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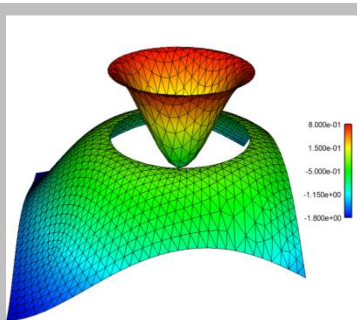

Time Integration Methods for the Enriched Conformal Decomposition Finite Element Method

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U.S. DEPARTMENT OF ENERGY

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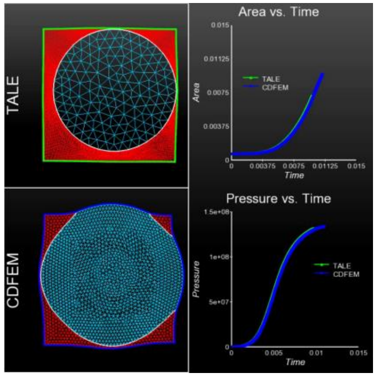
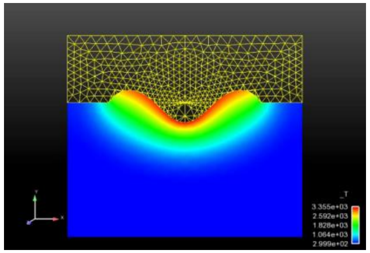
Motivation

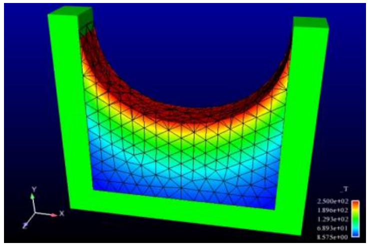
- Numerous problems with moving or topologically complex interfaces with discontinuous physics and fields



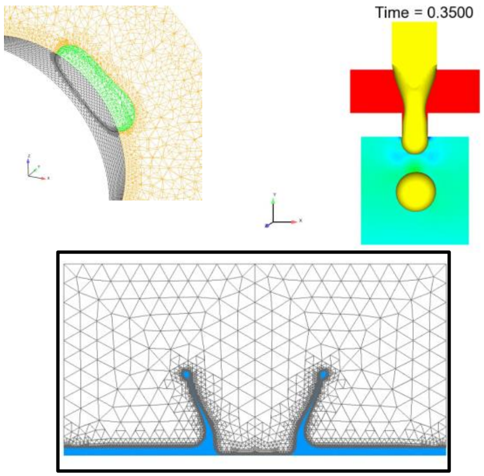
Conductive burn of energetic materials



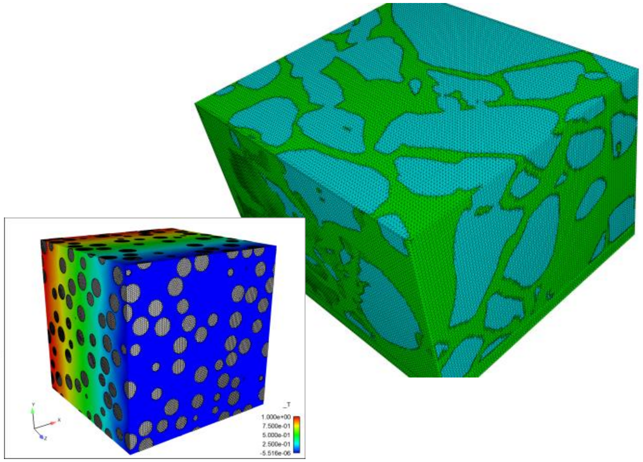
Laser welding



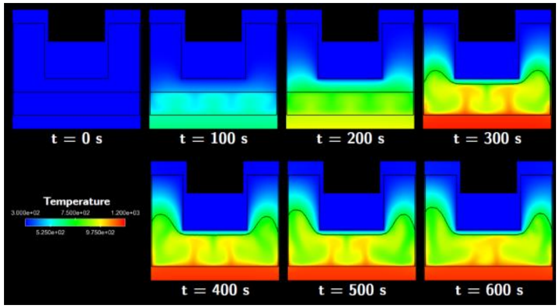
Material death



Capillary Hydrodynamics



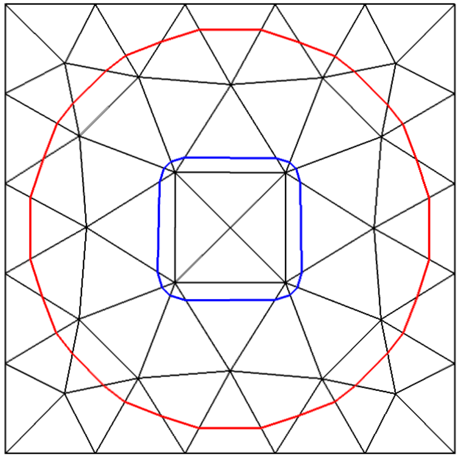
Transport in topologically complex domains including composite energetic materials and batteries

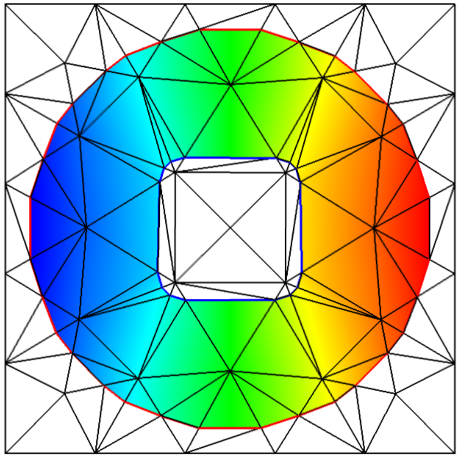


Organic Material Decomposition (OMD) with coupled porous and low Ma flow

Conformal Decomposition Finite Element Method (CDFEM)

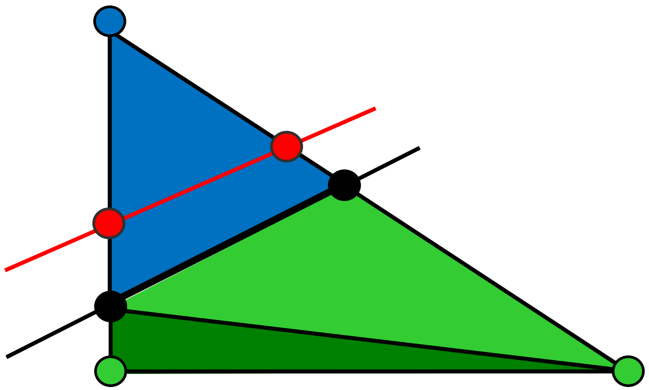
- Simple Concept
  - Use one or more level set fields to define materials or phases
  - Decompose non-conformal elements into conformal ones
  - Obtain solutions on conformal elements
- Related Work
  - Li et al. (2003) FEM on Cartesian Grid with Added Nodes
  - Ilinca and Hetu (2010) Finite Element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



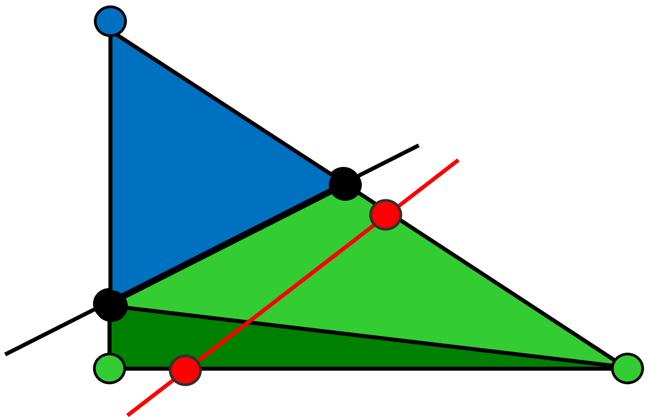


Moving Interfaces in Enriched Finite Element Methods

- 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

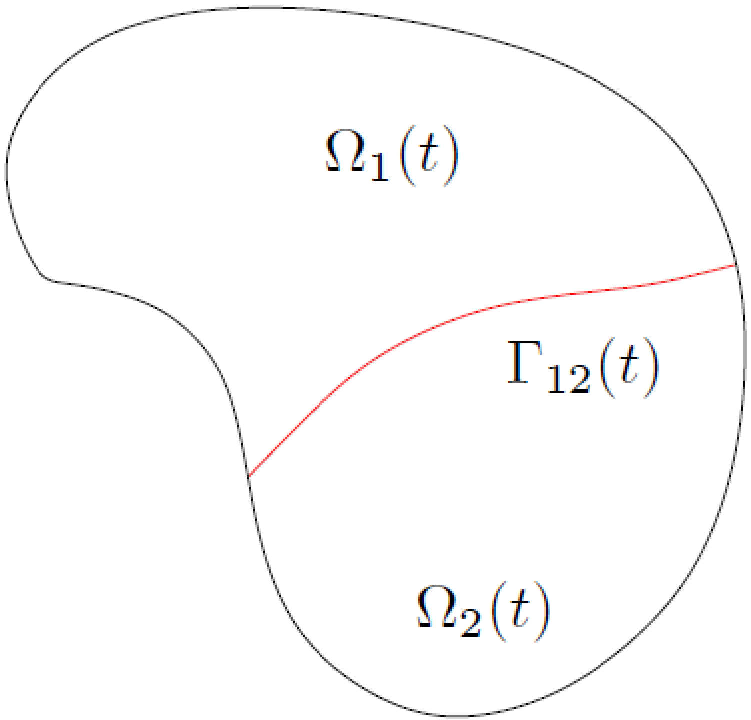
- Level Set Equation for interface motion

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

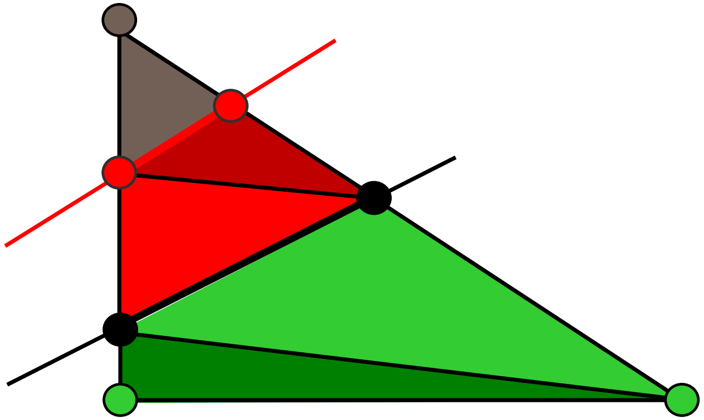
- Scalar advection-diffusion

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

- 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

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

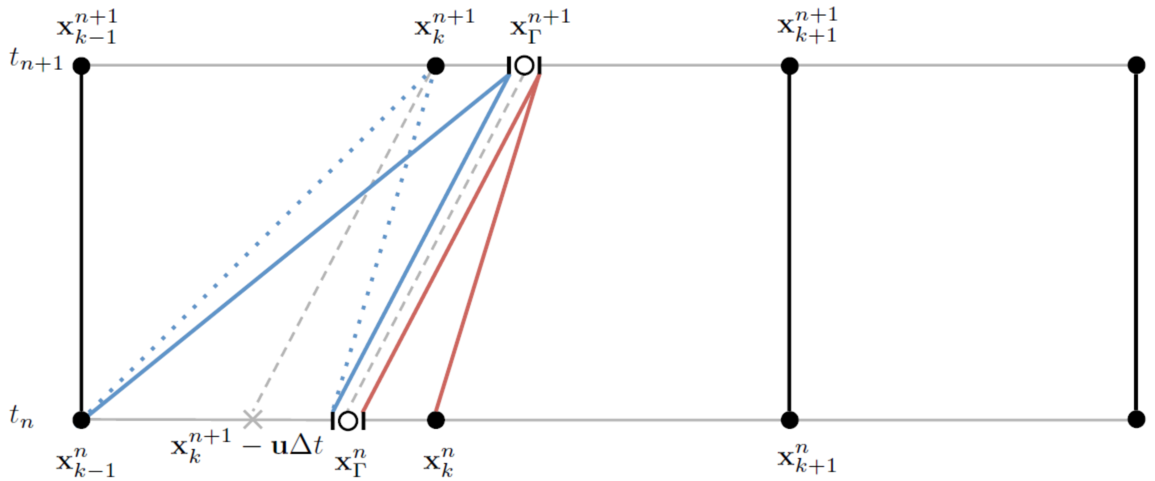
  - Careful formation of the time term evaluates fields at times when that field is present, $\psi_J^{n+1}(\mathbf{x})$ when $\mathbf{x} \in \Omega_J^{n+1}$and $\psi_I^n(\mathbf{x})$ when $\mathbf{x} \in \Omega_I^n$
  - However, this does involve differencing across material boundaries: ψ_J^{n+1}-ψ_I^n 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

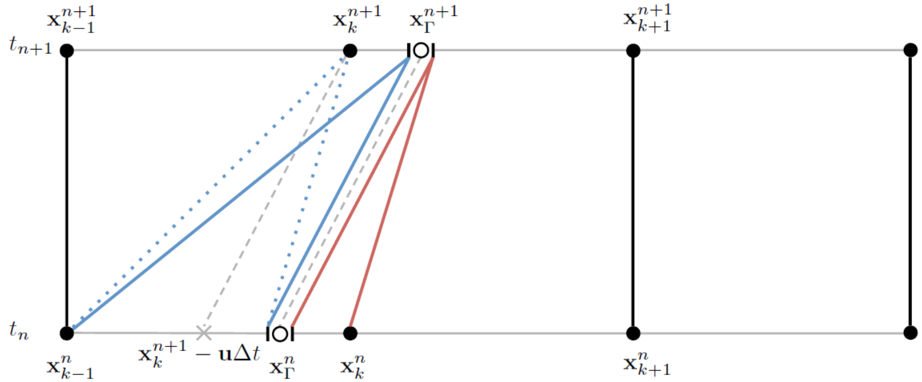
- Extrapolation from previous location
  - Essentially method by Henke et al. (2014) for XFEM (termed semi-Lagrangean)

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

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

$S^{n+1}(\mathbf{x})$ 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

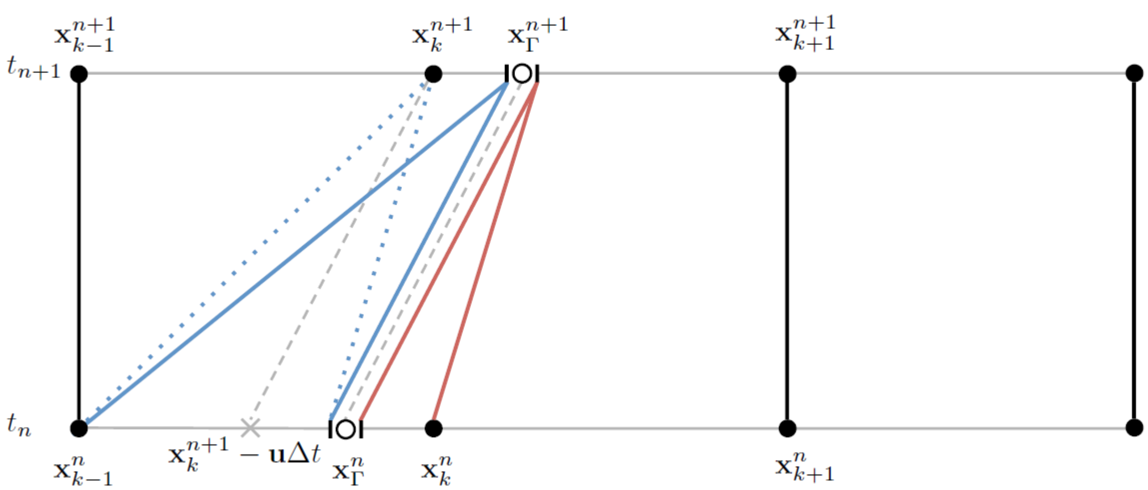


Approach for Dynamic Discretizations: Interface Extrapolation (IE)

- 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: 2[nd] 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

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

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

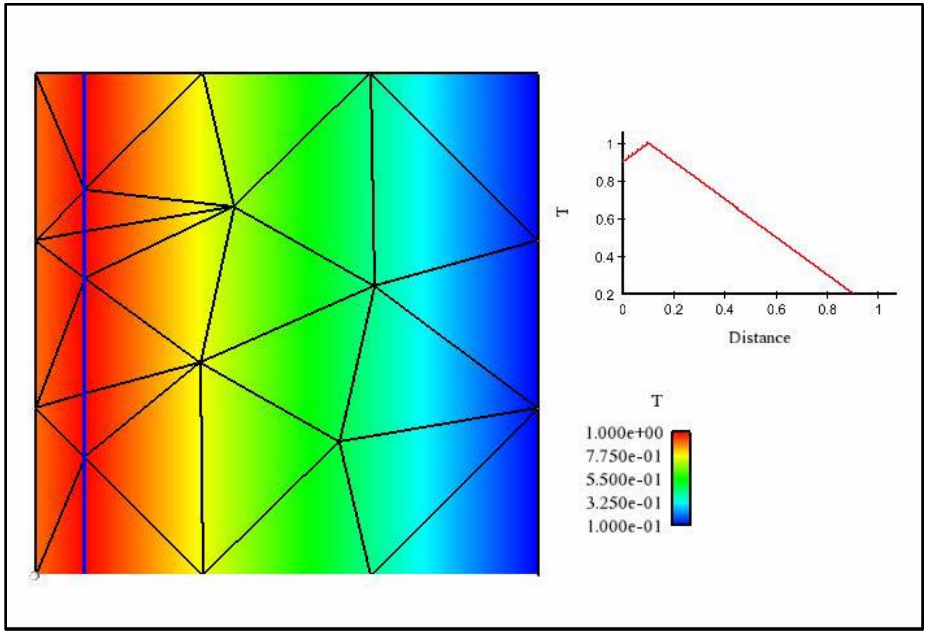
Approach for Dynamic Discretizations: Method Summary

- 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

- Constant advection 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

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

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

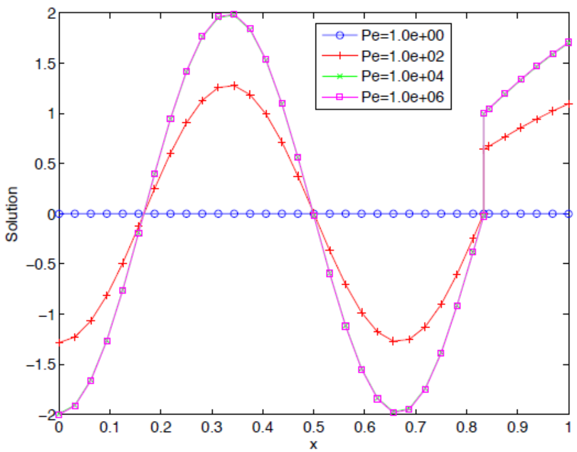
$$\Delta(t) = 2\exp(-t/c_t)/(\beta c_x c_t) \qquad s(x,t) = \begin{cases} 0, & \phi \leq 0 \\ -\frac{2}{\beta c_x c_t^2} \exp(-t/c_t), & \phi > 0 \end{cases}$$

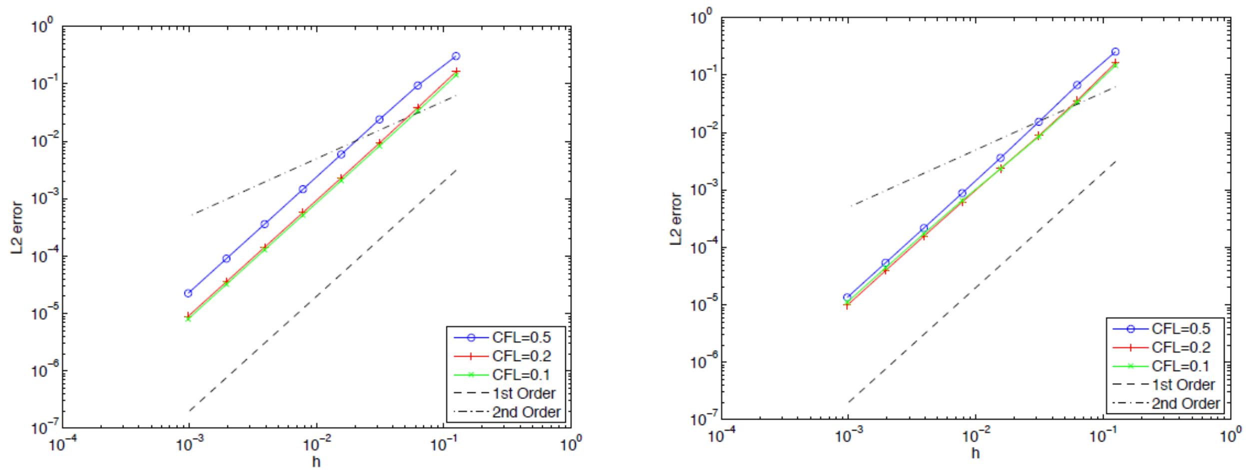
  - Examine convergence with in space and time for various Courant numbers

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

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

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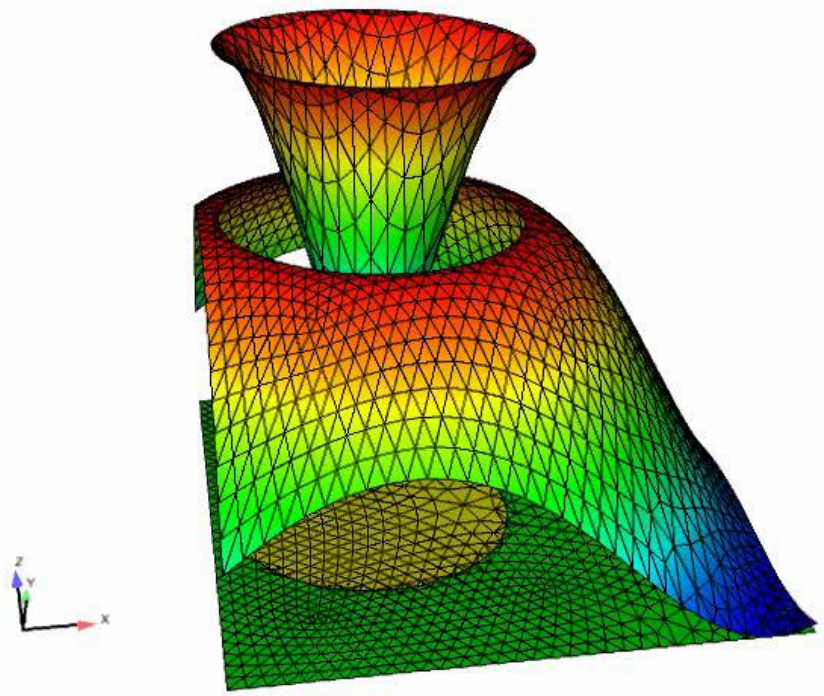
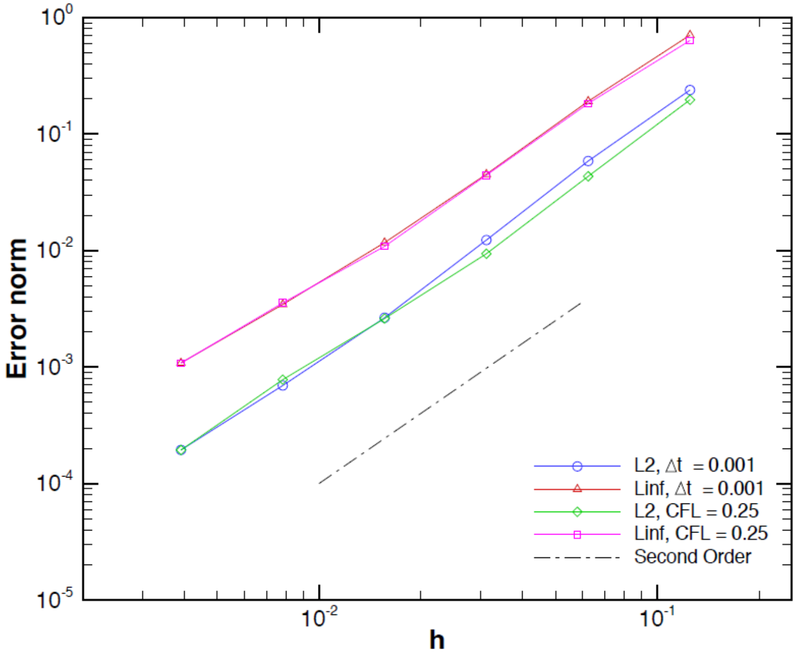
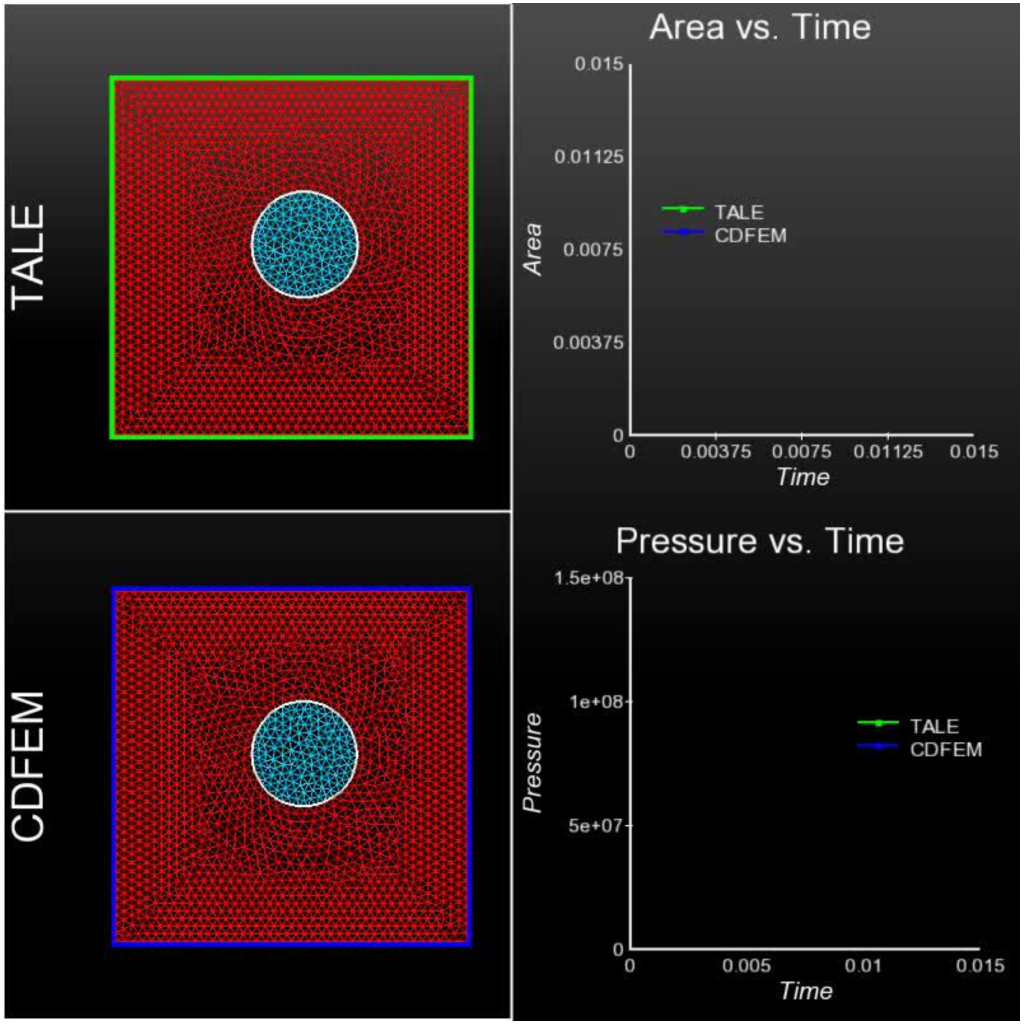




Convergence plot for the 2-D advection-diffusion problem with contact resistance, using the BDF2 time integrator

Comparison Between TALE and CDFEM Simulation of Burning, Deformable Solid

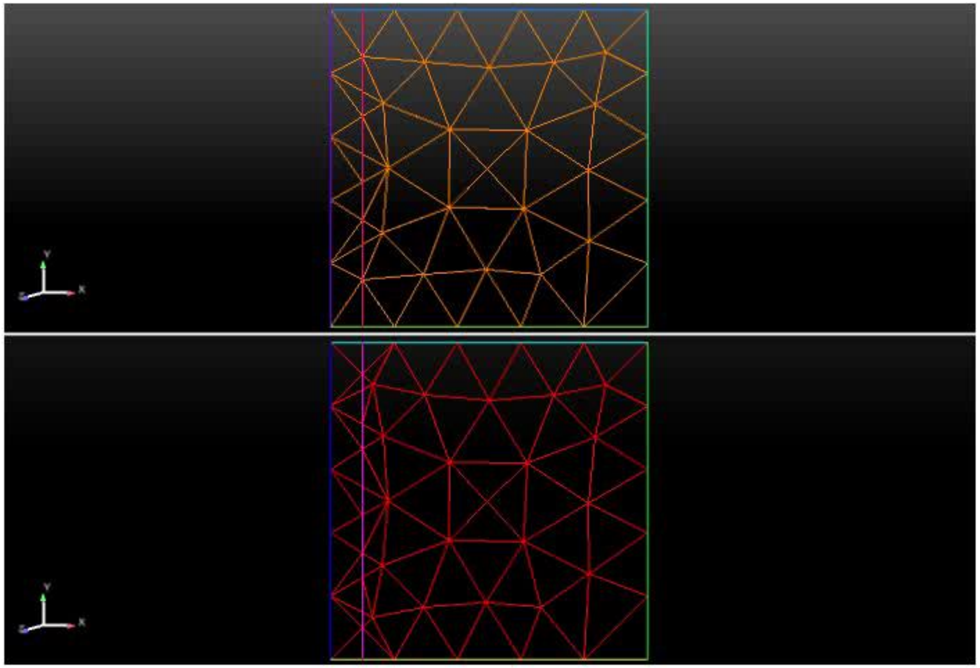


Summary

- Capturing arbitrary discontinuities on moving interfaces
  - All enriched methods require specialized method for handling dynamic discretization
- Subdomain Integration
  - Requires integration over domains that conform with both new and old interface locations
  - Not sufficient for strongly discontinuous fields
- Interface Extrapolation
  - Capable of optimal accuracy with arbitrary discontinuities
  - Extrapolation of weakly discontinuous fields are strongly discontinuous
  - Not uniquely defined in higher dimensions
- Moving Mesh
  - Capable of optimal accuracy for arbitrary discontinuities
  - Implementation somewhat complicated for Crank-Nicolson (but straightforward for BDF2)

CDFEM with Guaranteed Quality

- Uses mixture of decomposition and moving nodes of background mesh
  - Based on edge cut bounds
  - Improved minimum angle and condition number of resulting linear system of equations



XFEM - CDFEM Requirements Comparison for Thermal/Fluids

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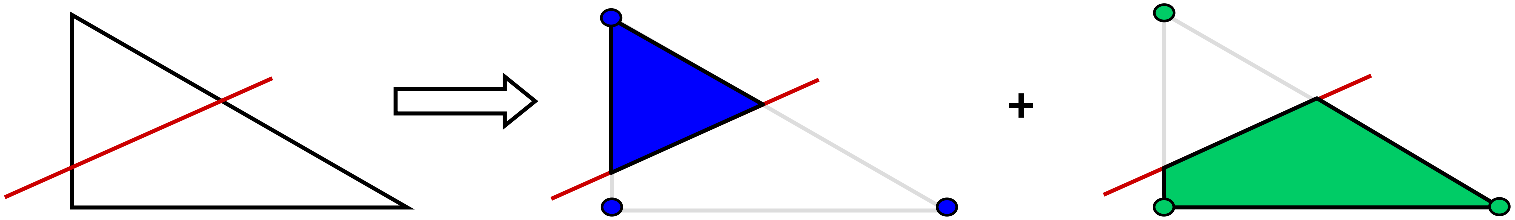
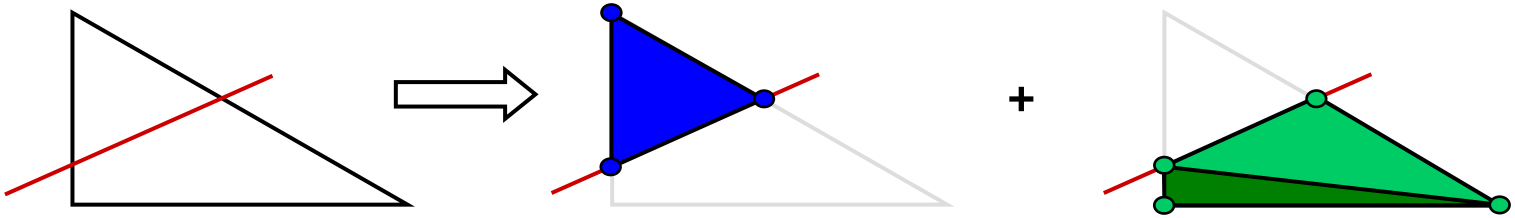
	XFEM	CDFEM
Volume Assembly	Conformal subelement integration, specialized element loops to use modified integration rules	Standard Volume Integration
Surface Flux Assembly	Specialized volume element loops with specialized quadrature	Standard Surface Integration
Phase Specific DOFs and Equations	Different variables present at different nodes of the same block	Block has homogenous dofs/equations that may differ from block to block
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

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