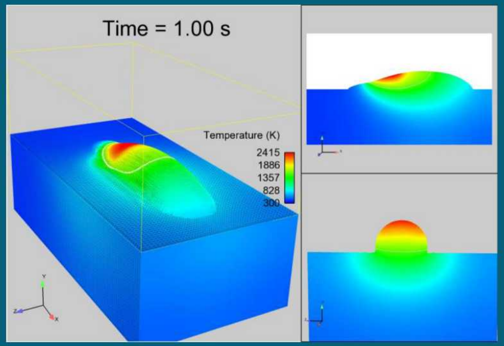
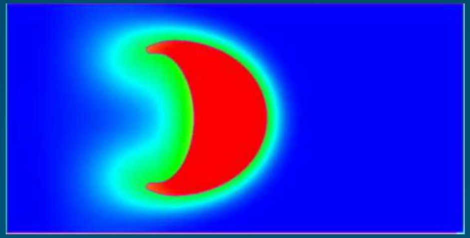
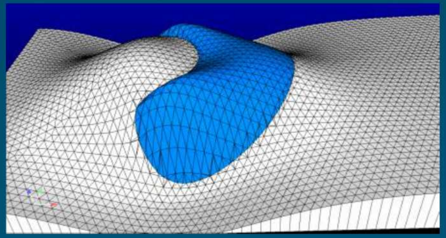
Sandia National Laboratories

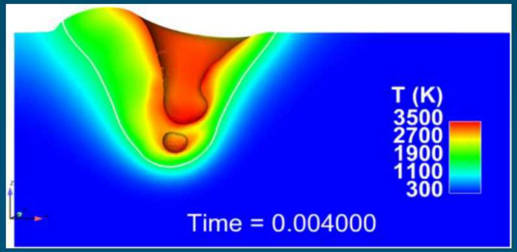
SAND2019-3229C

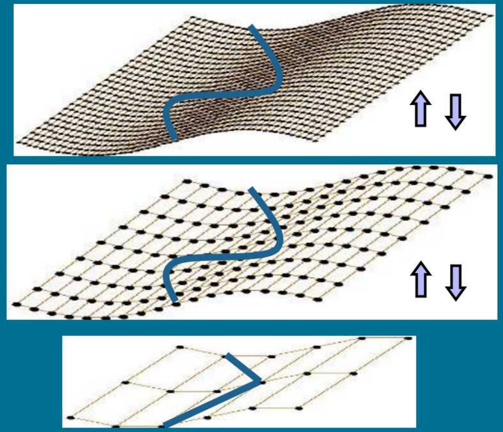
Assessment of the Accuracy and Conditioning of an Extended Conformal Decomposition Finite Element Method for Fluid-Fluid Interfaces











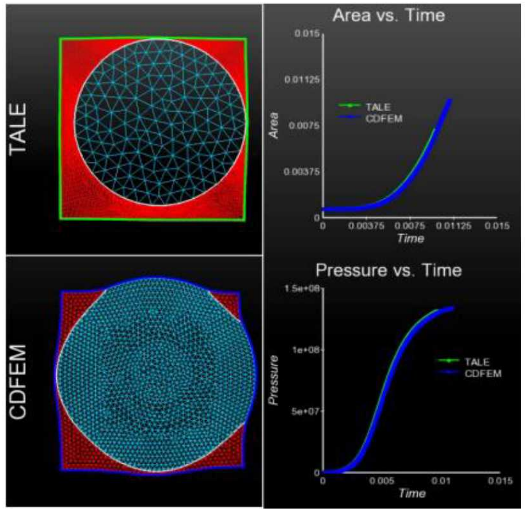
PRESENTED BY

David R. Noble

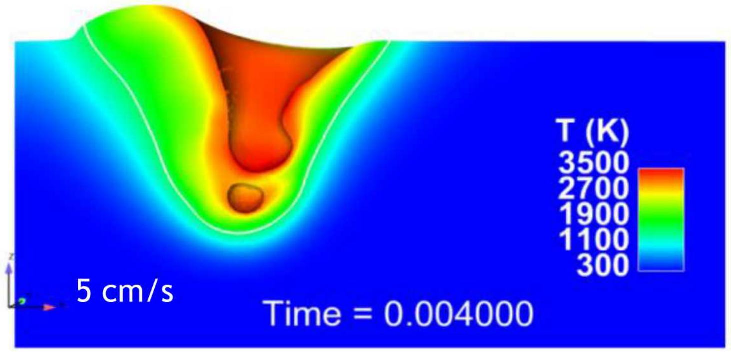
U.S. DEPARTMENT OF ENERGY NNSA

Motivation

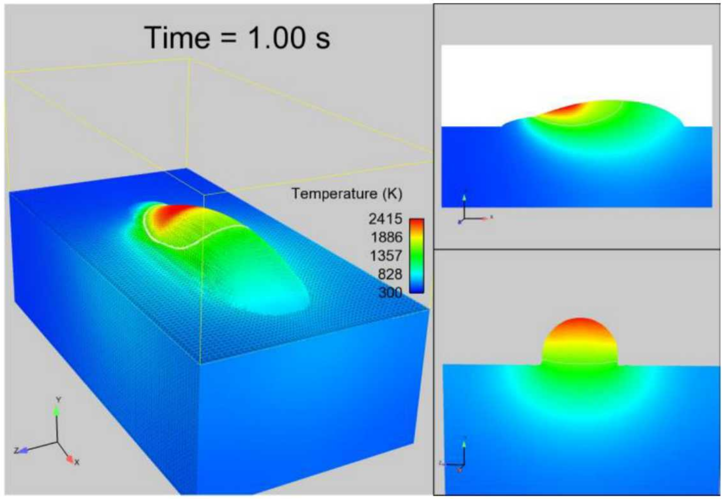
Numerous fluids problems with moving or topologically complex interfaces with discontinuous physics and fields



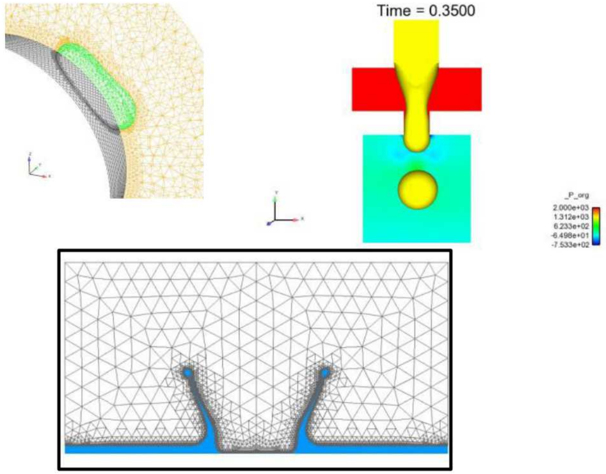
Conductive burn
of energetic materials



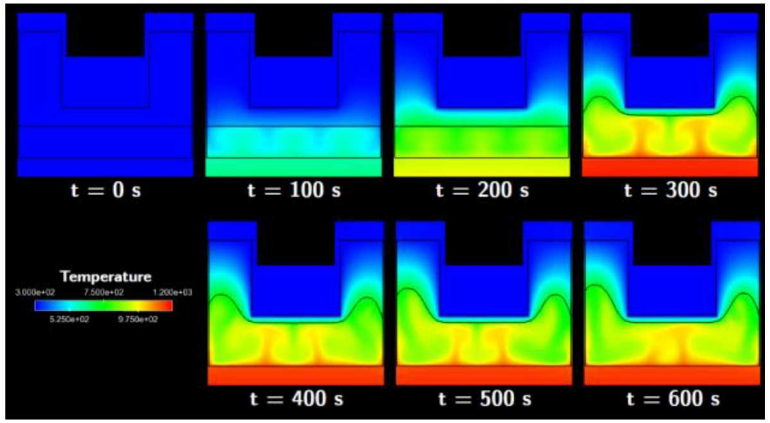
Laser welding



Additive Manufacturing



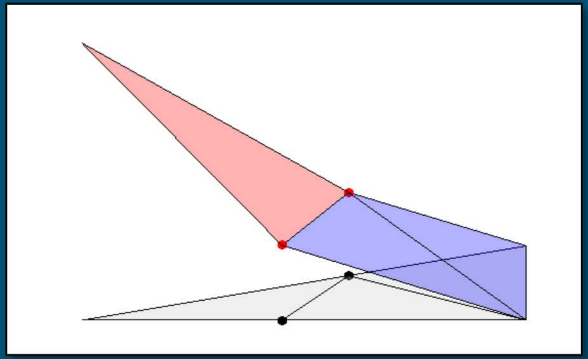
Capillary Hydrodynamics



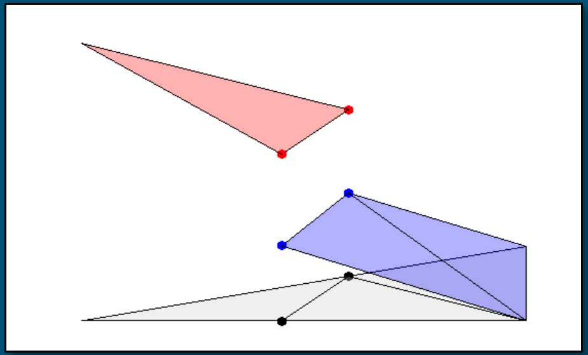
Organic Material Decomposition (OMD)
with coupled porous and low Ma flow

Interfacial Discontinuities in Sandia Applications

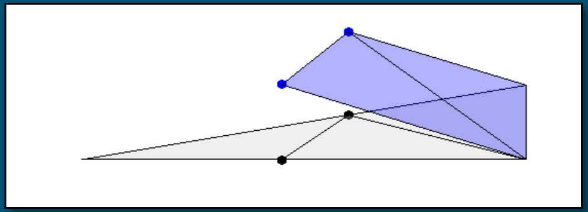
Weak Discontinuities
- Temperature due to discontinuous conductivity
- Velocity due to discontinuous viscosity
- Pressure due to discontinuous body forces
- Displacement due to discontinuous moduli



Strong Discontinuities
- Pressure due to capillary forces
- Displacement due to fracture



One-sided Fields
- Transport in evolving domains
- Multiphysics transport



Conformal Decomposition Finite Element Method (CDFEM)

Simple Concept (Noble, et al. 2010)

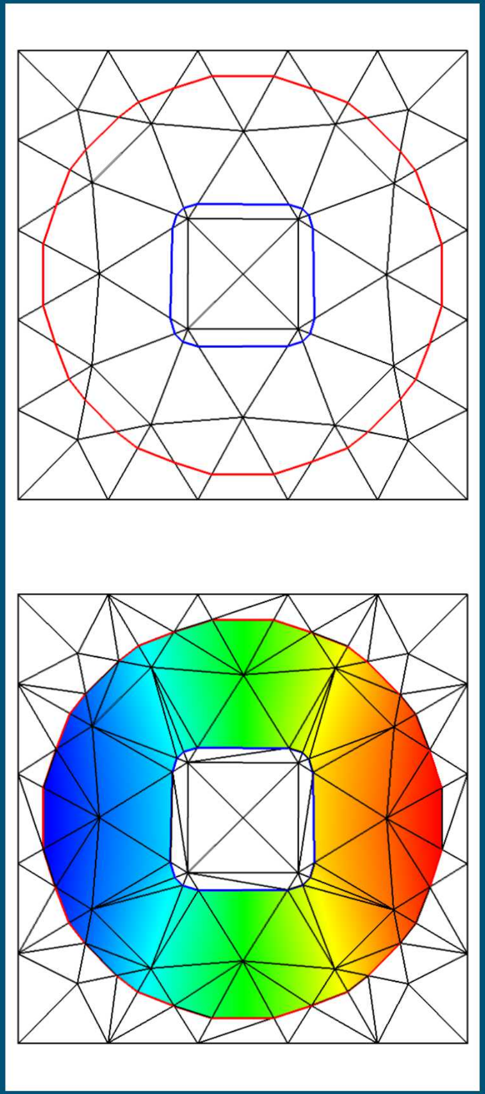
- Use one or more level set fields to define materials or phases
- Decompose non-conformal elements into conformal ones
- Obtain solutions on conformal elements
- Use single-valued fields for weak discontinuities and double-valued fields for strong discontinuities

Capability 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)

Implementation Properties

- Similar to finite element adaptivity
- Uses standard finite element assembly including data structures, interpolation, quadrature



But What About the Low Quality Elements?

Resulting meshes

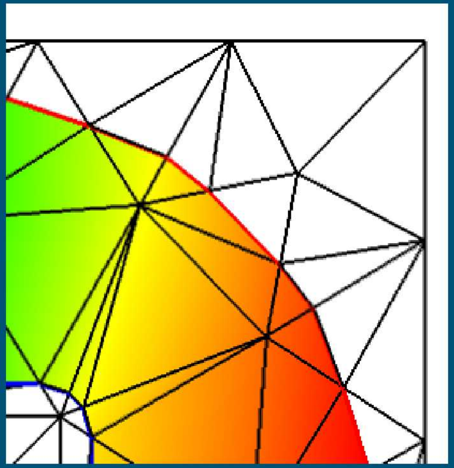
- ✗ Infinitesimal edge lengths
- ✗ Arbitrarily high aspect ratios (small angles)
- ✓ Can introduces obtuse angles. Can be avoided by cutting largest angle.

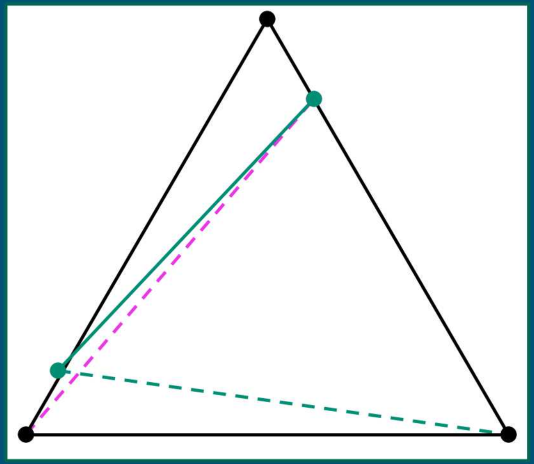
Consequences

- ✗ Condition number of resulting system of equations
- ✓ Interpolation error. Previous work has shown this is not an issue.
- ? Other concerns: stabilized methods, suitability for solid mechanics, Courant number limitations, capillary forces

Questions

- How serious is the issue with the matrix conditioning?
- What can be done to mitigate this issue?

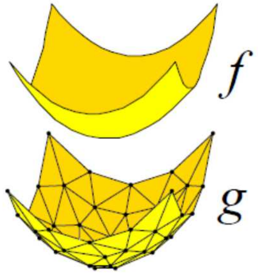


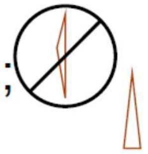
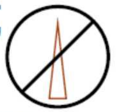
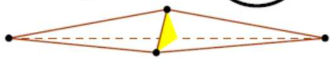


Impact of Mesh Quality

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.  

Punchline: Poor quality sliver CDFEM elements do not produce accuracy issues, but do produce poorly conditioned matrices.

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

Time-discretization scheme (2nd Order in Space and Time)

Momentum Prediction

$$\int_{\Omega^n} (\nabla \cdot \tilde{\mathbf{u}})\, w_i \mathrm{d}\Omega = 0,$$

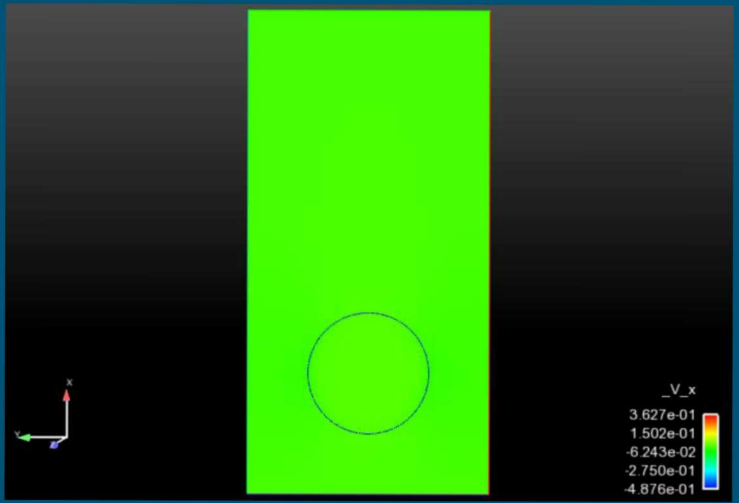
$$\int_{\Omega^n} \rho \left(\frac{\frac{3}{2}\tilde{\mathbf{u}} - 2\mathbf{u}^n + \frac{1}{2}\mathbf{u}^{n-1}}{\Delta t} + (\tilde{\mathbf{u}} \cdot \nabla)\,\tilde{\mathbf{u}} \right) \cdot \mathbf{w}_i \mathrm{d}\Omega$$
$$+ \int_{\Omega^n} -P\mathbf{I} + \mu \left(\nabla \tilde{\mathbf{u}} + \nabla \tilde{\mathbf{u}}^t\right) \cdot \nabla \mathbf{w}_i \mathrm{d}\Omega$$
$$+ \int_{\Gamma_f^n} \sigma \left((\mathbf{I} - \mathbf{nn}) + \Delta t \underline{\nabla} \tilde{\mathbf{u}}\right) \cdot \nabla \mathbf{w}_i \mathrm{d}\Gamma = 0,$$

Levelset Advection

$$\int_{\Omega^n} \left(\frac{\frac{3}{2}\phi^{n+1} - 2\phi^n + \frac{1}{2}\phi^{n-1}}{\Delta t} + \tilde{\mathbf{u}} \cdot \nabla \phi^{n+1} \right) w_i \mathrm{d}\Omega = 0$$

Conformal Decomposition

- Decompose mesh to conform to updated level set
- Compute mesh “velocity”



Momentum Correction

$$\int_{\Omega^{n+1}} (\nabla \cdot \mathbf{u}^{n+1})\, w_i \mathrm{d}\Omega = 0,$$

$$\int_{\Omega^{n+1}} \rho \left(\frac{\frac{3}{2}\mathbf{u}^{n+1} - 2\mathbf{u}^n + \frac{1}{2}\mathbf{u}^{n-1}}{\Delta t} + \left(\left(\mathbf{u}^{n+1} - \dot{\mathbf{x}}\right) \cdot \nabla\right) \mathbf{u}^{n+1} \right) \cdot \mathbf{w}_i \mathrm{d}\Omega$$
$$+ \int_{\Omega^{n+1}} -P\mathbf{I} + \mu \left(\nabla \mathbf{u} + \nabla \mathbf{u}^t\right)^{n+1} \cdot \nabla \mathbf{w}_i \mathrm{d}\Omega$$
$$+ \int_{\Gamma_f^{n+1}} \sigma \left((\mathbf{I} - \mathbf{nn}) + \Delta t \underline{\nabla} \left(\mathbf{u}^{n+1} - \tilde{\mathbf{u}}\right)\right) \cdot \nabla \mathbf{w}_i \mathrm{d}\Gamma = 0,$$

Verification (capillary wave decay)

Perturb two-phase interface with sinusoidal disturbance

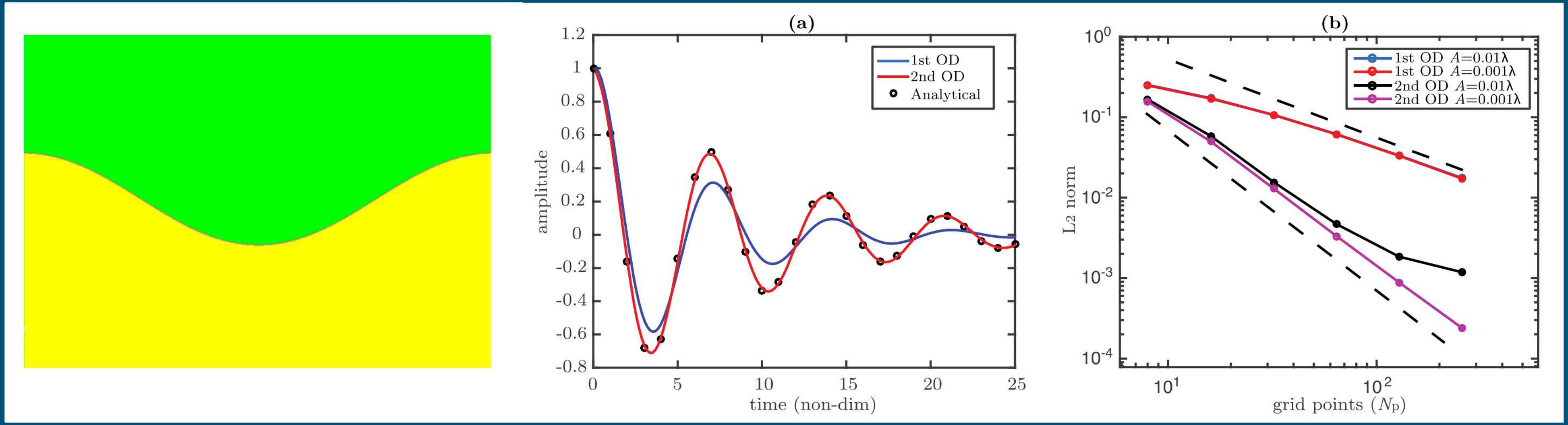
Interface shape should decay with specific frequency and rate (Prosperetti, 1981) at small amplitudes

Accurate prediction of capillary wave frequency and amplitude decay

CDFEM discretization of interface accurately captures surface tension dynamics

2nd order convergence in space and time

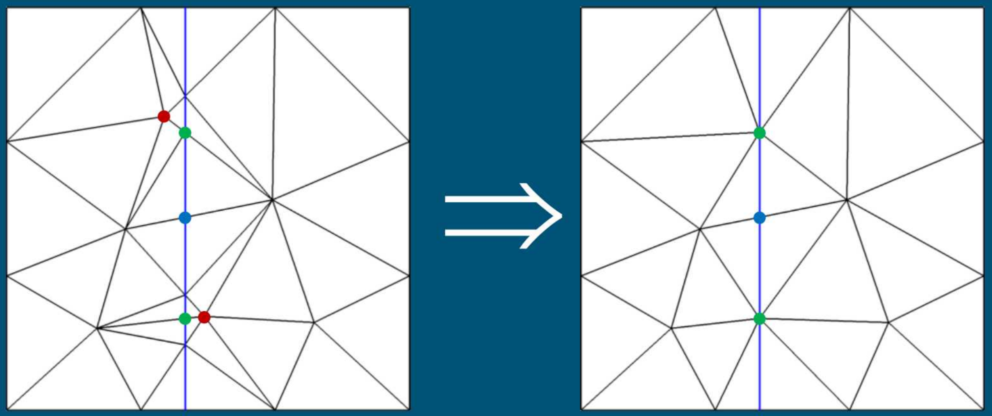
Interface Dynamics **Convergence**



Strategies to Circumvent Poor CDFEM Conditioning

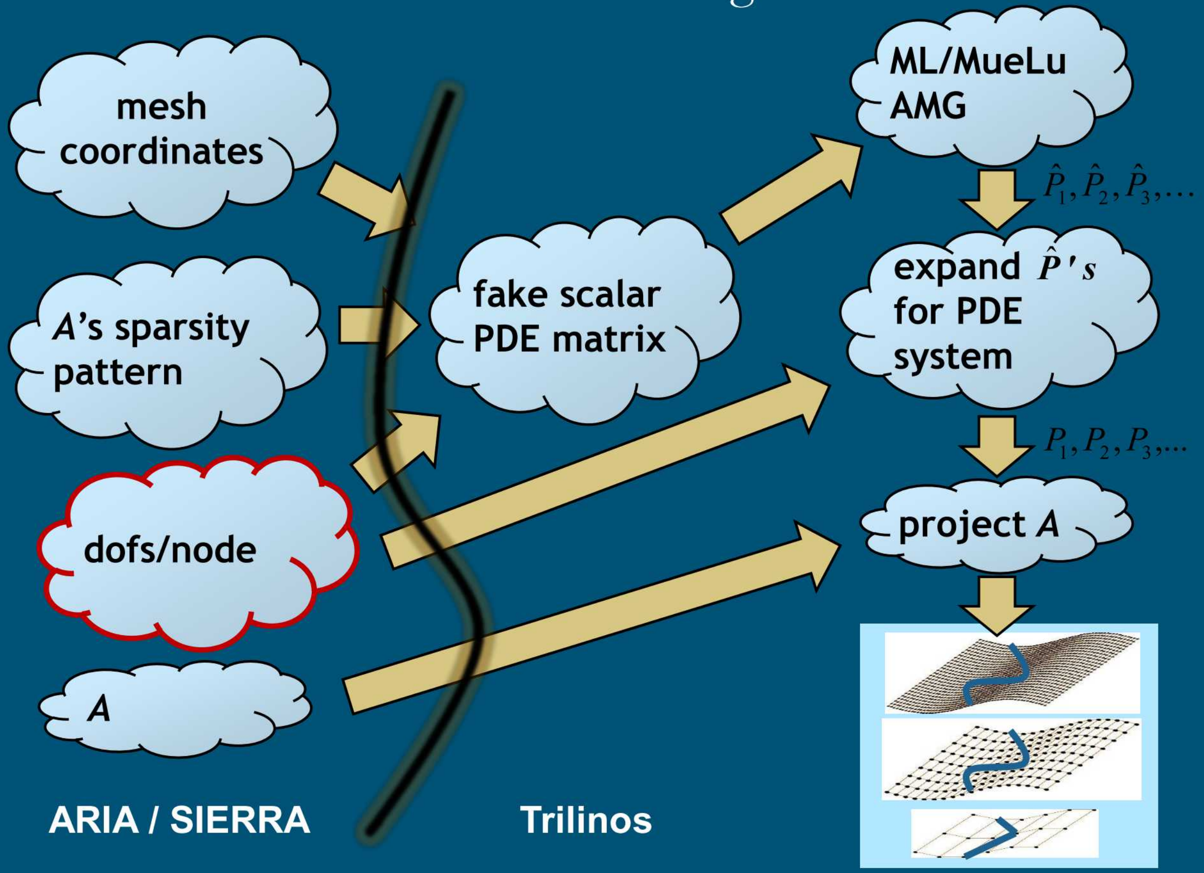
Coarsen by Snapping "bad" nodes

- Determine edge cut locations using level set
- When any 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, •→•)



Specialized Preconditioners

- Extended AMG solver in Trilinos to handle discontinuous variables on irregular meshes



Constraining CDFEM to Recover "XFEM"

- CDFEM Approximation

$$u(x) = \sum_{i \in P} u_i^P w_i^{subelement}(x) + \sum_{i \in CDFEM} u_i^{CDFEM} w_i^{subelement}(x)$$

- XFEM Approximation

$$u(x) = \sum_{i} u_i^P w_i(x) + \sum_{i \in XFEM} u_i^{XFEM} w_i^{XFEM}(x)$$

- Constrain CDFEM System of Equations

$$A_{CDFEM} \begin{bmatrix} u^P \\ u^{CDFEM} \end{bmatrix} = b^{CDFEM}, u^{CDFEM} = C_P u^P + C_{XFEM} u^{XFEM}$$

- Produce XFEM System of Equations

$$\begin{bmatrix} u^P \\ u^{CDFEM} \end{bmatrix} = M \begin{bmatrix} u^P \\ u^{XFEM} \end{bmatrix} \rightarrow M = \begin{bmatrix} I & 0 \\ C_P & C_{XFEM} \end{bmatrix}$$

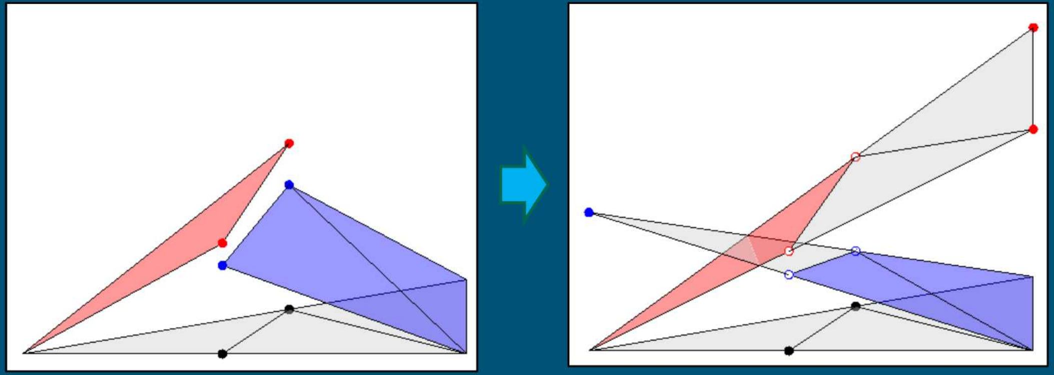
$$A_{XFEM} \begin{bmatrix} u^P \\ u^{XFEM} \end{bmatrix} = b^{XFEM}$$

$$A_{XFEM} = M^t A_{CDFEM} M, b^{XFEM} = M^t b^{CDFEM}$$

"XFEM" Spaces to Use for Coarsening

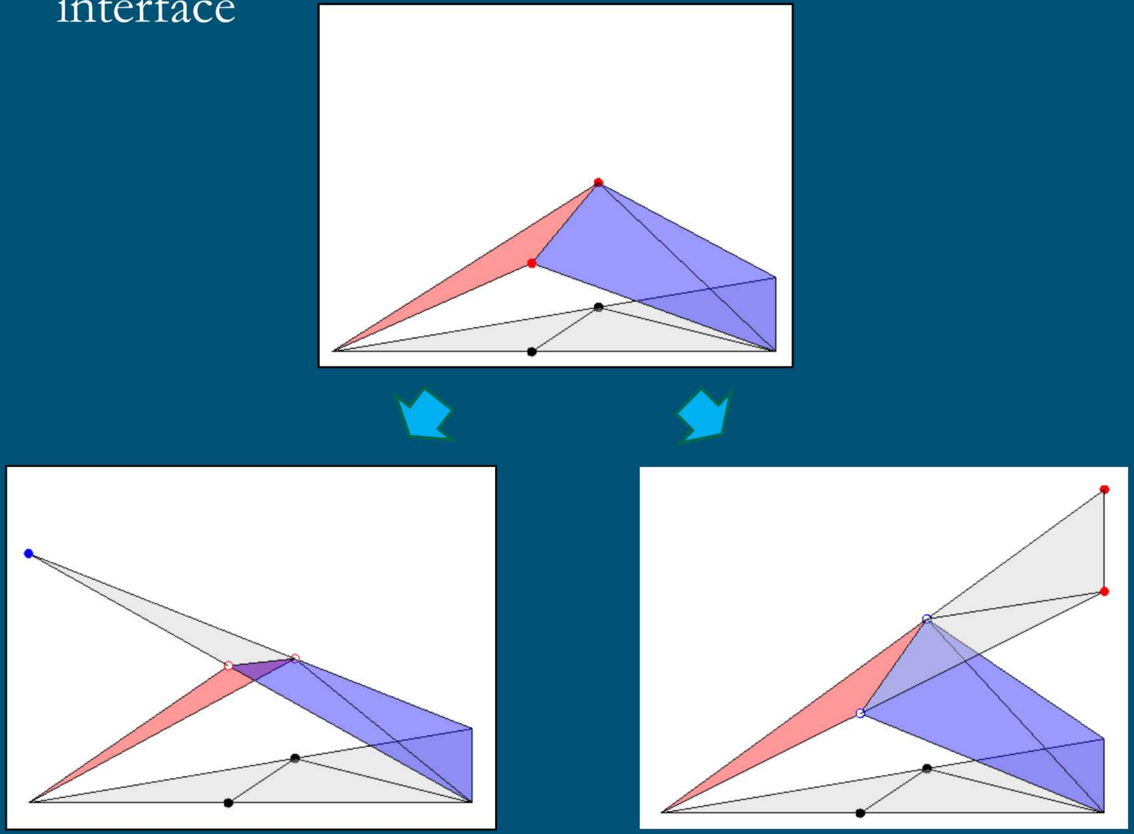
For Strong Discontinuities

- Heaviside XFEM Enrichment
- Replace/constrain CDFEM DOFs with enriched values on the parent nodes on both sides of interface



For Weak Discontinuities

- Piecewise linear ridge "C0 XFEM" enrichment
- Replace/constrain CDFEM DOFs with enriched values on the parent nodes from one side of the interface



2D Steady Taylor Vortex MMS Problem

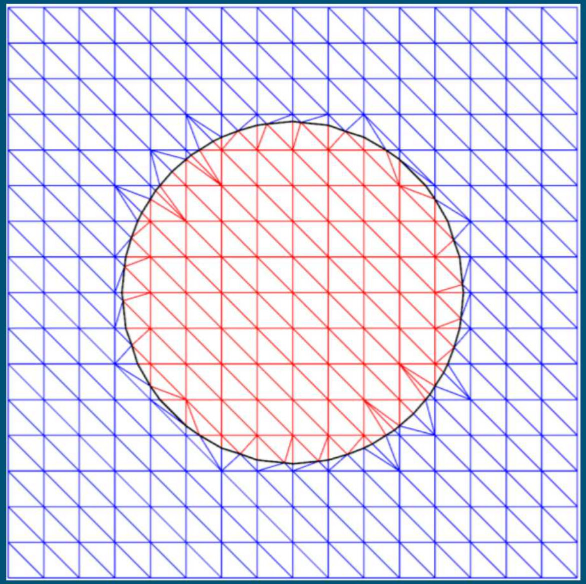
Simple Steady Velocity-Pressure Problem

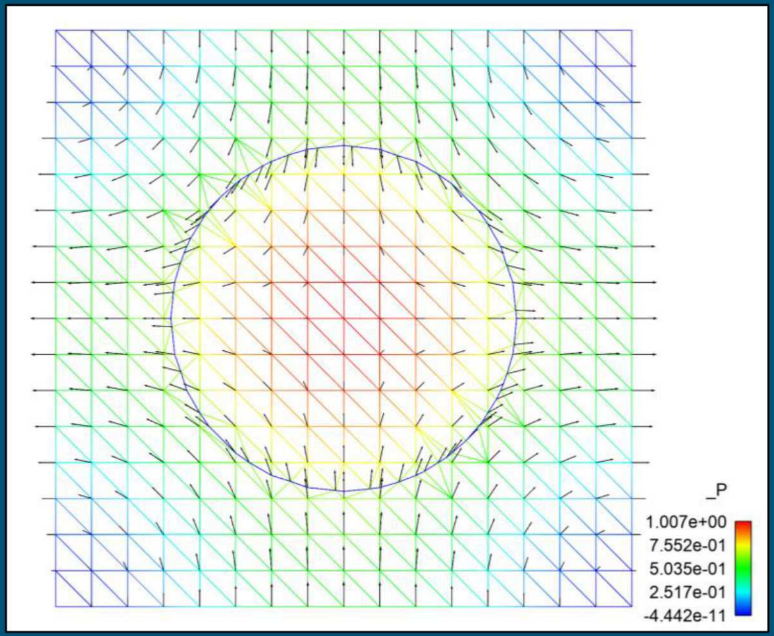
- Problem is continuous everywhere
- Introduce interface with C0-continuous velocity and either C0-continuous or discontinuous pressure
- Test accuracy and matrix conditioning

$$\int_\Omega (\boldsymbol{\rho}\mathbf{u}\cdot\nabla\mathbf{u} \ -\mathbf{F})\, w_i \ \ d\Omega + \int_\Omega (-P\mathbf{I} + \mu(\nabla\mathbf{u} + \nabla\mathbf{u}^t))\cdot\nabla w_i d\Omega = 0$$

$$\mathbf{u} = (-\cos(\pi x)\sin(\pi y)\,,\,\sin(\pi x)\cos(\pi y)) \quad \mathbf{F} = \frac{2\pi^2\mu}{\rho}\mathbf{u}$$

$$p = -\frac{1}{4}(\cos(2\pi x) + \cos(2\pi y))$$

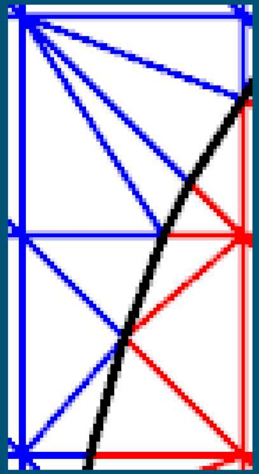




2D Steady Taylor Vortex MMS Results

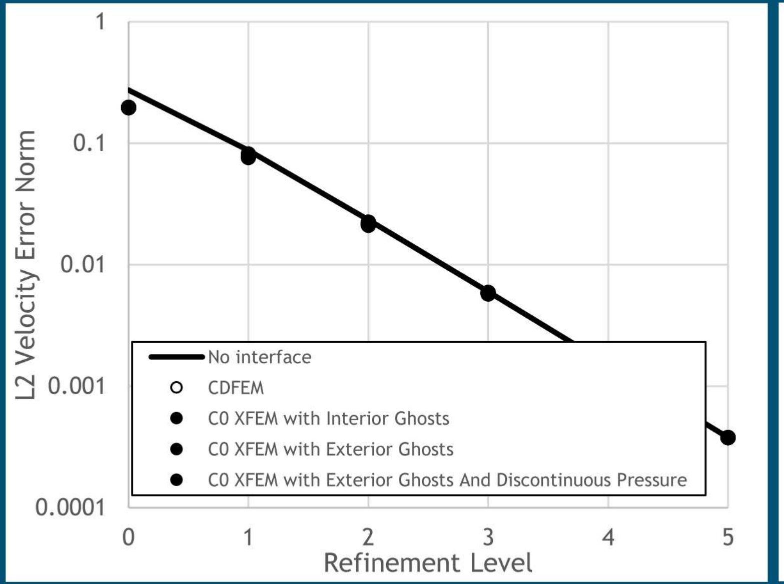
Formulations

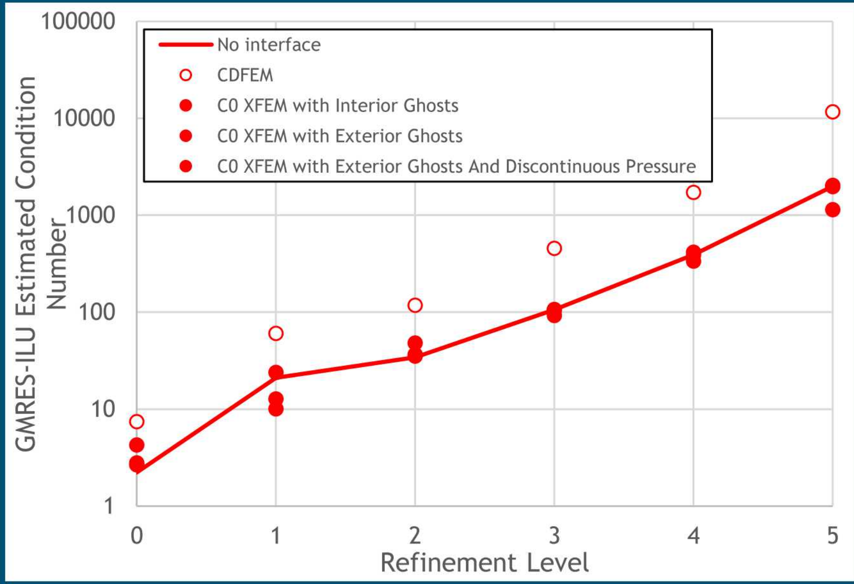
- CDFEM: Added velocity and pressure DOFs on interface nodes
- C0 XFEM: Added velocity and pressure DOFs on parent nodes of cut elements (either inside or outside)
- C0 XFEM and Discontinuous Pressure: Added velocity DOFs on outside parent nodes of cut elements and added pressure DOFs on parent nodes on both sides of interface

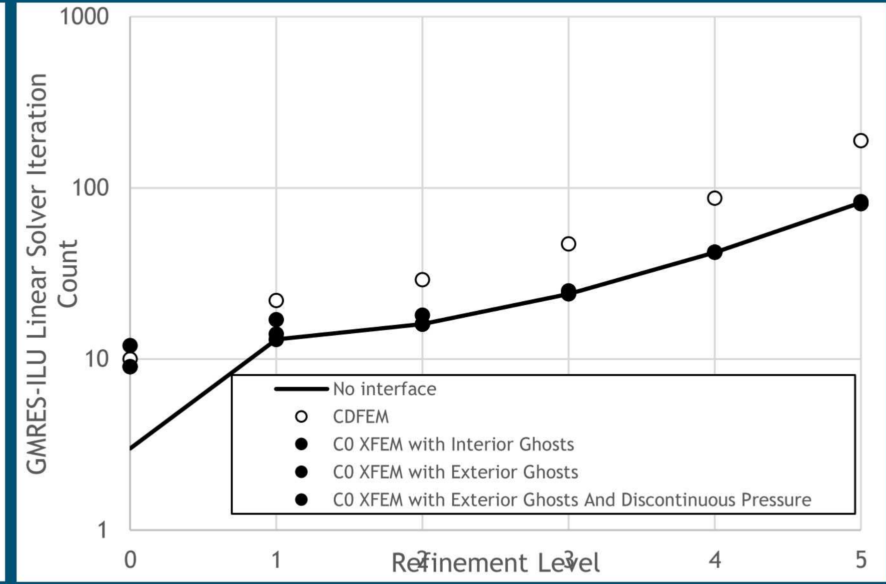


Results

- Optimally convergent for all formulations
- Little to no difference based on velocity enrichment of interior or exterior nodes
- Little to no difference based on XFEM Heaviside enriched pressure or continuous pressure
- XFEM shows significantly better conditioning and 2-3x reduction in number of linear solver iterations



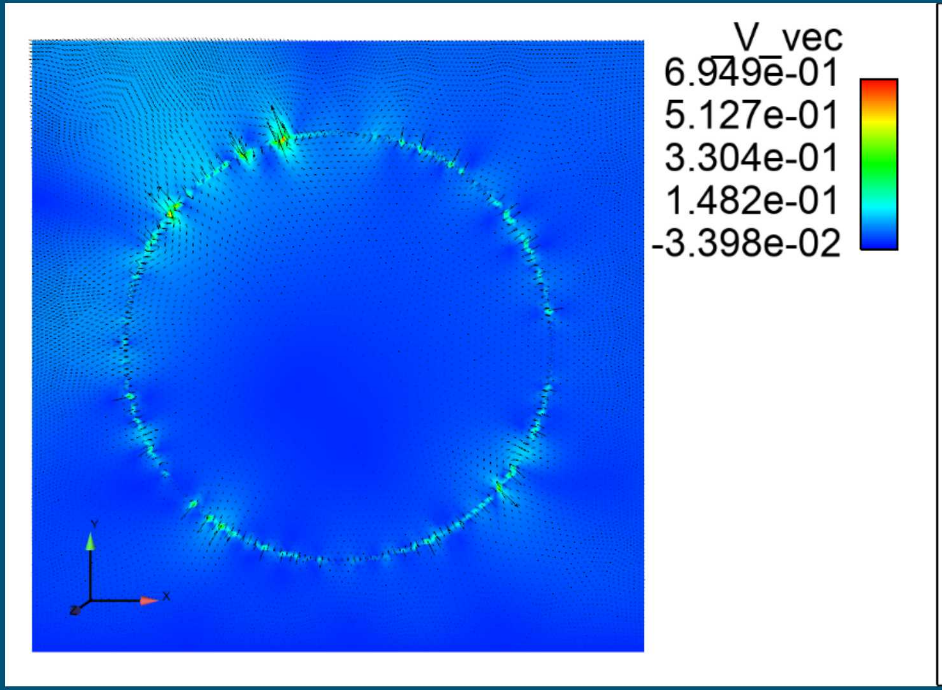


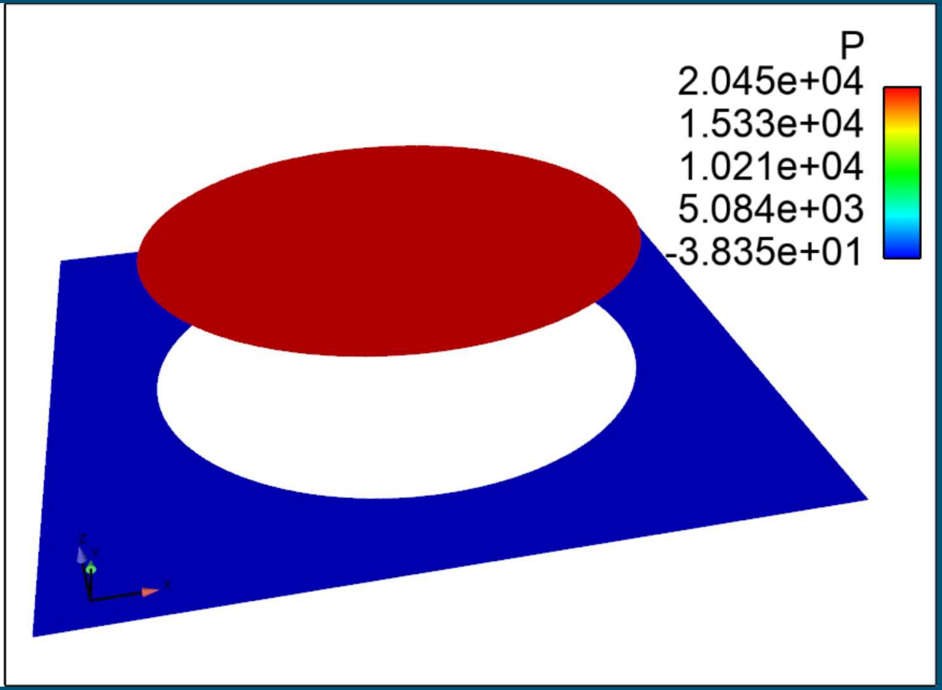


Steady-state test problem: Static Drop

$$\int_\Omega \mathbf{u}\cdot\nabla\mathbf{u}\, w_i\, d\Omega + \int_\Omega (-P\mathbf{I} + \mu(\nabla\mathbf{u} + \nabla\mathbf{u}^t))\cdot\nabla w_i d\Omega + \int_\Gamma \underbrace{\sigma((\mathbf{I}-\mathbf{nn})}_{\text{Laplace-Beltrami surface tension}} + \underbrace{\Delta t_{CA}\underline{\nabla}\mathbf{u})}_{\text{semi-implicit stabilization}}\cdot\nabla w_i d\Gamma = 0$$

Semi-implicit term, Hysing (2006), accounts for impact of velocity on interface shape/curvature

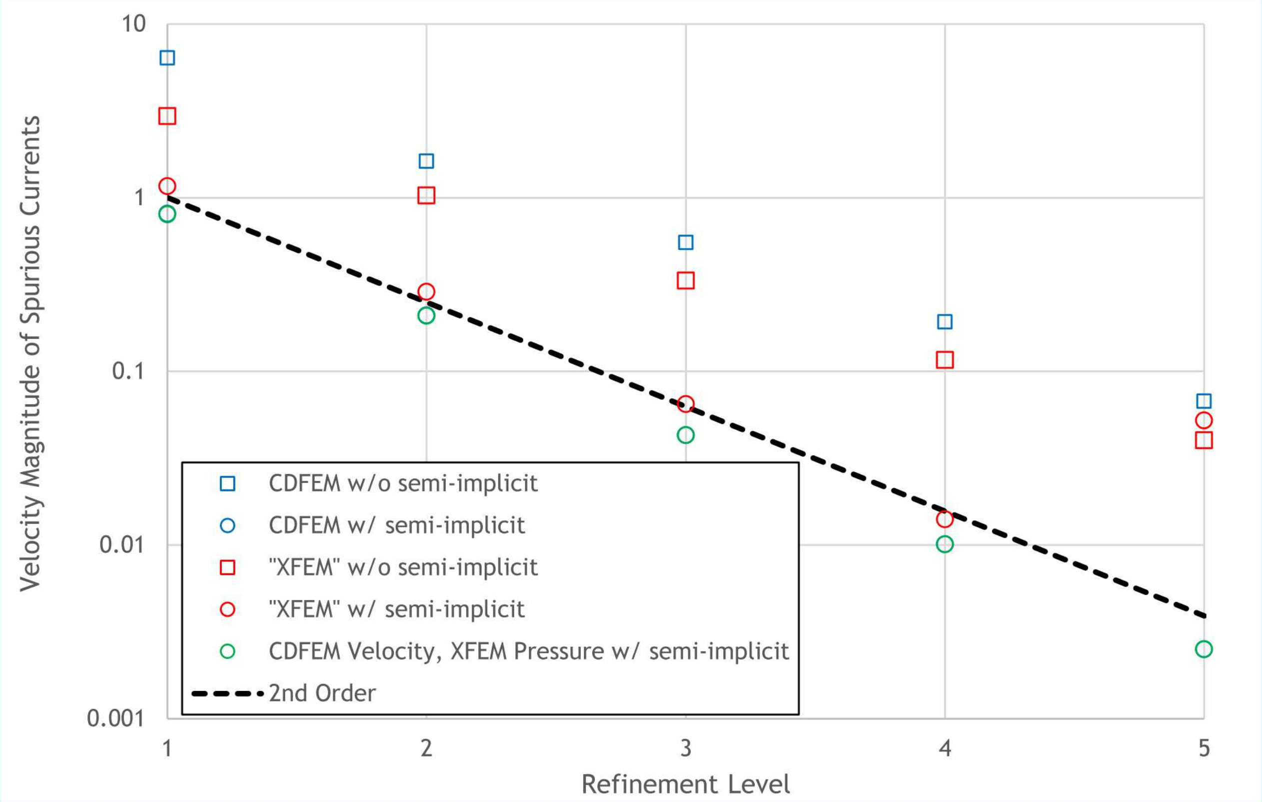


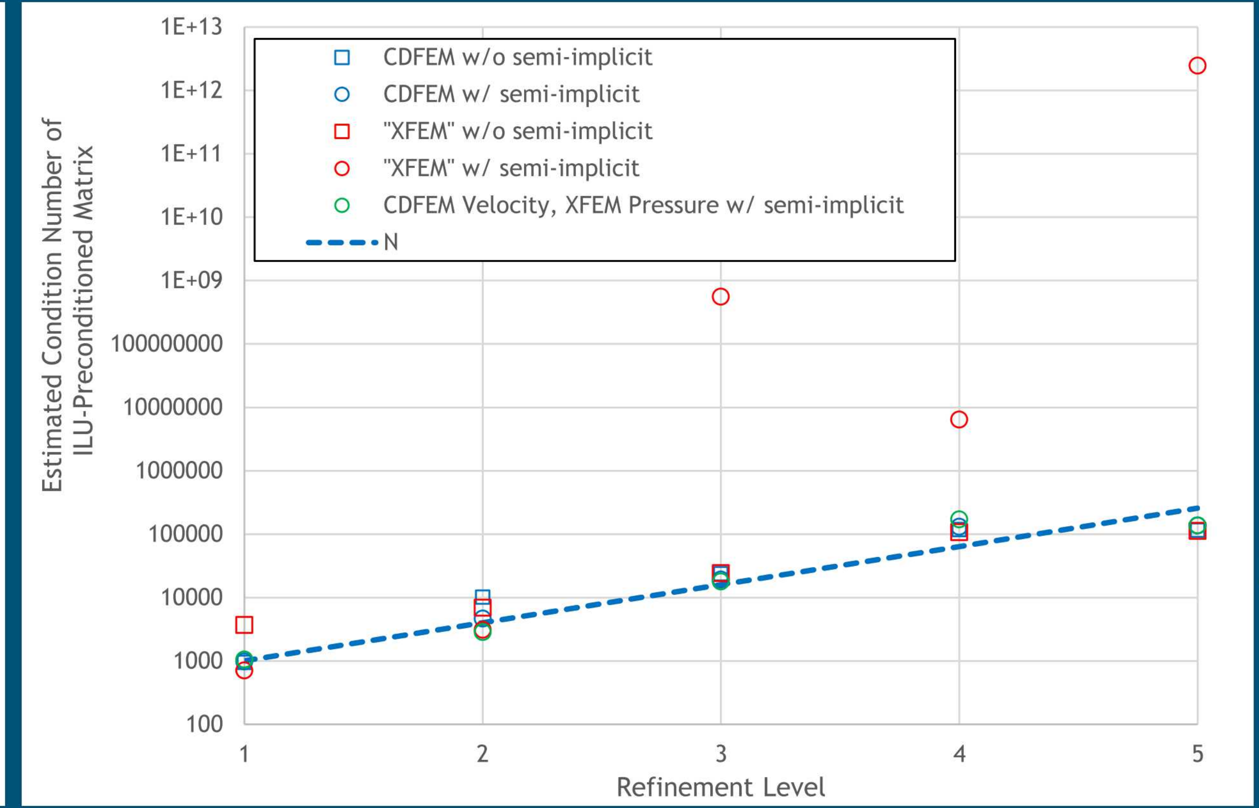


$$\Delta t_{CA} = \frac{D\mu}{\sigma}$$

$$\text{La} = \frac{\rho\sigma D}{\mu^2} = 5000$$

Static Drop With Mesh Refinement





Interaction between "XFEM" space and semi-implicit stabilization term

- Semi-implicit term leads to 2nd order convergence of spurious currents
- When combined with "XFEM" space (XFEM Heaviside for pressure, "C0 XFEM" for velocity), it appears that the velocity "locks", leading to very poorly conditioned system
- CDFEM velocity and Heaviside XFEM pressure is well-behaved, but not significantly better than CDFEM

Summary/Conclusions

- CDFEM useful as discretization or preprocessor for recovering other enriched spaces
  - Other enriched spaces recovered by constraining CDFEM DOFs
- Projection to "XFEM" Space Sometimes Beneficial
  - For weakly and strongly discontinuous scalar transport problems, solver cost reduced by 3-5x
  - For Taylor-Vortex problem (velocity-pressure), solver cost reduced by 2-3x
  - In all cases, only very small reduction in accuracy due to coarser space
- Projection to "XFEM" Space Can Be Problematic
  - Never shows better conditioning or lower solver cost for static bubble problem
  - Very poor conditioning when combined with semi-implicit stabilization term
    - Issues are associated with "C0-XFEM" Velocity enrichment, not Heaviside XFEM Pressure Enrichment
    - Richer CDFEM space does not show same issues