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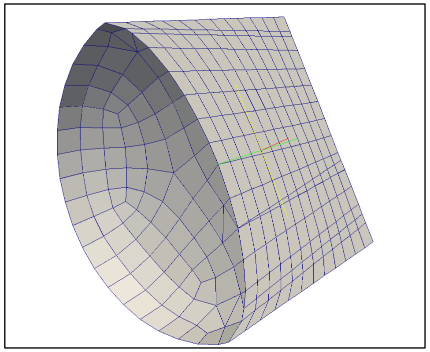
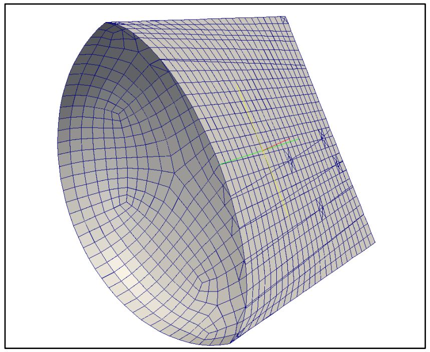
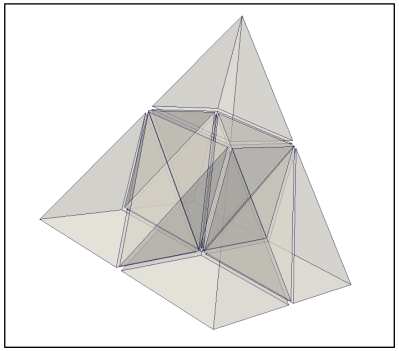
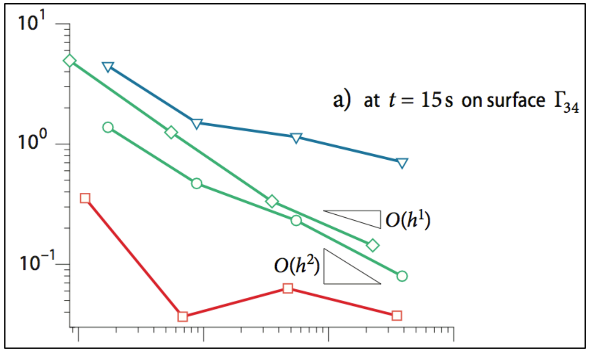

III. Solution Verification

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April 2014

U.S. DEPARTMENT OF ENERGY

NNSA National Nuclear Security Administration

Solution Verification

- In the Intro, we discussed the error model:

$$Q(h) = Q + C\,h^p$$

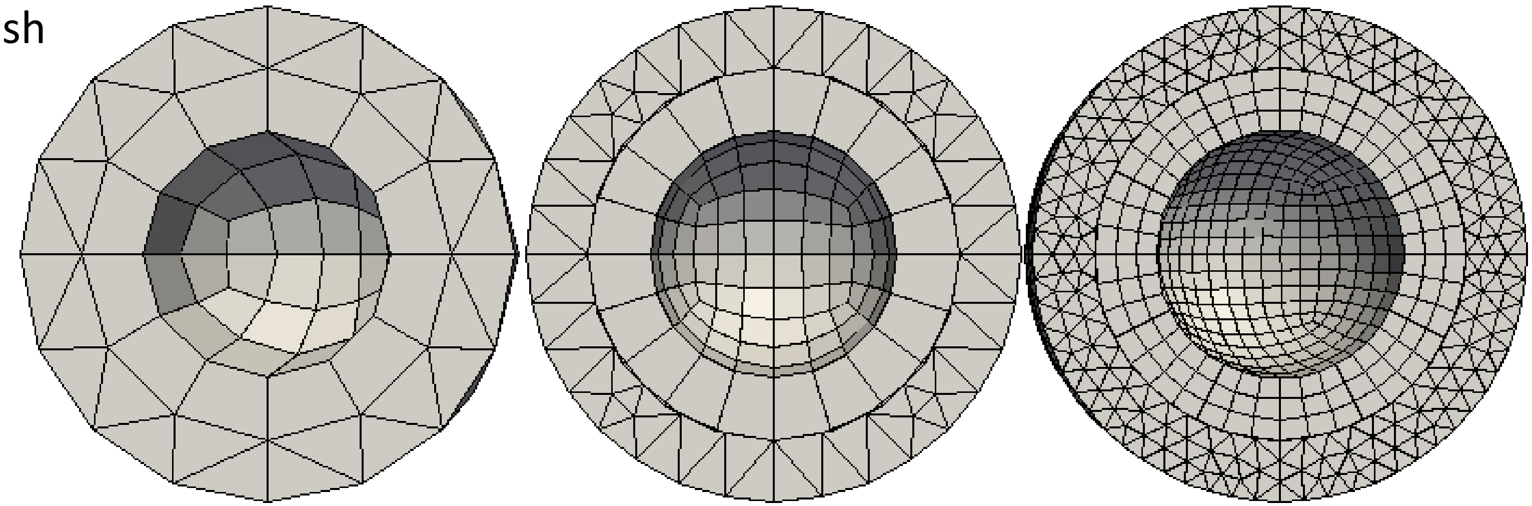
- When the true solution (*Q*) is unknown, we need solutions computed on 3 meshes to estimate *Q*.
  - This is a costly exercise, but is general and robust
- In this part, we discuss:
  - How we generate the meshes (UMR)
  - Further details on extrapolation
  - Basic examples of solution verification
  - What can go wrong
  - Complex examples: interpreting the results

Uniform Mesh Refinement (UMR)

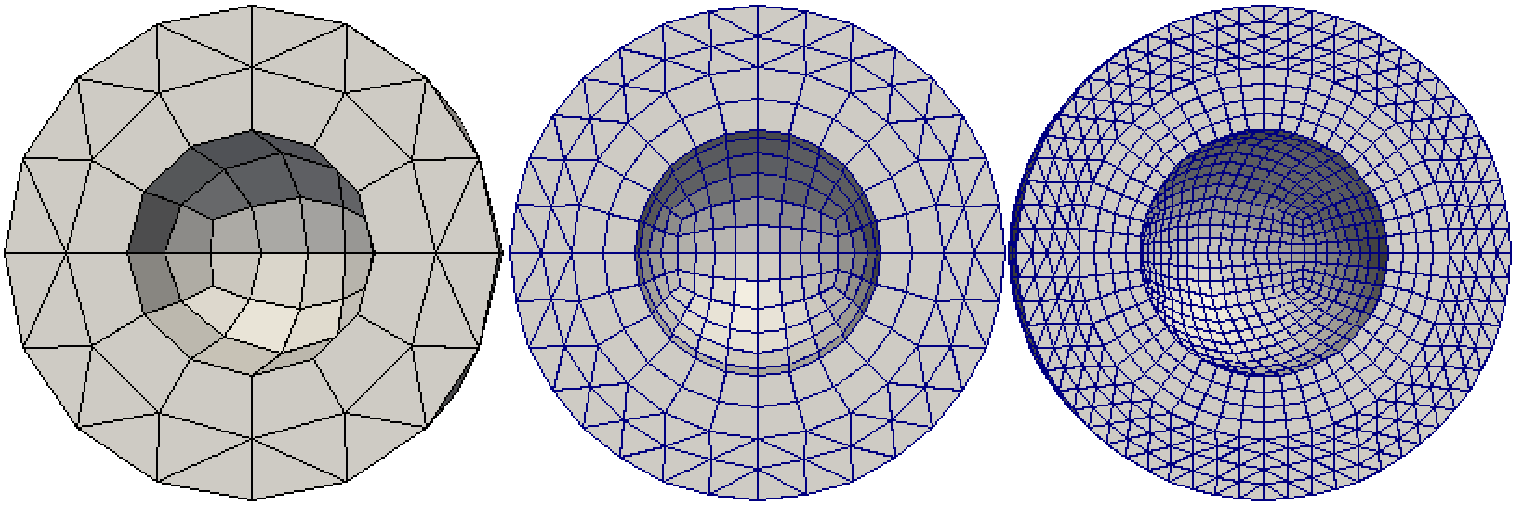
- We assume that someone has already built a mesh
- Ideally the CAD geometry should be preserved
- Multiple meshes are needed to assess convergence
  - Ideally the mesh size should be uniformly reduced
  - Geometric resolution should improve
- Tools for making finer (and coarser meshes):
  - Remeshing using the mesh generator (Cubit)
  - Uniform refinement by regular subdivision of each element (Percept or Cubit)
  - Mesh scaling to generate coarser or finer meshes (Cubit)

UMR: Example Meshes

Remesh



Refine (8x)

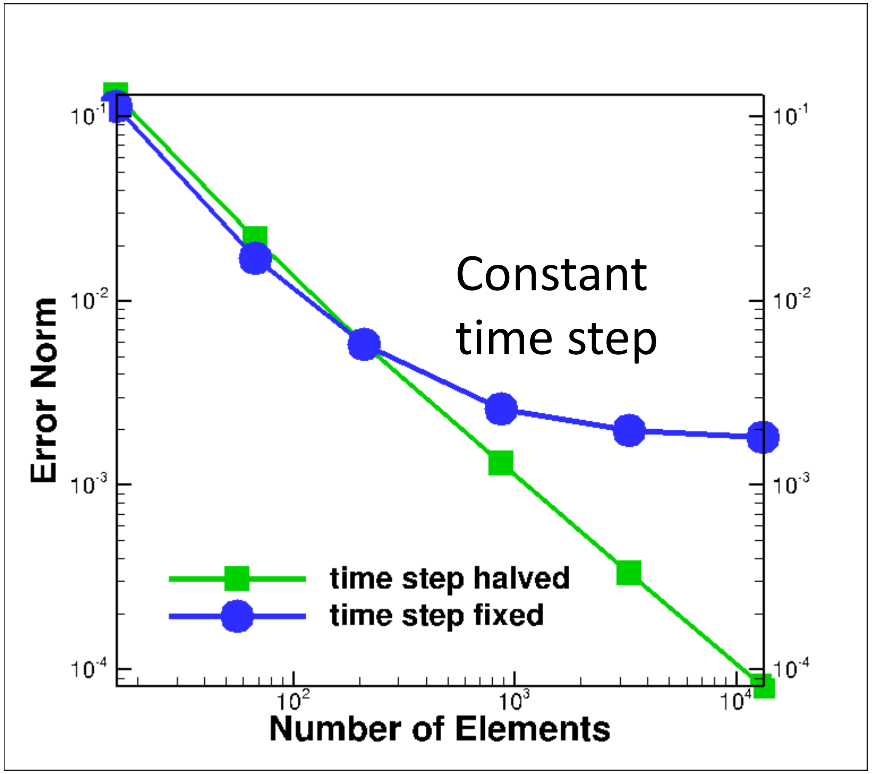


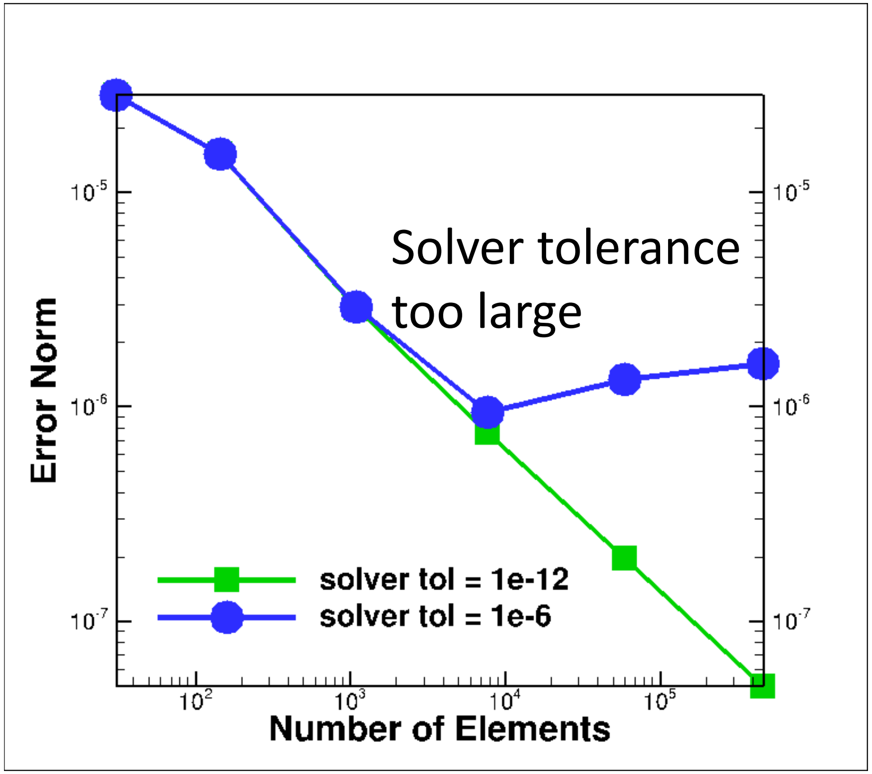
Handling Numerical Controls

- Most of the cost of UMR convergence studies arises from the use of increasingly finer meshes
- Many other numerical knobs should be controlled:
  - Time step size
  - Linear solver tolerances
  - Search tolerances (contact)
  - View factor resolution (enclosure radiation)
  - Iterative convergence for nonlinear & coupled physics
- Best practice: do a sensitivity study on the coarse mesh of all other numerical controls
  - Which are most sensitive?
  - What are sufficiently small tolerances?

Example: Numerical Controls

- We demonstrate the effect of not refining the time step or adequately controlling the linear solver tolerance





Using the Error Model for Extrapolation

- 3 parameters (*Q*,*C*,*p*) => need 3 equations
- Main assumptions:
- Ideally choose common mesh size ratio (*r*) – typically 2
- But can still handle non-uniform mesh size case
- Resulting solution – note that rate (*p*) depends mainly on <u>ratio of the changes in QoI</u>

$$Q(h) = Q + C\,h^p$$

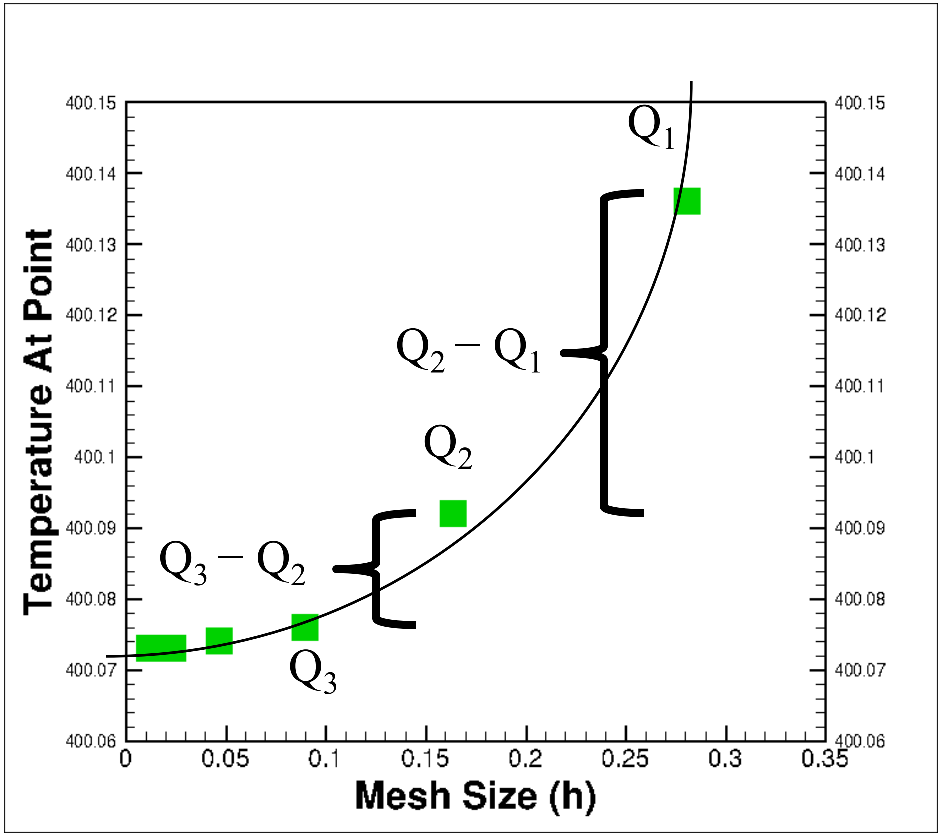
$$h_1 > h_2 > h_3, \quad r = \frac{h_1}{h_2} = \frac{h_2}{h_3}$$

$$p = \log\left(\frac{Q_2 - Q_1}{Q_3 - Q_2}\right) / \log(r)$$

$$C = \frac{Q_2 - Q_1}{h_2^p - h_1^p}$$

$$Q = Q_1 - C\,h_1^p$$

Extrapolation in Pictures



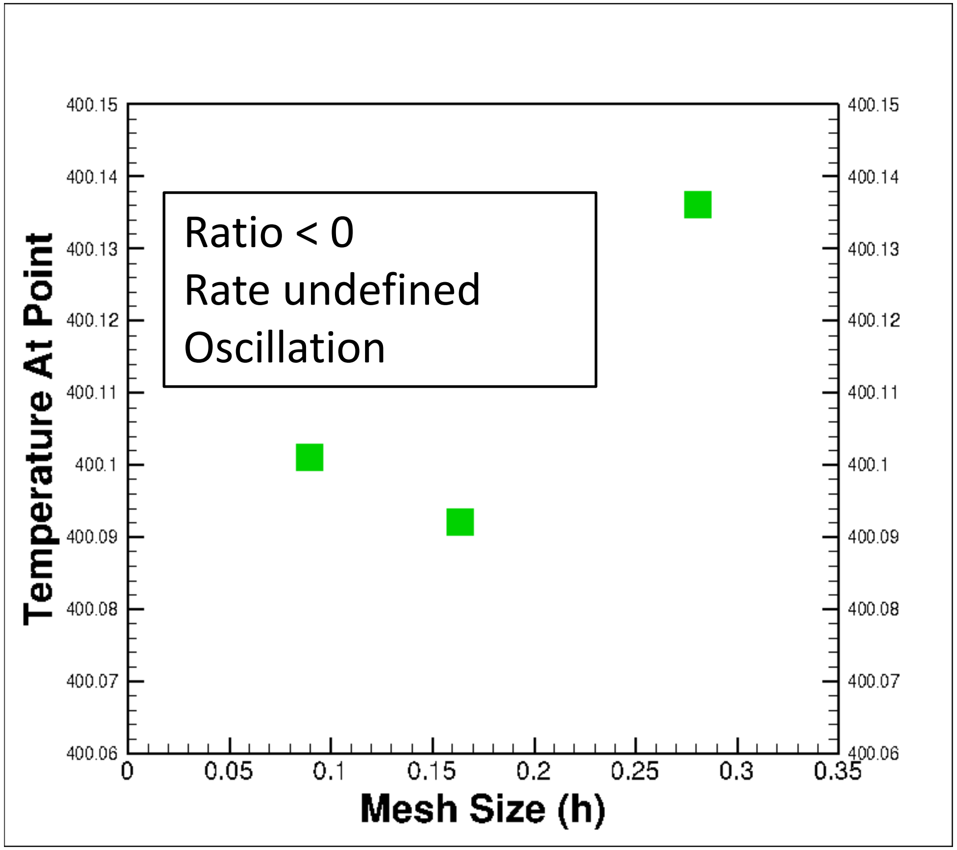
- Compute Q(h) for three mesh levels: $h_1>h_2>h_3$
- Compute differences
- Compute ratio
- Compute rate (p)

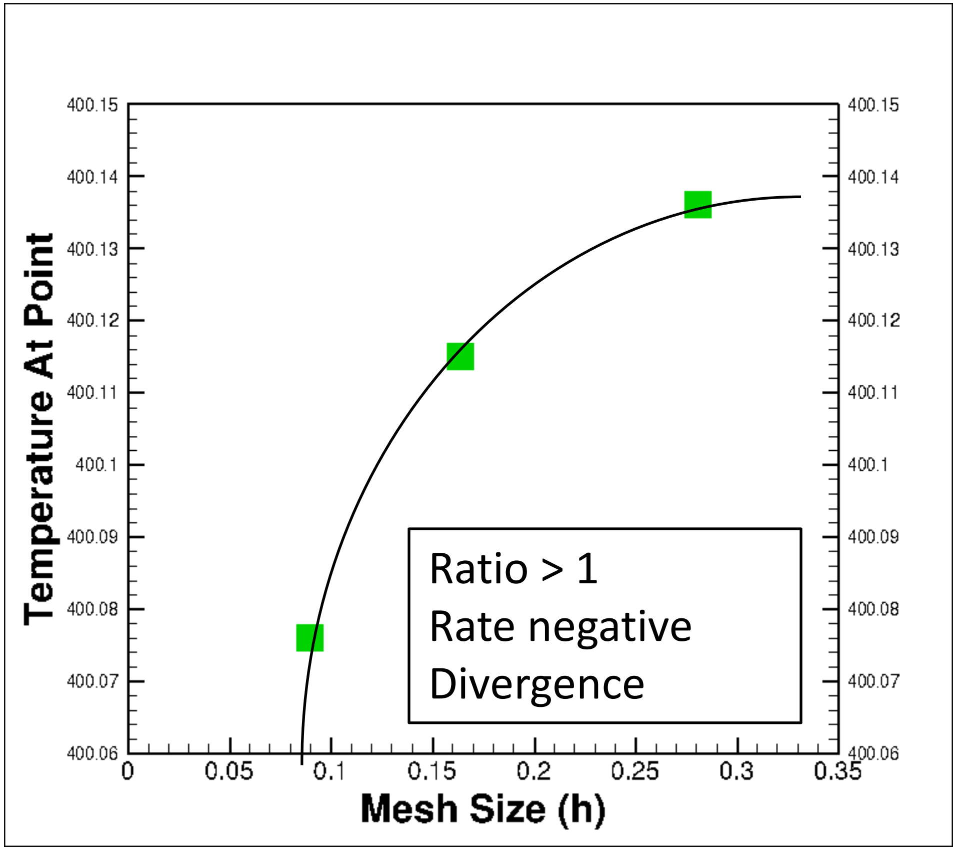
$$\text{Ratio} = (Q_2 - Q_1) / (Q_3 - Q_2) = r^p$$

$$\text{p} = \log(\text{Ratio}) / \log(r)$$

Question: when will the rate (p) be positive?

What Can Go Wrong





In these cases, should consider additional meshes, or investigate numerical controls

Extrapolation by Numbers

- Extrapolation using data

Nodes	h	Q(h)	Ratio	p	Q(extrap)
45	0.281	400.136			
225	0.164	400.092			
1377	0.090	400.076	2.777	1.473	400.056
9537	0.047	400.074	6.779	2.761	400.073
70785	0.024	400.073	2.630	1.395	400.072
545025	0.012	400.073	4.130	2.046	400.073

Temperature at Point

Nodes	h	Q(h)	Ratio	p	Q(extrap)	Error
45	0.281	-0.564				78.34%
225	0.164	-1.991				17.04%
1377	0.090	-2.293	4.728	2.241	-2.604	3.64%
9537	0.047	-2.358	4.657	2.219	-2.400	0.83%
70785	0.024	-2.373	4.387	2.133	-2.380	0.21%
545025	0.012	-2.376	4.173	2.061	-2.378	0.06%

Integrated Heat Flux

- Repeat the extrapolation for each set of 3 meshes
- Monitor the rate of convergence
- Use the extrapolated value to estimate the error for each mesh

What Can Cause Lower Rates of Convergence in Practice

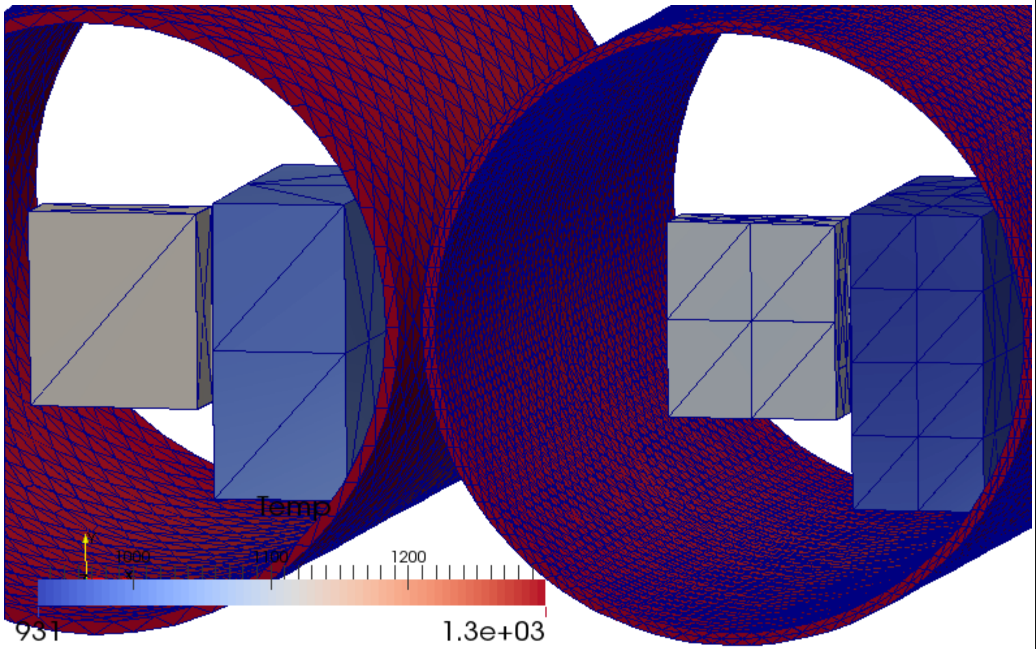
- Sources of error that alter the expected rate
  - Geometric features (reentrant corners)
  - Material discontinuities (jumps in gradients)
  - Shocks (jumps in solution values)
  - Inconsistent initial/boundary conditions
  - Poor mesh quality (initial mesh or from mesh deformation)
  - Irregular source terms (switching on/off)
  - Phase change / material failure (element death)
  - Undetected errors in the computer model

How to Estimate Mesh Size

- Often meshes are complex, unstructured
- We can use the case of a uniform mesh to generate an expression for an approximate mesh size
- Let *h* be the mesh size, *N* be the number of elements
  - 1D: $1/N = h$.
    - Think of a line with N elements.
  - 2D: $1/N = h^2$. $h = N^{-1/2}$
    - Think of a square with $N = (1/h)(1/h)$ elements
  - 3D: $1/N = h^3$. $h = N^{-1/3}$
    - Think of a cube with $N = (1/h)(1/h)(1/h)$ elements
  - General formula: $h = N^{-1/\mathrm{dim}}$

Example: Transient Thermal

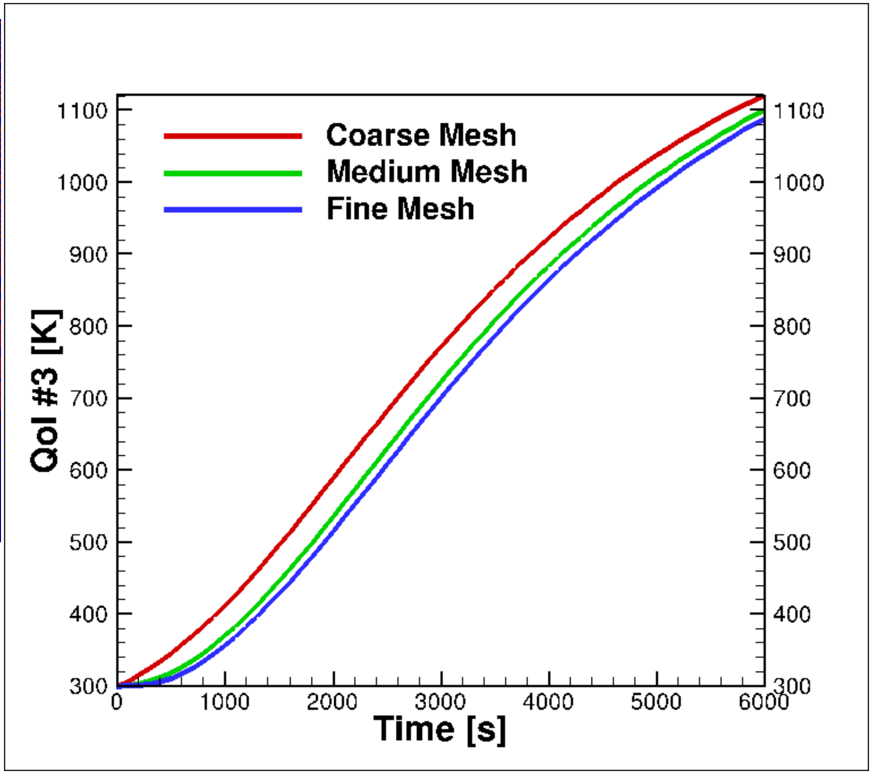
- Mock AFF for solution verification (metal case, foam, mock components, temperature-dependent properties)



coarse

medium

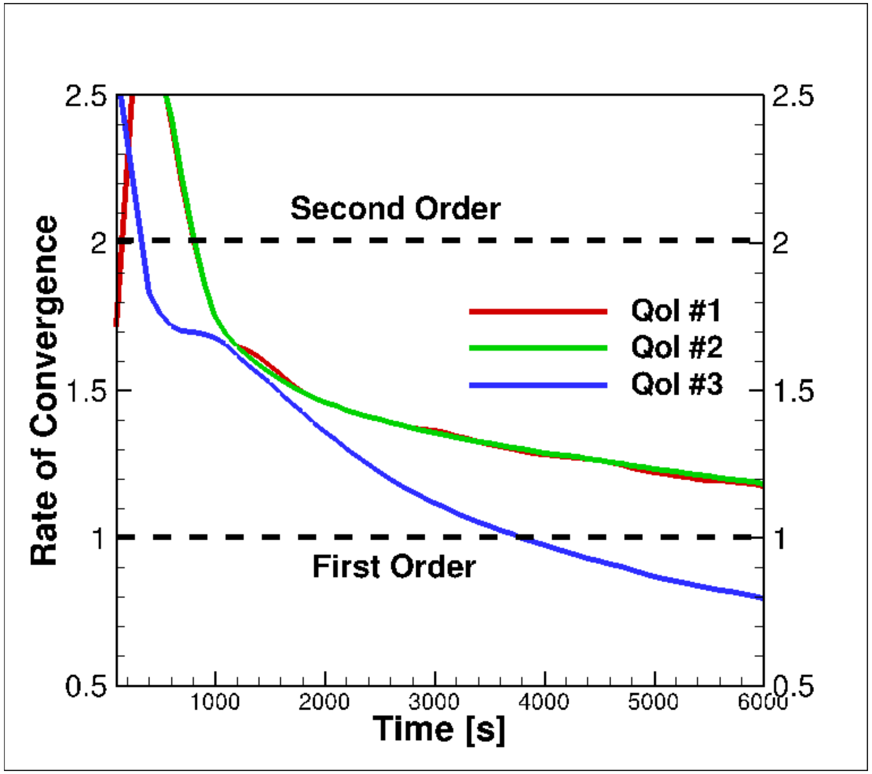
- QoIs: max/min/average temperature on part, temperature at point

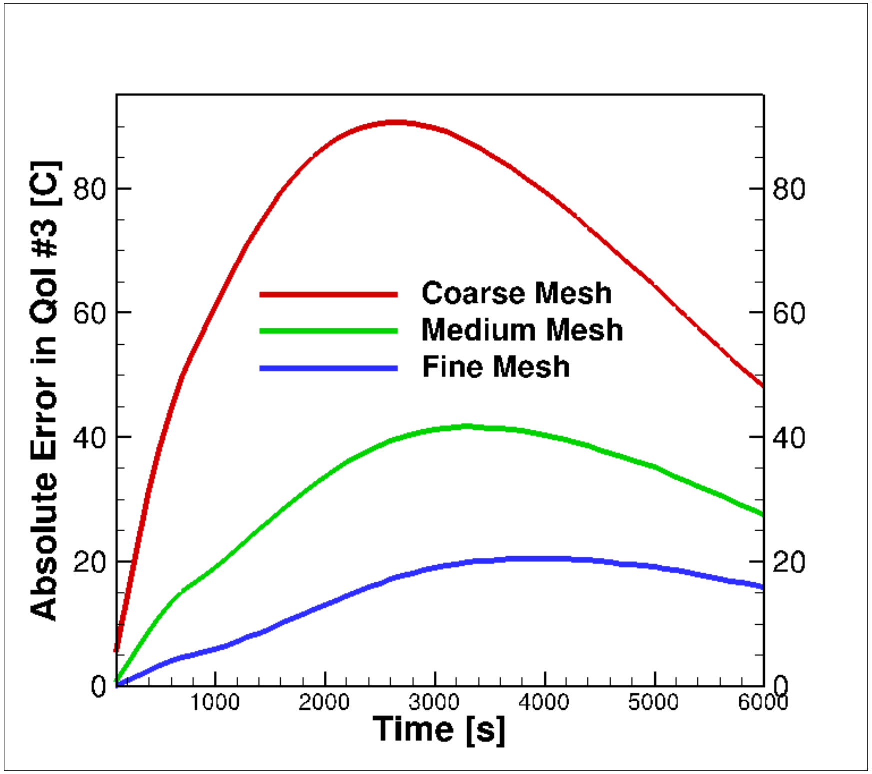


Example QoI history

Example: Transient Thermal (2)

- Convergence rates can vary over time
- Extrapolation enables quantification of errors in QoIs

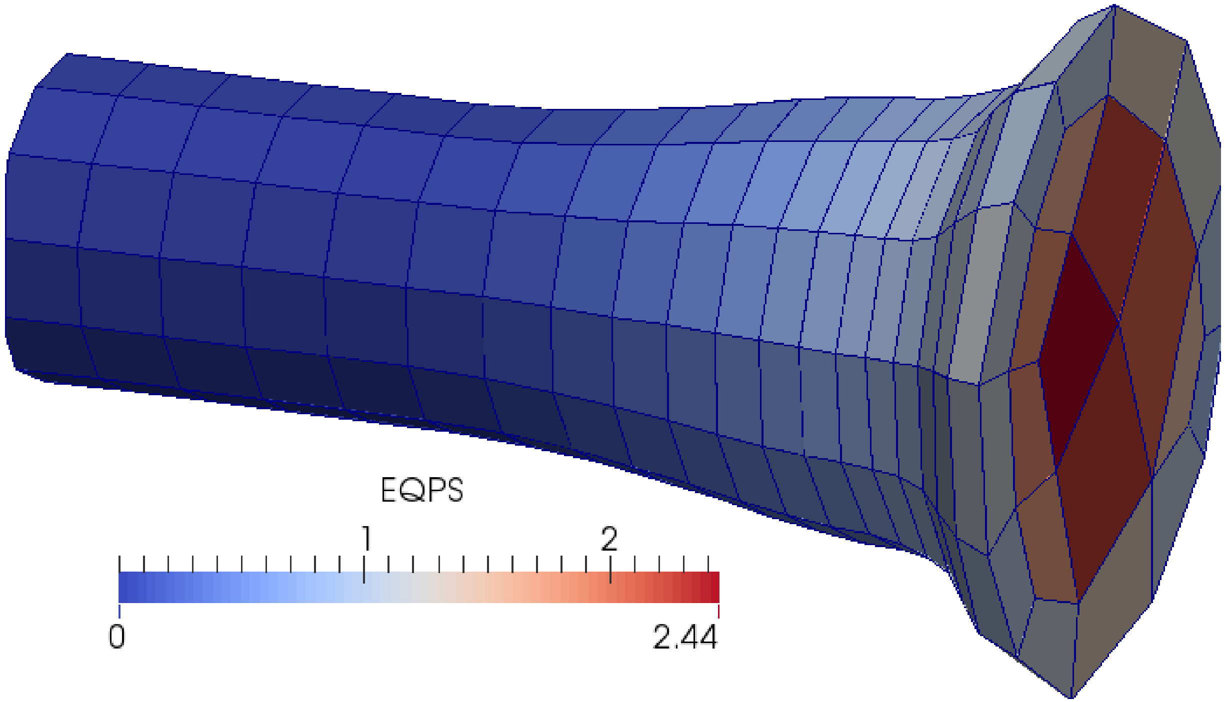




Example: Explicit Dynamics

- Taylor bar impact test (elastic-plastic deformation)
- QoIs: time history of axial displacement, force
- Four hex meshes were used (coarsest shown)

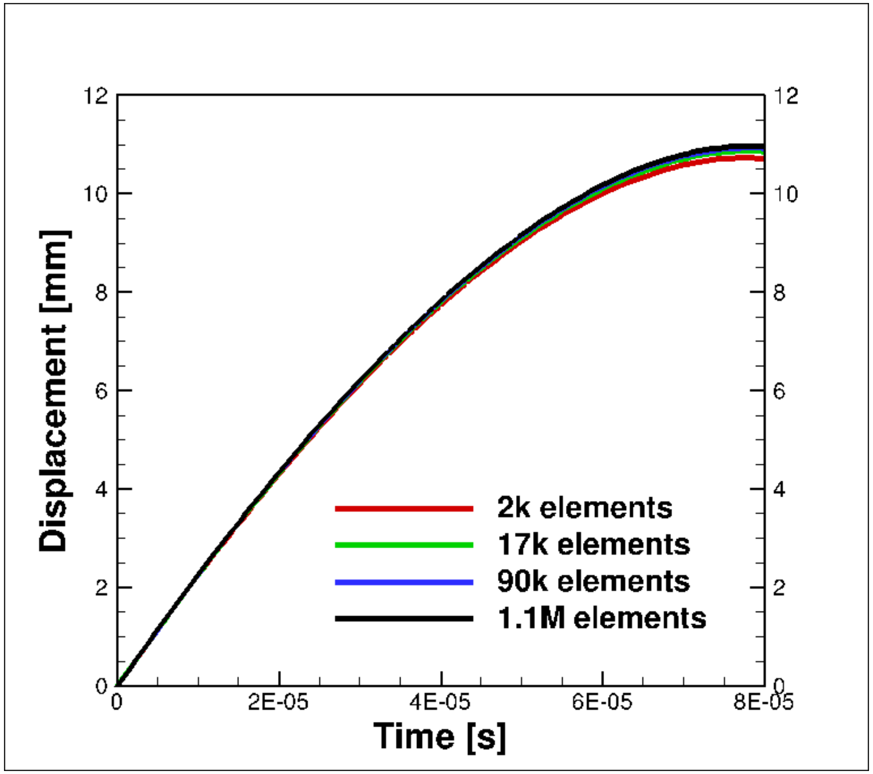
Displace.
QoI

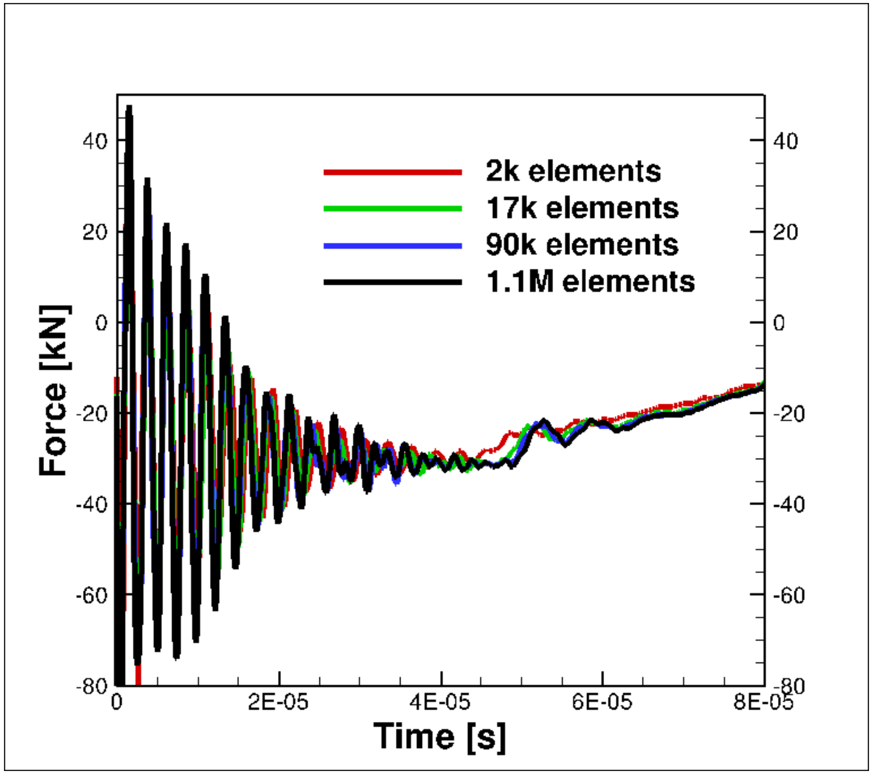


Force QoI

Example: Explicit Dynamics (2)

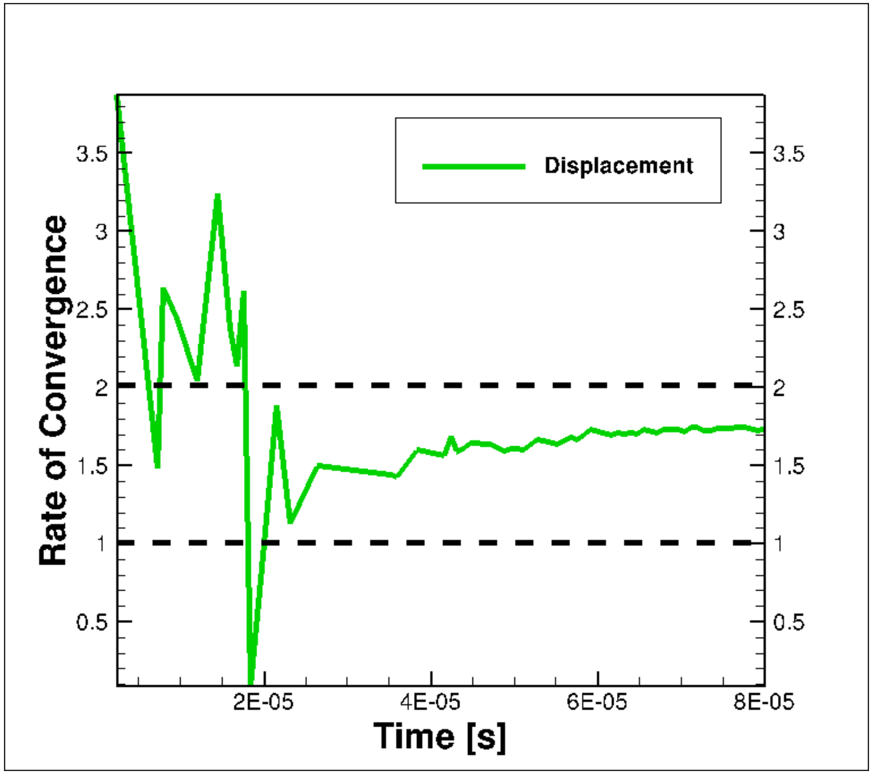
- These QoIs exhibit very different behavior
- Overlaying the plots does not quantify numerical error

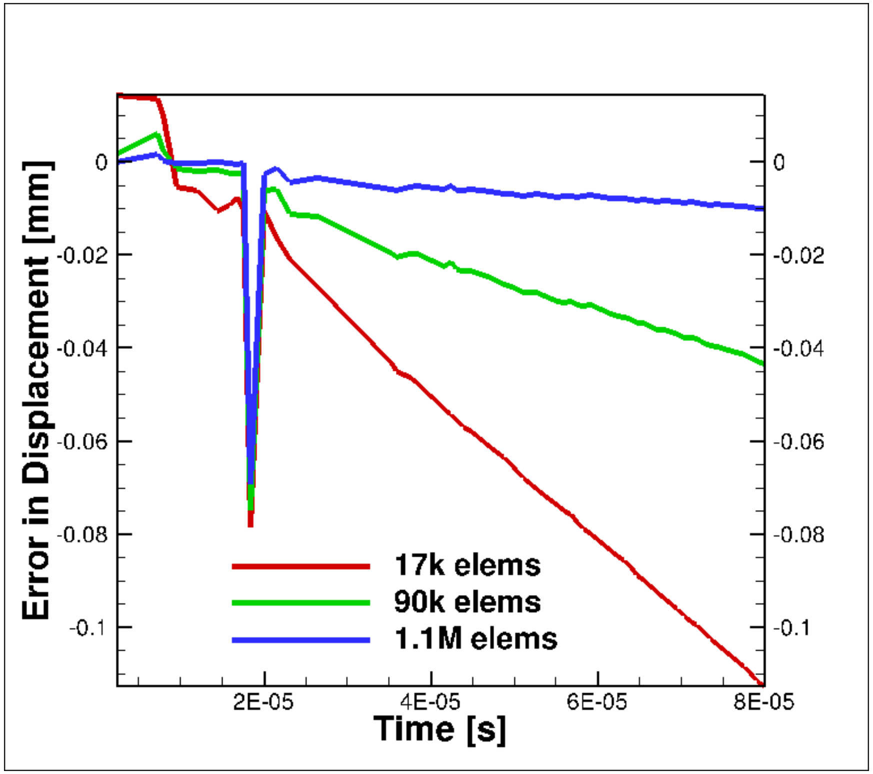




Example: Explicit Dynamics (3)

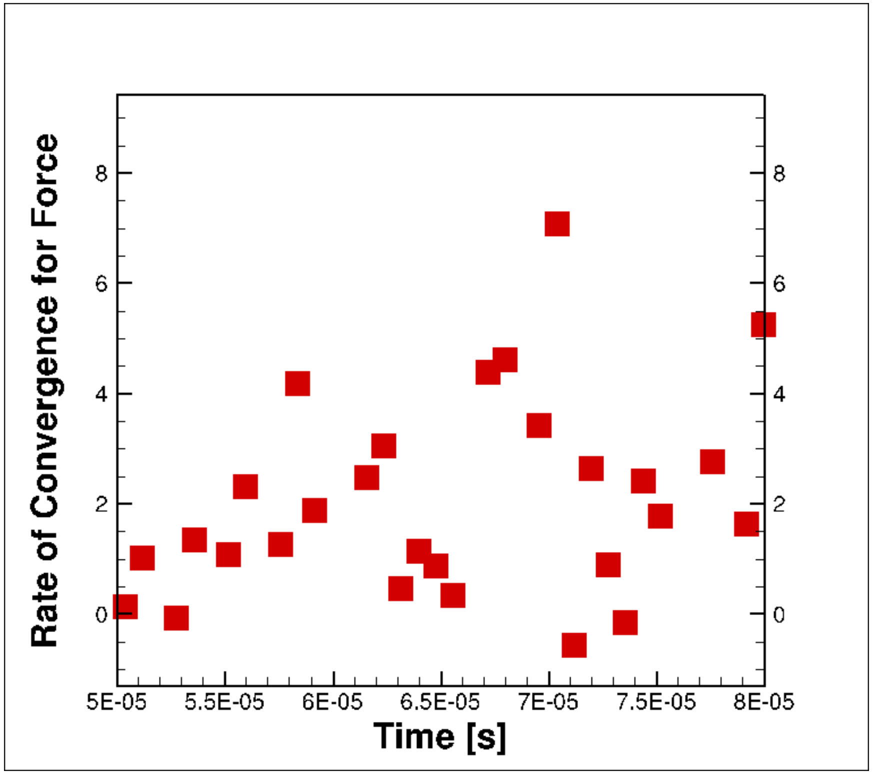
- Displacement exhibits convergence at most times
- The rate of convergence is less than the optimal (2)

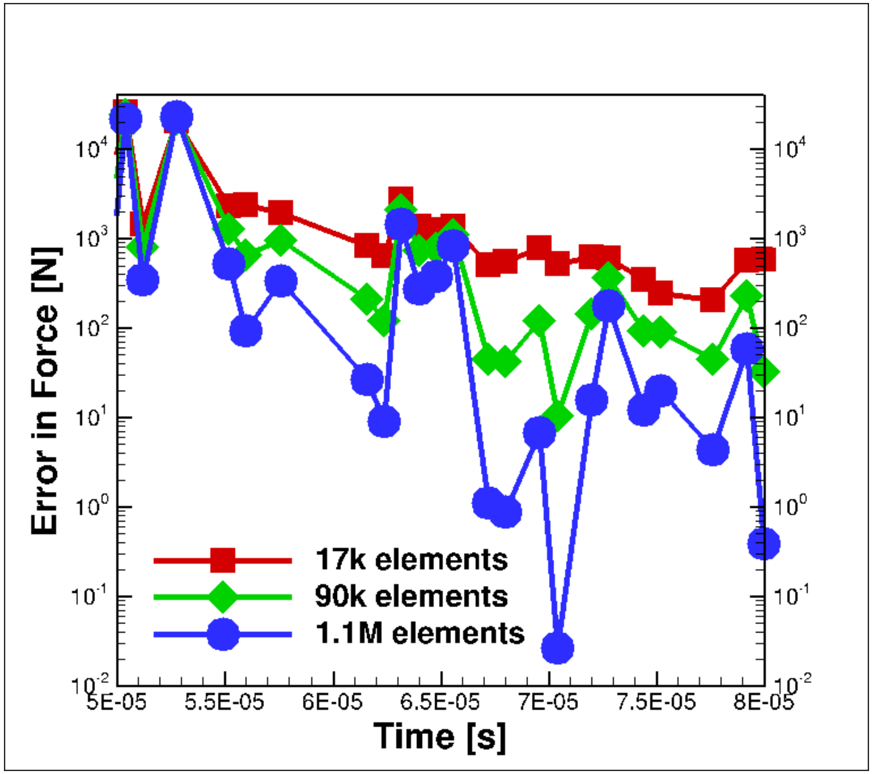




Example: Explicit Dynamics (4)

- Reaction force is initially highly oscillatory
- Later in time extrapolation works – but in a limited way

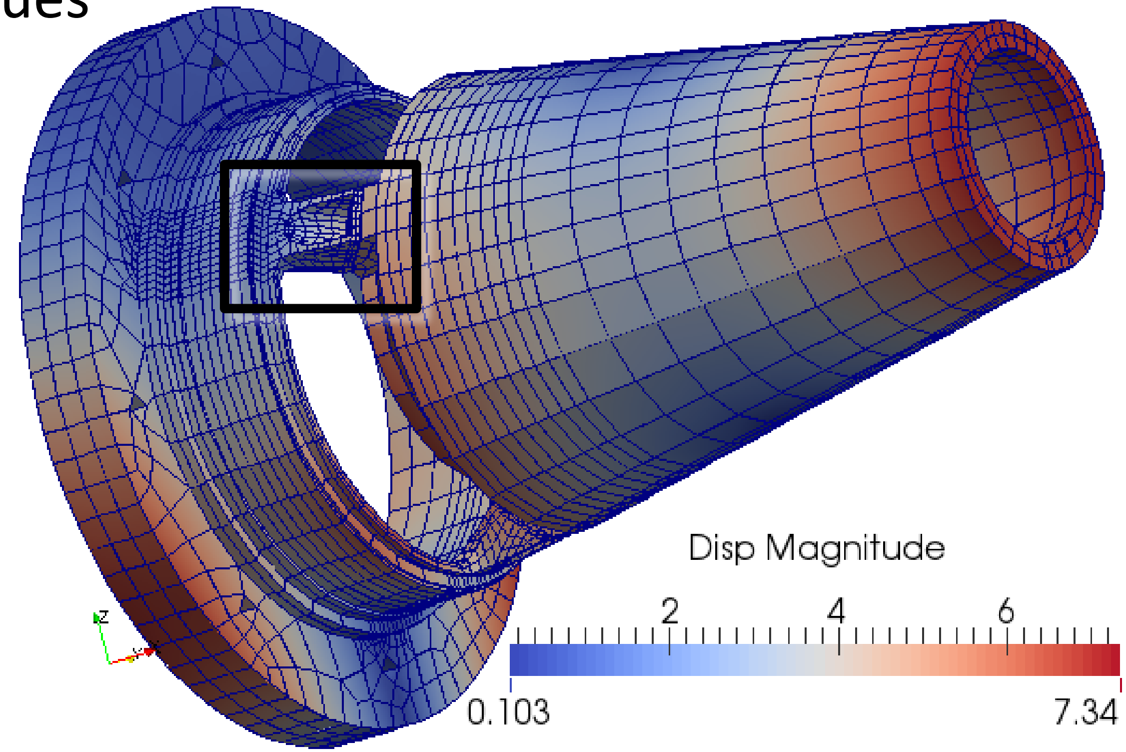




The Example Problem: Solution Verification for Modal Analysis

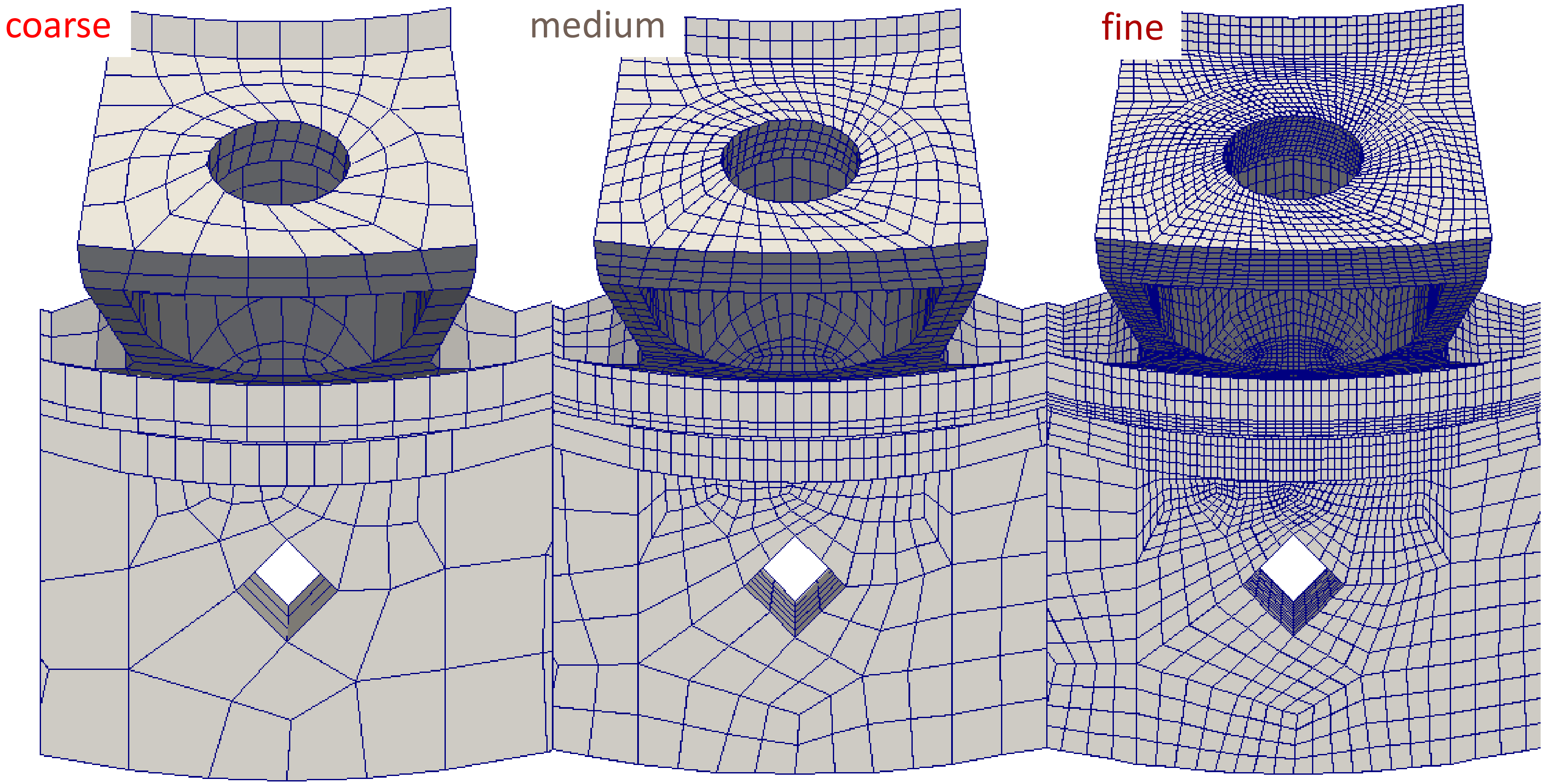
- This problem has a complex mesh, but few numerical controls (only solver tolerance, contact search tolerance)
- QoIs are the eigenvalues

Next slide we will zoom to the region indicated



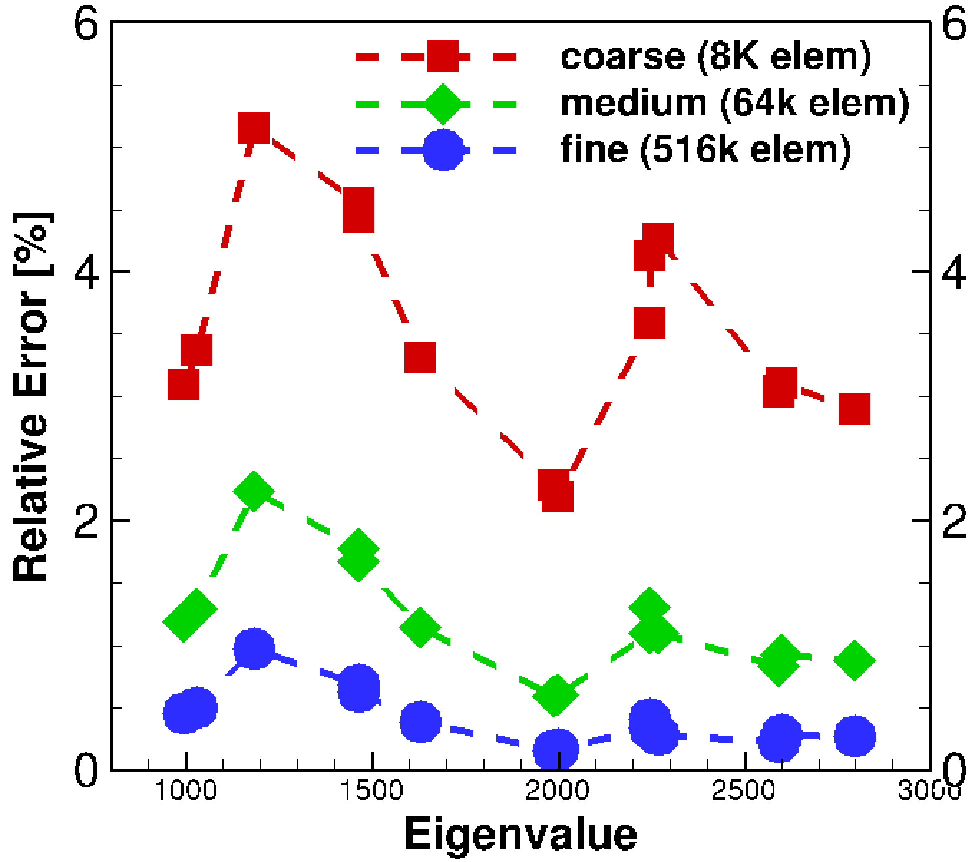
The Example Problem: Generation of Refined Meshes

- We used Sierra/Percept to generate refined meshes



The Example Problem: Numerical Error Estimates

- Errors from extrapolation (first 14 nonzero frequencies)



- In this case, we see convergence for all frequencies
- This allows us to assess the accuracy of each mesh
- Suitable accuracy depends on the application and other uncertainties (parametric, validation data, etc.)

Summary of Solution Verification

- Clearly define the quantity of interest (QoI) and the level of acceptable numerical error
- Conduct uniform mesh refinement (UMR) studies to quantify the numerical error in QoIs
- Use extrapolation when possible to assess convergence of QoIs and numerical error
- When errors and convergence rates are indeterminate, investigate
  - Numerical controls
  - Factors that may affect convergence
  - Further mesh refinement