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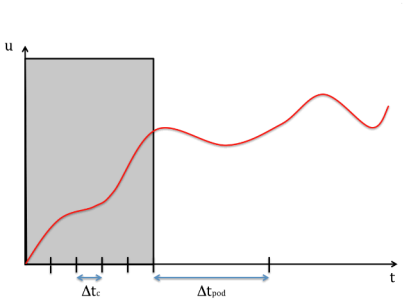

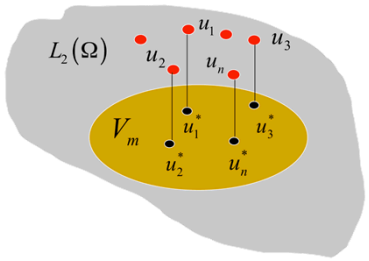

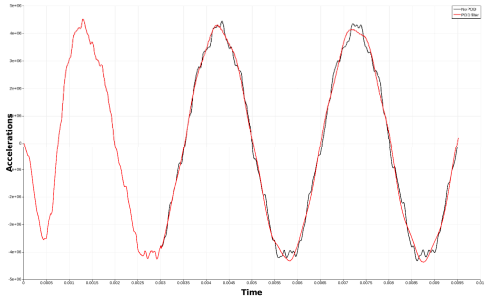

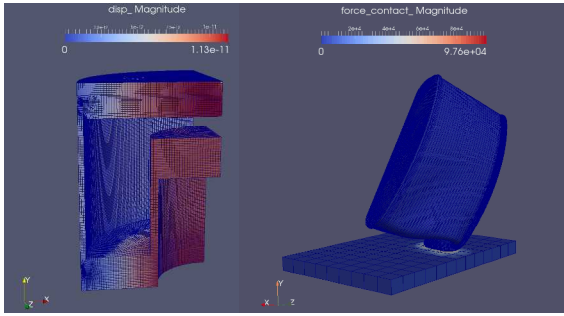

A Multiscale Mass Scaling Approach For Accelerating Explicit Dynamics Computations Using Proper Orthogonal Decomposition

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Sandia National Laboratories

U.S. DEPARTMENT OF ENERGY

National Nuclear Security Administration

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Outline

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- Governing equations
- Multiscale mass scaling approach
- Proper Orthogonal Decomposition (POD)
- Numerical Results
- Conclusions
- Final Remarks
- Acknowledgments
- References

Motivation

Objective: Reduce the computational time of our explicit dynamics simulations while maintaining accuracy in the solution.

- Incorporating fine scale details into a large scale model presents many computational challenges.

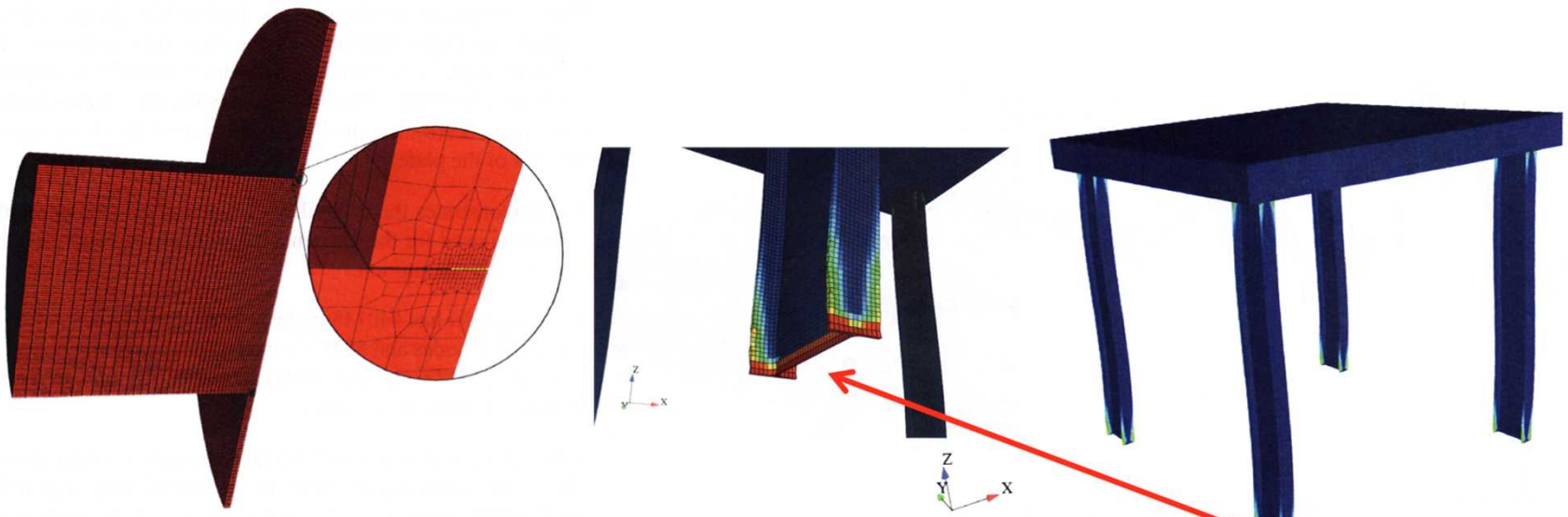

Figure 5.8. Fine mesh of plug drop specimen showing detail of weld region

Motivation

- Refining the finite element mesh to capture these details can result in a very large model.
- In explicit time integration, the critical time step is governed by the smallest elements in the model. As defined by Richtmeyer and Morton (1967) for explicit finite element methods, this critical time step is:

$$\Delta t_c \leq \frac{l}{c}$$

where Δt_c is the critical time step, l is the characteristic length of an element in a finite element mesh and c is the material sound speed.

- High level of refinement can lead to extremely small time steps.

Motivation

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- A wide variety of problems need high spatial resolution as opposed to temporal resolution.
- Many times the contributions of the low frequencies dynamics of the system are the ones of most interest, not necessarily the high-frequency dynamics themselves.
- Our goals center in performing an efficient decomposition of the problem into coarse and fine scales.
- We will attempt to improve performance, and maintain accuracy by allowing special treatment of each of those scales.

Governing equations

Starting with the initial boundary value problem (IBVP) describing the deformation of a solid body over time is given as

$$\nabla \cdot \boldsymbol{\sigma} + \rho \boldsymbol{b} = \rho \ddot{\boldsymbol{u}} \text{ in } \Omega$$

$$\boldsymbol{\sigma} \boldsymbol{n} = \boldsymbol{\tau} \text{ on } \Gamma_\tau$$

$$\boldsymbol{u} = \bar{\boldsymbol{u}} \text{ on } \Gamma_u$$

$$\dot{\boldsymbol{u}}(\boldsymbol{x}, 0) = \boldsymbol{v}_0(\boldsymbol{x})$$

$$\boldsymbol{u}(\boldsymbol{x}, 0) = \boldsymbol{u}_0(\boldsymbol{x})$$

where Ω is the physical domain with boundary Γ, ρ is the density of the material, $\boldsymbol{b}$ is a body force, $\ddot{\boldsymbol{u}}$ is the acceleration, $\boldsymbol{u}$ is the displacement, and $\boldsymbol{\tau}$ represents traction. The unit normal vector on the boundary is denoted as $\boldsymbol{n}$. Furthermore, $\Gamma_u \cap \Gamma_t = \emptyset$ and $\Gamma = \Gamma_u \cup \Gamma_t$. The initial displacement and velocity fields are denoted as $\boldsymbol{u}_0$ and $\boldsymbol{v}_0$, respectively.

Governing equations

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It is assumed that the Cauchy stress $\boldsymbol{\sigma}$ is given from a constitutive equation that relates the stress to the strain $\boldsymbol{\varepsilon}$ and its rates as

$$\boldsymbol{\sigma}(\boldsymbol{x},t) = \boldsymbol{F}\left(\boldsymbol{\varepsilon}(\boldsymbol{x},t), \frac{\partial \boldsymbol{\varepsilon}(\boldsymbol{x},t)}{\partial t}, ..., \frac{\partial^n \boldsymbol{\varepsilon}(\boldsymbol{x},t)}{\partial t^n}\right),$$

where the specific form of $\boldsymbol{F}$ is determined by the material model used.

Taking the variational form of the IBVP presented before, and discretizing using finite elements, we obtain the following semi-discrete system of equations in vector form

$$[M]\{\ddot{u}\} = \{f_{ext}\} - \{f_{int}\}.$$

$$[M]\{\ddot{u}\} = \{f\}.$$

This will be the starting point to describe and derive our approach.

Multiscale mass scaling approach

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Consider the acceleration vector $\{\ddot{u}\}$ to be in a finite dimensional space $U^n = U_f^n \oplus U_c^n$, where U_f^n and U_c^n represent the fine scale space and coarse scale space, respectively. Then, accelerations can be represented as

$$\{\ddot{u}\} = \{\ddot{u}^c\} + \{\ddot{u}^f\},\ \{\ddot{u}^c\} \in U_c^n \quad , \{\ddot{u}^f\} \in U_f^n,$$

where the dominant low frequency accelerations are captured in $\{\ddot{u}^c\}$, and the high frequency ones are contained in $\{\ddot{u}^f\}$. Assume that $U_c^n = \text{span}(\{\phi\}_i)_{i=1}^m$. Then, the coarse scale accelerations can be represented as

$$\{\ddot{u}^c\} = [\Phi]\{\ddot{q}\},$$

where $[\Phi]$ represents a matrix whose columns are the vectors $\{\phi\}_i$ and $\{\ddot{q}\}$ is a vector of coefficients whose dimension is that of the coarse space. Now we can express the semi-discrete governing equations as

$$\{f\} = [M]\{\ddot{u}^c\} + [M]\{\ddot{u}^f\}.$$

Multiscale mass scaling approach

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An expression for the coarse accelerations can be obtained using a Galerkin approach. That is, finding the coarse accelerations that satisfy

$$[\Phi]^T(\{f\} - [M]\{\ddot{u}^c\}) = 0,$$

which is equivalent to the following orthogonality condition between the coarse and fine scale accelerations.

$$\{\ddot{u}^c\}^T[M]\{\ddot{u}^f\} = 0, \ \forall \ \{\ddot{u}^c\} \in U_c^n, \{\ddot{u}_f^n\} \in U_f^n.$$

Defining a matrix $[M_c] = [\Phi]^T[M][\Phi]$, we get

$$[\Phi]^T\{f\} - [M_c]\{\ddot{q}\} = \{0\},$$

from which we can obtain the coarse scale acceleration coefficients as

$$\{\ddot{q}\} = [M_c]^{-1}[\Phi]^T\{f\}.$$

Then, the coarse scale acceleration vector can be written as

$$\{\ddot{u}^c\} = [\Phi][M_c]^{-1}[\Phi]^T\{f\}.$$

Multiscale mass scaling approach

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Now the coarse scale acceleration vector can be written as

$$\{\ddot{u}^c\} = [\Phi][M_c]^{-1}[\Phi]^T\{f\}.$$

The fine scale component of the inertial force can now be computed as

$$\begin{aligned}
[M]\{\ddot{u}^f\} &= \{f\} - [M]\{\ddot{u}^c\} \\
&= \{f\} - [M][\Phi][M_c]^{-1}[\Phi]^T\{f\} \\
&= ([I] - [M][\Phi][M_c]^{-1}[\Phi]^T)\{f\} \\
&= [P]\{f\},
\end{aligned}$$

where $[P] = [I] - [M][\Phi][M_c]^{-1}[\Phi]^T$ is an orthogonal matrix projection.

Multiscale mass scaling approach

The next step in the formulation is to scale the mass matrix of the high frequency accelerations as to increase the critical time step. To this end, we introduce a modified mass matrix defined as

$$[\widetilde{M}] = [\alpha][M],$$

where $[\alpha]$ is a diagonal scaling matrix whose components are defined as

$$\alpha_i = \begin{cases} \frac{(\Delta t)^2}{4} \left(\frac{\hat{K}_i}{M_i} \right)_{\text{max over i}} & \text{if } \Delta t > \Delta t_c \\ 1 & \text{otherwise.} \end{cases}$$

Here, Δt is a user-defined time step, $\hat{K}_i$ is an element nodal stiffness, and M_i is the element lumped mass at Node i.

Multiscale mass scaling approach

The fine scale accelerations can now be expressed as

$$\{\ddot{u}^f\} = [\widetilde{M}]^{-1}[P]\{f\}.$$

The total acceleration vector is obtained as

$$\{\ddot{u}\} = [\Phi][M_c]^{-1}[\Phi]^T\{f\} + [\widetilde{M}]^{-1}[P]\{f\}.$$

Multiscale mass scaling approach

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How do we build this matrix $[\Phi]$?

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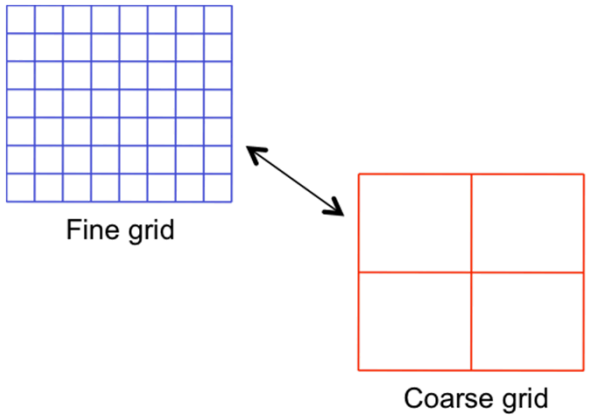
Multigrid approach



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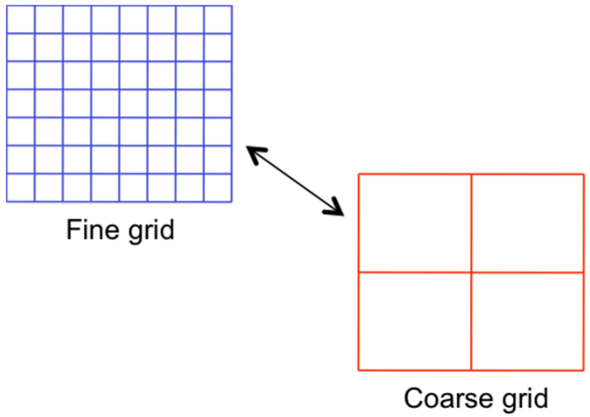
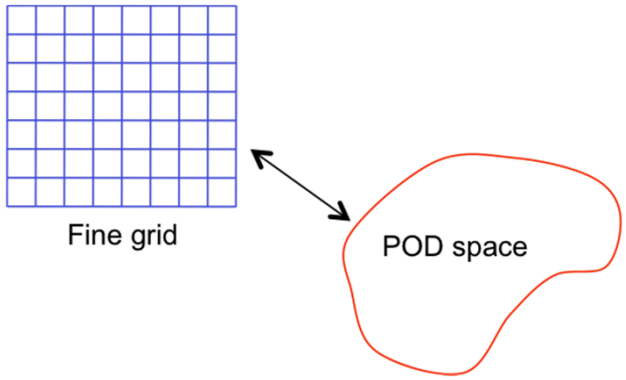


Proper Orthogonal Decomposition approach



Proper Orthogonal Decomposition

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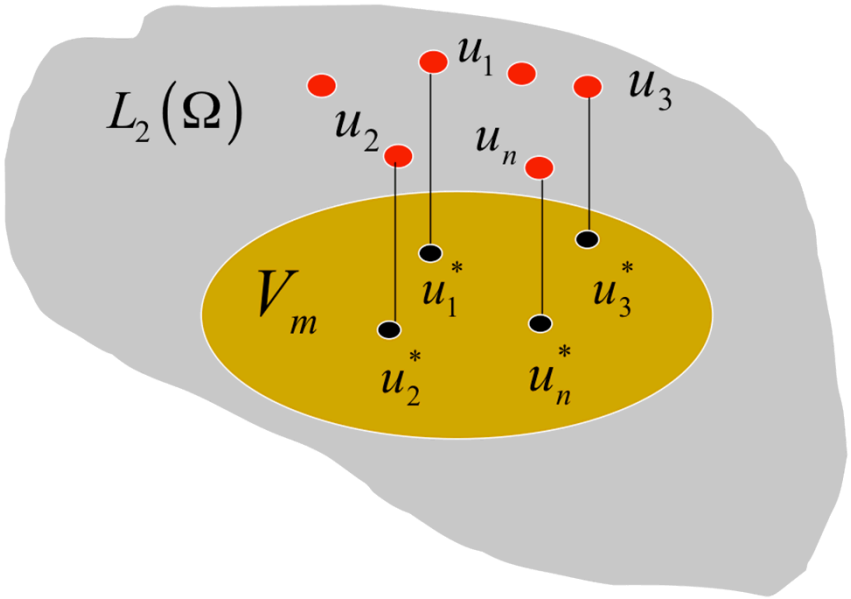
- Proper Orthogonal Decomposition (POD) has been widely used for data analysis and reduced order modeling.
- The main objective of POD is to obtain a low dimensional orthogonal basis for representing an ensemble of high dimensional data.
- POD makes no assumptions about the linearity of the problem to which is applied, so it can be used with any type of nonlinear problem.
- Berkooz, Holmes and Lumley (1993) showed that the eigenvalues associated with the POD modes are related to the kinetic energy of the system.
- Consequently, POD modes are good candidates for building the coarse space represented by the interpolation matrix $[\Phi]$

Proper Orthogonal Decomposition

Given an ensemble of functions $\{\boldsymbol{u}_k\}_{k=1}^n \in L_2$. The main goal in POD is to find a sequence of subspaces such that the average distance between the members of the ensemble and these subspaces is minimal.



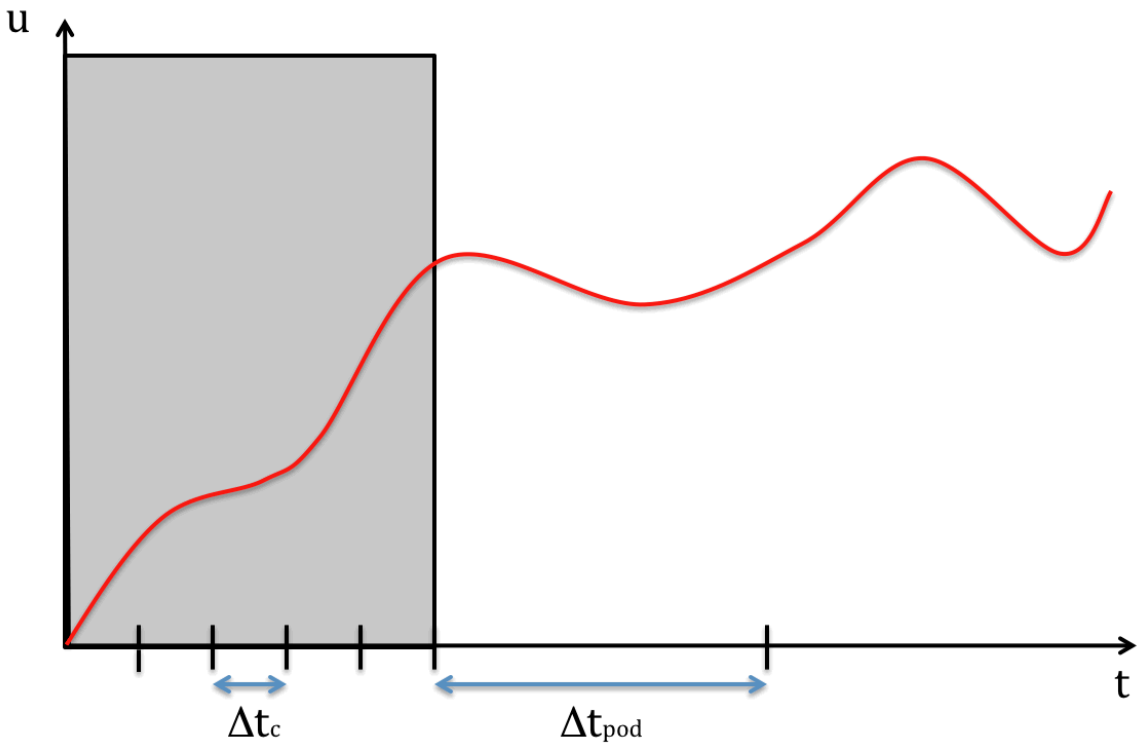
In other words, find finite dimensional representations of the form:

$$\hat{\boldsymbol{u}}(\boldsymbol{x}) = \sum_{j=1}^{m} a_j \boldsymbol{\phi}_j(\boldsymbol{x})$$

where $\boldsymbol{\phi}_j(\boldsymbol{x})$ denotes the j^{th} POD mode and a_j is a scalar coefficient.

Proper Orthogonal Decomposition

- In this work, the ensemble of functions needed to compute the POD modes were taken as the displacements obtained at early time steps of the full scale simulation.
- These functions turn out to be snapshots of the displacement solution vectors at specific times during the simulation.



Numerical Results

- What effect does this approach have on the accelerations?

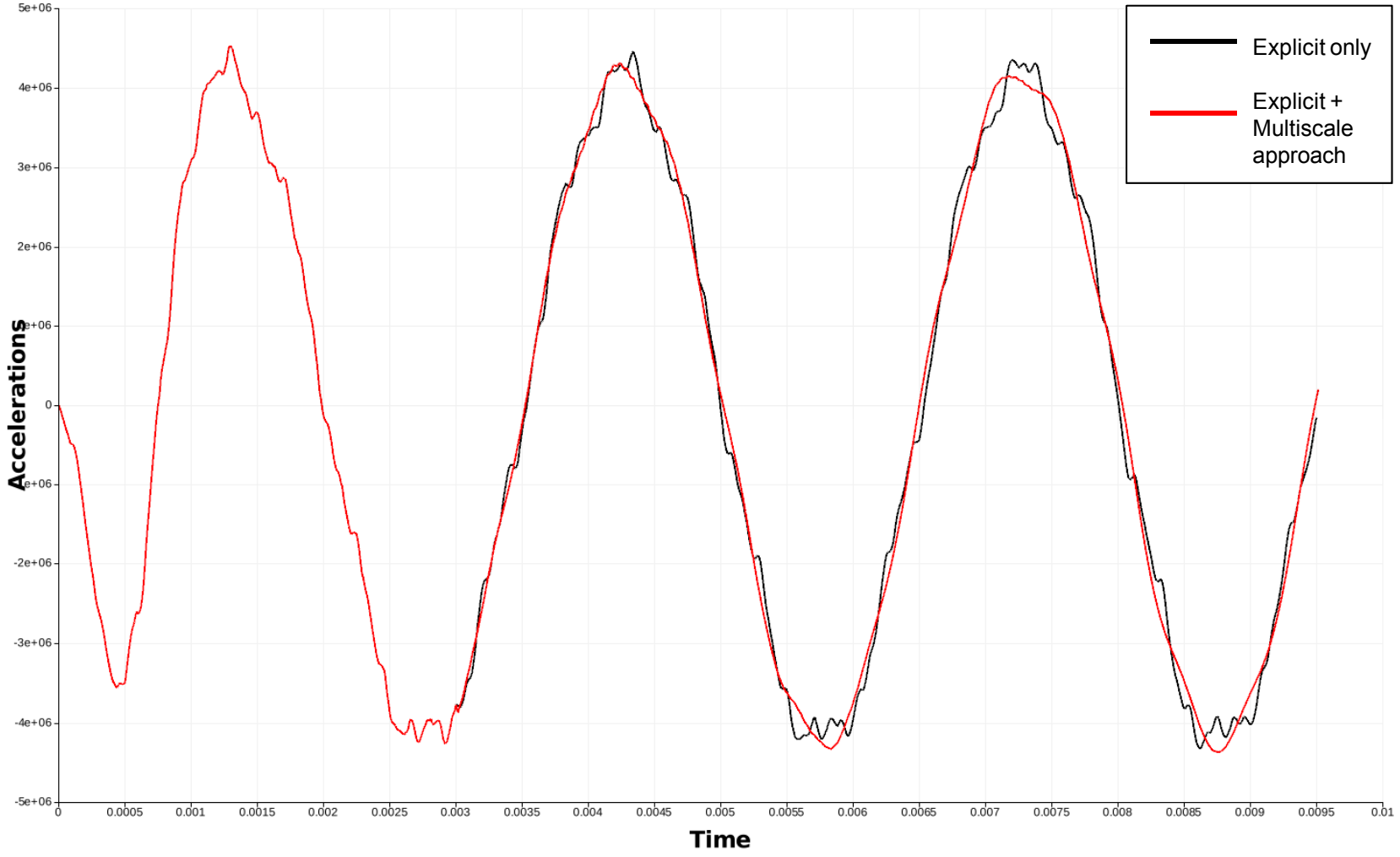
Numerical Results

- What effect does this approach have on the accelerations? Remember:

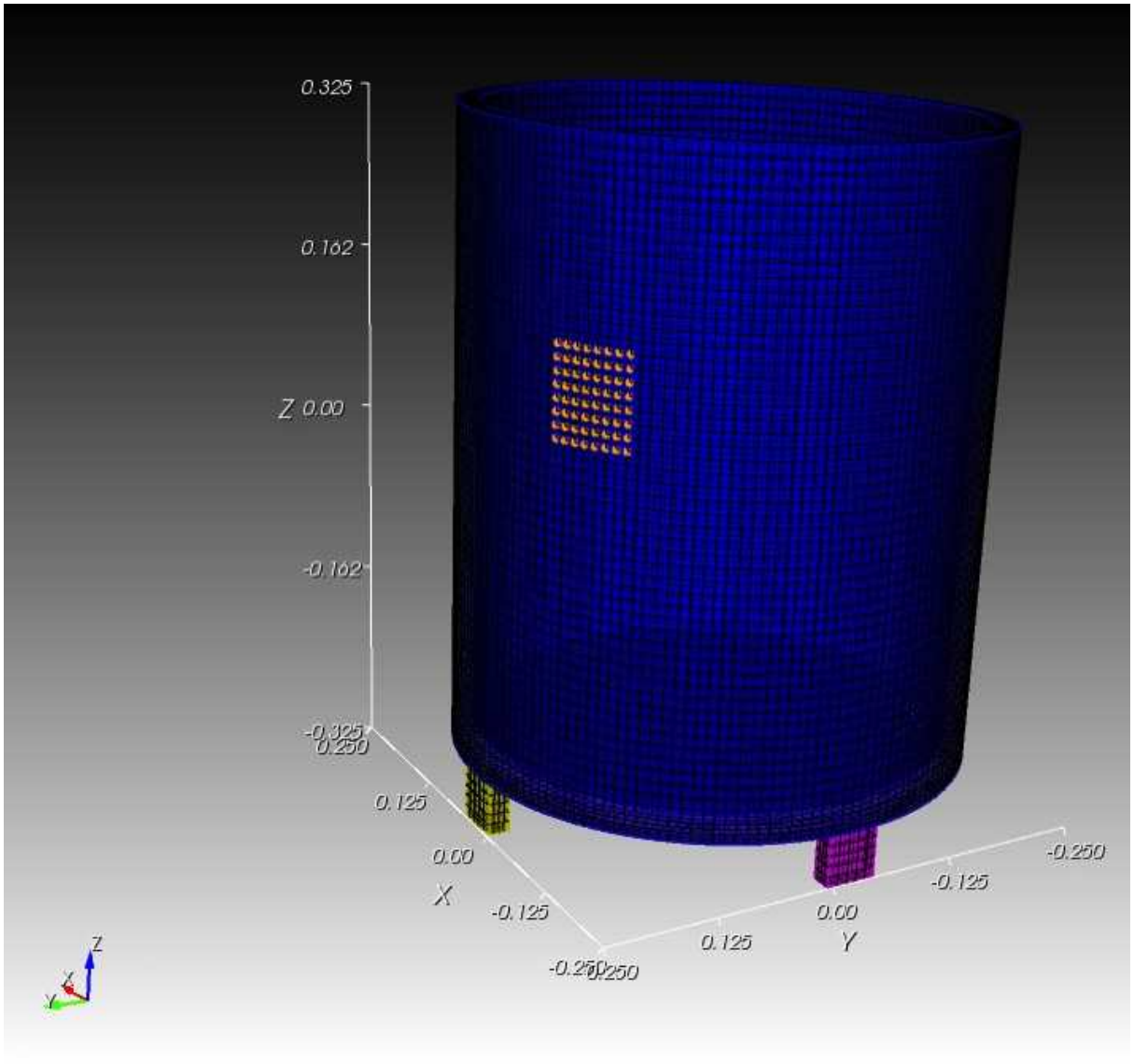
$$\{\ddot{u}\} = [\Phi][M_c]^{-1}[\Phi]^T\{f\} + [\widetilde{M}]^{-1}[P]\{f\}$$

Numerical Results

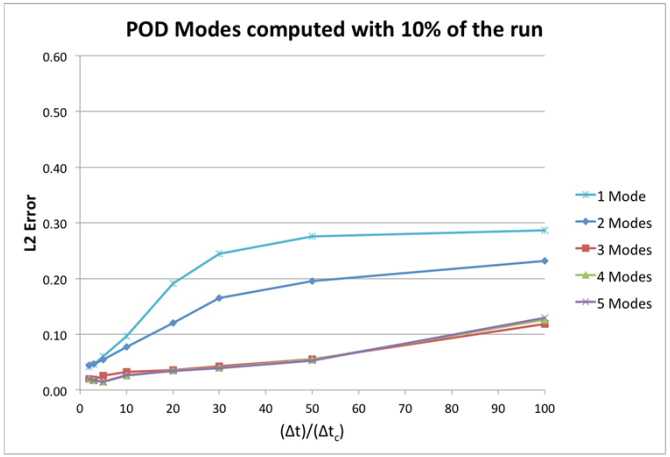
- What effect does this approach have on the accelerations?



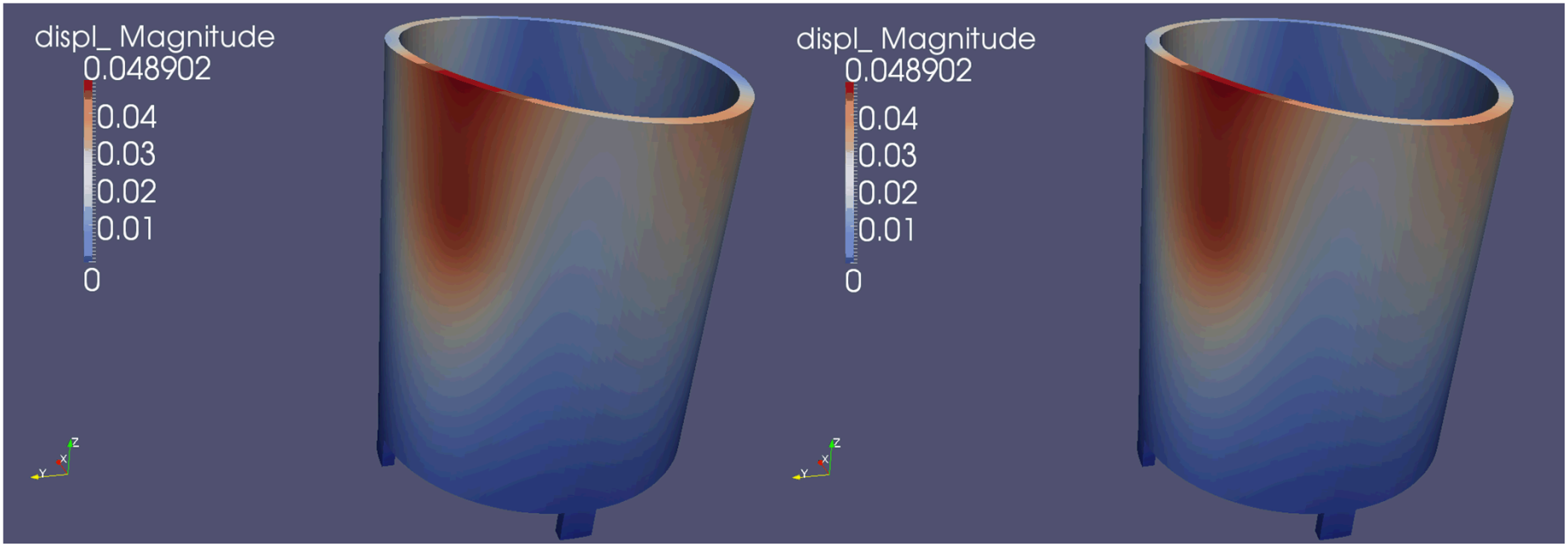
Numerical Results – Example 1



- Linear elastic material
- Fixed displacements in bottom of legs.
- Load on selected nodes increases linearly over time.
- Termination time is 5×10^{-4} s
- ~45K HEX8 elements



Numerical Results – Example 1



(a) (b)

- Displacement magnitude at a time of 5×10^{-4} s: a) using conventional central difference algorithm; b) using multiscale approach with 10 snapshots, 5 POD modes and $3(\Delta t_c)$ time step.

Numerical Results – Example 1

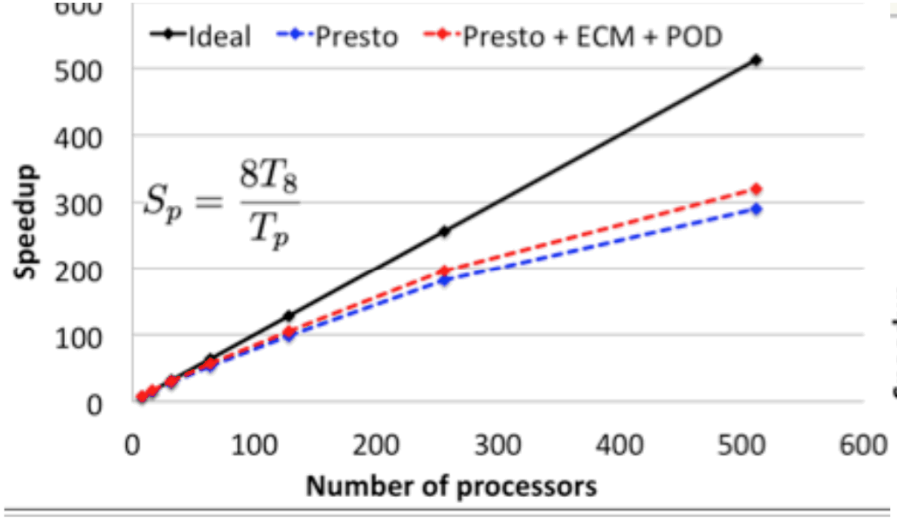
Table 1: POD modes computed at 10% of the simulation time

(a) Performance improvements for total simulation time

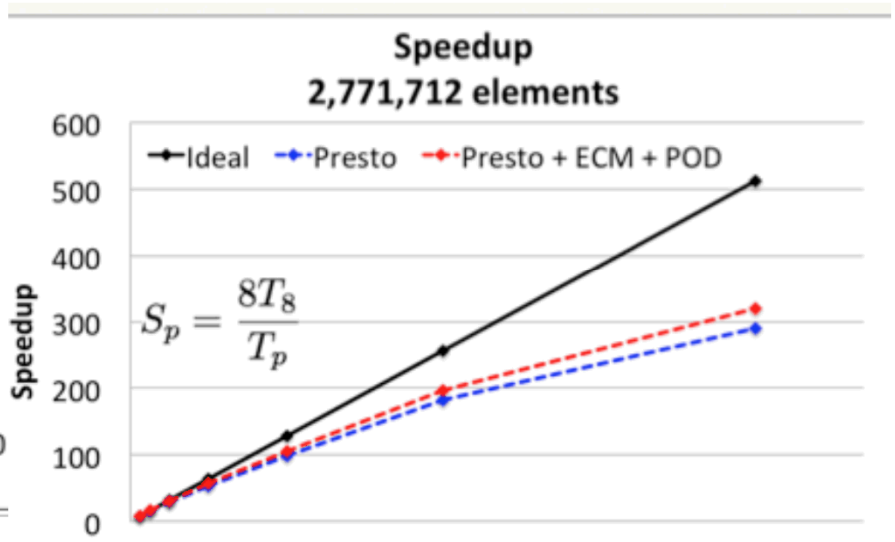
Method	Time step (s)	CPU time (s)	PIF	Von Mises Stress relative error %
Explicit dynamics	Δt_c	2396.29	-	-
Multiscale explicit dynamics using 5 POD modes	$3(\Delta t_c)$	1176.92	2.04	1.58%
	$10(\Delta t_c)$	582.33	4.11	2.24%
	$20(\Delta t_c)$	448.76	5.34	3.14%

Numerical Results – Example 1

- **Parallel computing**



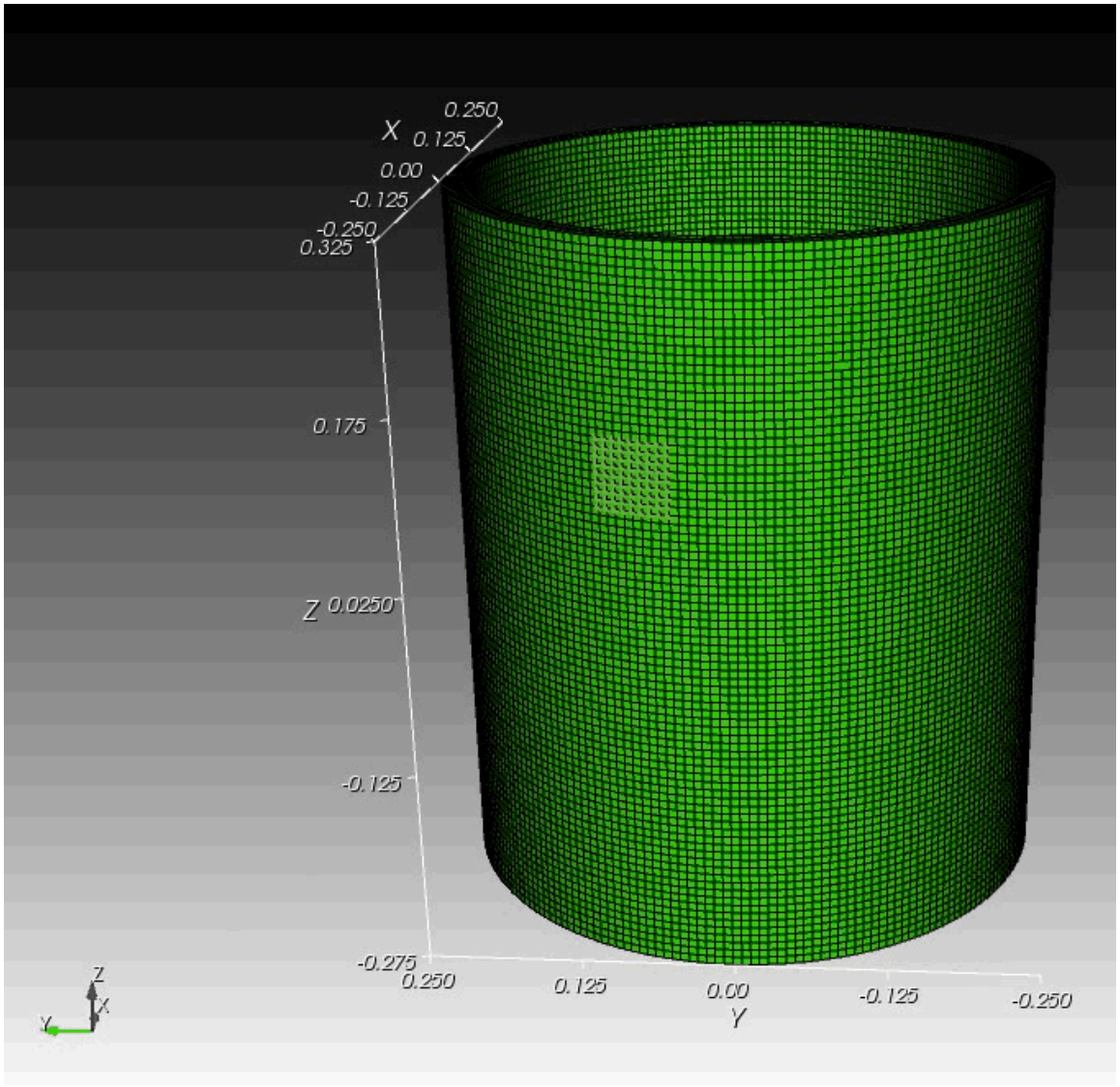
(a)



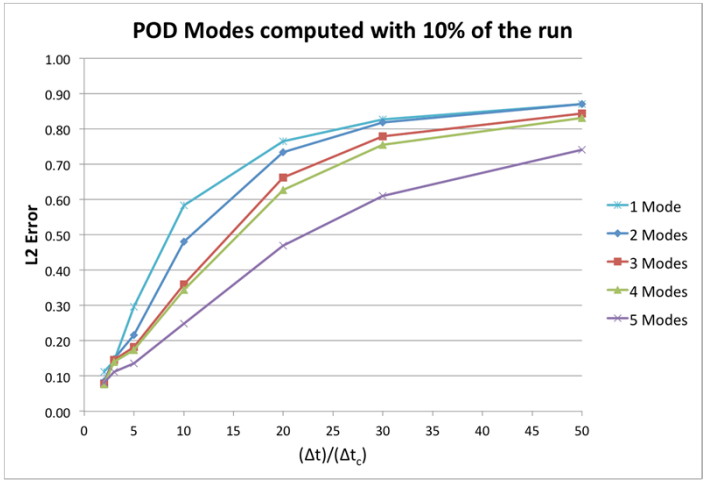
(b)

- a) Speedup and b) Efficiency results for 2,771,712 element problem in Example 1

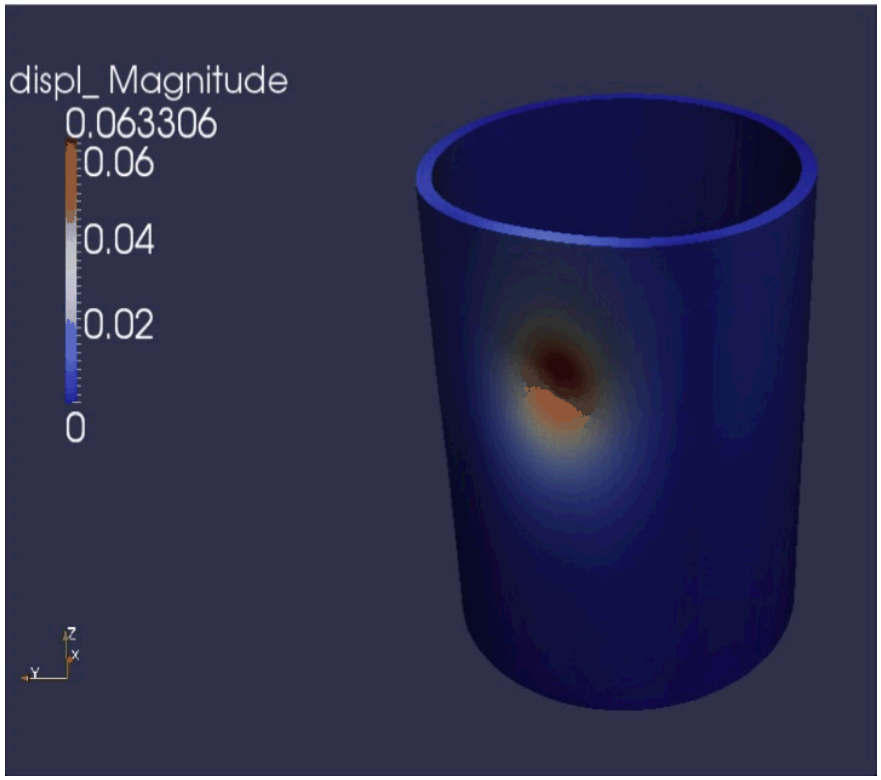
Numerical Results – Example 2



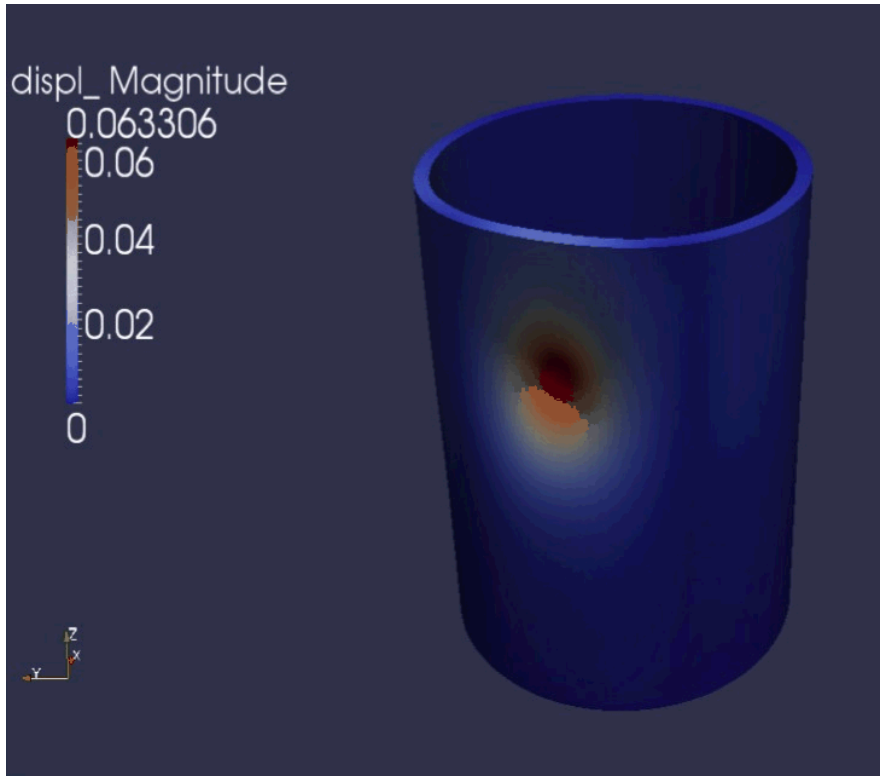
- Elastic-plastic non-linear material
- Bottom of cylinder fixed.
- Load on selected nodes varies linearly over time.
- Termination time is 5×10^{-4} s
- ~44K HEX8 elements



Numerical Results – Example 2



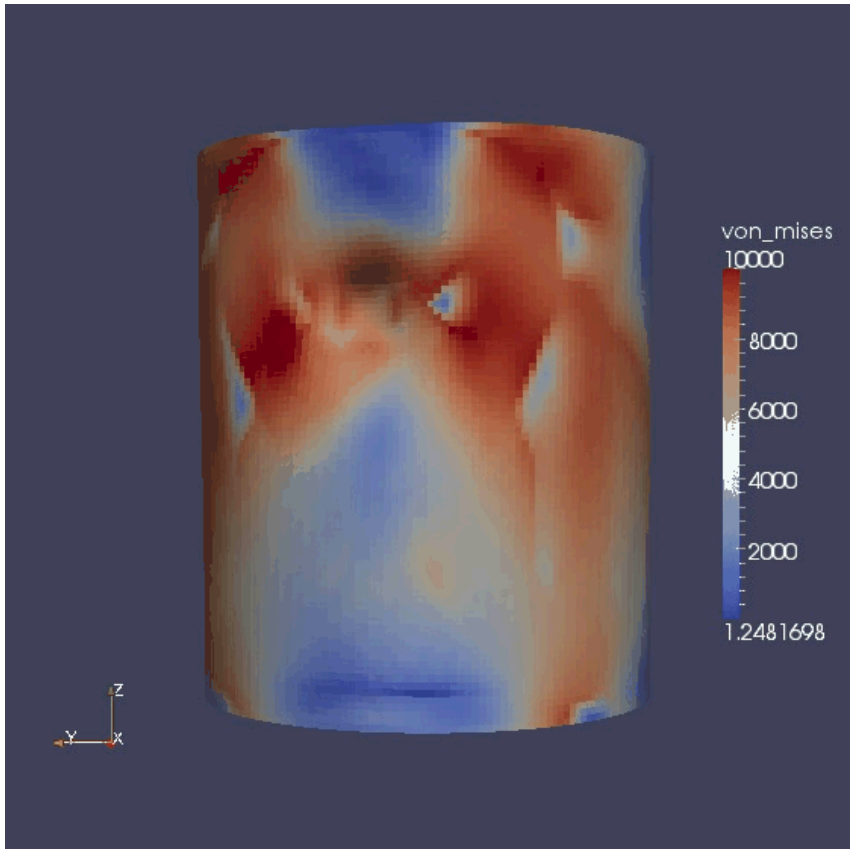
(a)



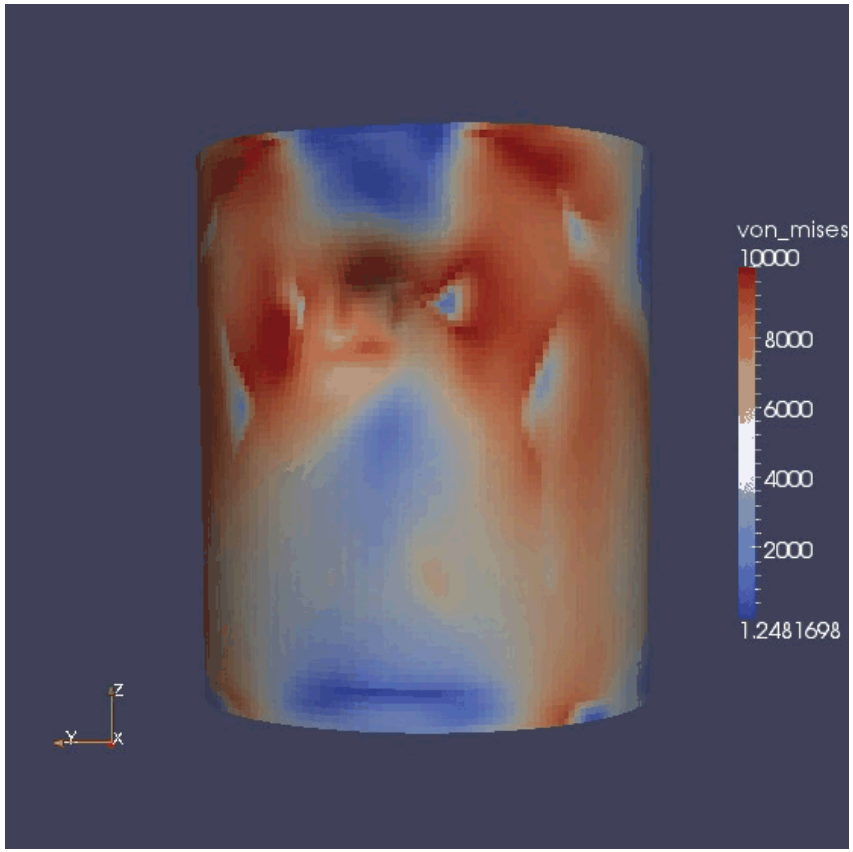
(b)

- Displacement magnitude results at termination time of 5×10^{-4} s: a) using conventional central difference algorithm; b) using multiscale approach with 20 snapshots and 5 POD modes.

Numerical Results – Example 2



(a)



(b)

- Von Mises results at termination time of 5×10^{-4} s: a) using conventional central difference algorithm; b) using multiscale approach with 20 snapshots and 5 POD modes.

Numerical Results – Example 2

Table 1: POD modes computed at 10% of the simulation time

(a) Performance improvements for total simulation time

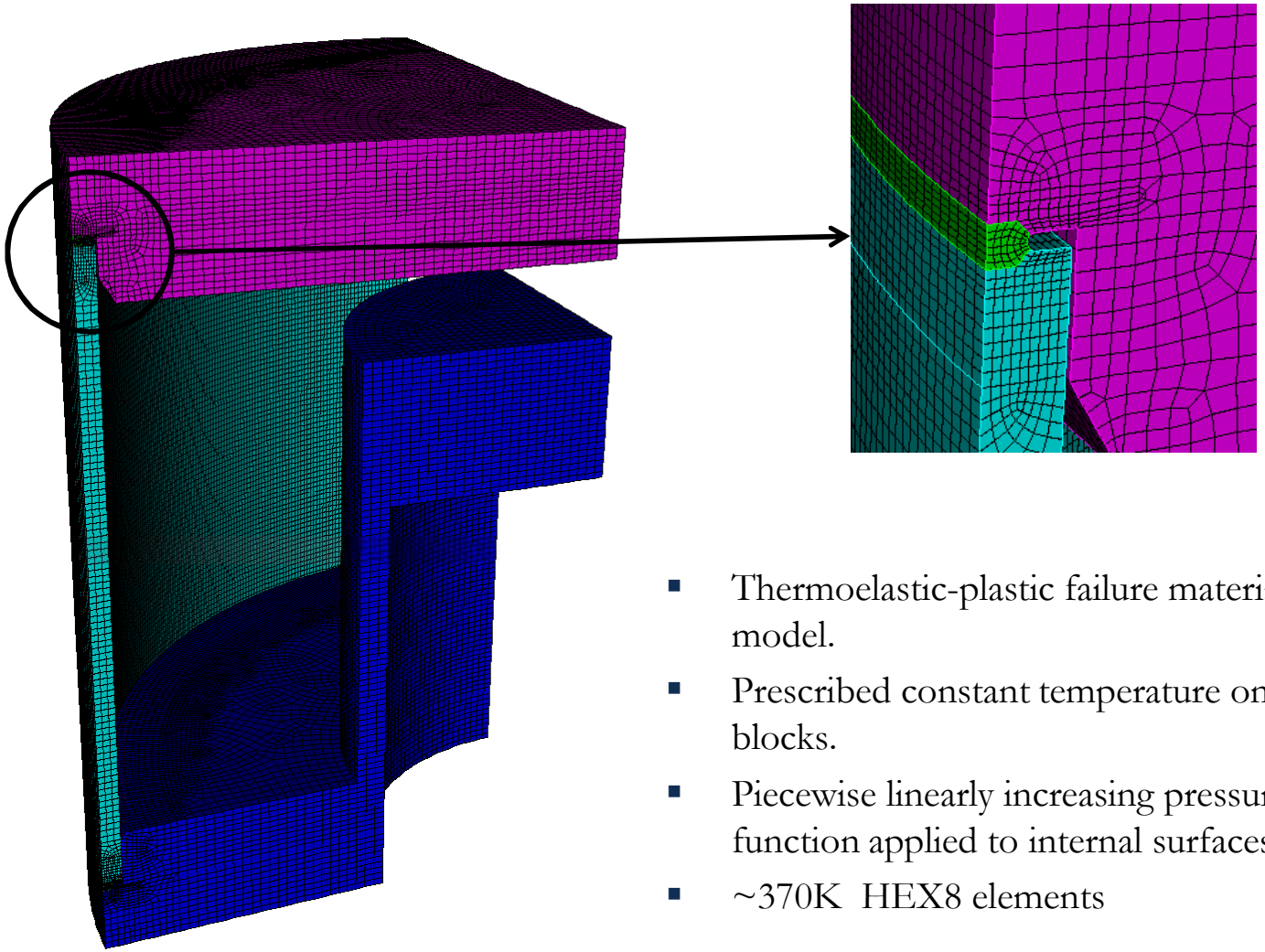
Method	Time step (s)	CPU time (s)	PIF	Displacement relative error %
Explicit dynamics	Δt_c	3014.24	-	-
Multiscale explicit dynamics using 5 POD modes	$2(\Delta t_c)$	2135.01	1.41	8.09%
	$3(\Delta t_c)$	1587.55	1.90	11.14%
	$5(\Delta t_c)$	1068.09	2.82	13.57%

POD modes refresh

Table 2: Multiscale approach using 5 POD modes and POD modes refresh

	Performance Improvement Factor		Displacement relative error %	
Time step Δt_c	POD modes not recomputed	POD modes recomputed	POD modes not recomputed	POD modes recomputed
$2(\Delta t_c)$	1.41	1.12	8.09	5.67
$3(\Delta t_c)$	1.90	1.59	11.14	6.52
$5(\Delta t_c)$	2.82	2.22	13.57	8.23

Numerical Results – Example 3



- Thermoelastic-plastic failure material model.
- Prescribed constant temperature on all blocks.
- Piecewise linearly increasing pressure function applied to internal surfaces.
- ~370K HEX8 elements

Numerical Results – Example 3

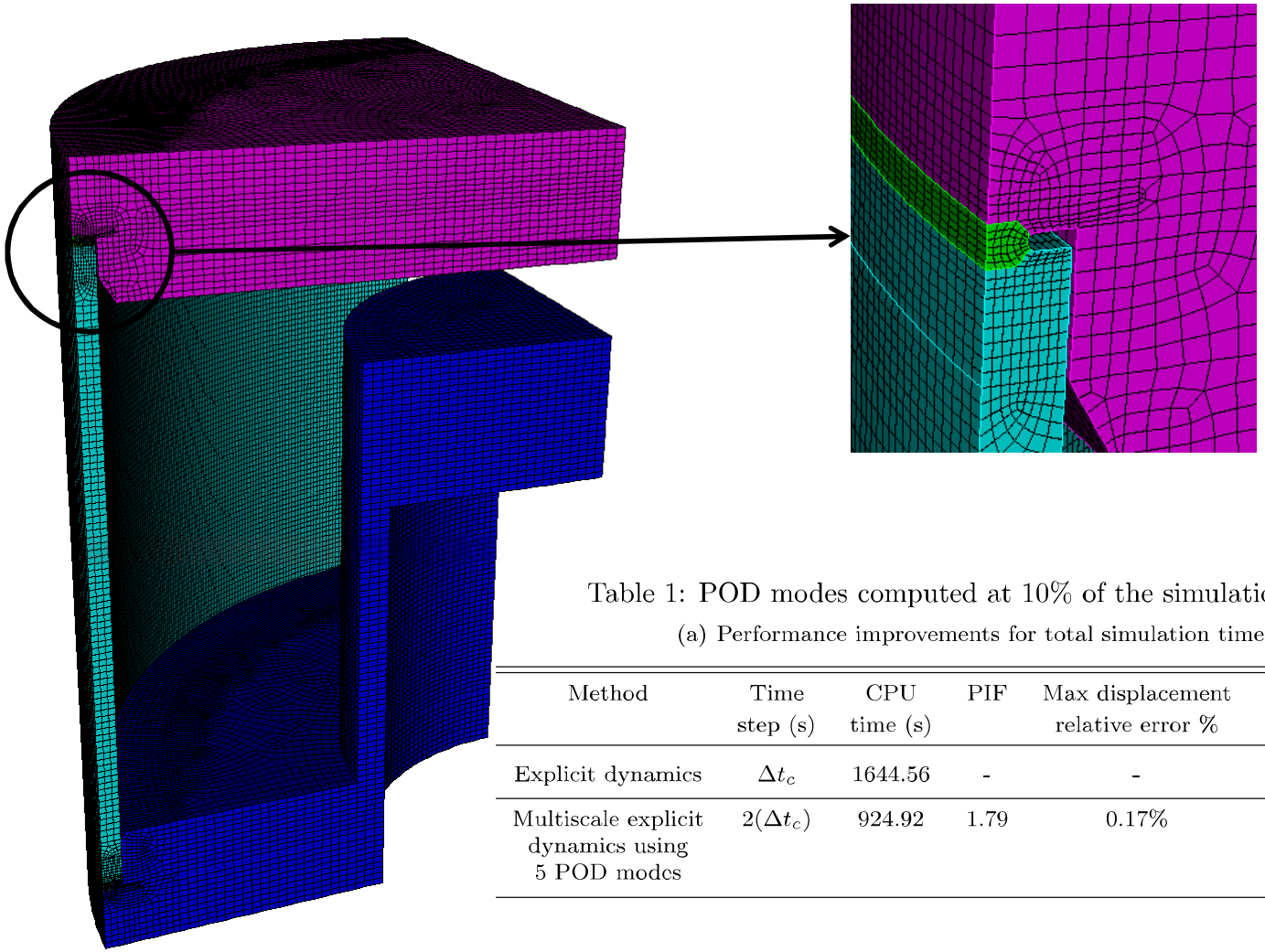
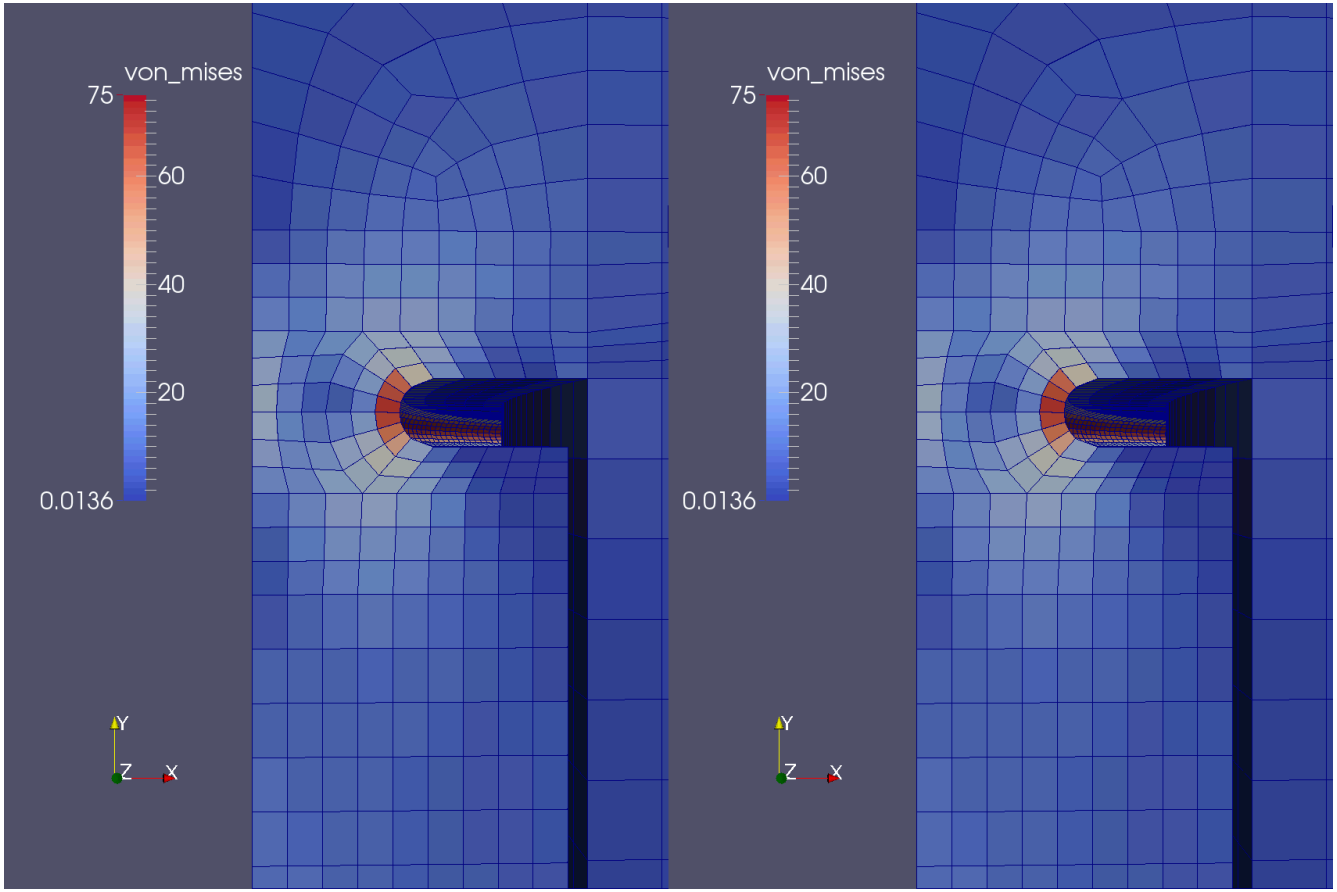


Table 1: POD modes computed at 10% of the simulation time

(a) Performance improvements for total simulation time

Method	Time step (s)	CPU time (s)	PIF	Max displacement relative error %	Max Von Mises relative error %
Explicit dynamics	Δt_c	1644.56	-	-	
Multiscale explicit dynamics using 5 POD modes	$2(\Delta t_c)$	924.92	1.79	0.17%	0.14%

Numerical Results – Example 3



(a) (b)

- Von Mises results at termination time of 1×10^{-4} s: a) using conventional central difference algorithm; b) using multiscale approach with 15 snapshots collected in initial 10% of the simulation, and 5 POD modes.

Conclusions

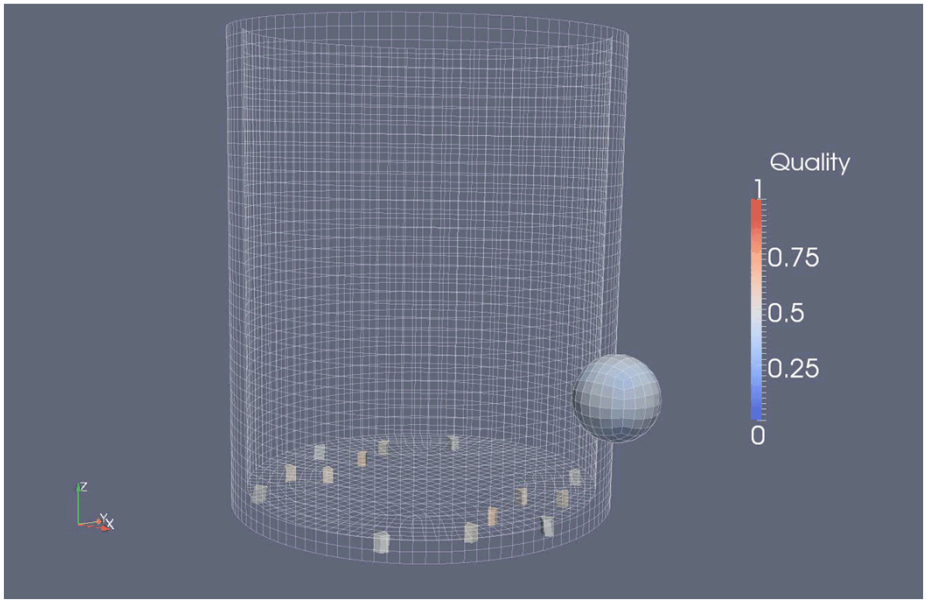
- Reduced the computational time of our explicit dynamics simulations while maintaining accuracy in the solution, for problems dominated by low frequency responses over time. This was accomplished with our multiscale mass scaling approach using proper orthogonal decomposition.
- In some cases, significantly larger time steps were achieved, without compromising accuracy.
- Using a larger number of POD modes to build the coarse space decreased the error in the solution.
- Increasing the number of snapshots used to build the POD modes led to smaller errors.
- Accuracy was improved by refreshing the POD modes during the simulation.
- The implementation of this multiscale mass scaling approach proved to be very scalable, adhering to SIERRA Mechanics code standards.

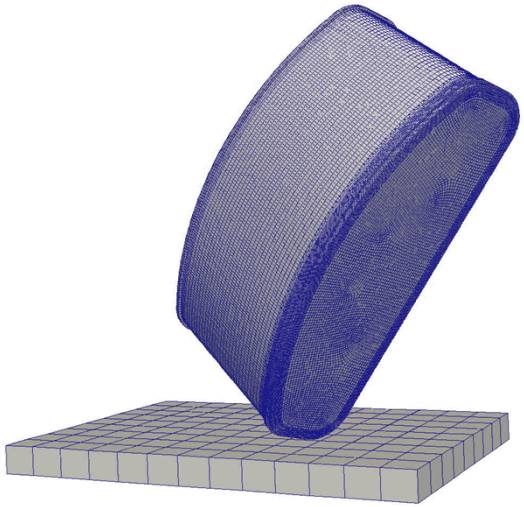
Future directions

- We should focus on improving the overall robustness of this method by studying how the difference sources of error influence accuracy and stability.
- Understanding how the different sources of error relate to each other and affect the solution of the problem can help in choosing more appropriate coarse time step estimates.
- Explore new ideas that can provide further guidance in choosing an appropriate amount of snapshots and POD modes "on the fly" during a simulation, and that can guarantee accuracy while still delivering performance improvements.
- Selective block implementation of this approach might also improve performance and increase accuracy.
- We have observed that problems involving contact still present a big challenge.

Future directions

- Can we tackle these problems with this approach?





Acknowledgments

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- Cornell University
  - Prof. Wilkins Aquino
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Questions?

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