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A Conformal Decomposition Method for Thermal-Fluid Transport Problems with Complex or Dynamic Topology

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ESRF Review
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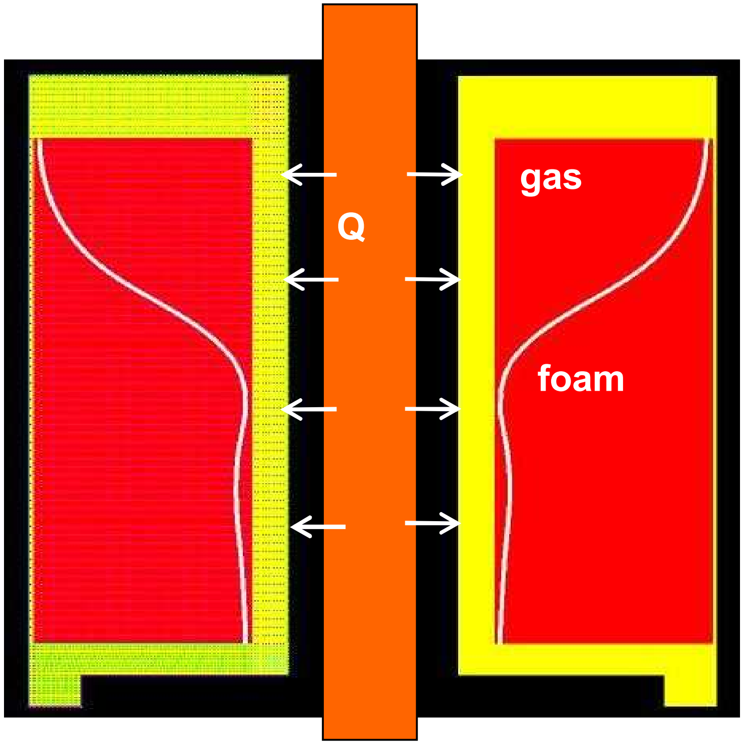
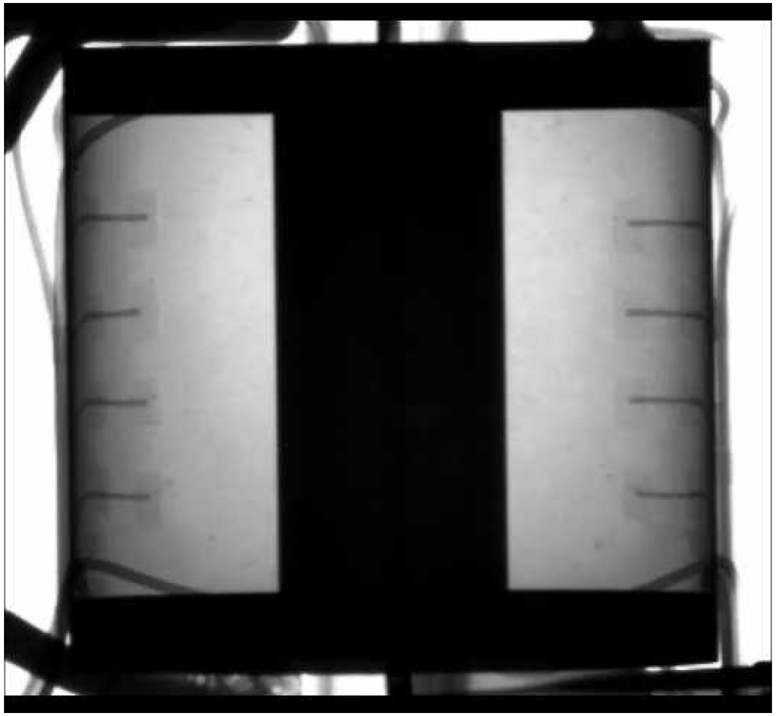
Motivation: Need for predictive capability for dynamic interfacial transport

Problems in the Assured Safety and Security Focus Areas are characterized by transport in domains with complex and/or dynamic topology.

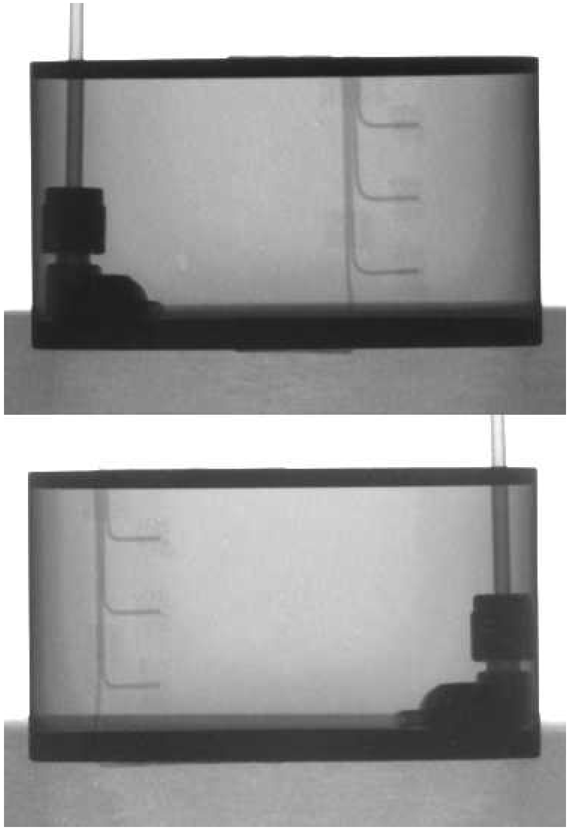
Example: Liquefaction in Foam Decomposition Complicates Pressurization Simulations

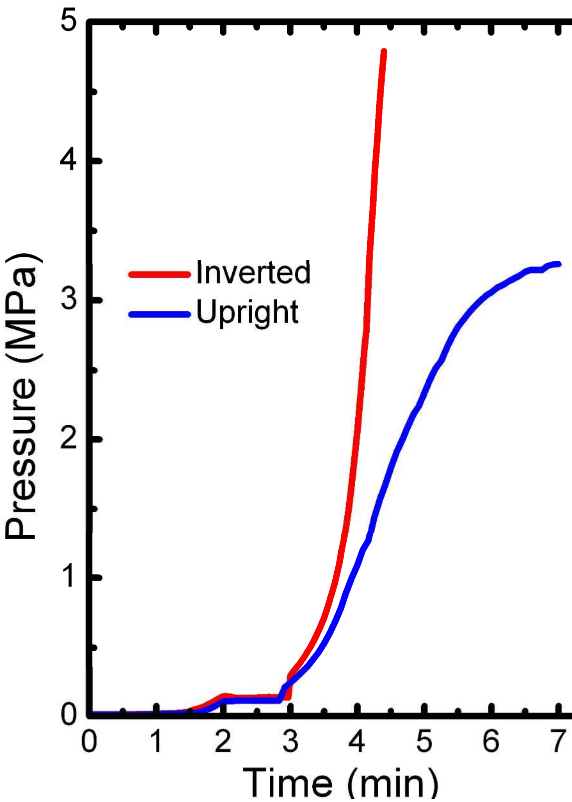




Motivation: Dynamic interfaces, cont'd

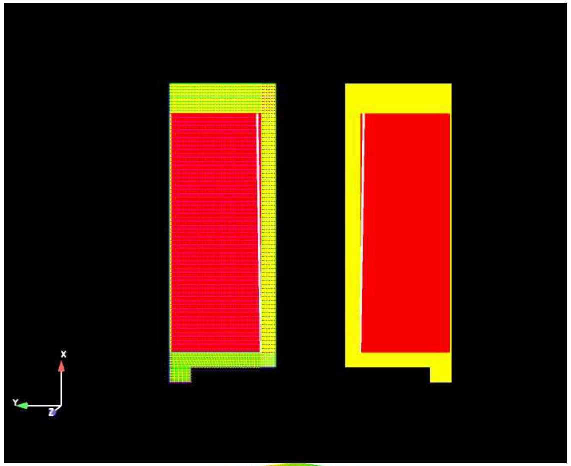
Dynamics Of Liquefaction Of Decomposing Foam Affects Pressurization



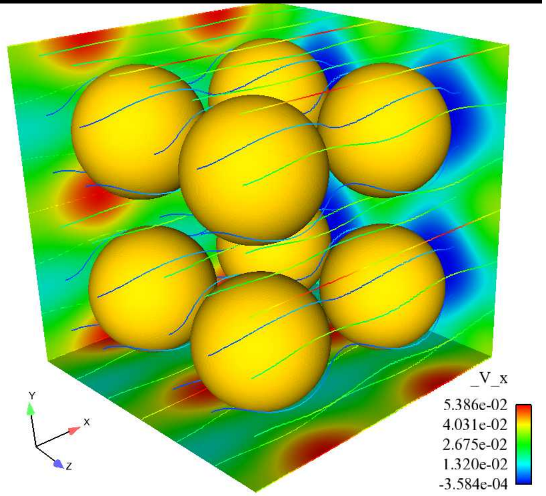


Motivation: Dynamic and complex interfacial transport

- **Problem Class: Dynamic Interface Problems**
  - **Typical application area for level set or VOF methods**
  - **Examples: multiphase flow and phase change problems like foam decomposition, aluminum relocation, and spilling fuels.**
  - **Benefits**
    - Difficult, if not impossible, to address using ALE



- **Problem Class: Topologically Complex, but Stationary Interfaces**
  - **A less obvious application area**
  - **Examples: conduction in composite materials, single phase flow in porous media**
  - **Benefits**
    - Avoid conformal mesh generation
    - Avoid contact between disparate meshes



Finite Element Methods for Interfaces in Fluid/Thermal Applications

- **Boundary Fitted Meshes**
  - Supports wide variety of interfacial conditions accurately
  - Requires boundary fitted mesh generation
  - Not feasible for arbitrary topological evolution (ALE)
    - Mesh quality degrades with evolution, phase breakup and merging are precluded.
- **eXtended Finite Element Methods (XFEM)**
  - Dolbow et al. (2000), Belytchko et al. (2001)
  - Successfully applied to numerous problems ranging from crack propagation to phase change to multiphase flow
  - Supports weak conditions accurately, mixed and Dirichlet conditions are actively researched (Dolbow et al.)
  - Avoids boundary fitted mesh generation
  - Supports general topological evolution (subject to resolution requirements)
- **Generalized Finite Element Methods (GFEM)**
  - Strouboulis et al. (2000)
  - Combination of standard finite element and partition of unity enrichment
- **Immersed Finite Element Methods**
  - Li et al. (2003)
  - Supports selected jumps across material boundaries (discontinuous gradient or value)

- **Conformal Decomposition Finite Element Method (CDFEM)**
  - **Enrichment by adding nodes along interfaces**

Level Sets in Finite Elements: Extended Finite Element Method

- **Extended Finite Element: Finite Element Method for Embedded Interfacial Jumps**
  - **Dolbow et al (2000)**
- **Enrich elements containing discontinuities**
  - **Add extra degrees of freedom, a_i**

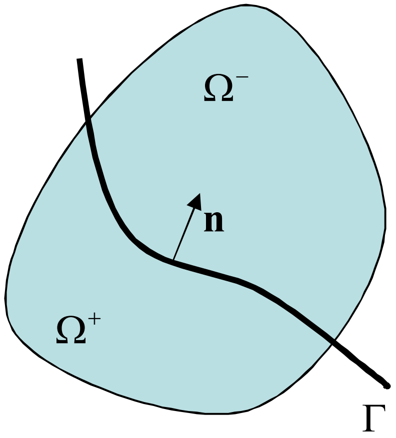
$$T = \sum_i N_i T_i + \sum_i N_i g_i a_i$$

  - **Basis functions for extended dofs have two parts**
  - **Standard continuous variation within element, N_i**
  - **Discontinuous extending function, g_i**
  - **Typical form for discontinuous value**

$$g_i(x) = H(\phi(x)) - H(\phi_i), \quad \phi_i \equiv \phi(x_i)$$

  - **Typical form for discontinuous gradient**

$$g_i(x) = |\phi(x)| - |\phi_i|$$



Extended Finite Element Method

- **Features**
  - **Enforces continuity across element faces**
    - Enrichment is nodal
  - **Element contributions are discontinuous**

    Element contribution to residual

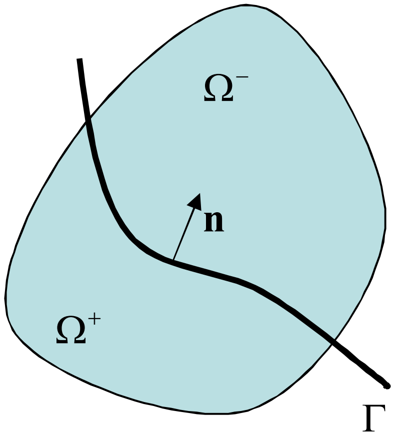
$$R_i = -\int_{\Omega} \nabla N_i \cdot k \nabla T \, d\Omega$$

becomes

$$R_i = -\int_{\Omega^-} \nabla N_i \cdot k \nabla T \, d\Omega - \int_{\Omega^+} \nabla N_i \cdot k \nabla T \, d\Omega$$

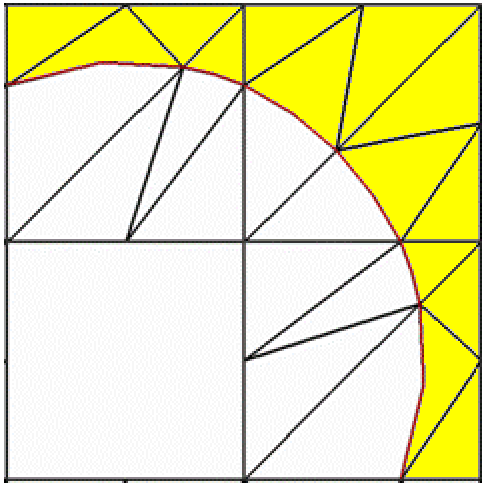
$$-\int_{\Gamma} N_i^+ \mathbf{n} \cdot \mathbf{Q}^+ \, d\Omega + \int_{\Gamma} N_i^- \mathbf{n} \cdot \mathbf{Q}^- \, d\Omega$$

- Weight functions are discontinuous
- Gradients are discontinuous
- Requires conformal integration



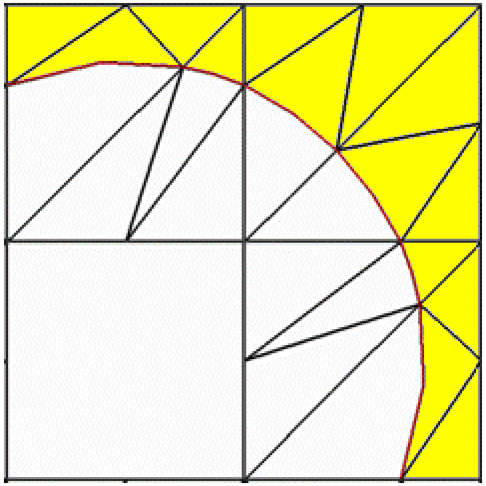
Extended Finite Element Method – Implementation in production codes

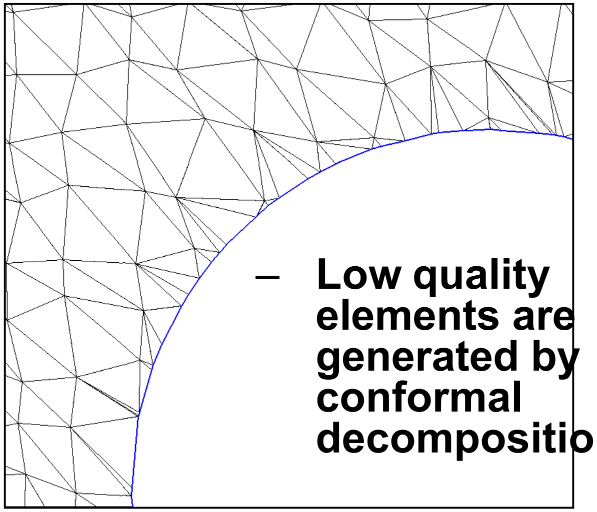
- **Code Requirements (for fully integrated elements)**
  - **Conformal integration**
    - Integration conforms to phases present in element
    - Varying number of integration points depending on phase distribution
  - **Enriched Basis**
    - Active degrees of freedom (dofs) depend on phase distribution
    - Varying numbers of dofs at nodes
    - Subset of dofs active at each integration point
  - **Boundary conditions**
    - Dirichlet BC's are problematic (research area)
    - Interfacial flux conditions are a new class of boundary conditions (part volume, part bc)
  - **General**
    - Increasingly complicated for multiple phases (beyond 2)
    - Must be implemented at element assembly level



Beyond XFEM: Conformal Decomposition Finite Element Methods (CDFEM)

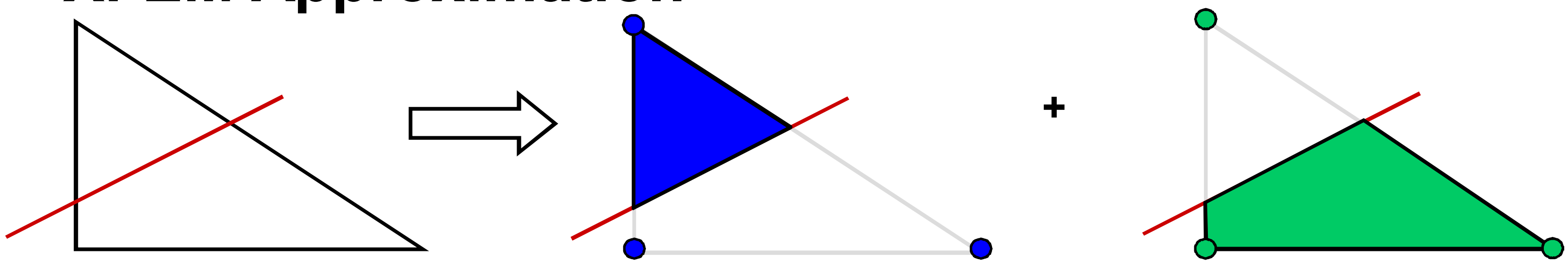
- **Simple Concept**
  - **Decompose non-conformal elements into conformal ones**
  - **Obtain solution on conformal elements**
- **Related Work**
  - **Li et al. (2003) FEMCGAN: FEM on Cartesian Grid with Added Nodes**
    - Focus on Cartesian Grid. Considered undesirable because it lost original matrix structure.
- **Properties**
  - **Supports wide variety of interfacial conditions accurately (identical to boundary fitted mesh)**
  - **Avoids boundary fitted mesh generation**
  - **Supports general topological evolution (subject to resolution requirements)**
  - **Requires modified matrix structure (additional elements)**
    - Similar to finite element adaptivity
  - **Uses standard finite element assembly including data structures, interpolation, and quadrature**
- **Questions**
  - **Accuracy? Conformal elements can have vanishing quality.**
  - **Relationship to XFEM?**



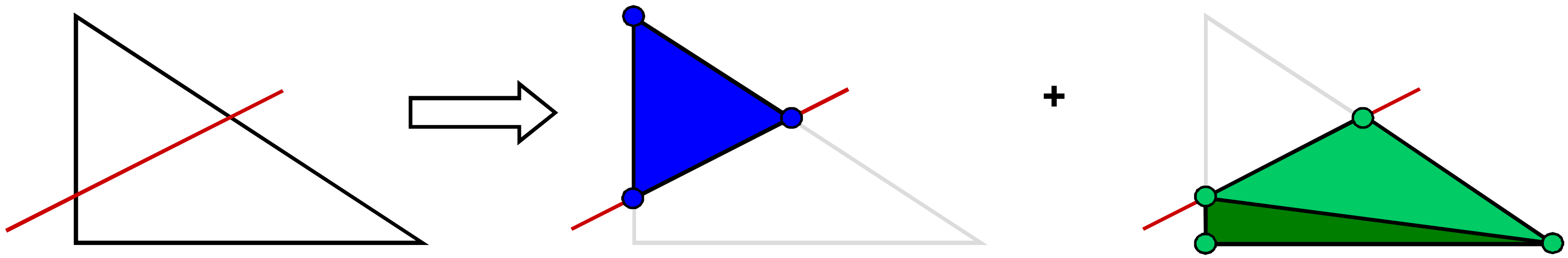


XFEM – CDFEM Comparison

- **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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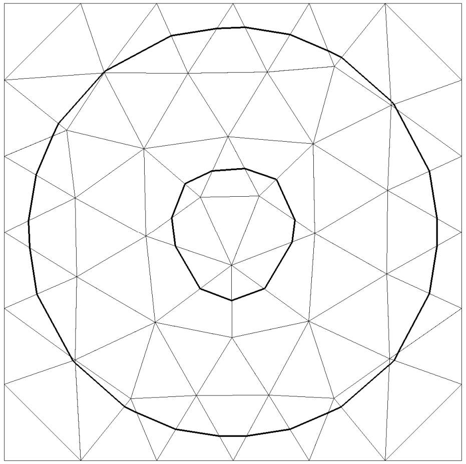
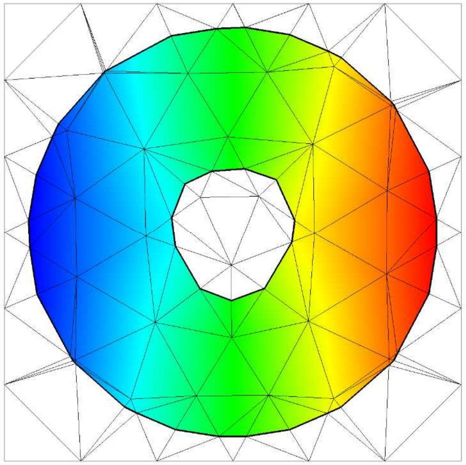
XFEM – CDFEM Comparison, cont'd

- **Approximation**
  - **CDFEM space contains XFEM space**
    - Accuracy of CDFEM no less than XFEM? Li et al. (2003)
    - 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 the decomposition can be performed once on the input mesh

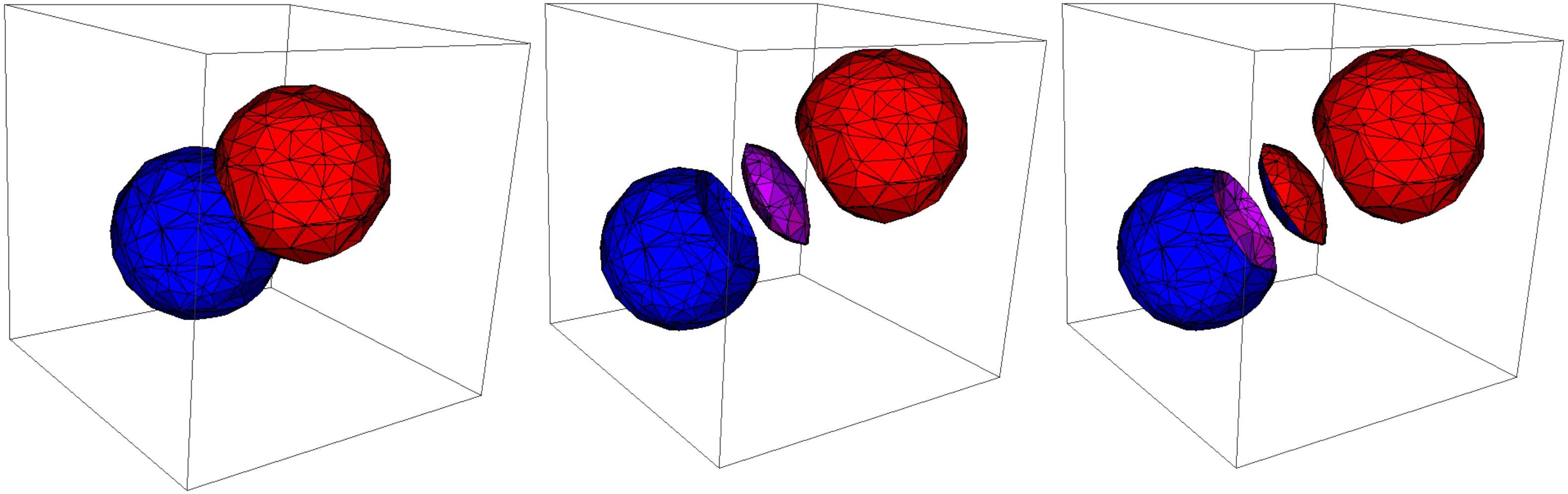
CDFEM Implementation

- **For Steady State Problems**
  - **Stationary Interfaces**
    - Conformal decomposition can be performed once
    - Provides test of accuracy, performance, and implementation
- **For Transient Problems**
  - **Must perform decomposition based on current interface location**
    - Level set provides convenient description
  - **Similar requirements to adaptive refinement**
    - Dynamic data structures, matrix graph
    - Prolongation of solution to new nodes
  - **Transparent to physics code (Element assembly)**





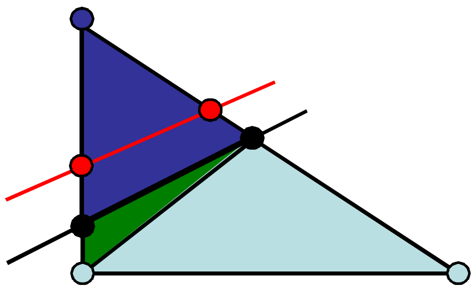
Multiphase CDFEM Status



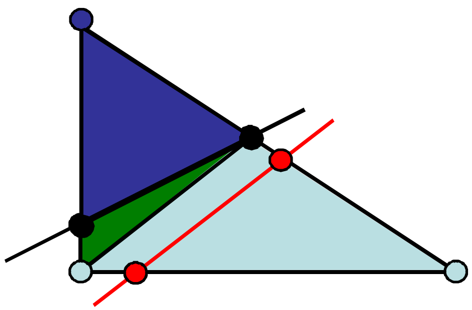
- **Aria/Krino able to run conformally decomposed problems**
  - Static decomposition of blocks and sidesets
  - Creation of sideset on interface for bc application
  - Phase specific material properties, equations, source terms, etc.
  - Parallel
  - Multiple phases defined by multiple level set fields
  - Mixed Elements (LBB) Tris/Tets
- **TODO**
  - Dynamic decompositions
  - Combined h-adaptivity – CDFEM
  - Condensation support for recovering XFEM

Moving CDFEM Goals

- **How do we handle the moving interface?**



- **What do we do when nodes change sign?**



- **Goals**
  - Try to recover moving mesh case for moving interface
  - Try to preserve minima, maxima
- **Proposal**
  - Prolongation: Set “old” value to value of nearest point on interface
  - Dynamics: Use ALE style (u-dxdt) for advection term

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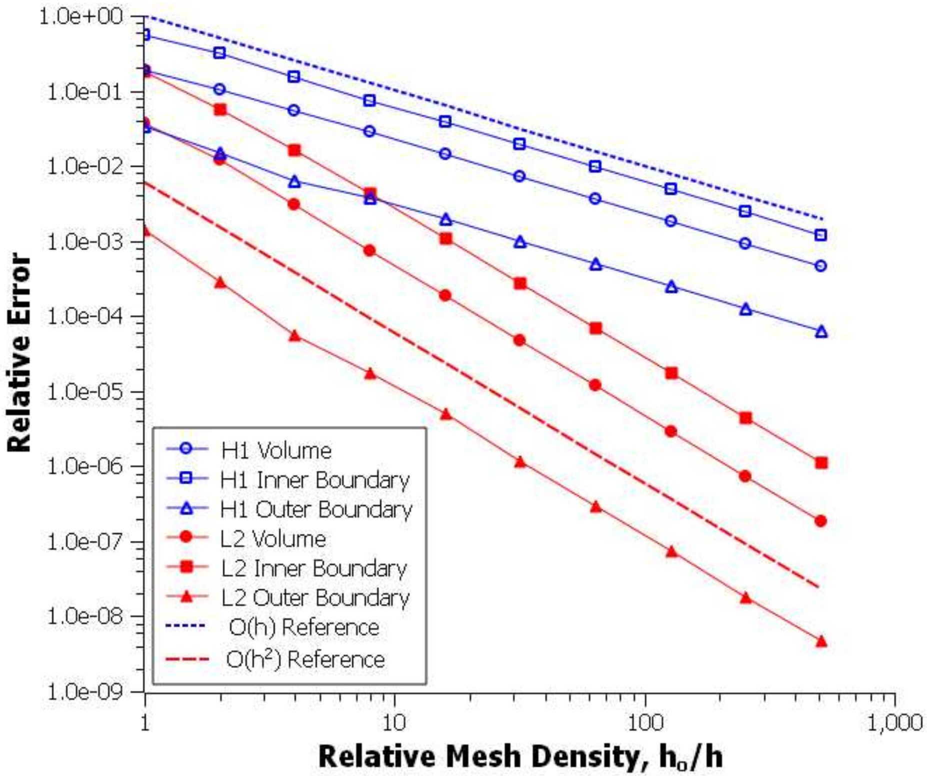
CDFEM Verification

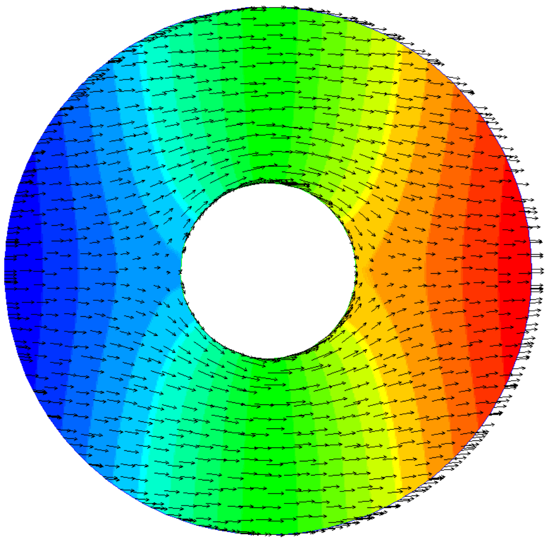
- **Two-Dimensional Potential Flow About a Cylinder (static)**
  - Analytical solution provides quantitative measure of accuracy
    - Accuracy of velocity potential and its gradient computed in volume and on interface
  - Allows experiments with various boundary conditions
- **Three-Dimensional Potential Flow About a Sphere (static)**
- **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

Results documented with journal article: Noble, Newren, Lechman, “A Conformal Decomposition Finite Element Method for Modeling Stationary Fluid Interface Problems”, International Journal for Numerical Methods in Fluids (accepted, 2009)

CDFEM Simulation of Steady, Potential Flow about a Circular Cylinder

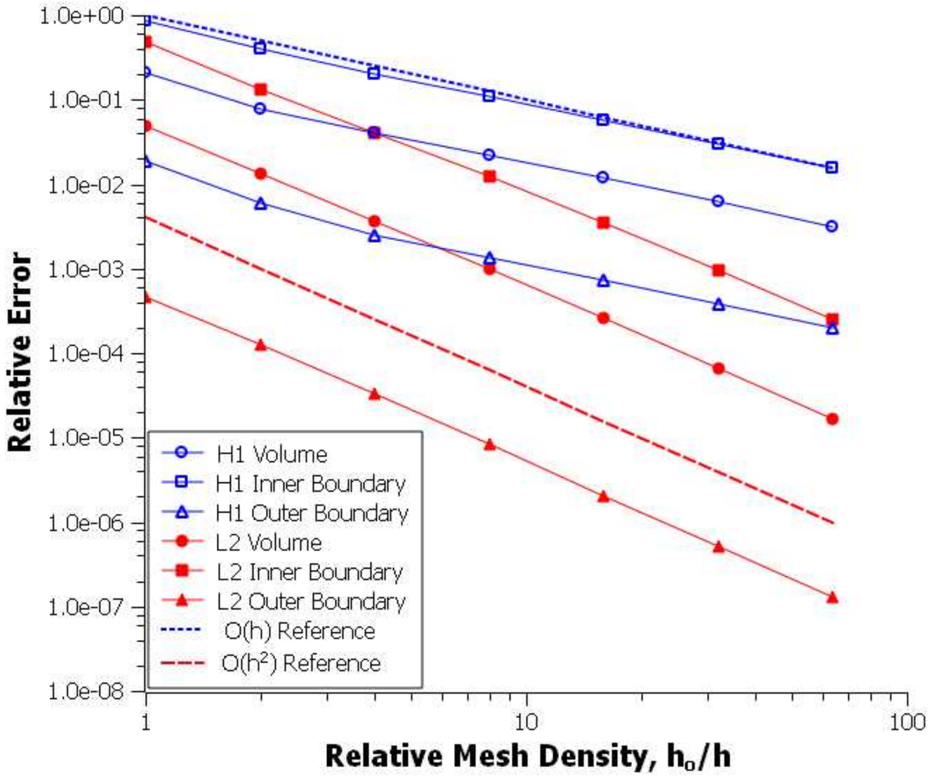
- Embedded curved boundaries
- Dirichlet BC on outer surface, Natural BC on inner surface
- Optimal convergence rates for solution and gradient both on volume and boundaries

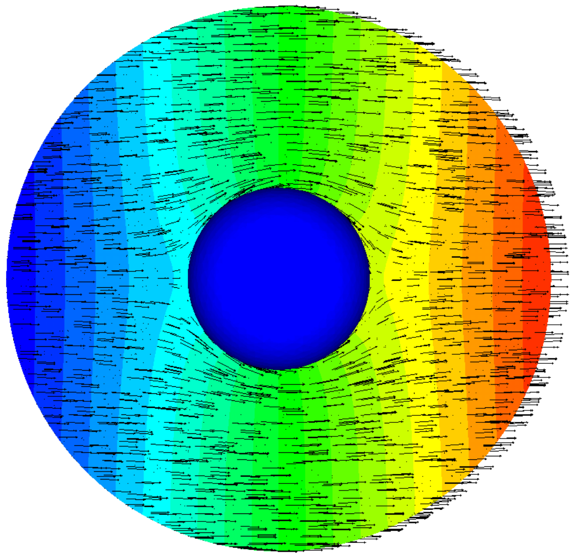




CDFEM Simulation of Steady, Potential Flow about a Sphere

- 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





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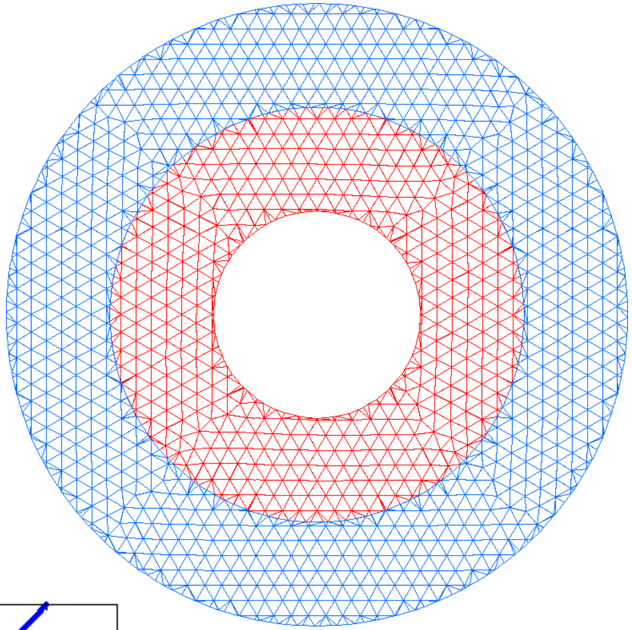
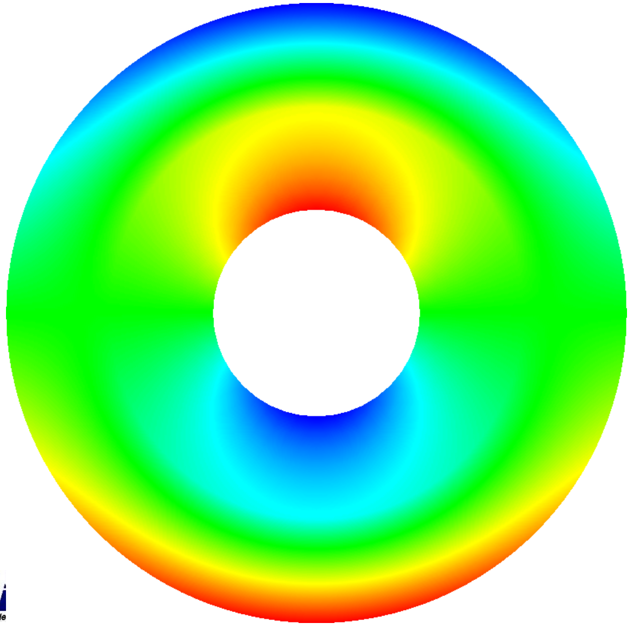
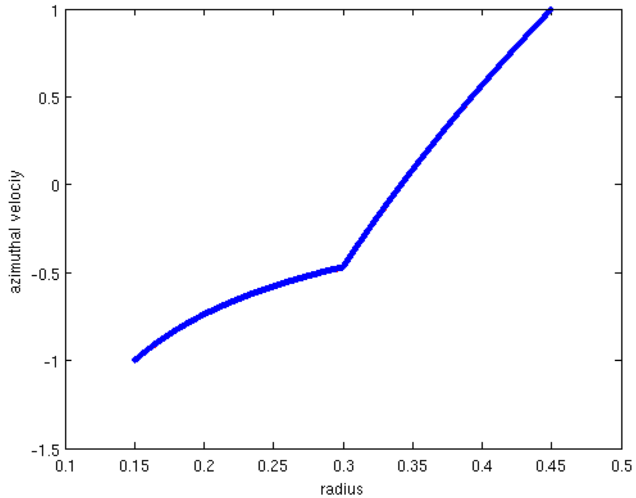
CDFEM Simulation of Steady, Fluid-Fluid Interface Problem: Couette Flow

- Two-Phase Flow between concentric cylinders
  - Counter-rotating cylinders
  - 4:1 viscosity ratio
  - No surface tension
- Dirichlet conditions on inner and outer surfaces, weak discontinuity along interface
- Cut regular, unstructured mesh along outer, inner, and interfacial radii

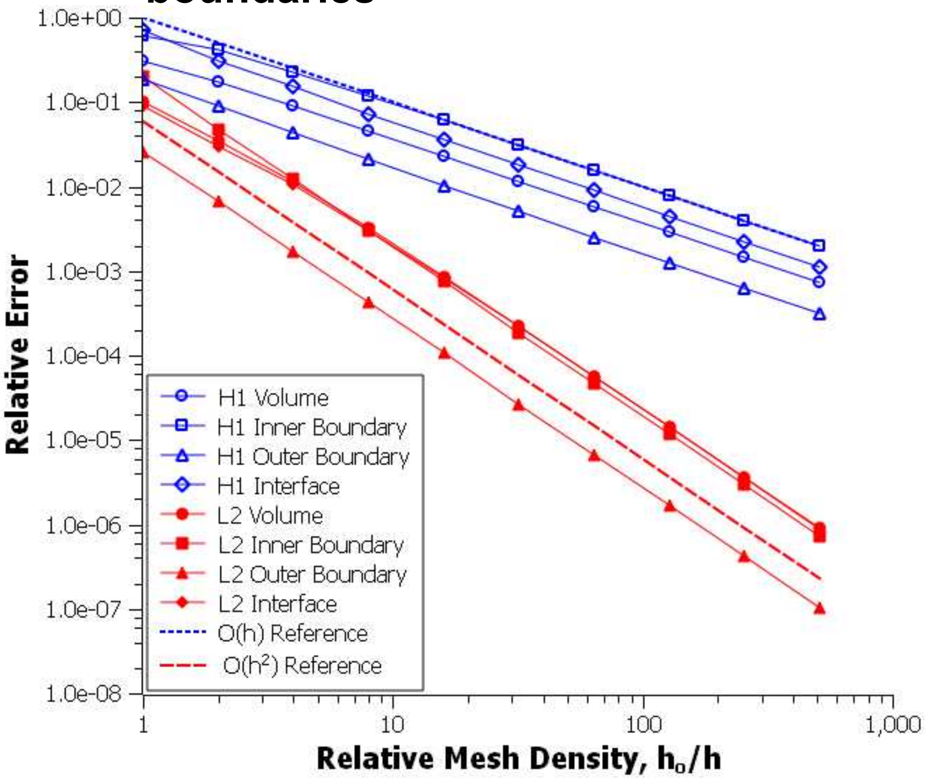


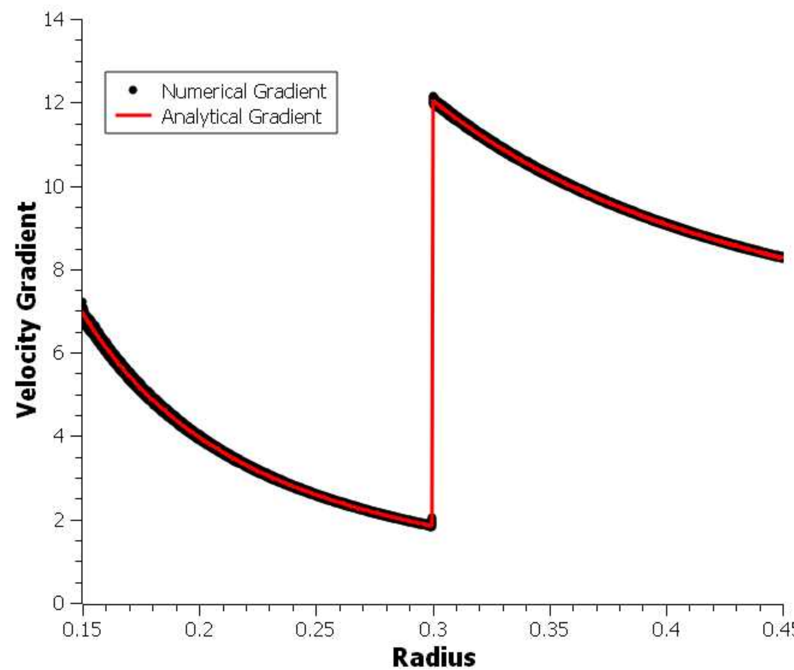




CDFEM Simulation of Steady, Fluid-Fluid Interface Problem: Couette Flow

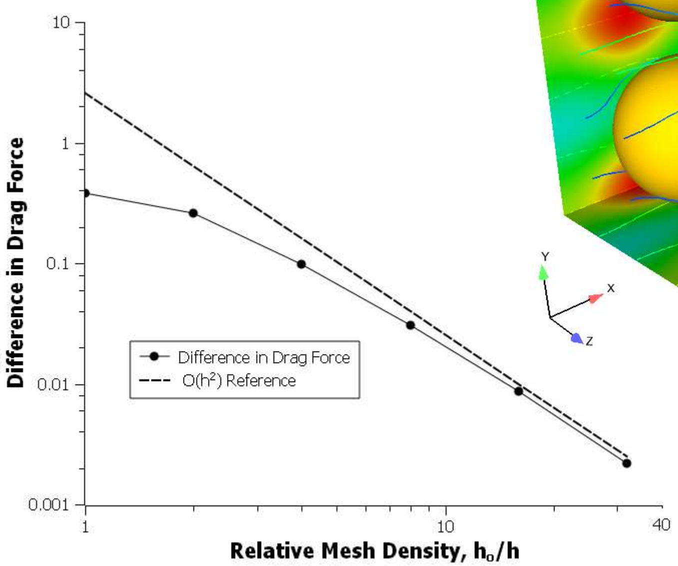
- **Embedded curved boundaries**
- **Dirichlet BC on inner and outer surface**
- **Weak discontinuity in velocity captured sharply and accurately**
- **Optimal convergence rates for solution and gradient both on volume and boundaries**

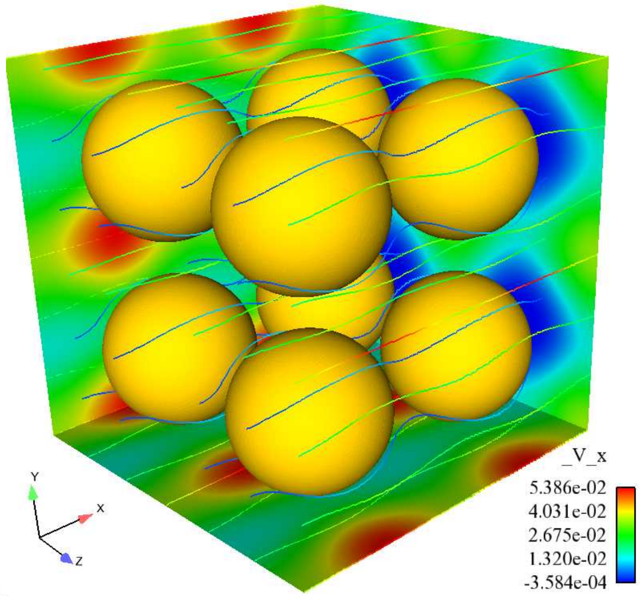


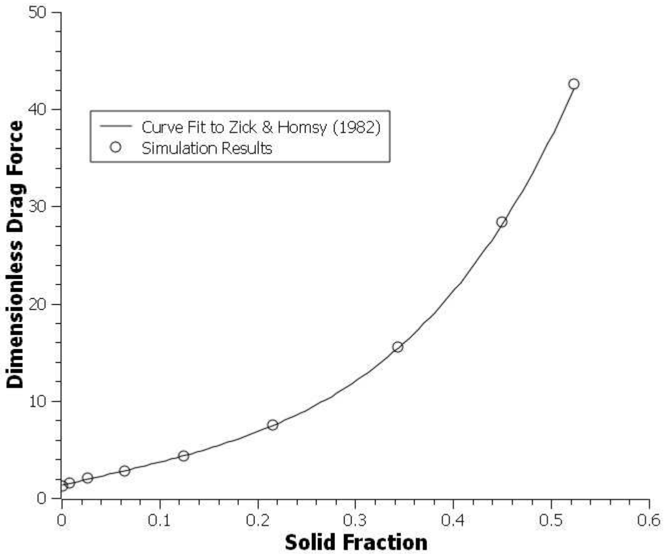


CDFEM Simulation of Steady, Viscous Flow about a Periodic Array of Spheres

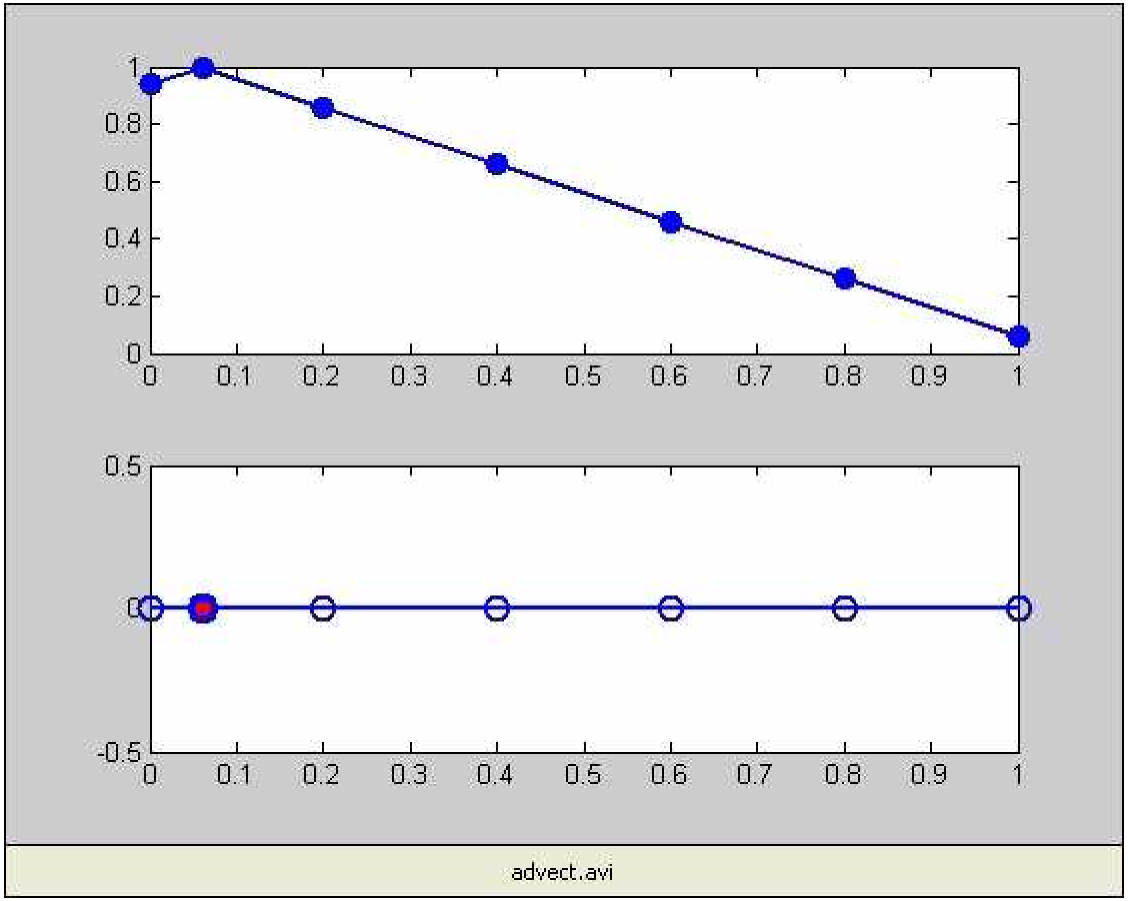
- Embedded curved boundaries
- Dirichlet BC on sphere surface
- Accurate results right up to close packing limit
- Sum of nodal residuals provides accurate/convergent measure of drag force





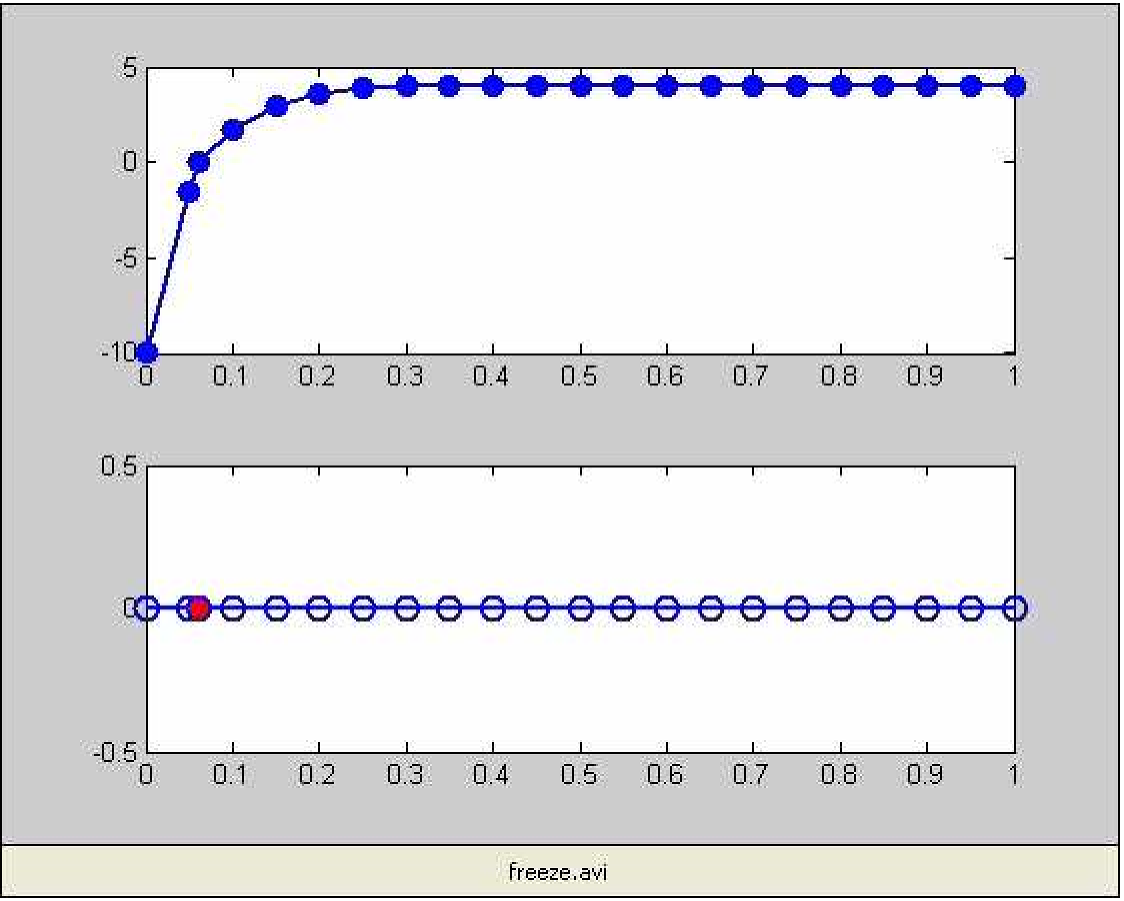


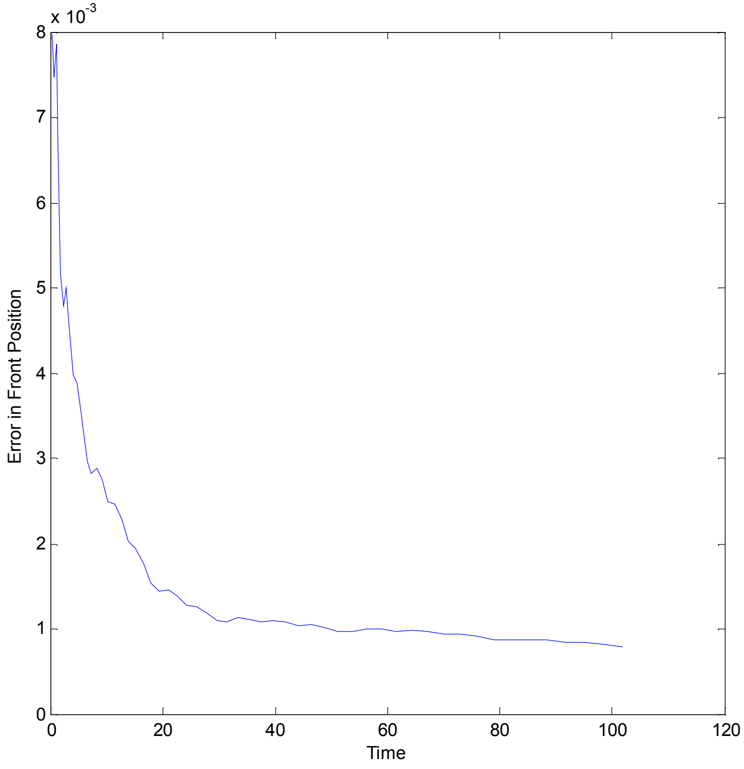
Dynamic CDFEM: 1-D Advection of a Piecewise Linear Field



- Exact preservation of linear field
- Does not pollute Max-Min

Dynamic CDFEM: 1-D Phase Change





– **Great agreement with exact solution**

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Summary and Conclusions

- **CDFEM - Theory**
  - Recovers XFEM when added nodes are constrained to lie in XFEM space
  - Demonstrates optimal rates of convergence for both Neumann and Dirichlet BC on curved surfaces
- **CDFEM – Practice**
  - Simple method for handling arbitrary interfacial discontinuities
    - Transparent to underlying finite element assembly
  - Optimal convergence rates obtained for both volume and surface quantities for Dirichlet, Neumann, and mixed boundary conditions
- **Project Status**
  - Parallel CDFEM for multiphysics is implemented, tested and documented.
  - Dynamic CDFEM is developed and tested in 1-D MATLAB
  - Dynamic CDFEM in SIERRA under development

New ESRF project aimed at development/application of these ideas for material liquefaction and relocation

Relevant Publications and Presentations

- Noble, Newren, Lechman, "A Conformal Decomposition Finite Element Method for Modeling Stationary Fluid Interface Problems", *International Journal for Numerical Methods in Fluids* (accepted, 2009)
- Noble, Lechman, "Verification of a Conformal Decomposition Finite Element Method for Steady Fluid Flows" to be presented at the *10th U.S. National Congress for Computational Mechanics*, Columbus, OH (2009)
- Holdych, Noble, Secor, "Quadrature Rules for Triangular and Tetrahedral Elements with Generalized Functions", *International Journal for Numerical Methods in Engineering,* **73**, 1310-1327 (2008)
- Noble, "Modeling Steady State Fluid Interface Problems Using the Conformal Decomposition Finite Element Method (CDFEM)", Presented at the *14th International Conference on Finite Elements in Flow Problems*, Santa Fe, NM (2007)
- Holdych, Noble, "Integration Techniques for Extended Finite Element Methods", Presented at the *7th World Congress on Computational Mechanics*, Los Angeles, CA (2006)
- Noble, Sun, "Modeling Decomposed Foam Dynamics using a Level Set - Extended Finite Element Approach", presented at *APS Division of Fluid Dynamics*, Chicago, IL (2005)