

Overview of Encore

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Sandia National Laboratories

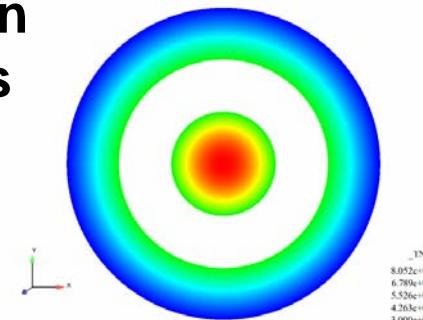
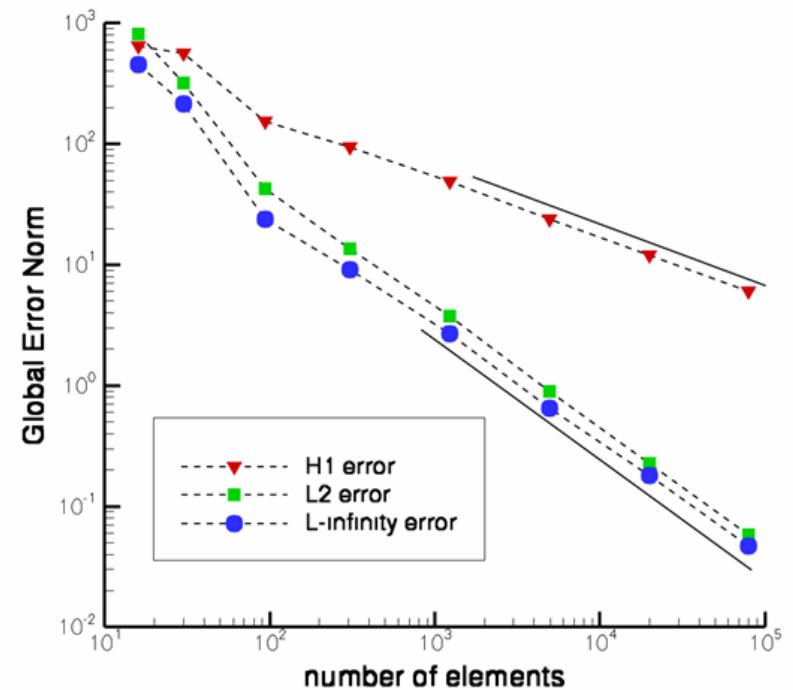


Outline

- **Code and solution verification**
- **Feature coverage tool**
- **Transition to Trilinos (STK_Encore)**
- **Mesh adaptivity**
- **Uncertainty quantification (UQ) using random fields**
- **FY11 Encore roadmap**

Code Verification Support

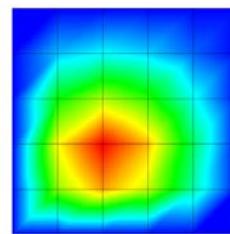
- Generic function interface
 - Analytic functions
 - Text strings: “ $x+y$ ”
 - User subroutines
 - Mesh based field functions
 - FE interpolation of solution fields
- Error metrics
 - Integration point based (integrals, max norm)
 - Nodal/element based
- Generate forcing terms for verification by method of manufactured solutions



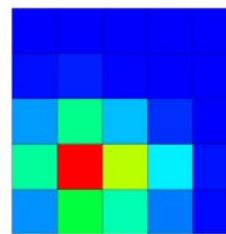


Solution Verification Support

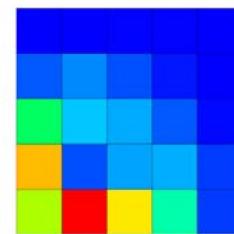
- Read in solution from output files
 - Currently IO is limited to ExodusII
- Interpolation of solutions between different grids
- Error metrics based on comparison of solutions from different meshes
- Compute convergence rates
 - Global error metrics
 - Local spatial convergence



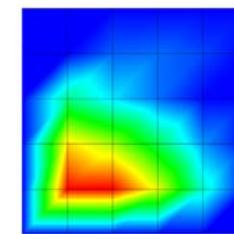
Coarse grid solution



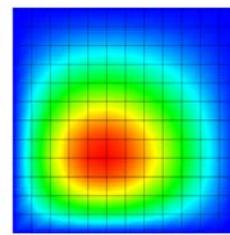
L2 error



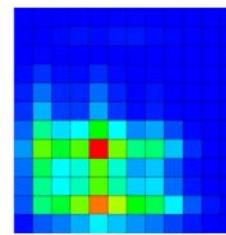
H1 error



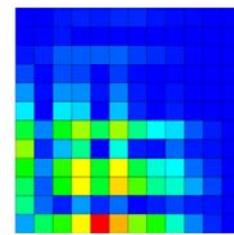
Nodal error



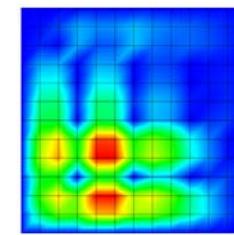
Fine grid solution



L2 error



H1 error



Nodal error



Feature Coverage Tool

Analyst questions (PCMM level):

- In how many tests is a feature used?
- In which test suite?
- In which tests, in what context?
- Are two features tested together?

Developer needs coverage of:

- Every suboption, string, or algorithm knob is included
- Multiphysics code coupling
- Multiple test suites (regression, verification, acceptance, etc.)



Example Output

- Filter: Against specific Sandia application (input deck)
- Test suite: verification, features versus tests (242)



Transition to STK_Encore

- **Encore (FY08-present) is a component in Sandia's SIERRA Mechanics suite**
 - Built on the SIERRA Framework
 - Developed as part of DOE/ASC program
 - Restrictive licensing (not open source)
 - Code base strongly tied to SIERRA
- **STK_mesh (FY10-present): Sierra Toolkit is started**
 - next generation of SIERRA Framework
 - Fully Open Source and released as part of Trilinos

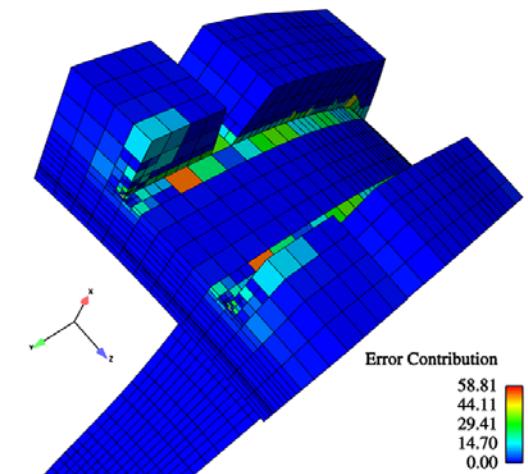
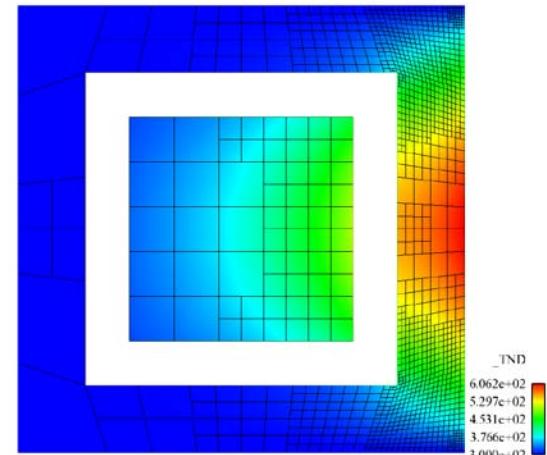


STK_Encore

- **STK_Encore (FY10-present): next generation version of Encore**
 - Developed to support multiple customers (ASC, NEAMS, CASL)
 - Rewritten on top of STK (Sierra ToolKit)
 - Open source licensing
 - Design goals:
 - Quick and easy code and solution verification
 - Support non-Sierra workflows and formats
 - Command line interface
 - Scripting API (python or other dynamic languages)
 - C/C++ Library API

Mesh Adaptivity

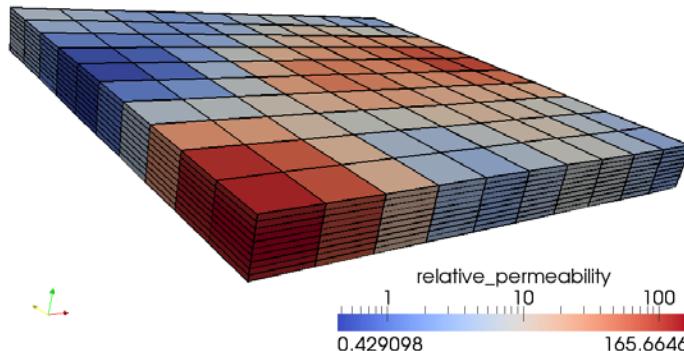
- Encore supports both uniform and adaptive mesh refinement
- Uniform refinement is used (in parallel) to generate meshes for solution verification
 - FY11: joint project with Cubit meshing team to include CAD geometry in uniform refinement
 - Can also enrich to higher order elements for verification
- Adaptive refinement generates locally refined meshes to efficiently reduce numerical error
 - FY11: adaptive tetrahedral refinement will be implemented in STK_Encore
 - Encore contains some basic error indicators that can be used to drive adaptivity (recovery/averaging, residuals)





UQ using Random Fields

- Support for spatial heterogeneous random fields (RFs) was added to Encore in FY10.
- Can be used to simulate material and boundary condition variability beyond random variables (which are uniform over space and time)
- RFs are characterized by a vector of random variables that are controlled using DAKOTA
- FY11: work will include interface to experimental data
- FY11: Encore UQ capability will be included in STK_Encore





Encore FY11 Roadmap

- Interface to Encore through
 - File IO (ExodusII)
 - LIME interface (using ModelEvaluator)
- Refine/Enrich for additional element types
- Grid to grid mapping/transfer of fields
- Dynamic language (Python) API
- Automated mesh convergence studies
 - Local Richardson Extrapolation (node/element level)
- Non-uniform refinement of simplex elements
- Non-uniform refinement of hexahedral elements (no hanging nodes)
- Boundary layer refinement of quad/hex element
- Scope and design of CAD geometry (NURBS) integration