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Conformal Decomposition Finite Element Method (CDFEM) Interface Tracking Technology for Full 3D, Parallel, Transient Capabilities in SIERRA Mechanics

David R. Noble
Thermal and Fluid Processes

Executive Summary

This set of annotated viewgraphs with executive summary provides a record of the completion of the FY10 Level 2 milestone #3606.

Milestone Description:

Free surface flows are found in many situations of interest to the nuclear weapons program, including manufacturing processes such as foaming, encapsulation, and welding, and flows associated with molten metals and liquefied organics that can result from abnormal thermal events. Robust methods of interface tracking in complex geometries are needed to enable accurate simulations of these processes. In this milestone, SNL will develop, implement, and apply a novel interface tracking technology, the CDFEM. SNL will demonstrate the application of this approach to a representative problem of high interest, transient melting and flow.

Completion Criteria:

A production capability within SIERRA Mechanics that can robustly track and remesh interfaces using the CDFEM approach. A demonstration of the capability for transient melting and flow in a representative geometry.

Certification Method:

A program review is conducted and its results are documented. The review will include members of the B61 LEP thermal analysis team.
Professional documentation, such as a report or a set of viewgraphs with a written summary, is prepared as a record of the milestone completion.

Contribution to the ASC Program:

Completion of this milestone will add a key technology for robust interface tracking to the SIERRA Mechanics tool set, and will capture the best attributes of each of level sets and ALE. Free-surface flows are encountered in numerous problems including encapsulation and laser welding processes, and flows that result from melting and liquefaction of materials in abnormal thermal environments.

The motivation for this work is to provide a robust interface tracking capability for analyzing complex and dynamic interface problems at Sandia. Increasingly, Sandia's problems of interest involve complex and/or dynamic interfaces. Complex interface problems can take advantage of interface capturing including level set methods to avoid boundary fitted mesh generation. Dynamic interface problems often require interface capturing because they involve evolving topology.

Previous work in Engineering Science at Sandia for dynamic interfaces has employed Arbitrary Lagrangian Eulerian (ALE), diffuse Level Set (LS), and eXtended Finite Element (XFEM) methods. Recently the Conformal Decomposition Finite Element Method (CDFEM) has been developed to try to capture the best features of ALE and LS methods. Specifically we seek to allow arbitrary interface evolution while retaining the clarity, robustness, and accuracy of mesh-based descriptions of both the interfacial and volumetric physics.

This milestone involves the development and implantation of CDFEM as well as the demonstration of the method on a representative problem involving melting and flow. A milestone kickoff meeting in January clarified the requirements of the milestone and defined the representative problem. The results of this work include the 2D and 3D simulations of a block of aluminum melting due to a hot enclosure with realistic material properties including density, specific heat, conductivity, and surface tension. The formation and effects of an oxide layer are deferred to future work.

The physics modeled in this work include energy conservation via an advection-diffusion equation, mass and momentum conservation via the Navier-Stokes equations, and interfacial advection via the level set advection equation. Advection stabilization via SUPG and pressure stabilization via PSPG are employed. The interface between the fluid and solid is modeled as a diffuse transition between solidus and liquidus temperatures. The interface between the aluminum and surrounding air is handled with CDFEM.

CDFEM is implemented in SIERRA. The capability is parallel and is capable of describing an arbitrary number of phases. The usage of CDFEM is covered with viewgraphs describing a sample melting problem. The syntax is intended to mimic boundary fitted mesh simulations as much as possible.

Simulations of melting and flow are significantly more complicated than static geometry simulations and have much higher resolutions requirements in both space and time. Work is needed on models, discretization, and stabilization to allow for cost effective techniques for probing only the physics of interest. Future work should include the implementation and testing of CDFEM for projection methods or splitting techniques that will have better parallel scalability than the fully coupled methods employed this year. Another complication in CDFEM is the degenerate of nearly degenerate elements produced by the decomposition. The strategy used in the demonstration calculations proved to be very robust.

Many aspects of CDFEM have been verified, showing that convergent solutions are obtained on arbitrary meshes. Other aspects still need to be verified in future work.

Demonstration calculations of melting Aluminum with and without flow due to a hot enclosure are presented in both 2D and 3D.

Milestone Review: Conformal Decomposition Finite Element Method (CDFEM) Interface Tracking Technology for Full 3D, Parallel, Transient Capabilities in SIERRA Mechanics

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Albuquerque, New Mexico

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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This presentation documents the completion of a Level II Milestone completed in FY10Q4.

Outline

- Milestone Definition
- Motivation
  - Relevant applications
  - Why Conformal Decomposition Finite Element (CDFEM)
- Methodology
  - Formulation/Implementation description
  - Capability description
  - Usage (Description/Documentation)
- Complications
- Results
  - Verification (completed and still needed)
  - Example problem
    - Melting and flow of Aluminum in hot enclosure
- Summary and Future Work

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Outline for the presentation. A key component of this work is the development, implementation, and testing of the Conformal Decomposition Finite Element Method (CDFEM). Comparisons are made with alternate methods for discretizing dynamic interfaces, which form when materials melt and flow. The details of how CDFEM is formulated and implemented are discussed. The usage/syntax for CDFEM is presented for a melting and flow problem. Some time is spent discussing the difficulties that are encountered in melting and flow simulations, including complications that are unique to CDFEM. Extensive verification has been performed on aspects of CDFEM and level set methods and highlights of this work are presented. Future verification needs are identified. Multiple simulations of melting and flow are presented for an Aluminum block subjected to hot surroundings. After summarizing the results, future work is identified.

FY10 Level II Milestone

Conformal decomposition finite element method (CDFEM) interface tracking technology for full 3D, parallel, transient capabilities in SIERRA Mechanics

Description:

Free surface flows are found in many situations of interest to the nuclear weapons program, including manufacturing processes such as foaming, encapsulation, and welding, and flows associated with molten metals and liquefied organics that can result from abnormal thermal events. Robust methods of interface tracking in complex geometries are needed to enable accurate simulations of these processes. In this milestone, SNL will develop, implement, and apply a novel interface tracking technology, the CDFEM. SNL will demonstrate the application of this approach to a representative problem of high interest, transient melting and flow.

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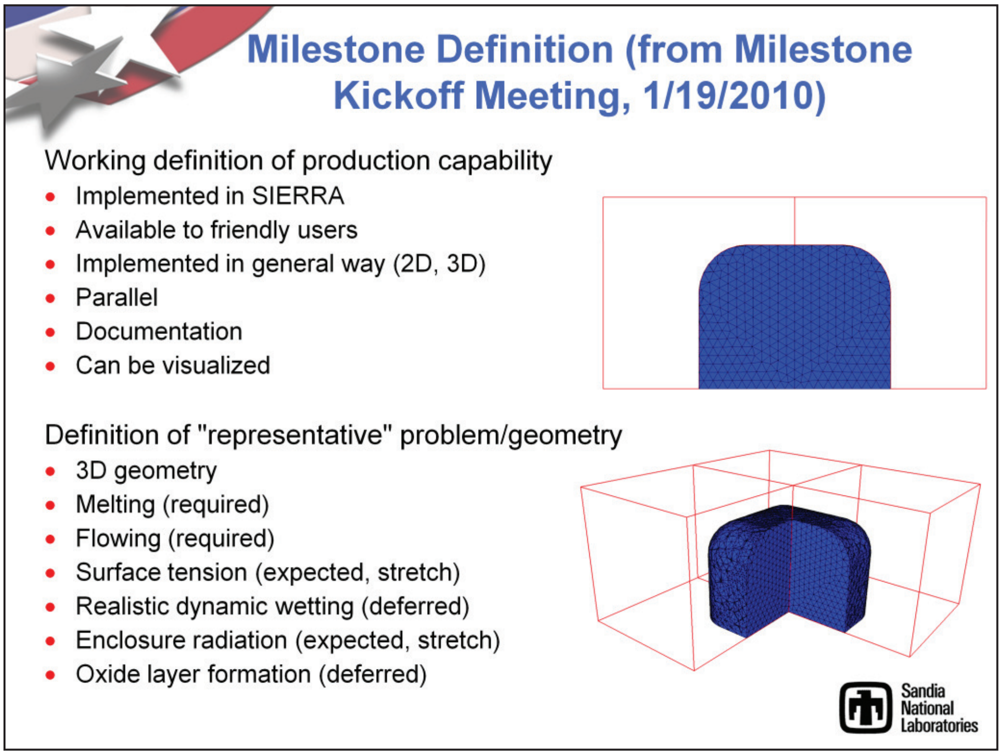
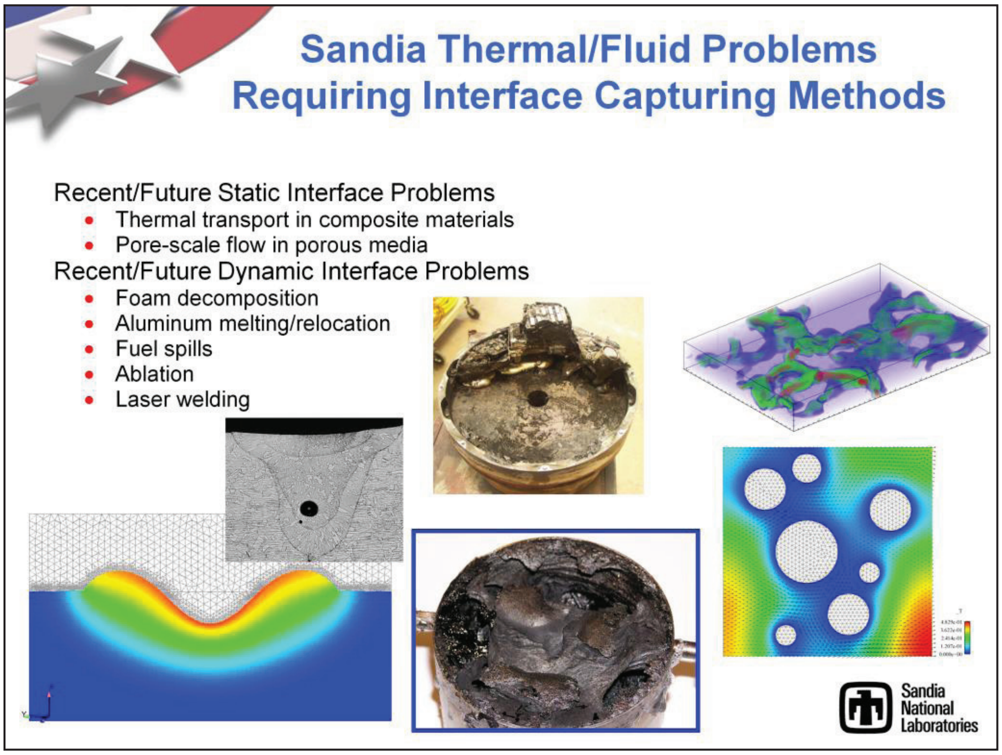
The text of the milestone.

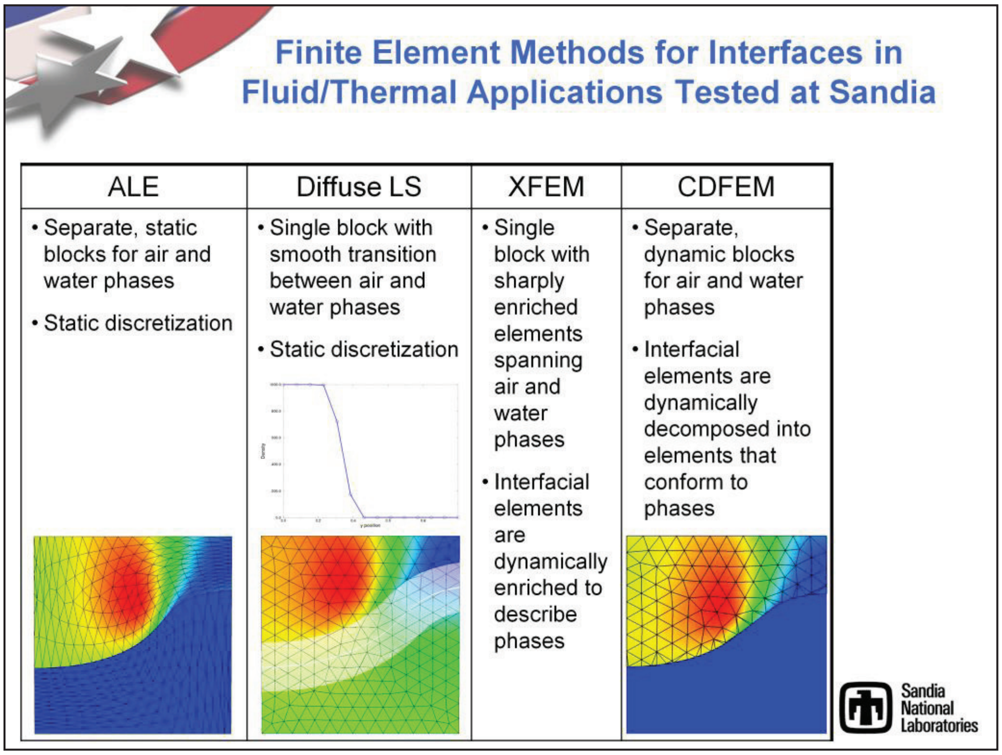


A meeting was held on 1/19/2010 to help clarify the milestone and its definition. A working definition of "production capability" and the "representative" problem and geometry was decided upon. This slide itemizes the requirements. It was decided that some items would not be part of the milestone and are labeled "deferred". Items labeled as "expected, stretch" are goals that exceed the requirements of the milestone, but are highly desirable in order to capture the relevant physics. The geometry is a rounded block of Aluminum subjected to hot surroundings.



Increasingly, Sandia's problems of interest involve complex and/or dynamic interfaces. Complex interface problems can take advantage of interface capturing including level set methods to avoid boundary fitted mesh generation. This is applicable to pore scale transport in geologic and engineered materials. Similar requirements are presented in thermal transport in composite materials.

Dynamic interface problems often require interface capturing because they involve evolving topology. A few years ago, these methods were pursued for predicting void formation in laser welding. Foam decomposition and liquefaction remains a problem of interest. Likewise, aluminum relocation is of interest in adverse environments. Similar challenges arise in the prediction of fuel spills and large scale ablation.



Several methods for dynamic interface problems including melting and flow have been developed, implemented, and tested at Sandia.

The traditional approach for these problems is to move the nodes of the mesh as the materials deform and flow using an Arbitrary Lagrangian Eulerian (ALE) method. While elements in ALE deform, they never change material. In this way the discretization is static.

Diffuse Level Set (LS) methods allow arbitrary topology change by providing a definition of the interfaces that can evolve in a mesh independent manner. The interfacial physics are smeared out however over a length scale that is typically a few times larger than element size. The method allows property variation, but the discretization is static with the same unknowns present in the elements regardless of the interface location.

Extended Finite Element Methods (XFEM) provide a sharp definition of the interface by enriching the elements that span the interface in order to capture both weak and strong discontinuities across the interface. In this way the discretization is dynamic as the unknowns can change depending on the materials present in an element.

CDFEM, by comparison, decomposes the existing elements into ones that conform to the interface and the resulting elements inherit the discretization that is appropriate for the material. In this way the elements change material (including the properties, equations, source terms, and fluxes) as the interface evolves.

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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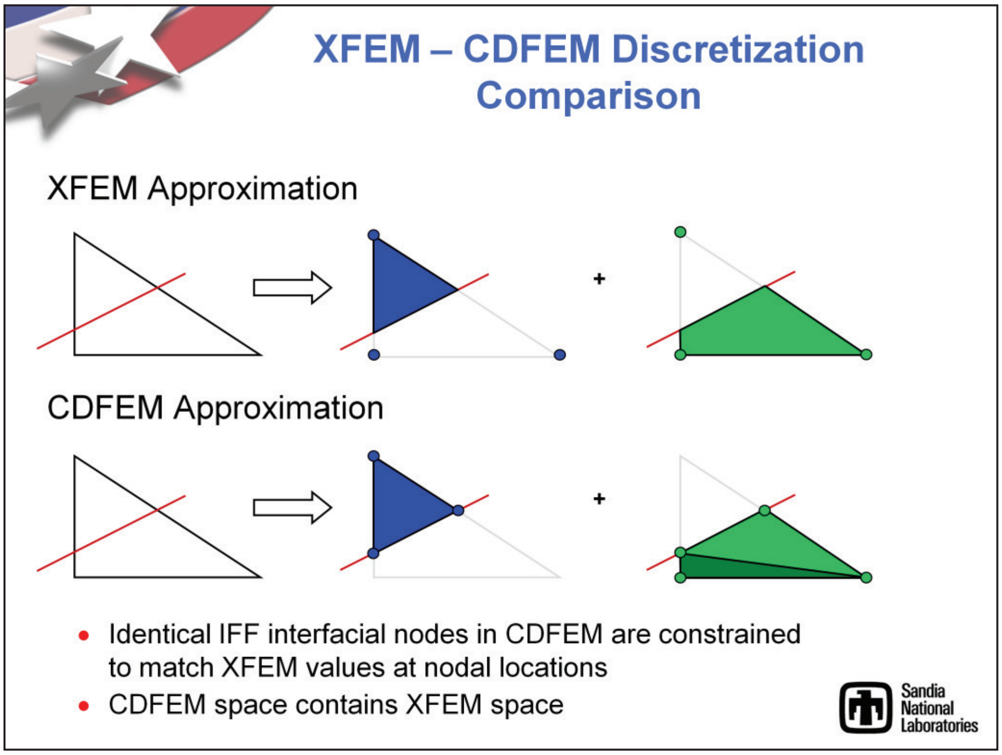
This slide evaluates the applicability of dynamic interface methods to the problem of melting and flow. In order to simulate melting and flow, the method must accommodate enclosure radiation on the evolving liquid interface, accurately address capillary hydrodynamics, and handle changes in topology as the liquid is formed and flows.

ALE readily handles all of the boundary conditions, including enclosure radiation, as well as the capillary hydrodynamics. However, the method cannot address the topology change or large deformation that are ubiquitous in melting and flow problems.

In diffuse LS methods, the interfacial physics are imposed using diffuse source terms that are activated on elements in the vicinity of the interface. Similarly, physical properties are assumed to transition smoothly across the interface. Because of this diffuse definition of the interface, it does not present a sharp definition of the enclosure radiation surfaces or, consequently, the temperature of these surfaces.

XFEM provides a sharp definition of the interface by enriching the elements that span the interface in order to capture both weak and strong discontinuities across the interface. Because the element assembly is based on subelements and their faces rather than elements and their faces, the method is fairly invasive to the code, however, requiring specialized code for both the volume and surface assembly.

By using standard finite elements, however, CDFEM allows for a dynamic discretization capable of describing sharp interfaces with minimal code changes.



Because XFEM is better known that CDFEM, it is useful to compare the discretizations. In XFEM, all unknowns are associated with the existing nodes of the input element. When an interface passes through an element, additional unknowns are added to the existing nodes in order to describe all of the materials present in the element. In contrast, CDFEM enriches the element by adding nodes on the interface between the materials.

These two discretizations can be made equivalent by constraining the CDFEM nodes to agree with values interpolated from the XFEM discretization. In this way, the discrete space of CDFEM contains the discrete space of XFEM. This has consequences for accuracy and boundary conditions. CDFEM is at least as accurate as XFEM with Heaviside enrichment. Dirichlet and flux boundary conditions are both readily applied in CDFEM, but can be challenging in XFEM.

Formulation: Thermal Transport

Conduction/Convection

- Advection – Diffusion

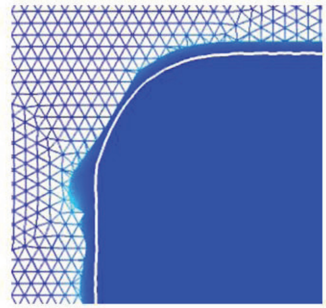
$$\rho c_p \frac{\partial T}{\partial t} + \rho u \cdot \nabla T = \nabla \cdot k \nabla T$$

- 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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The standard Galerkin formulation for thermal transport must be modified for the advection created by flow and for the mesh motion induced in CDFEM. In addition, advection stabilization (SUPG) is required to resolve sharp gradients in advection dominated flows. The stabilization parameter is calculated based on work by Shakib.

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

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

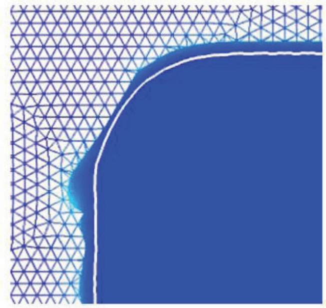
$$\int_\Omega \left[-P I + \mu\left(\nabla u + \nabla u^t\right)\right] \cdot \nabla N_i \, d\Omega - \int_\Omega \rho g \, N_i \, d\Omega + \int_\Gamma S \, N_i \, d\Gamma = 0$$

- 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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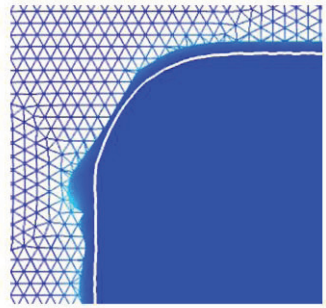
The flowing of the Aluminum melt is described by the Navier-Stokes equations. Using piecewise linear elements for both velocity and pressure necessitates the use of pressure stabilization. In the demonstration simulations, PSPG was used. Again SUPG is used for advection stabilization.

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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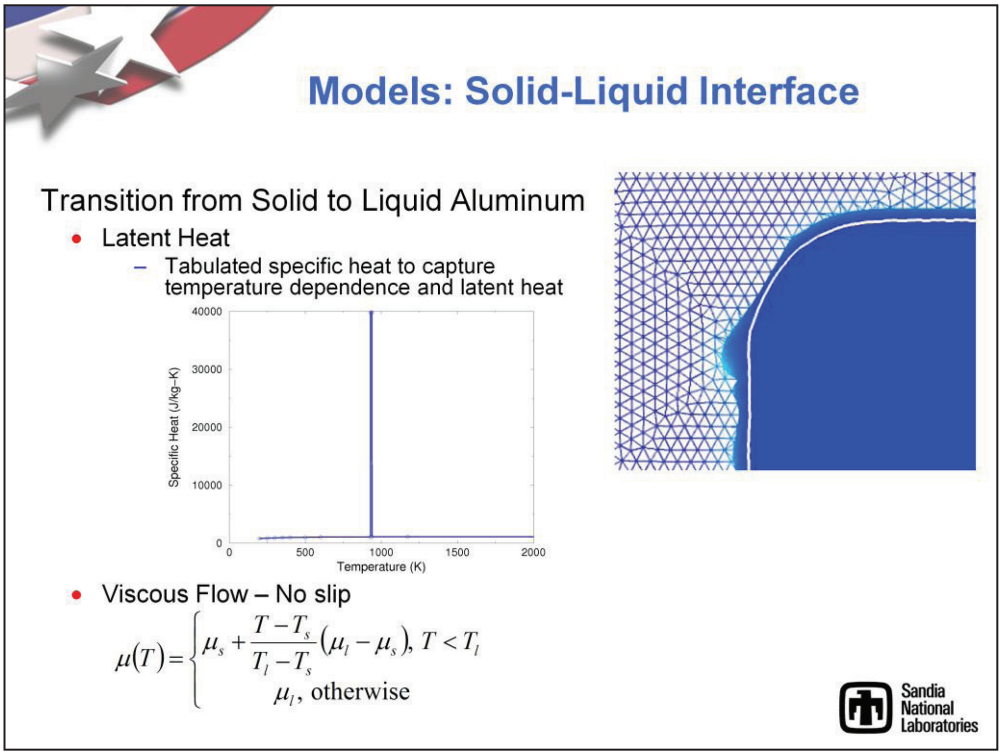
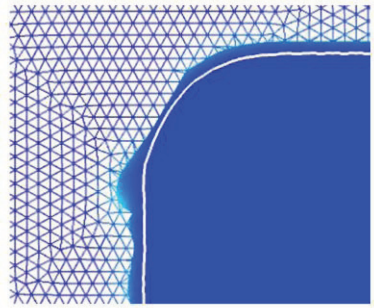
The interfacial motion is computed using a level set approach. The level set variable is initialized as a signed distance function. It evolves according to the advection equation using the local fluid velocity. Again SUPG is used for advection stabilization. While the advection correctly describes the motion of the interface, it does not preserve the signed distance property. Periodic renormalization restores this property. The renormalization procedure used in this work involves reconstructing the interface and computing the signed distance.



While the interface between the liquid aluminum and surrounding air is tracked with the level set field, the interface between the solid and liquid is modeled as a diffuse transition as the material temperature varies from the solidus to liquidus temperatures. Material properties are made a function of temperature in order to capture the interfacial physics. In order to capture the effect of the latent heat of fusion, the specific heat is modeled with a type of delta function acting over this temperature range. In order to transition from solid-like to fluid-like behavior the viscosity is ramped from a very large viscosity that produces rigid body motion to the actual viscosity of molten aluminum.

Models: Liquid-Air Interface



Capillary Force

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

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

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

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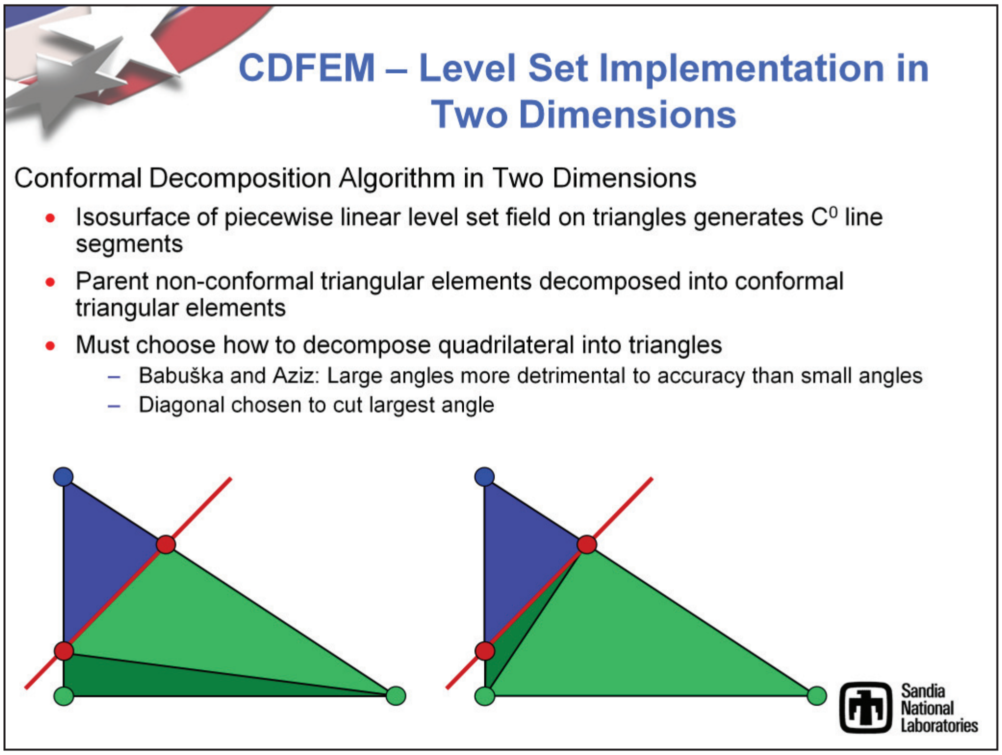
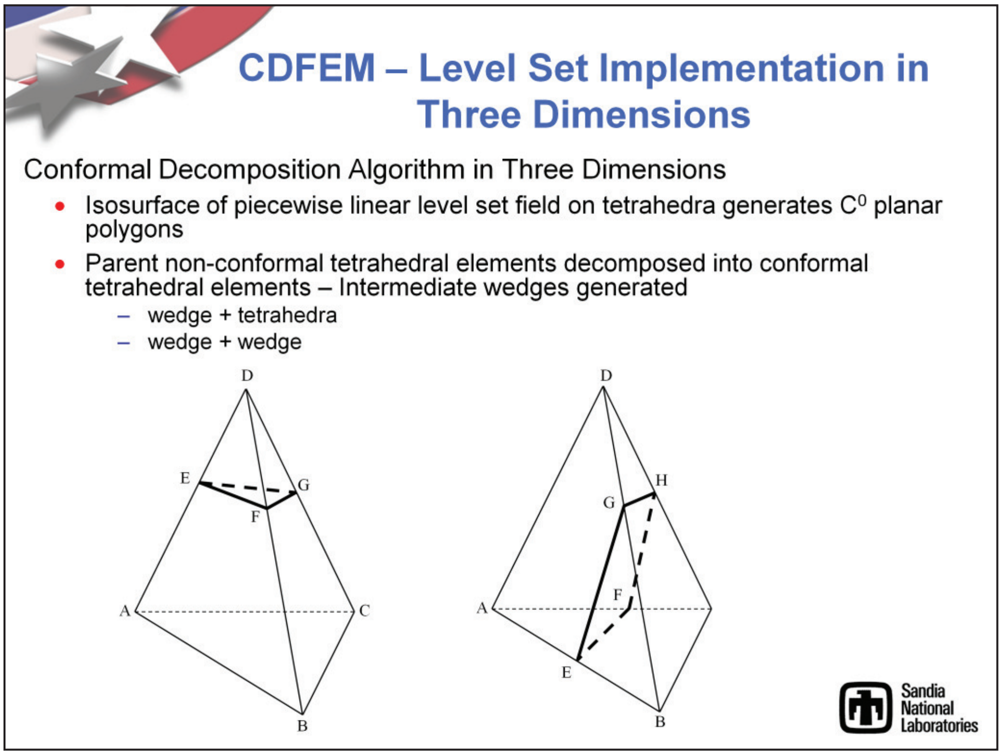
The interface between the liquid aluminum and surrounding air is tracked with the level set field. CDFEM decomposes the elements into ones that conform to the interface according to the zero isosurface of the level set field. Side sets are generated on the interface for applying interfacial boundary conditions. A jump in the normal stress across the interface is generated by surface tension. This curvature based traction is applied using integration by parts to avoid the explicit calculation of the curvature. Recent work by Hysing proposed a stabilization term that helps regularize the interface to avoid instabilities caused by the loose coupling between the momentum equations and the level set equations. The radiative transport on the interface is modeled in one of two ways. Either a simple radiative boundary condition or enclosure radiation is used. In the case of enclosure radiation, the viewfactors are recalulated every time step because the interface is evolving in time.



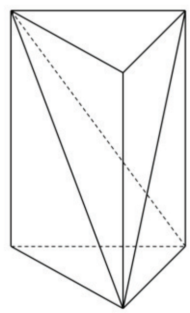
Description of the CDFEM algorithm in 2-D. The zero isosurface of the piecewise linear level set field consists of line segments. The interface is denoted in red. It segments the elements into two materials, indicated by the blue triangular region, and the green quadrilateral region. Parent non-conformal triangular elements are decomposed into triangular elements that conform to the interface. A choice must be made regarding the subdivision of the quadrilateral region into triangular elements. Babuska and Aziz found that large angles are more detrimental to accuracy than small angles. Consequently, the largest angle is cut.



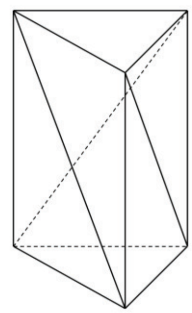
Description of the CDFEM algorithm in 3-D. The zero isosurface of the piecewise linear level set field consists of planar cuts through the tetrahedral elements. The resulting subelement shapes are determined by the number of nodes on either side of the interface. When the nodes are split 1-3, the parent tetrahedron is divided into a tetrahedron and a wedge. When the nodes are split 2-2, two wedges are formed.

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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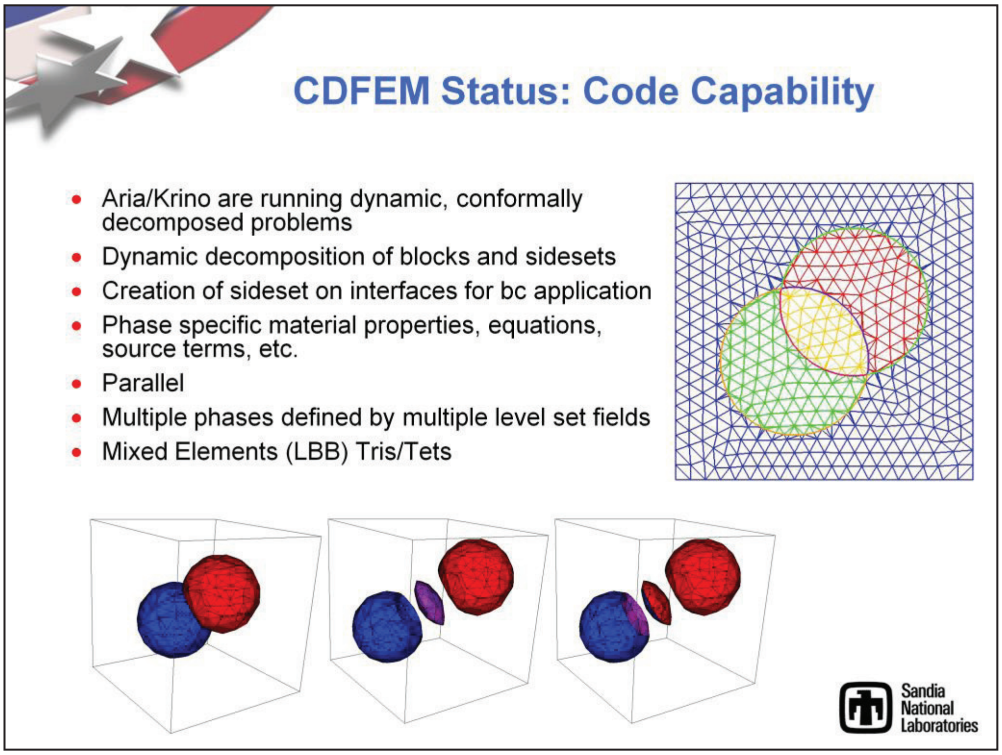
The wedges formed by the decomposition must be further broken into tetrahedra. Based on the earlier findings in 2-D we would seek to split the largest angles. Unfortunately, it is not always possible to accommodate this face-based criterion. This is because the face diagonals can form a Schonhard's polyhedron, which cannot be decomposed into tetrahedra with adding additional nodes, or Steiner points. The current algorithm therefore consists of cutting largest angle of interfacial faces, and a node-based algorithm for other faces. This is guaranteed to be decomposable into tetrahedra.

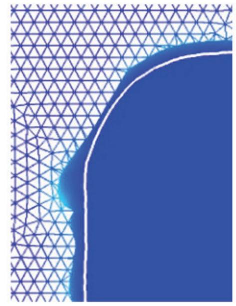


The conformal decomposition algorithms are implemented in the Sierra code krino. Aria assembles the equations on the decomposed elements just as if they came from a boundary fitted mesh generated by the user. The decomposed elements are placed in element blocks of common material. Sidesets are generated along block-block boundaries. Separate material specifications can be associated with each element block. The capability is implemented in parallel. The level set approach scales to any number of materials (or phases) including intersections of level set domains. While not tested extensively, mixed elements are also supported for LBB elements (i.e. piecewise linear pressure, quadratic velocity).

CDFEM Usage: Material Specification

- Just like conformal blocks:

```
BEGIN Aria Material Aluminum # Units in mks
   Density              = Constant Rho = 2700. # kg/m^3
   Specific Heat        = user_function name = Cp_Al \$
                          x = temperature      # J/kg-K
   Heat Conduction      = Fouriers_Law
   Thermal Conductivity = Constant K = 250.     # J/m-s-K
END
BEGIN Aria Material Air # Units in mks
   Density              = Constant Rho = 1.    # kg/m^3
   Specific Heat        = Constant Cp = 1000.  # J/kg-K
   Heat Conduction      = Fouriers_Law
   Thermal Conductivity = Constant K = 0.03     # J/m-s-K
END
BEGIN Aria Material Air_Aluminum_interface # Units in mks
   emissivity = constant E = 0.3
END
```



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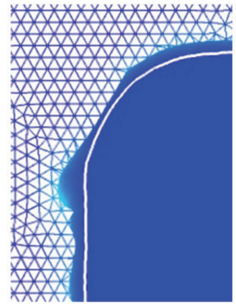
The material specification in CDFEM simulations is no different than in static geometry simulations. Separate material properties can be specified for each of the materials present in the problem.

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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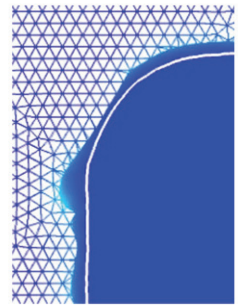
The term “phase” is used in CDFEM to specify a subdomain of one or more blocks that share a common identity. The specification of the phases is done through the “Finite Element Model”. Each phase is defined in terms of the level set field(s). In this example we define two phases, “Air” and “Aluminum” each of which is associated with opposite sides of the level set interface, LS. With these phases specified, each element block in the database can be subdivided into phase-specific blocks. The portion of block_1 that is in phase Air is denoted “block_1_Air”. Each of these phase specific blocks are then associated with a material block just as they are for static element blocks.

Along phase boundaries, sidesets are generated (called “surface” in Sierra). Two such surfaces are generated along the interface between Aluminum and Air. Both are one-sided sidesets, because they only touch elements of one of the phases. The sideset, “surface_block_1_Aluminum_Air” is generated on each of the sides of the elements in “block_1_Aluminum” that border the interface. Similarly, the sideset, “surface_block_1_Air_Aluminum” is generated on each of the sides of the elements in “block_1_Air” that border the interface. This is done so that the user can specify boundary conditions that apply to just one of the materials.

CDFEM Usage: Level Set Specification

- Level set equation system



```
BEGIN LEVEL SET INTERFACE LS
  Distance Variable = solution->LEVEL_SET
   BEGIN ANALYTIC INITIAL CONDITION my_ic
      Facets format = EXO filename = 2d_IC_facets.g
   END
END

BEGIN Equation System level_set
   Use Linear Solver gmres
   Nonlinear Solution Strategy = Newton
   Maximum Nonlinear Iterations = 10
   Nonlinear Residual Ratio Tolerance = 1.0e-6

   EQ Level_Set for Level_Set ON block_1          using Q1 WITH XFER
   EQ Level_Set for Level_Set ON block_1_Air      using Q1 WITH MASS ADV SUPG
   EQ Level_Set for Level_Set ON block_1_Aluminum using Q1 WITH MASS ADV SUPG

   EQ Momentum for Velocity on block_1_Air      using Q1 with XFER
   EQ Momentum for Velocity on block_1_Aluminum using Q1 with XFER
END
```

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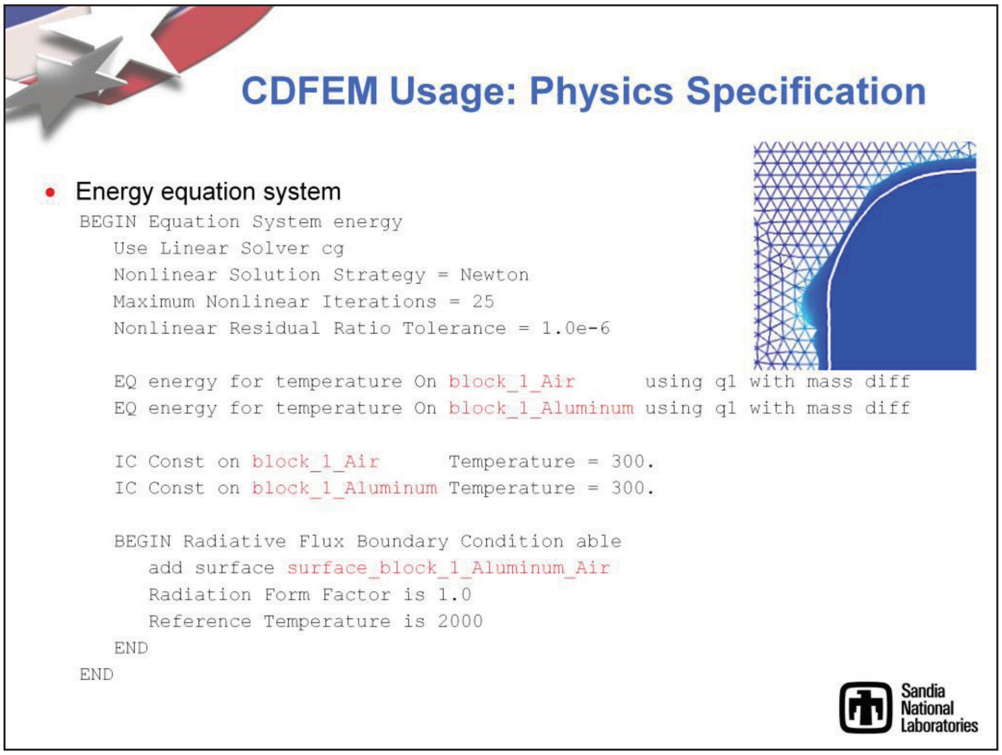
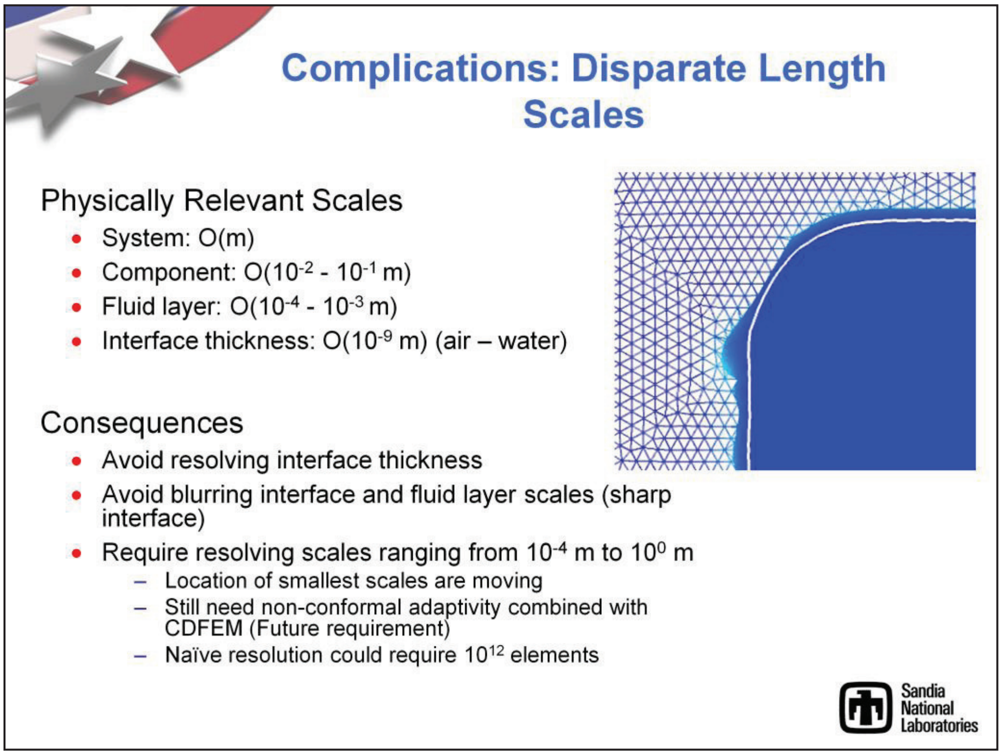
The level set interface, "LS", used in the phase specification, is defined with a short block that gives the level set variable name and optionally allows the specification of initial conditions on this field. Here, a set of facets, generated by Cubit, are used to compute the signed distance.

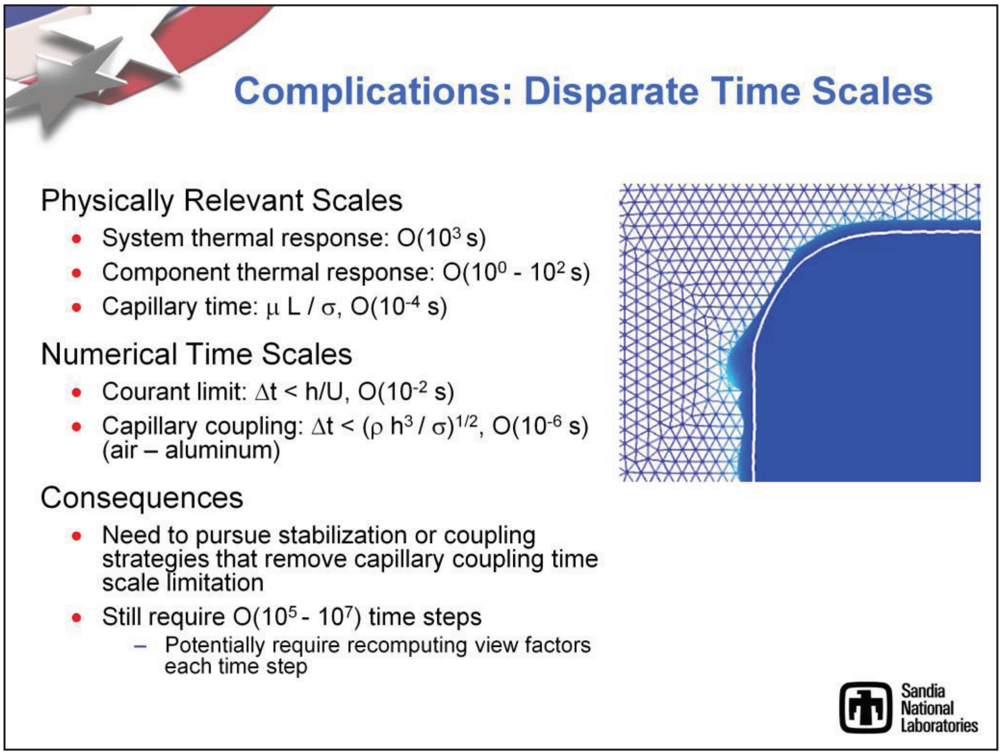
As described earlier, the level set field evolves according to an advection equation with mass, advection, and stabilization terms.



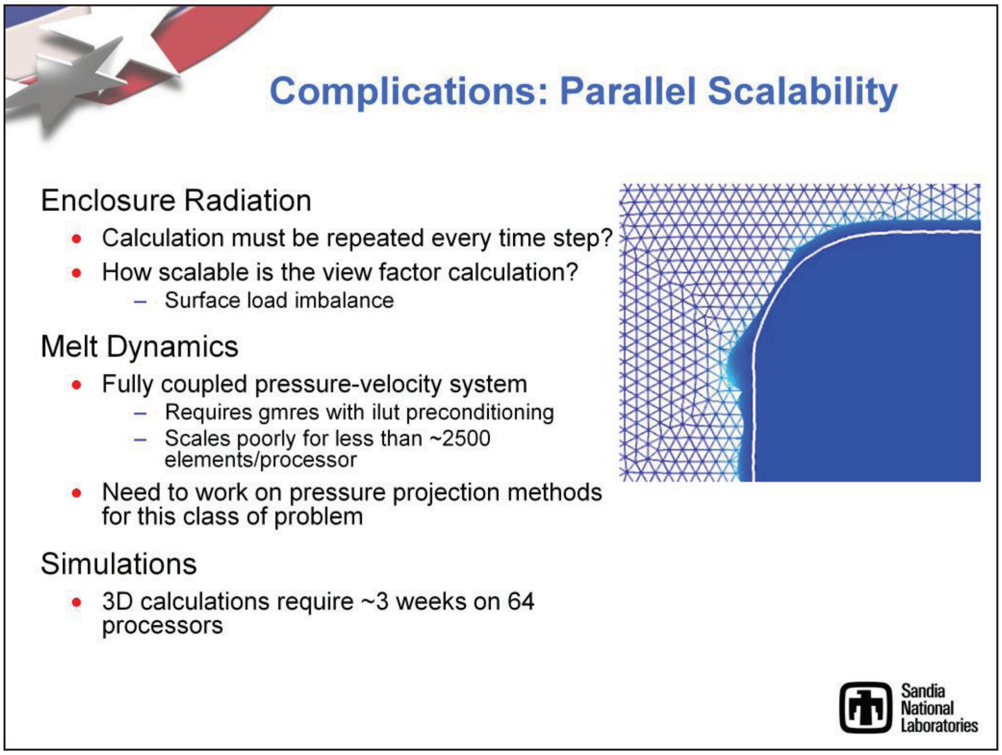
The specification of the physics is basically identical to that used in static geometry simulations. Just the names of the element blocks and surfaces are modified to refer to the phase-specific blocks and interfaces.



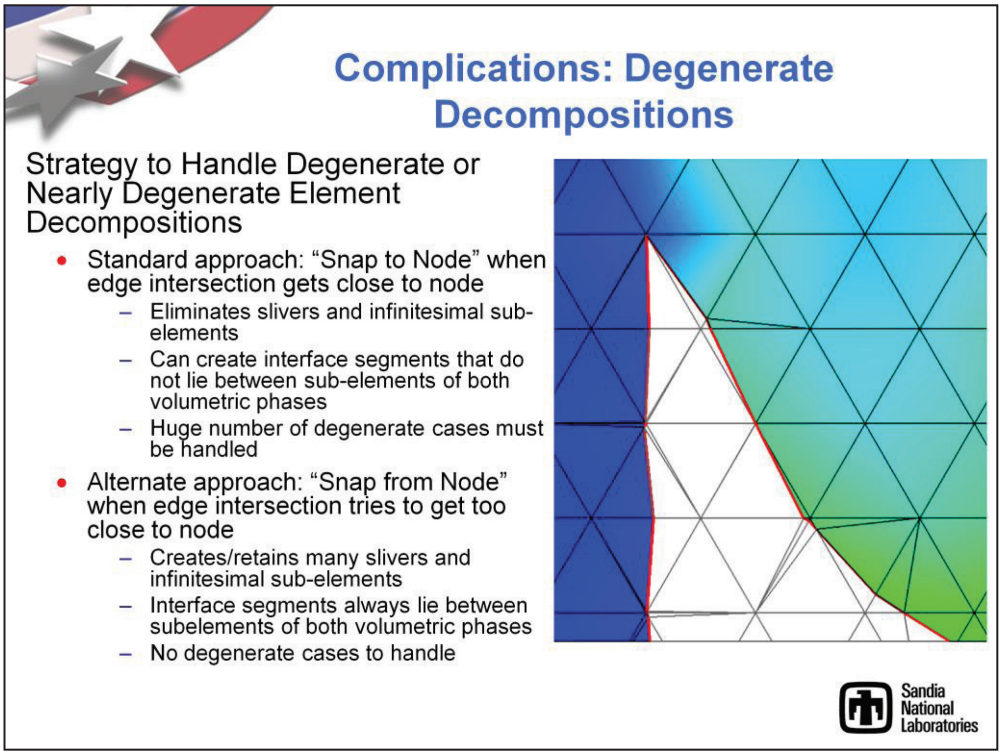
Simulations of melting and flow are considerably more complicated than static geometry ones. One of these complications is related to the disparate length scales introduced. Resolving physics on the interfacial scale is clearly prohibitive. Even when employing a sharp interface method, the thin fluid layer introduces scales much smaller than the features of the melting part. Since this layer is moving, we cannot provide adequate mesh resolution a priori. Instead future capability should allow a combination of non-conformal adaptivity and conformal decomposition. Currently, conformal decomposition cannot be combined with adaptivity.



Similar issues arise from the disparate time scales introduced in melting and flowing. The capillary time scale is many orders of magnitude shorter than the time scale of thermal response. Stability requires resolving this time scale, however. Mesh based scales like the Courant condition also can dramatically increase the number of time steps needed. Since the geometry is changing, the viewfactors must be recomputed which is expensive. Strategies that soften or eliminate stability restrictions are highly desirable to make melting and flow simulations tractable.

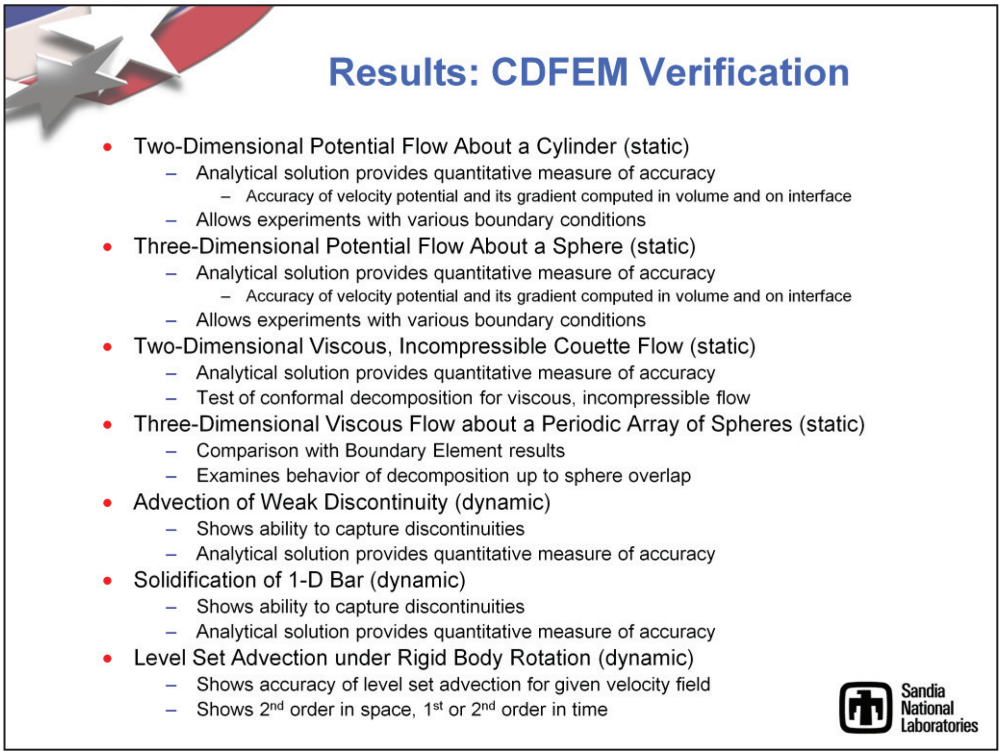


With the high cost of melting and flow simulations, we seek to use massively parallel machines to provide reasonable turn-around. But parallel scalability for this class of problems can be poor. Does enclosure radiation scale well with increased parallel processors, especially when the surfaces are located on a subset of the processors? Fully coupled pressure-velocity PSPG systems can be poorly conditioned requiring solvers and preconditions that scale poorly. Future work needs to examine pressure projection and splitting methods that reduce cost while maintaining accuracy and stability.



A complication that arises in CDFEM simulations relates to the way that degenerate or nearly degenerate decompositions are handled. Most published methods advocate removing slivers and infinitesimal elements by snapping the interface to the nearby node or edge. A huge number of degenerate and even pathological cases, however, can be generated using this strategy.

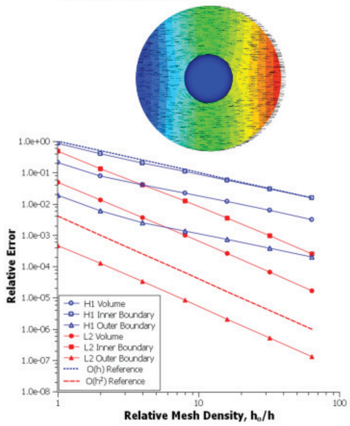
The simulations presented here use an alternate strategy that keeps the interface from getting too close to the nodes. This eliminates the degenerate cases. Both strategies can have undesirable consequences, however, in capillary hydrodynamics, which is highly sensitive to the interface curvature.



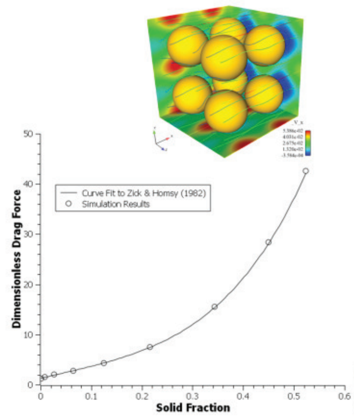
Extensive work has been done to verify the current CDFEM capability and level set advection.

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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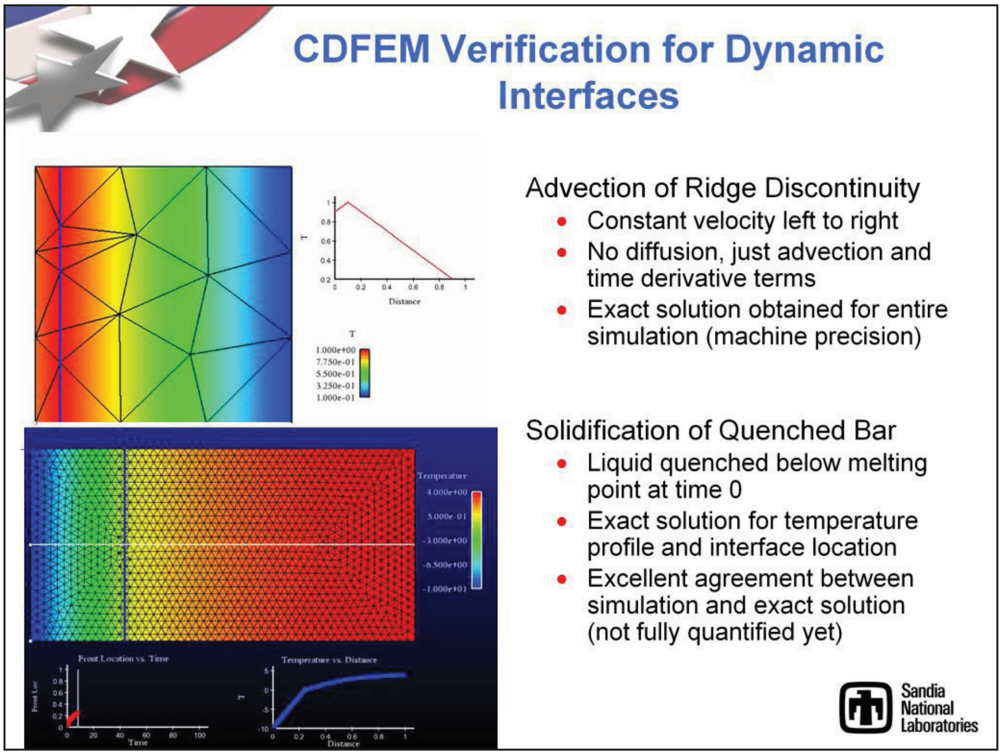
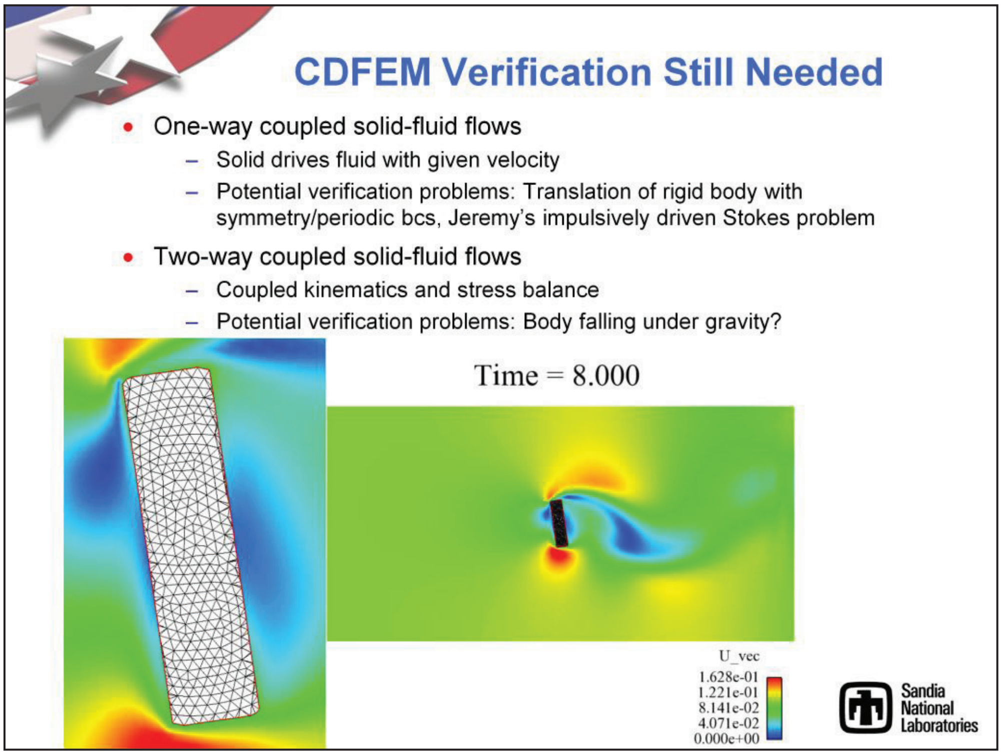
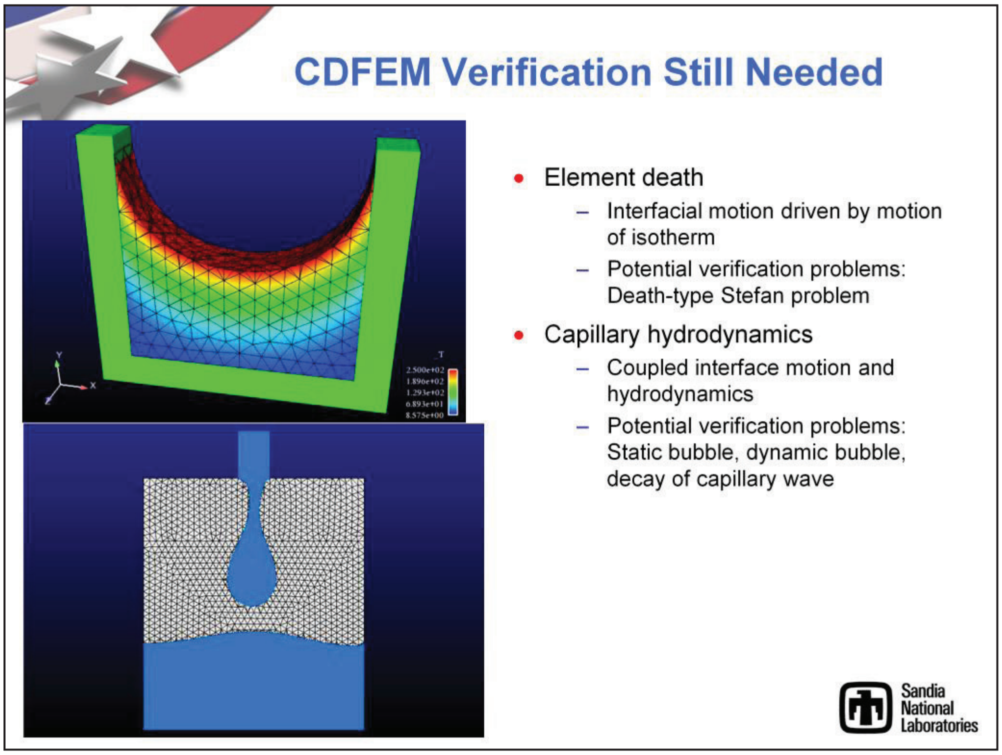
Two examples of static CDFEM verification.



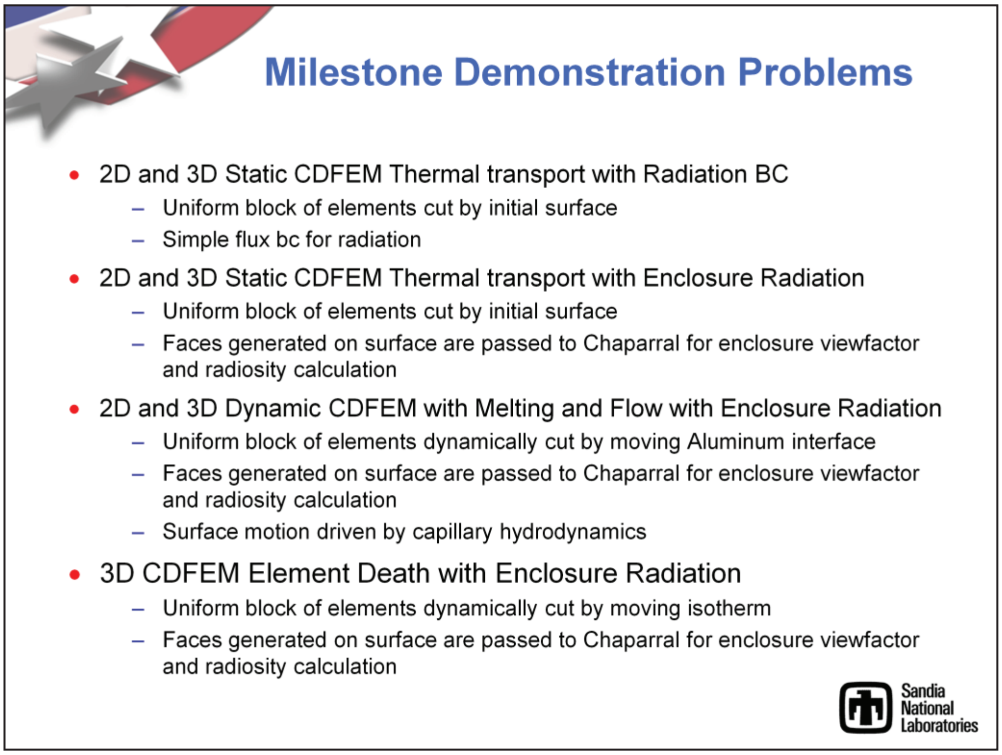
Two examples of transient CDFEM verification. The quantification of the accuracy of the bar solidification has not been completed.



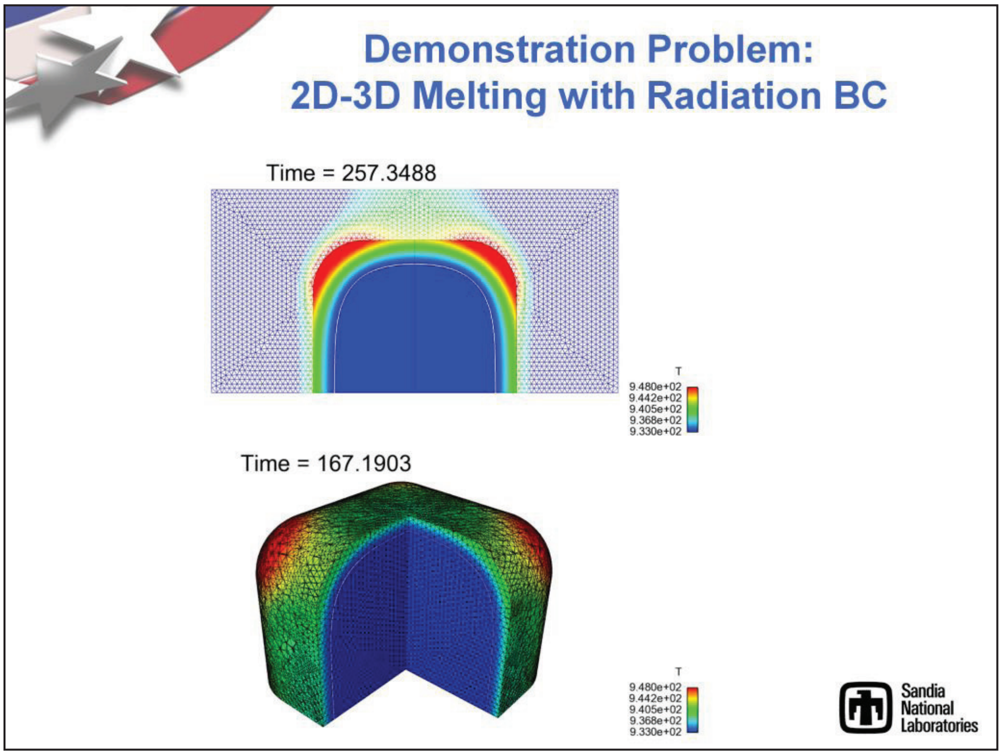
One aspect of CDFEM that has not been fully verified yet is solid-liquid flows.



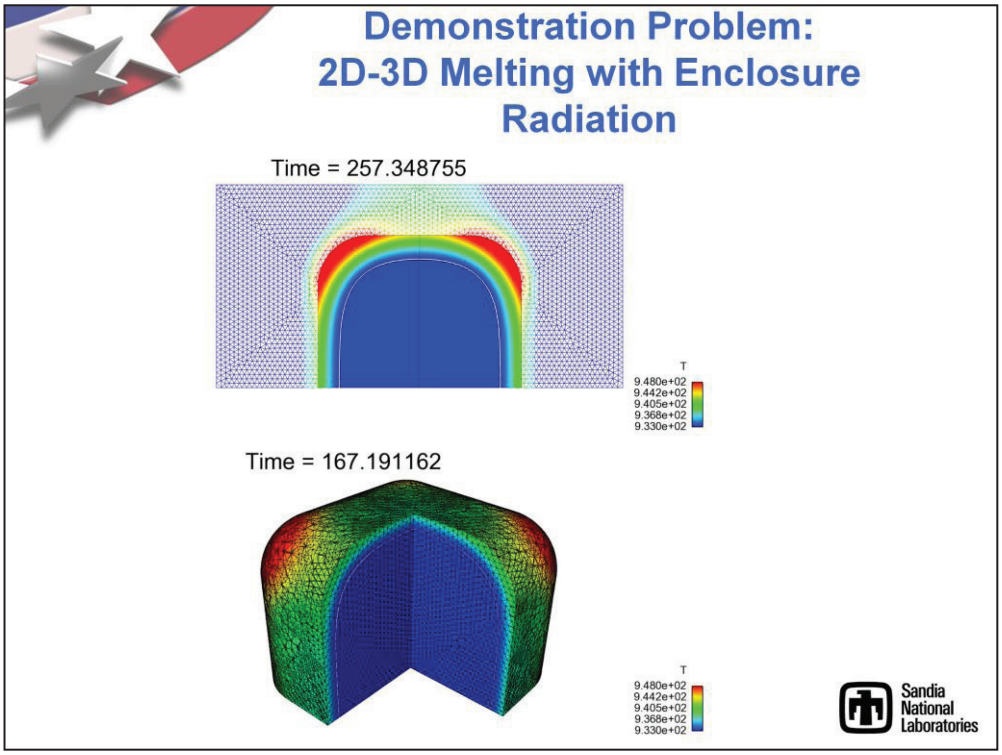
Other dynamic interface applications that have not been verified yet.



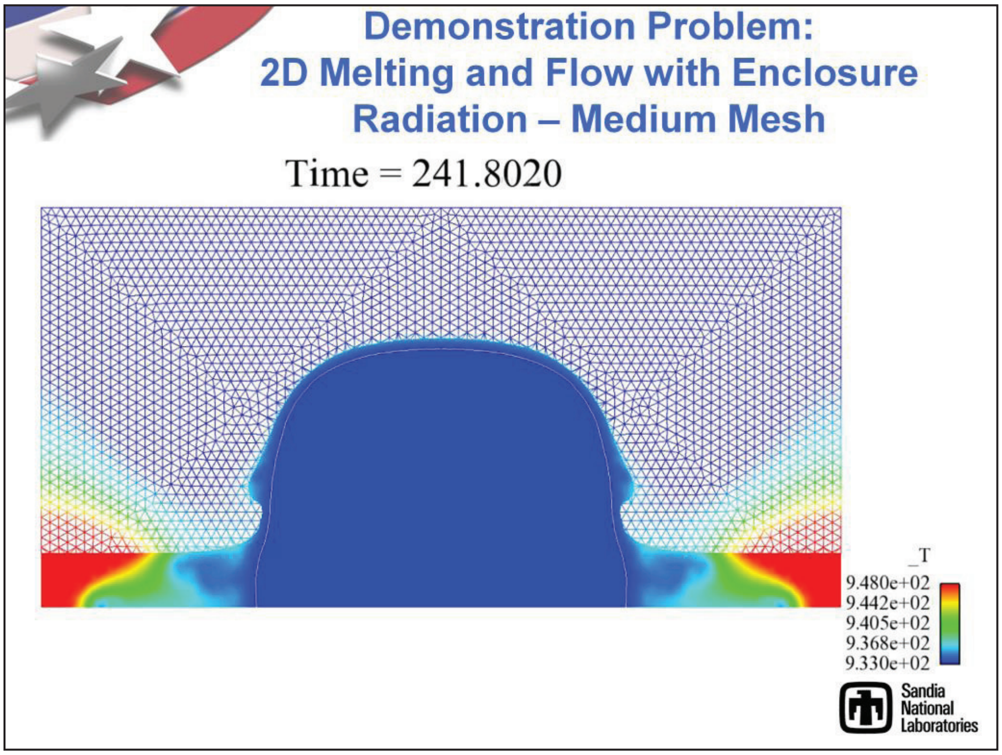
2-D and 3-D simulations of melting with or without flow and with radiation BC's or enclosure radiation were performed.



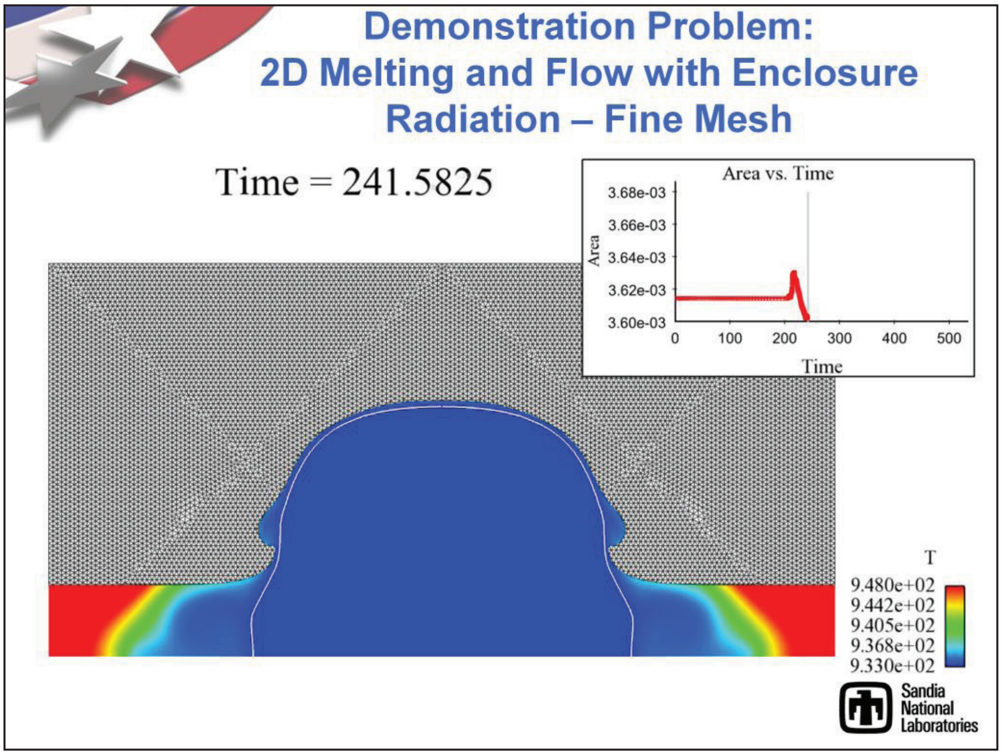
Demonstration of melting without flow due to a radiation BC. Block is 10cm across. The process of 3-D melting is faster for the same dimensions due to the increased surface to volume ratio.



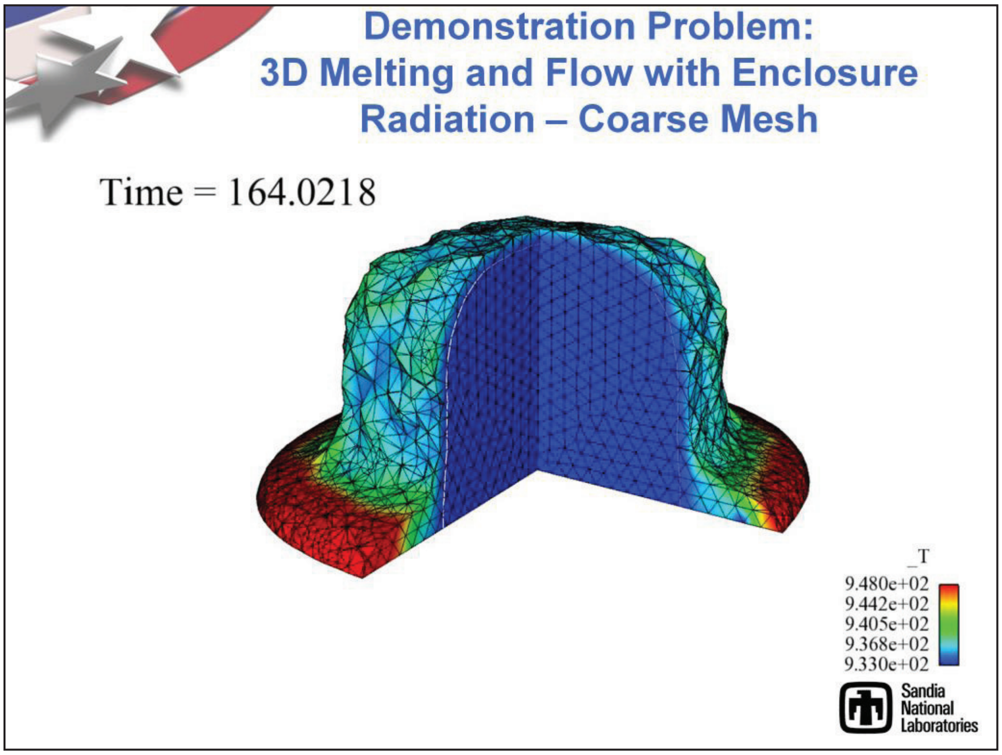
Demonstration of melting without flow due to a hot partial enclosure.



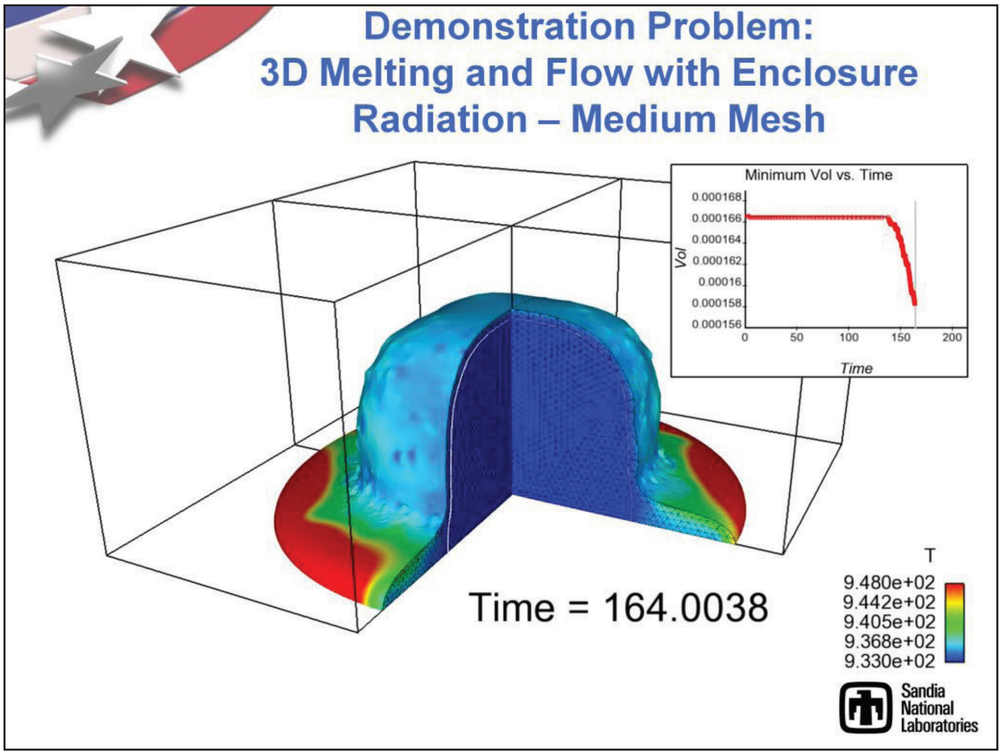
2-D simulation of melting and flow on medium mesh.



2-D simulation of melting and flow on fine mesh.



3-D simulation of melting and flow on coarse mesh.



3-D simulation of melting and flow on medium mesh. This simulation ran for over 2 weeks and only simulated a portion of the melting process.

Summary and Future Work

- CDFEM is Accurate for Static Interface Problems
  - Multiple verification tests performed
- CDFEM is Robust for Static/Dynamic Interface Problems
  - Runs for weeks handling 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 CDFEM for element death
  - 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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Supporting Material

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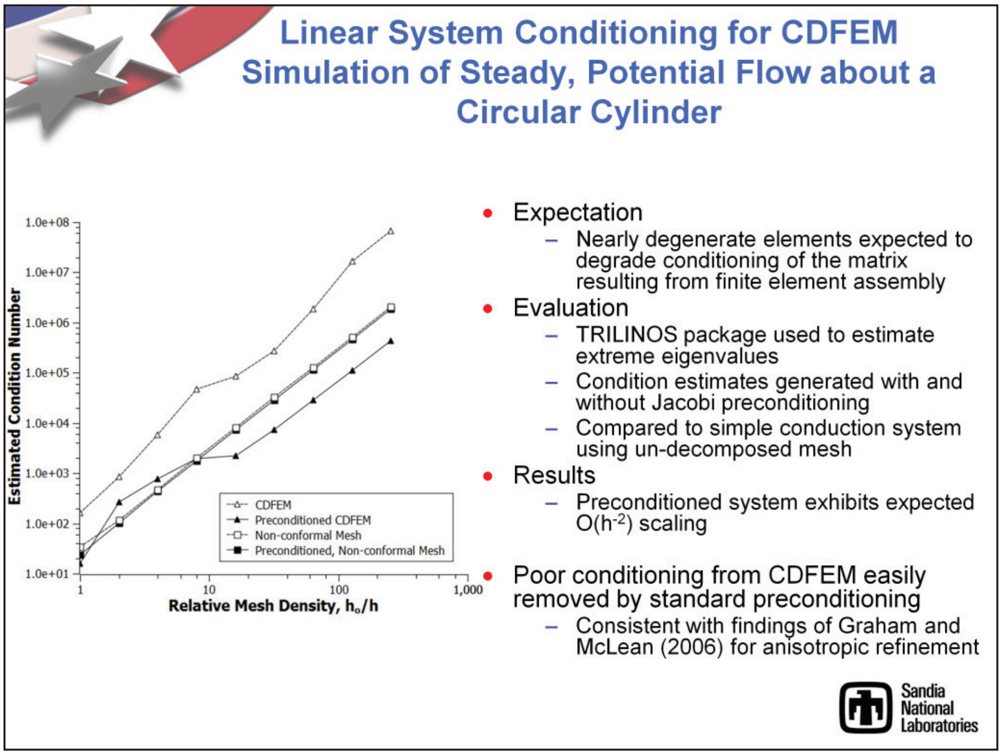

One concern raised by reviewers of CDFEM involves the conditioning of the resulting linear systems. This was explored for static CDFEM decompositions. Without preconditioning, the CDFEM system of equations showed significant growth in the condition number due to the nearly degenerate nodes. However, simple preconditioning removed this poor conditioning. This result is consistent with published results for anisotropic, non-conformal adaptivity where a similar issue arises.

XFEM Requirements Comparison for Thermal/Fluids and Solids

	Thermal/Fluids	Solids
Volume Assembly	Conformal subelement integration, specialized element loops to use modified integration rules	Single point integration regardless of enrichment
Surface Flux Assembly	Specialized volume element loops with specialized quadrature	Not normally required, single point integration when needed
Phase Specific DOFs and Equations	Different variables present at different nodes of the same block	Block has homogenous dofs/equations
Enrichment Types	Requires Heaviside enrichment for Pressure, Ridge enrichment for Velocity and Temperature	Requires only Heaviside enrichment for Displacement
BC's Required on Interface	All types, Dirichlet, Neumann, Mixed, Enclosure radiation	Normally none required

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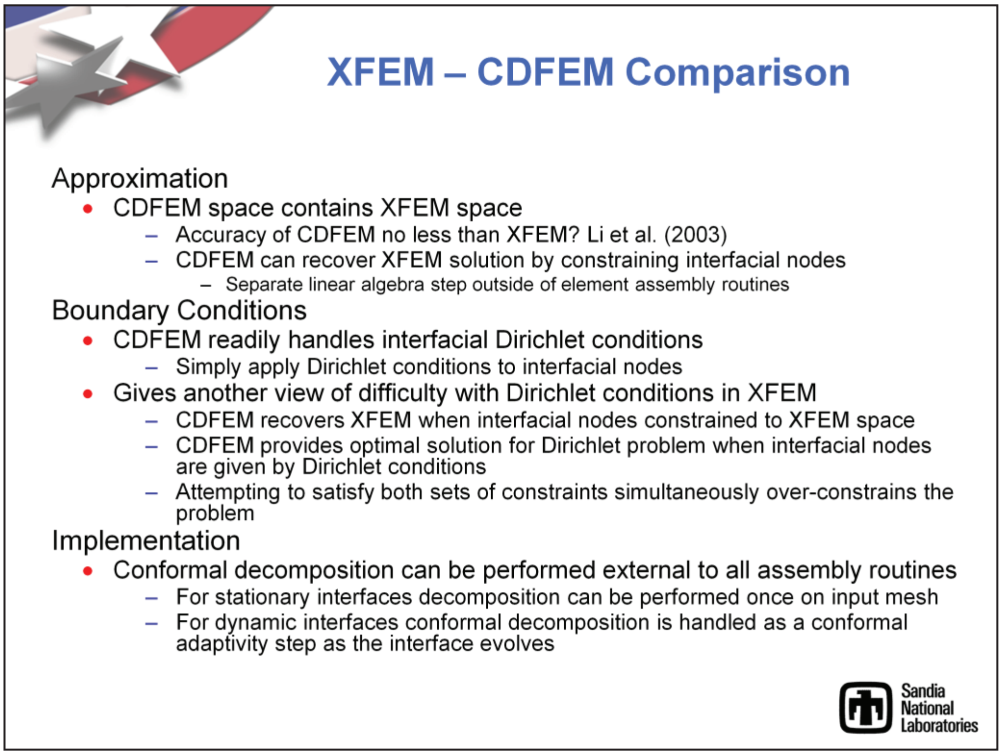
XFEM is being pursued in solid mechanics for dynamic interfaces. Here is a comparison of the requirements for thermal/fluids to those for solids when employing XFEM.



This is a theoretical comparison of XFEM and CDFEM.

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

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This is a comparison of the code requirements for XFEM and CDFEM for thermal/fluids applications.