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Motivation

- The Computational Mechanics Community lacks an Open Source Collaborative Coding Environment
- Sandia's production analysis codes (Sierra) would benefit from a computational mechanics test bed

Objective

- Provide an Open Source tool, useful for both internal and external collaboration
- Establish a path from research to the production codes, using an emphasis on common data structures via STK

Approach

- Build upon the strength of Trilinos – Open Source, modular, rich/diverse capabilities (trilinos.sandia.gov)
- Leverage existing agile component, transformational capabilities (Albany)
- Combine expertise from multiple centers (1400/1500/8200)

Key Features

- Sierra ToolKit (STK) mesh representation
- Parallel with Exodus I/O (STK)
- Full suite of solvers (NOX, Amesos, Belos)
- Library of finite elements (Intrepid)
- Multi-physics dependency management (Phalanx)
- Automatic Differentiation - AD (Sacado)
- Compute the jacobian of nonlinear residual (Newton's method)

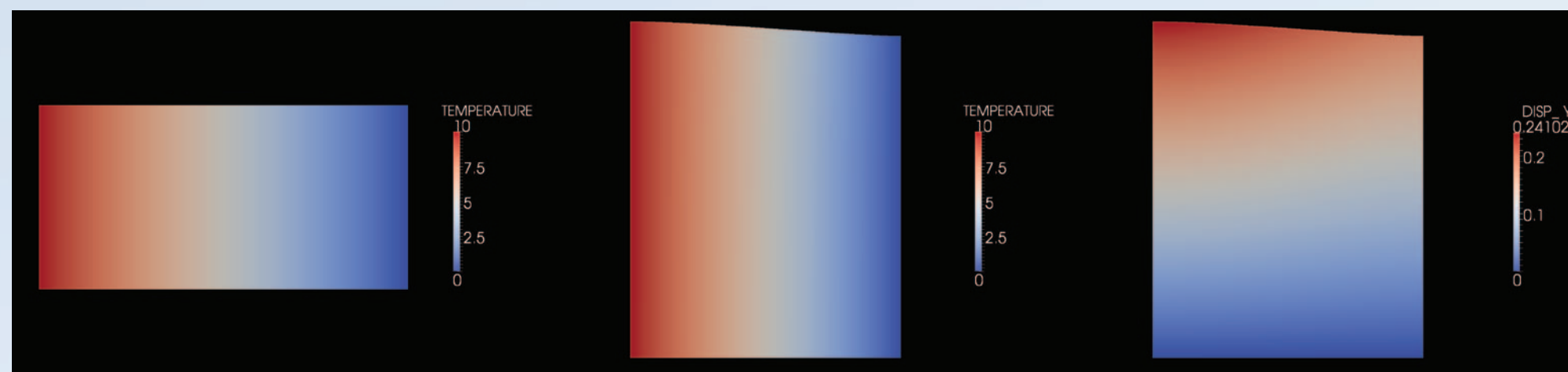
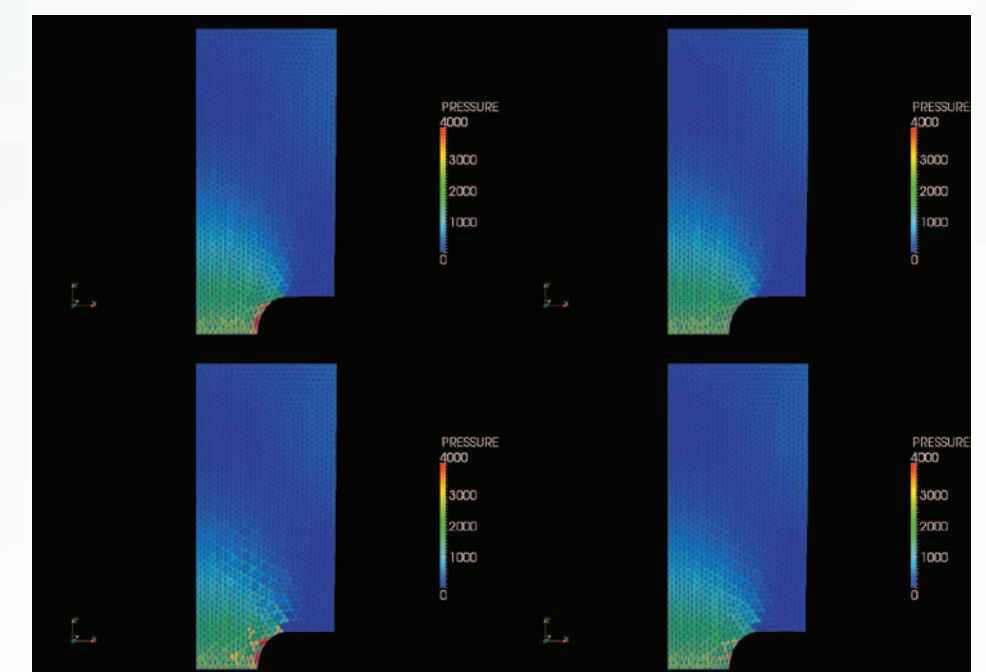
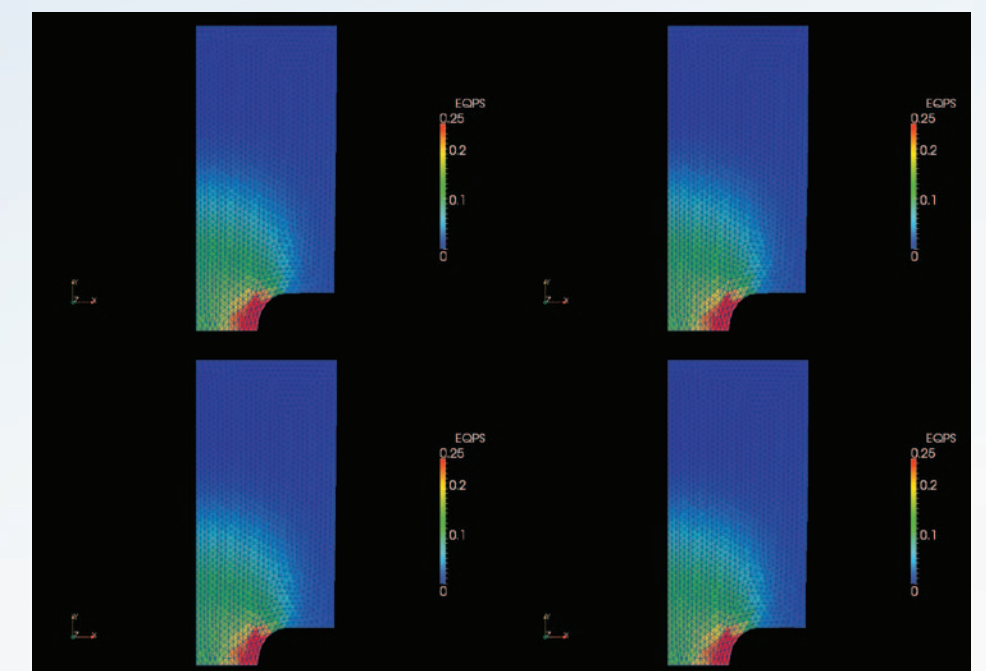
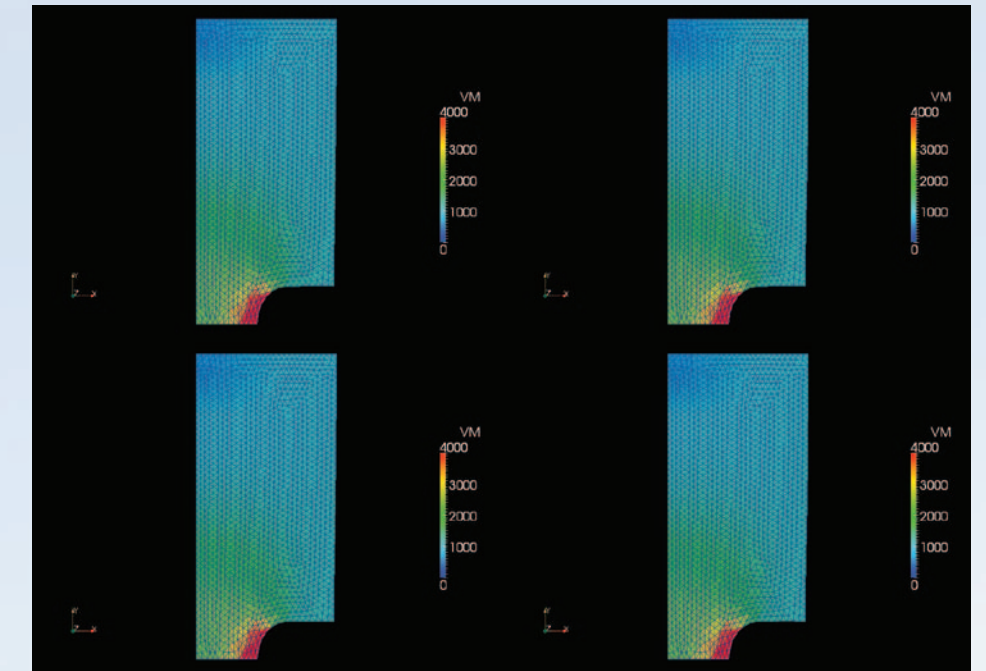
$$J = \frac{\partial R(u)}{\partial u}$$

- Given an energy, compute a conjugate stress (hyperelastic materials, variational principles)

$$P = \frac{\partial \Psi(F)}{\partial F}$$

- Embedded UQ – Stochastic Galerkin Finite Elements (Stokhos)
- Material Models – Library of Advance Materials for Engineering (LAME)

Element Formulation Investigation



Thermoelasticity Dependency Graph

AD Example

$$y = \sin(e^x + x \log x), \quad x = 2$$

$$\begin{aligned} x &\leftarrow 2 & \frac{dx}{dx} &\leftarrow 1 \\ t &\leftarrow e^x & \frac{dt}{dx} &\leftarrow t \frac{dx}{dx} \\ u &\leftarrow \log x & \frac{du}{dx} &\leftarrow \frac{1}{x} \frac{dx}{dx} \\ v &\leftarrow xu & \frac{dv}{dx} &\leftarrow u \frac{dx}{dx} + x \frac{du}{dx} \\ w &\leftarrow t + v & \frac{dw}{dx} &\leftarrow \frac{dt}{dx} + \frac{dv}{dx} \\ y &\leftarrow \sin w & \frac{dy}{dx} &\leftarrow \cos(w) \frac{dw}{dx} \end{aligned}$$

x	$\frac{d}{dx}$
2.000	1.000
7.389	7.389
0.301	0.500
0.602	1.301
7.991	8.690
0.991	-1.188

