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Enriched Finite Element Methods at Sandia National Laboratories for Multimaterial and Multiphysics Transport Problems with Complex or Dynamic Topology

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U.S. DEPARTMENT OF ENERGY

NNSA National Nuclear Security Administration

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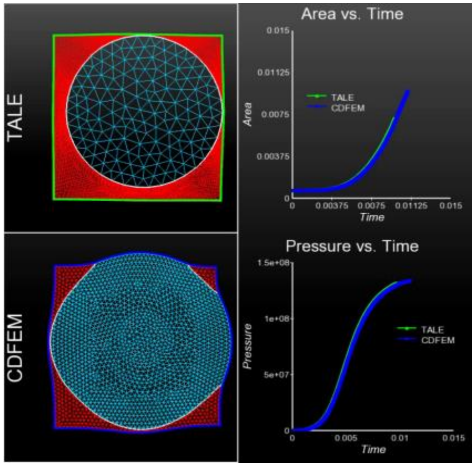
- Application to multimaterial and multiphysics transport problems with complex and dynamic topology
  - Battery performance: Scott Roberts, Brad Trembacki, Hector Mendoza
  - Laser Welding: Mario Martinez
  - Conductive burn of energetic materials: Bill Erikson
  - Capillary Wetting: Alec Kucala

Outline

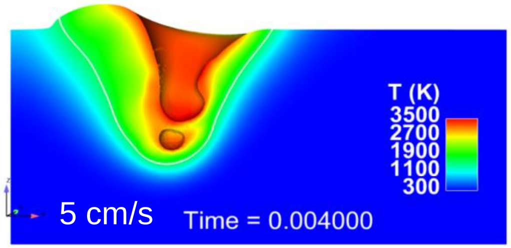
- Motivation
  - Multimaterial, multiphase, and/or multiphysics
  - Complex or dynamic topology
- Methodology
  - Enriched finite element methods
- Research Challenges and Solutions
  - Time stepping
  - Matrix conditioning
- Throughout: Solution Verification
- Future Work

Motivation

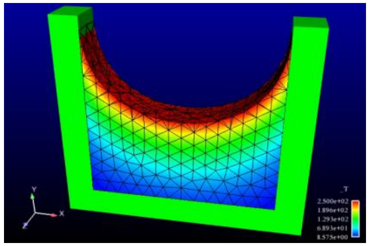
- Numerous problems with moving or topologically complex interfaces with discontinuous physics and fields



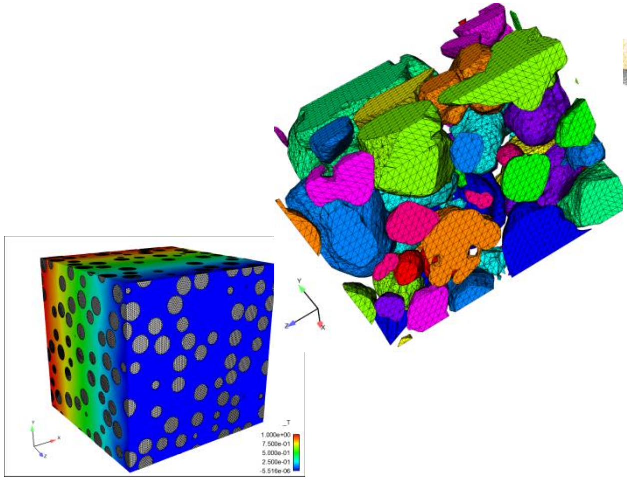
Conductive burn of energetic materials



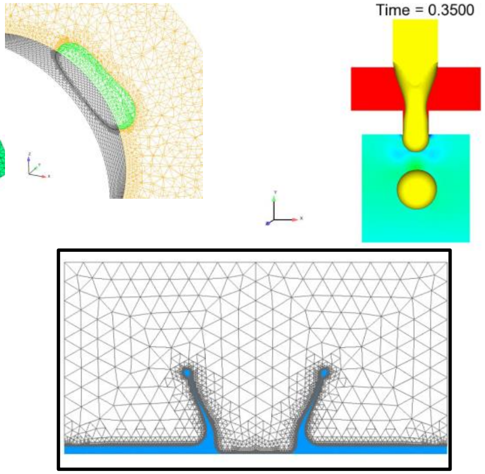
Laser welding



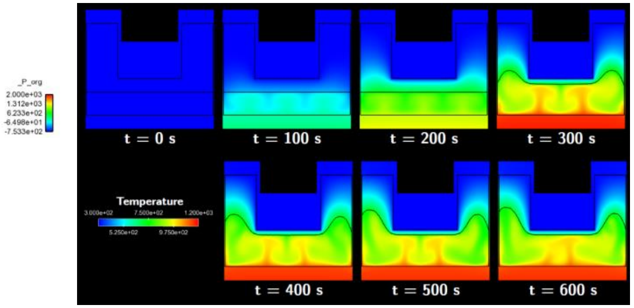
Material death



Transport in topologically complex domains including composite energetic materials and batteries

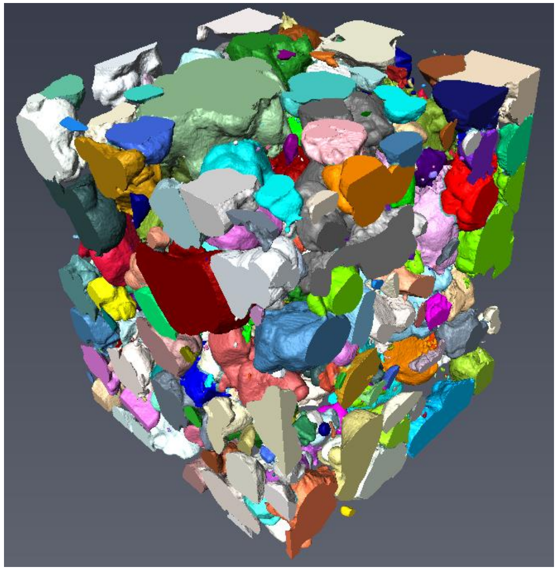


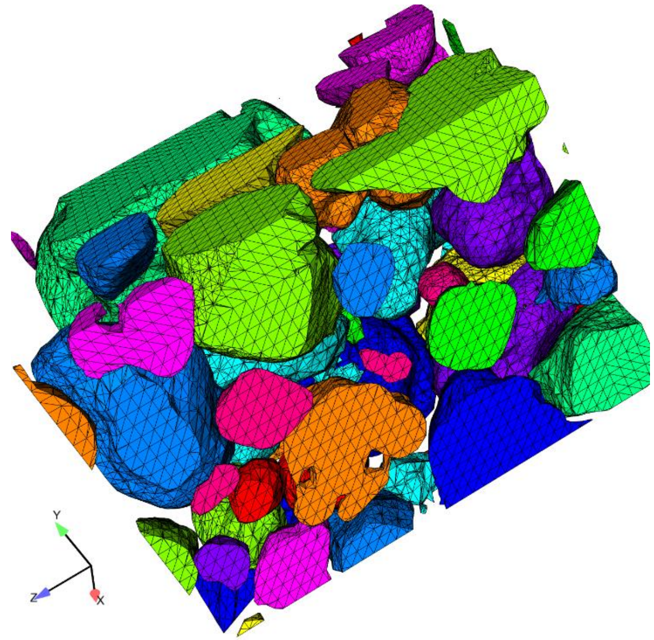
Capillary Hydrodynamics



Organic Material Decomposition (OMD) with coupled porous and low Ma flow

Prototypical Multimaterial Problem: Battery Performance

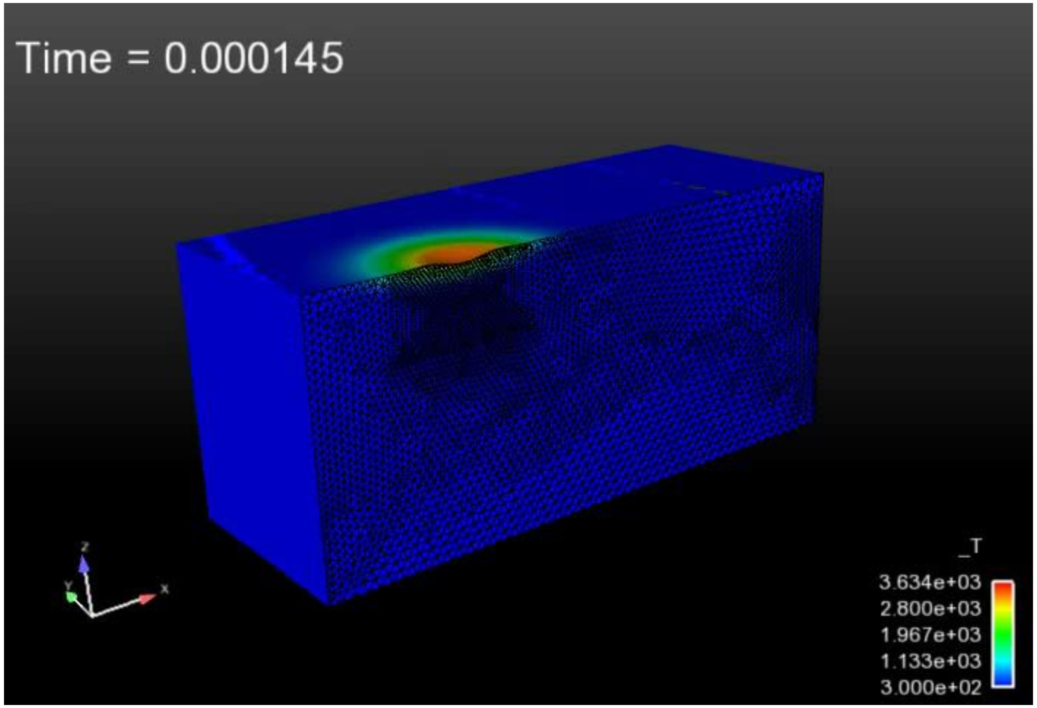


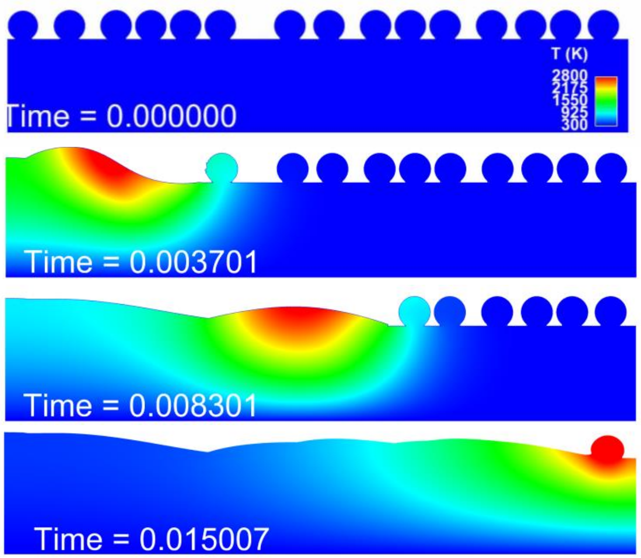


- Numerous materials in contact
  - Distinct anisotropic properties from grain to grain
- Complex Volumetric and interfacial physics
  - Electrochemistry, possibly with contact resistance at grain boundaries
- Static, but Complex Topology
  - Obtained from experimental image reconstruction
  - Precludes many automated meshing strategies

Prototypical Multiphase Problems: Laser Welding and Additive Manufacturing

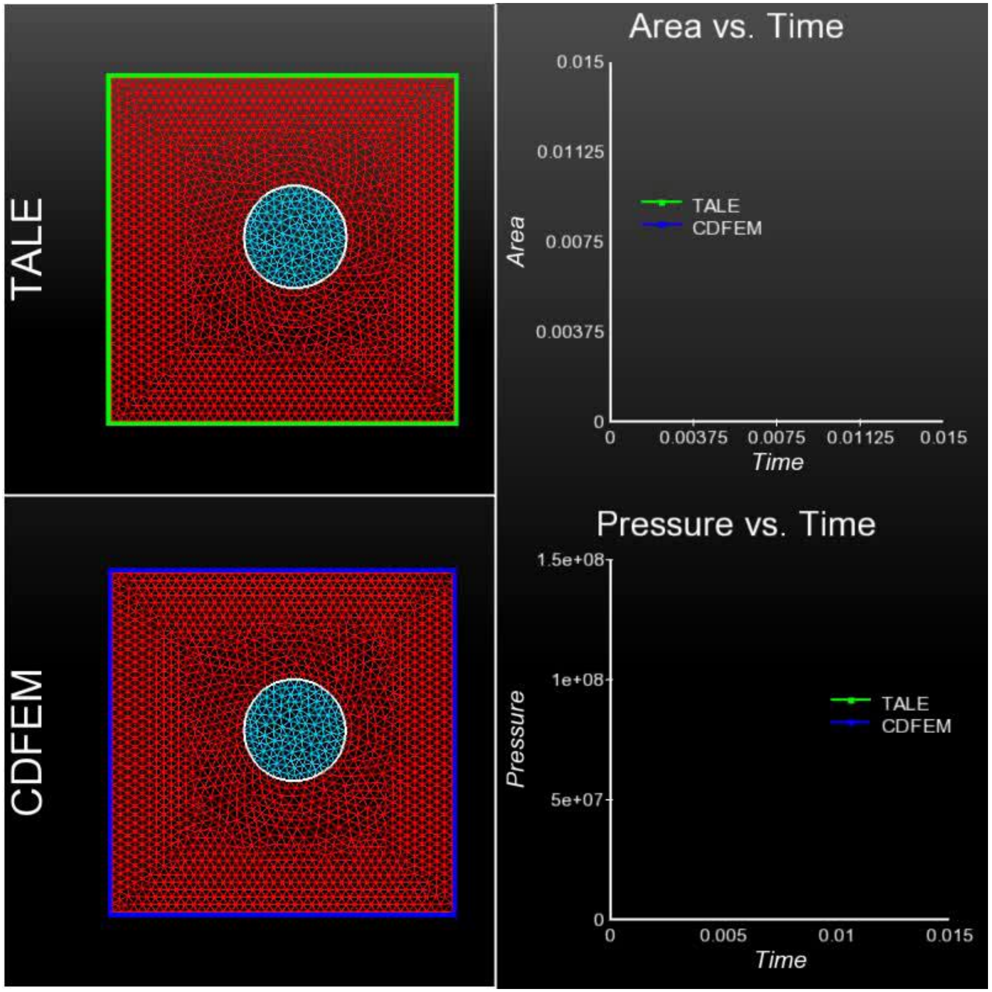
- Both laser welding and additive manufacturing via selective laser melting involve using a laser to apply intense heating over a very small area to metals
- Complex interfacial transport involving capillarity, laser heating, non-equilibrium vaporization, gives rise to dynamic, discontinuous physics and fields

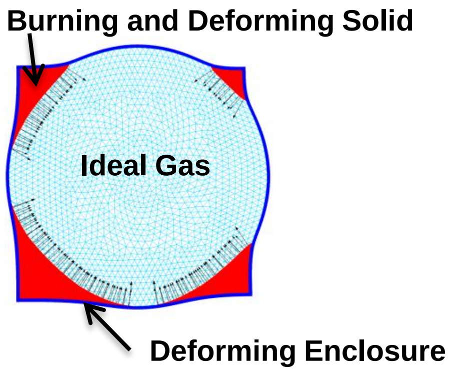




Additive Manufacturing via selective laser melting

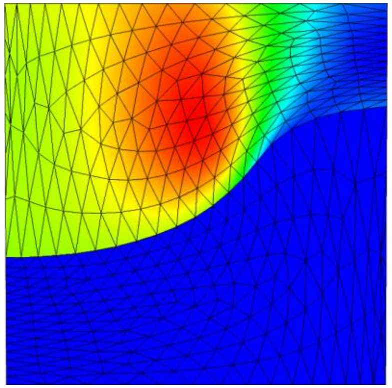
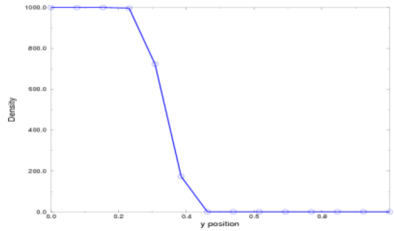
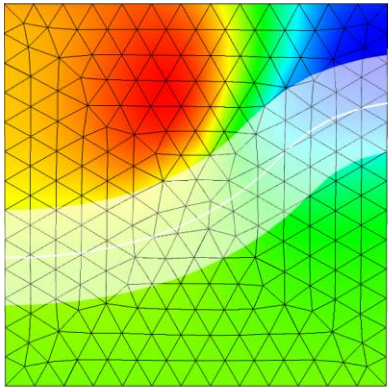
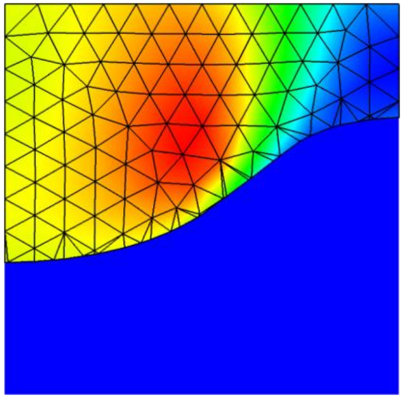
Prototypical Multiphysics Problem: Burning, Deformable Solid





- Disparate Volumetric Physics
  - 3 Distinct materials and physics – fluid, solid, and burning solid
  - DOFs discontinuous or one-sided
- Complex Interfacial Physics
  - Momentum balance, mass balance, burn front motion
  - Fronts moving with speed other than local velocity
- Dynamic Topology
  - Precludes simple moving mesh methods
  - Interfaces created and deleted dynamically

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

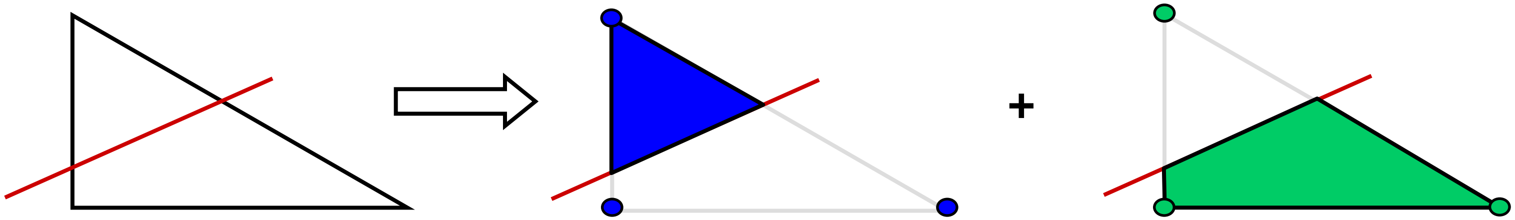
		Enriched Finite Element Methods	
ALE	**Diffuse LS**	**XFEM**	**CDFEM**
• Separate, static blocks for gas and liquid phases • Static discretization 	• Single block with smooth transition between gas and liquid phases • Static discretization  	• Single block with sharply enriched elements (weak or strong) spanning gas and liquid phases • Interfacial elements are dynamically enriched to describe phases	• Separate, dynamic blocks for gas and liquid phases • Interfacial elements are dynamically decomposed into elements that conform to phases 

Many Forms of Enriched Finite Element Methods for Discontinuous Transport Problems

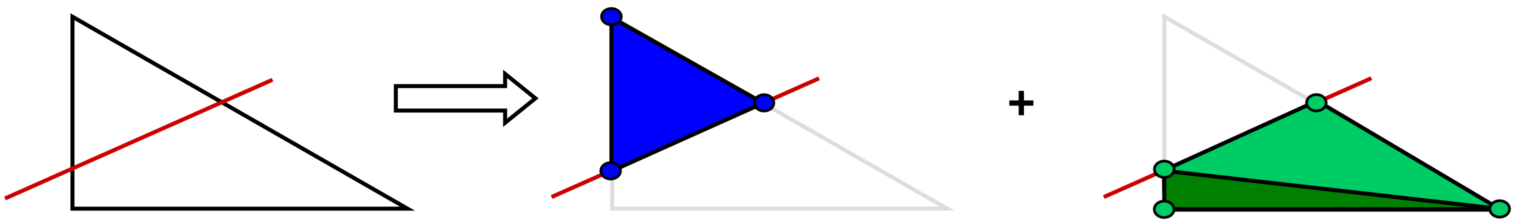
- Generalized Finite Element Methods (GFEM)
  - I. Babuška, G. Caloz, J.E. Osborn (1994)
  - Use non-polynomial shape functions to more accurately capture material response
  - May include continuous or discontinuous functions
- eXtended Finite Element Methods (XFEM)
  - N. Moës, J. Dolbow, T. Belytschko (1999)
  - Nodal enrichment using discontinuous functions
- Conformal Decomposition Finite Element Methods (CDFEM)
  - D.R. Noble, E.P Newren, J.B Lechman (2010)
  - Decompose background mesh into elements that conform to both the background elements and the implicit interfaces
  - Enrichment occurs via degrees of freedom at added interface nodes
  - Shape functions for nodes of background mesh are modified by conformal decomposition
- Hierarchical Interface-Enriched Finite Element Methods (HIEFEM)
  - S. Soghrati and P.H. Geubelle (2012)
  - Retain unaltered shape functions for nodes of background mesh
  - Enrichment occurs via degrees of freedom at added interface nodes

XFEM – CDFEM Discretization Comparison

- XFEM Approximation



- CDFEM Approximation



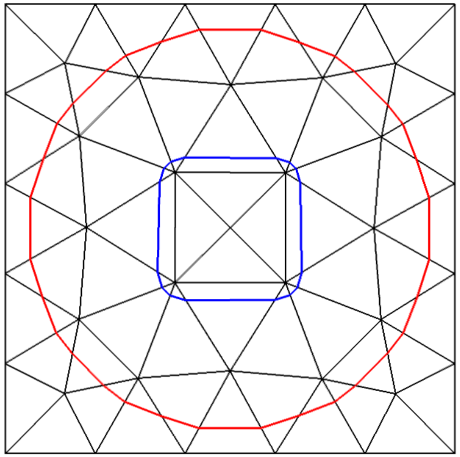
  - Identical IFF interfacial nodes in CDFEM are constrained to match XFEM values at nodal locations
  - CDFEM space contains XFEM space
    - CDFEM is no less accurate than XFEM (Li et al., 2003)
    - XFEM can be recovered from CDFEM by adding constraints

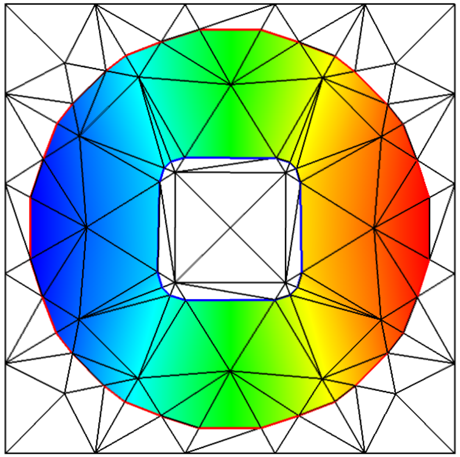
XFEM - CDFEM Requirements Comparison

	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

Conformal Decomposition Finite Element Method (CDFEM)

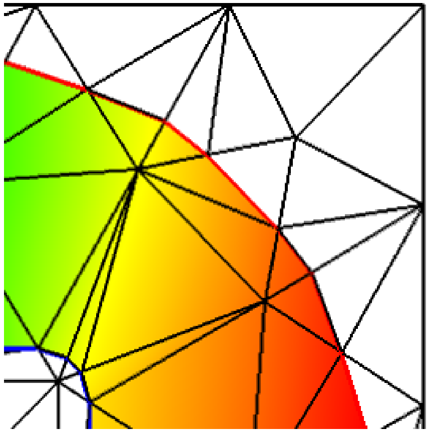
- Simple Concept (Noble, et al. 2010)
  - Use one or more level set fields to define materials or phases
  - Decompose non-conformal elements into conformal ones
  - Obtain solutions on conformal elements
- Related Work
  - Li et al. (2003) FEM on Cartesian Grid with Added Nodes
  - Ilinca and Hetu (2010) Finite Element Immersed Boundary
  - S. Soghrati and P.H. Geubelle (2012) Interface Enriched Finite Element
- 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

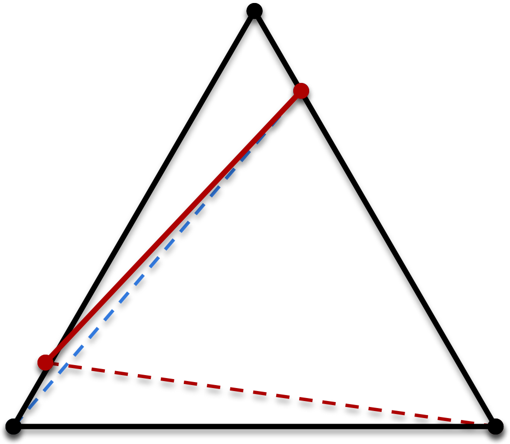




But What About the Low Quality Elements?

- Resulting meshes
  - Infinitesimal edge lengths
  - Arbitrarily high aspect ratios (small angles)
  - Introduces obtuse angles. Depending on cutting strategy, large angles can approach 180^o
- Consequences
  - Condition number of resulting system of equations
  - Interpolation error
  - Other concerns: stabilized methods, suitability for solid mechanics, Courant number limitations, capillary forces
- Questions
  - How serious are these issues?
  - What can be done to mitigate them?

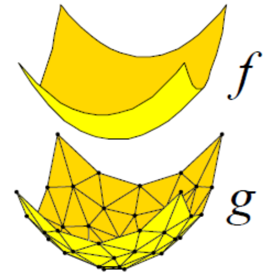


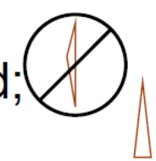
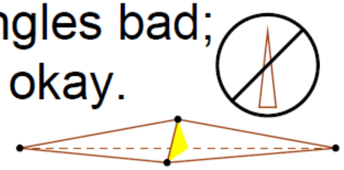


Impact of Mesh Quality

Three Criteria for Linear Elements

Let f be a function.
Let g be a piecewise linear interpolant of f over some triangulation.

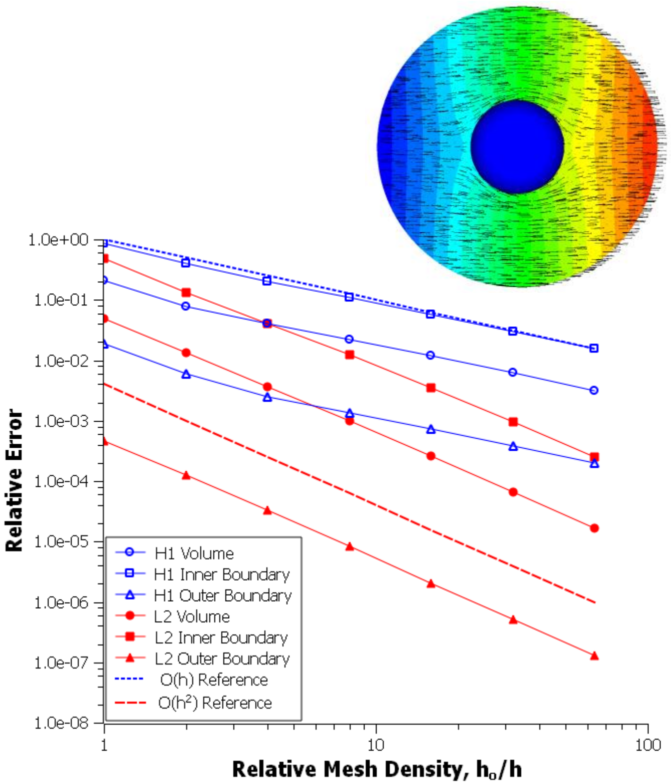


Criterion	
Interpolation error $\|\| f - g \|\|_\infty$	Size very important. Shape only marginally important.
Gradient interpolation error $\|\| \nabla f - \nabla g \|\|_\infty$	Size important. Large angles bad; small okay. 
Element stiffness matrix maximum eigenvalue λ_{max}	Small angles bad; large okay. 

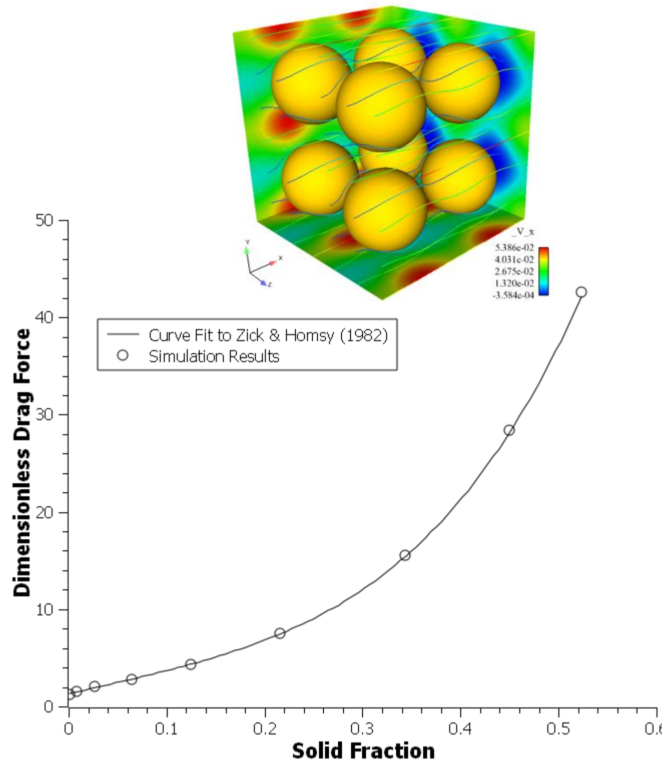
Reprinted from “What is a Good Finite Element?” by Jonathan Richard Shewchuk

Static Interface CDFEM Verification

- 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

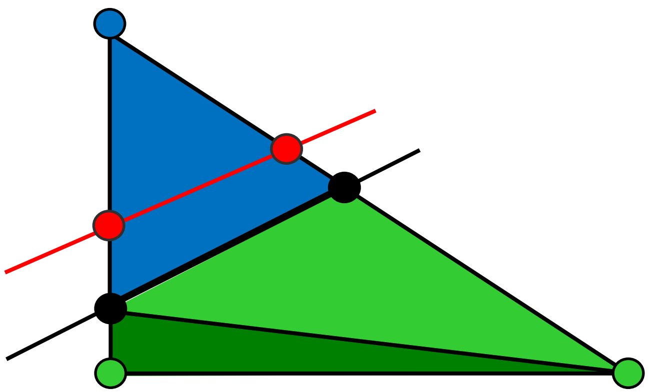


Research Challenges

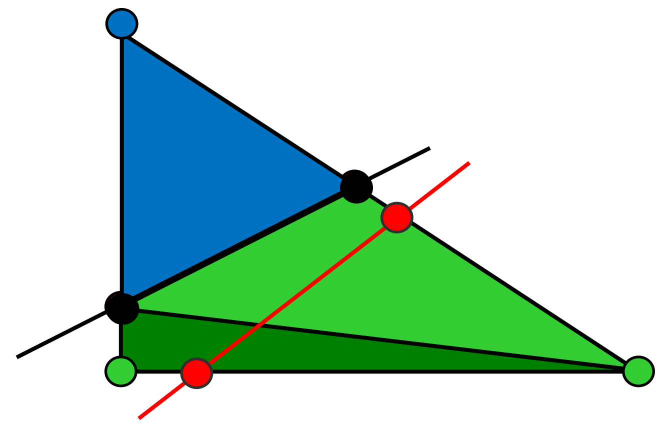
- Time stepping
  - How to handle dynamic unknowns as interface evolves
- Matrix conditioning
  - Issue common to “all” enriched finite element methods
  - Linearly dependent system of equations if produced as support vanished for enriched degrees of freedom
    - Same as small angle issue
- Physics-geometry coupling
  - How to develop full Newton methods when unknowns are dynamic within a nonlinear iteration loop
  - Ongoing work in this area
- Stabilized enriched finite elements
  - Little work has been done here

Research Challenge: Evolving Interfaces in Enriched Finite Element Methods

- How do we handle the moving interface?



- What do we do when nodes change material?



- This is an issue for all enriched finite element methods
  - CDFEM
  - XFEM – Issue when nodes change material

Model Problem: Scalar Advection-Diffusion

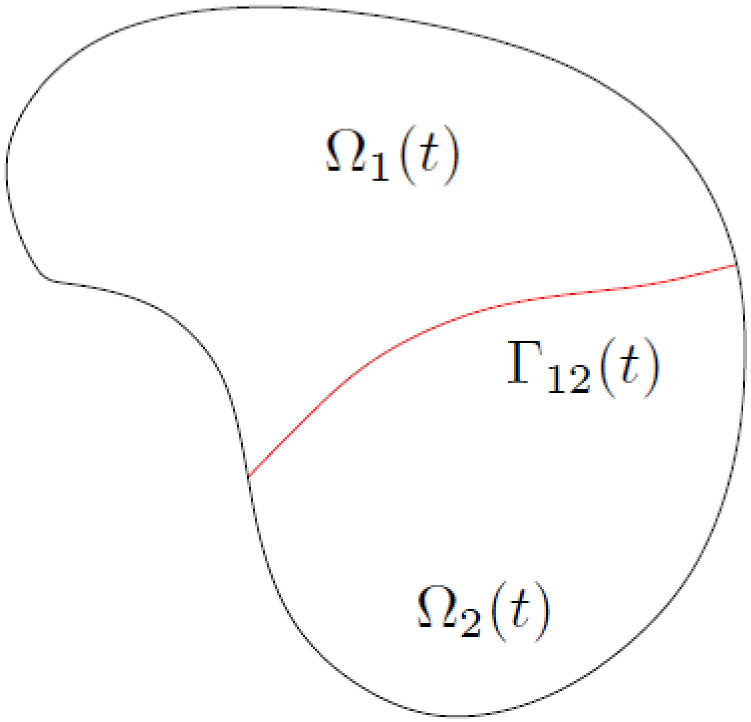
- Level Set Equation for interface motion

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

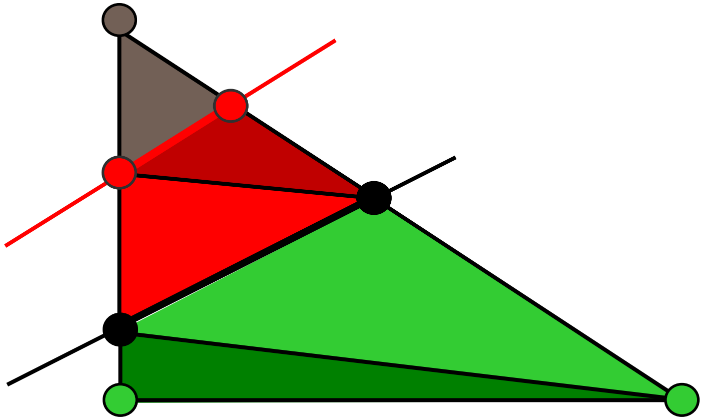
- Scalar advection-diffusion

$$\frac{\partial \psi}{\partial t} + \mathbf{u} \cdot \nabla \psi - \alpha \nabla^2 \psi = s(\mathbf{x}, t)$$

- Allow arbitrary discontinuities in fields across interface
  - Discontinuous value and gradient



Approach for Dynamic Discretizations: Subdomain Integration



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

$$\Omega_1^n \cap \Omega_1^{n+1} \quad \Omega_1^n \cap \Omega_2^{n+1}$$
$$\Omega_2^n \cap \Omega_1^{n+1} \quad \Omega_2^n \cap \Omega_2^{n+1}$$

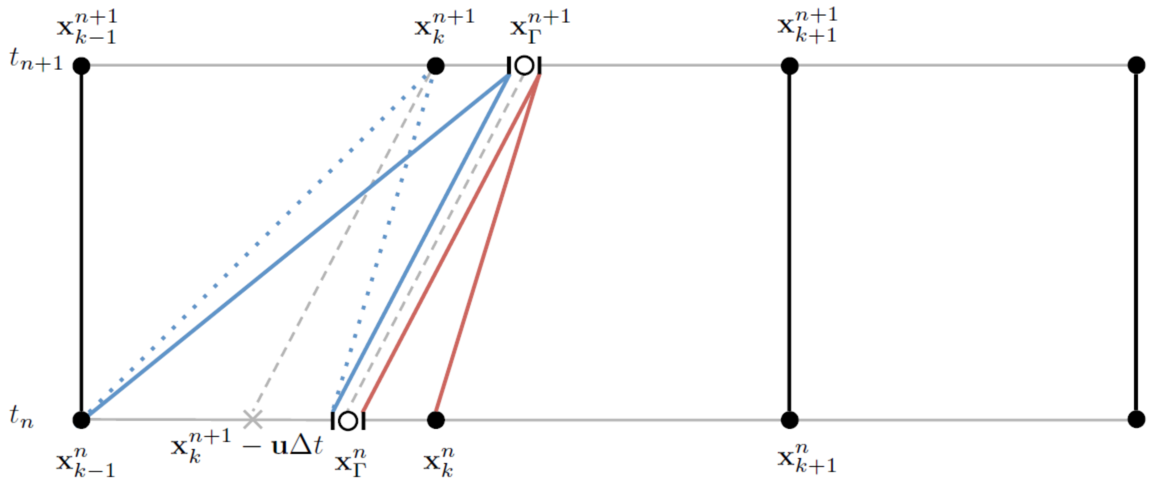
  - Scalar advection – Backward Euler

$$\int_\Omega \left(\frac{\partial \psi}{\partial t} + \mathbf{u} \cdot \nabla \psi \right) w_i \mathrm{d}\Omega = \sum_I \sum_J \int_{\Omega_I^n \cap \Omega_J^{n+1}} \left(\frac{\psi_J^{n+1} - \psi_I^n}{\Delta t} + \mathbf{u} \cdot \nabla \psi_J^{n+1} \right) w_i \mathrm{d}\Omega$$

  - Careful formation of the time term evaluates fields at times when that field is present, $\psi_J^{n+1}(\mathbf{x})$ when $\mathbf{x} \in \Omega_J^{n+1}$ and $\psi_I^n(\mathbf{x})$ when $\mathbf{x} \in \Omega_I^n$
  - However, this does involve differencing across material boundaries: ψ_J^{n+1}-ψ_I^n when $I \neq J$
  - Proposed by Fries and Zilian (2009) but shown to be insufficient for strong discontinuities by Henke et al. (2014)

Approach for Dynamic Discretizations: Semi-Lagrangian Advection

- Semi-Lagrangian advection
  - Discretize time and advection terms simultaneously to avoid dispersive errors
    $$\int_\Omega \left(\frac{\partial \psi}{\partial t} + \mathbf{u}\cdot\nabla\psi\right) w_i \mathrm{d}\Omega = \int_\Omega \frac{D\psi}{Dt} w_i \mathrm{d}\Omega \approx \sum_J \int_{\Omega_J^{n+1}} \frac{\psi_J^{n+1}(\mathbf{x}) - \psi_J^n(\mathbf{x}^*)}{\Delta t} w_i \mathrm{d}\Omega$$
  - For straight line characteristics: $\mathbf{x}^* = \mathbf{x} - \mathbf{u}\Delta t$
  - Quantity $\psi_J^n(\mathbf{x}^*)$ evaluated by interpolation
    - May be overly diffusive
  - Avoids differencing across material boundaries by tracing back to previous location
  - Less clear how to handle arbitrary interface motion (i.e. phase change)



Approach for Dynamic Discretizations: Extrapolation from Previous Location

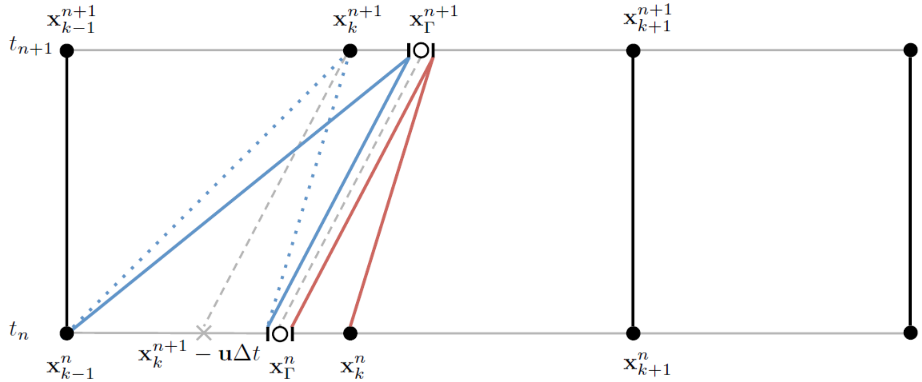
- Extrapolation from previous location
  - Essentially method by Henke et al. (2014) for XFEM (termed semi-Lagrangean)

$$\int_\Omega \frac{D\psi}{Dt} w_i \mathrm{d}\Omega \approx \sum_J \int_{\Omega_J^{n+1}} \left(\frac{\psi_J^{n+1}(\mathbf{x}) - \hat{\psi}_J^n(\mathbf{x})}{\Delta t} + \mathbf{u} \cdot \nabla \psi_J^{n+1}(\mathbf{x}) \right) w_i \mathrm{d}\Omega$$

$$\hat{\psi}_{J,k}^n = \begin{cases} \psi_J^n(\mathbf{x}_k), & S^n(\mathbf{x}_k) = S^{n+1}(\mathbf{x}_k) \\ \psi_J^n(\mathbf{x}^*) + (\mathbf{x}_k - \mathbf{x}^*) \cdot \nabla \psi_J^n(\mathbf{x}^*), & S^n(\mathbf{x}_k) \neq S^{n+1}(\mathbf{x}_k) \end{cases}$$

$S^{n+1}(\mathbf{x})$ is set of all materials present at $\mathbf{x}$

  - Allows time and advection terms to be handled separately
  - Avoids differencing across material boundaries by tracing back to previous location
  - Involves extrapolation from previous location to current location
  - Extrapolation may be poorly defined because of multi-valued gradient in 2-D and 3-D
  - Even for weakly discontinuous fields, the extrapolated field is strongly discontinuous

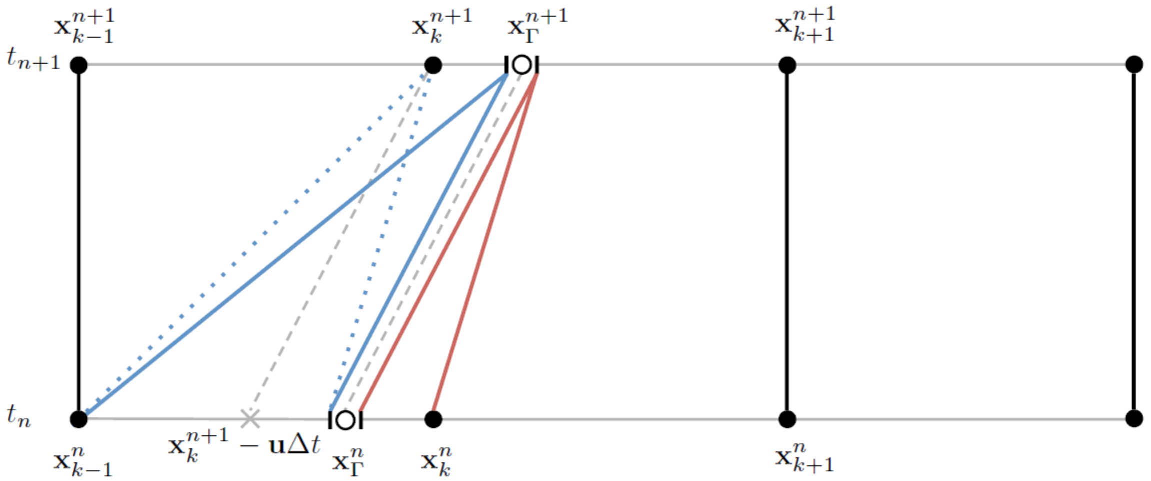


Approach for Dynamic Discretizations: Interface Extrapolation (IE)

- Extrapolation from closest point on previous interface

$$\hat{\psi}^n_{J,k} = \begin{cases} \psi^n_J(\mathbf{x}_k), & S^n(\mathbf{x}_k) = S^{n+1}(\mathbf{x}_k) \\ \psi^n_J(P^n(\mathbf{x}_k)) + (\mathbf{x}_k - P^n(\mathbf{x}_k)) \cdot \nabla\psi^n_J(P^n(\mathbf{x}_k)), & S^n(\mathbf{x}_k) \neq S^{n+1}(\mathbf{x}_k) \end{cases}$$

  - Point $P^n(\mathbf{x})$ is the nearest point to $\mathbf{x}$ on the previous interface
  - Identical to extrapolation from previous location in 1-D if CFL<1
  - Extrapolation may be poorly defined due to discontinuous gradient in 2-D and 3-D
  - Even for weakly discontinuous fields, the extrapolated field is strongly discontinuous



Approach for Dynamic Discretizations: Moving Mesh (MM)

- Uses Arbitrary Lagrangian Eulerian (ALE) technology for moving meshes
  - Relates time derivative following a moving point to the time derivative fixed in space

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

$$\left.\frac{\partial \psi}{\partial t}\right|_{x} = \left.\frac{\partial \psi}{\partial t}\right|_{\xi} - \dot{\mathbf{x}} \cdot \nabla\psi$$

$$\int_{\Omega} \frac{D\psi}{Dt} w_i \mathrm{d}\Omega \approx \sum_J \int_{\Omega_J^{n+1}} \left(\frac{\psi_J^{n+1}(\mathbf{x}) - \psi_J^n(\mathbf{X})}{\Delta t} + (\mathbf{u} - \dot{\mathbf{x}}) \cdot \nabla\psi_J(\mathbf{x}) \right) w_i \mathrm{d}\Omega \quad \dot{\mathbf{x}} = \frac{\mathbf{x} - \mathbf{X}}{\Delta t}$$

- Using the closest point projection

$$\int_{\Omega} \frac{D\psi}{Dt} w_i \mathrm{d}\Omega \approx \sum_J \int_{\Omega_J^{n+1}} \left(\frac{\psi_J^{n+1}(\mathbf{x}) - \tilde{\psi}_J^n(\mathbf{x})}{\Delta t} + (\mathbf{u} - \dot{\mathbf{x}}(\mathbf{x})) \cdot \nabla\psi_J^{n+1}(\mathbf{x}) \right) w_i \mathrm{d}\Omega$$

$$\tilde{\mathbf{x}}_k^n = \begin{cases} \mathbf{x}_k, & S^n(\mathbf{x}_k) = S^{n+1}(\mathbf{x}_k) \\ P^n(\mathbf{x}_k), & S^n(\mathbf{x}_k) \neq S^{n+1}(\mathbf{x}_k) \end{cases} \quad \begin{aligned} \tilde{\psi}_{J,k}^n &= \psi_J^n(\tilde{\mathbf{x}}_k^n) \\ \tilde{\psi}_J^n(\mathbf{x}) &= \sum_k \tilde{\psi}_{J,k}^n w_k \end{aligned} \quad \dot{\mathbf{x}}(\mathbf{x}) = \sum_k \frac{\mathbf{x}_k^{n+1} - \tilde{\mathbf{x}}_k^n}{\Delta t} w_k$$

- Recovers semi-Lagrangian in limit of $\dot{\mathbf{x}} = \mathbf{u}$

Approach for Dynamic Discretizations: 2nd Order Interface Extrapolation (IE)

- Second order time accuracy via Crank-Nicolson (CN)
  - Straightforward to average advection operator

$$\sum_J \int_{\Omega_J^{n+1}} \left(\frac{\psi_J^{n+1}(\mathbf{x}) - \hat{\psi}_J^n(\mathbf{x})}{\Delta t} + \mathbf{u} \cdot \frac{\nabla \psi_J^{n+1}(\mathbf{x}) + \nabla \hat{\psi}_J^n(\mathbf{x})}{2} \right) w_i \mathrm{d}\Omega$$

- Second order time accuracy via BDF2
  - Requires extrapolation of n-1 state

$$\sum_J \int_{\Omega_J^{n+1}} \left(\frac{\frac{3}{2}\psi_J^{n+1}(\mathbf{x}) - 2\hat{\psi}_J^n(\mathbf{x}) + \frac{1}{2}\hat{\psi}_J^{n-1}(\mathbf{x})}{\Delta t} + \mathbf{u} \cdot \nabla \psi_J^{n+1}(\mathbf{x}) \right) w_i \mathrm{d}\Omega$$

Approach for Dynamic Discretizations: 2nd Order Moving Mesh (MM)

- Second order time accuracy via Crank-Nicolson (CN)
  - Dynamic domain requires integral to evaluated at half plane

$$\sum_J \int_{\Omega_J^{n+\frac{1}{2}}} \left(\frac{\psi_J^{n+1}(\mathbf{x}) - \tilde{\psi}_J^n(\mathbf{x})}{\Delta t} + (\mathbf{u} - \dot{\mathbf{x}}(\mathbf{x})) \cdot \frac{\nabla \psi_J^{n+1}(\mathbf{x}) + \nabla \tilde{\psi}_J^n(\mathbf{x})}{2} \right) w_i \mathrm{d}\Omega$$

$$\mathbf{x}_k^{n+\frac{1}{2}} \equiv \frac{1}{2}(\tilde{\mathbf{x}}_k^n + \mathbf{x}_k^{n+1})$$

- Second order time accuracy via BDF2
  - Requires nearest point projection of n-1 state

$$\sum_J \int_{\Omega_J^{n+1}} \left(\frac{\frac{3}{2}\psi_J^{n+1}(\mathbf{x}) - 2\tilde{\psi}_J^n(\mathbf{x}) + \frac{1}{2}\tilde{\psi}_J^{n-1}(\mathbf{x})}{\Delta t} + (\mathbf{u} - \dot{\mathbf{x}}(\mathbf{x})) \cdot \nabla \psi_J^{n+1}(\mathbf{x}) \right) w_i \mathrm{d}\Omega$$

$$\dot{\mathbf{x}}(\mathbf{x}) = \sum_k \frac{\frac{3}{2}\mathbf{x}_k^{n+1} - 2\tilde{\mathbf{x}}_k^n + \frac{1}{2}\tilde{\mathbf{x}}_k^{n-1}}{\Delta t} w_k$$

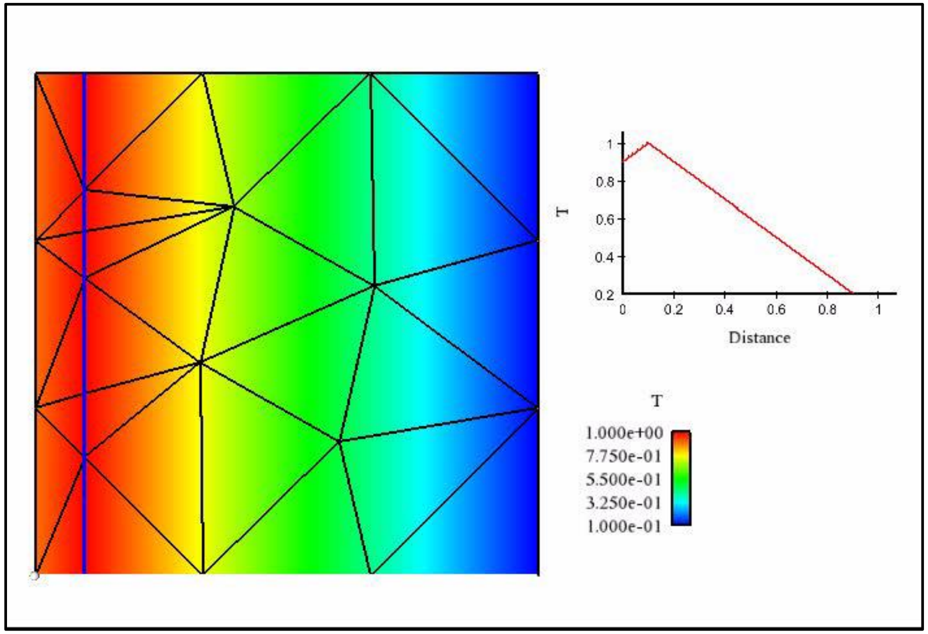
Approach for Dynamic Discretizations: Method Summary

- Capturing arbitrary discontinuities on moving interfaces
  - All enriched methods require specialized method for handling dynamic discretization
- Subdomain integration
  - Requires decomposition with respect to old and new configurations
  - Differences across material boundaries
  - Not convergent for strong discontinuities (Henke et al. 2014)
- Interface Extrapolation
  - Poorly defined at element boundaries in higher dimensions due to discontinuous gradient
  - The extrapolation of a weak discontinuity is strongly discontinuous
  - 2^{nd} order versions straightforward to implement
- Moving Mesh
  - Only requires value, not gradient from nearest point, so it is well defined in higher dimensions
  - Crank-Nicolson requires assembly over mid-plane configuration
  - 2^{nd} order time accuracy is straightforward via BDF2

Results: Patch Tests

- Constant advection of a strong discontinuity
  - Subdomain integration method does not converge (Henke et al. 2014)
  - Both interface extrapolation and moving mesh achieve machine precision

- Constant advection of a weak discontinuity
  - All proposed methods should achieve machine precision (Subdomain integration not tested.)



Results: MMS for 1-D Advection-Diffusion with Strong and Weak Discontinuity from Contact Resistance

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- Constant advection of a sinusoid
  - Trivial level set solution for constant advection velocity

$$\phi(x,t) = (x - x_0) - ut$$

  - Method of manufacture solutions for advection-diffusion with both strong and weak discontinuity

$$\psi(x,t) = \begin{cases} \kappa \sin(c_x[x - (x_0 + ut)]) \exp(-t/c_t), & \phi \le 0 \\ \sin(c_x[x - (x_0 + ut)]/\kappa) \exp(-t/c_t) + \Delta, & \phi > 0 \end{cases}$$

$$\alpha_l \frac{\partial \psi}{\partial x}\bigg|_{\phi=0^-} = \alpha_r \frac{\partial \psi}{\partial x}\bigg|_{\phi=0^+} = \beta \left(\psi|_{\phi=0^+} - \psi|_{\phi=0^-} \right)$$

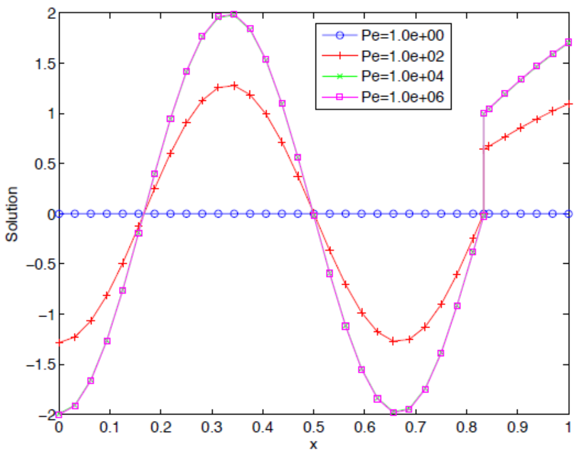
$$\Delta(t) = 2\exp(-t/c_t)/(\beta c_x c_t) \qquad s(x,t) = \begin{cases} 0, & \phi \le 0 \\ -\frac{2}{\beta c_x c_t^2} \exp(-t/c_t), & \phi > 0 \end{cases}$$

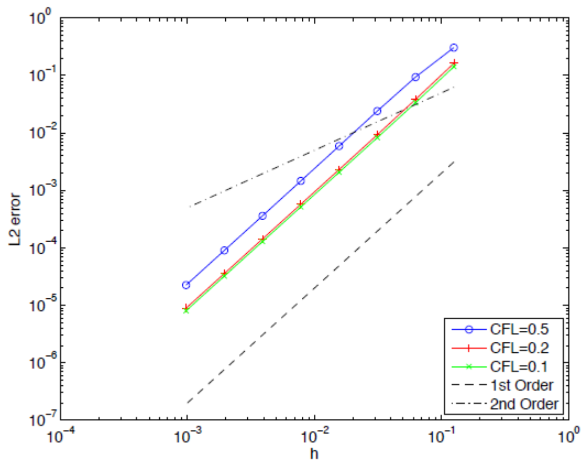
  - Examine convergence with in space and time for various Courant numbers

$$\mathcal{E}_{L_2,\Omega} = \|\psi^h - \psi(\mathbf{x},t)\|_\Omega = \left(\int_\Omega \left(\psi^h - \psi(\mathbf{x},t)\right)^2 \mathrm{d}\Omega \right)^{1/2}$$

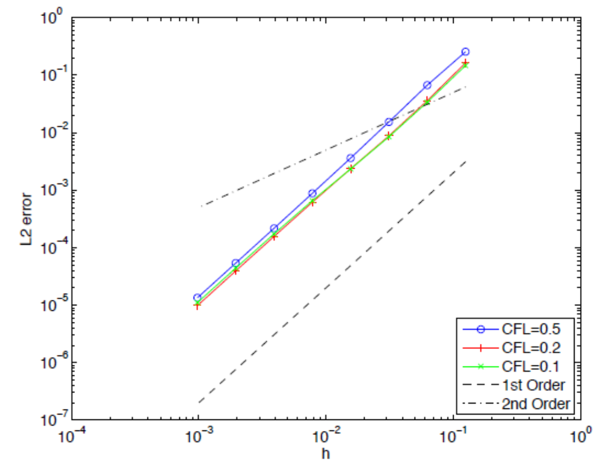
Results: MMS for 1-D Advection-Diffusion with Strong and Weak Discontinuity from Contact Resistance

- Constant advection advection of a sinusoid
  - 2nd order convergence using BDF2 for either Interface Extrapolation or Moving Mesh methods



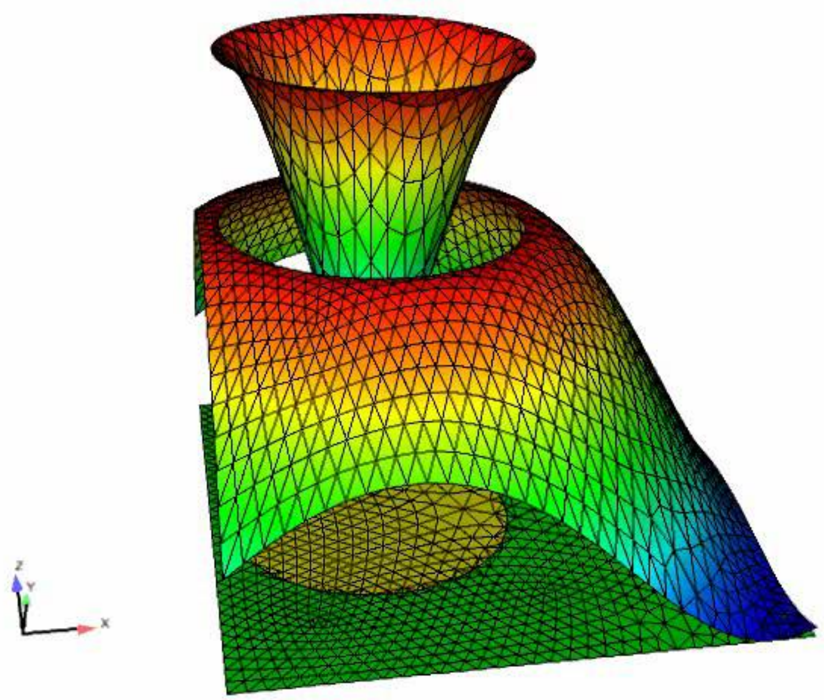


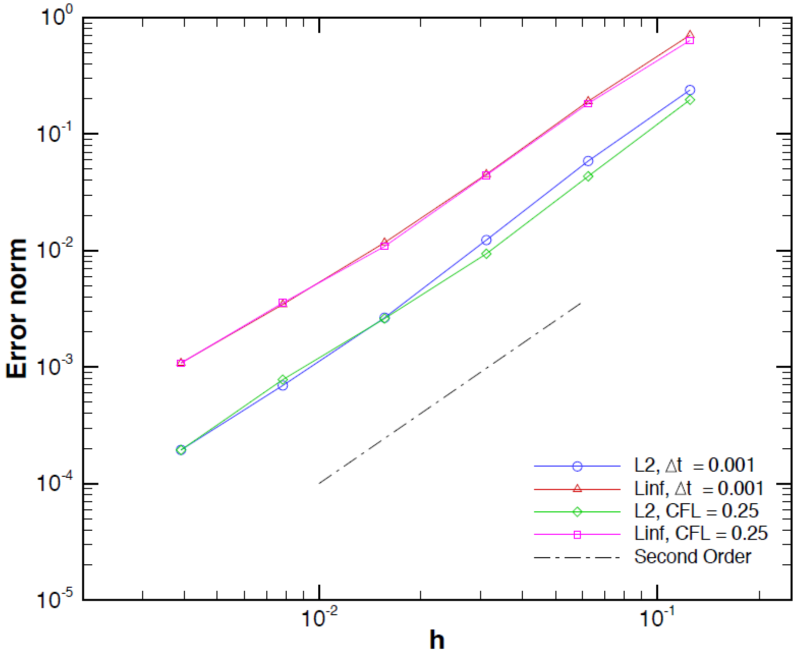
(a) Moving mesh (MM)



(b) Interface extrapolation (IE)

Verification via MMS for 2D Advection-Diffusion with a Sharp Discontinuity





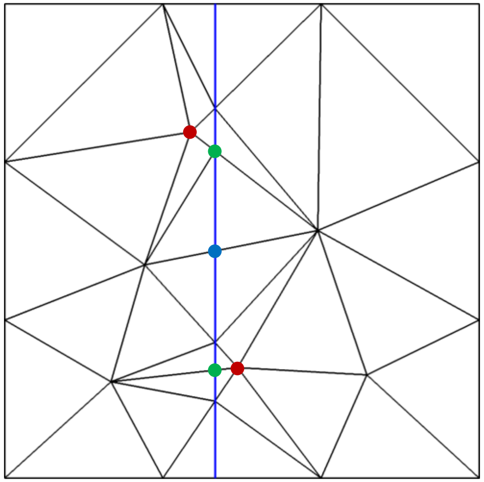
Convergence plot for the 2-D advection-diffusion problem with contact resistance, using the BDF2 time integrator

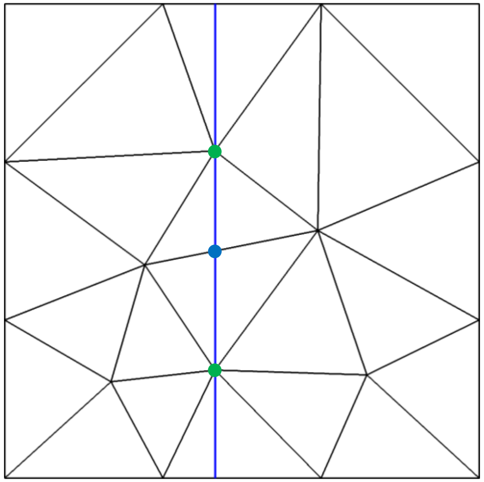
Research Challenge: Circumventing Poor Conditioning of Enriched System of Equations

- Common issue to GFEM, XFEM, cutFEM, CDFEM
  - Linearly dependent as support vanishes
  - Small angle poor conditioning in CDFEM
- Previously published solutions
  - Moës et al. (2002) – Snapping interface to nodes in XFEM
    - Modifies geometry by moving interface
- Proposed solutions
  - Guaranteed quality CDFEM – Snap background mesh to interface
    - Avoids disturbing interface location
    - Difficult to implement (or impossible) near boundaries or other interfaces
  - Specially designed preconditioners based on hierarchical basis

Guaranteed Quality Conformal Decomposition Finite Element Method (CDFEM)

- Simple Concept
  - Determine edge cut locations using intersection of level set and edge
  - When any of the edges of a node are cut below a specified ratio, move the node to the closest edge cut location (snap background mesh nodes to interface, •→•)
- Related Work
  - Moës et al. (2002) – Snapping interface to nodes in XFEM
  - Labelle and Shewchuk (2007) - Isosurface stuffing for guaranteed quality meshes that conform to an isosurface
  - Rangarajan and Lew (2012) - Universal Meshes for guaranteed quality triangulations that conform to a smooth surface



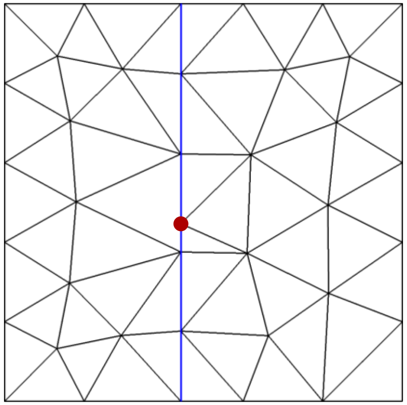


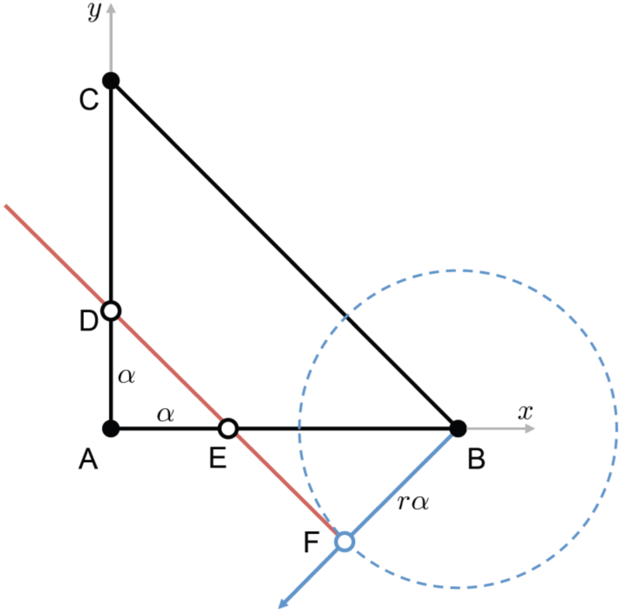
Choosing the Edge Snap Tolerance in 2D

- How High Can the Snap Tolerance Be?
  - Can we push this so that no edge get cut, only snapped? NO
- Maximum snap tolerance for non-degenerate triangles
  - Cannot allow all nodes of an element to snap to the interface
  - Maximum snap tolerance, α, in terms of maximum to minimum edge length ratio, r

$$\alpha = \frac{\sqrt{2}r - 1}{2r^2 - 1}$$

  - Maximum snap tolerance of 0.41 for equilateral triangle mesh and 1/3 for structured mesh



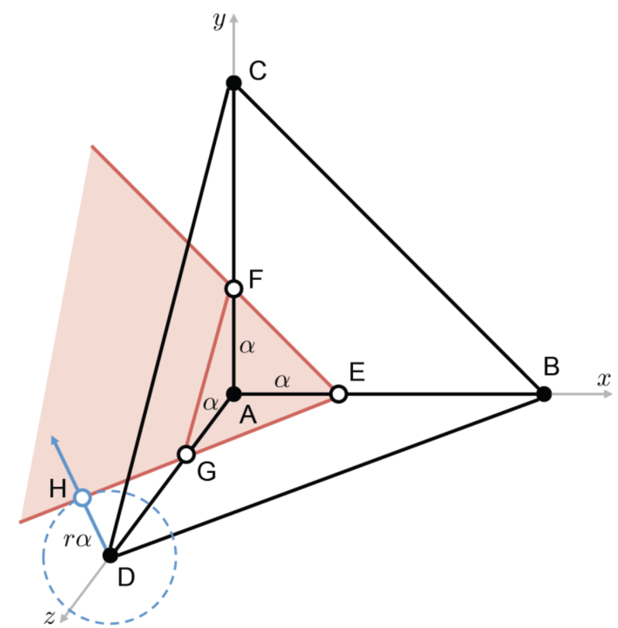


Choosing the Edge Snap Tolerance in 3D

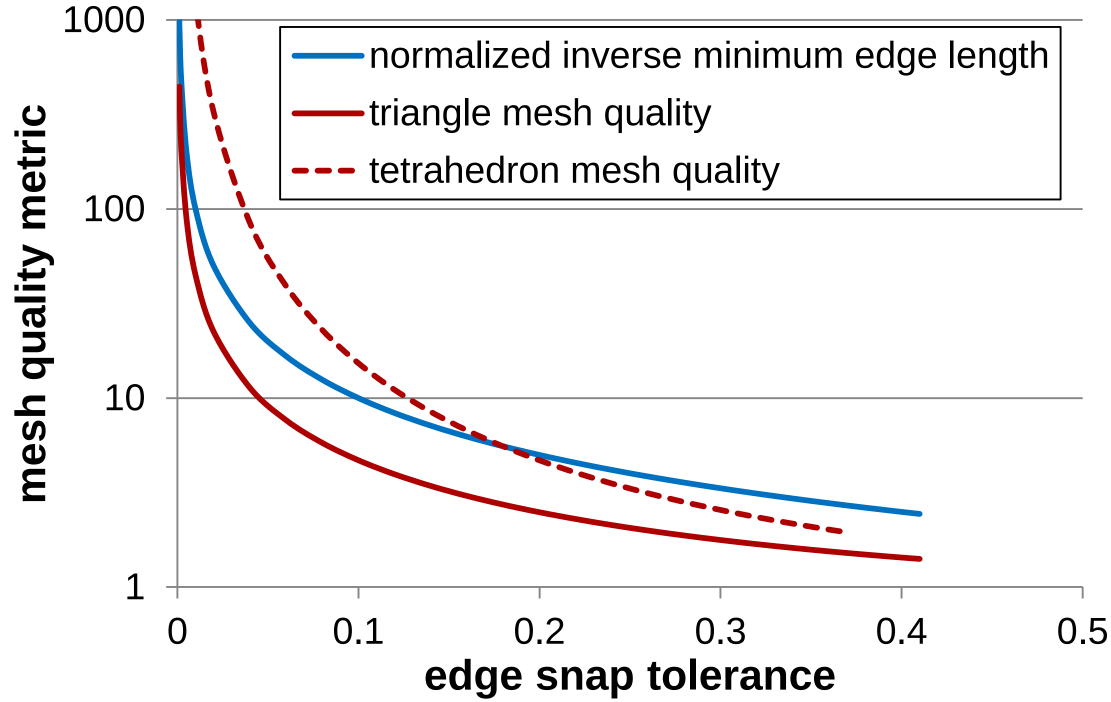
- Maximum snap tolerance for non-degenerate tetrahedral mesh
  - Cannot allow all nodes of an element to snap to the interface
  - Maximum snap tolerance, α, in terms of maximum to minimum edge length ratio, r

$$\alpha = \frac{\sqrt{3}r - 1}{3r^2 - 1}$$

  - Maximum snap tolerance of 0.37 for equilateral tetrahedron mesh and 0.29 for structured mesh



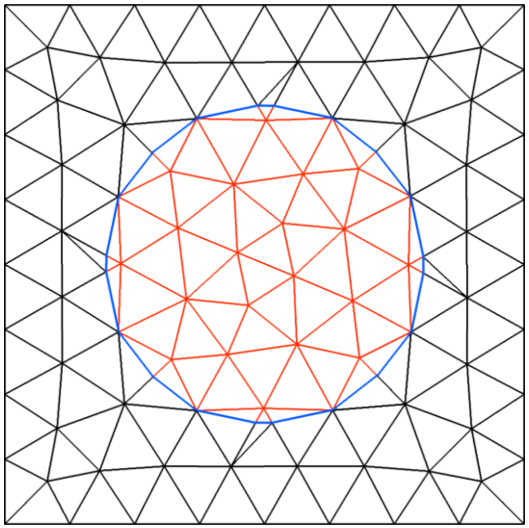
Guaranteed Mesh Quality As a Function of Edge Snap Tolerance

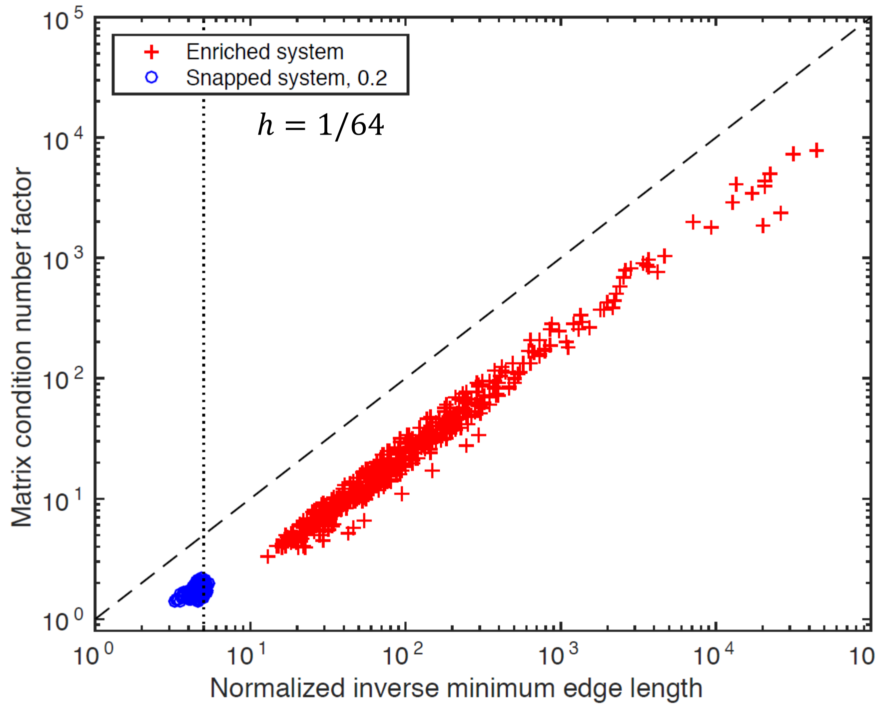


- Mesh quality measures
  - Normalized inverse minimum edge length, λ
  - Element quality (Berzins 1998)

    triangles: $Q_w = \frac{1}{12\sqrt{3}A}\left(\sum_e h_e\right)^2$ tetrahedrons: $Q_w = \frac{1}{1296\sqrt{2}V}\left(\sum_e h_e\right)^3$
  - For snap tolerance of 0.2 for equilateral triangle, λ=5, Q_w=2.49
  - For snap tolerance of 0.1 for equilateral tetrahedron, λ=10, Q_w=15.3

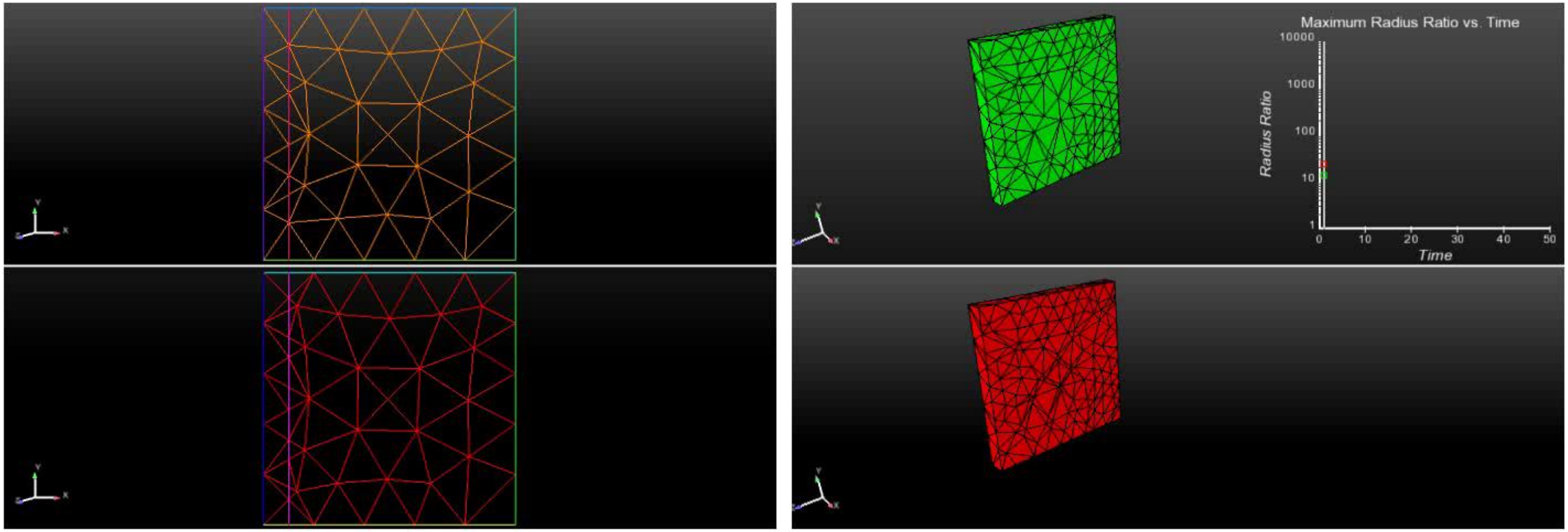
Quantitative Improvement in Condition Number and Minimum Edge Length in 2D





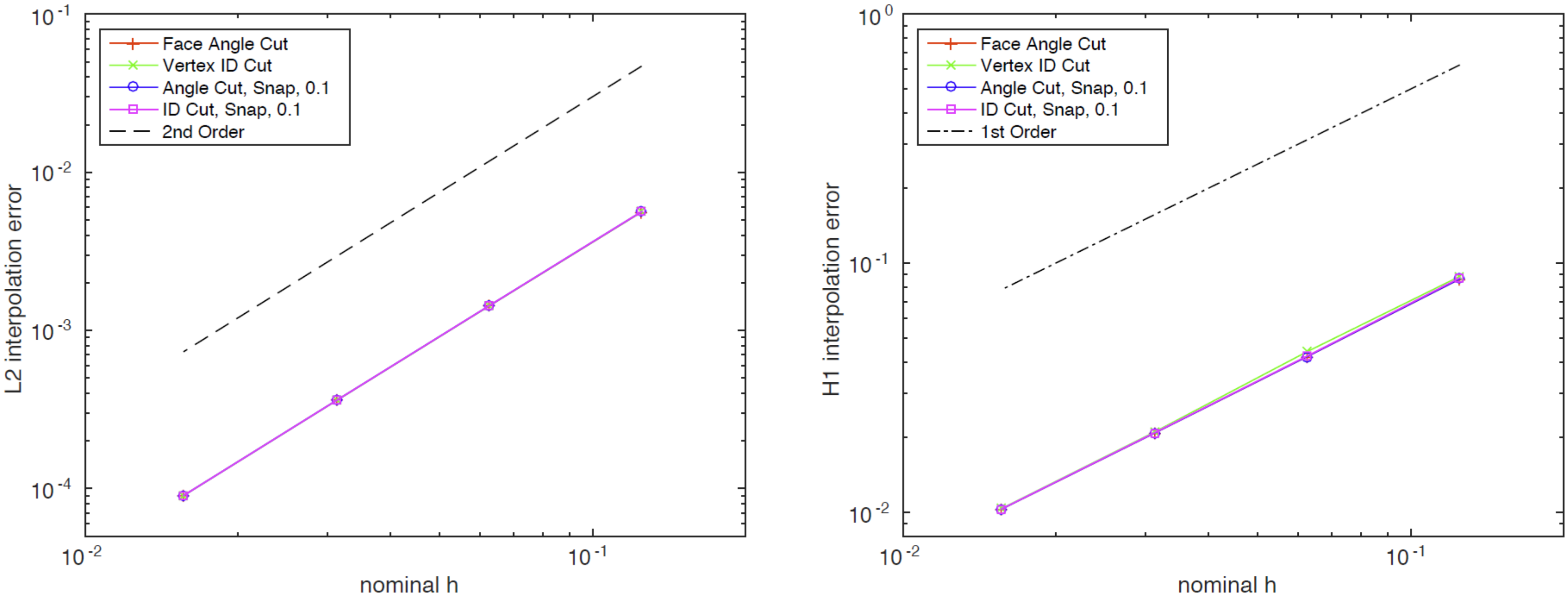
- Test
  - Perform 500 decompositions for circle with random radius with and without snapping
  - Evaluate minimum edge length and condition number of Laplacian matrix
- Results
  - Without snapping, both minimum edge length and condition number shows many orders of variation. These quantities are highly correlated.
  - Snap tolerance of 0.2 reduces inverse minimum edge length and condition number to small multiples of uncut mesh values.

Qualitative Improvement Obtained by Snapping Nodes to Interface



- Improved angles, edge lengths, element volumes, radius ratio

Convergence of Interpolation Error in 3D



- Test
  - Decomposed mesh for sphere of radius $(\pi+1)/10$
  - Evaluate interpolation error with mesh refinement for function:

$$f(x,y) = (x - x_c)^2 + (y - y_c)^2 + (z - z_c)^2 - r^2$$

- Results
  - Solution error decreases at expected rates regardless of snapping or face cutting strategy
  - In fact, neither snapping or face cutting has a significant effect on the interpolation error as compared to mesh refinement

Creating Well-Conditioned Systems Without Modifying the Mesh Geometry

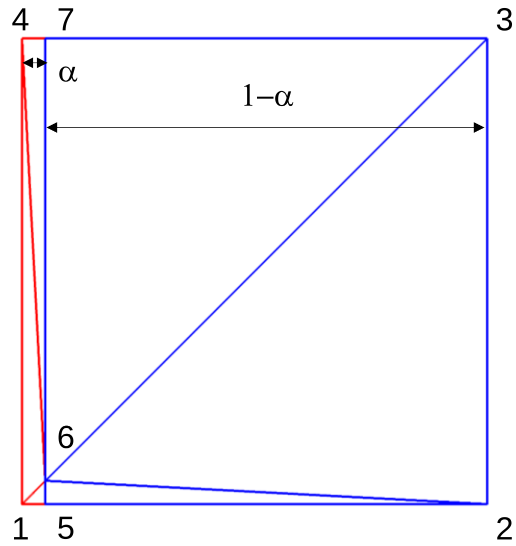
- Motivation
  - With multiple interfaces or near external boundaries slivers are unavoidable
- Ideas considered
  - Some form of stabilization?
    - Ghost penalty stabilization has been shown to eliminate poor conditioning in XFEM and cutFEM methods
  - Change of variables
    - Constrain added CDFEM nodes to have values in XFEM space of functions
      - Conceptually involves introducing constraints for CDFEM added nodes in terms of unknowns located at parent nodes
      - This produces well-conditioned systems for 1-sided problems!
    - Use hierarchical basis for added CDFEM nodes
      - Can be formed as either actual change of variables or as preconditioner for unaltered CDFEM system

Prototype poorly conditioned problem

- Modified Poisson Equation

  $$cT = \nabla^2 T$$

  - Mass-like and Laplacian term
  - Vary interface position, α



- Matrix (α=0.001)

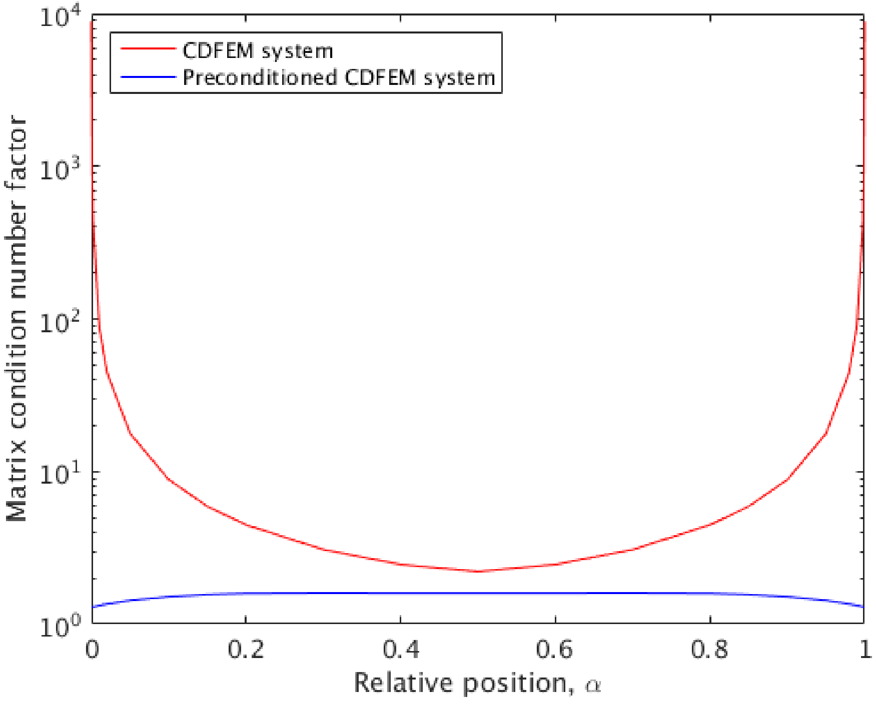
0.4995	0	0	0.0005	-0.0005	-0.4995	0
0	0.0011	-0.0005	0	-0.0000	-0.0005	0
0	-0.0005	0.0012	0	0	0.0001	-0.0005
0.0005	0	0	0.4995	0	-0.0005	-0.4995
-0.0005	-0.0000	0	0	0.5005	-0.5000	0
-0.4995	-0.0005	0.0001	-0.0005	-0.5000	1.0012	-0.0005
0	0	-0.0005	-0.4995	0	-0.0005	0.5006

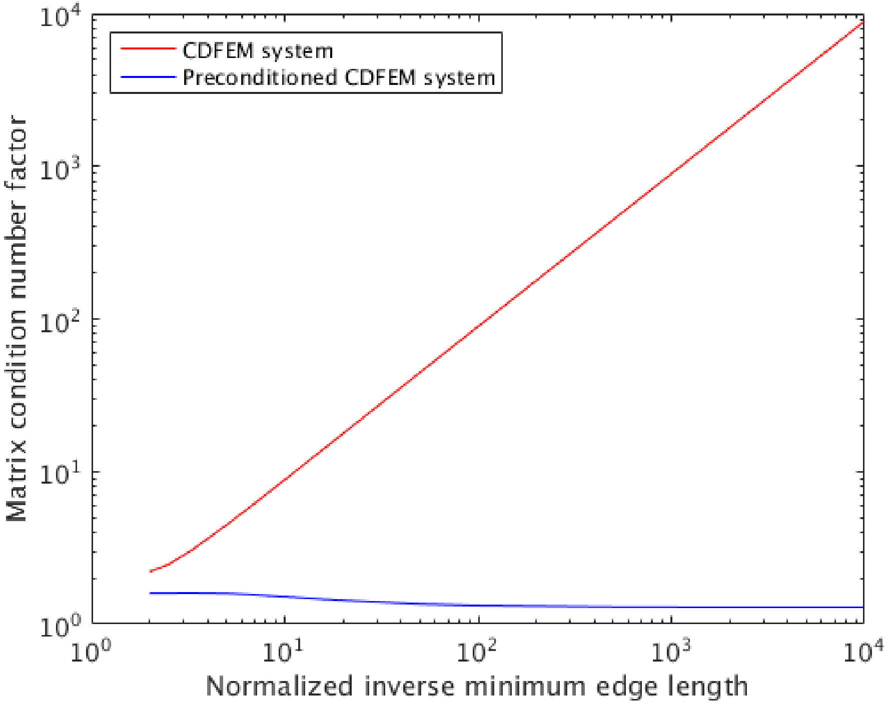
$$\times \frac{1}{0.001}$$

  - Growing disparity of row and column scales
  - Sliver elements generate penalty between nearby nodes

Conditioning of Prototype problem

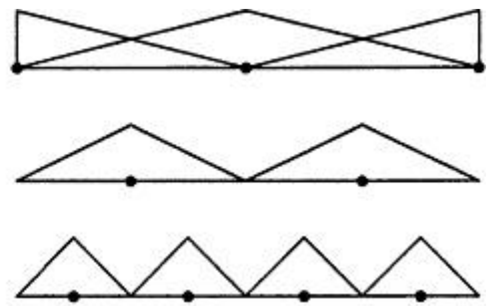
- Condition number ~ $1/(\alpha - \alpha^2)$
- Not helped by Jacobi preconditioning
- However, preconditioner based in hierarchical basis yields condition number nearly independent of edge cut position, α





Hierarchical Basis Functions

Standard Linear Lagrange Basis Functions



Linear Hierarchical Basis Functions

- Both have same approximation space

  $T = c\hat{T}$, T=Standard unknowns, $\hat{T}$=Hierarchical unknowns

- With only 1 level (CDFEM) the condition number for hierarchical basis ($\hat{A}$) is independent of added node location, unlike standard basis (A) (with Jacobi preconditioning)

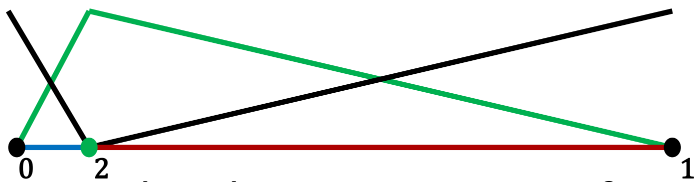
$$AT = b \quad \rightarrow \quad Ac\hat{T} = b$$
$$c^t Ac\,\hat{T} = c^t b \;\rightarrow\; \hat{A}\hat{T} = \hat{b}$$

- Can be posed as preconditioner of original system

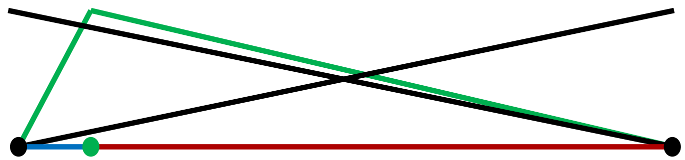
$$\hat{M}^{-1} = \hat{L}\hat{L}^t \qquad \hat{L}^t\hat{A}\hat{L} = L^t A L \;\text{ if }\; L = c\hat{L}$$

Application of Hierarchical Basis Functions to CDFEM Added Nodes – Hierarchical Basis

- CDFEM Basis Functions for weak discontinuities

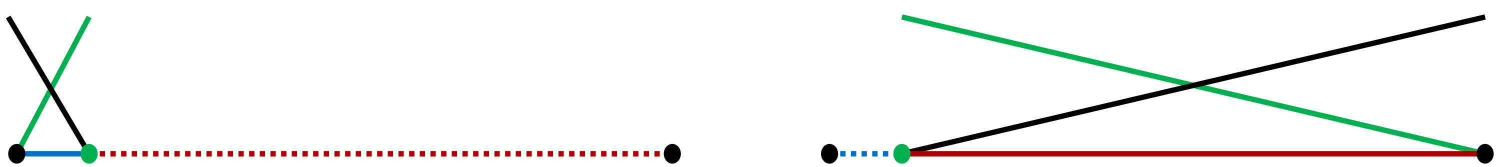


- Hierarchical Basis Functions for weak discontinuities

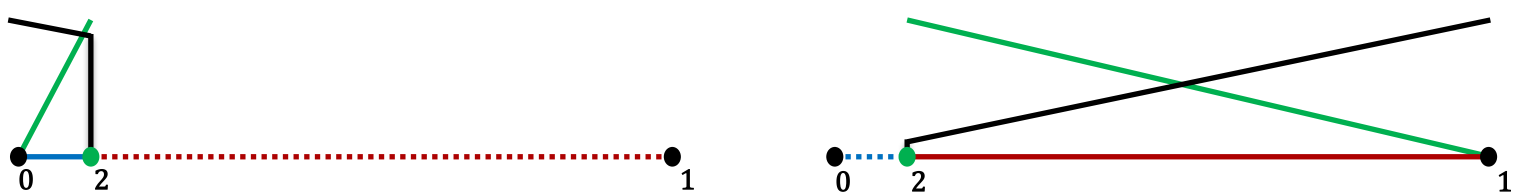


$$T_2 = (1-\alpha)T_0 + \alpha T_1 + \hat{T}_2$$

- CDFEM Basis Functions for strong discontinuities



- Hierarchical Basis Functions for strong discontinuities



$$T_2 = (1-\alpha)T_0 + \hat{T}_2$$

$$T_2 = \alpha T_1 + \hat{T}_2$$

Application of Hierarchical Basis Functions to CDFEM Added Nodes – Linear Algebra

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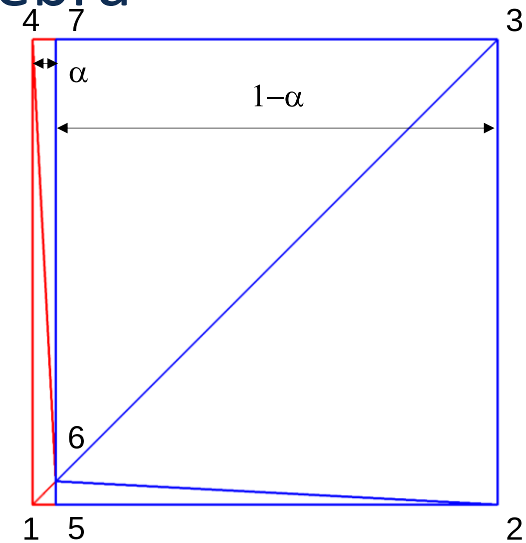
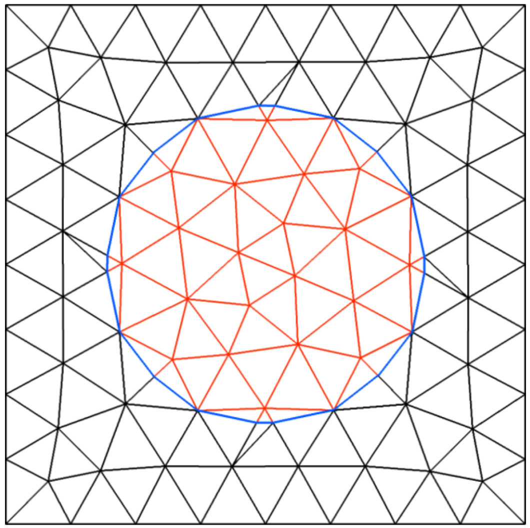
$$c = \begin{bmatrix} 1 & & & & & & \\ & 1 & & & & & \\ & & 1 & & & & \\ & & & 1 & & & \\ 1-\alpha & \alpha & & & 1 & & \\ 1-\alpha & & \alpha & & & 1 & \\ & & \alpha & 1-\alpha & & & 1 \end{bmatrix}$$

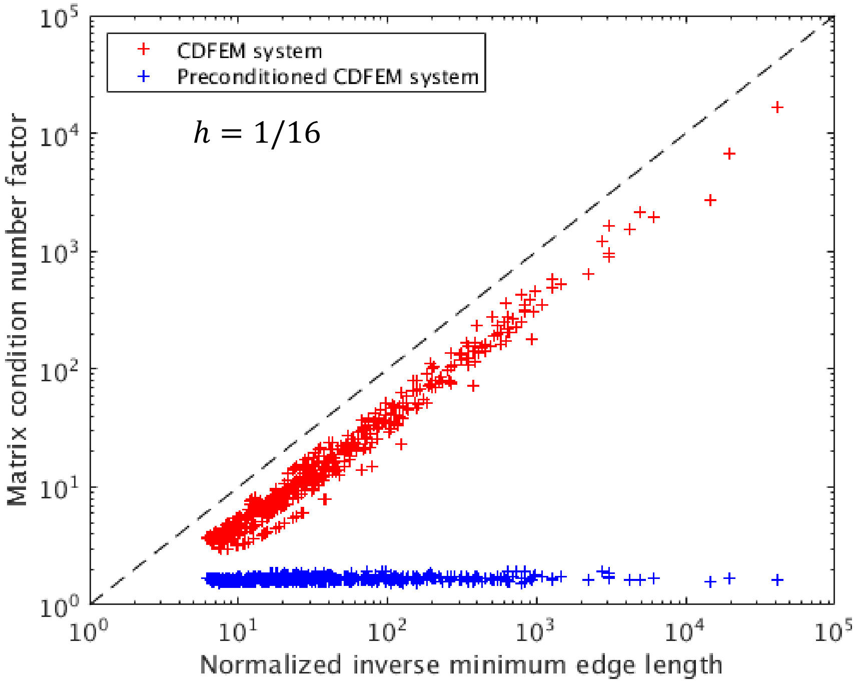


- Transformation from hierarchical to standard basis (c) is built edge by edge
- Hierarchical matrix preconditioner also readily approximated in terms of α based on scale of diagonal
- End result is that poor conditioning due to CDFEM slivers is removed

$$L^t AL = \begin{pmatrix} 1.1667 & -0.4583 & 0.0833 & -0.4583 & 0.0000 & 0.0369 & -0.0145 \\ -0.4583 & 1.0833 & -0.4583 & 0 & 0.0158 & -0.0303 & 0 \\ 0.0833 & -0.4583 & 1.1667 & -0.4583 & -0.0158 & 0.0342 & 0.0013 \\ -0.4583 & 0 & -0.4583 & 1.0833 & 0 & -0.0303 & 0.0184 \\ 0.0000 & 0.0158 & -0.0158 & 0 & 0.5000 & -0.4995 & 0 \\ 0.0369 & -0.0303 & 0.0342 & -0.0303 & -0.4995 & 1.0002 & -0.0005 \\ -0.0145 & 0 & 0.0013 & 0.0184 & 0 & -0.0005 & 0.5001 \end{pmatrix}$$

Quantitative Improvement in Condition Number using Hierarchical Basis (HB) Preconditioner





- Test
  - Perform 500 decompositions for circle with random radius with and without HB preconditioner
  - Evaluate minimum edge length and condition number of modified Poisson matrix
- Results
  - Condition number of HB preconditioned matrix is nearly independent of minimum edge length

Summary: Matrix Conditioning

- Findings
  - Slivers do indeed cause poor conditioning
  - Poor conditioning is removed using concepts from hierarchical basis
- Consequences
  - Only removes poor conditioning from slivers, not from overall problem size
    - Require ML preconditioner for overall system
  - Sliver conditioning is also handled by incomplete factorization
    - Limited usefulness in parallel
- On-going work
  - Implement and test hierarchical preconditioners for strongly discontinuous problems
  - Implement preconditioners in production code
- Impact
  - Key part of large scale, parallel scalable solution strategy

Future Work

- Research Topics
  - Coupling between interface motion and physics
    - Capillary dominated flows
    - Fluid-structure interaction (particularly stiff fluids)
    - Full Newton strategies and discrete space requirements
  - Stabilized enriched finite elements
  - Using enriched finite element methods to eliminate user-generated meshes
    - Remove costly step in analysis
    - Allows dynamic interfaces include topology optimization
- Exciting applications
  - Traditional analysis has focused on static, meshable geometries
  - Exascale computing opens up possibilities to address more problems with increasing complexity and geometric fidelity
    - Requires scalable algorithms both in problem size and processor count