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A Dynamic Conformal Decomposition Finite Element Method (CDFEM) for Capillary Hydrodynamics

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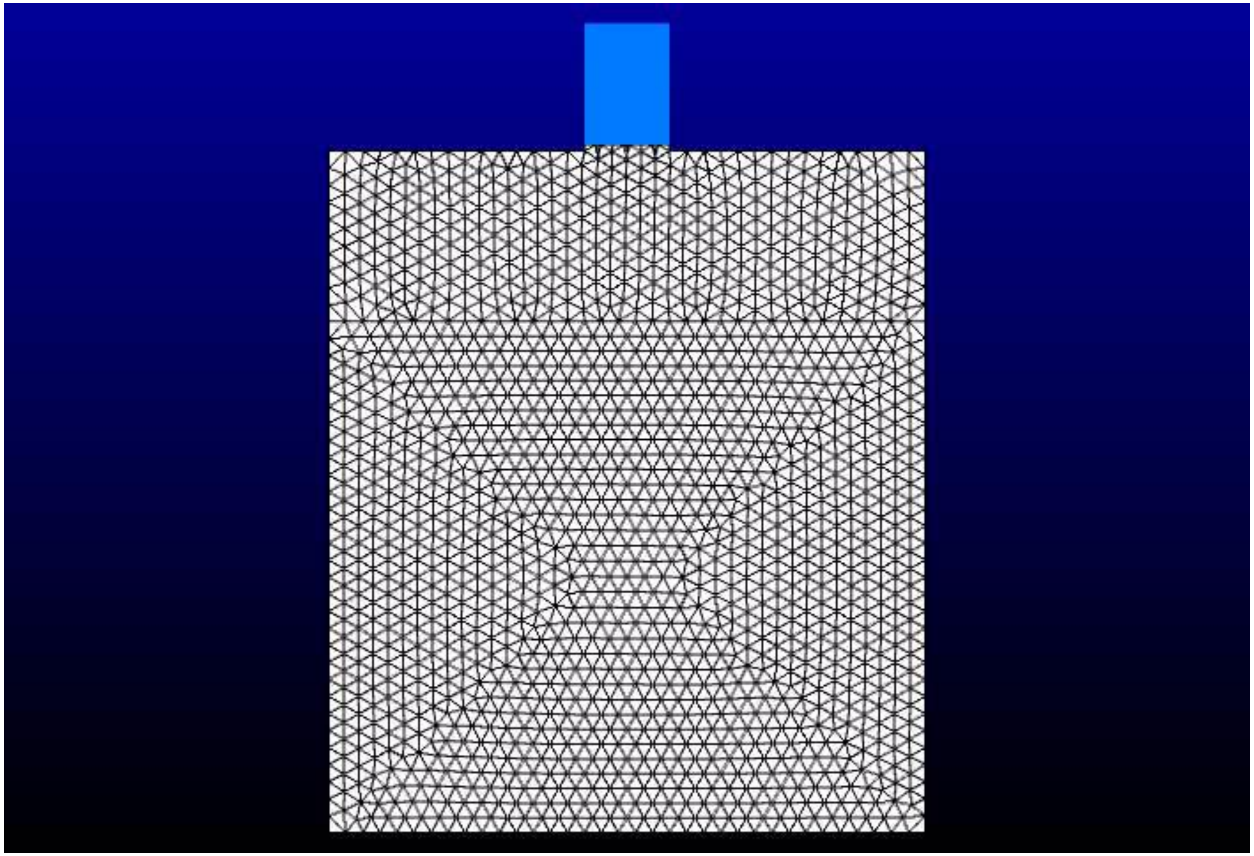
Target Application: Capillary Hydrodynamics

Target Application

- Problems where fluid dynamics and capillary forces are important



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Methodology: Conformal Decomposition Finite Element Method (CDFEM)

Simple Concept

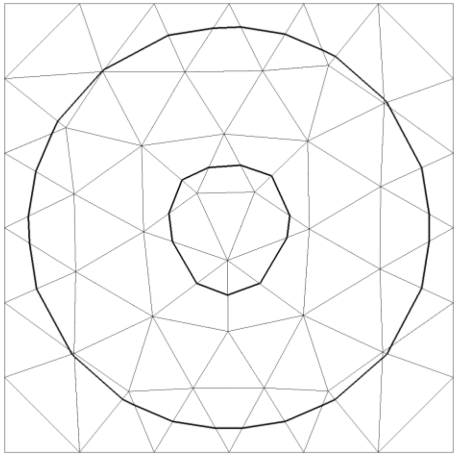
- Use one or more level set fields to define materials or phases
- Decompose non-conformal elements into conformal ones
- Obtain solutions on conformal elements

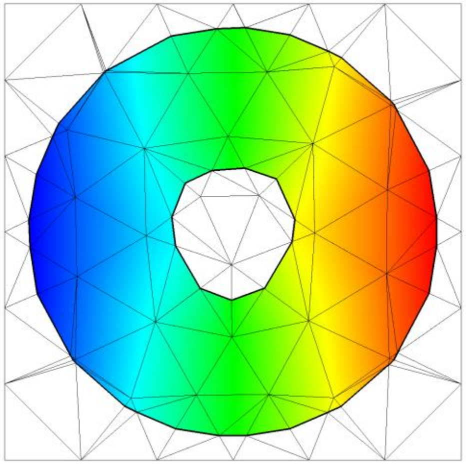
Related Work

- Li et al. (2003) FEM on Cartesian Grid with Added Nodes
  - Focus on Cartesian Grid. Considered undesirable because it lost original mesh structure.
- Ilinca and Hetu (2010) Finite Element Immersed Boundary
  - Focus on solid-fluid with Dirichlet BCs

Properties

- Supports wide variety of interfacial conditions (identical to boundary fitted mesh)
- Avoids manual generation of boundary fitted mesh
- Supports general topological evolution (subject to mesh resolution)
- Similar to finite element adaptivity
- Uses standard finite element assembly including data structures, interpolation, quadrature





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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

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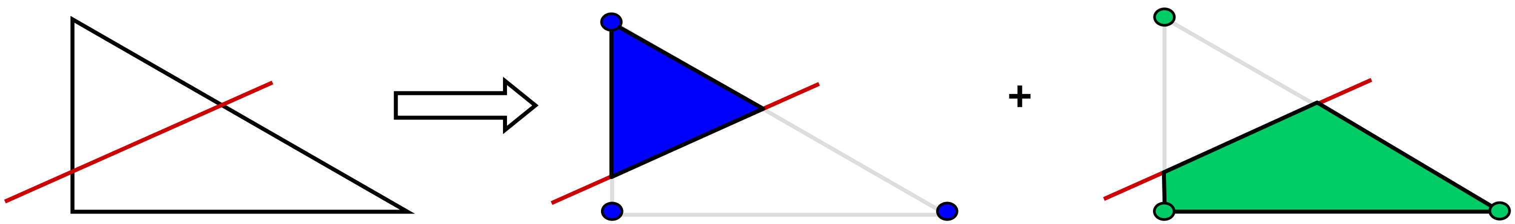
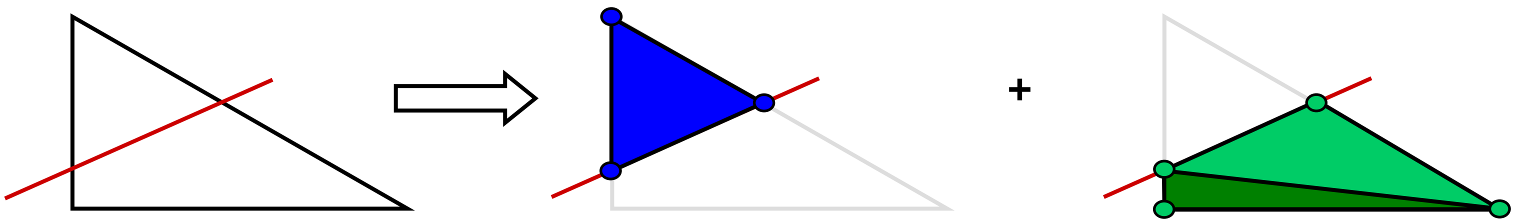
XFEM – CDFEM Discretization Comparison

XFEM Approximation



CDFEM Approximation



- Identical IFF interfacial nodes in CDFEM are constrained to match XFEM values at nodal locations
- CDFEM space contains XFEM space
  - CDFEM is no less accurate than XFEM (Li et al., 2003)
  - XFEM can be recovered from CDFEM by adding constraints

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

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

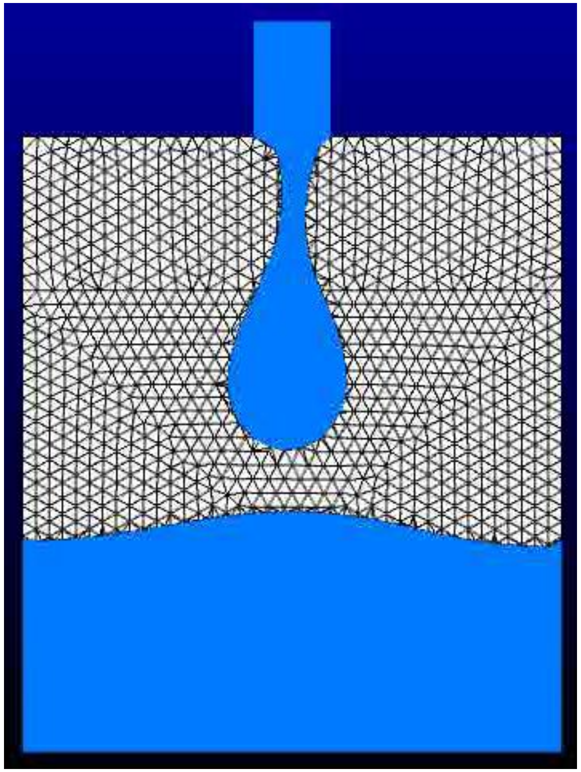
$$\int_\Omega \left[-P\,I + \mu\left(\nabla u + \nabla u^t\right)\right] \cdot \nabla N_i \, d\Omega - \int_\Omega \rho g \, N_i \, d\Omega + \int_\Gamma S\, N_i \, d\Gamma = 0$$

- 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

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



Formulation: Interface Dynamics

Level Set Equation

- Advection equation

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

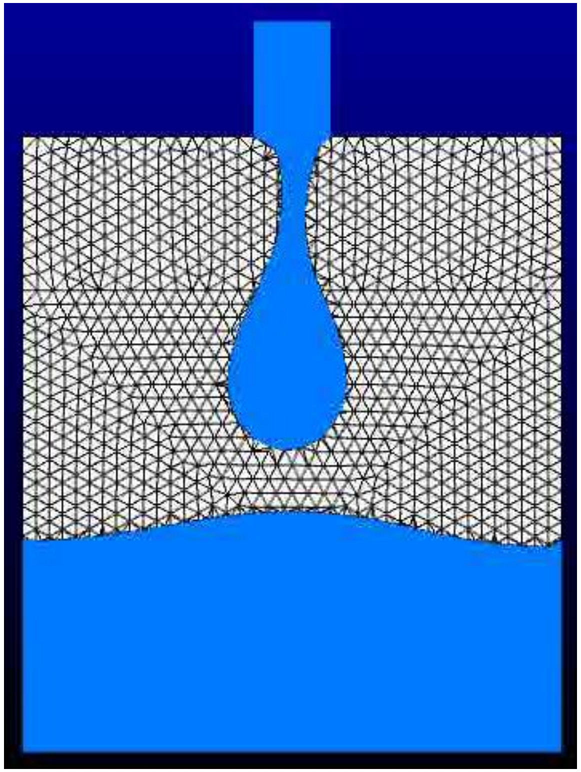
- Galerkin, Backward Euler

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

- 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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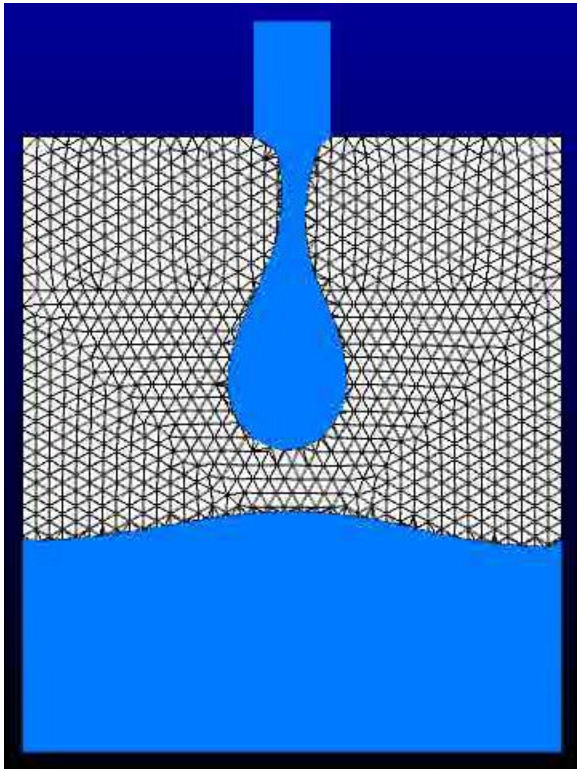
Models: Liquid-Air Interface

Capillary Force

- Same model used in ALE simulations
  - Jump in stress due to interfacial tension
  - Laplace-Betrami implementation avoids second derivatives

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



Interface Stabilization

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

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

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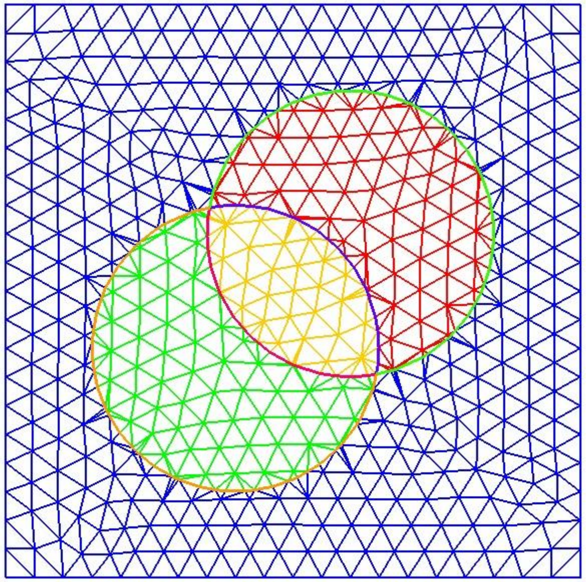
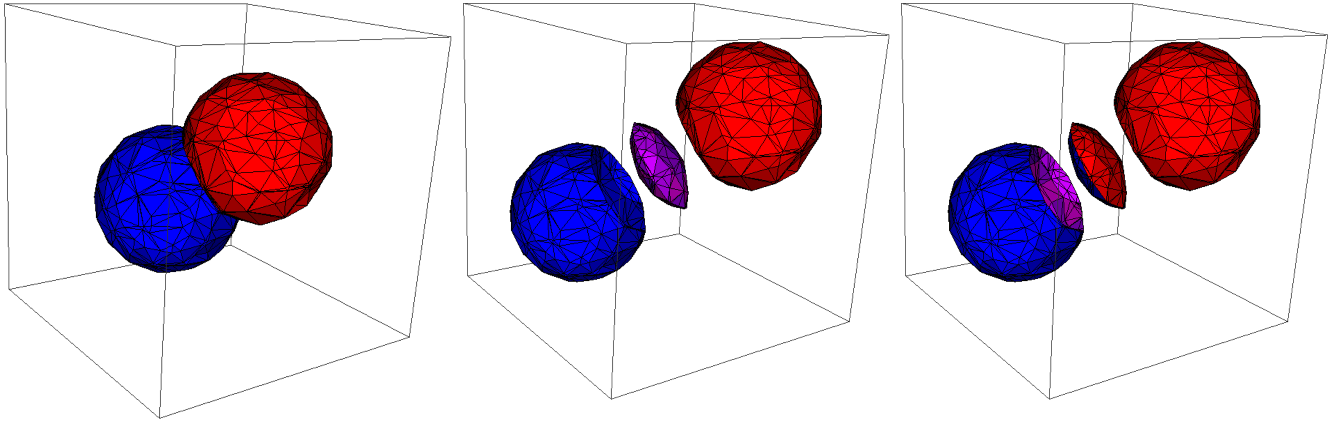
CDFEM for Static Interfaces

- Level set function generated for desired geometry
  - Multiple phases defined by multiple level set fields
- Non-conformal elements that intersect the level set undergo conformal decomposition
  - Dynamic decomposition of blocks and sidesets
  - Creation of sideset on interfaces for bc application
  - Phase specific material properties, equations, source terms, etc.
- Other features
  - Parallel
  - Mixed Elements (LBB) Tris/Tets





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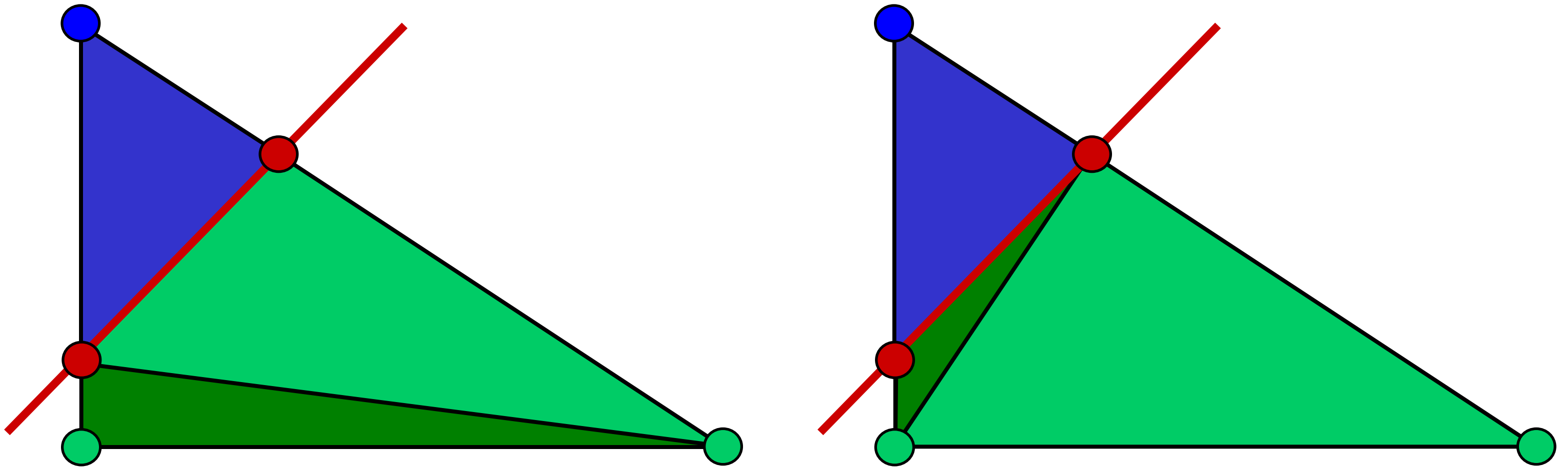
CDFEM – Level Set Implementation in Two Dimensions

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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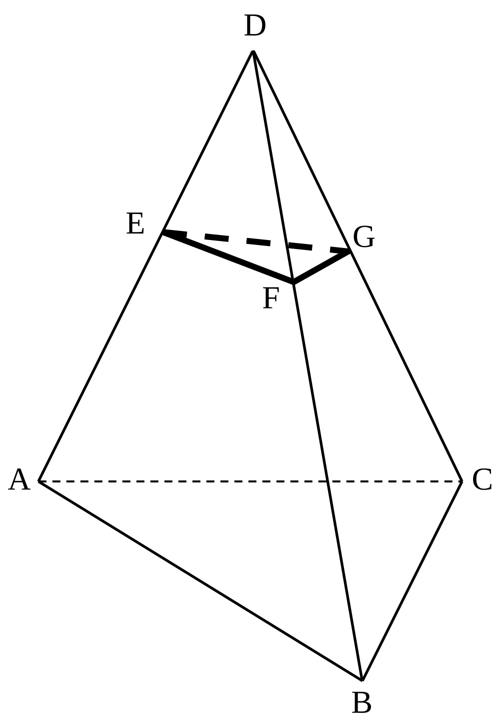
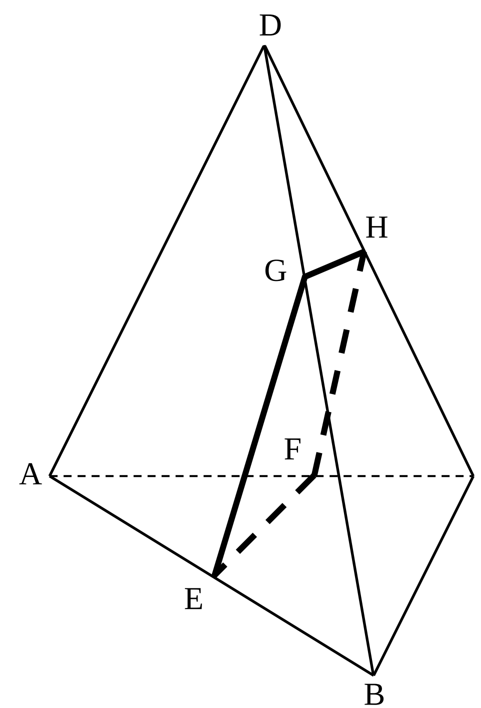
CDFEM – Level Set Implementation in Three Dimensions

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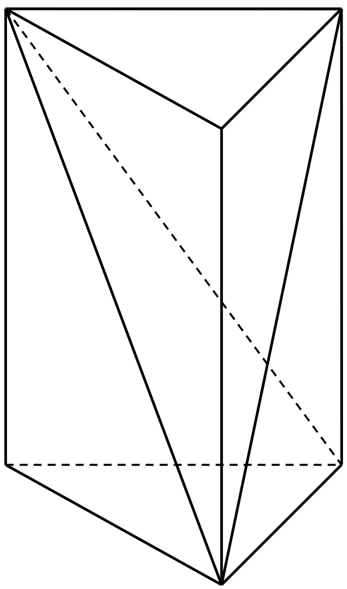
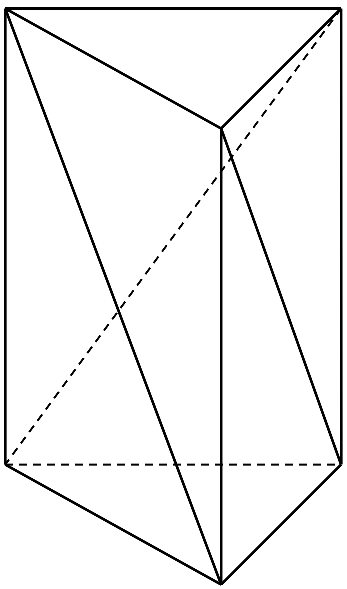
CDFEM – Level Set Implementation in Three Dimensions – cont'd

- 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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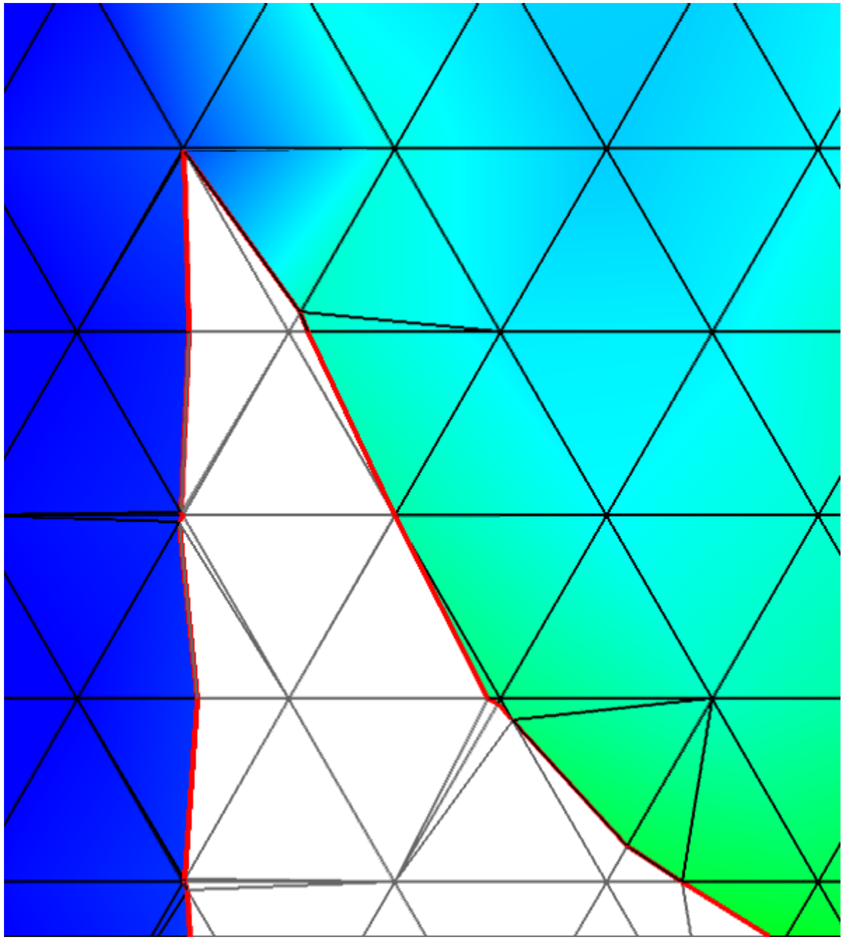
Complications: Degenerate Decompositions

Strategy to Handle Degenerate or Nearly Degenerate Element Decompositions

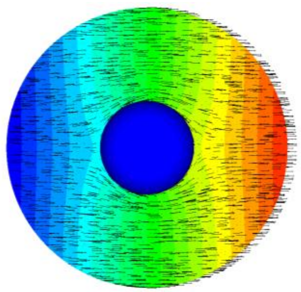
- Standard approach: “Snap to Node” when edge intersection gets close to node
  - Eliminates slivers and infinitesimal sub-elements
  - Can create interface segments that do not lie between sub-elements of both volumetric phases
  - Huge number of degenerate cases must be handled
- Alternate approach: “Snap from Node” when edge intersection tries to get too close to node – Ilinca and Hetu (2010)
  - Creates/retains many slivers and infinitesimal sub-elements
  - Interface segments always lie between subelements of both volumetric phases
  - No degenerate cases to handle

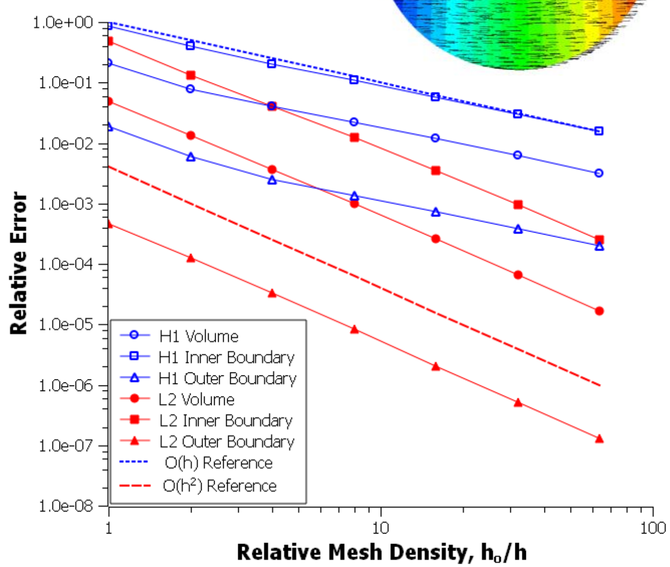


CDFEM Verification for Static Interfaces

Steady Potential Flow about a Sphere

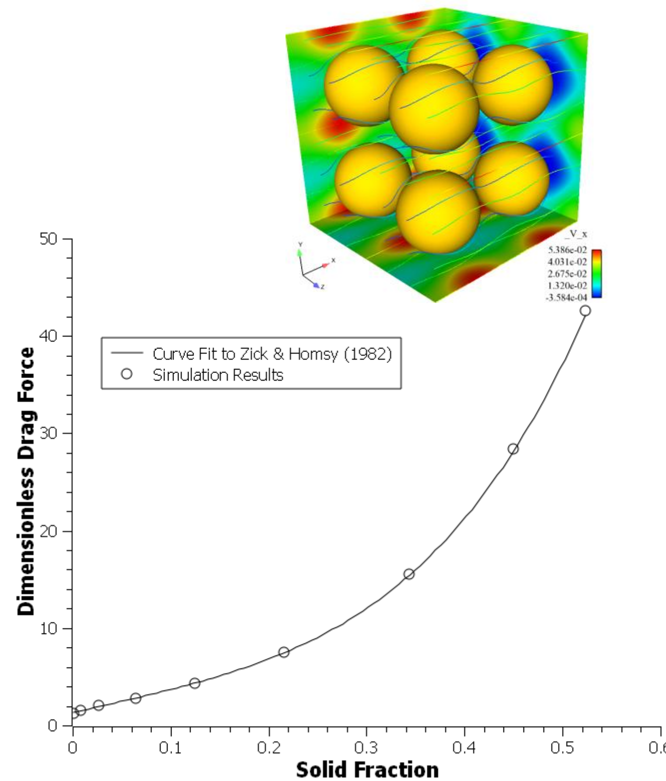
- Embedded curved boundaries
- Dirichlet BC on outer surface, Natural BC on inner surface
- Optimal convergence rates for solution and gradient both on volume and boundaries





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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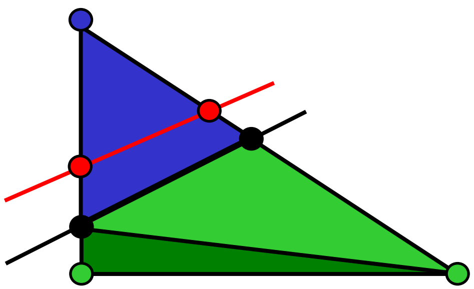
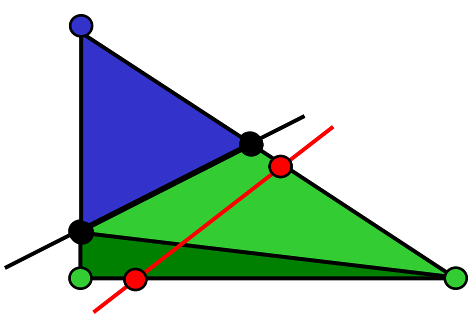
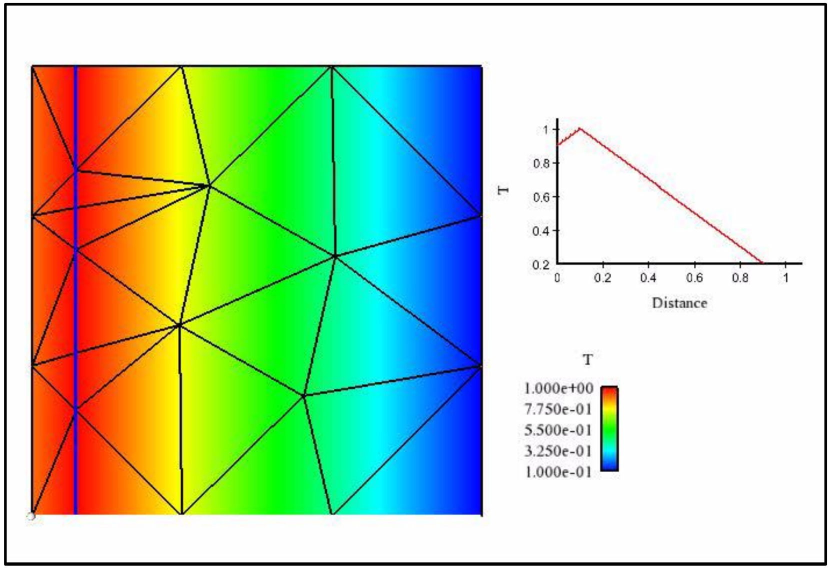
CDFEM for Moving Interfaces

- How do we handle the moving interface?



- What do we do when nodes change sign?





Patch Test: Exact preservation of discontinuous gradient with constant advection

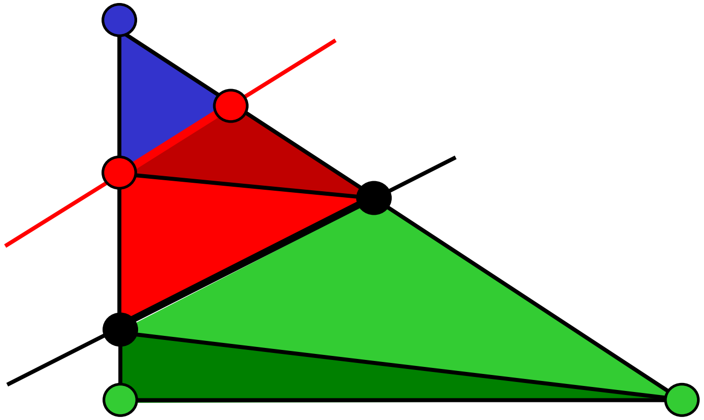
Approach for Dynamic Discretizations Due to Moving Interfaces: Dynamic Subdomains

- XFEM – Immersed Interface Approach
  - Integration done over the 4 subdomains

$$\Omega_{++} \equiv \Omega_+^n \bigcap \Omega_+^{n+1} \qquad \Omega_{--} \equiv \Omega_-^n \bigcap \Omega_-^{n+1}$$

$$\Omega_{+-} \equiv \Omega_+^n \bigcap \Omega_-^{n+1} \qquad \Omega_{-+} \equiv \Omega_-^n \bigcap \Omega_+^{n+1}$$

  - Constant advection – Backward Euler

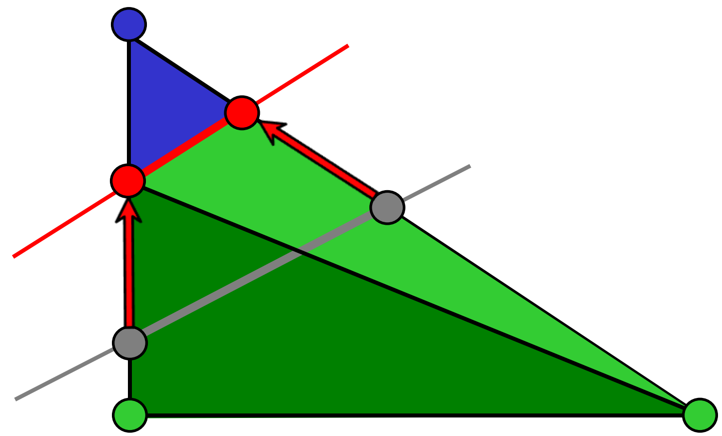


$$\int_\Omega \left(\frac{\partial \psi}{\partial t} + u \cdot \nabla \psi \right) N_i \, d\Omega = 0 \Rightarrow R_i = \int_\Omega \left(\frac{\psi^{n+1} - \psi^n}{\Delta t} + u \cdot \nabla \psi^{n+1} \right) N_i \, d\Omega$$

$$R_i = \int_{\Omega_{++}} \left(\frac{\psi_+^{n+1} - \psi_+^n}{\Delta t} + u \cdot \nabla \psi_+^{n+1} \right) N_i \, d\Omega + \int_{\Omega_{--}} \left(\frac{\psi_-^{n+1} - \psi_-^n}{\Delta t} + u \cdot \nabla \psi_-^{n+1} \right) N_i \, d\Omega +$$

$$\int_{\Omega_{+-}} \left(\frac{\psi_-^{n+1} - \psi_+^n}{\Delta t} + u \cdot \nabla \psi_-^{n+1} \right) N_i \, d\Omega + \int_{\Omega_{-+}} \left(\frac{\psi_+^{n+1} - \psi_-^n}{\Delta t} + u \cdot \nabla \psi_+^{n+1} \right) N_i \, d\Omega$$

Approach for Dynamic Discretizations Due to Moving Interfaces: Mesh Motion



- ALE – CDFEM Approach
  - Consider deforming domain
  - Apply chain rule to time derivative

$$\left.\frac{\partial \psi}{\partial t}\right\|_{\xi} = \left.\frac{\partial \psi}{\partial t}\right\|_{\mathbf{x}} + \left.\frac{\partial \mathbf{x}}{\partial t}\right\|_{\xi} \cdot \nabla_{\mathbf{x}} u$$

  - Constant advection – Backward Euler

$$\int_{\Omega} \left(\frac{\partial \psi}{\partial t} + u \cdot \nabla \psi \right) N_i \, d\Omega = 0 \Rightarrow R_i = \int_{\Omega} \left(\left.\frac{\partial \psi}{\partial t}\right\|_{\xi} + (\mathbf{u} - \dot{\mathbf{x}}) \cdot \nabla \psi \right) N_i \, d\Omega$$

$$R_i = \int_{\Omega_+^{n+1}} \left(\frac{\psi_+^{n+1}(\xi) - \psi_+^{n}(\xi)}{\Delta t} + u \cdot \nabla \psi_+^{n+1} \right) N_i \, d\Omega + \int_{\Omega_-^{n+1}} \left(\frac{\psi_-^{n+1}(\xi) - \psi_-^{n}(\xi)}{\Delta t} + u \cdot \nabla \psi_-^{n+1} \right) N_i \, d\Omega$$

  - Requires integration only over new decomposition
  - Requires definition of mesh velocity, $\dot{\mathbf{x}}$
    - Current algorithm: If edge cut previously, node moved along edge, otherwise find nearest node on the old interface

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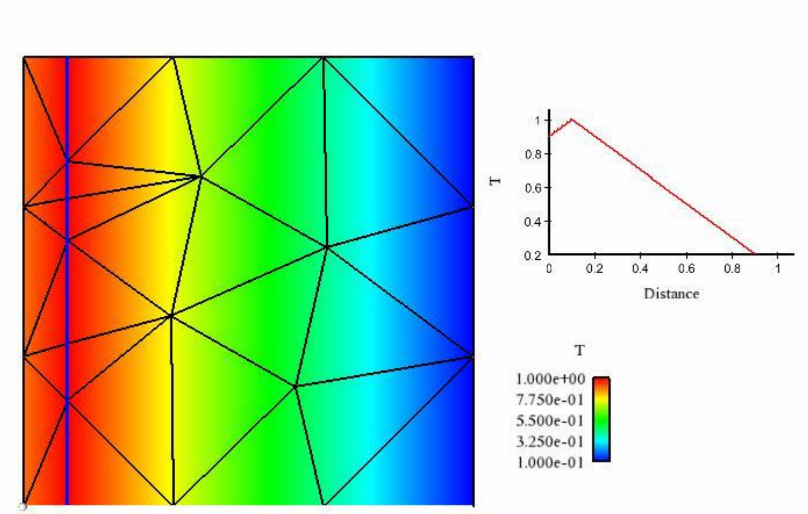
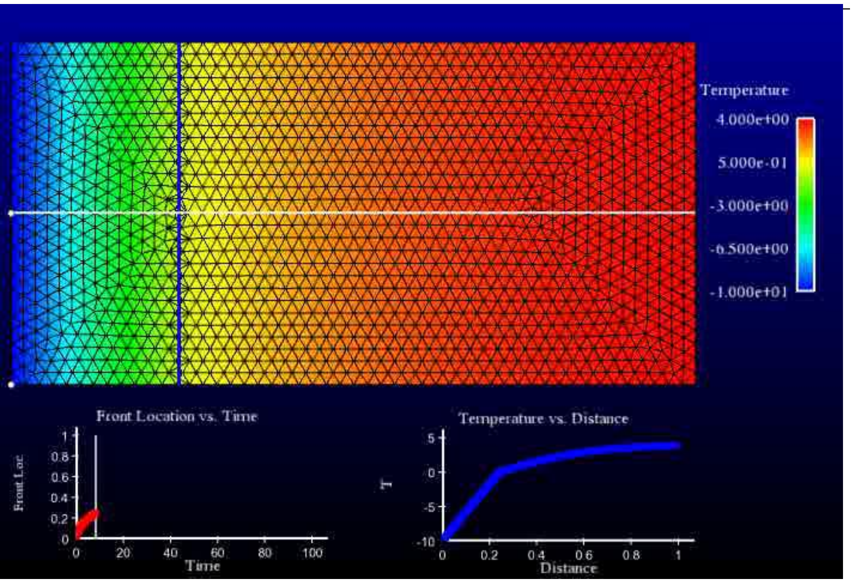
CDFEM Verification for Dynamic Interfaces



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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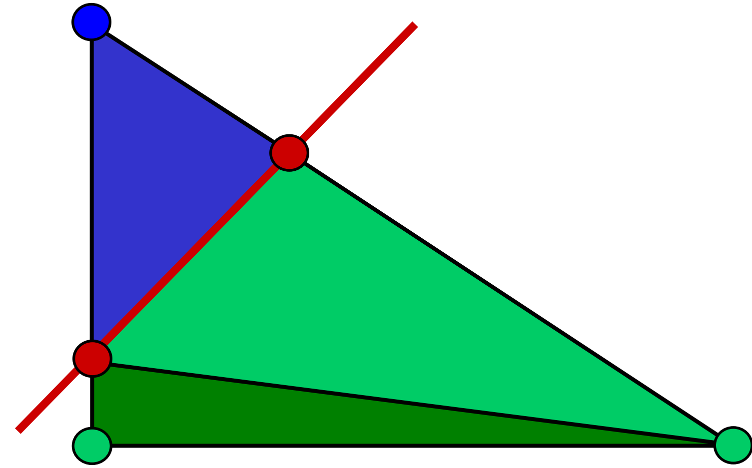
Level Set Approximation Space

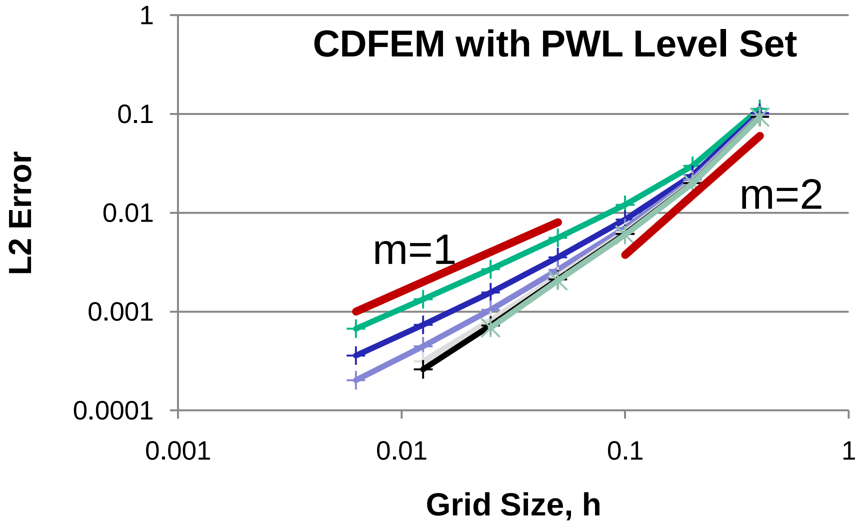
- What space should be used for the Level Set field?
- Apparently not given much consideration in XFEM or immersed interface approaches
  - Not proposed as a field to be enriched, instead standard piecewise linear (PWL) field is deemed sufficient
- Natural space in CDFEM is PWL on the subelements, not on the non-conformal parent element (SubPWL)
  - These subelements, however, can describe non-linear (non-planar) interfaces on the parent element
- What are the consequences of the different spaces?
- How can CDFEM recover PWL on the parent element?
- Are there ramifications for the velocity field?

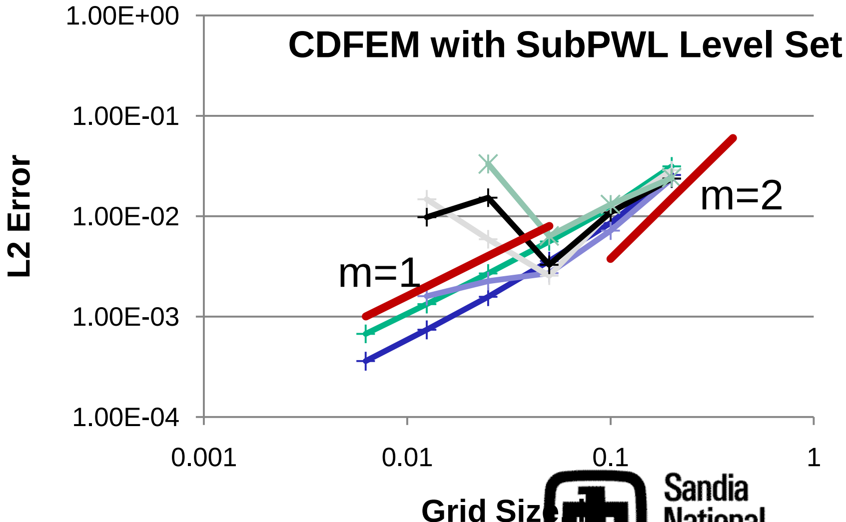


Benchmark: Level Set Advection

- Test: Pure advection of level set field
  - Test 1: Advection of level set field on fixed mesh
  - Test 2: Advection of level set field on CDFEM mesh (PWL decomposition with SubPWL level set field)
  - Test 3: Advection of constrained level set field on CDFEM mesh (PWL decomposition with PWL level set field)

- Results: Both Test 1 and 3 show optimal convergence rate while Test 2 does not
  - Mismatch between decomposition space and level set space appears detrimental to stability/convergence





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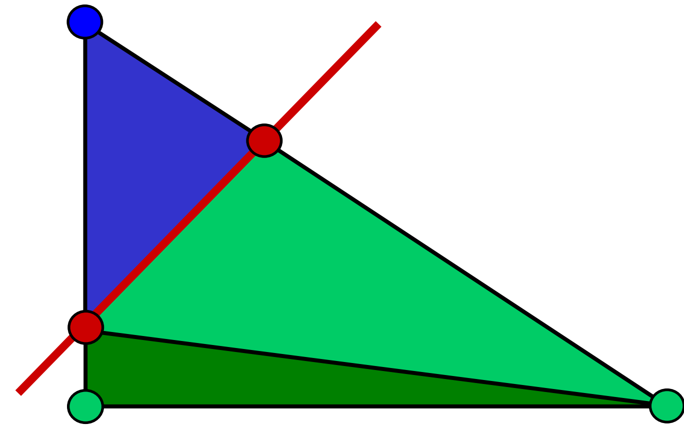
PWL Level Set Field: Consequences for Velocity Space

- Assume that because decomposition is PWL, then the Level Set Field should be PWL



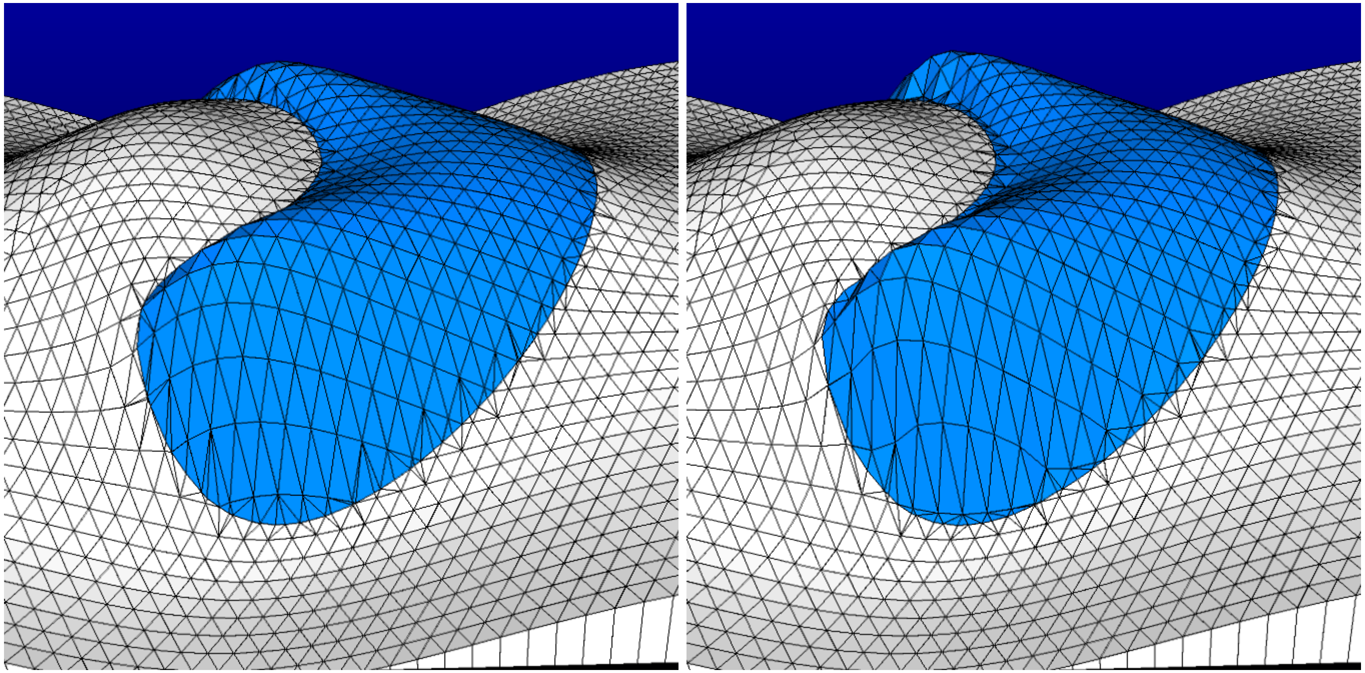
$$\frac{\partial \phi}{\partial t} + u \cdot \nabla \phi = 0 \rightarrow \phi^{n+1} = \phi^{n+1} + \Delta t\, u \cdot \nabla \phi$$

- For new level set field to remain PWL:

$$u \cdot \nabla \phi \sim \mathrm{PWL} \rightarrow \nabla (u \cdot \nabla \phi) = c \rightarrow n \cdot \nabla u = c$$

  - This requires the normal velocity gradient to be continuous across the interface!
  - This is definitely not a requirement for satisfying the conservation equations
  - Failing to satisfy this requirement can lead to a mismatch between the level set advection and the resulting interface location
  - Such a mismatch can lead to spurious currents (non-zero velocity that yield no interface motion)
- Possible solution – constrain entire velocity to be PWL
  - Equivalent to not enriching velocity gradient in XFEM – Found to be necessary by Fries and Zilian

Capillary Hydrodynamics: Consequences of Velocity Space



- Tests: Static bubble and rising bubble
  - Test show sub-optimal, in fact, unstable behaviour for unconstrained velocity space
  - Constrained velocity space is overly diffusive, unable to sharply capture the physically discontinuous velocity gradient
  - Constraint is excessive in that it removes discontinuity in both the normal and tangential gradient in velocity

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Summary

- CDFEM is Accurate for Static Interface Problems
  - Multiple verification tests performed
  - Method expected to be at least as accurate as XFEM
- CDFEM is Robust for Static/Dynamic Interface Problems
  - Handles arbitrary interface topology in 2d and 3d
- CDFEM usage of Moving Mesh Time Derivative Appears Optimal
  - Less work than decomposition/integration over intersections of old and new subdomains
  - Exactly satifies advection patch test and provides optimal convergence rates for pure advection
- XFEM and CDFEM decompositions normally require piecewise linear level set fields
  - Possible that normal velocity inherits this limitation
  - Possible reason that enriched velocity gradient formulations have shown less than desirable stability/convergence
  - Constrained CDFEM simulations show desired stability and convergence