SAND2014-19112C

Recent Advances in Code Verification of Sierra Solid Mechanics and Structural Dynamics

85th Shock & Vibration Symposium

DS: Navy Enhanced Sierra Mechanics Session

October 28, 2014

James V. Cox, Garth M. Reese, & Kendall H. Pierson

Sandia National Laboratories

Sandia National Laboratories is a multi-program laboratory operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

U.S. DEPARTMENT OF ENERGY

National Nuclear Security Administration

Introduction

- Objective of verification: build *credibility* in our modeling & simulation results.

  credibility – the quality or power of inspiring belief (MW Dic.)

- Oberkampf & Roy, 2010: "The fundamental elements that build credibility in computational results are:

  (a) quality of the analysts conducting the work,

  (b) quality of physics modeling,

  (c) verification and validation activities, and

  (d) uncertainty quantification and sensitivity analyses."

Introduction

code verification

- O&R: "*Verification* is the process of assessing software correctness and numerical accuracy of the solution to a given mathematical model.

solution verification

- *Validation* is the process of assessing the physical accuracy of a mathematical model based on comparisons between computational results and experimental data."

- Why is verification important for the analysts?
  - Increased confidence in the results – analysts and customers
  - Code is assumed to be verified when:
    - Calibrating models
    - Validating models
    - Quantifying uncertainty of models
    - Performing any type of certification work

Verification Activities

Elements of Software Quality

- Automated
- Flexible
- Cross-platform
- Continuous and nightly

- Performance at scale
- Memory and cpu time use
- Representative models
- Automated, repeatable

- Static Analysis
- Coverage Analysis

- Version Control
- Code Reviews/Pair Programming
- Unit, Integration and System Testing
- Requirements
- Project Management
- Training
- etc

Verification Strategy

- Sierra categories of verification problems ("simple to complex")
  1. *Sanity*
  2. *Symmetry*
  3. *Conservation*
  4. *Code-to-code comparison*
  5. *Discretization error* – compares 1 simulation to 1 analytical solution
  6. *Convergence* – examines convergence behavior, but < EQ test
     - Inexact reference solution (*e.g.*, analytical solution based upon LE)
     - Asymptotic analysis of rate
     - Richardson extrapolation to obtain higher order approximation
  7. *Error quantification* – examines convergence rate with exact analytical solution
     - Preferred by the verification community because of its ability to reveal errors in the application code.

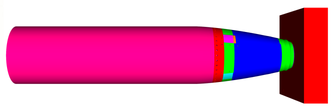
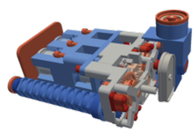
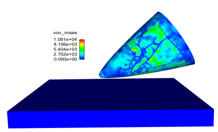
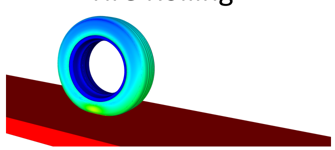
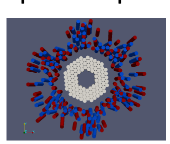
Regression Test Results

Software verification depends critically on a solid regression test suite.

Multiple platforms, multiple compilers, unit, integration and system level tests.

Site	Build Name	Update Files	Build Error	Build Warn	Test NotRun/Skipped	Test Fail	Test Pass
Production - TLCC2							
uno-login3	master-intel-12.1-release-openmpi-1.6-mkl				0	0	8590
chama-login8	master-intel-12.1-release-openmpi-1.6-mkl		0	6	0	1	8710
sierra101	master-intel-12.1-release-openmpi-1.6.4-mkl		0	6	0	0	11451^{+1}
Production - TLCC							
glory-login2	master-intel-12.1-release-openmpi-1.4.3-mkl		0	6	0	0_{-2}	8582^{+2}
Production - Cielo							
mzlogin01e	master-intel-12.1.xe6-release-vendor		0	0	0	22^{+22}	915_{-22}
Production - Sequoia							
bgq-b1	master-gcc-4.7.2.bgqwrapper-release-mpich-bgq-wrapper-essl		0	0	0	10_{-3}	8509
Production - SRN Desktop							
sierra105	master-intel-12.1-release-intelmpi-4.1-mkl		0	6	0	0	11423
installdir-create-sierra105	master-intel-12.1-release-intelmpi-4.1-mkl						
Production - SCN Desktop (RH5)							
sierra002	master-intel-12.1-release-intelmpi-4.1-mkl		0	6	0	0	11423
installdir-create-sierra002	master-intel-12.1-release-intelmpi-4.1-mkl						
Production - Training							
macsierra01	master-darwin-4.7.macports-release-openmpi-1.6.4	332	0	0	0	1	8540
Production - Development compilers							
sierra104	master-gcc-4.7.2-debug-openmpi-1.6.4		0	0	0	0	11353
sierra103	master-gcc-4.7.2-release-openmpi-1.6.4		0	0	0	0	11391

Performance Test Suite

Problem	Machine (# Proc)	Original 4.28 (seconds)	VOTD 4.33.2 (seconds)	VOTD 4.33.4 (seconds)	Speedup (total)
Crush 	Chama (32)	4535	883	844	**5.37x**
Shock of electronics 	Chama (32)	1449	616	689	**2.10x**
impact 	Chama(32)	7634	3480	3574	**2.14x**
Tire Rolling 	Chama(16)	3928	1082	1085	**3.62x**
crush	Chama(32)	1027	460	499	**2.06x**
Coupled impulse 	Chama(64)	141266	18182	18234	**7.75x**

Verification Assessment

EXAMPLE

Feature Coverage Tool (FCT) – an automated tool for determining the coverage of our verification test suite (VERT) with respect to analysis capabilities

- ➢ Developers apply to assess testing gaps
- ➢ Analysts apply to assess test coverage of capabilities applied in an analysis
- ➢ b−version has weaknesses
- ○ false positives & negatives
- ○ no verification test type
- ○ does not know intent of test

Solid Mechanics VOTD - verification tests (subset of adagio_rtest presto_rt

C

/ Commands / **Begin Sierra <jobidentifier>** / Begin Function <functionname>

Coverage	Command	Tests
68.6%	⊞ Begin Definition For Function <functionname>	81
0%	⊞ Begin Developer Spring Support Section <spring_…	0
11.1%	⊞ Begin Feti Equation Solver <solver name>	42
36.7%	⊞ Begin Finite Element Model <label>	333
75%	⊟ Begin Function <functionname>	246
100%	Abscissa {=|Are|Is} <name: string+>	169
0%	Abscissa Offset {=|Are|Is} <abscissa_offset: real>	0

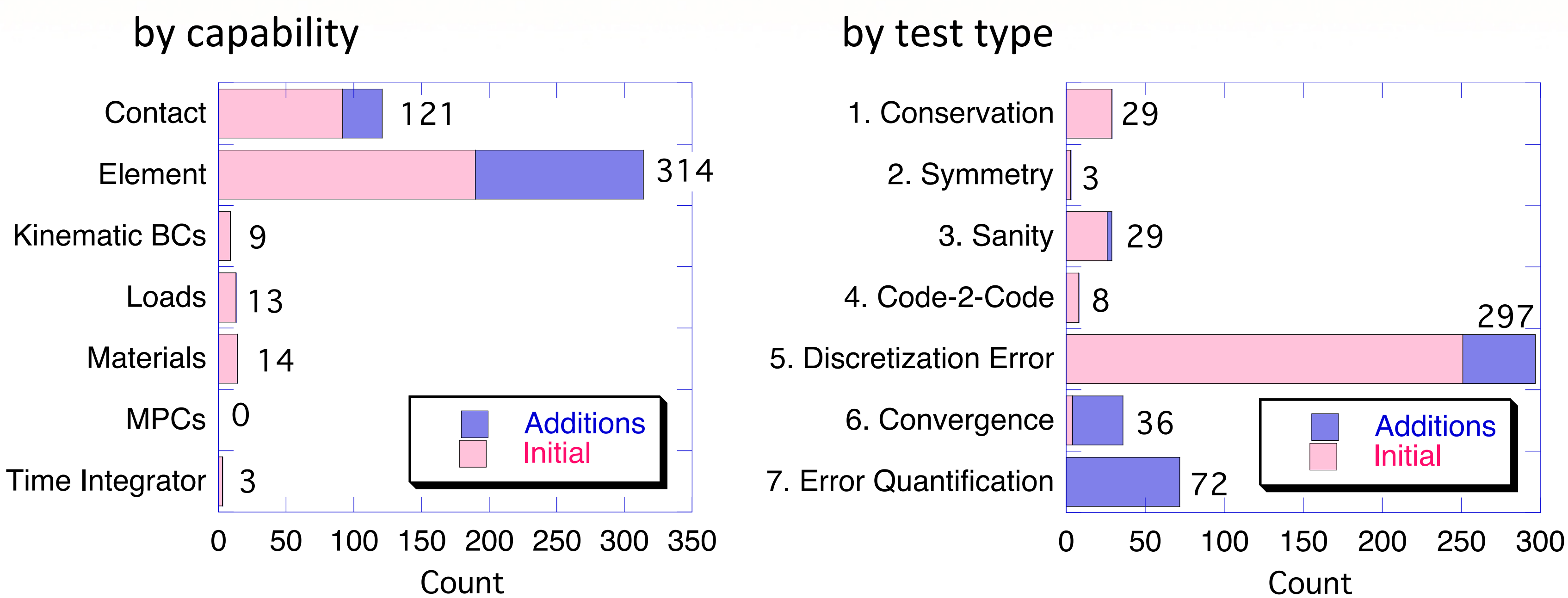
100%	⊟ Formulation {=|Are|Is} {Composite_Tet|Enhanced_Strain|Fully_Integrated|Mean_Quadrature|Q1P0|Selective_Deviatoric|Thickshell|Void|Xfem}	37
100%	{THICKSHELL}	8
100%	{SELECTIVE_DEVIATORIC}	2
100%	{FULLY_INTEGRATED}	5
100%	{MEAN_QUADRATURE}	7
100%	{ENHANCED_STRAIN}	14
100%	{Q1P0}	1

Actual count ~ 26 → (7)

Verification Assessment

Solid Mechanics – Sierra/SM

- Verification tests



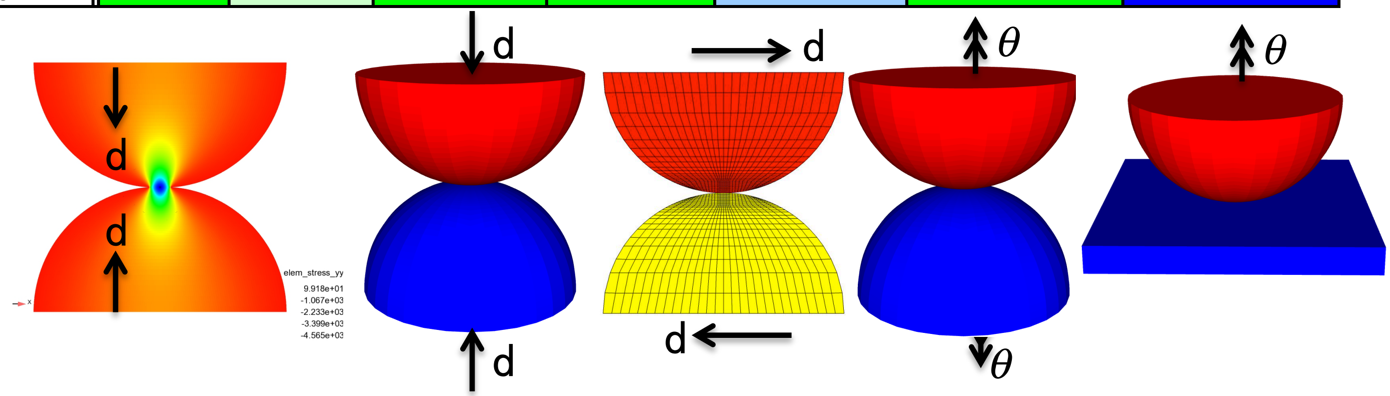
- Coverage additions include:
  - Contact convergence tests
  - Element linear elastic and finite deformation patch tests
  - Element finite deformation, error quantification tests
  - Element convergence tests (solid cantilever beam)

Verification

Progress on Contact Convergence Tests

- ~ work by Ben R.
- ~ work in progress
- ~ in v-manual as 2nd results
- ~ in v-manual

		Problem	Hertz	Hertz	Hertz	Mindlin	Mindlin	Lubkin	Lubkin
		Geometry	cyl-cyl	cyl-cyl	sph-sph	cyl-cyl	cyl-cyl	sph-sph	sph-pl
		Time Dep.	QS	QS	QS	QS	QS	QS	QS
		Deform.	LE	LE	LE	LE	LE	LE	LE
		Load/case	U	U	U	U	T	U	U
		Material	Elas	Neo	Elas	Elas	Elas/Neo	Elas	Elas
Contact	El. Topo.	Int. & ε inc							
Node-face	Hex 8	mq so							
		full so							
face-face		mq so							
		full so							

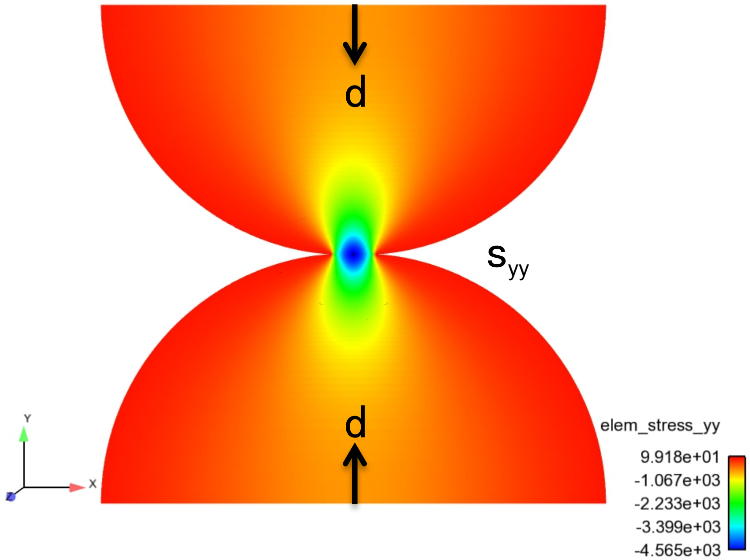


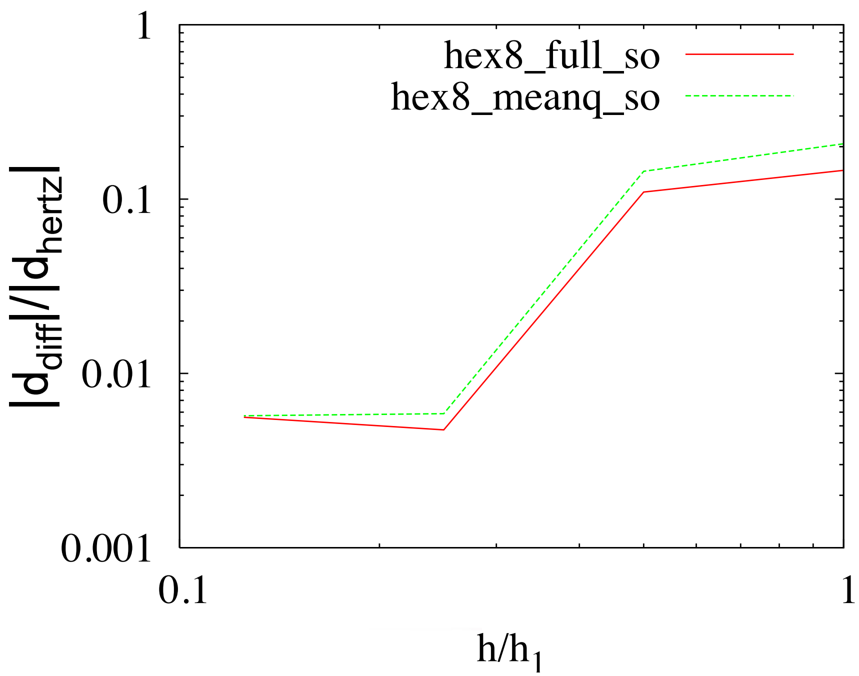
- All tests gave differences with the inexact analytical solutions ≤ 3%
- Resorted to asymptotic analysis to estimate rates of convergence.
- Observed convergence rates were better without friction

Contact Convergence Tests

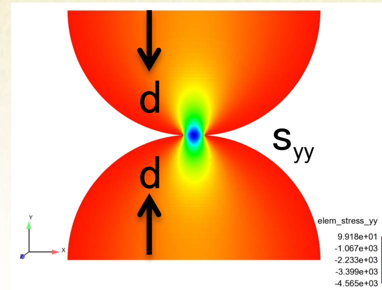
Hertz cylinder-cylinder

- A first step in contact convergence testing
- Initial comparison with Hertz solution
- Inexact reference solution -> non-monotonic convergence to a constant difference



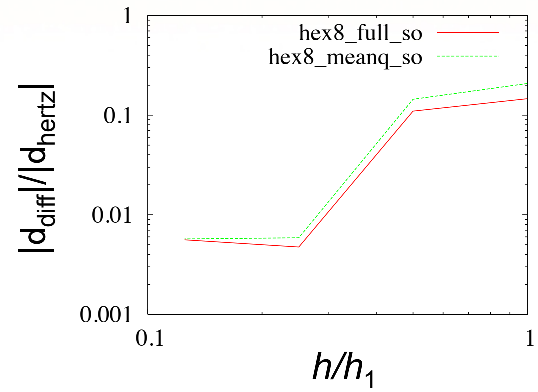


Contact Convergence Tests



- Cylinder-cylinder contact
  - Addition of asymptotic analysis

FEM solutions $\{f_{h_i}\}_{i=1}^{5}$ → Using Hertz for reference solution $f_{diff_i} = f_{h_i} - f_{hertz}$ →



Using power series form

$$f_{h_i} = f_{exact} + ch^p + O\left(h^{p+1}\right)$$

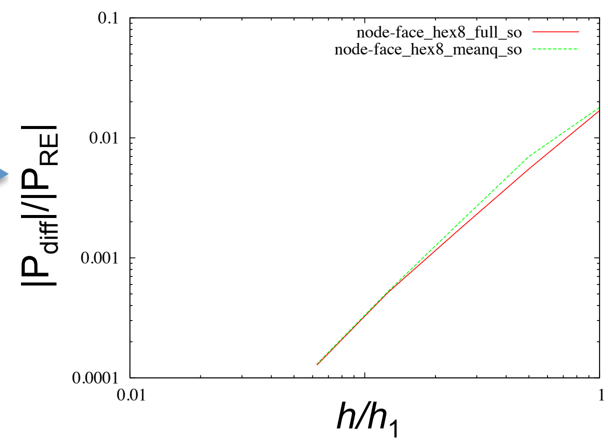
Assume $\{f_{h_i}\}$ in asymptotic range

$$f_{h_i} = \tilde{f}_{exact} + ch^p$$

Using sets of 3 meshes solve for *p*, *c*, and $\tilde{f}_{exact}$

meanq_so: *p* ~ 1.11, 1.86, 1.84

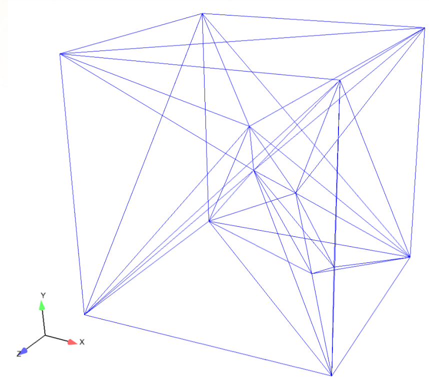
full_so: *p* ~ 1.57, 1.69, 1.62



Finite Deformation Patch Tests

Example of secondary benefits of verification

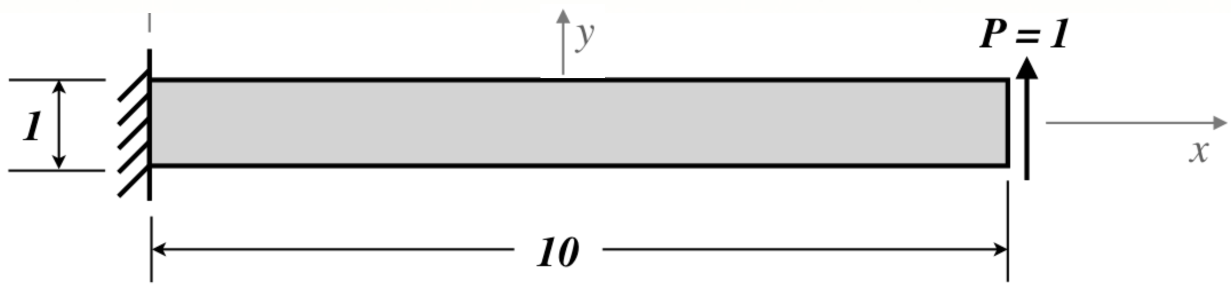
- Finite Deformation tests address $O(1\%)$ and $O(100\%)$ strains
- Quasistatic with displacement boundary conditions
- Exact solutions calculated for hypo- and hyper-elasticity
- Relative accuracy should "approach" the machine epsilon
- All hex and tet elements had relative errors $\leq O(10^{-12})$ except 1 – the composite Tet10
- Investigation -> culprit was a legacy single precision mesh combined with an element sensitivity to mid-edge node position.
- Gradient calculation was analytical and assumed mid-edge nodes were exactly at middle of straight edges.
- Use cases of concern:
  - geometry conformal meshing – mid-edge node conforming to curved surface
  - graded meshing – with graded mid-edge placement)



Slender Cantilever Beam Problem

Example of a weaker element convergence test

Geometry & Boundary Conditions



Material

Homogeneous and isotropic elastic

Young's modulus = 1E6

Poisson's ratio = 0.3

Consistent units assumed

Initial Conditions

Zero displacements, strains, and stresses

Conceptual & Mathematical Model Assumptions

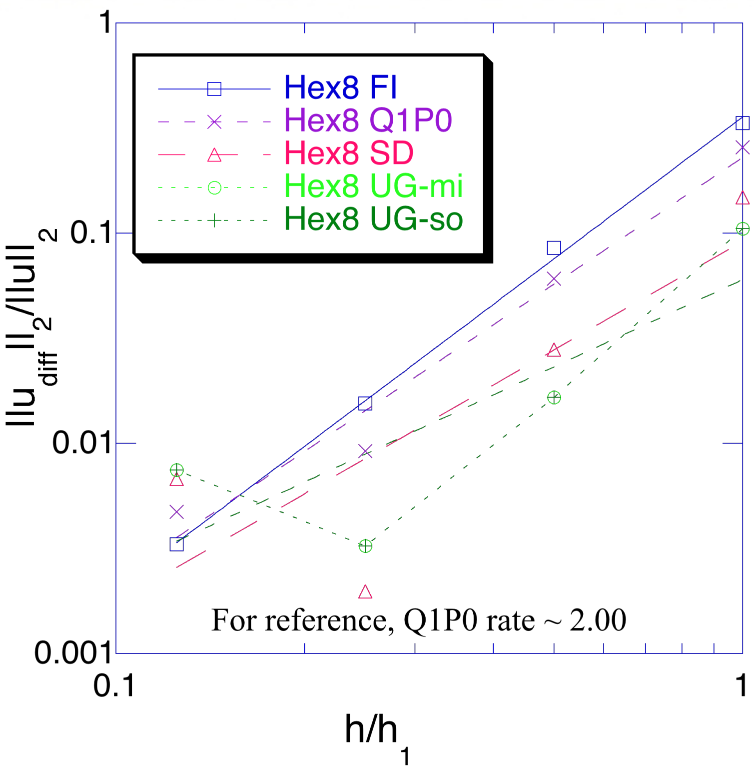
Static analysis

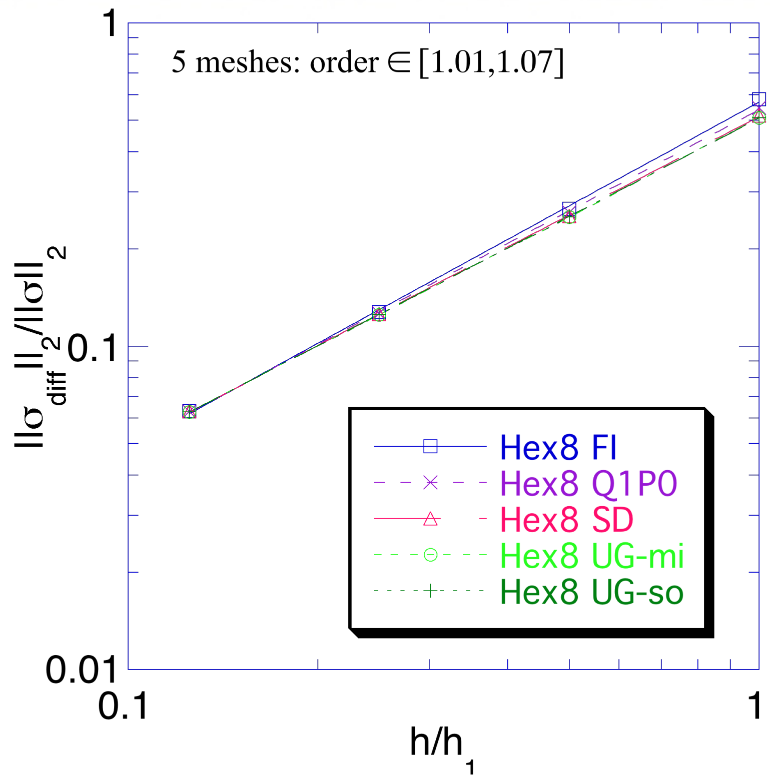
Linear behavior

Reference solution based upon Euler-Bernoulli beam theory

Slender Cantilever Beam Problem

- *convergence results for 5 hex element types*
- *Meshes: cube elements with 2, 4, 8, and 16 through depth*

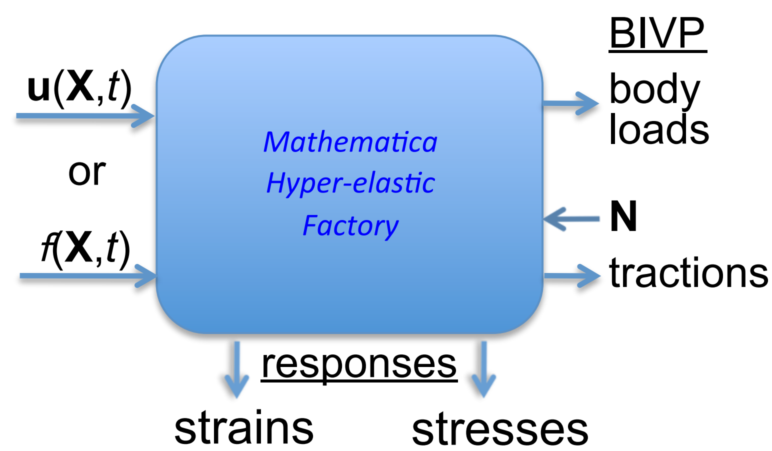




Error Quantification Testing Efforts

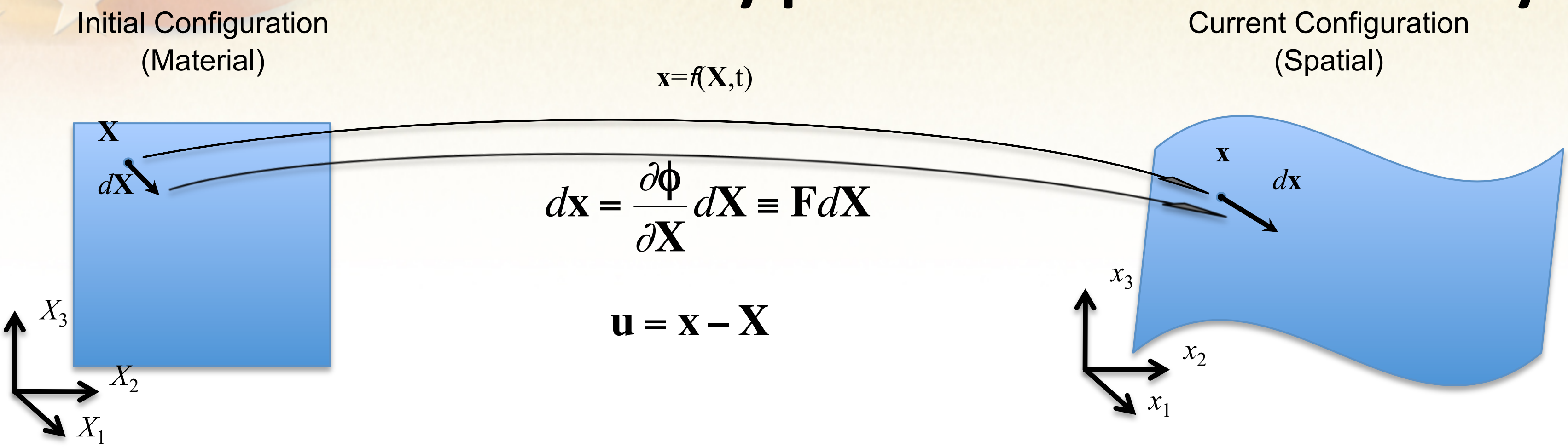
- Manufactured solution motivations
  - Limit of inexact reference solution studies
  - Finite deformation (FD)
  - Contact with larger contact areas
  - Contact with FD
  - V&V community considers “error quantification” tests the most rigorous

- Manufacturing Scope
  - Quasistatics or dynamics
  - Currently limited to hyper-elasticity and hypo-elasticity
  - Displacement and/or traction BCs



2nd implementation in stk_mms

Mathematica Hyperelastic Factory



$$d\mathbf{x} = \frac{\partial \phi}{\partial \mathbf{X}} d\mathbf{X} \equiv \mathbf{F} d\mathbf{X}$$

$$\mathbf{u} = \mathbf{x} - \mathbf{X}$$

Right Cauchy-Green Deformation Tensor

$\mathbf{C}=\mathbf{F}^T\mathbf{F}$

$$d\mathbf{x}_1 \cdot d\mathbf{x}_2 = d\mathbf{X}_1 \cdot \mathbf{C} d\mathbf{X}_2$$

Lagrangian or Green strain Tensor

$$\mathbf{E} = \frac{1}{2}(\mathbf{C} - \mathbf{I}) \qquad \frac{1}{2}(d\mathbf{x}_1 \cdot d\mathbf{x}_2 - d\mathbf{X}_1 \cdot d\mathbf{X}_2) = d\mathbf{X}_1 \cdot \mathbf{E} d\mathbf{X}_2$$

2nd Piola-Kirchoff Stress via a hyperelastic constitutive model

Isotropic material examples

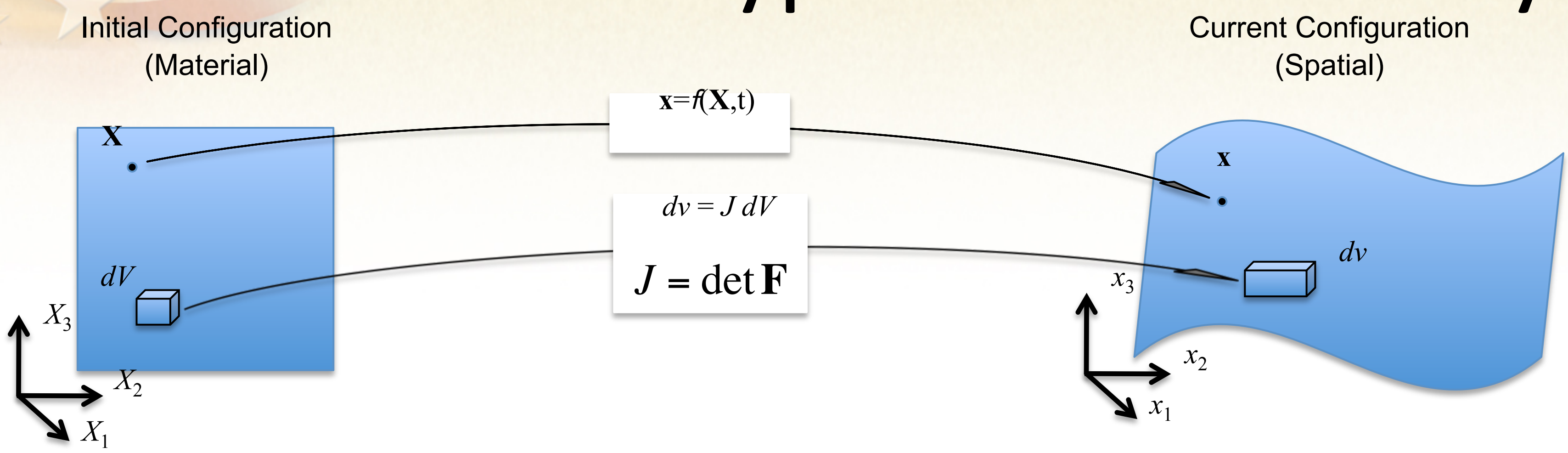
$$\mathbf{S}(\mathbf{C}) = 2\frac{\partial \Psi}{\partial \mathbf{C}} \qquad \mathbf{S} = \lambda\left(\ln\left(III_c^{1/2}\right)\right)\mathbf{C}^{-1} + \mu\left(\mathbf{I} - \mathbf{C}^{-1}\right)$$

Compressible Neo-Hookean material

$$\mathbf{S}(\mathbf{E}) = 2\frac{\partial \Psi}{\partial \mathbf{E}} \qquad \mathbf{S} = \lambda(tr\mathbf{E})\mathbf{I} + 2\mu\mathbf{E}$$

St. Venant-Kirchhoff material

Mathematica Hyperelastic Factory



2nd Piola-Kirchoff Stress — 1st Piola-Kirchoff Stress — Cauchy Stress

$\mathbf{S} \xrightarrow{\;\mathbf{P} = \mathbf{F}\mathbf{S}\;}$ (area vector) $\mathbf{P} \xrightarrow{\;\boldsymbol{\sigma} = J^{-1}\mathbf{P}\mathbf{F}^{T}\;}$ (force vector) $\mathbf{s}$

$\mathbf{S} \xrightarrow{\;\boldsymbol{\sigma} = J^{-1}\phi_*[\mathbf{S}] = J^{-1}\mathbf{F}\mathbf{S}\mathbf{F}^{T}\;} \mathbf{s}$

Conservation of linear momentum

$$DIV\,\mathbf{P} + \mathbf{f}_0 = \mathbf{0} \qquad div\,\boldsymbol{\sigma} + \mathbf{f} = 0$$

$$\mathbf{f}_0 = -DIV\,\mathbf{P} \xleftarrow{\;\mathbf{f}_0 = J\mathbf{f}\;} \mathbf{f} = -div\,\boldsymbol{\sigma}$$

Traction boundary conditions

$$\mathbf{t}_0 = \mathbf{P}\cdot\mathbf{N} \xleftarrow{\;t_0 = t\left(\frac{da}{dA}\right)\;} \mathbf{t} = \boldsymbol{\sigma}\cdot\mathbf{n}$$

Analytical expressions yield code for Sierra/SM user subroutines

Error Quantification Verification Efforts

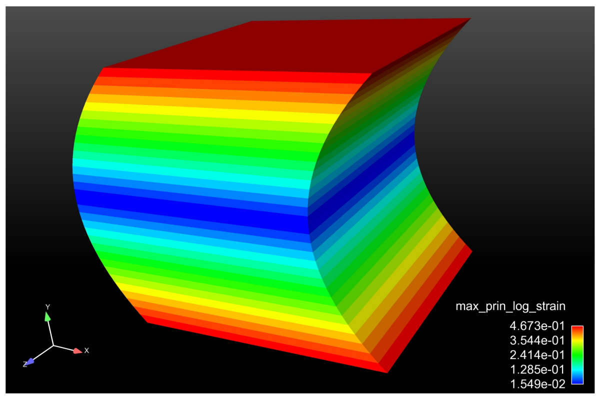
Initial Adagio Test

- **u** 2nd order (patch tests + 1)
- 30 constants -> 3 (test poly_2a)

$u_x = aY^2,\ u_y = bZ^2,\ u_z = cX^2$

Test 2a1

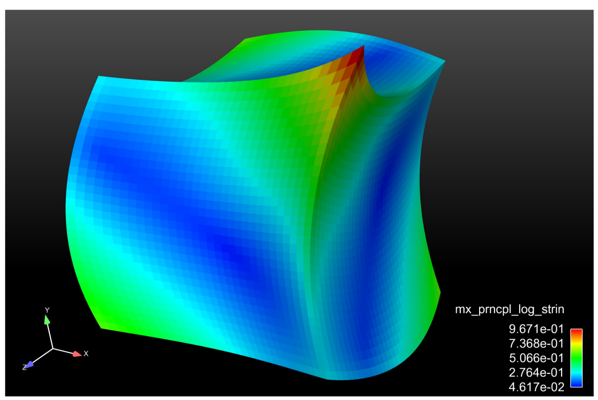
$a \neq 0$



…

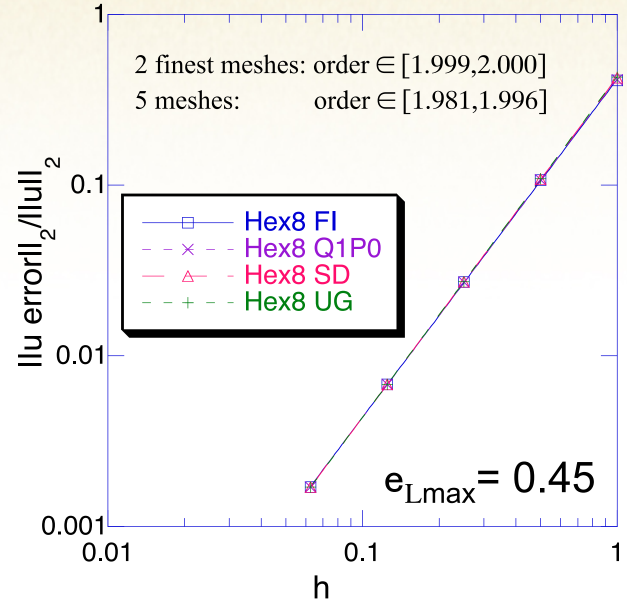
Test 2a2

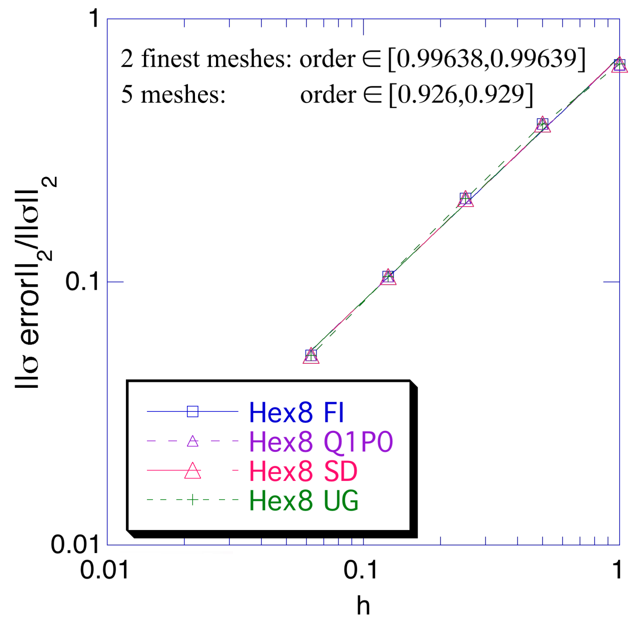
$a,b \neq 0$



Test 2a3

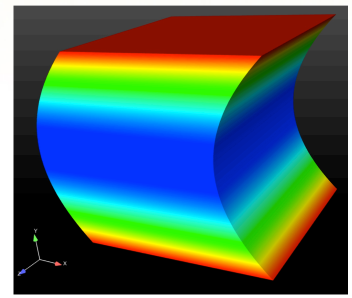
$a,b,c \neq 0$

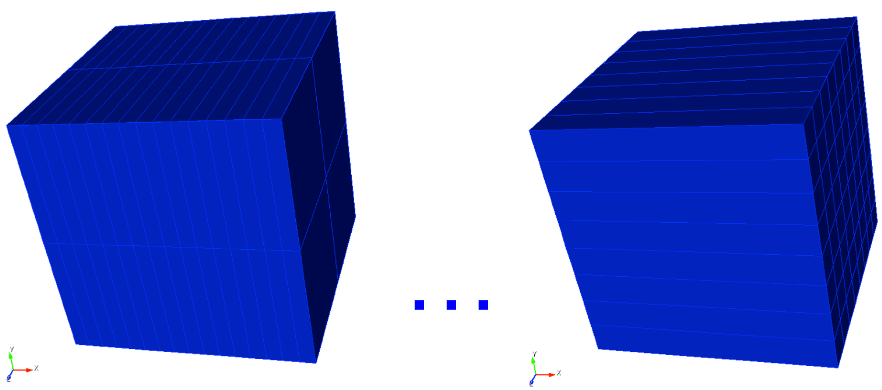


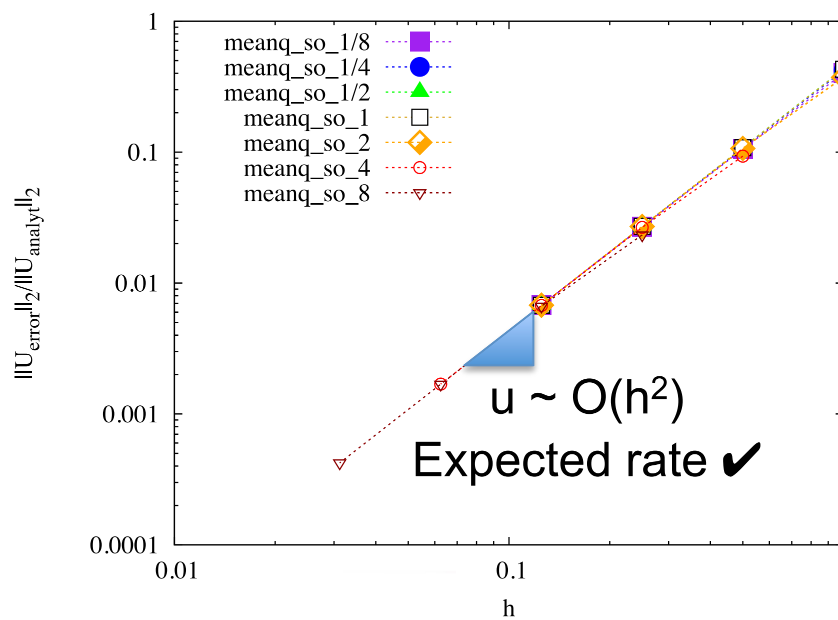


Sierra/SM Verification

- Aspect Ratio Tests
  - Motivated by issue with an impact problem
    Analyses with different aspect ratios gave different results in a limited mesh convergence study.
  - Three aspect ratio test groups added, each had:
    4 Hex8 elements x 7 aspect ratios x 4 meshes
    = 112 analyses



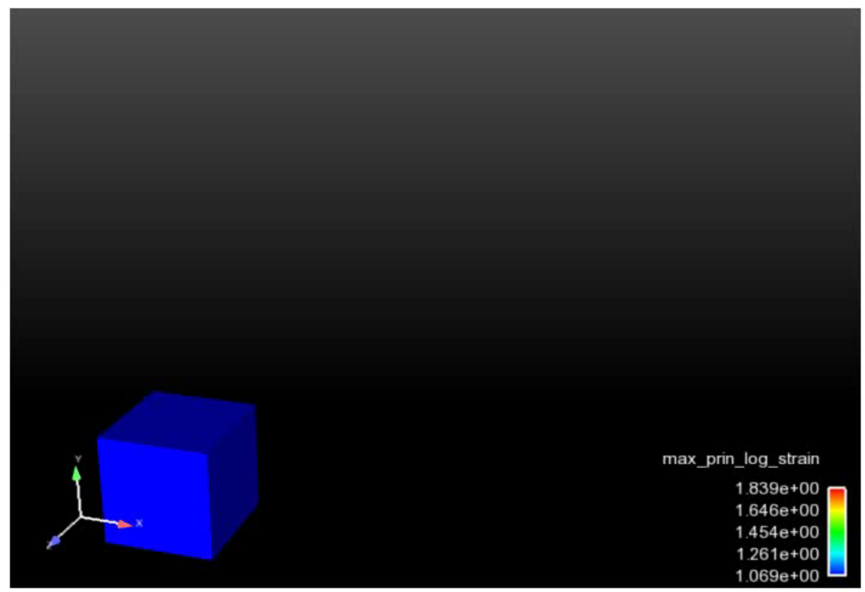




Sierra/SM Verification

- Aspect ratio tests continued
  - Previous case limited to non-zero gradient in one direction
  - Combine a deformation and rigid body rotation
  - Two test cases *O*(2%) and *O*(200%) logarithmic strains
  - Deformation mapping yields a quadratic displacement field as:

    $u_i = atr^2$ where a ~ arbitrary scale constant, *t* ~ time, and *r* ~ radius to origin
  - Rotation 60 degrees about a cube diagonal



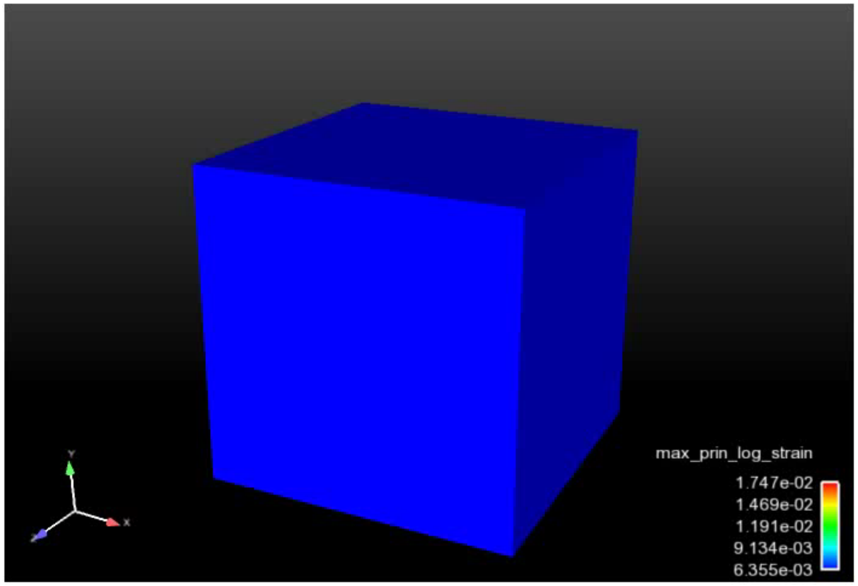
O(2%) Deformation case

O(200%) Deformation case

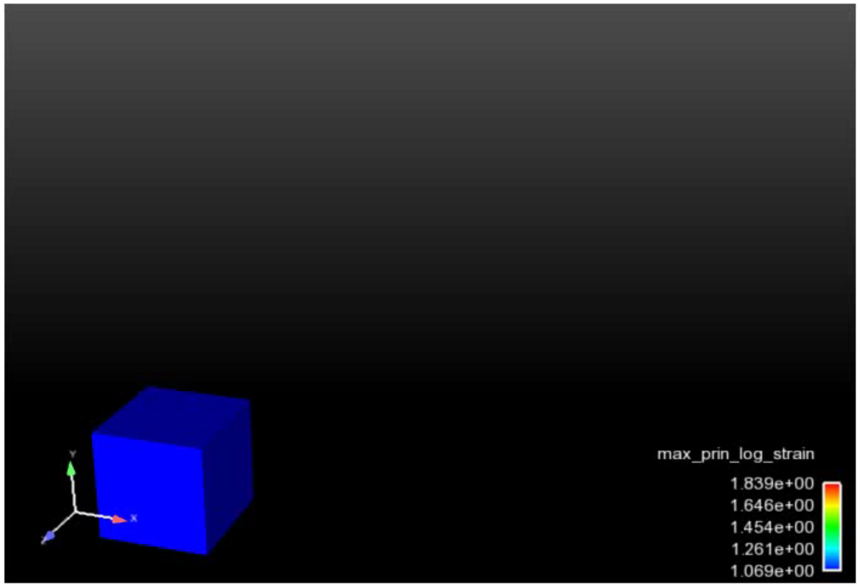
Sierra/SM Verification

- Aspect ratio tests continued
  - Previous case limited to non-zero gradient in one direction
  - Combine a deformation and rigid body rotation
  - Two test cases *O*(2%) and *O*(200%) logarithmic strains
  - Deformation mapping yields a quadratic displacement field as:

    $u_i = atr^2$ where a ~ arbitrary scale constant, *t* ~ time, and *r* ~ radius to origin
  - Rotation 60 degrees about a cube diagonal



O(2%) Deformation case



O(200%) Deformation case

On-going work

- *Convergence testing using classical solutions*
  - *Temporal integration testing*
- *Convergence testing using manufactured solutions*
  - *Application to contact*
  - *Application to problems with hypoelastic material models*
    - *the plot thickens with constitutive relationships having an incremental form and given in terms of rate of deformation tensor and objective stress rates –*
  - *Application to more complex material models?*
  - *Application to solid dynamics*

Closing comments

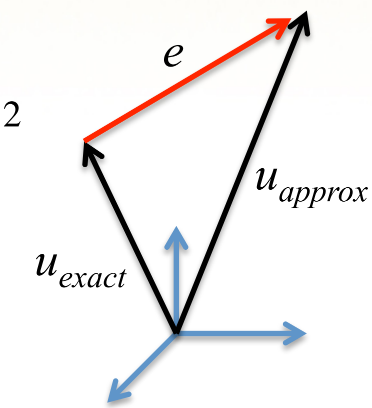
- *Original test suite:*
  - *lots of discretization error tests (subset in the manual)*
  - *Lacked needed "convergence tests" and adequate coverage*
- *We have recently added 150+ tests*
- *More importantly we have addressed some key gaps with respect to "convergence tests" and capabilities*
- *Issues identified have been revised in code*
- *Recent tests => good code quality, but there are gaps in the evidence*
- *On-going verification work needs to address coverage needs from FCT and basic capabilities*

Extra/Unused Sprint Slides Follow…

Introduction

- *Background*
  - L_2-norm (our measure of size)

$$\left\| u_{approx} - u_{exact} \right\|_2 = \left\{ \int_\Omega \left[u_{approx}(x) - u_{exact}(x) \right]^2 d\Omega \right\}^{1/2}$$



  - Convergence rate
    - by theory or assumption we express the error in power form as:

$$\|e_h\| = \|u_h - u_{exact}\| = ch^p + O(h^{p+1})$$

where h ~ measure of element size *(or time step),*

u_h ~ approximate solution for element size h

Introduction

- *Background continued*
  - *Observed rate of convergence (or order of accuracy)*
    - *We seek numerical results in the asymptotic range, i.e., where $O(h^{P+1})$ term can be neglected giving*

      $$\|e_h\| \cong c h^p$$

      taking the log of both sides gives

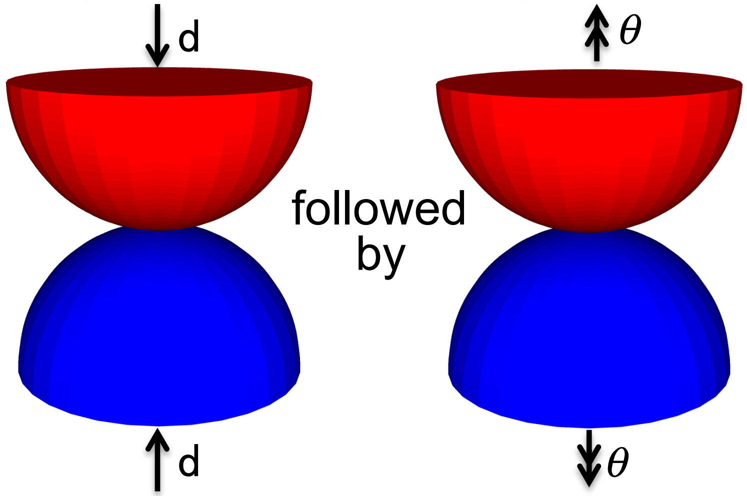
      $$\log(\|e_h\|) \cong \log(c) + p \log(h)$$

      slope on log-log plot yields observed rate of convergence
- Expected convergence rates for 8-noded hex elements
  - Displacements: p=2 → ½ mesh refinement gives ¼ error
  - Stresses: p=1 → ½ mesh refinement gives ½ error

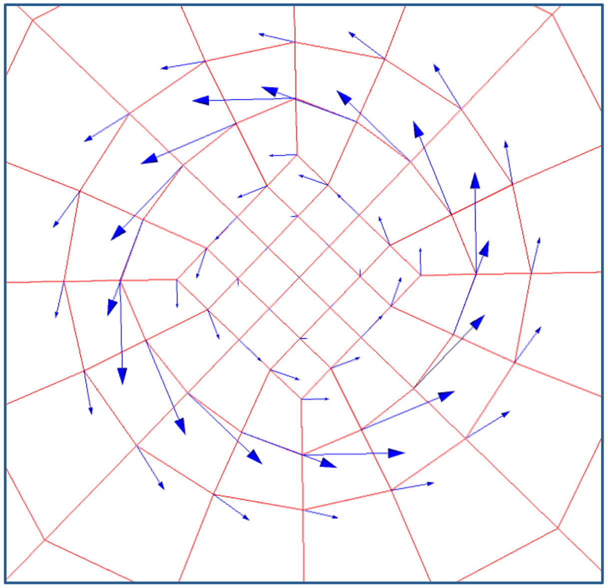
Contact Convergence Tests

Lukin *et al*. sphere-sphere tests – "Hertz with a twist"

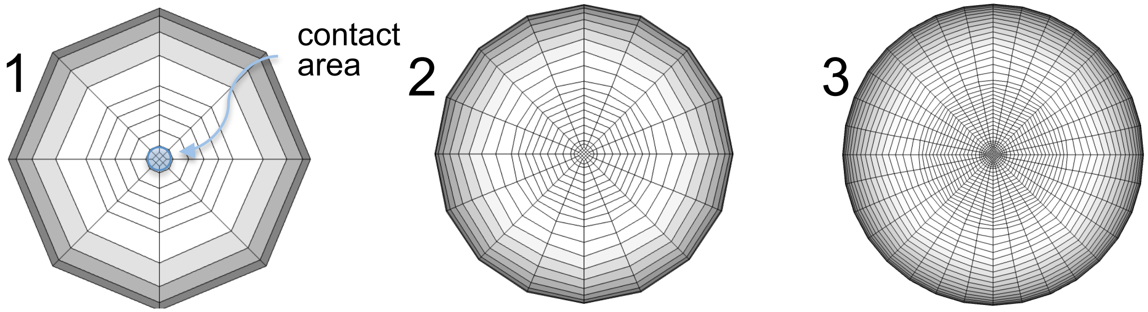
– Hertz compression twist



Nodal contact forces
Mesh 2

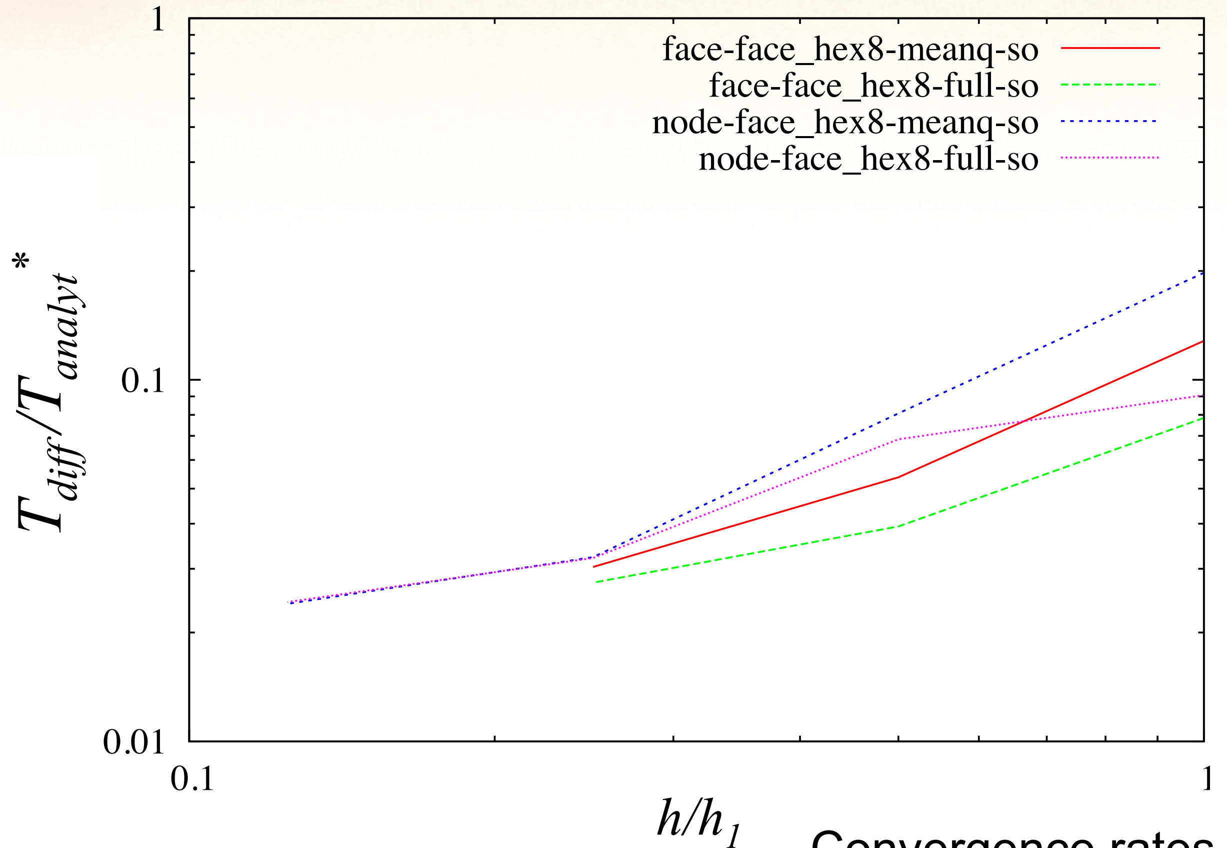


– Mesh sequence



Contact Convergence Tests

Lubkin *et al.* sphere-sphere tests – “Hertz with a twist”



Convergence rates from asymptotic analysis

	Meanq-so	Full
face/face	1.68, 1.84	3.16, 2.02
node/face	1.37, 2.36	4.80, 0.27

* Approximate analytical solution from: Segalman, Starr, and Heinstein (2005)