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A Conformal Decomposition Finite Element Method for Melting and Flowing Aluminum

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Outline

- Motivation
  - Applications that require Interface Capturing
  - Why Conformal Decomposition Finite Element (CDFEM)
- Methodology
  - Formulation/Implementation description
  - Capability description
  - Usage (Description/Documentation)
- Complications
- Results
  - Verification (completed and still needed)
  - Demonstration problem
    - Melting and flow of Aluminum in hot enclosure
- Summary and Future Work

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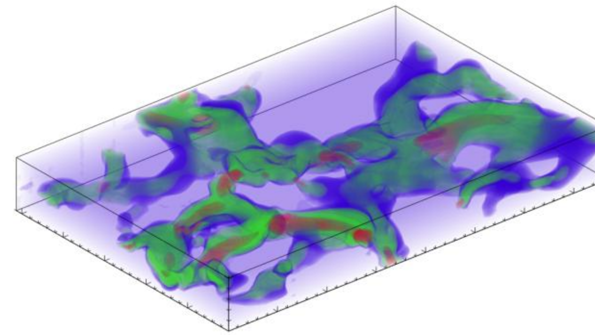
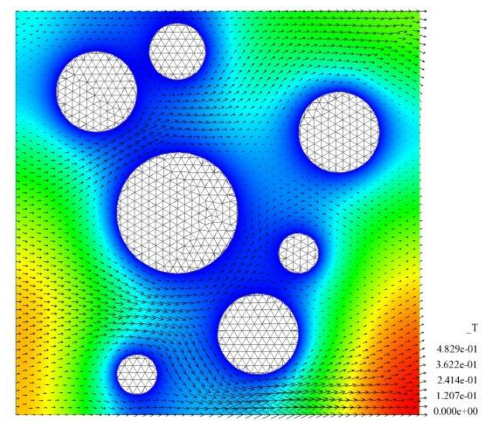
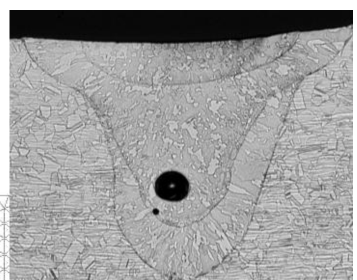
Sandia Thermal/Fluid Problems Requiring Interface Capturing Methods

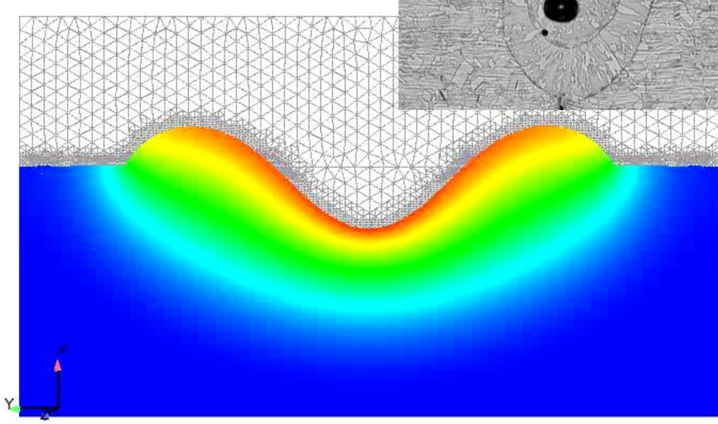
Recent/Future Static Interface Problems
- Thermal transport in composite materials
- Pore-scale flow in porous media

Recent/Future Dynamic Interface Problems
- Foam decomposition
- Aluminum melting/relocation
- Fuel spills
- Ablation
- Laser welding









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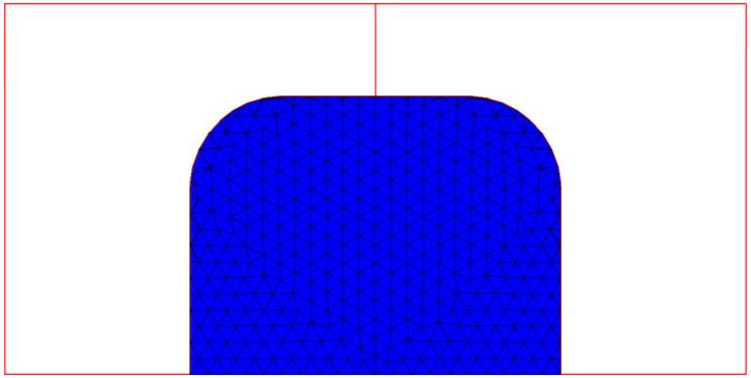
Melting and Flowing Aluminum in a Representative Geometry

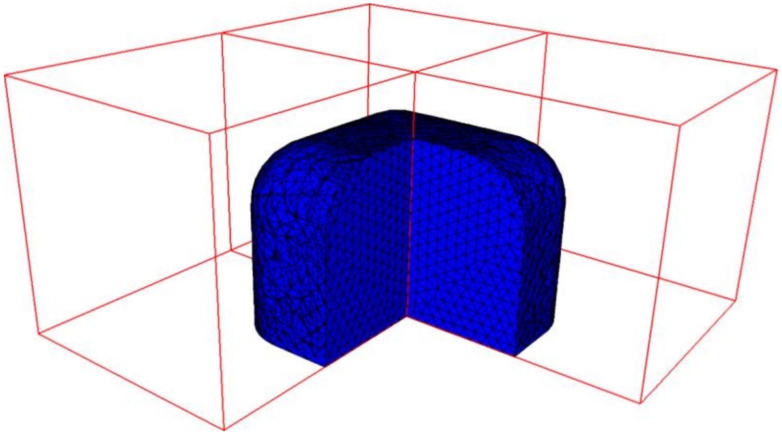
Melting and Flowing Aluminum

- 2-D and 3-D 10cm rounded block

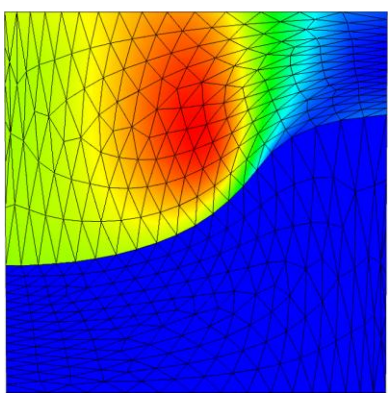
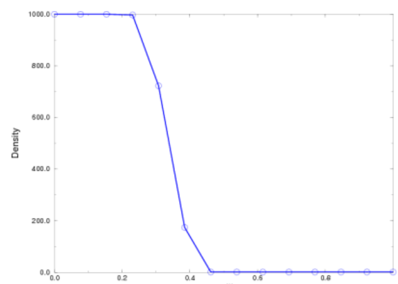


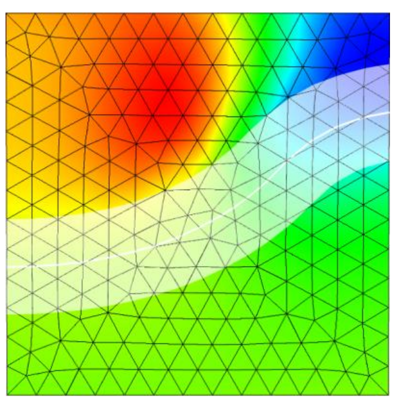
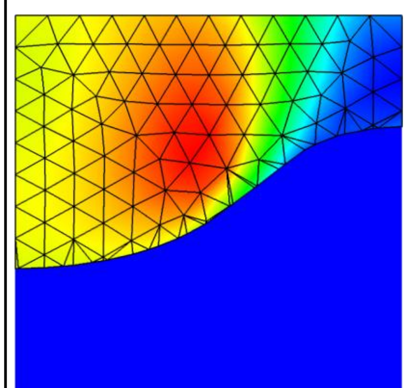
Physics

- Melting
  - Solid, liquid and surrounding air
  - Discontinuous material properties produces weak discontinuities in temperature, velocity
- Flowing
  - Navier-Stokes in liquid and air, rigid solid
- Surface tension
  - Capillary force along liquid-air interface
  - Strong discontinuity in pressure
- Enclosure radiation
  - Hot, isothermal surroundings radiating through optically thin air
- Realistic dynamic wetting (omitted)
- Oxide layer formation (omitted)



Finite Element Methods for Interfaces in Fluid/Thermal Applications Tested at Sandia

<table>
<tr><th>ALE</th><th>Diffuse LS</th><th>XFEM</th><th>CDFEM</th></tr>
<tr>
<td>• Separate, static blocks for air and water phases
• Static discretization
</td>
<td>• Single block with smooth transition between air and water phases
• Static discretization


</td>
<td>• Single block with sharply enriched elements spanning air and water phases
• Interfacial elements are dynamically enriched to describe phases</td>
<td>• Separate, dynamic blocks for air and water phases
• Interfacial elements are dynamically decomposed into elements that conform to phases
</td>
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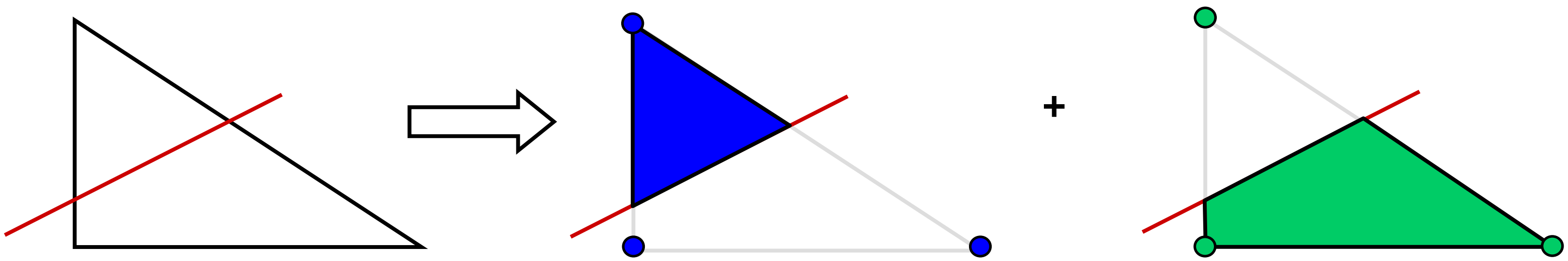
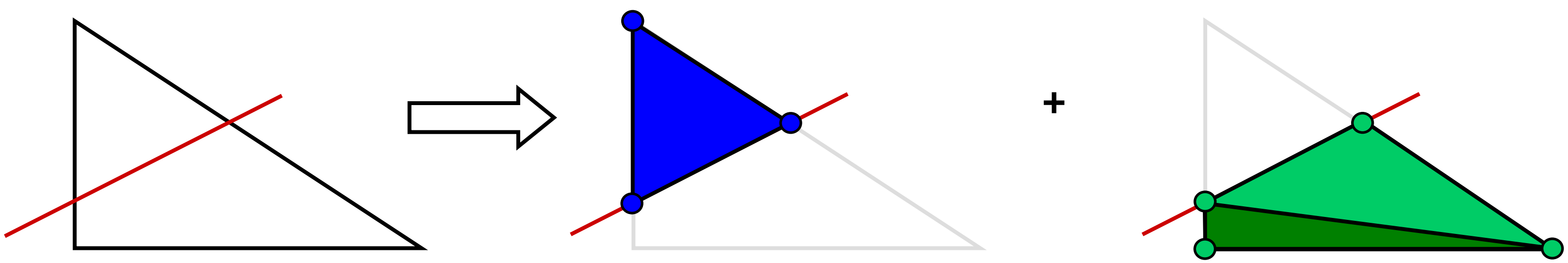
XFEM – CDFEM Discretization Comparison

XFEM Approximation



CDFEM Approximation



- Identical IFF interfacial nodes in CDFEM are constrained to match XFEM values at nodal locations
- CDFEM space contains XFEM space

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XFEM – CDFEM Comparison

Approximation

- CDFEM space contains XFEM space
  - Accuracy of CDFEM no less than XFEM Li et al. (2003)
  - CDFEM may be less stable than XFEM
  - CDFEM can recover XFEM solution by constraining interfacial nodes
    - Separate linear algebra step outside of element assembly routines

Boundary Conditions

- CDFEM readily handles interfacial Dirichlet conditions
  - Simply apply Dirichlet conditions to interfacial nodes
- Gives another view of difficulty with Dirichlet conditions in XFEM
  - CDFEM recovers XFEM when interfacial nodes constrained to XFEM space
  - CDFEM provides optimal solution for Dirichlet problem when interfacial nodes are given by Dirichlet conditions
  - Attempting to satisfy both sets of constraints simultaneously over-constrains the problem

Implementation

- Conformal decomposition can be performed external to all assembly routines
  - For stationary interfaces decomposition can be performed once on input mesh
  - For dynamic interfaces conformal decomposition is handled as a conformal adaptivity step as the interface evolves

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XFEM - CDFEM Requirements Comparison for Thermal/Fluids

	XFEM	CDFEM
Volume Assembly	Conformal subelement integration, specialized element loops to use modified integration rules	Standard Volume Integration
Surface Flux Assembly	Specialized volume element loops with specialized quadrature	Standard Surface Integration
Phase Specific DOFs and Equations	Different variables present at different nodes of the same block	Block has homogenous dofs/equations
Dynamic DOFS and Equations	Require reinitializing linear system	Require reinitializing linear system
Various BC types on Interface	Dirichlet BCs are research area	Standard Techniques available

Formulation: Thermal Transport

Conduction/Convection

- Advection – Diffusion

$$\rho c_p \frac{\partial T}{\partial t} + \rho u \cdot \nabla T = \nabla \cdot k \nabla T$$

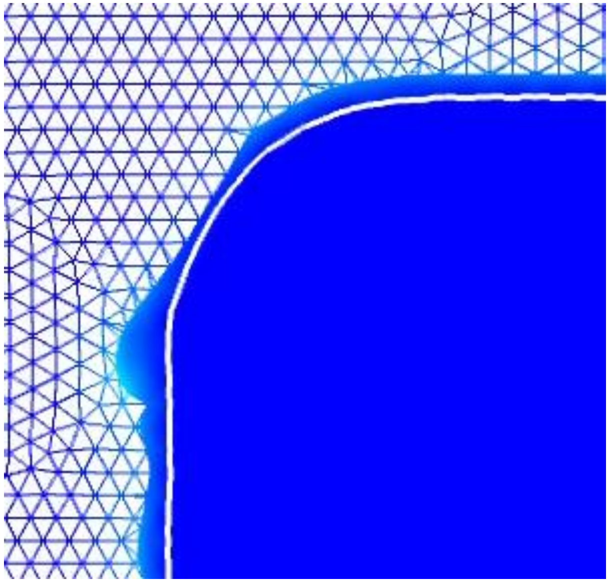
- Galerkin, Backward Euler, Dynamic geometry introduces moving mesh term

$$\int_\Omega \rho c_p \frac{T - T^n}{\Delta t} N_i \, d\Omega + \int_\Omega \rho (u - \dot{x}) \cdot \nabla T \, N_i \, d\Omega +$$

$$\int_\Omega k \nabla T \cdot \nabla N_i \, d\Omega + \int_\Gamma q \cdot n \, N_i \;\; d\Gamma = 0$$

- SUPG stabilization

$$N_i \Rightarrow N_i + \tau_T \, u \cdot \nabla N_i, \; \tau_T = \left[\left(\frac{2}{\Delta t} \right)^2 + u_i g_{ij} u_j + 12 \alpha^2 g_{ij} g_{ij} \right]^{-\frac{1}{2}}$$



Formulation: Melt Dynamics

Navier - Stokes

- Incompressible, Newtonian

$$\nabla \cdot u = 0,\ \rho \frac{\partial u}{\partial t} + \rho u \cdot \nabla u = -\nabla P + \nabla \cdot \mu\left(\nabla u + \nabla u^t\right) + \rho g$$

- Galerkin, Backward Euler, Moving mesh term

$$\int_\Omega \rho \frac{u - u^n}{\Delta t} N_i \, d\Omega + \int_\Omega \rho\left(u - \dot{x}\right) \cdot \nabla u \, N_i \, d\Omega +$$

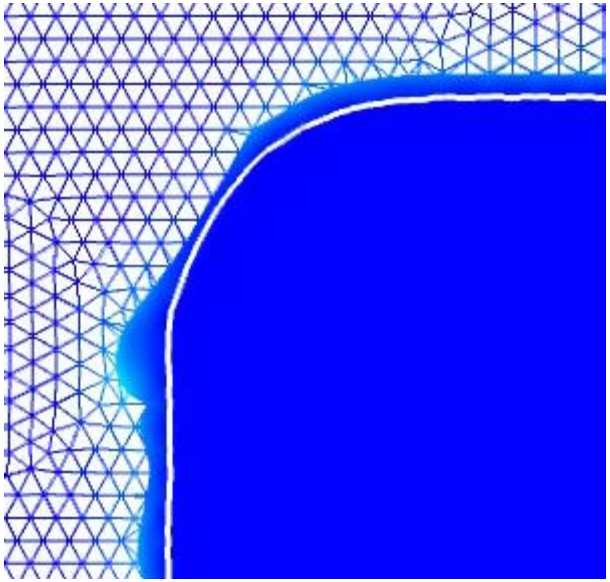
$$\int_\Omega \left[-P\,I + \mu\left(\nabla u + \nabla u^t\right)\right] \cdot \nabla N_i \, d\Omega - \int_\Omega \rho g \, N_i \, d\Omega + \int_\Gamma S \, N_i \, d\Gamma = 0$$

- PSPG stabilization

$$\int_\Omega \nabla \cdot u \, N_i \, d\Omega + \int_\Omega \tau_u \left[-\nabla P + \rho g\right] \cdot \nabla N_i \, d\Omega = 0$$

- SUPG stabilization

$$N_i \Rightarrow N_i + \tau_u \, u \cdot \nabla N_i,\ \tau_u = \left[\left(\frac{2}{\Delta t}\right)^2 + u_i g_{ij} u_j + 12\left(\frac{\mu}{\rho}\right)^2 g_{ij} g_{ij}\right]^{-\frac{1}{2}}$$



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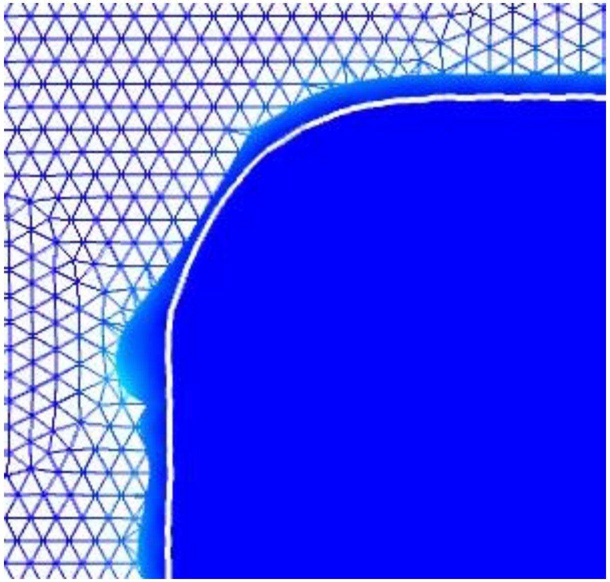
Formulation: Interface Dynamics



Level Set Equation

- Advection equation

$$\frac{\partial \phi}{\partial t} + u \cdot \nabla \phi = 0$$

- Galerkin, Backward Euler

$$\int_{\Omega} \frac{\phi - \phi^n}{\Delta t} N_i \, d\Omega + \int_{\Omega} u \cdot \nabla \phi \, N_i \, d\Omega = 0$$

- SUPG stabilization

$$N_i \Rightarrow N_i + \tau_\phi u \cdot \nabla N_i, \; \tau_\phi = \left[\left(\frac{2}{\Delta t} \right)^2 + u_i g_{ij} u_j \right]^{-\frac{1}{2}}$$

- Periodic renormalization
  - Compute nearest distance to interface

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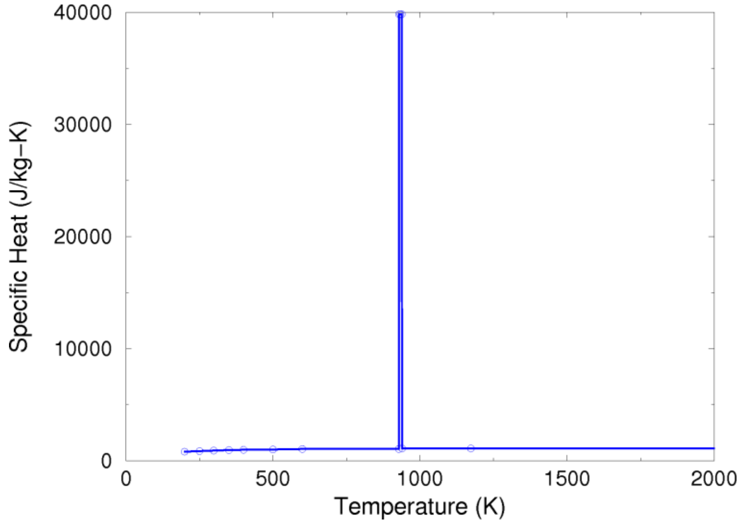
Models: Solid-Liquid Interface

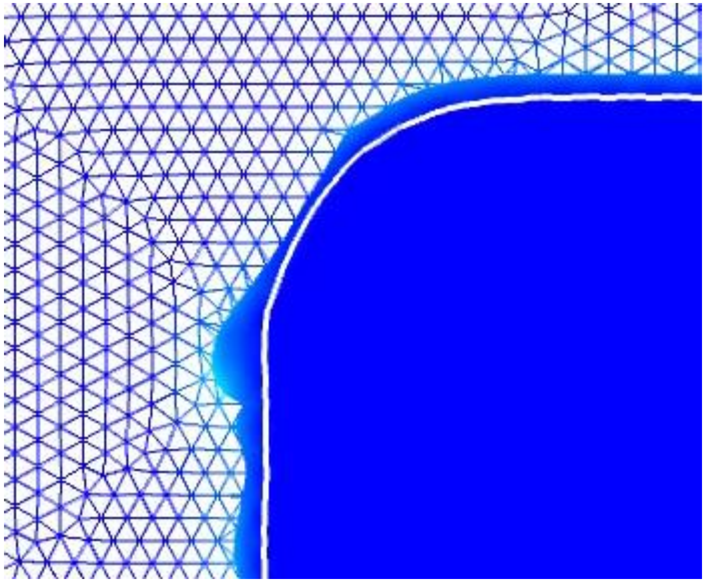
Transition from Solid to Liquid Aluminum

- Latent Heat
  - Tabulated specific heat to capture temperature dependence and latent heat



- Viscous Flow – No slip

$$\mu(T)=\begin{cases}\mu_s+\dfrac{T-T_s}{T_l-T_s}(\mu_l-\mu_s), & T<T_l\\ \mu_l, & \text{otherwise}\end{cases}$$



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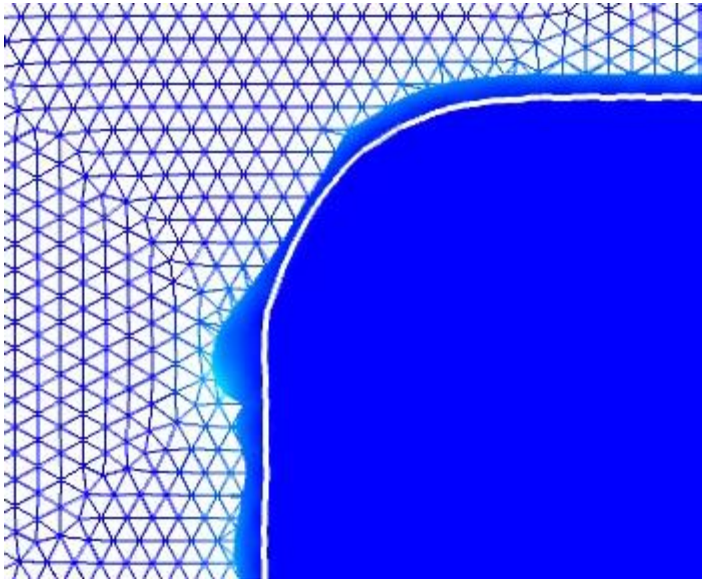
Models: Liquid-Air Interface

Capillary Force

- Same model used in ALE simulations
  - Jump in stress due to interfacial tension

$$\int_\Gamma \left(\gamma\kappa \mathbf{n} + \nabla_s \gamma\right) N_i \; d\Gamma = \int_\Gamma \gamma \nabla_s N_i \; d\Gamma, \; \nabla_s \equiv \left(\mathbf{I} - \mathbf{nn}\right)\nabla$$



Interface Stabilization

- Surface viscosity type stabilization
  - Based on recent paper by Hysing

$$\int_\Gamma \mu_{surf} \nabla_s u \cdot \nabla N_i \; d\Gamma$$

Radiation

- Simple radiation boundary condition

$$\int_\Gamma \varepsilon\sigma \left(T^4 - T_e^4\right) N_i \; d\Gamma$$

- Enclosure radiation
  - Enclosure temperature 2000K
  - Repeat viewfactor calculation every time step

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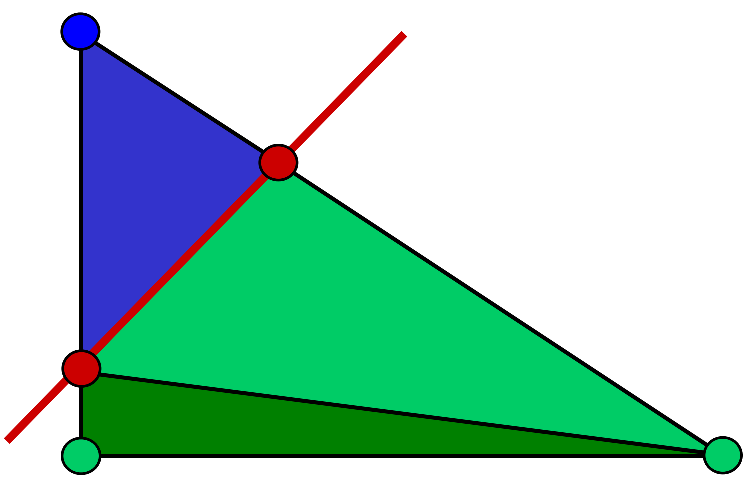
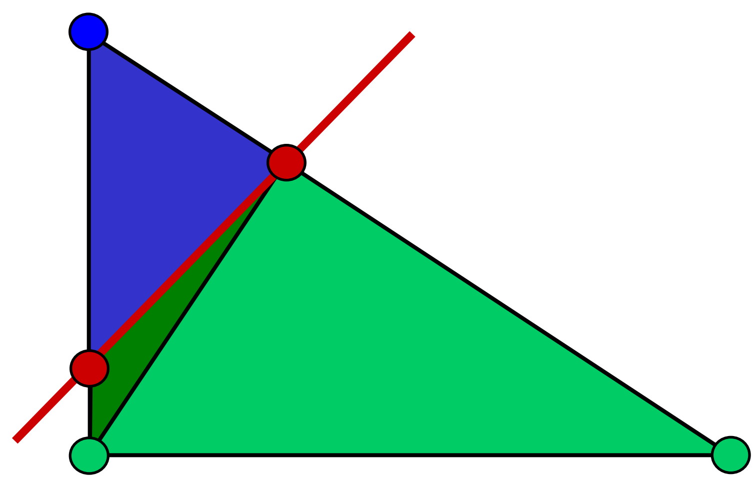
CDFEM – Level Set Implementation in Two Dimensions

Conformal Decomposition Algorithm in Two Dimensions

- Isosurface of piecewise linear level set field on triangles generates C^0 line segments
- Parent non-conformal triangular elements decomposed into conformal triangular elements
- Must choose how to decompose quadrilateral into triangles
  - Babuška and Aziz: Large angles more detrimental to accuracy than small angles
  - Diagonal chosen to cut largest angle





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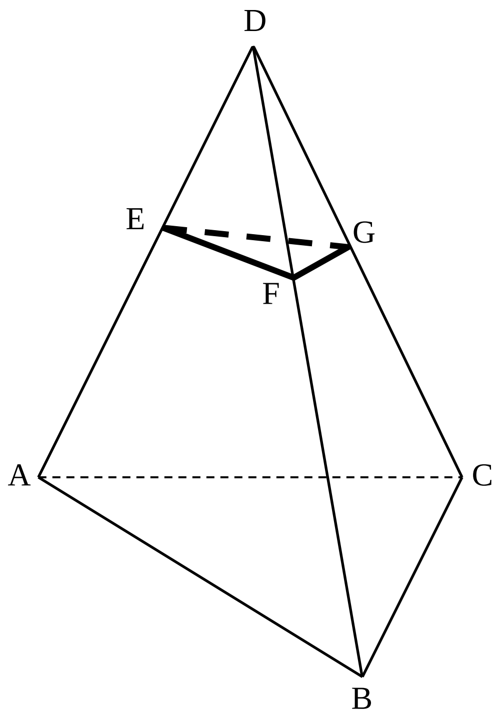
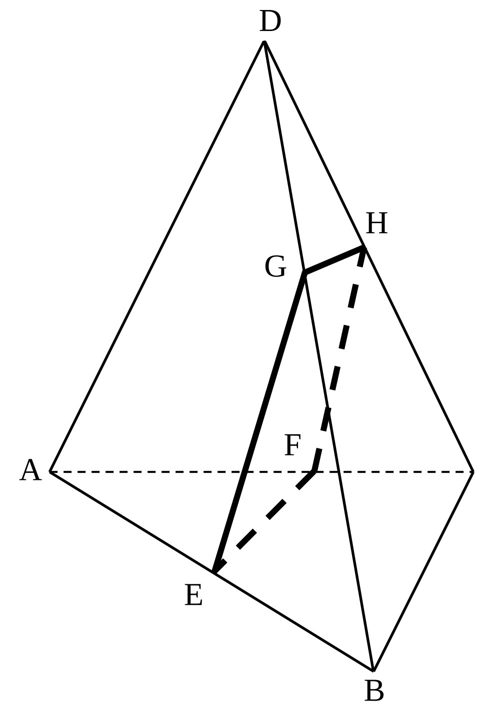
CDFEM – Level Set Implementation in Three Dimensions

Conformal Decomposition Algorithm in Three Dimensions

- Isosurface of piecewise linear level set field on tetrahedra generates C^0 planar polygons
- Parent non-conformal tetrahedral elements decomposed into conformal tetrahedral elements – Intermediate wedges generated
  - wedge + tetrahedra
  - wedge + wedge





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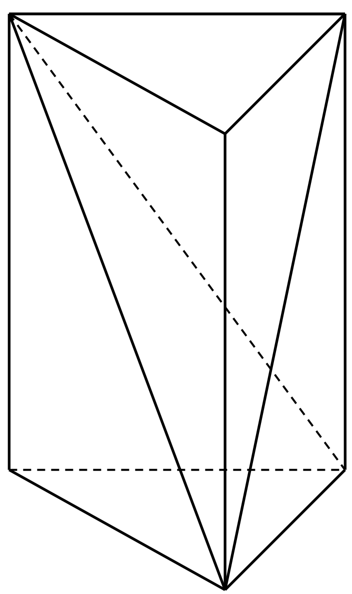
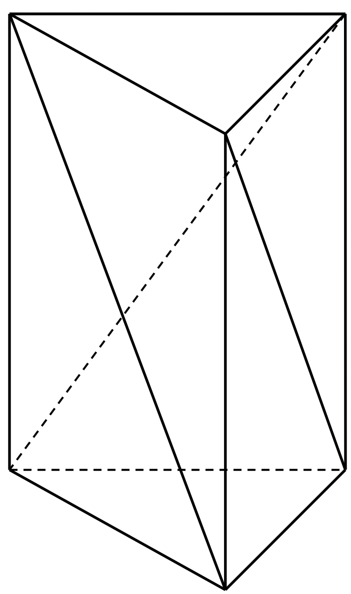
CDFEM – Level Set Implementation in Three Dimensions – cont'd

- Decompose faces of wedges into triangles and then generate tetrahedra
  - Desired strategy is again to choose the diagonals to cut largest angles
  - Non-tetrahedralizable wedge called Schonhardt's polyhedron may be generated
  - Current strategy depends on face
    - Interfacial faces – cut largest angle, Non-interfacial faces – select node with largest level set magnitude (prefers edges that are not aligned with interface)



Wedge amenable to generation of tetrahedra



Schonhardt's Polyhedron – Non-tetrahedralizable without Steiner points

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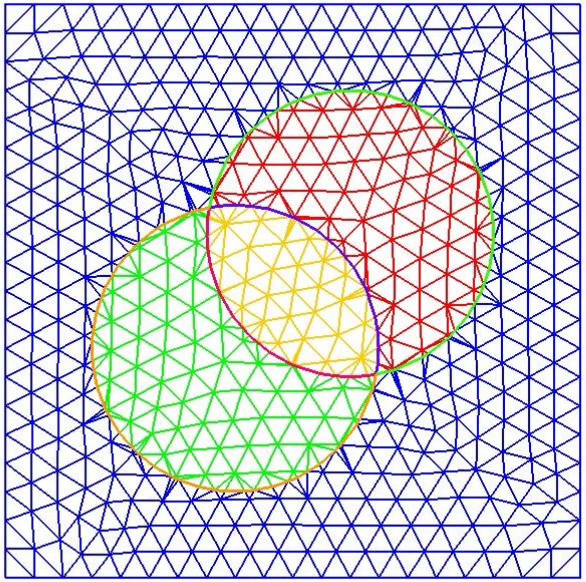
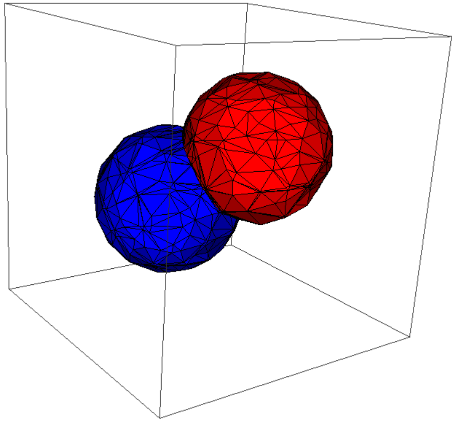
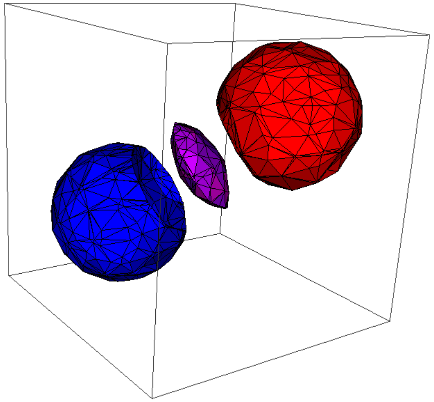
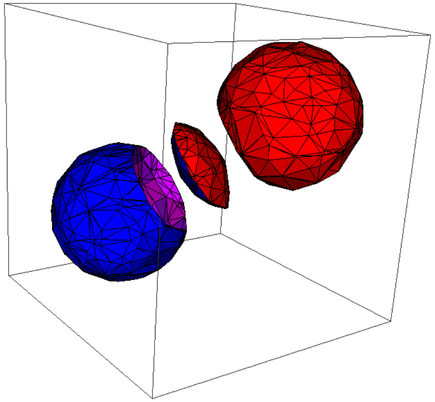
CDFEM Status: Code Capability

- Aria/Krino are running dynamic, conformally decomposed problems
- Dynamic decomposition of blocks and sidesets
- Creation of sideset on interfaces for bc application
- Phase specific material properties, equations, source terms, etc.
- Parallel
- Multiple phases defined by multiple level set fields
- Mixed Elements (LBB) Tris/Tets









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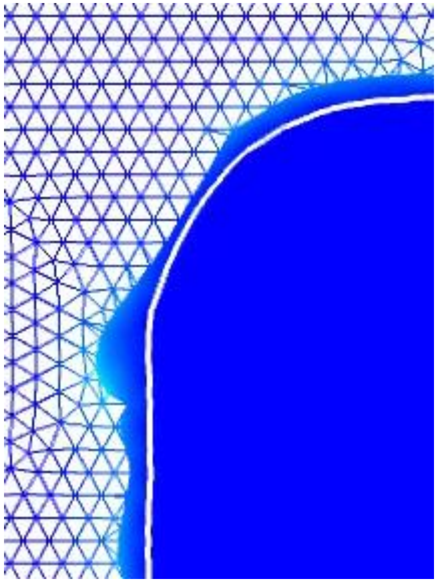
CDFEM Usage: FEM Model Specification

- Linking level set function with phases and materials:



```
BEGIN FINITE ELEMENT MODEL Melting-Flow
   database name = 3d_box.g
   BEGIN Parameters For Phase Air
      where LS is positive
   END
   BEGIN Parameters For Phase Aluminum
      where LS is negative
   END
   BEGIN Parameters For Block block_1_Air
      Material Air
   END
   BEGIN Parameters For Block block_1_Aluminum
      Material Aluminum
   END
   BEGIN Parameters For Surface surface_block_1_Aluminum_Air
      Material Air_Aluminum_interface
   END
END FINITE ELEMENT MODEL Melting-Flow
```

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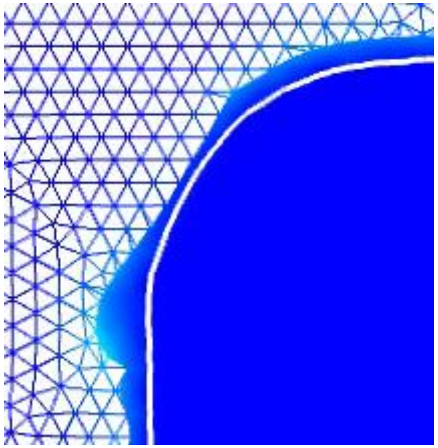
CDFEM Usage: Physics Specification



- Energy equation system

```
BEGIN Equation System energy
   Use Linear Solver cg
   Nonlinear Solution Strategy = Newton
   Maximum Nonlinear Iterations = 25
   Nonlinear Residual Ratio Tolerance = 1.0e-6

   EQ energy for temperature On block_1_Air      using q1 with mass diff
   EQ energy for temperature On block_1_Aluminum using q1 with mass diff

   IC Const on block_1_Air      Temperature = 300.
   IC Const on block_1_Aluminum Temperature = 300.

   BEGIN Radiative Flux Boundary Condition able
      add surface surface_block_1_Aluminum_Air
      Radiation Form Factor is 1.0
      Reference Temperature is 2000
   END
END
```

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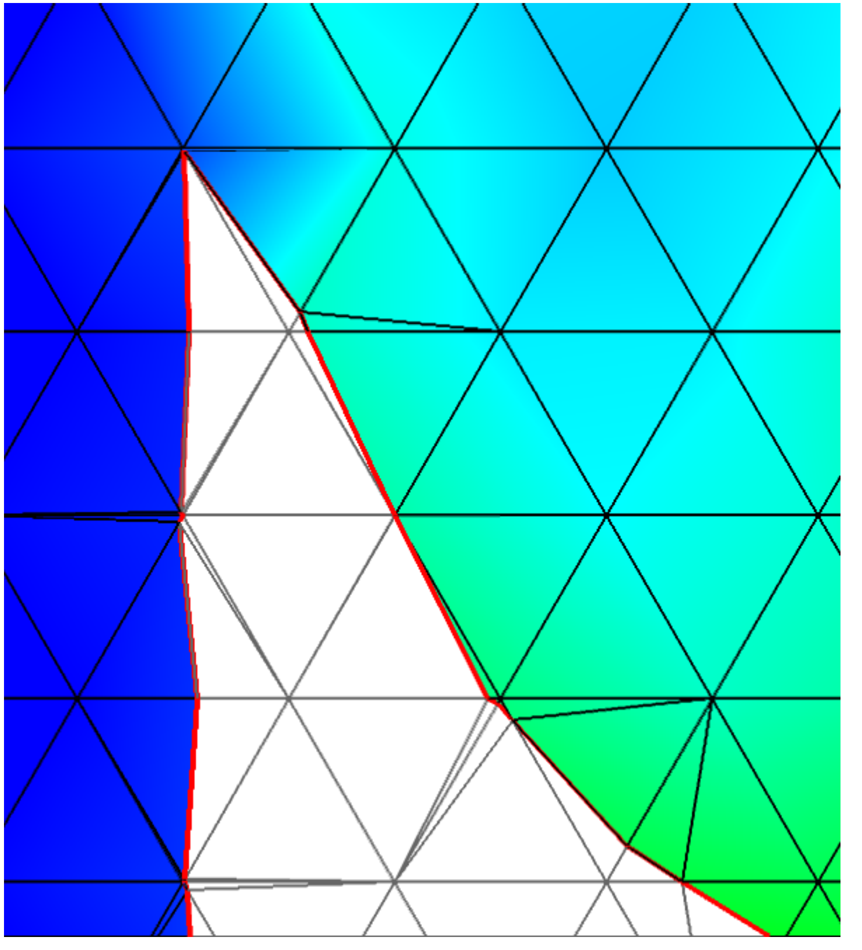
Complications: Degenerate Decompositions

Strategy to Handle Degenerate or Nearly Degenerate Element Decompositions

- Standard approach: “Snap to Node” when edge intersection gets close to node
  - Eliminates slivers and infinitesimal sub-elements
  - Can create interface segments that do not lie between sub-elements of both volumetric phases
  - Huge number of degenerate cases must be handled
- Alternate approach: “Snap from Node” when edge intersection tries to get too close to node
  - Hetu (2009)
  - Creates/retains many slivers and infinitesimal sub-elements
  - Interface segments always lie between subelements of both volumetric phases
  - No degenerate cases to handle



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Results: CDFEM Verification

- Two-Dimensional Potential Flow About a Cylinder (static)
  - Analytical solution provides quantitative measure of accuracy
    - Accuracy of velocity potential and its gradient computed in volume and on interface
  - Allows experiments with various boundary conditions
- Three-Dimensional Potential Flow About a Sphere (static)
  - Analytical solution provides quantitative measure of accuracy
    - Accuracy of velocity potential and its gradient computed in volume and on interface
  - Allows experiments with various boundary conditions
- Two-Dimensional Viscous, Incompressible Couette Flow (static)
  - Analytical solution provides quantitative measure of accuracy
  - Test of conformal decomposition for viscous, incompressible flow
- Three-Dimensional Viscous Flow about a Periodic Array of Spheres (static)
  - Comparison with Boundary Element results
  - Examines behavior of decomposition up to sphere overlap
- Advection of Weak Discontinuity (dynamic)
  - Shows ability to capture discontinuities
  - Analytical solution provides quantitative measure of accuracy
- Solidification of 1-D Bar (dynamic)
  - Shows ability to capture discontinuities
  - Analytical solution provides quantitative measure of accuracy
- Level Set Advection under Rigid Body Rotation (dynamic)
  - Shows accuracy of level set advection for given velocity field
  - Shows 2^{nd} order in space, 1^{st} or 2^{nd} order in time

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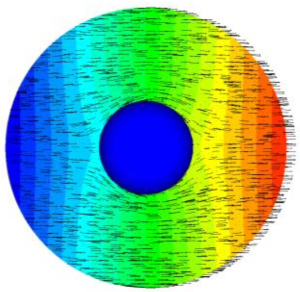
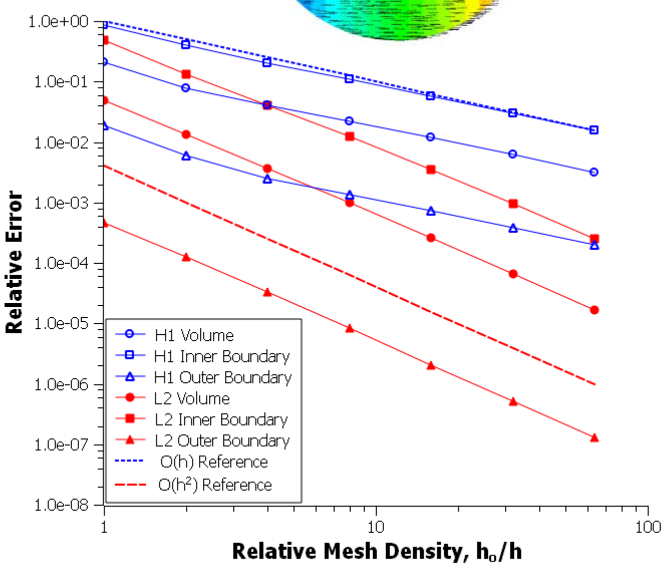
CDFEM Verification for Static Interfaces

Steady Potential Flow about a Sphere

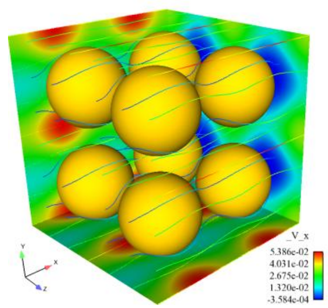
- Embedded curved boundaries
- Dirichlet BC on outer surface, Natural BC on inner surface
- Optimal convergence rates for solution and gradient both on volume and boundaries

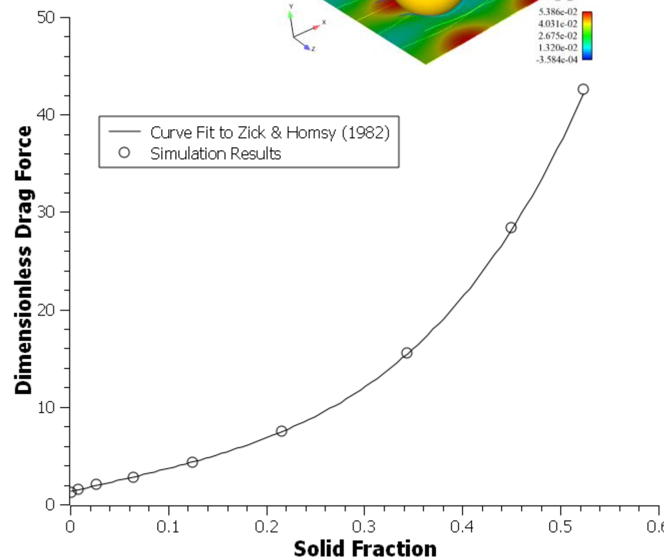




Steady, Viscous Flow about a Periodic Array of Spheres

- Embedded curved boundaries
- Dirichlet BC on sphere surface
- Accurate results right up to close packing limit
- Sum of nodal residuals provides accurate/convergent measure of drag force





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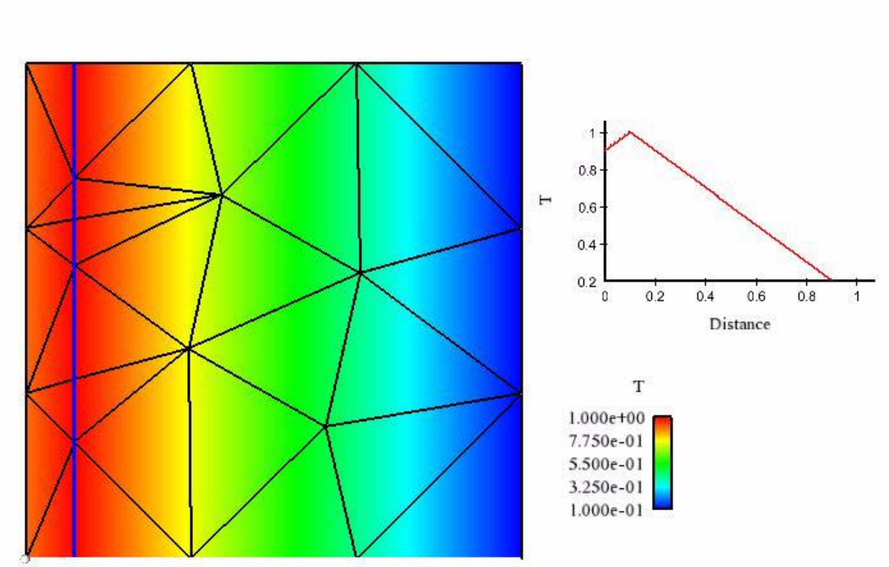
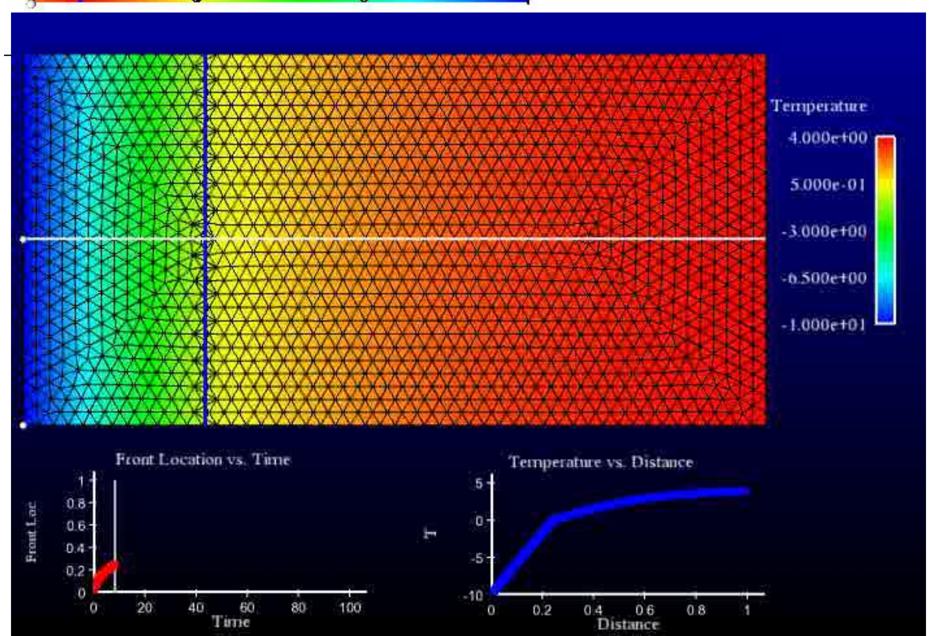
CDFEM Verification for Dynamic Interfaces





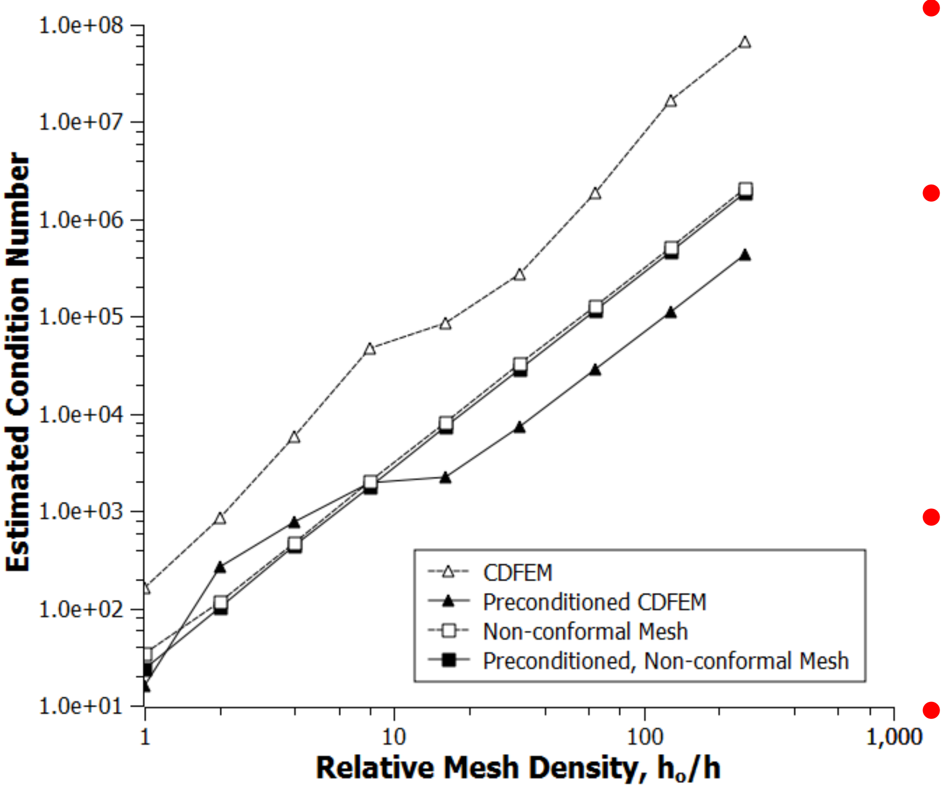
Advection of Ridge Discontinuity

- Constant velocity left to right
- No diffusion, just advection and time derivative terms
- Exact solution obtained for entire simulation (machine precision)

Solidification of Quenched Bar

- Liquid quenched below melting point at time 0
- Exact solution for temperature profile and interface location
- Excellent agreement between simulation and exact solution (not fully quantified yet)

Linear System Conditioning for CDFEM Simulation of Steady, Potential Flow about a Circular Cylinder

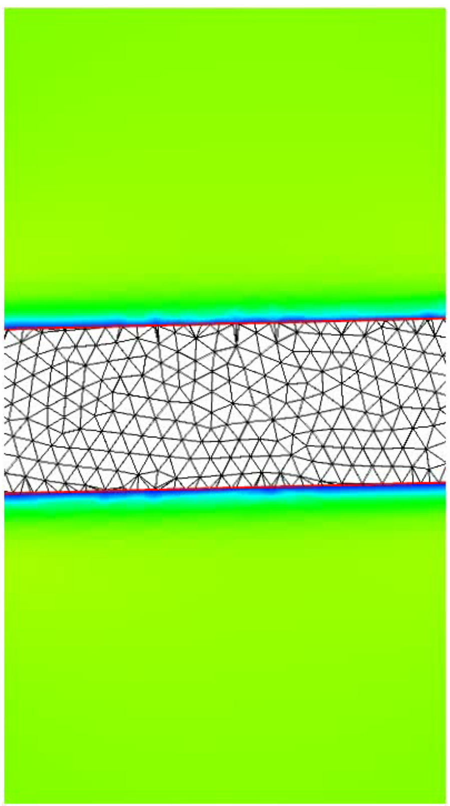


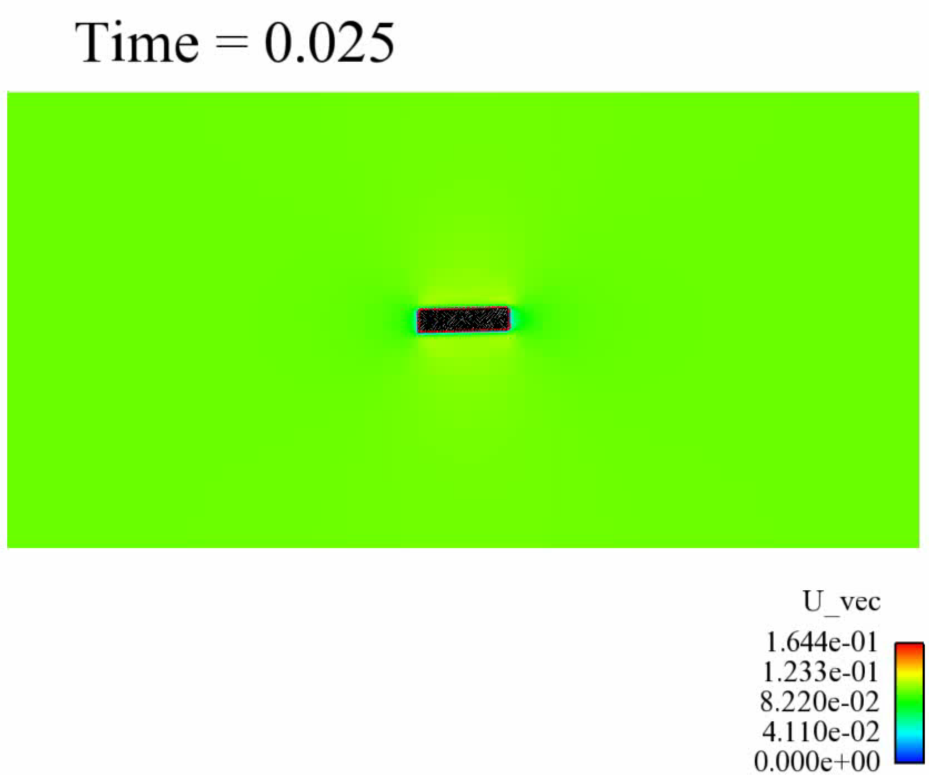
- Expectation
  - Nearly degenerate elements expected to degrade conditioning of the matrix resulting from finite element assembly
- Evaluation
  - TRILINOS package used to estimate extreme eigenvalues
  - Condition estimates generated with and without Jacobi preconditioning
  - Compared to simple conduction system using un-decomposed mesh
- Results
  - Preconditioned system exhibits expected $O(h^{-2})$ scaling

- Poor conditioning from CDFEM easily removed by standard preconditioning
  - Consistent with findings of Graham and McLean (2006) for anisotropic refinement

CDFEM Verification Still Needed

- One-way coupled solid-fluid flows
  - Solid drives fluid with given velocity
  - Potential verification problems: Translation of rigid body with symmetry/periodic bcs, Jeremy's impulsively driven Stokes problem
- Two-way coupled solid-fluid flows
  - Coupled kinematics and stress balance
  - Potential verification problems: Body falling under gravity?





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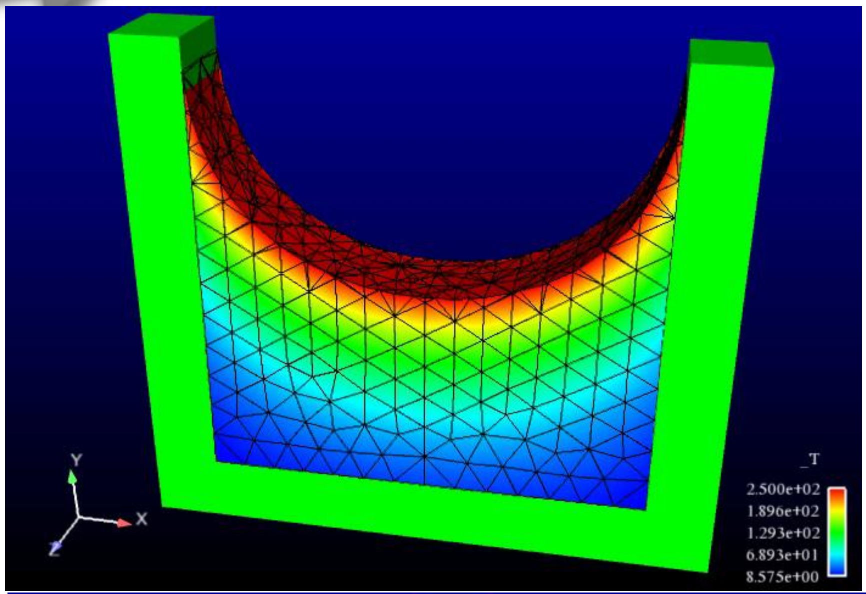
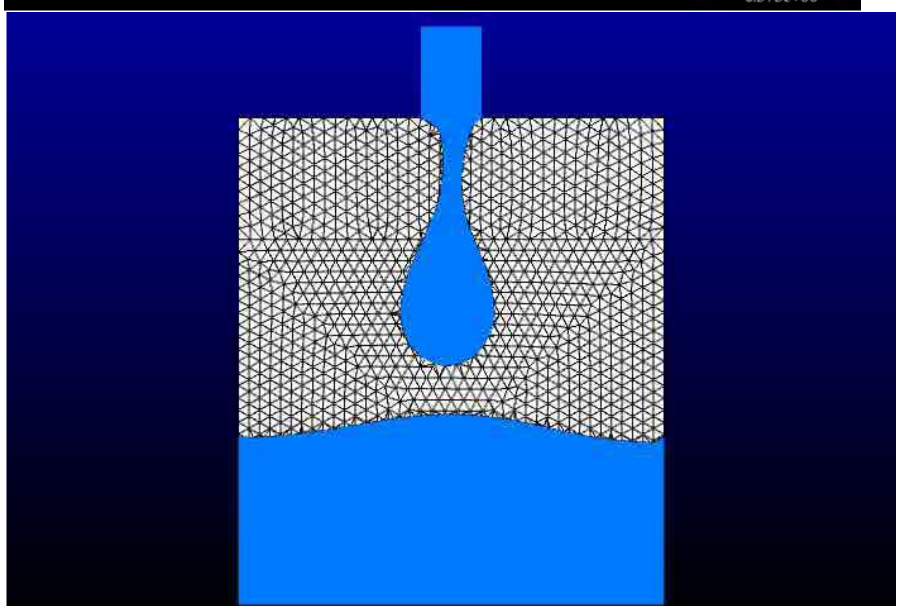
CDFEM Verification Still Needed





- Element death
  - Interfacial motion driven by motion of isotherm
  - Potential verification problems: Death-type Stefan problem
- Capillary hydrodynamics
  - Coupled interface motion and hydrodynamics
  - Potential verification problems: Static bubble, dynamic bubble, decay of capillary wave

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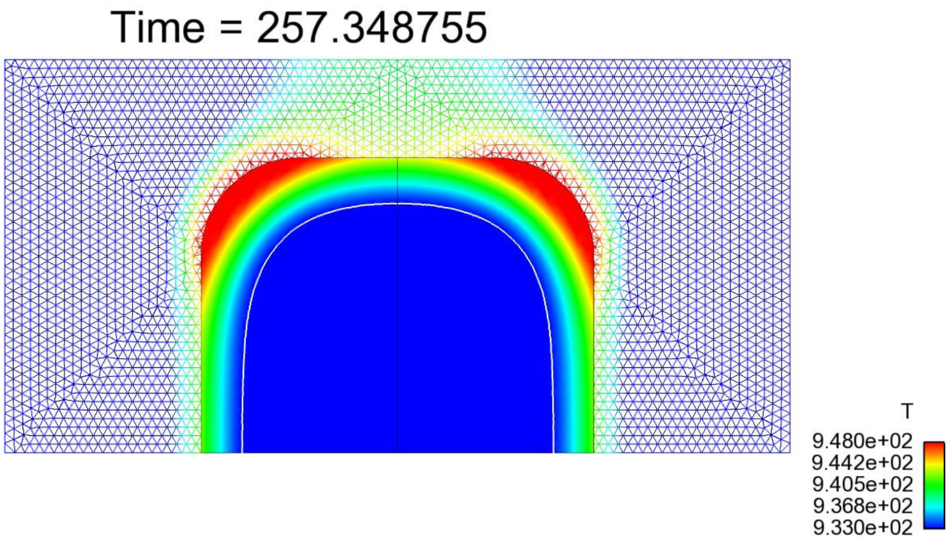
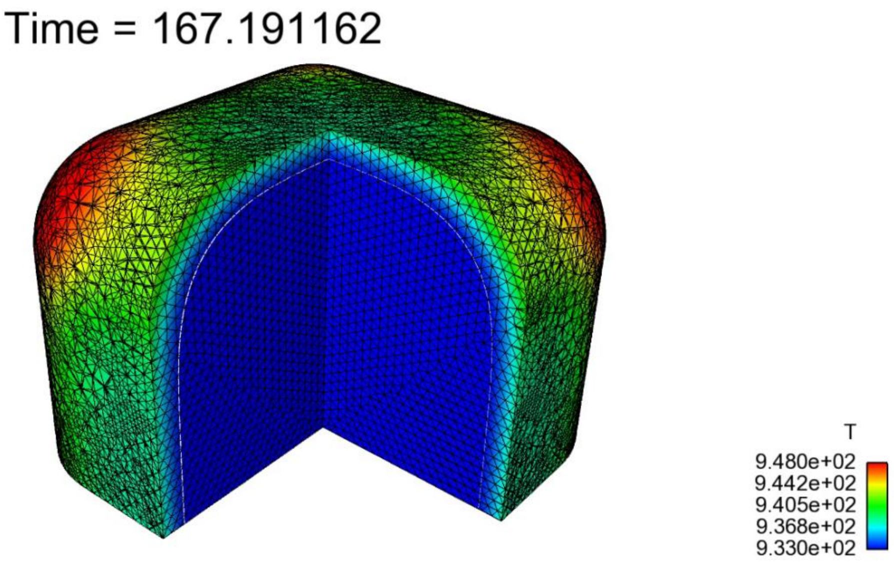
Demonstration Problems

- 2D and 3D Static CDFEM Thermal transport with Enclosure Radiation
  - Uniform block of elements cut by initial surface
  - Faces generated on surface are passed to Chaparral for enclosure viewfactor and radiosity calculation
  - Shows ability to support face-based transport on static CDFEM surface
- 2D and 3D Dynamic CDFEM with Melting and Flow with Enclosure Radiation
  - Uniform block of elements dynamically cut by moving Aluminum interface
  - Faces generated on surface are passed to Chaparral for enclosure viewfactor and radiosity calculation
  - Surface motion driven by capillary hydrodynamics
  - Shows ability to support face-based transport on dynamic CDFEM surface

Demonstration Problem: 2D-3D Melting with Enclosure Radiation





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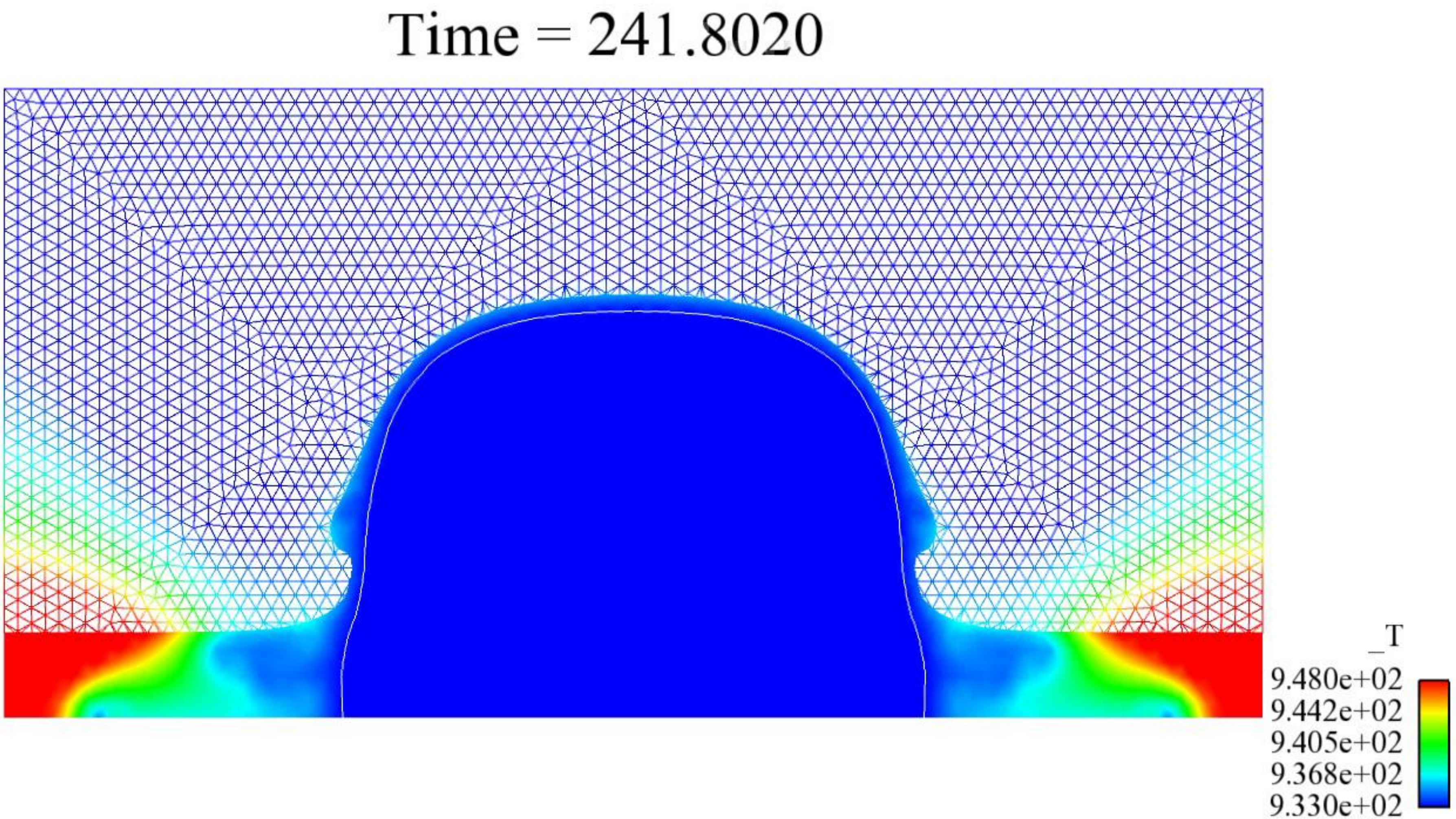
Demonstration Problem: 2D Melting and Flow with Enclosure Radiation – Medium Mesh



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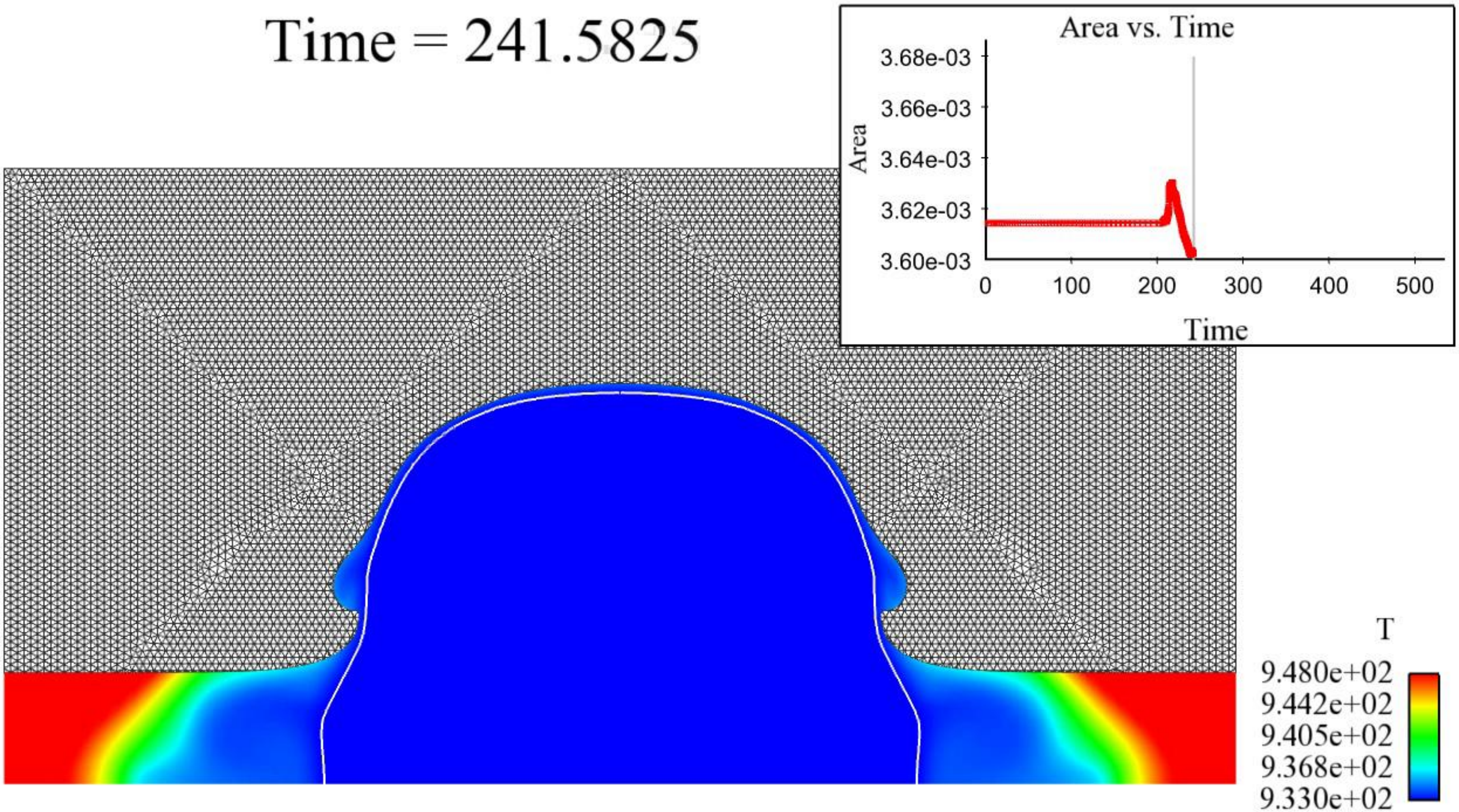
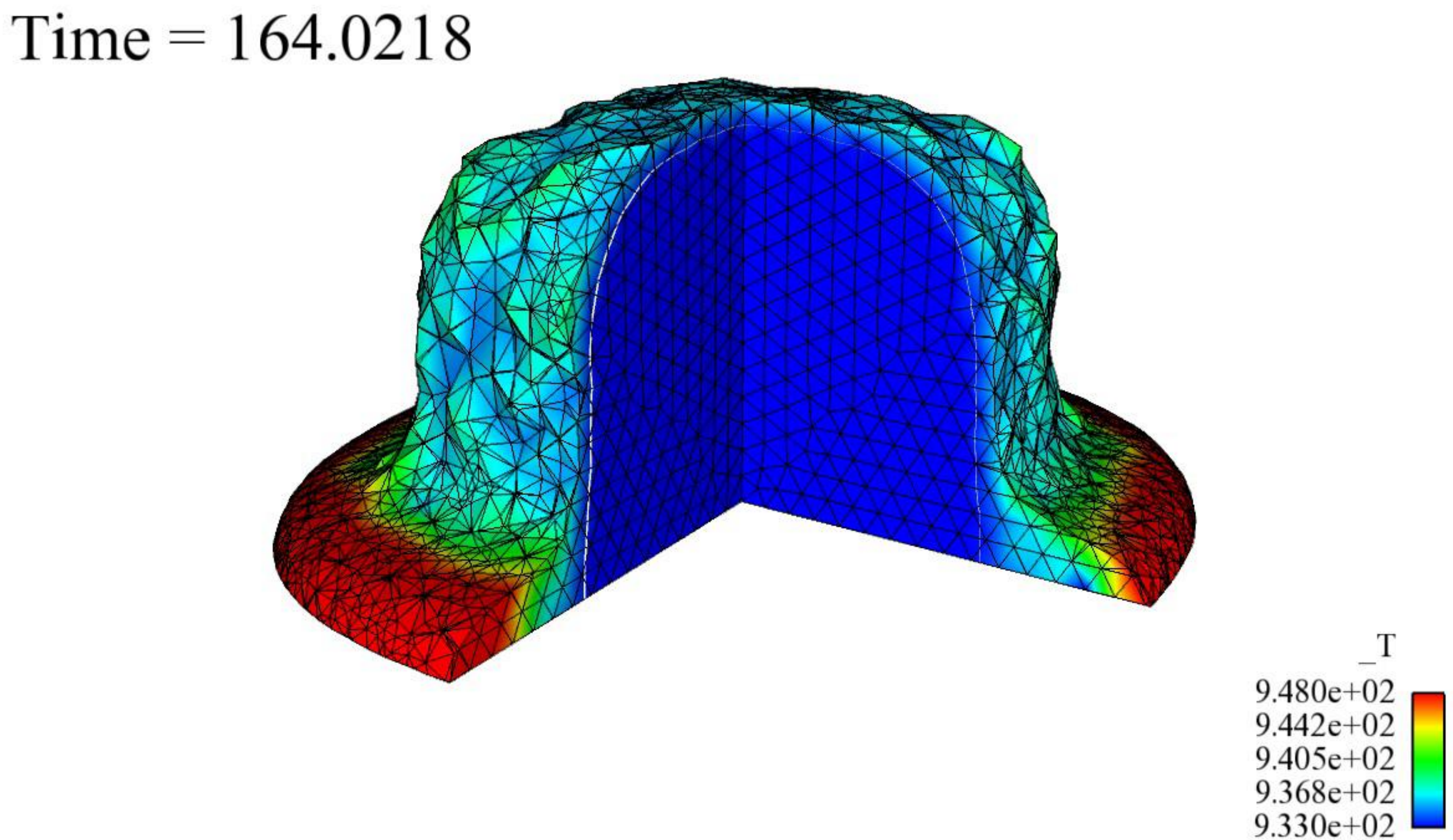
Demonstration Problem: 2D Melting and Flow with Enclosure Radiation – Fine Mesh



Demonstration Problem: 3D Melting and Flow with Enclosure Radiation – Coarse Mesh



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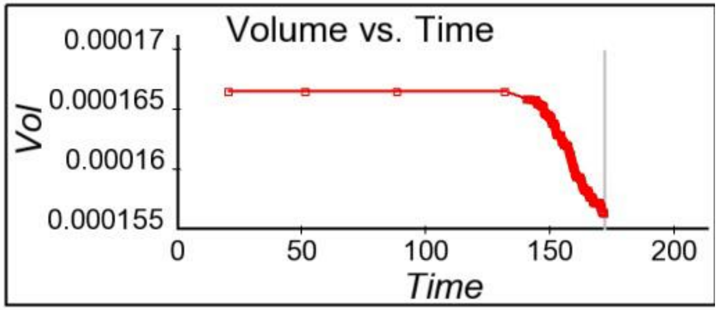
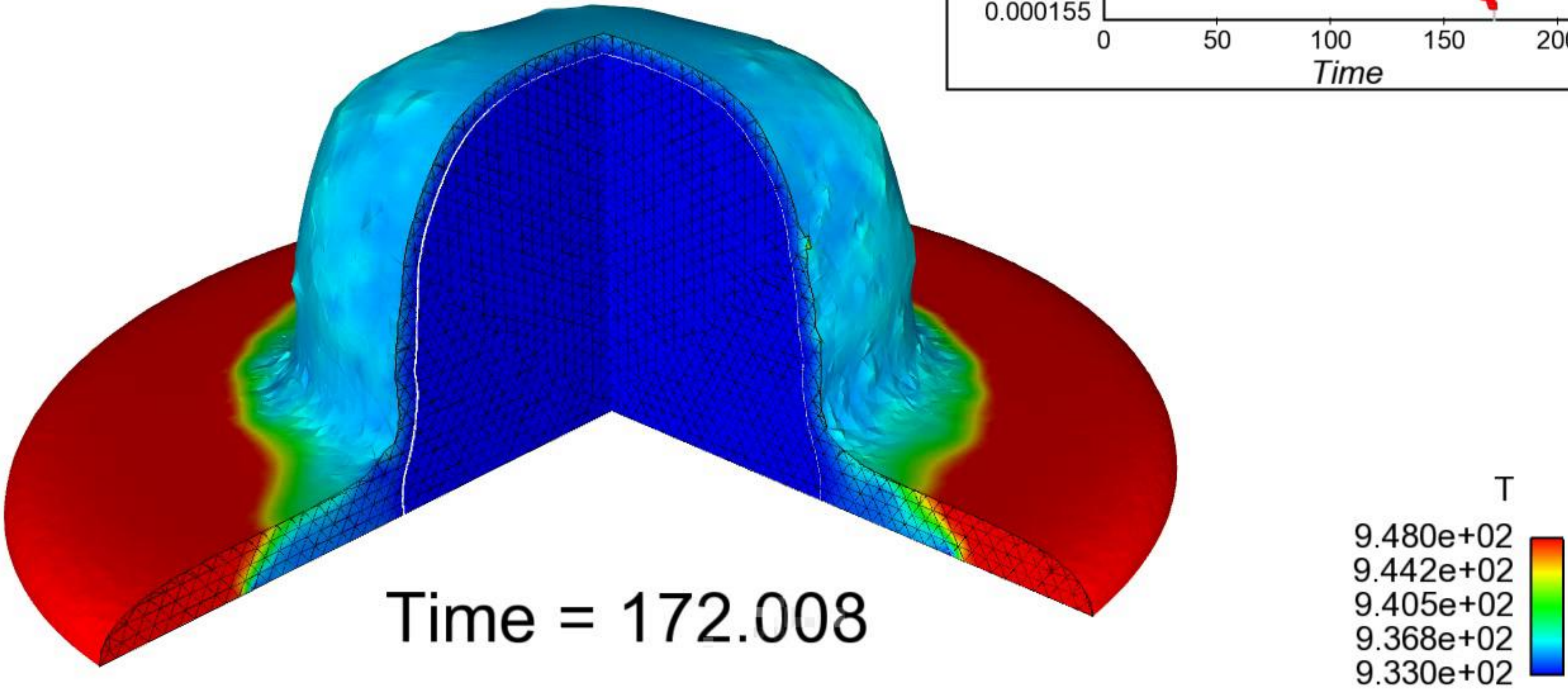
Demonstration Problem: 3D Melting and Flow with Enclosure Radiation – Medium Mesh





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Summary and Future Work

- CDFEM is Accurate for Static Interface Problems
  - Multiple verification tests performed
- CDFEM is Robust for Static/Dynamic Interface Problems
  - Arbitrary topology handled
  - Verification underway
  - Stability/stabilization being studied
- CDFEM Provides Flexible Approach for Interfacial Physics
  - Allows capillary forces, enclosure radiation on moving fluid interfaces with no additional code
- Future/Ongoing Work
  - Finish transient verification suite
  - Examine pressure and advection stabilization for nearly degenerate elements
  - Develop/implement/verify generalized interface evolution strategy
  - Develop/implement combination of non-conformal adaptivity and CDFEM
  - Develop splitting/projection strategies for pressure-velocity system in CDFEM

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