SAND2011-1180C

A Conformal Decomposition Finite Element Methods (CDFEM) for Melting and Flowing Aluminum

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This work was performed at Sandia National Laboratories. Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy under Contract DE-AC04-94AL85000.

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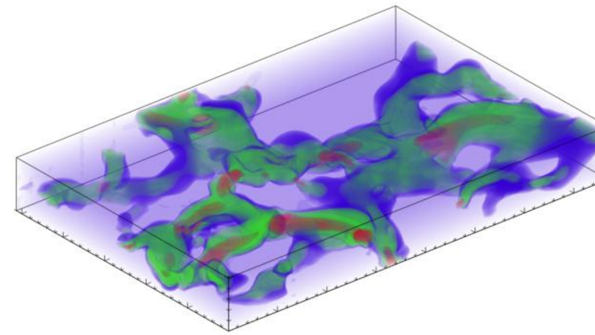
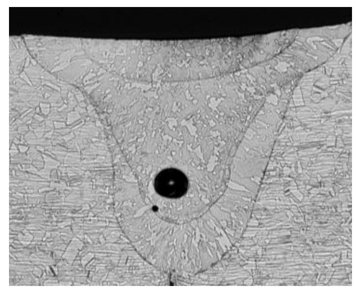
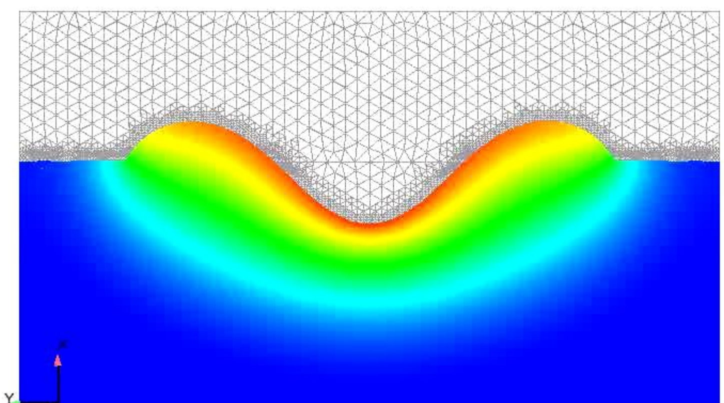
Thermal/Fluid Problems Requiring Interface Capturing Methods

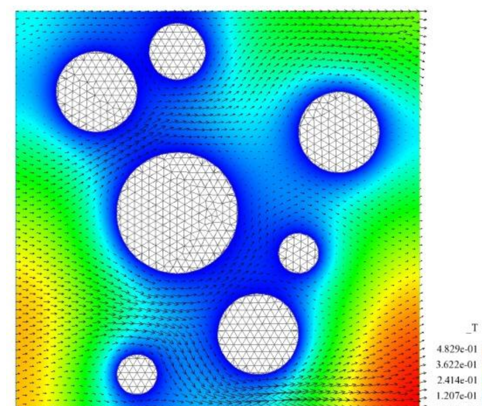
Recent/Future Static Interface Problems
- Thermal transport in composite materials
- Pore-scale flow in porous media

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









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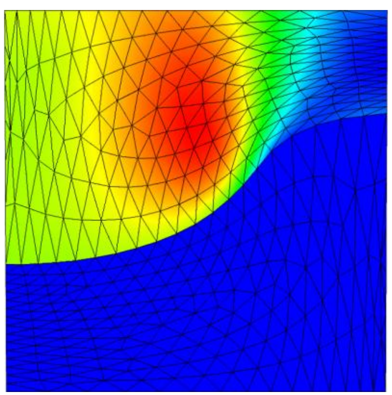
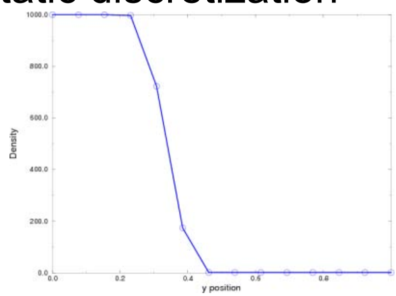
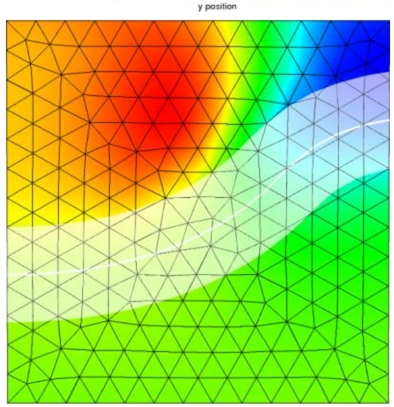
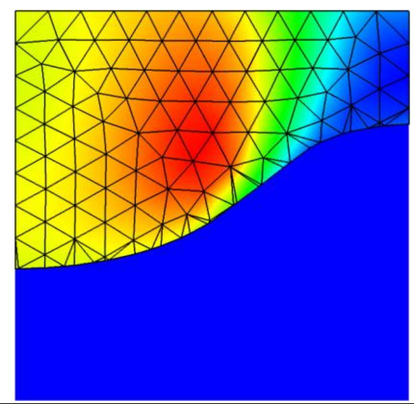
Finite Element Methods for Interfaces in Fluid/Thermal Applications Tested at Sandia

ALE	Diffuse LS	XFEM	CDFEM
• Separate, static blocks for air and water phases • Static discretization 	• Single block with smooth transition between air and water phases • Static discretization  	• Single block with sharply enriched elements spanning air and water phases • Interfacial elements are dynamicall y enriched to describe phases	• Separate, dynamic blocks for air and water phases • Interfacial elements are dynamically decomposed into elements that conform to phases 

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Method Requirements Comparison for Melting and Flow

Reqt./Method	ALE	Diffuse LS	XFEM	CDFEM
Enclosure Radiation	Existing capability	Not possible (could try interface reconstruction and diffuse source)	Requires specialized code (to make implicit surfaces part of enclosure)	Existing capability
Capillary Hydro-dynamics	Existing capability	Existing specialized capability (Properties and sources depend on level set)	Requires specialized code (Heaviside pressure, Ridge Temperature and Velocity, sub-element integration)	Existing capability
Topology Change	Not possible (could try automated remeshing)	Existing specialized capability	Existing specialized capability	Existing specialized capability
Notes	Ideal method for small deformation with complex volumetric and interfacial physics	Ideal method for large deformation with single volume physics and simple interfacial physics	Better interface physics than diffuse LS, single volume physics, invasive to code	Allows large deformation without compromising physics description

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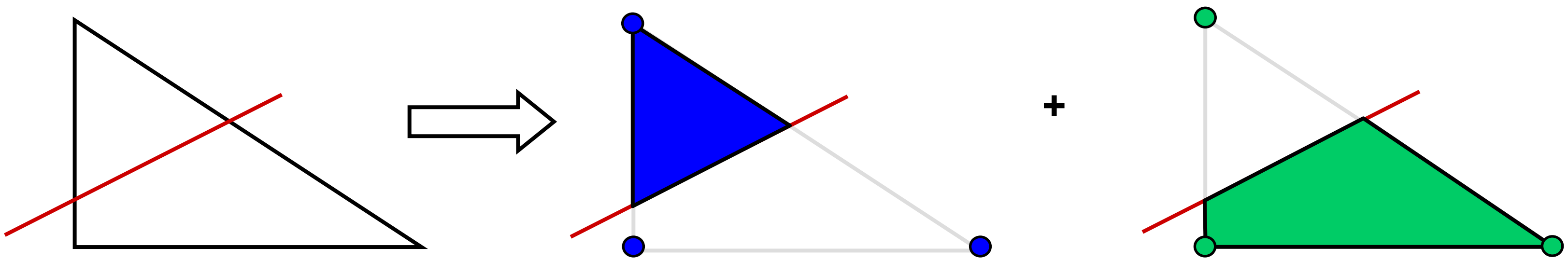
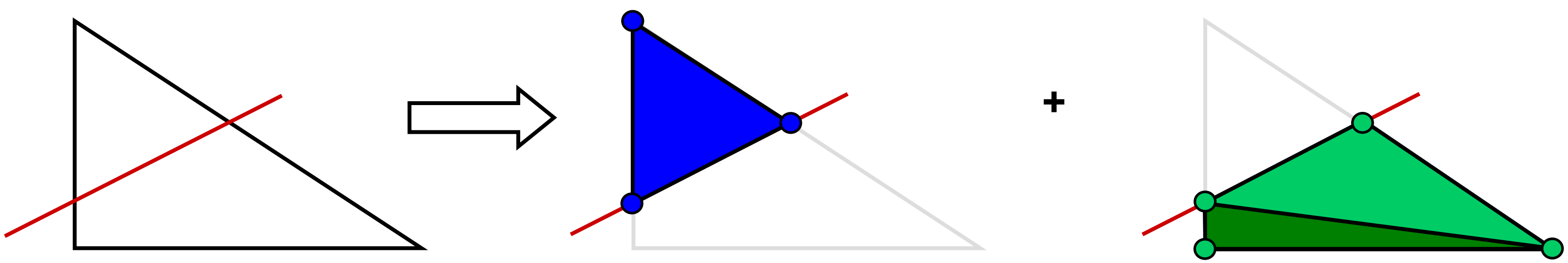
XFEM – CDFEM Discretization Comparison

XFEM Approximation



CDFEM Approximation



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

Formulation: Thermal Transport

Conduction/Convection

- Advection – Diffusion

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

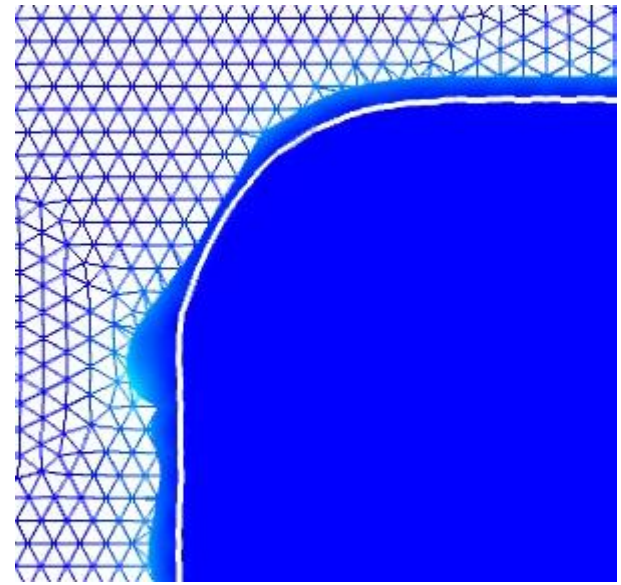
- Galerkin, Backward Euler, Dynamic geometry introduces moving mesh term

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

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

- SUPG stabilization

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



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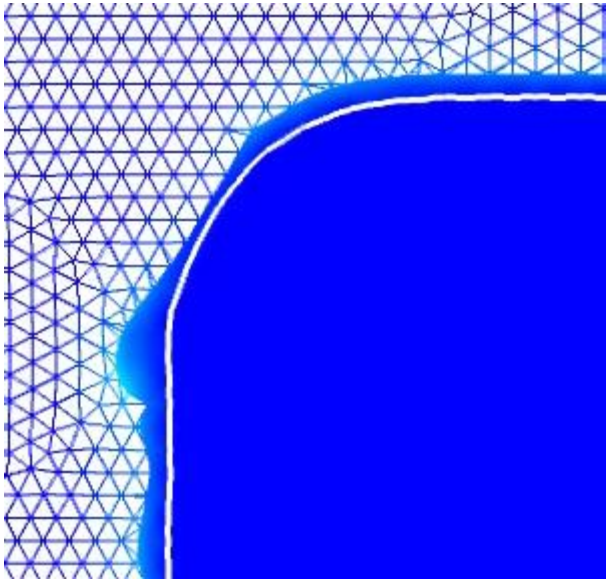
Formulation: Melt Dynamics



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

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

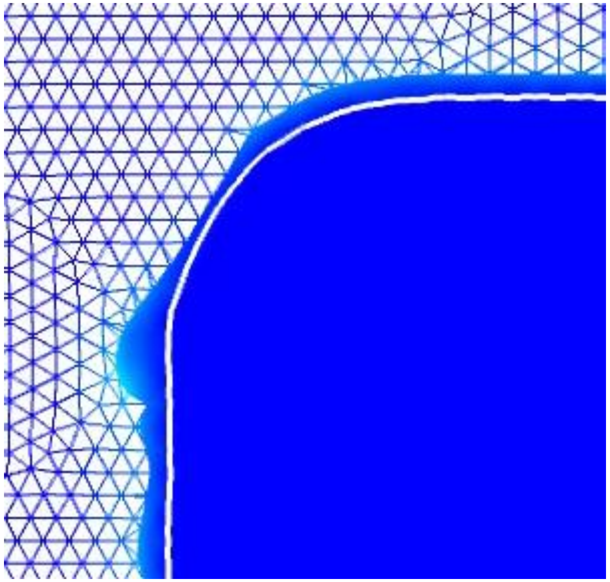
- Galerkin, Backward Euler

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

- 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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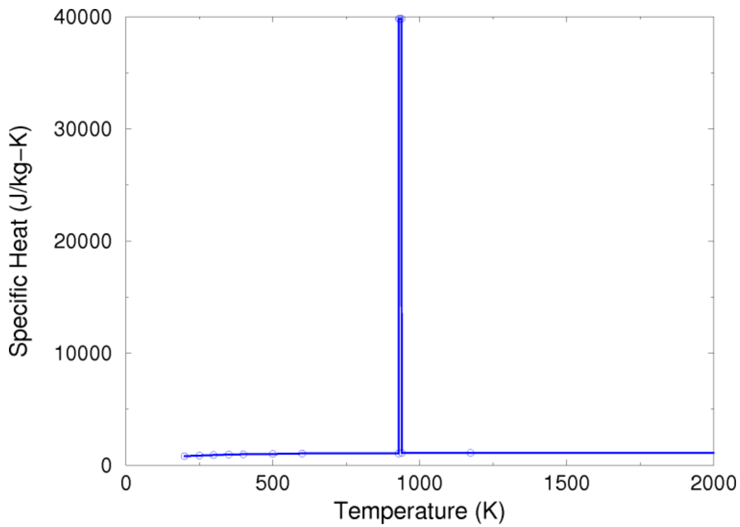
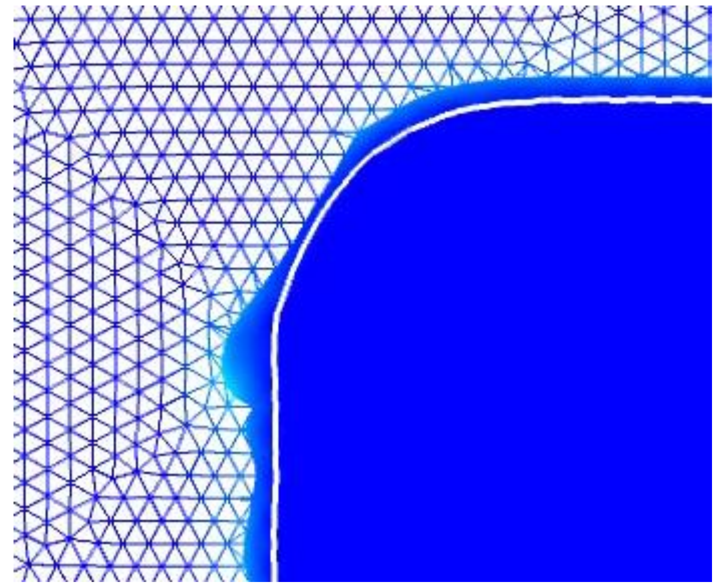
Models: Solid-Liquid Interface

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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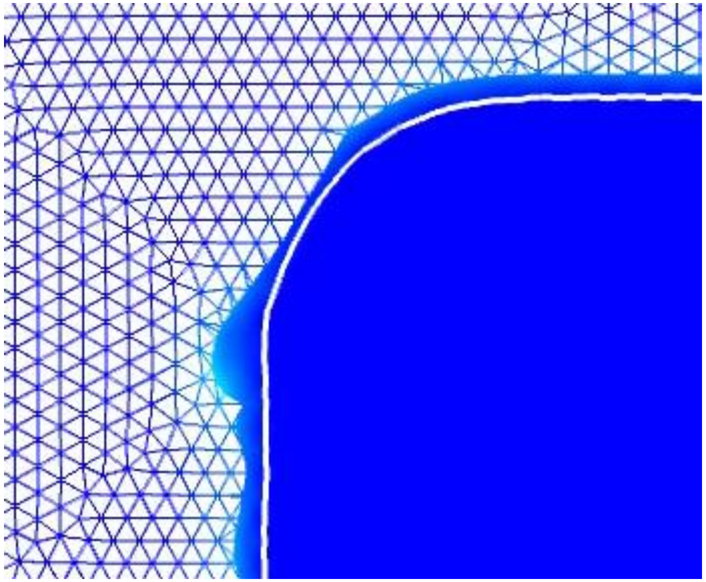
Models: Liquid-Air Interface

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

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

Radiation

- Simple radiation boundary condition

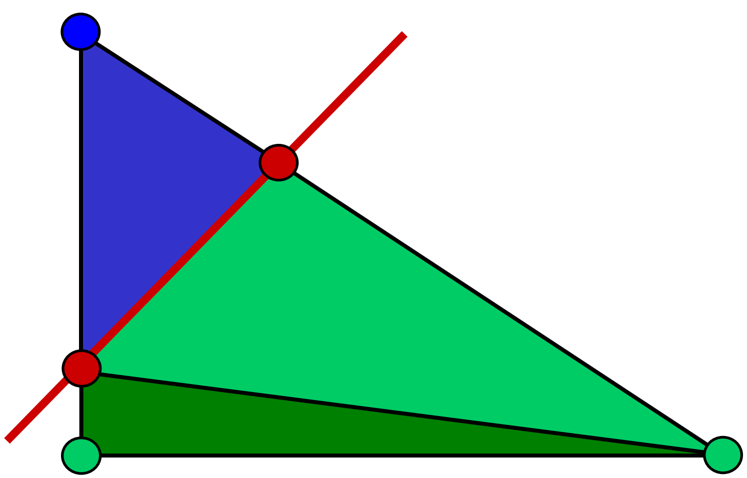
$$\int_{\Gamma} \varepsilon\sigma \left(T^4 - T_e^4\right) N_i \; d\Gamma$$

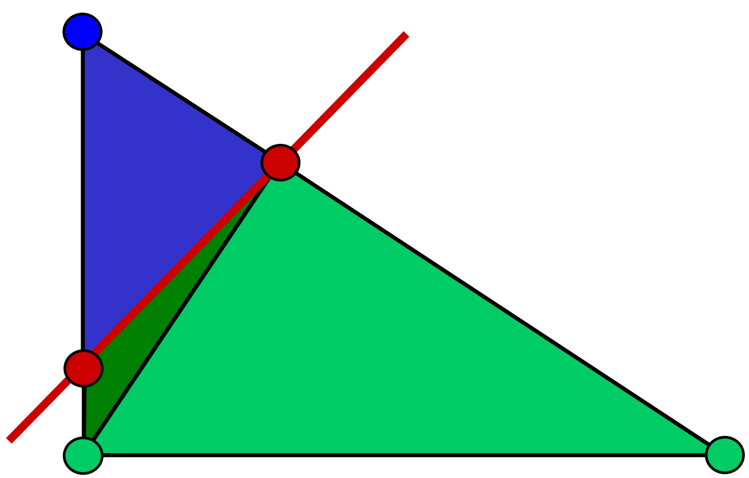
- Enclosure radiation
  - Enclosure temperature 2000K
  - Repeat viewfactor calculation every time step

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

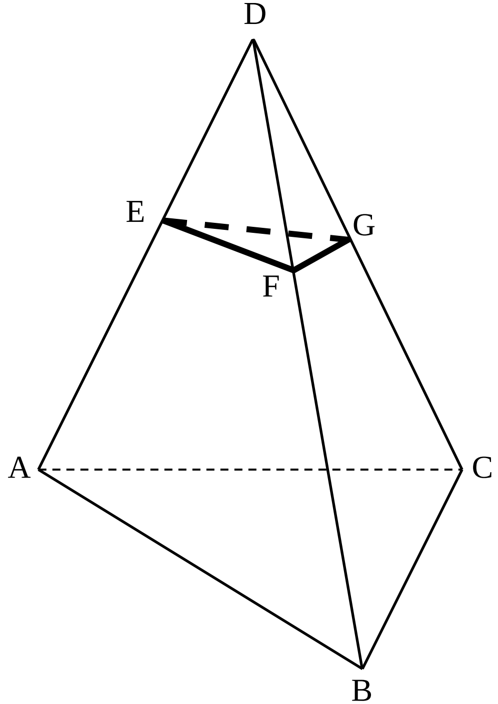


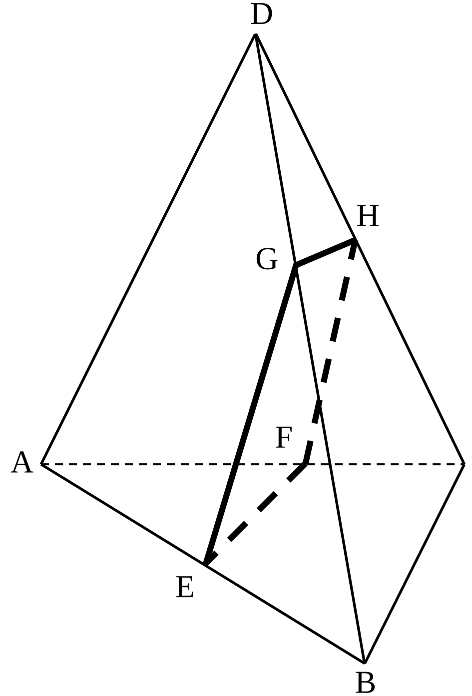


CDFEM – Level Set Implementation in Three Dimensions

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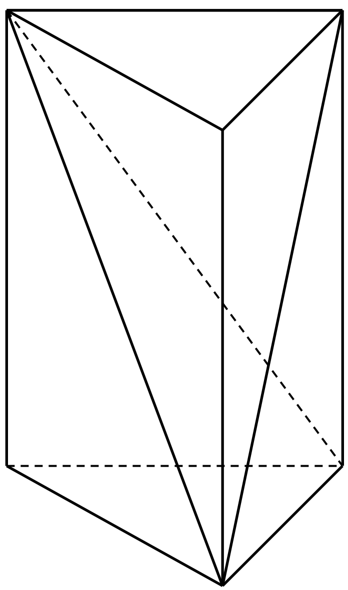
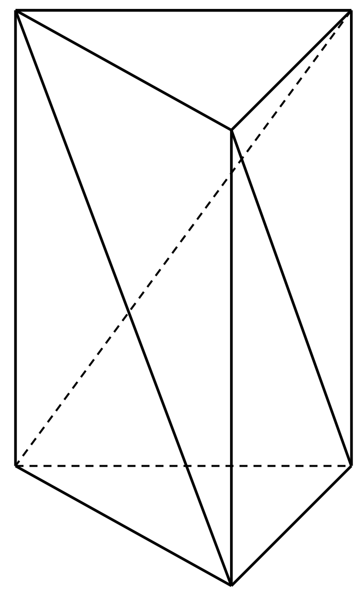
CDFEM – Level Set Implementation in Three Dimensions – cont'd

- 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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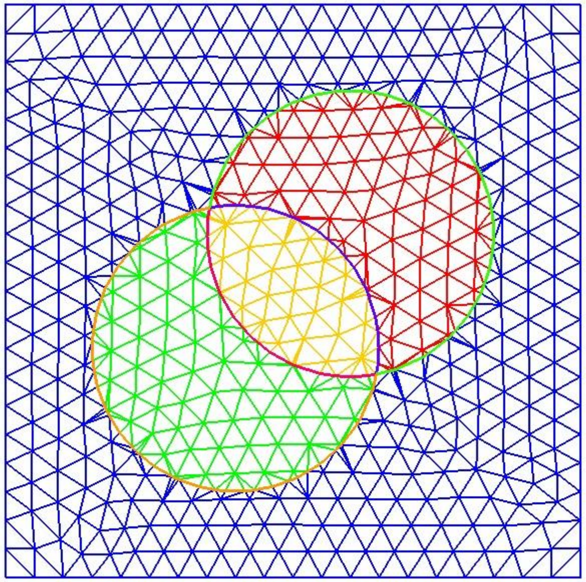
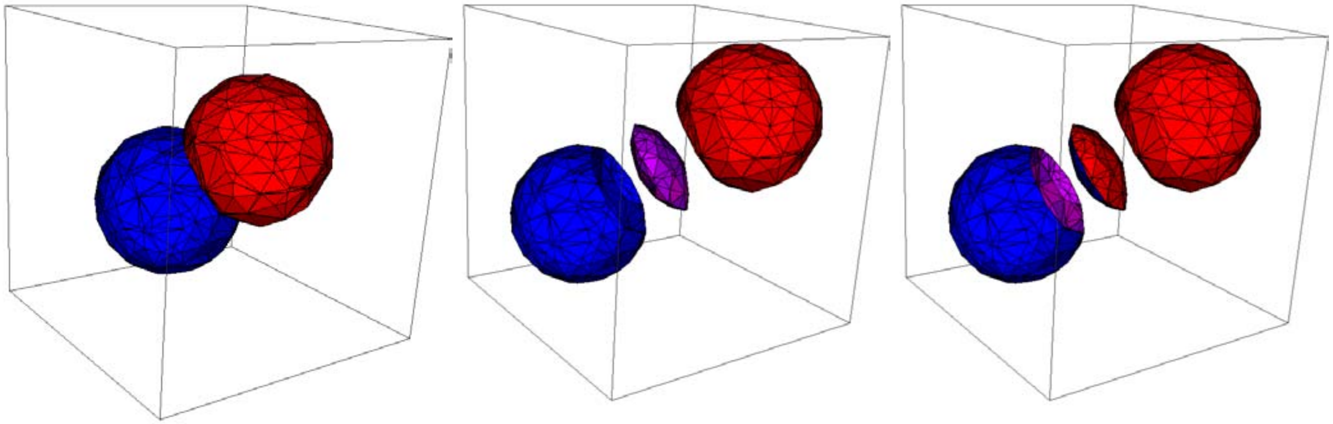
CDFEM Status: Code Capability

- 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

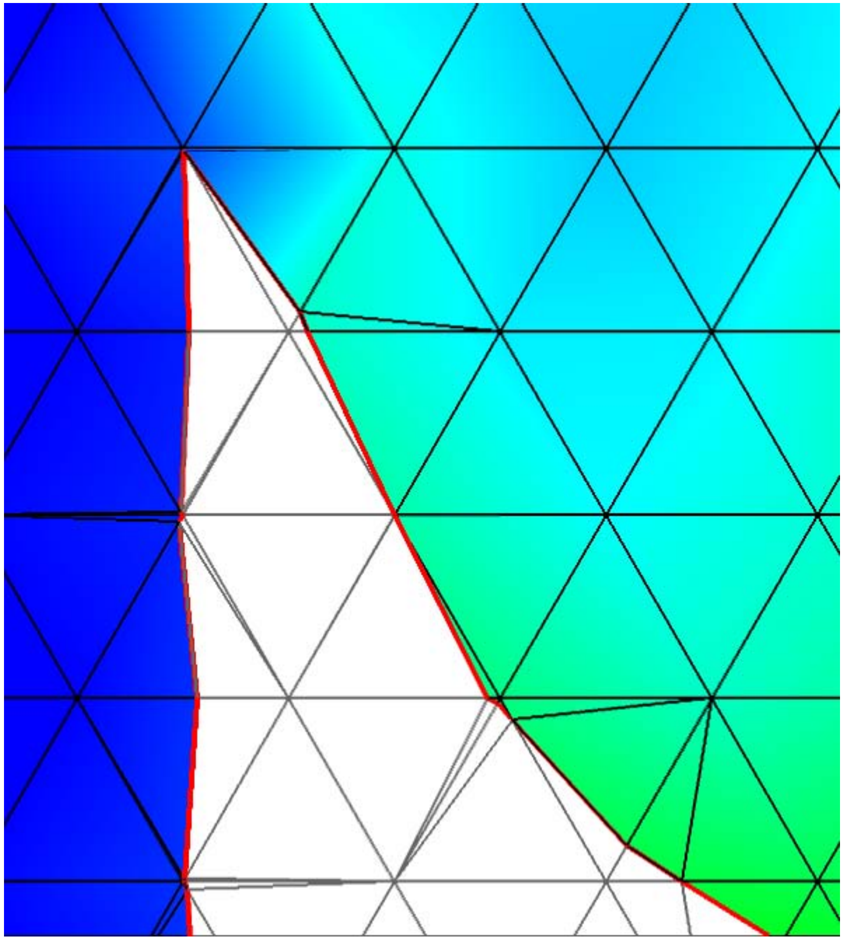




Complications: Degenerate Decompositions

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 et al.
  - Creates/retains many slivers and infinitesimal sub-elements
  - Interface segments always lie between subelements of both volumetric phases
  - No degenerate cases to handle

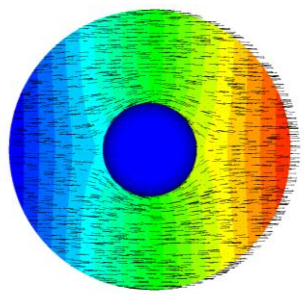


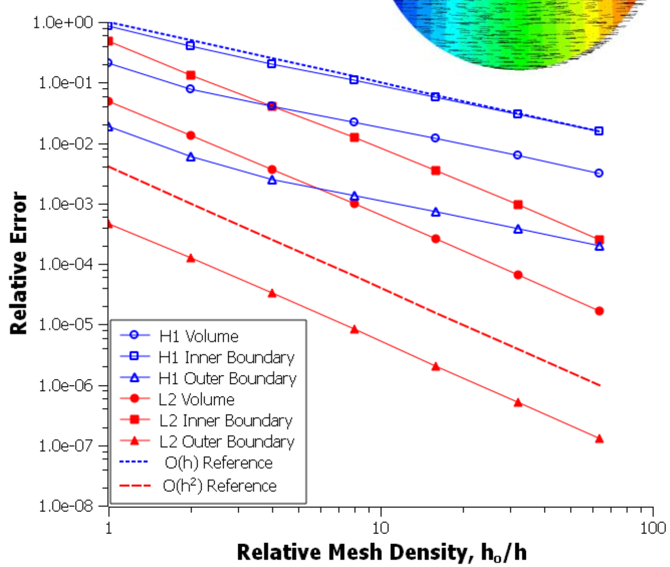
Results: CDFEM Verification

- 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 2nd order in space, 1st or 2nd order in time

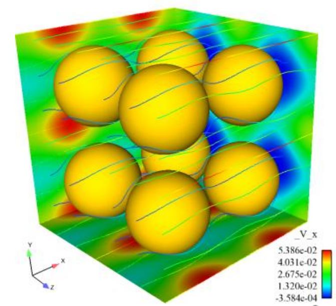
CDFEM Verification for Static Interfaces

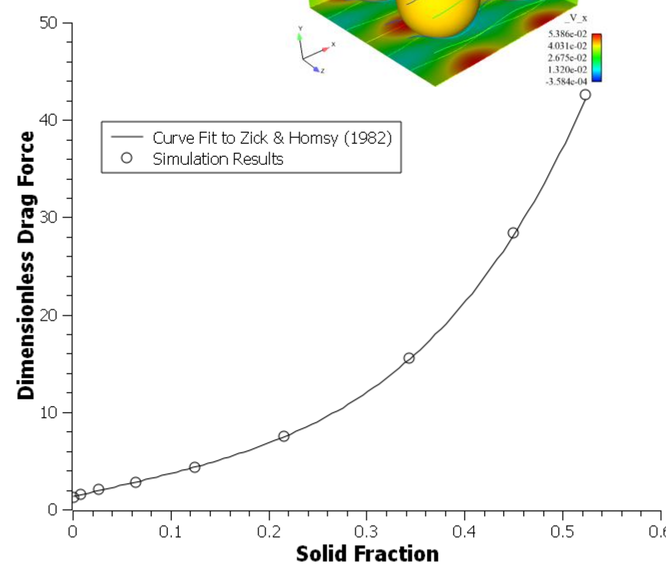
Steady Potential Flow about a Sphere
- Embedded curved boundaries
- Dirichlet BC on outer surface, Natural BC on inner surface
- Optimal convergence rates for solution and gradient both on volume and boundaries





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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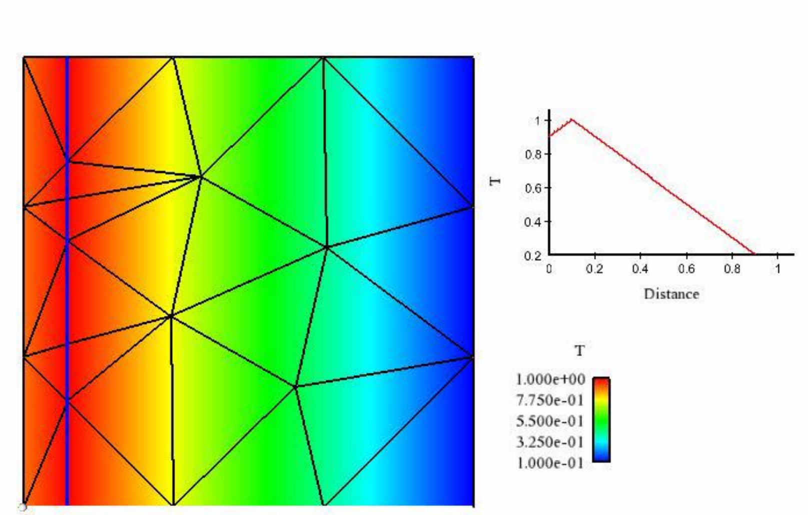
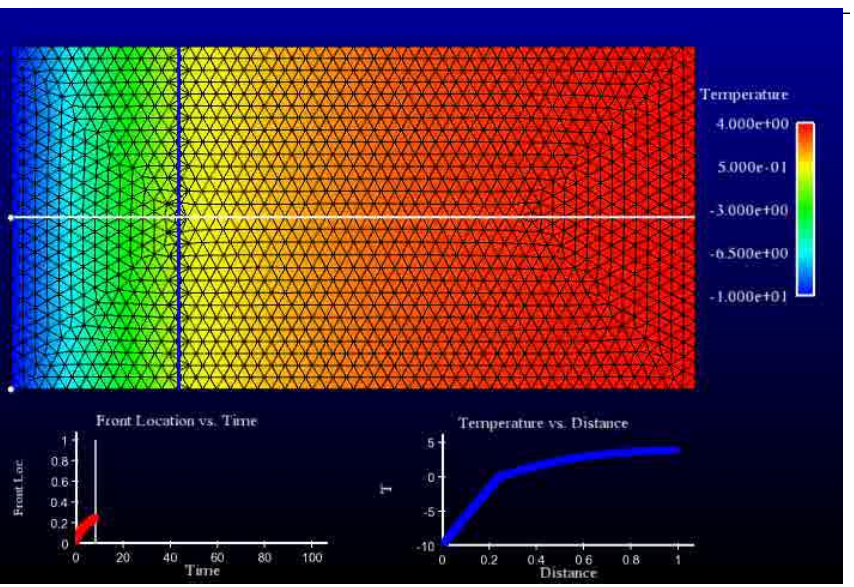
CDFEM Verification for Dynamic Interfaces



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)

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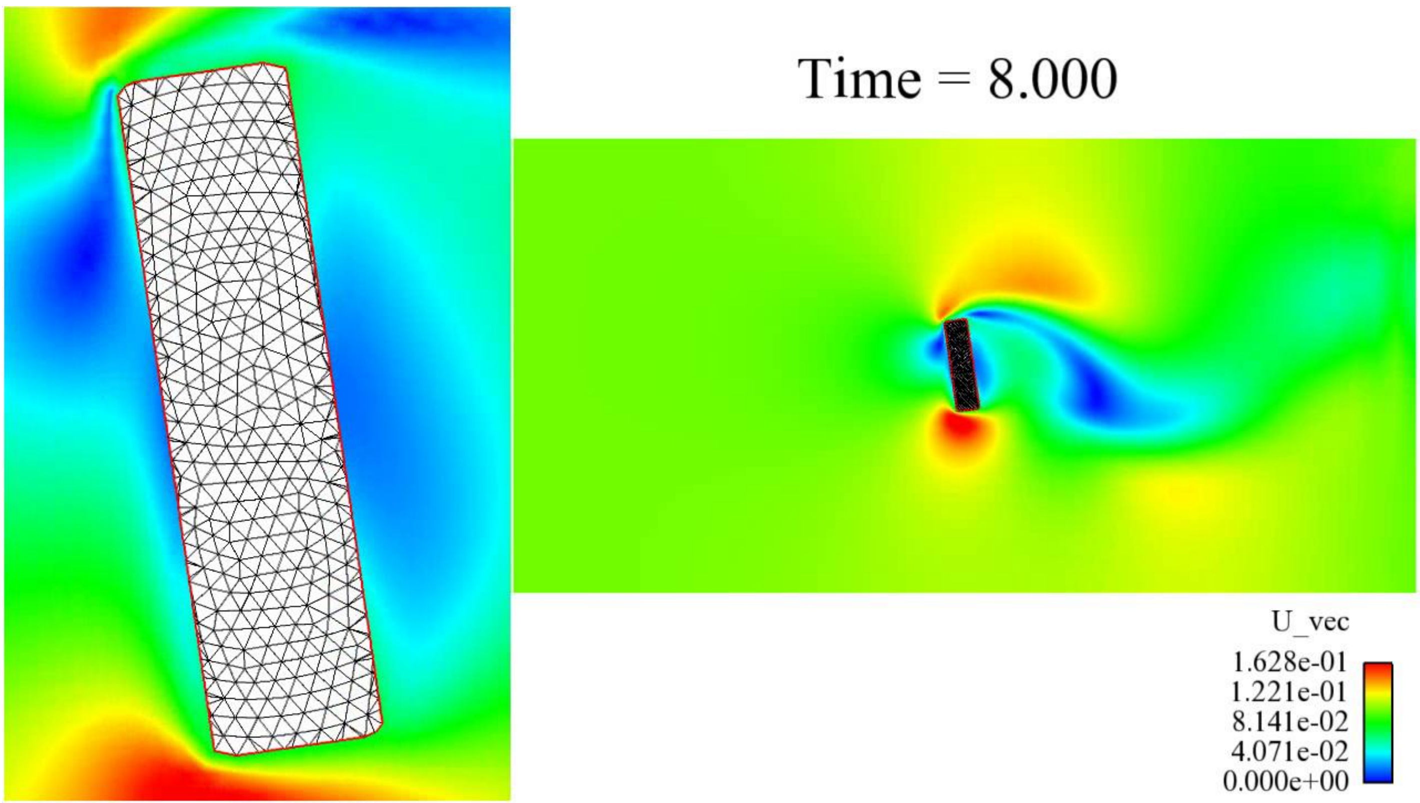
CDFEM Verification Still Needed

- 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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Aluminum Melting 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 used for enclosure viewfactor and radiosity calculation

- 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 used for enclosure viewfactor and radiosity calculation
  - Surface motion driven by capillary hydrodynamics

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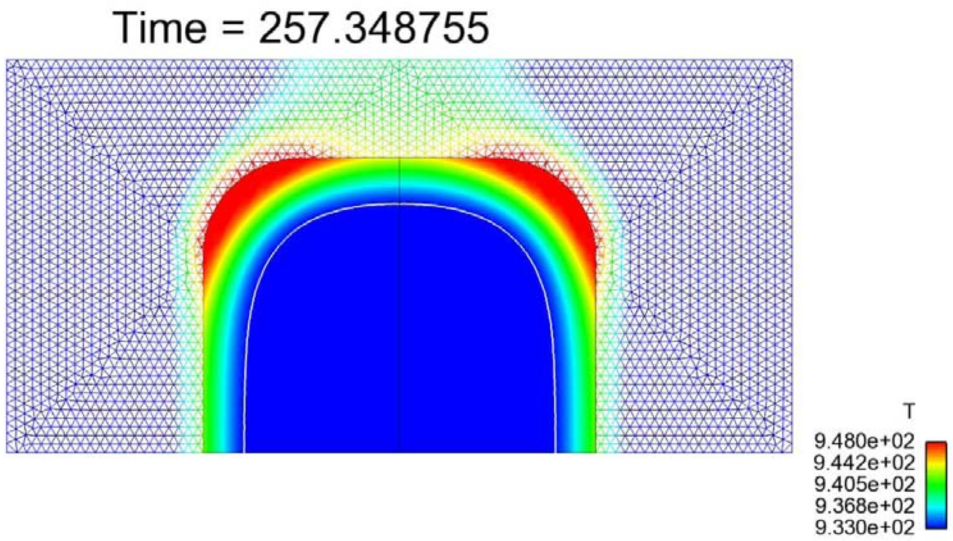
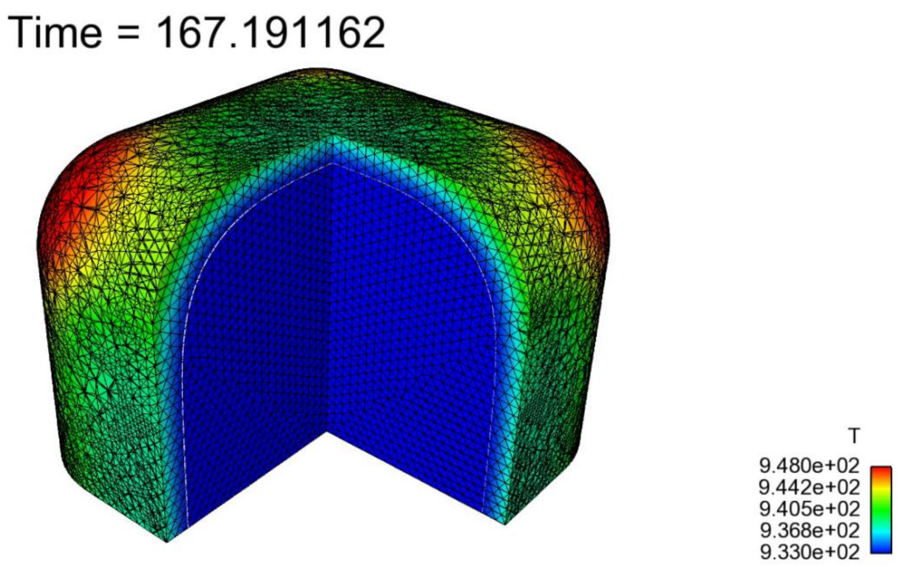
Demonstration Problem: 2D-3D Melting with Enclosure Radiation





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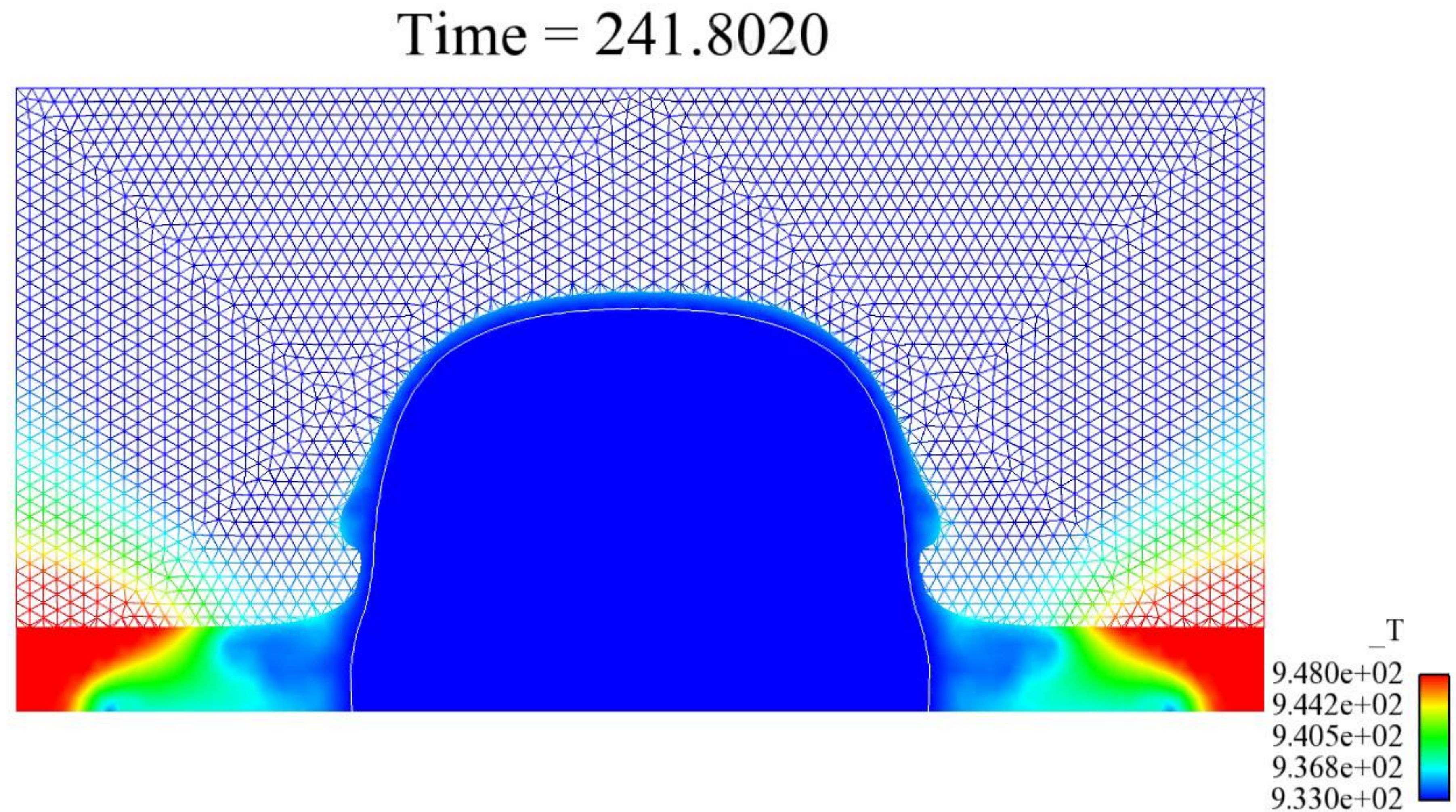
Demonstration Problem: 2D Melting and Flow with Enclosure Radiation – Medium Mesh



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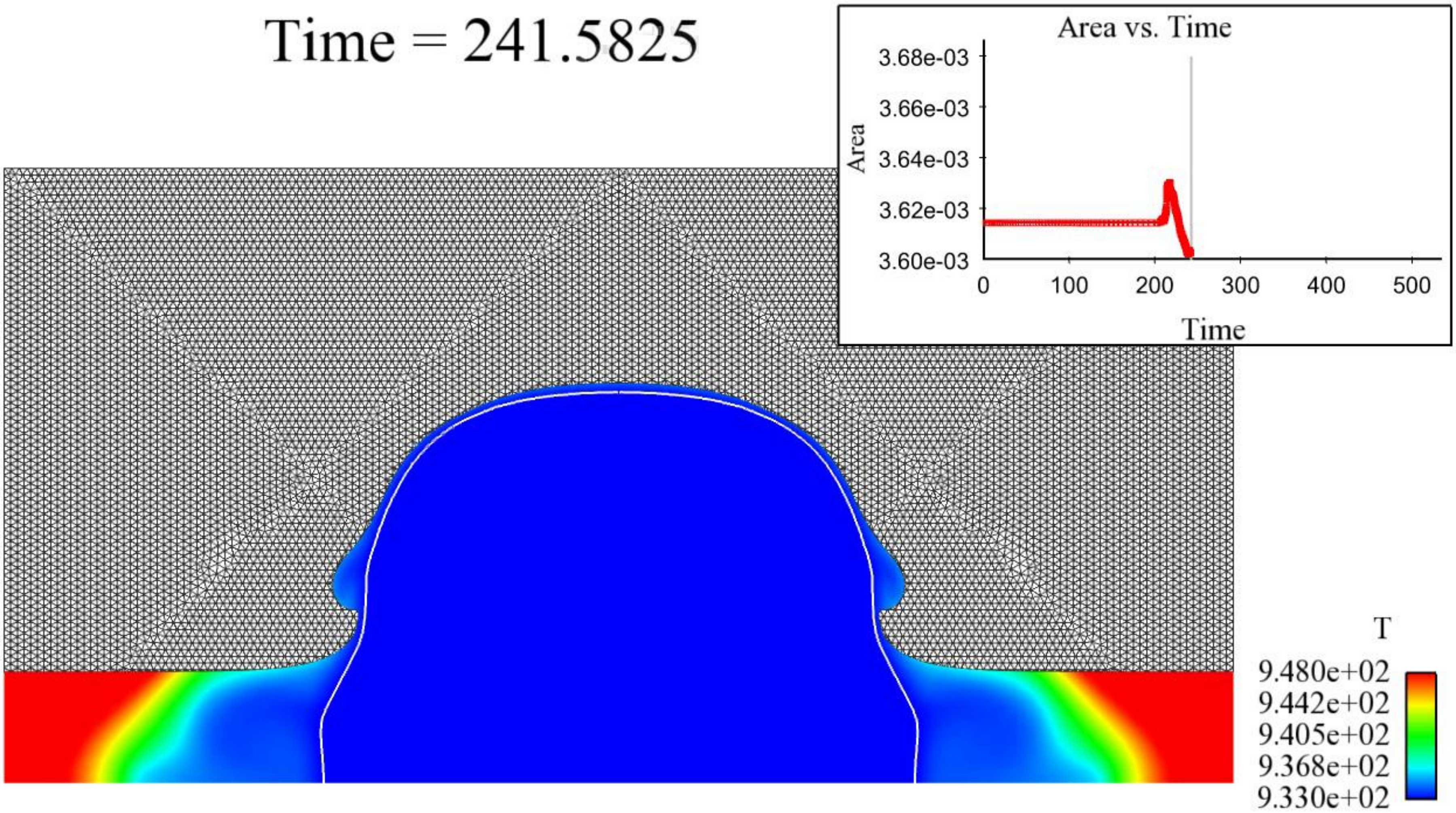
Demonstration Problem: 2D Melting and Flow with Enclosure Radiation – Fine Mesh



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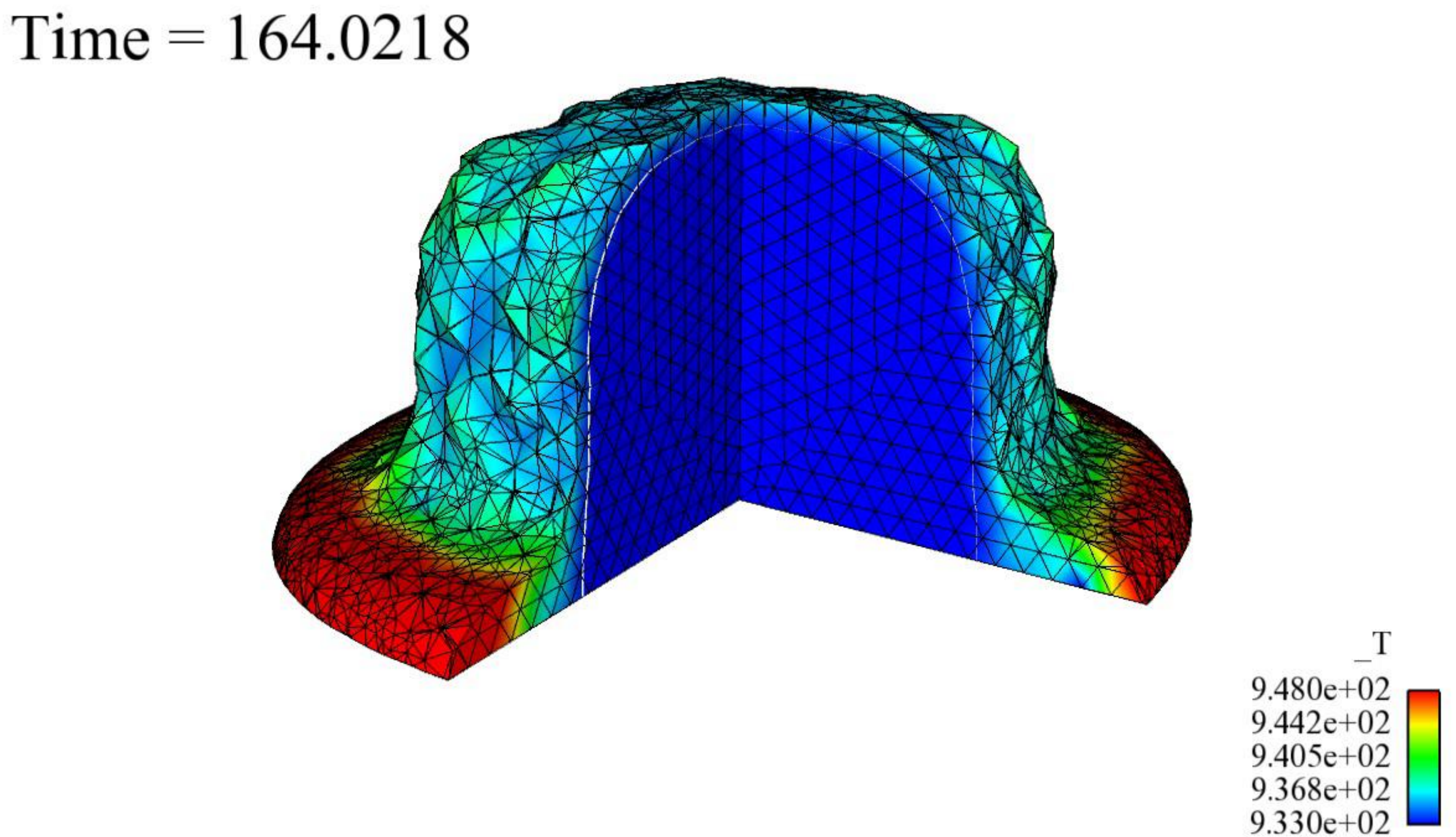
Demonstration Problem: 3D Melting and Flow with Enclosure Radiation – Coarse Mesh



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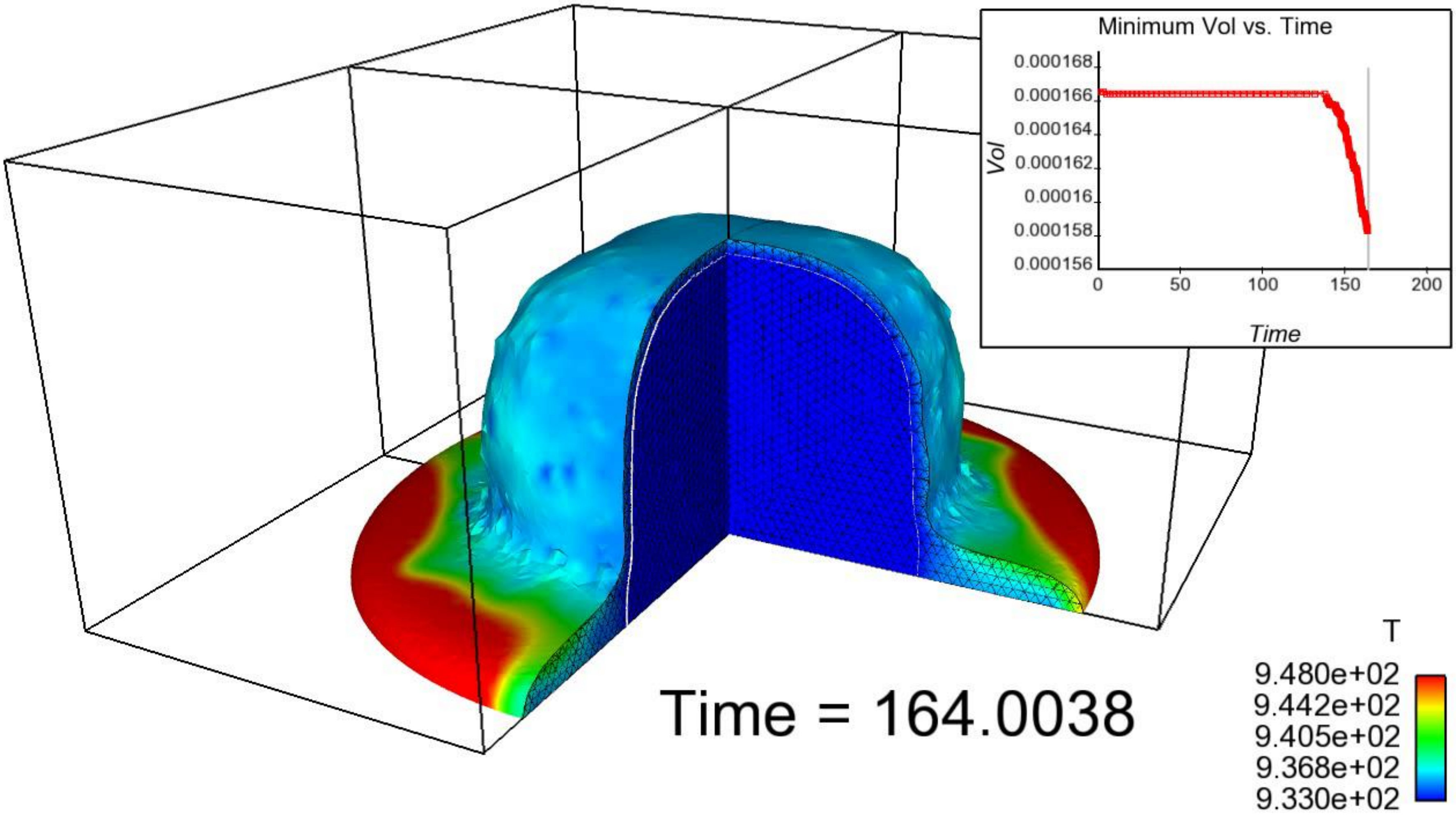
Demonstration Problem: 3D Melting and Flow with Enclosure Radiation – Medium Mesh



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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
  - Handles arbitrary interface topology in 2d and 3d
- CDFEM Provides Flexible Approach for Interfacial Physics
  - Allows 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
  - Explore relationship between velocity discretization and level set discretization and impact on stability

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