Coupled physics using Albany and PUMI

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Introduction
Previous Albany + PUMI applications

Albany + PUMI have already been used successfully for:

- Thermomechanical simulations of dielectric deep trenches.
- Creep + Thermo-elastoplasticity for flip-chip packages.
- Error estimation/adaptation for uncertain flows.
- Large deformation elastoplasticity simulations.

Applications currently run through AlbanyT executable.
i.e. Albany executable is the ‘driver’ at the highest level.

Motivation to use Albany as a library

Simulation workflows:

- Want to control software components from a high-level driver.
- Albany - FEM analysis / advanced analysis features.
- PUMI - parallel mesh services / mesh adaptation.
- Other codes - advanced capabilities / additional physics.

Application examples:

- Additive manufacturing with evolving geometries.
- One-way coupled physics.
- Dislocation dynamics coupling to finite element methods.
- Adaptive simulations with goal-oriented error estimation.
Adaptive simulation workflows
Using Albany as a library
Code structure
Application-specific executables

Replace ‘Driver’ box with newly developed application

- Retain rich set of physics already implemented in Albany.
- Flexibility to implement new application specific drivers.
- Less interference with AlbanyT application development.

Potential overhead associated with this approach:

- Potential for some ‘overlap’ code.
- Code-base becomes more spread out.
Dislocation Dynamics
Overview


- Dislocation segments/loops embedded in domain.
- Initial dynamics of dislocation segments/loops solved for in infinite domain.
- FEM simulation modifies dynamics to account for effect of finite domain.
Proposed workflow

1. Compute new location of dislocation segment nodes.
2. Generate FEM mesh such that a mesh vertex is placed at each dislocation segment node location.
3. Pre-process FEM mesh + dislocation segment nodes to compute appropriate traction and displacement BCs.
5. Using FEM solution info - compute forces acting on dislocation segment nodes.
6. Repeat.
Software components - ParaDis

- Parallel dislocation dynamics code.
- Originally developed at LLNL.
- Solves dynamics of dislocations in infinite domain.
- Can be modified to account for finite domains.

Figure 2: https://pls.llnl.gov/people/divisions/physics-division/condensed-matter-science-section/eos-and-materials-theory-group/projects/dislocation-dynamics-for-single-crystal-plasticity-of-bcc-metals
Software components - Simmetrix

- Finite element mesh generation
- Mesh generation conformal to segment nodes.
- Query intersection of dislocation segments with FEM domain boundary.

Figure 3: Random dislocation segments in a cube
Software components - Albany

- Parallel finite element analysis engine.
- Incorporate traction + displacement boundary conditions.

Figure 4: Stress induced by single dislocation segment
Flow of data

ParaDis

- Passes segment information (node locations) to

Simmetrix

- Generates FEA mesh for

Pre-processor

- Generates BCs for

Albany

- Provides segment force information to
Goal-oriented error estimation and mesh adaptation
Proposed workflow

1. Build \( p \)-order finite element linear algebra and discretization data structures.

2. Compute the solution to the primal problem using \( p \)-order finite elements.

3. Enrich linear algebra and discretization data structures to account for \( p + 1 \)-order finite elements.

4. Compute global error estimate \( \mathcal{E} \approx J(u) - J(u^h) \).

5. Localize error estimate at the mesh entity level.

6. Adapt the mesh based on localized error estimates.

7. Repeat.
Software components - Albany

- Parallel finite element analysis engine.
- Compute the FEM solution to the primal problem.
- Compute the FEM solution to the dual problem.
- Compute local contributions to the error.

Figure 5: Example primal solution
Figure 6: Example dual solution
Software components - SCOREC

- Large suite of parallel mesh services.
- Unstructured mesh adaptation.
- Parallel partitioning and load balancing.
Builds p-order data
Builds p+1-order data
Solves primal FEM problem
Solves dual FEM problem
Estimates error
Updates mesh data
Adapts mesh

Albany

u^H
z^h

SCOREC
Questions?
Thank you!