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# Towards Verification and Validation of Thermal Mechanical Failure

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## Background and Objective

Weapon system analyses, especially high consequence ones, depend on verified and validated (V&V) simulation codes. Part of the V&V process is solution verification, in which results for responses of interest are shown to converge as the mesh is refined. This allows the error in a simulated response due to spatial discretization to be estimated and ideally shown to be small relative to other sources of error and uncertainty in the analysis. Current projects require quasi-static mechanical and coupled thermal mechanical analysis capabilities. ADAGIO, Sandia's implicit structural mechanics code, is the appropriate code to use to meet this requirement. However, this code has not had as much V&V work completed as have more mature analysis codes, to demonstrate its readiness to apply to high consequence weapon system analyses. The Advanced Scientific Computing (ASC) program funds V&V projects each year to help deploy, test, and verify Sandia analysis code capabilities. One of FY12's current projects is focused on V&V of thermal mechanical failure. As ARIA, the Sandia thermal analysis code, is more mature, we are focusing on verifying the mechanical code, ADAGIO.

The goal is to demonstrate that we can solve thermal mechanical problems using ADAGIO for the mechanical solution, and ARIA for the thermal solution, and that results will converge as the mesh, time step, and convergence tolerance are refined. In order for thermal mechanical problems to be considered, the thermal and mechanical parts must be verified to satisfy the same criteria independently, as well as capabilities specifically engaged for fully coupled analyses (problems that include thermal-mechanical interactions). Our ADAGIO solution verification work begins with simple test problems, then addressing more complex problems that include plasticity, contact, failure, and thermal mechanical coupling. This work focuses on solution verification in ADAGIO for different element types and formulations to show that as the mesh is refined, the metric of interest converges to a solution. Where possible we compare simulation results to analytic results or test data to validate the model, but the focus is more on solution verification.

## Theory and Procedure

Model geometry and meshing were done using Cubit meshing tool. The two problems completed so far are:

1. Sphere with a pressure of 350 MPa applied to the inner wall
2. Cantilever beam with a point load of 3600 N applied to the beam's free end

Problems in process:

3. Cylindrical compression specimen, compressed to a displacement of 12.7 mm
4. Cantilever beam with tied contact, point load of 3600 N applied to the beam's free end

Meshes were refined by reducing the element size by half in each direction for each refinement. A total of 4 meshes were generated for each problem. Both models were meshed using 8-node hexahedral elements and 10-node tetrahedral elements. Figure 1 shows sample hexahedral and tetrahedral meshes used in this study. Six different element formulations, or numerical integration rules, were paired with the two element types to obtain a comparison of convergence rates. Table 1 lists the element formulations used, along with their characteristics.

From the simulation results, a convergence study was conducted for each element and formulation pair to determine the convergence rate for the response of interest. The convergence rate ***p*** determines how fast the discretization error goes to zero as the mesh is refined, and here a constant grid refinement ratio ***r*** is assumed, defined by

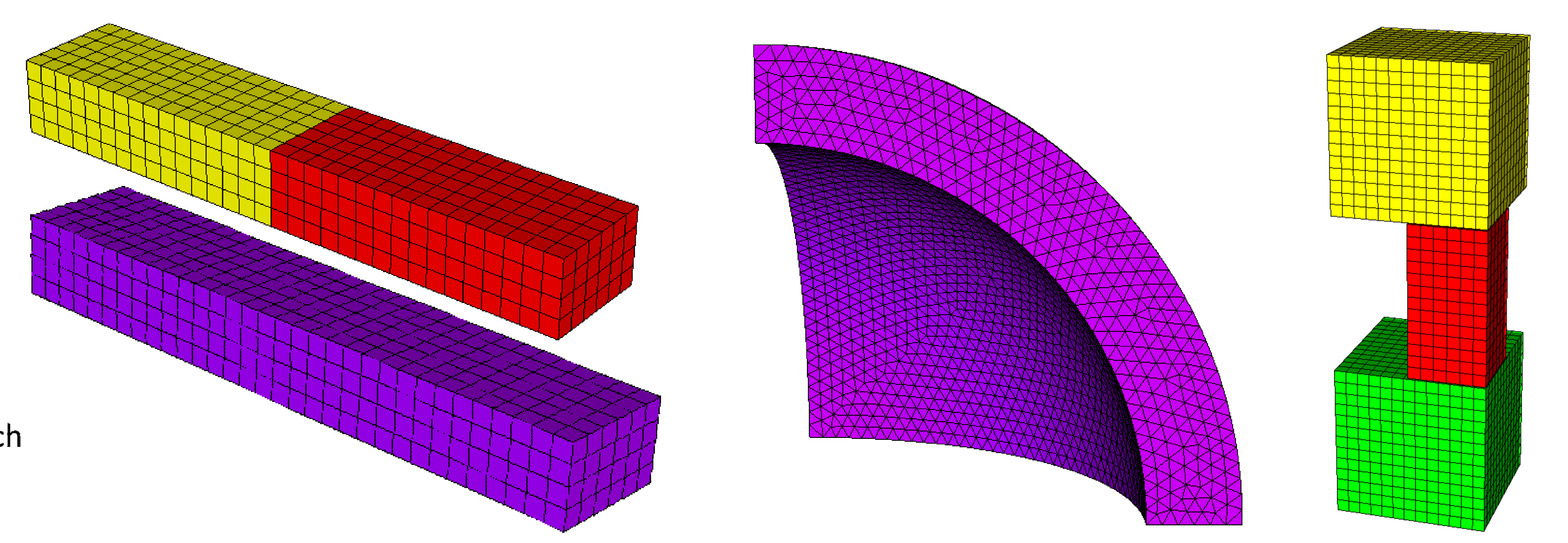
$$r = h_2/h_1$$

where $h_n$ is the grid spacing on successively finer grids. Using the grid refinement ratio, the convergence rate ***p*** can be obtained from three solutions $f_n$ on successively finer grids by

$$p = ln\left(\frac{f_3 - f_2}{f_2 - f_1}\right)/\ln(r)$$

Richardson Extrapolation was used to estimate the true solution to calculate the convergence rate curve. Richardson extrapolation ($f_{h=0}$) is a method of obtaining a higher-order estimate of a solution at zero-grid spacing from a series of lower-order discrete values, defined by

$$f_{h=0} = f_1 + \frac{f_1 - f_2}{r^p - 1}$$



Cantilever Beam, with and without tied contact — Pressurized Sphere — Compression Specimen

Figure 1. Sample hexahedral and tetrahedral meshes used in this study

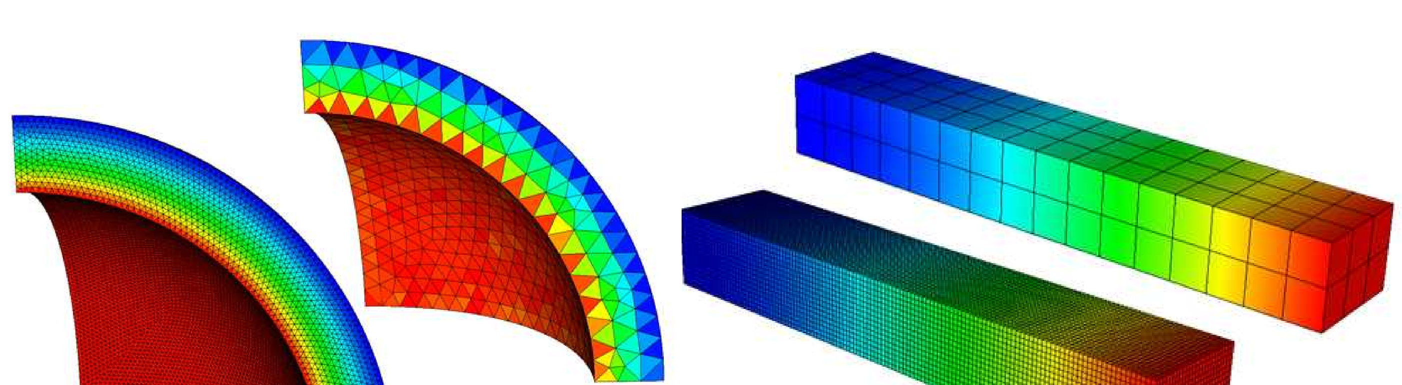
| Formulation | Element | Characteristics |
|---|---|---|
| Single Integration | HEX8 | One integration point |
| | TETRA10 | |
| Fully Integrated | HEX8 | 8 integration points, 2x2x2 Gauss Rule |
| Selective Deviatoric | HEX8 | Deviatoric parameter = 1, 8 integration points, pressure term is averaged |
| q1p0 | HEX8 | Pressure and deviatoric stresses evaluated separately, single integration for pressure, 2x2x2 Gauss rule for deviatoric stress |
| Composite_tet | TETRA10 | 5 integration points |

Table 1. Element formulations used in this study

## Results and Conclusions

Following completion of the simulations for each element type and formulation, convergence studies were conducted based on the following metrics for each model

1. Sphere: radial stress at the inner wall
2. Cantilever beam: beam displacement at the free end



Metrics for Convergence
Left: Radial stress at the sphere's inner wall
Right: Displacement at the beam's free end

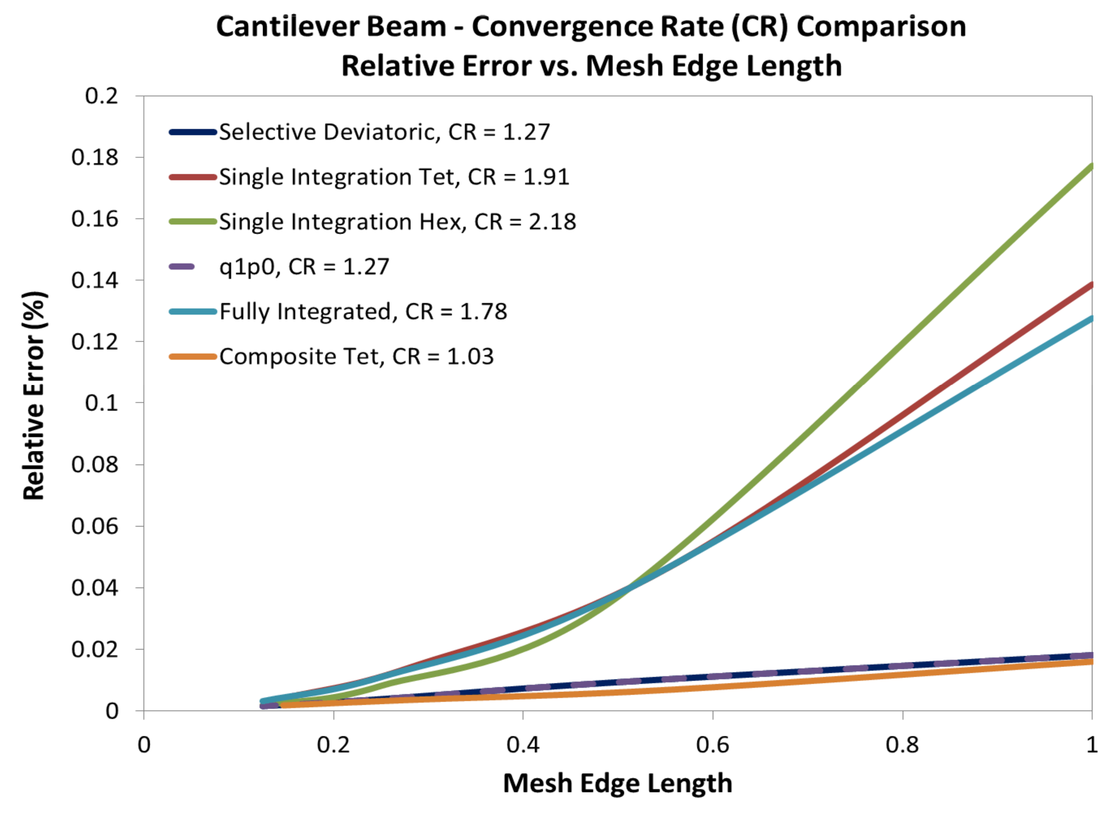
It is expected that order of convergence for displacements and global quantities like strain energy should have convergence rates of order 2. Since strain and stress are calculated based on the derivative of displacement, is it expected that the convergence rate for local quantities like stress and strain should be of order 1. However, results show some variation in convergence rate calculations. In some cases rate of mesh refinement may not have been uniform, or elements may have been more distorted in some models more than others, both can effect the convergence rates. Further convergence rate calculations, using additional metrics such as strain energy, should help to determine if these results are consistent for each element type and formulation.

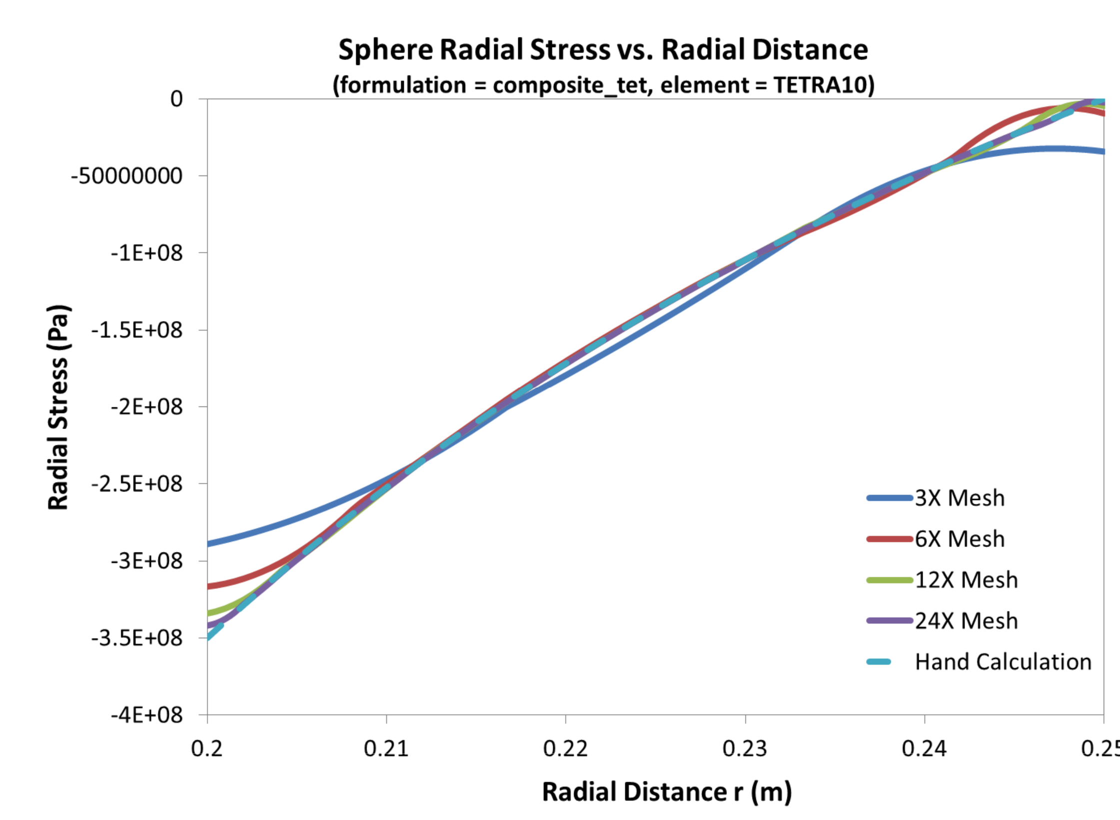
**Convergence Results for the Elastic Sphere**

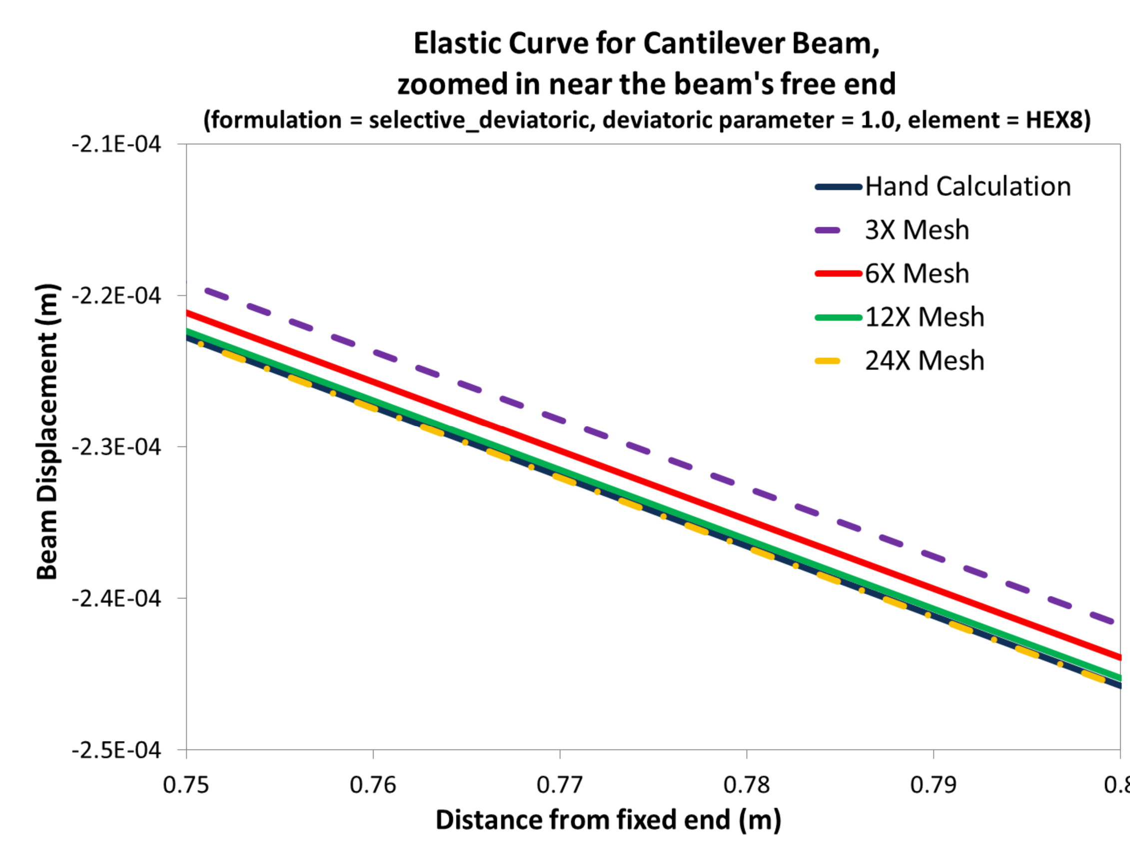
| Formulation | Element | Convergence Rate | Richardson Extrapolation | Relative Error, 24X Mesh |
|---|---|---|---|---|
| Fully Integrated | HEX8 | 0.99 | -35.01994 MPa | 0.032% |
| Q1P0 | HEX8 | 0.98 | -35.03077 MPa | 0.033% |
| Single Integration default | HEX8 | 0.97 | -35.03567 MPa | 0.033% |
| Selective Deviatoric (Deviatoric Parameter = 1) | HEX8 | 0.97 | -35.0333 MPa | 0.033% |
| Composite Tet | TETRA10 | 0.40 | -38.29665 MPa | 0.096% |
| Single Integration default | TETRA10 | 0.33 | -39.46557 MPa | 0.13% |

**Convergence Results for the Elastic Cantilever Beam**

| Formulation | Element | Convergence Rate | Richardson Extrapolation | Relative Error, 24X Mesh |
|---|---|---|---|---|
| Fully Integrated | HEX8 | 1.78 | $-2.46117 \times 10^{-4}$ m | 0.0032% |
| Q1P0 | HEX8 | 1.27 | $-2.46211 \times 10^{-4}$ m | 0.0016% |
| Single Integration default | HEX8 | 2.18 | $-2.46109 \times 10^{-4}$ m | 0.0018% |
| Selective Deviatoric (Deviatoric Parameter = 1) | HEX8 | 1.27 | $-2.46 \times 10^{-4}$ m | 0.0016% |
| Composite Tet | TETRA10 | 1.03 | $-2.46597 \times 10^{-4}$ m | 0.0019% |
| Single Integration default | TETRA10 | 1.91 | $-2.463 \times 10^{-4}$ m | 0.0041% |

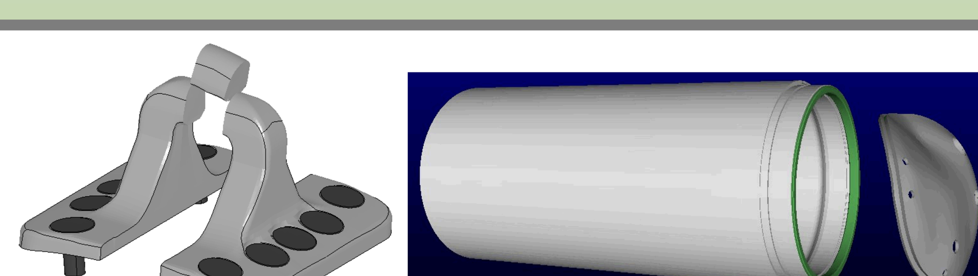



## Future Work

Current progress of this project has only focused on the solution verification of simple mechanical problems. Future work will involve more complex test problems to more accurately simulate model behavior in real problems of interest. Current problems in progress include tension specimens pulled to failure and compression specimens with sliding contact. Additional test problems with tied contact used to connect parts in which meshes don't align, pressurized vessels with threaded covers (which simulate some weapon cases), pressurized welded enclosures using surface failure models, and coupled thermal mechanical models will also be studied. All these capabilities are required to assess the nuclear safety of existing weapons in abnormal environments, and to support redesign efforts (like Life Extension Programs) intended to improve the nuclear safety of systems in the stockpile.



Future models to be investigated
Left: Lifting lug pulled to failure
Right: Threaded joint coming apart due to pressurization

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NNSA National Nuclear Security Administration

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