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Albany: A multiphysics application based on Trilinos

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Trilinos User's Group Meeting
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CSRI, Sandia-NM

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Albany is

- **a parallel, implicit, unstructured-grid finite element code,**
- **that uses "as many Trilinos packages as possible" in a single code**
- **to demonstrate advanced engineering analysis capabilities across a wide range of physics applications.**

- **Albany illustrates how to integrate Trilinos packages in a general way to create a highly-featured parallel application including**
  - Discretization services (Intrepid, Shards, STK, Seacas)
  - Linear solvers and preconditioners (Stratimikos, Belos, ML, MueLu)
  - Advanced nonlinear analysis (Piro, NOX, LOCA)
  - Leading edge software construction/engineering capabilities (Phalanx, TBGP, integrated build/test)

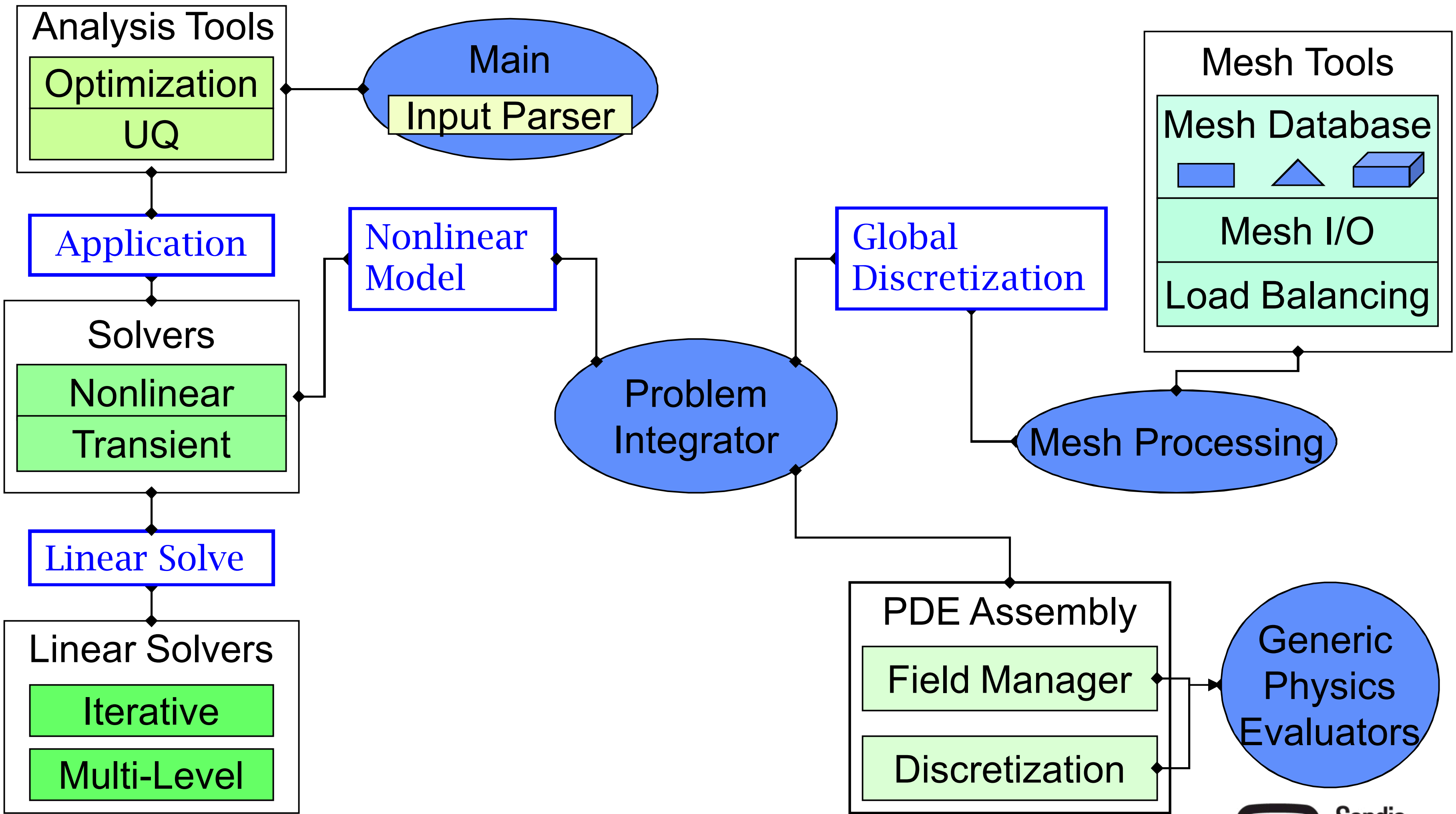
Trilinos packages enabled in AlbanySettings.cmake

ThyraTpetraAdapters
Ifpack2
MueLu
Teuchos
Shards
Sacado
Epetra
EpetraExt
Ifpack
AztecOO

Amesos
Anasazi
Belos
ML
Pamgen
Phalanx
Intrepid
NOX
Stratimikos
Thyra

OptiPack
GlobiPack
Seacas
Stokhos
Isorropia
Piro
STK
Teko
Zoltan
Rythmos
MOOCHO

Albany high level design



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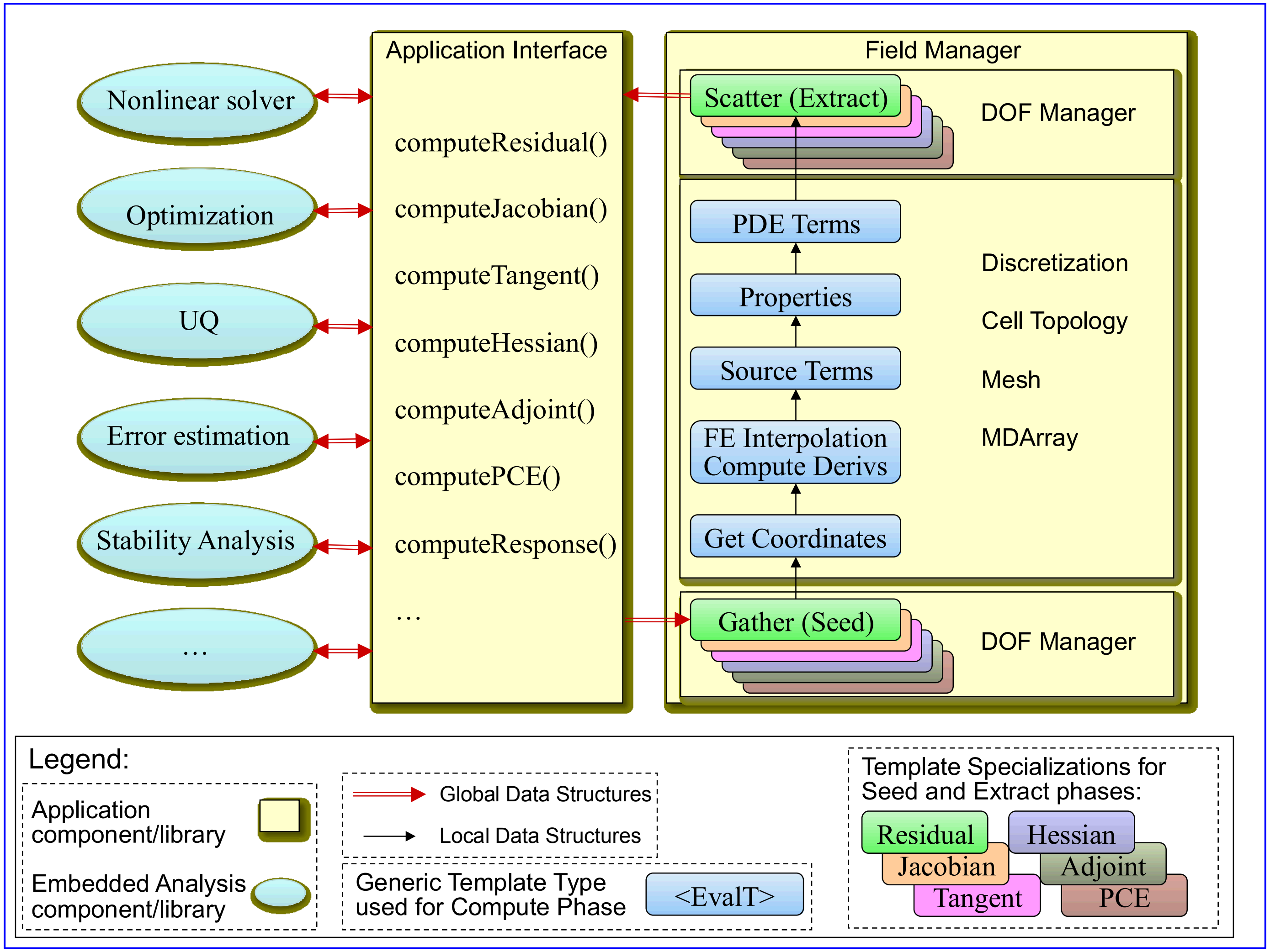
Albany generic physics interface



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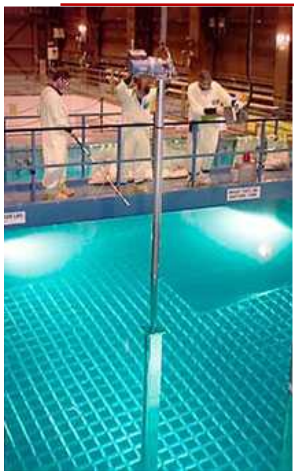
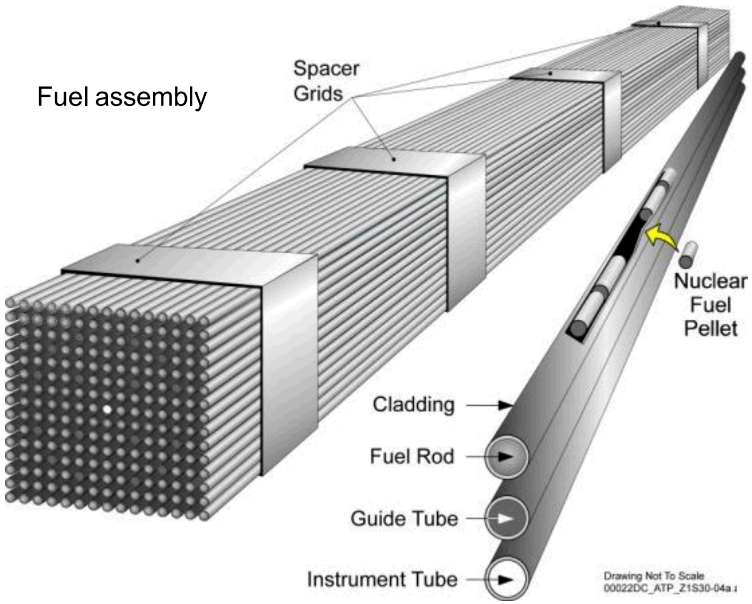
Albany multiphysics

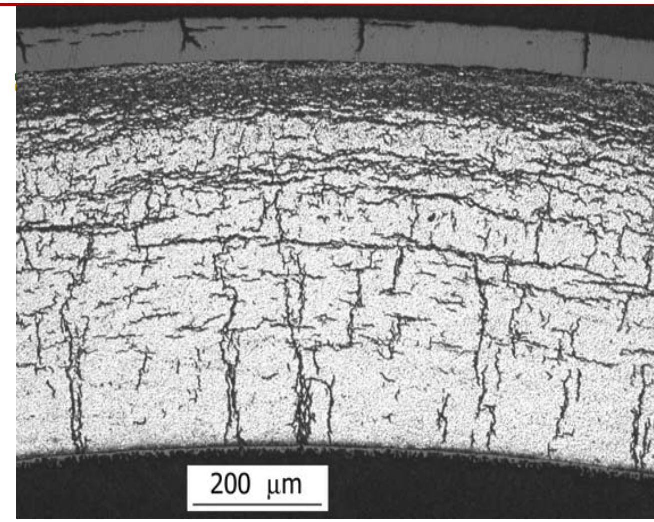
- **Test suite comprised of ~230 problems. Selected examples include:**
- **Computational mechanics**
  - elasticity, J2 plasticity, thermomechanics, unsaturated poroelasticity, thermo-poro-mechanics, diffusion-deformation, cladding Zry4 hydride reorientation, gradient damage, rate independent hardening minus recovery (RIHMR)
- **Fluids**
  - compressible Navier-Stokes, finite element for land ice experiments (FELIX), coupled reactor, vortex shedding, Rayleigh-Bernard
- **Diffusion, misc**
  - heat equation, PoissonSchrodinger, Cahn Hilliard / Elasticity, continuation, load and displacement stepping problems

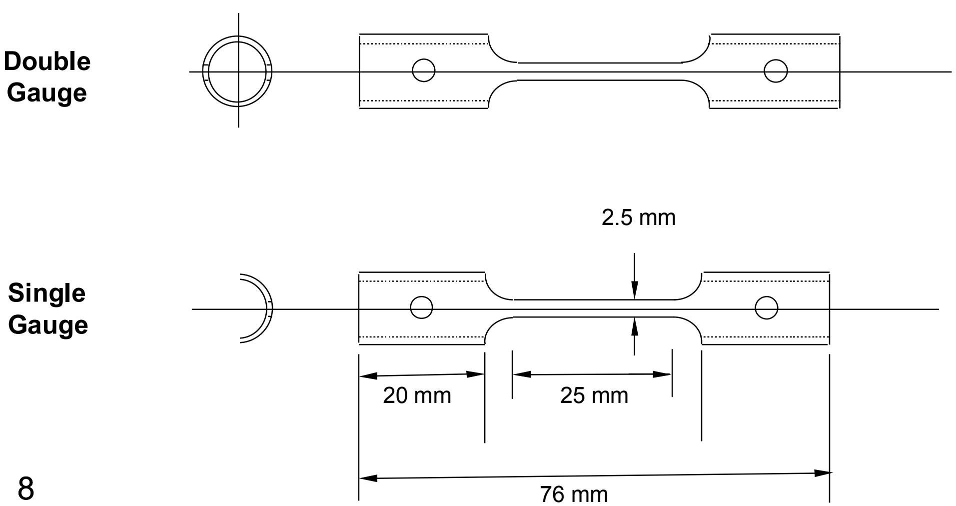
Selected Albany Application Examples

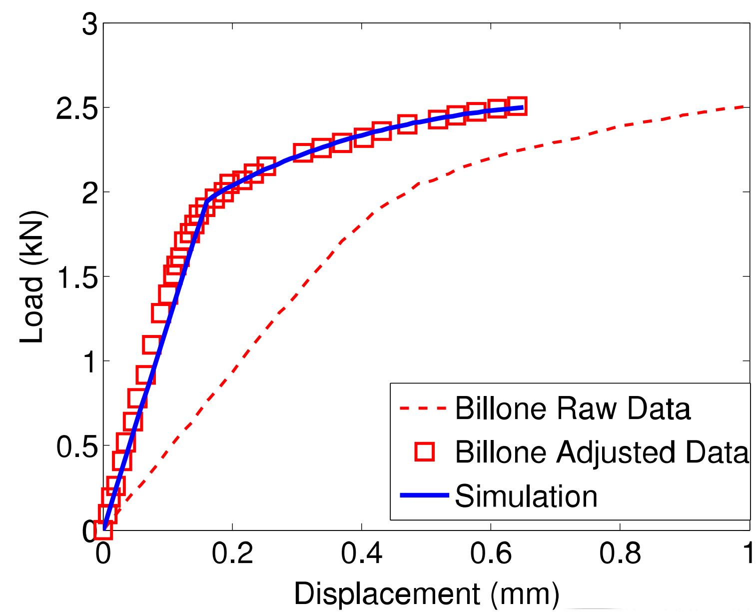
Used reactor fuel handling



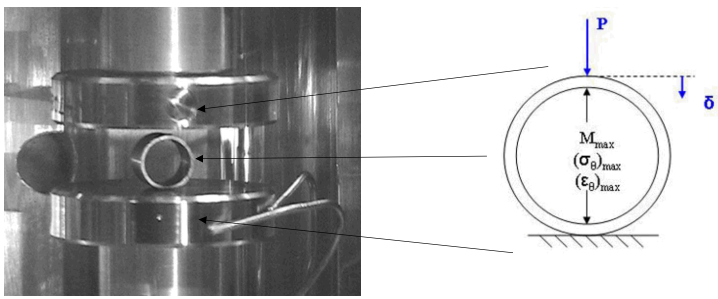




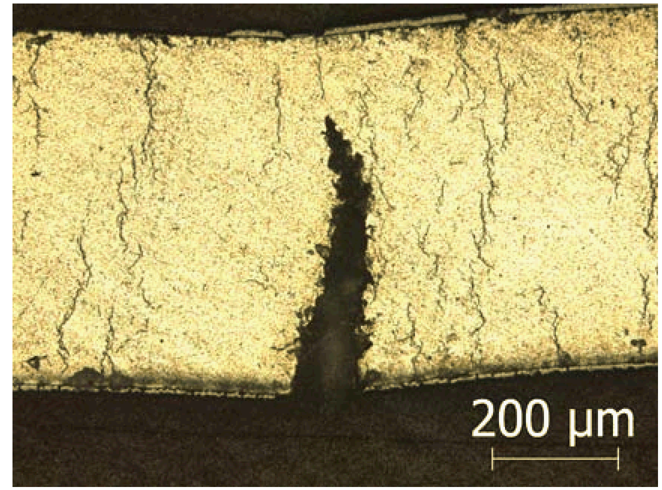




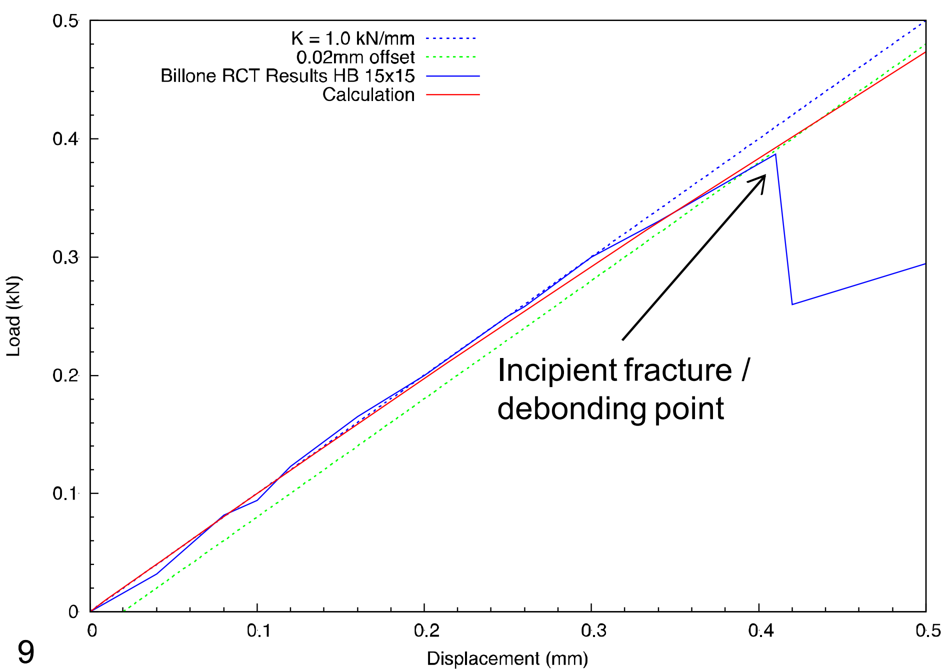
Predict cladding behavior



Ring Compression Test Fixture



Billone, et.al. 2012



- **Excellent agreement was obtained with experiments on actual fuel samples, up to the point of sample failure**

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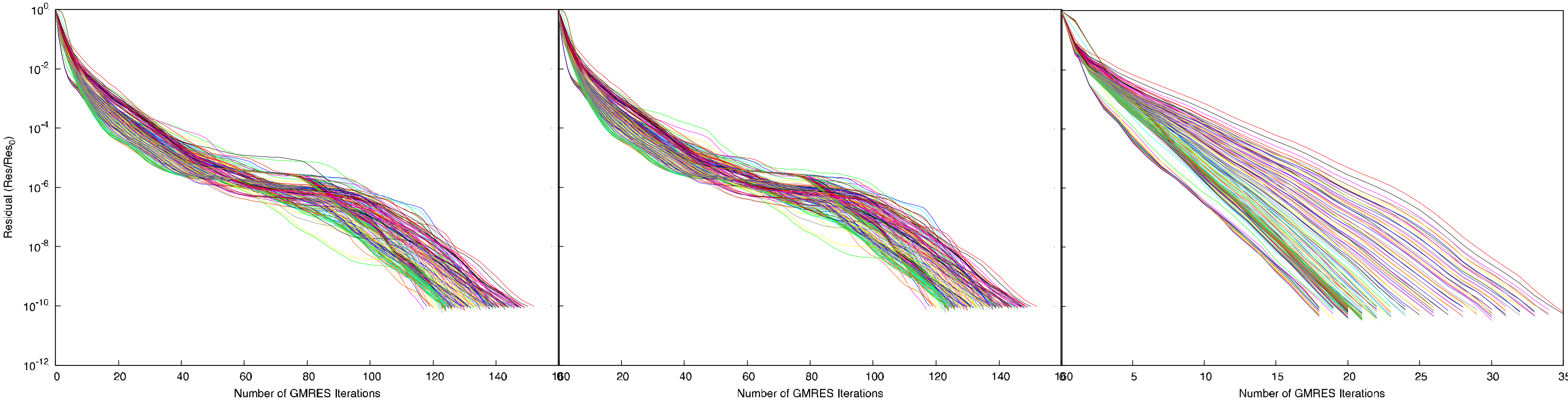
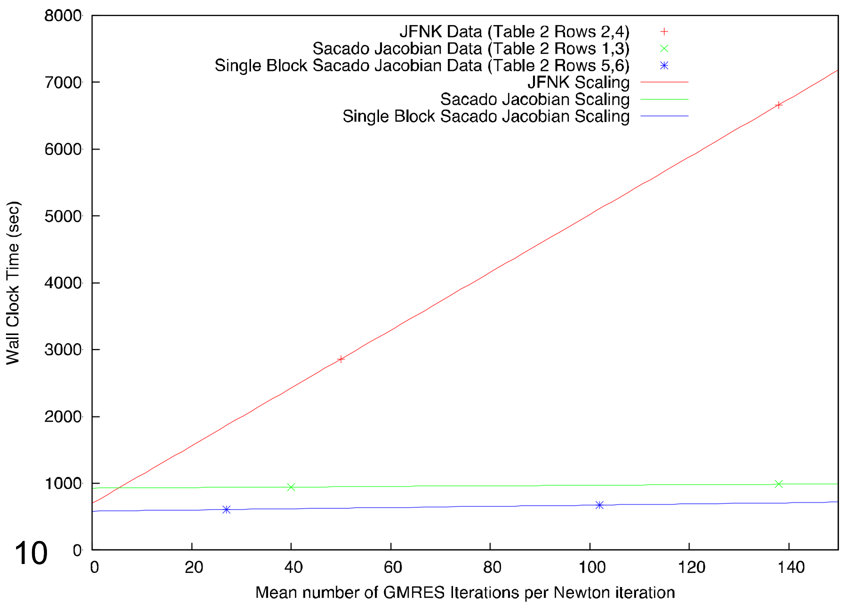
Using state of the art analysis capabilities



Teko BGS/ML

Teko BGS/ML JFNK

ML



Albany features found most impactful:

- **Rapid model implementation**
- **Extensive collection of existing physics capabilities that are easily "reused"**
- **Wide variety of solvers and preconditioners can be brought to bear on the problem**
- **Everything needed "under one roof": LOCA continuation, parallel load balancing, SA and UQ (TriKota), multiple Jacobian strategies, etc**

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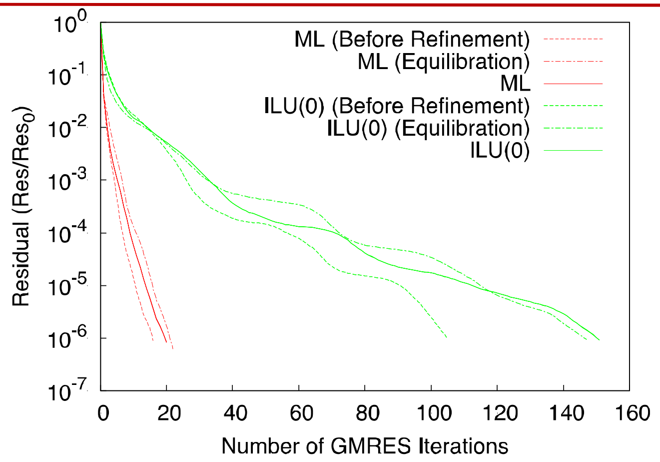
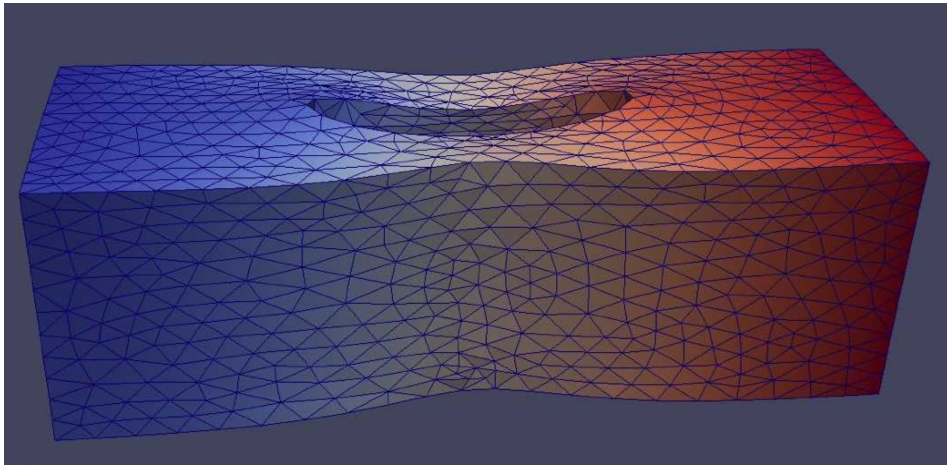
Adaptive elasticity

- **Elastic deformation of a rectangular bar**
- **Continuation problem: location of right boundary is the continuation parameter**
- **Zienkiewicz-Zhu error indicator drives refinement near hole**
- **Preconditioned Belos (GMRES)solver used inside LOCA**
- **Consider ILU(0) and AMG (SA) – Albany communicates rigid body modes (null space info) to ML**

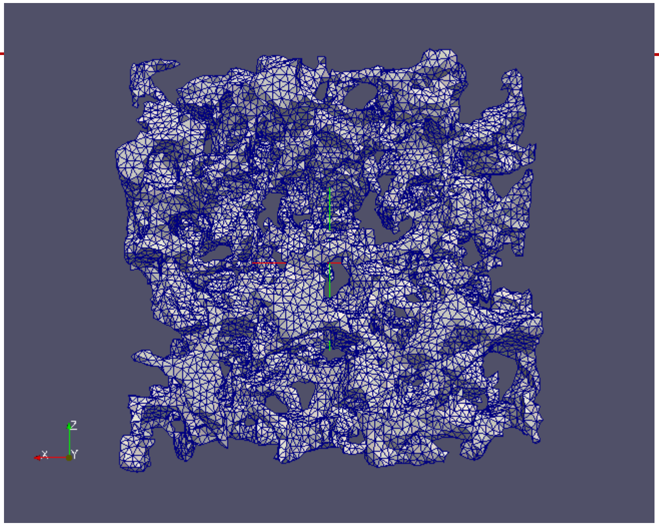


Convergence: Comparing preconditioning options

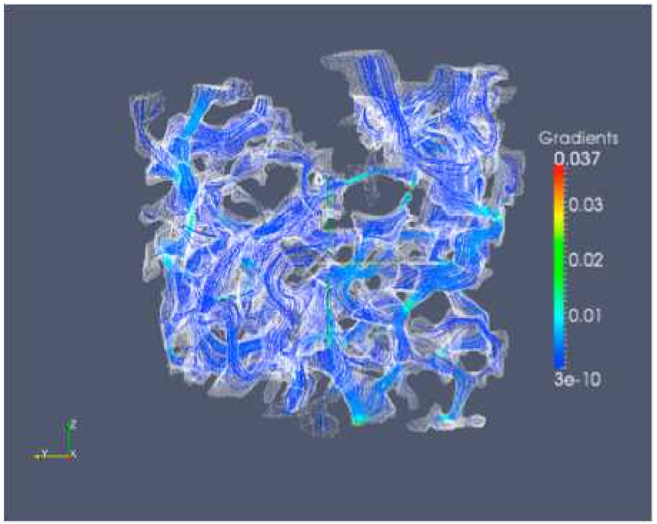


Bar deformation: Mesh adapts to reduce error (ZZ)

LCM: Estimating Effective Thermal Conductivity from Microstructures



Mesh generated from CT images of 12% porosity Fontainnebleau sandstone (from Teng-fong Wong)



Single-phase Thermal Diffusion simulation on CT Images

- Volume averaging effective thermal conductivity

$$\boldsymbol{k}_\theta = \phi^{\mathrm{f}} \boldsymbol{k}_\theta^{\mathrm{f}} + (1 - \phi^{\mathrm{f}}) \boldsymbol{k}_\theta^{\mathrm{s}}$$

(cf. Preisig & Prevost, IJGGC 2011)

- Homogenized effective conductivity via Eshelby equivalent inclusion method (for spherical inclusions)

$$\boldsymbol{k}_\theta = \left(k_\theta^f + \frac{\phi^{\mathrm{f}} (k_\theta^{\mathrm{s}} - k_\theta^{\mathrm{f}}) k_\theta^{\mathrm{f}}}{(k_\theta^{\mathrm{s}} - k_\theta^{\mathrm{f}}) \phi^{\mathrm{f}} + k_\theta^{\mathrm{f}}} \right) \boldsymbol{I}$$

(cf. Zhou & Meschke, IJNAMG 2013)

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See Sun, Ostien, Salinger, International Journal for Numerical and Analytical Methods in Geomechanics, 2013

LCM: Optimal Stabilization Parameter Estimation

1D poromechanics governing equation

$$c\frac{\partial^2 \hat{p}}{\partial x^2} = \frac{\partial \hat{p}}{\partial t}, \qquad c = \frac{k}{\mu}\frac{M'H}{H + \nu\beta M'}; M' = \frac{M(K + 4G/3)}{K + 4G/3 + B^2 M}$$

Three node stencil (standard Galerkin method)

$$- \hat{p}_{A-1} + 2\hat{p}_A - \hat{p}_{A-1} + \frac{h^2}{6\vartheta c \Delta t}(\hat{p}_{A-1} + 4\hat{p}_A + \hat{p}_{A+1}) = 0$$

Three node stencil (Stabilized Galerkin method)

$$-\hat{p}_{A-1} + 2\hat{p}_A - \hat{p}_{A-1} + \frac{h^2}{12\vartheta c \Delta t}[(2-\gamma)\hat{p}_{A-1} + (8+2\gamma)\hat{p}_A + (2-\gamma)\hat{p}_{A+1}] = 0$$

Growth/decay rate

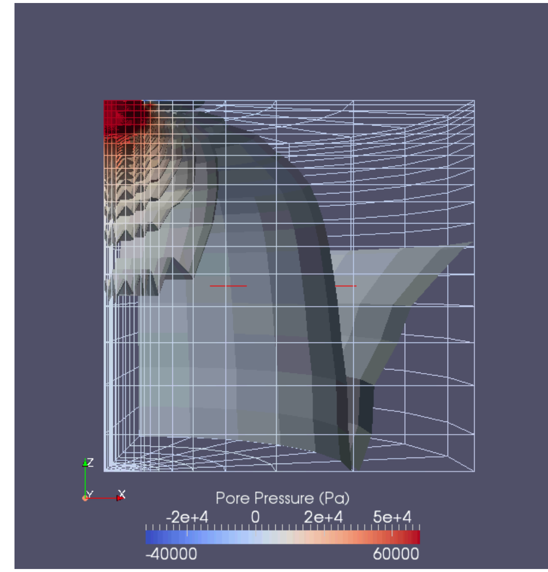
$$\cosh \frac{h}{(\sqrt{\vartheta c \Delta t})^h} = \frac{(1 + h^2/\vartheta c \Delta t)(4+\gamma)/6}{(1 - h^2/\vartheta c \Delta t)(2-\gamma)/12}$$

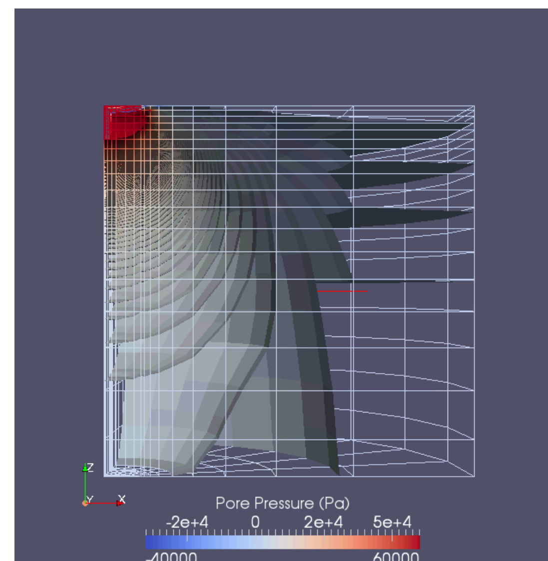
To have real growth/decay rate, we need

$$\gamma > 2 - 12\frac{\vartheta c \Delta t}{h^2} > 0 \qquad \gamma = \left(2 - 6\frac{\vartheta c \Delta t}{h^2}\right)\left(\frac{1}{2} + \frac{1}{2}\tanh\left(2 - 12\frac{\vartheta c \Delta t}{h^2}\right)\right)$$

Safety factor

Turn off stabilization without introducing switch

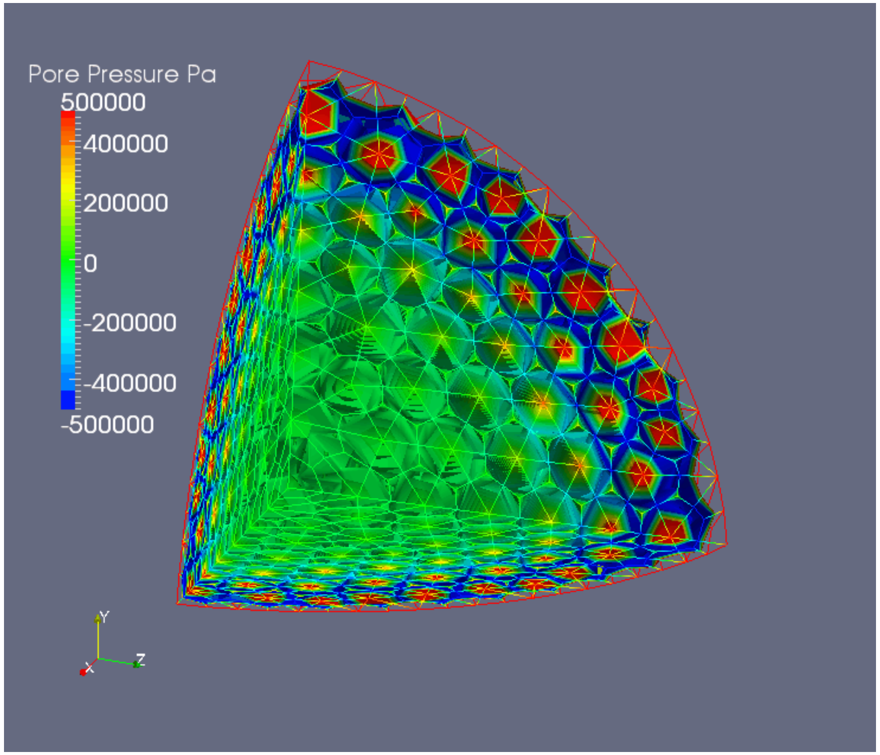




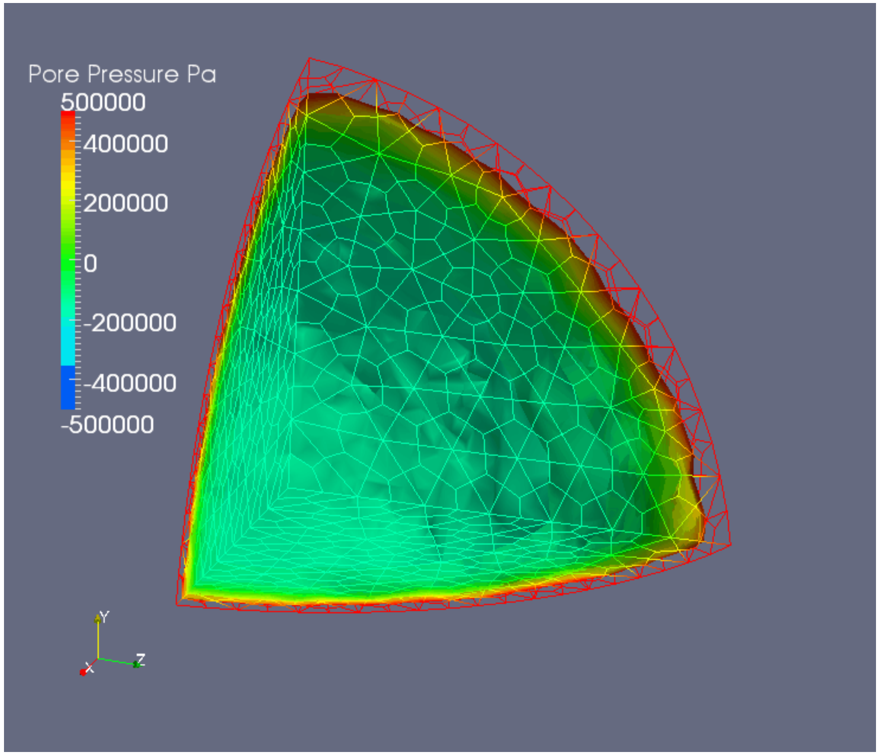
Thermo-hydro-mechanical Responses of Porous Sphere in Thermal Reservoir

Under-diffusion with spurious patterns

Diffusion with estimated optimal stabilization



Pore Pressure computed with standard Galerkin FEM

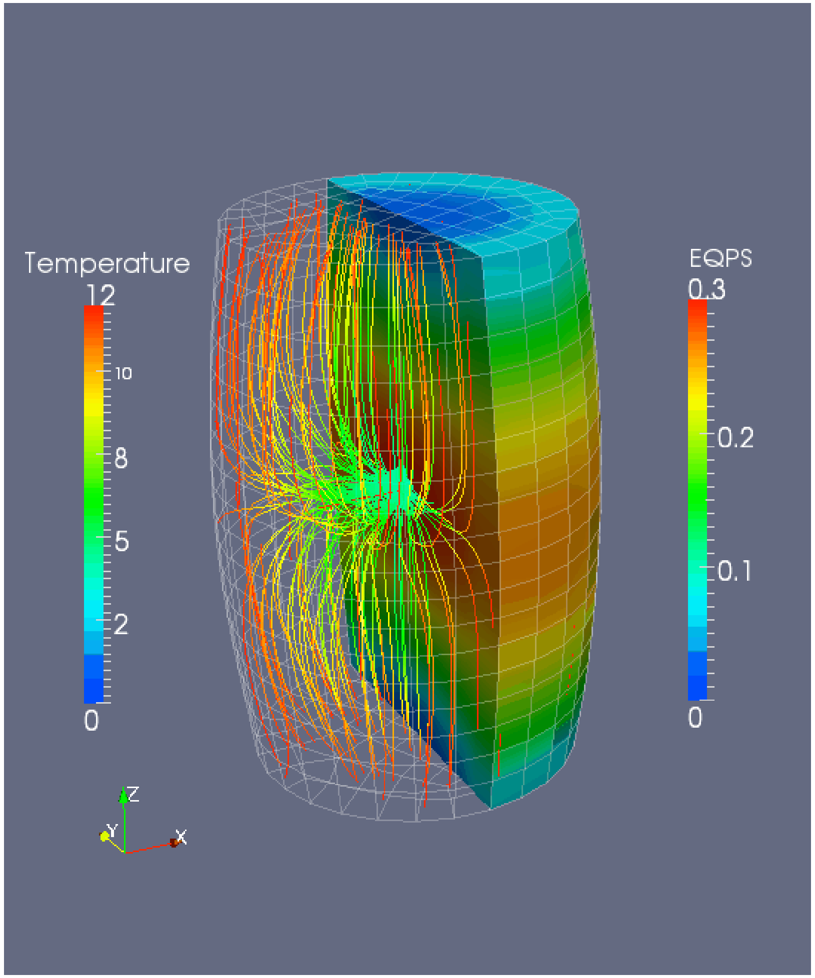


Pore Pressure computed with Stabilized FEM

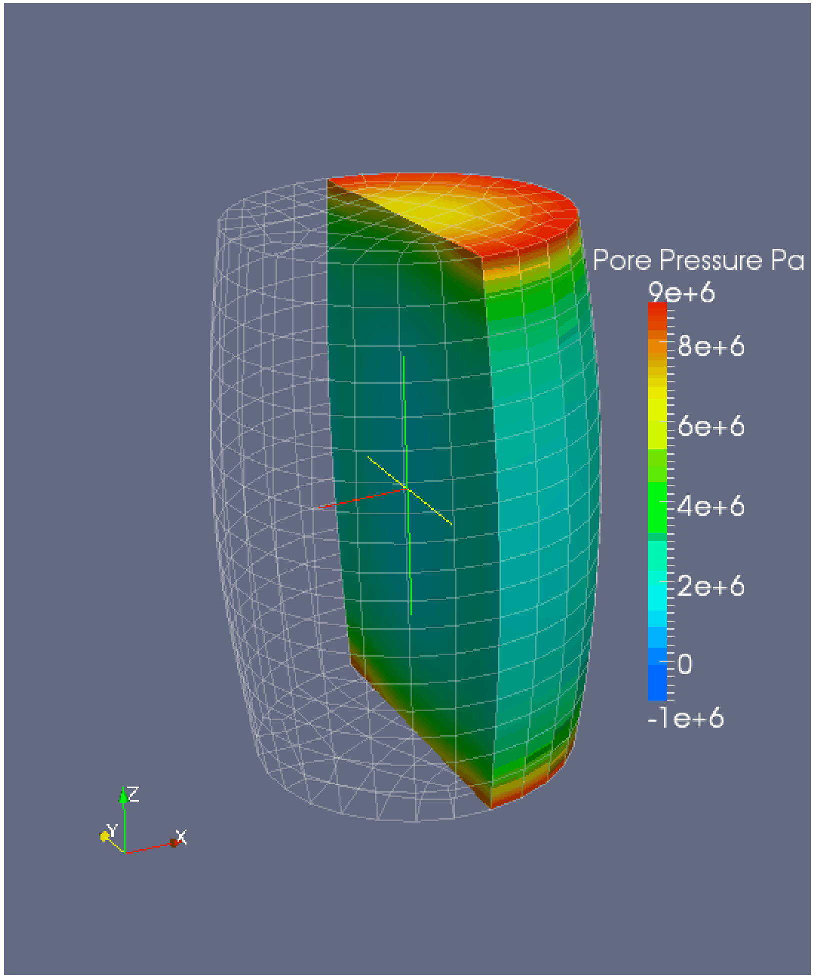
Note: we do not impose shape pore pressure gradient.

Unconfined Compression Test of Cold Thermo-sensitive Porous Media at Room Temperature

Temperature & equivalent plastic strain

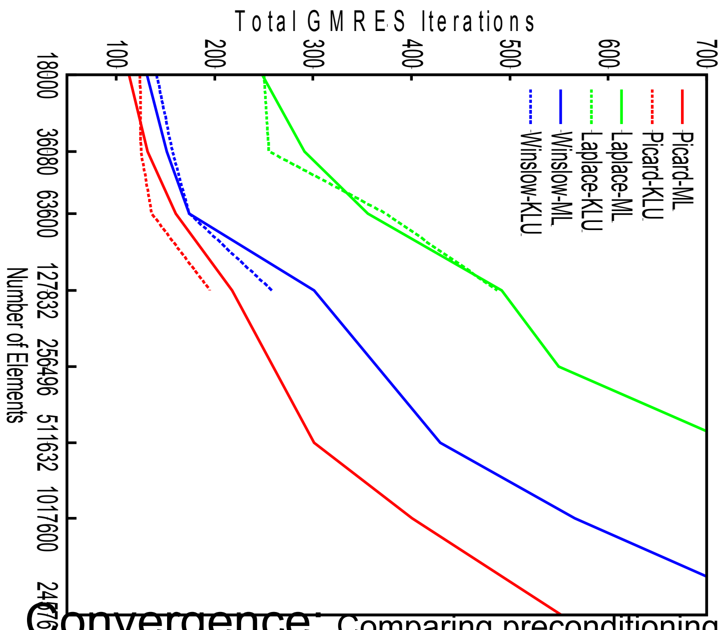


Pore Pressure



ALE methods R&D

- Rapid development of Laplace Beltrami ALE mesh adaptation strategy
- Collection of Trilinos solvers, preconditioners, and continuation strategies supports algorithmic experimentation
- Goal: add FieldManager to Alegra and directly "share" remesh evaluators between Albany and Alegra



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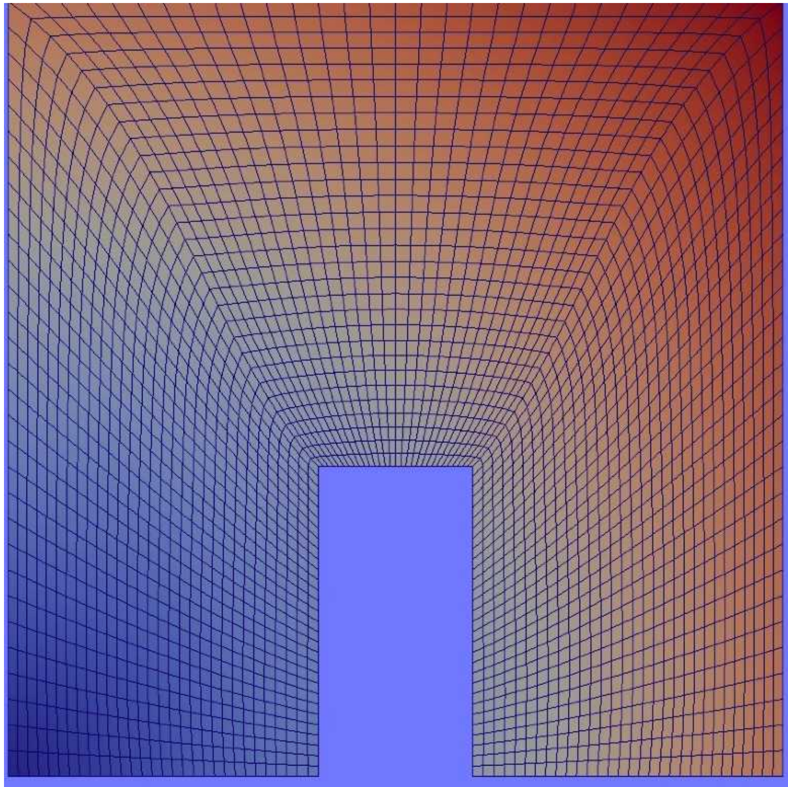
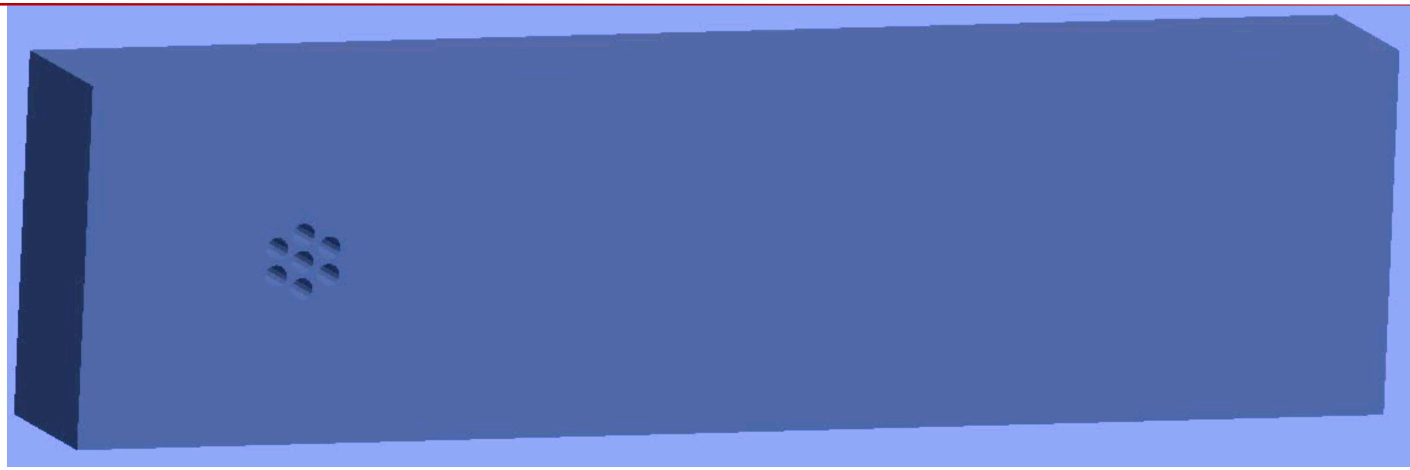
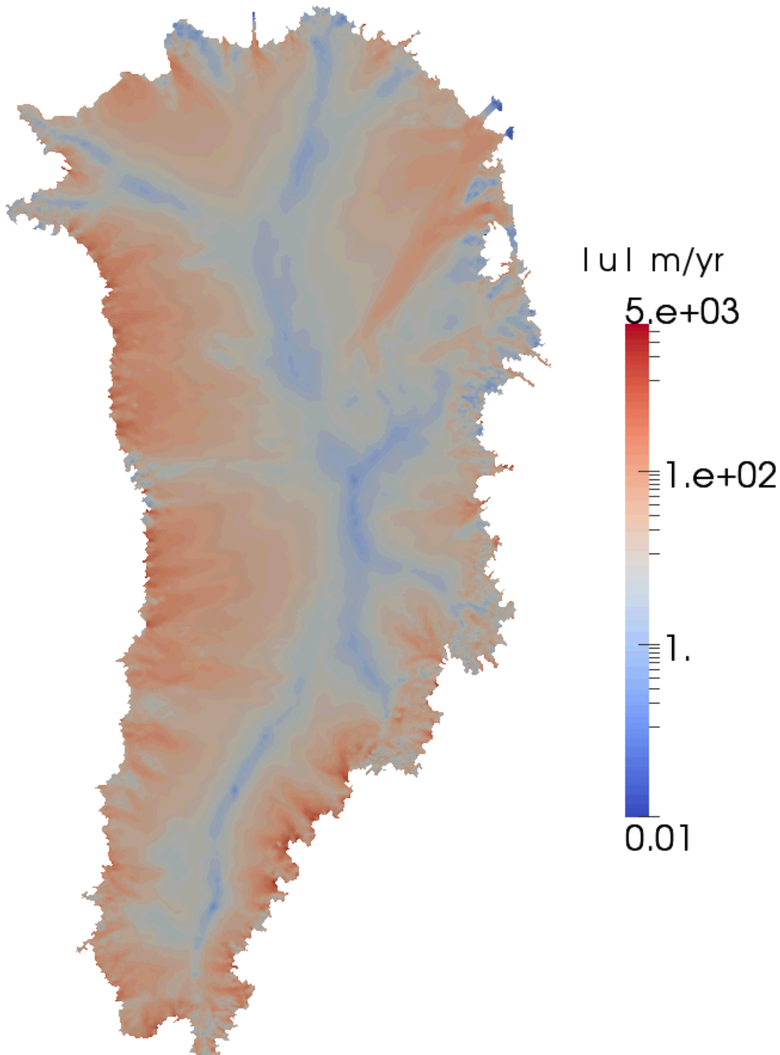


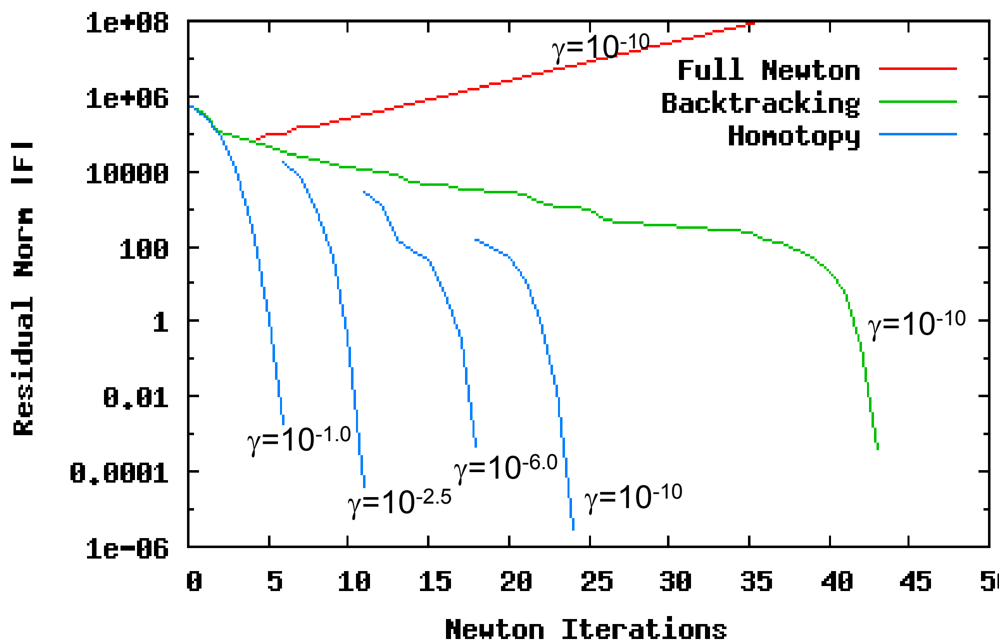
von Karman vortex



- Navier-Stokes problem
- Rythmos time integration: Implicit RK – 1 step Θ (trapezoidal)
- Corresponding bifurcation solution (critical velocity 60.254)

FELIX (Finite Element Land Ice eXperiments)

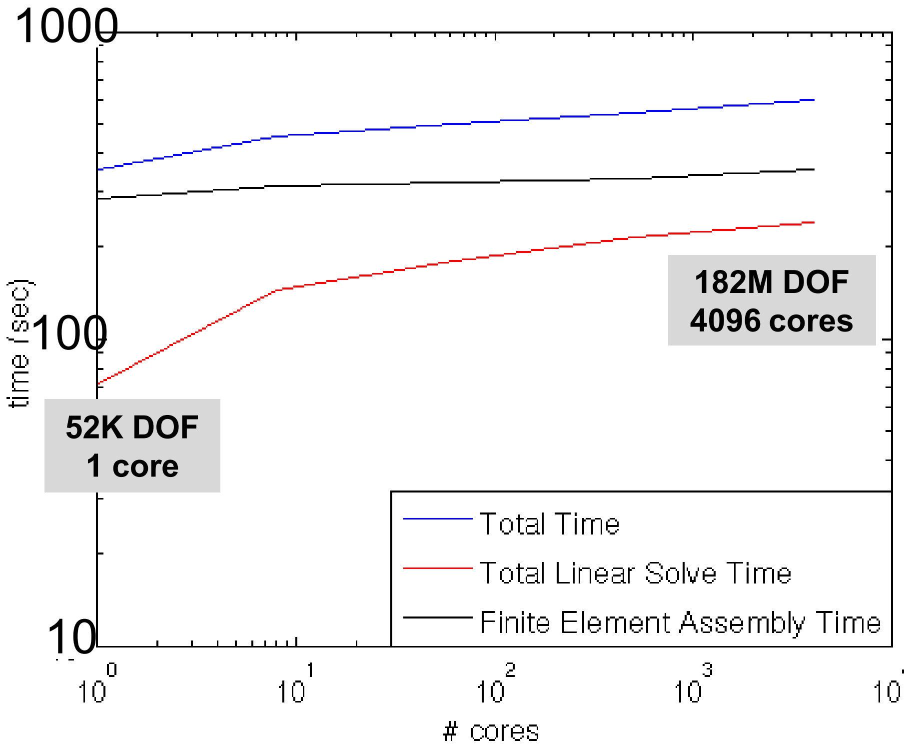


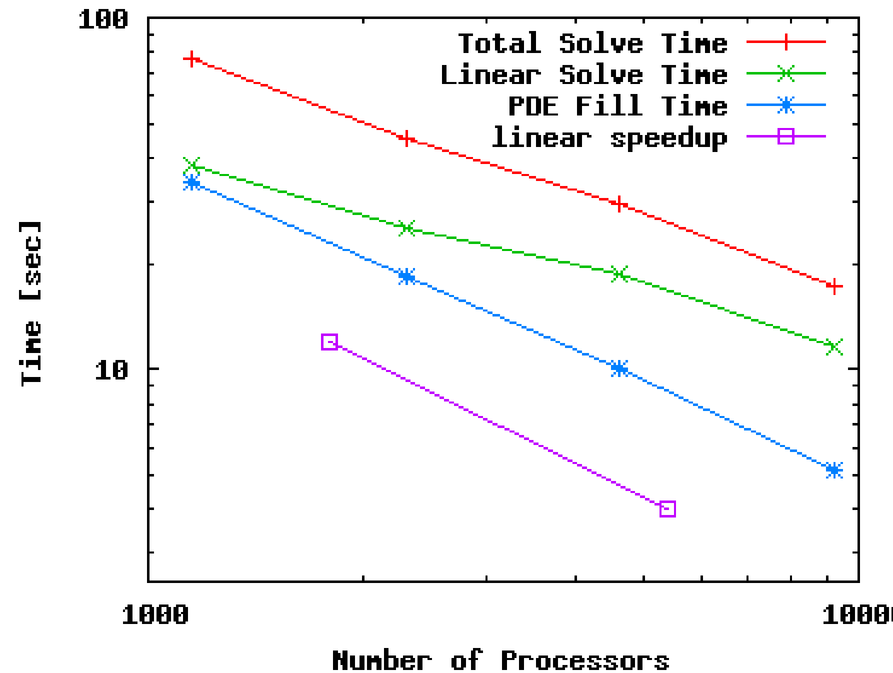


Robustness: Full Newton Method augmented with Homotopy Continuation

Greenland ice sheet, surface velocity magnitude (m/yr)

Scalability: Initial Data (On Hopper)





Weak Scaling on ISMIP Test problem:

- 60% Efficiency after 4096x scale-up
- Finite Element Assembly nearly constant
- Linear algebra fast but not constant
- Results by: Ray Tuminaro

Strong Scaling on gis2km steady solve:

- 4.5x speed-up on 8x processors
- Absolute times are small
- Setup/PostProcessing cost not shown
- Results by: Pat Worley

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Further information

- Albany download web page: https://software.sandia.gov/albany
- Albany paper, A. Salinger et. al., "Albany: A Component-Based Partial Differential Equation Code Built on Trilinos," SAND-2013-8430-J (submitted to ACM-TOMS) and references contained therein
- Getting started doc: https://software.sandia.gov/albany/gettingStarted.pdf
- Points of contact: Glen Hansen, gahanse@sandia.gov, Andy Salinger, agsalin@sandia.gov