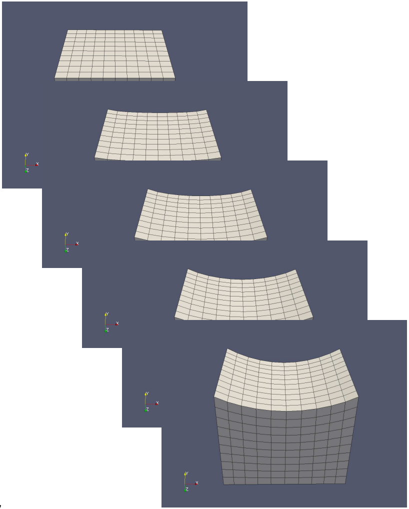
- Run full-order model in Albany to generate training data
- Construct modal basis
- Construct sample mesh

Online Stage

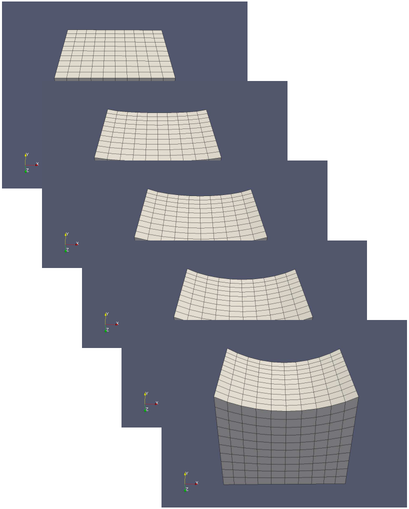
- Run reduced-order model in Albany
- Post-process results

Run FOM to Generate Training Data

Poisson Ratio $\nu = 0.25$



Poisson Ratio $\nu = 0.30$

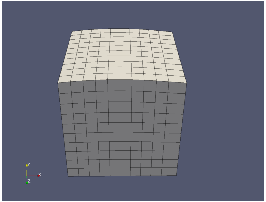


Unlimited Release

Create Modal Basis

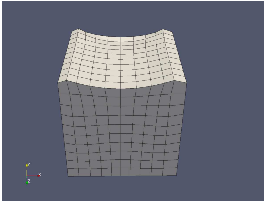
Run AlbanyRBGen executable

- Uses Proper Orthogonal Decomposition (POD) to create a basis



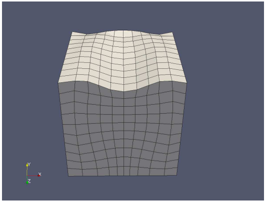
Mode 1

…



Mode 3

…



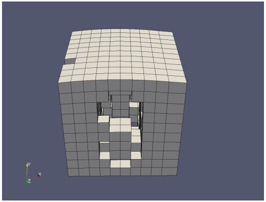
Mode 5

…

Create Sample Mesh

Run AlbanyMeshSample executable

- Uses a greedy algorithm to select nodes that best represents the full basis
- 400 sample nodes (out of 1331 total nodes) for a 35 mode basis



Mode 1

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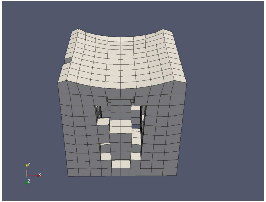
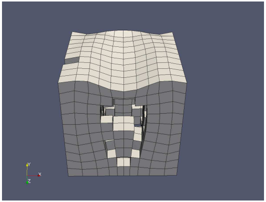


Mode 3

...



Mode 5

...

Run Reduced-Order Model in Albany

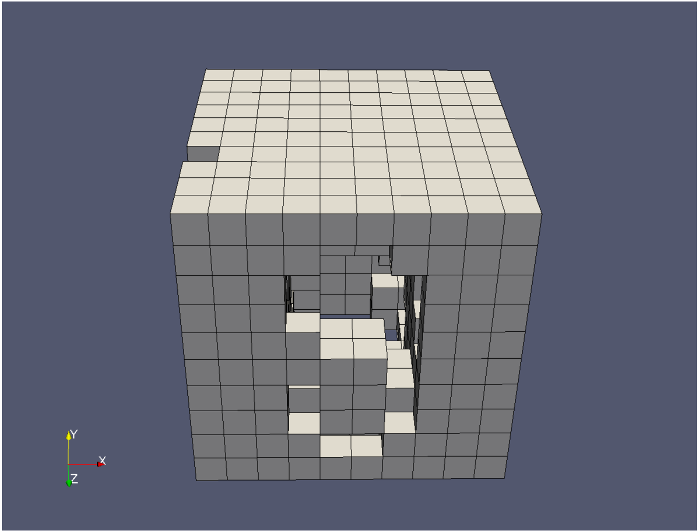
Run ROM at point not in training data

- Poisson Ratio $\nu = 0.2857$

Modify the Albany input file:

- Specify the Exodus file containing the basis
- Add a Model Order Reduction section to the input file
- Specify various options such as the number of modes
- Possibly change the linear solver
  - FOM - typically involves a large, sparse system
  - ROM - involves a small, dense system

Galerkin ROM, 30 Modes, 400 Sample Nodes



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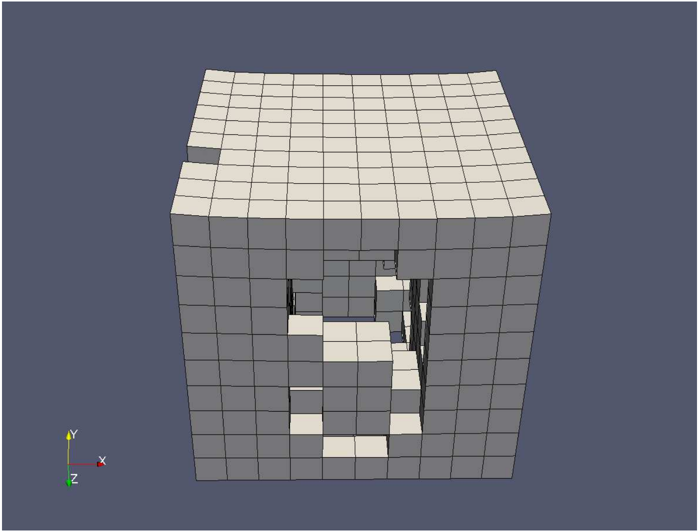

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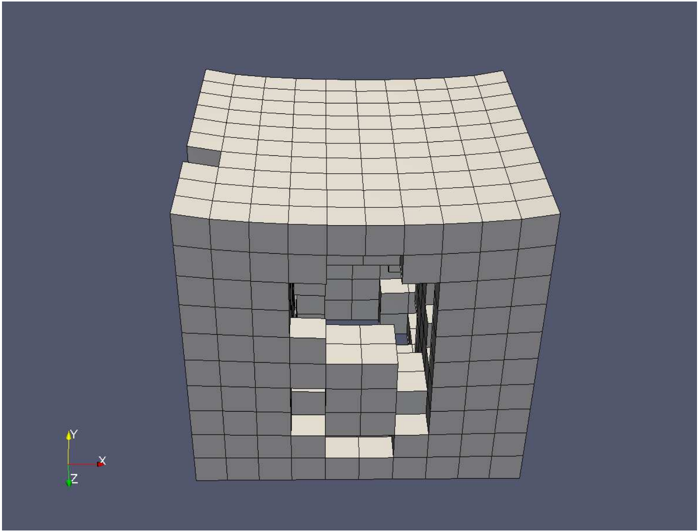

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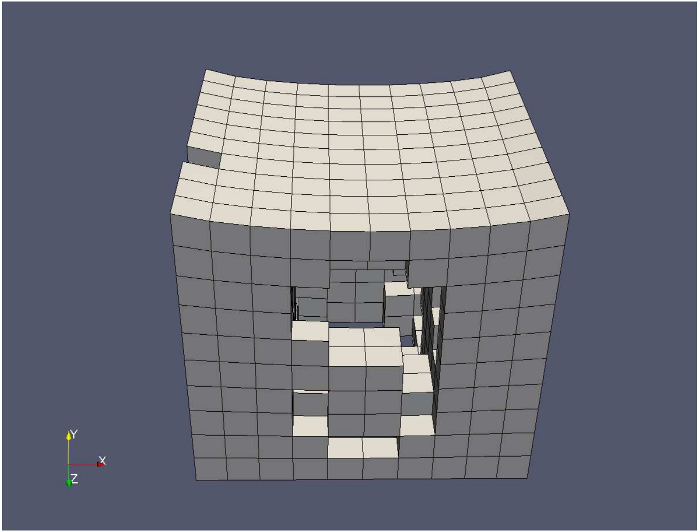

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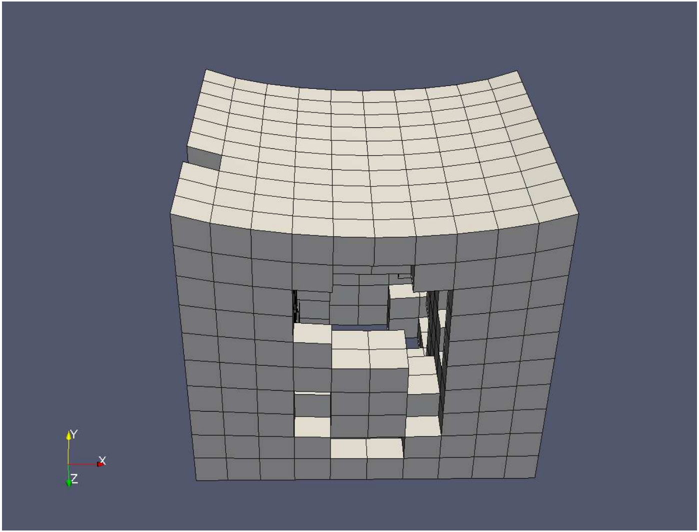

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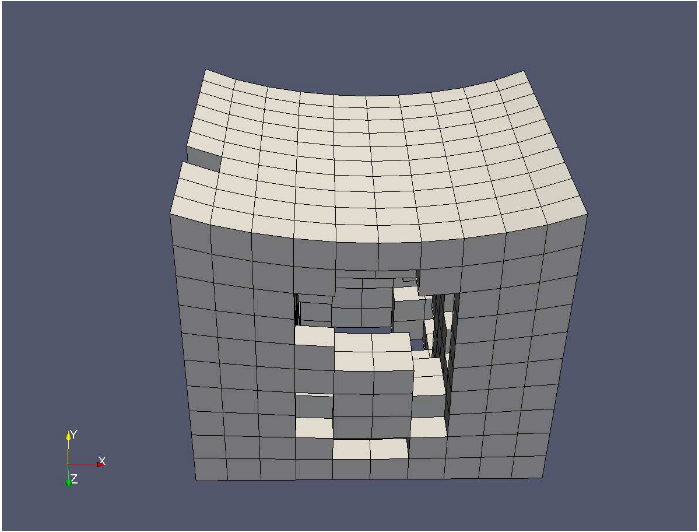

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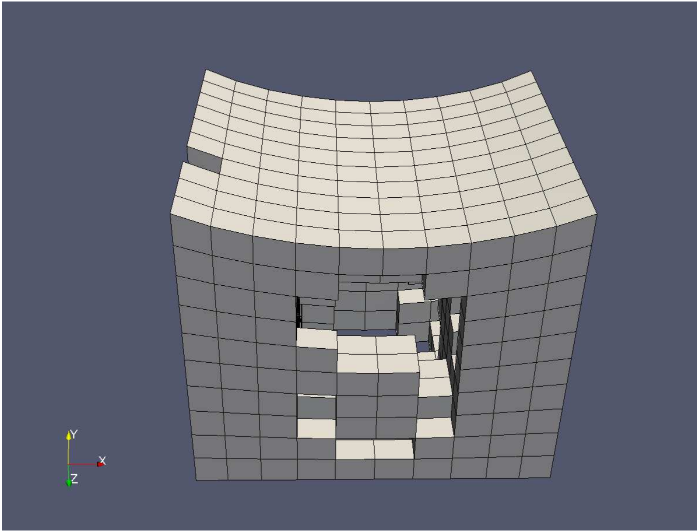

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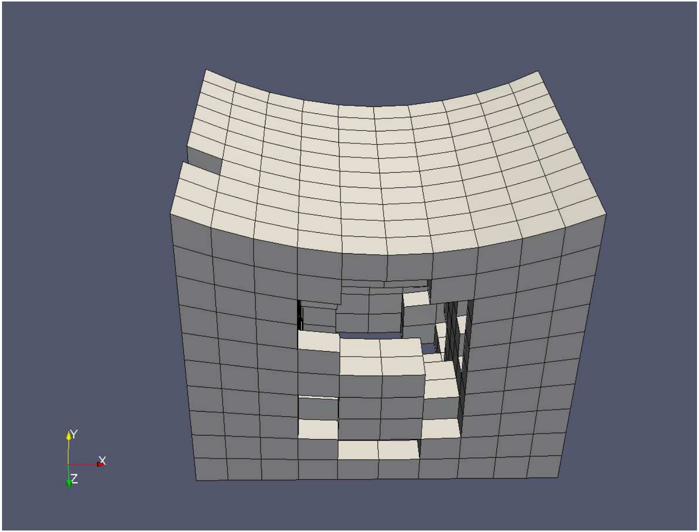

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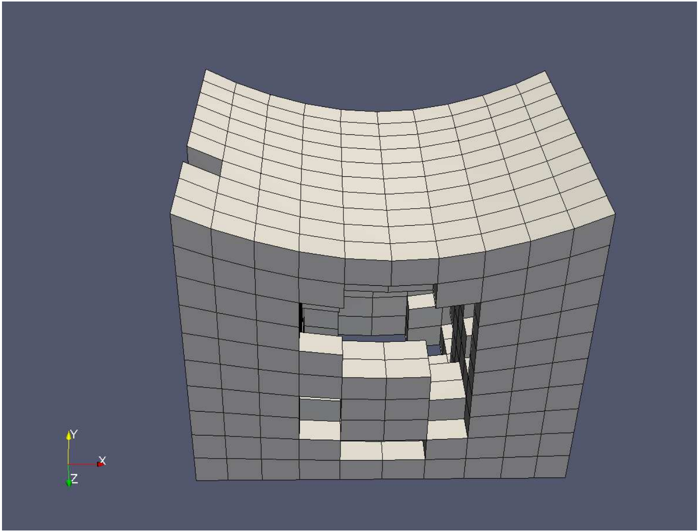

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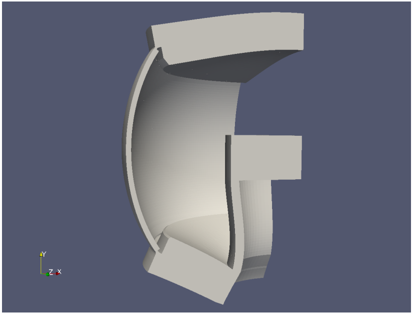
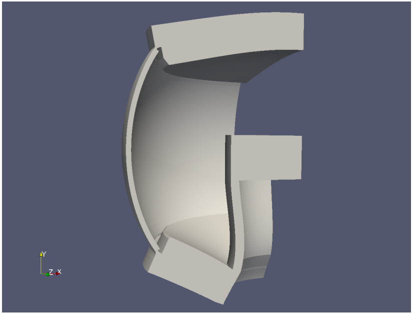
Current work is focused on creating ROMs for complex mechanical and coupled thermal-mechanical systems of interest at Sandia

- Predictive Capability Assessment Project (PCAP) test case



Full-Order Model



Galerkin ROM, no truncation, no hyper-reduction

Current and Future Work

Model Reduction capabilities in Albany are being improved and extended

- LSPG ROMs have improved handling of boundary conditions
- Preconditioned LSPG ROMs have been implemented using IFPACK to try to improve the accuracy and robustness of ROMs
- Investigating structure preserving constraints that may improve the accuracy of the ROMs

Questions?