SAND2022-6751C

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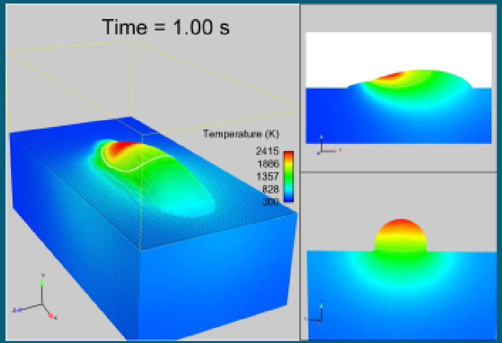
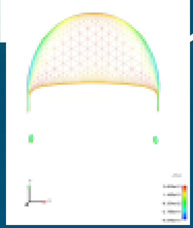
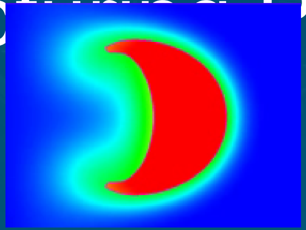
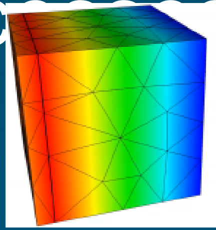
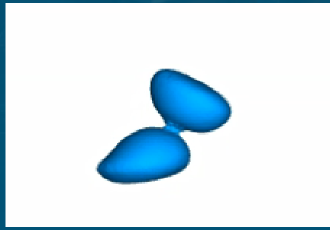
The Conforming Transient h-r Unstructured Adaptive Mesh Refinement (cThruAMR) Method for Multiphysics Simulations of Manufacturing Processes

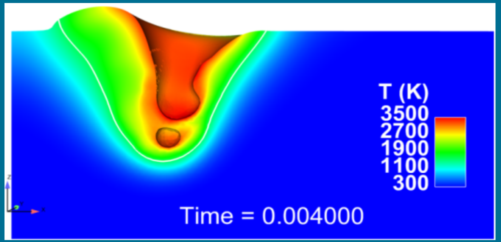












PRESENTED BY

David R. Noble

U.S. DEPARTMENT OF ENERGY NNSA

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Quality Discretizations for Manufacturing Processes

Motivation

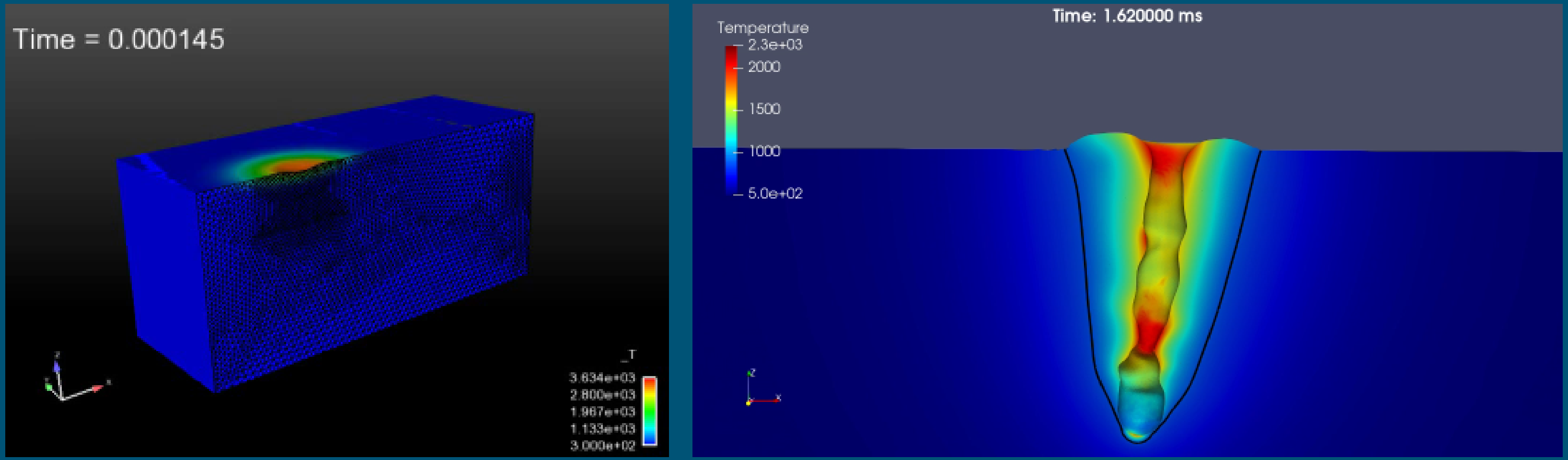
- Numerous manufacturing problems with moving interfaces with discontinuous physics and fields

Solution

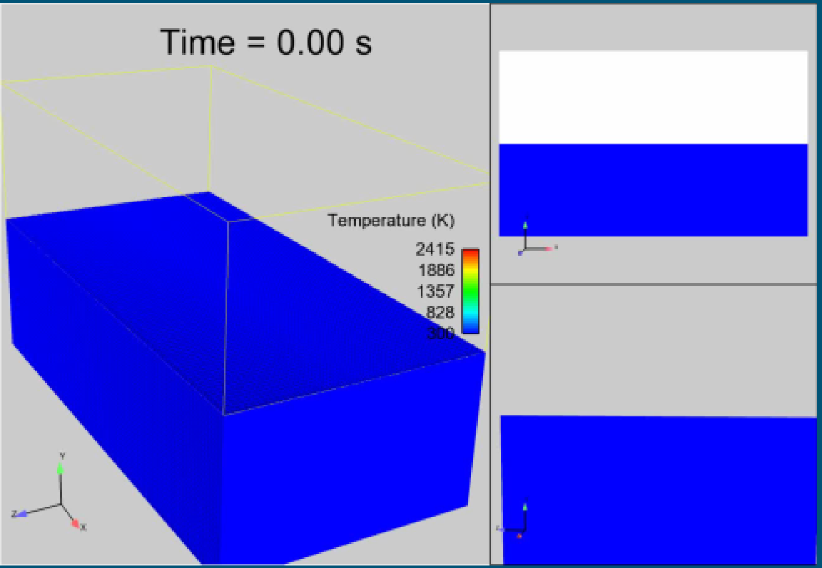
- cThruAMR - Conforming, transient, h-r unstructured adaptive mesh refinement

Related Work

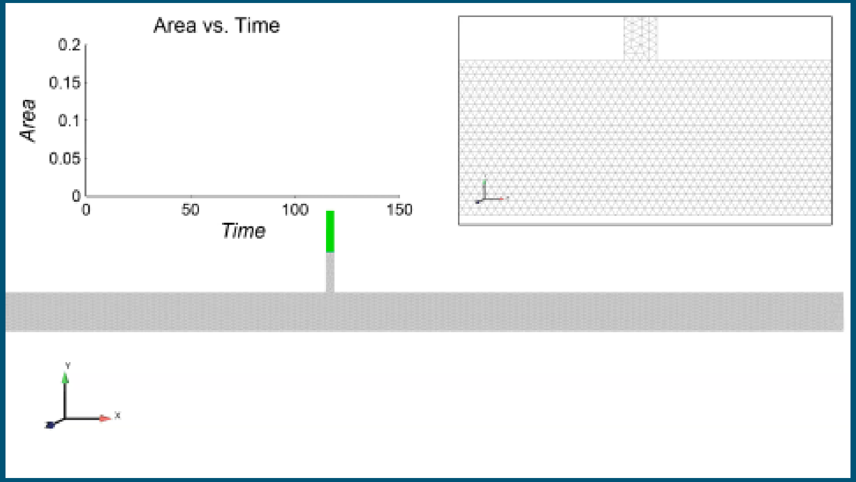
- CISAMR – Conforming to Interface Structured Adaptive Mesh Refinement (Soghrati)



Laser welding

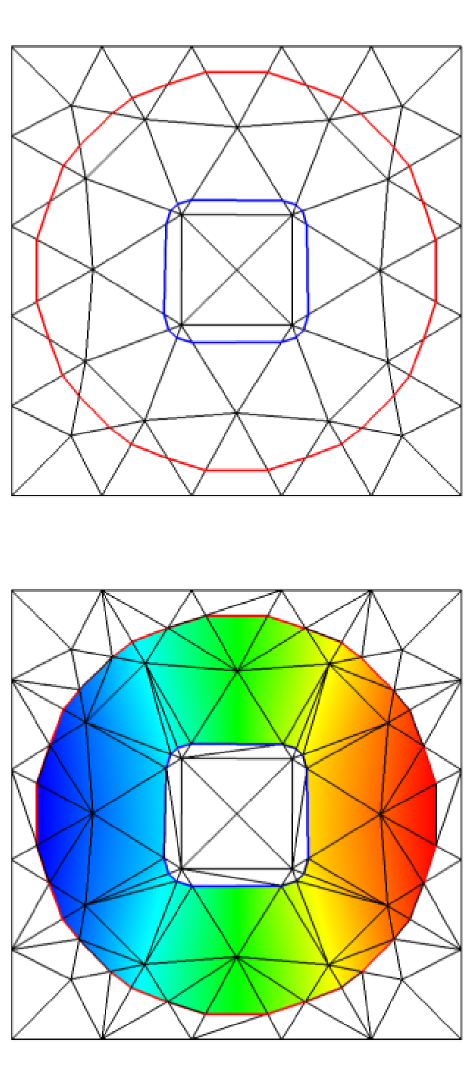


LENS Additive Manufacturing



Direct Write

Conforming 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-conforming elements into conforming ones
- Obtain solutions on conforming finite elements
- Use single-valued fields for weak discontinuities and double-valued fields for strong discontinuities

Related Work
- Li et al. (2003) FEM on Cartesian Grid with Added Nodes
- IGFEM, HIFEM (Soghrati, et al. 2012), DE-FEM (Aragon and Simone, 2017)

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

CDFEM is conforming transient unstructured h-adaptivity

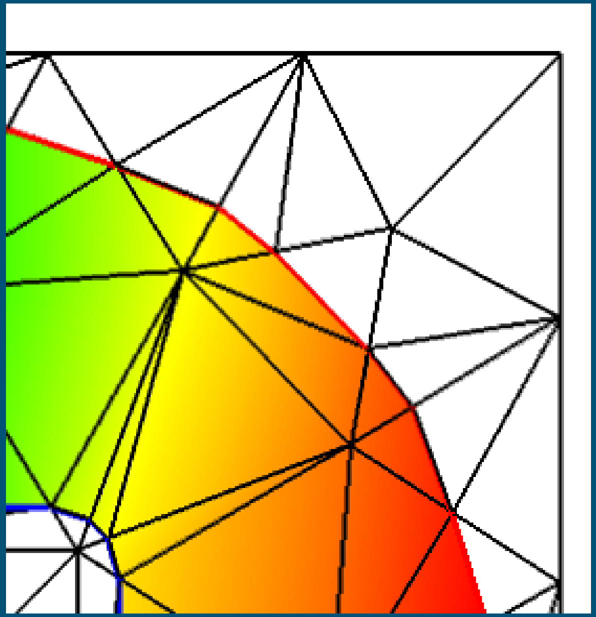
But What About the Low Quality Elements?

Resulting meshes

- ❌ Infinitesimal edge lengths
- ❌ Arbitrarily high aspect ratios (small angles)

Consequences

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



Question

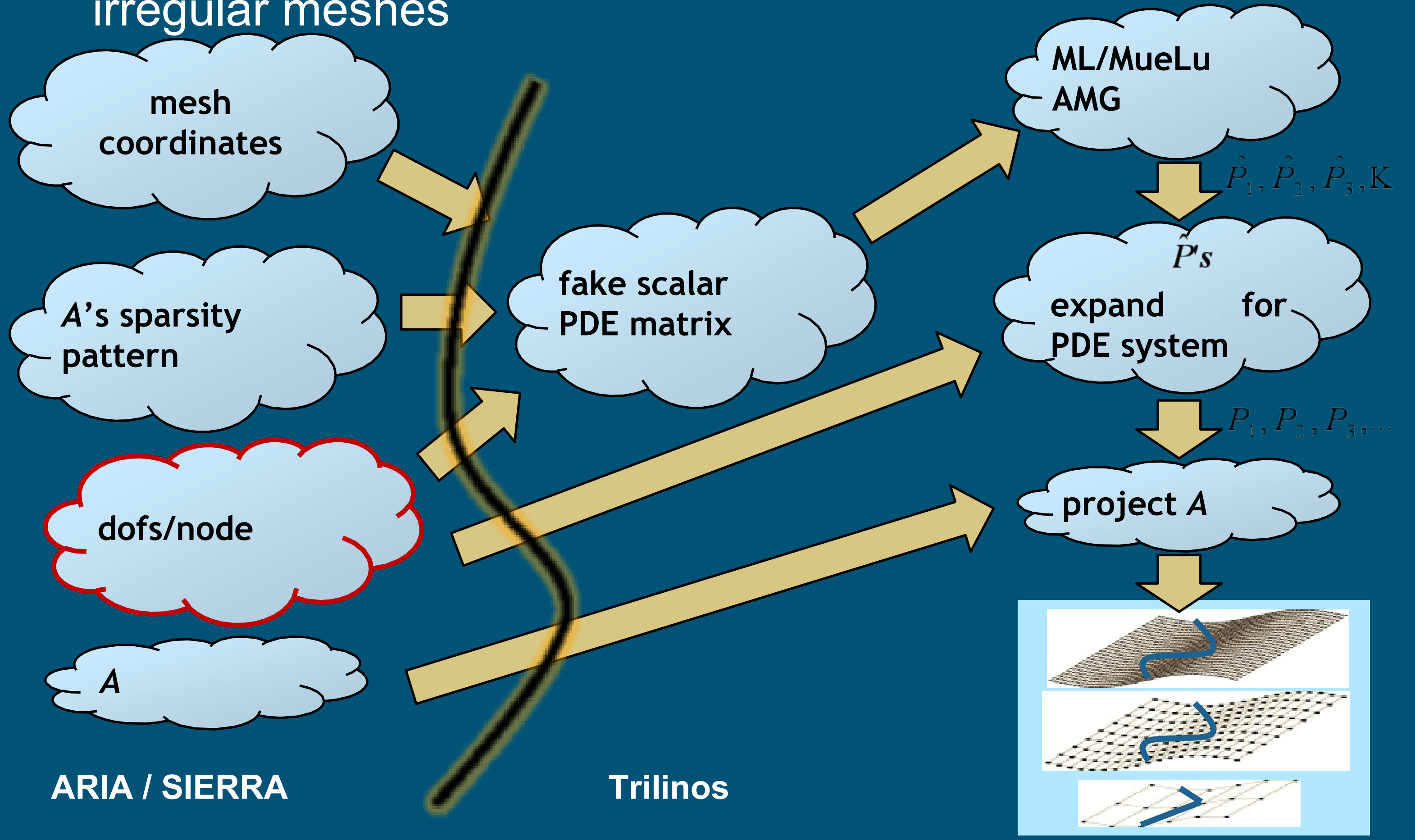
- By adding conforming r-refinement (node motion) in addition to conforming h-refinement, can these problems be alleviated?

Solver Strategies to Circumvent Poor CDFEM Conditioning

mesh → discretization → assembly → solve

Specialized Preconditioners

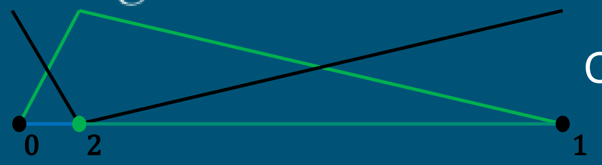
- Extended algebraic multigrid (AMG) solver in Trilinos to handle discontinuous variables on irregular meshes



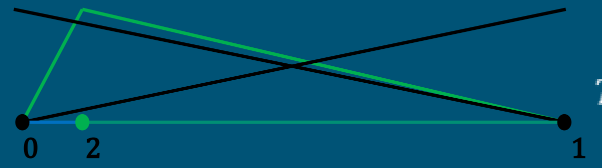
num nodes	ILU precond		mod ML precond	
	avg its	lin. sys. time	avg its	lin. sys. time
15K	90.1	20.0	11.5	10.0
60K	218.3	473.5	21.8	44.0
238K	318.2	3198.4	21.0	256.4
948K	580*	> 10 hrs	27.2	997.2

Change of Variables for Improving Discretization Quality

Change to hierarchical interface DOFs



CDFEM Basis in 1-D



Hierarchical Basis in 1-D

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

$T = c\hat{T}$, 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)

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

Can be posed as preconditioner of original system

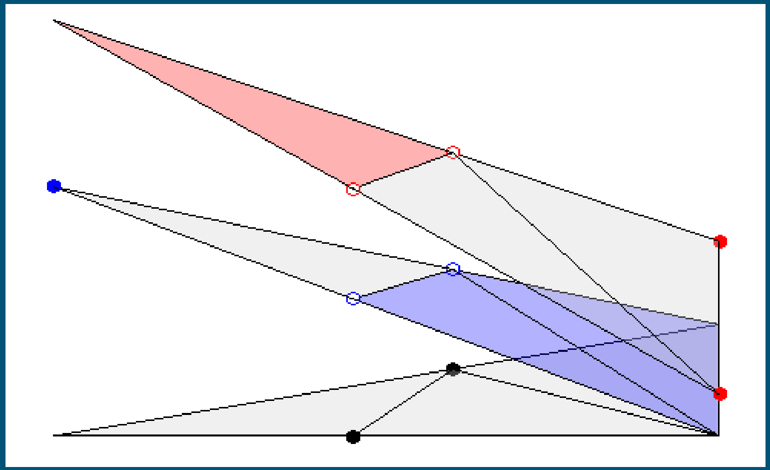
$$M^{-1} = c\hat{M}^{-1}c^t \quad \hat{M}^{-1} = \hat{L}\hat{L}^t \quad \hat{L}^t\hat{A}\hat{L} = L^t A L \;\text{ if }\; L = c\hat{L}$$

Coarsen the interface enrichment

- Assemble conforming (poor quality) elements
- Constrain solution to coarser space (like XFEM space)

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

$$A_{XFEM}\begin{bmatrix} u^P \\ u^{XFEM} \end{bmatrix} = b^{XFEM},\; M = \begin{bmatrix} I & 0 \\ C_P & C_{XFEM} \end{bmatrix}$$



Conforming r-refinement (snapping) as a Strategy for Improving Discretization Quality

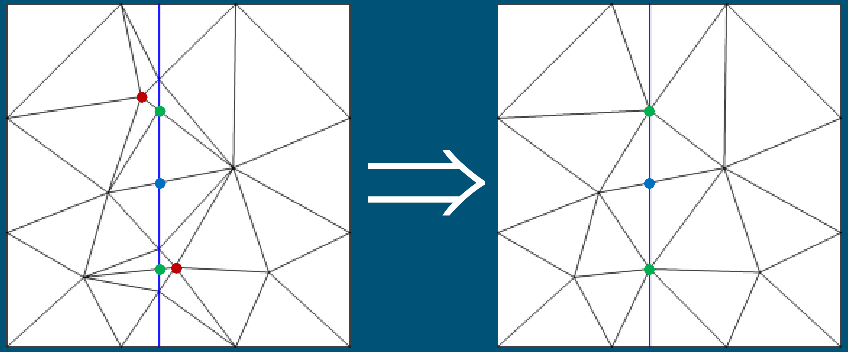
mesh → discretization → assembly → solve

Previous Work

- Labelle and Shewchuk (2007) on Isosurface Stuffing
- Soghrati et al (2017) on CISAMR
- Sanchez-Rivadeneira et al (2020) on stable GFEM with snapping

Our Previous Algorithm

- 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, •→•)

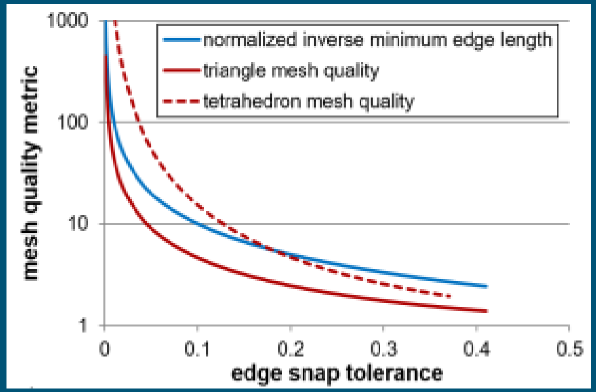


Even small snap tolerance effective at improving quality

- Provable element quality
  - Element quality metric (Berzins 1998)

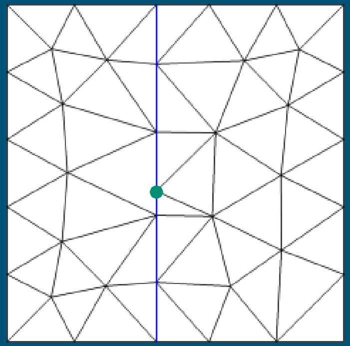
$$Q_w = \frac{1}{1296\sqrt{2}V}\left(\sum_e h_e\right)^3$$

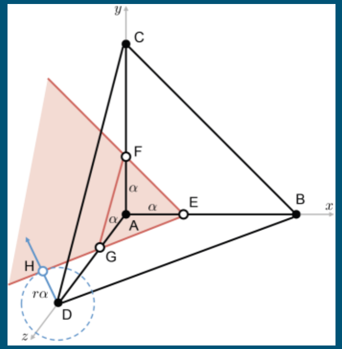
  - For snap tolerance of 0.1, Q_w=15.3



Selection of Snap Tolerance

- Cannot allow all nodes of an element to snap to the interface





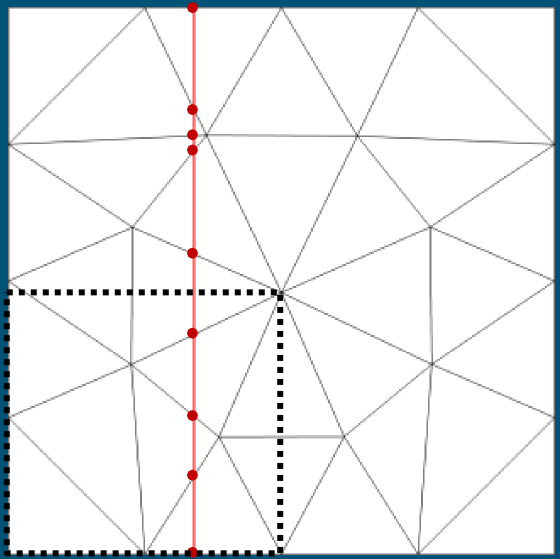
$$\alpha = \frac{\sqrt{3}r - 1}{3\,r^2 - 1}$$

- Maximum snap tolerance of 0.33 for BCC tet mesh (lengths of 1 and $\sqrt{3}/2$), 0.29 for right angle tet mesh (lengths of 1 and $\sqrt{2}$)
- Maximum $\alpha \to 0$ as $r \to \infty$

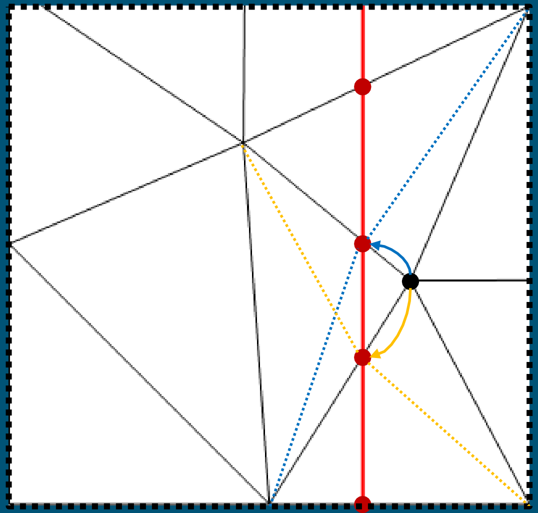
Algorithm: Snap When Quality is Better than Cutting

Snap when element quality of snapping is better than the element quality if the intersection points are cut into the mesh

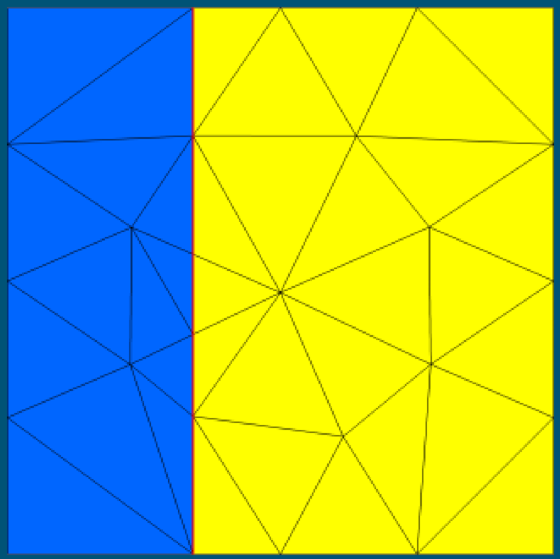
- The estimated cutting quality for a node is the minimum quality of the elements that would be produced by cutting each edge using the node at its intersection point
- The snapping quality for a node and intersection point is the minimum quality of the elements if the node is moved to that intersection point
- If the snapping quality is better than the estimated cutting quality, then the node is a candidate for snapping to that intersection point
- Select and snap the candidates that are higher quality than any of the neighboring snap candidates, reintersect edges, repeat until all candidate snaps are performed



Mesh with intersecting interface

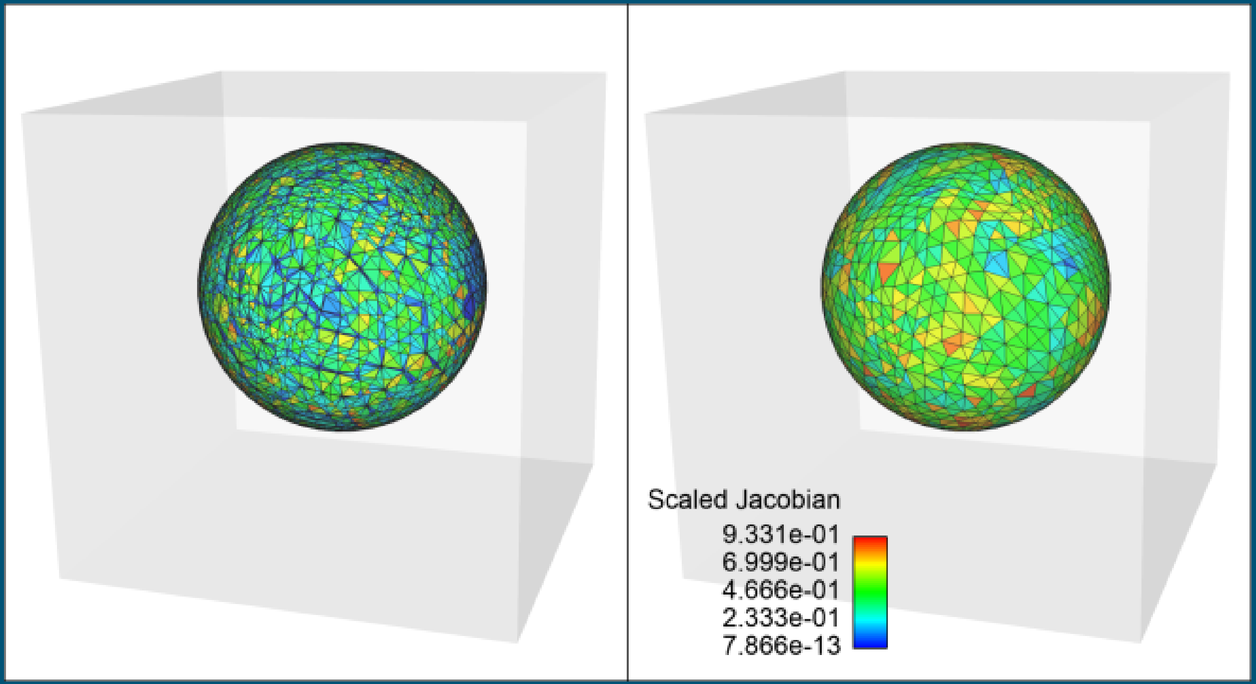


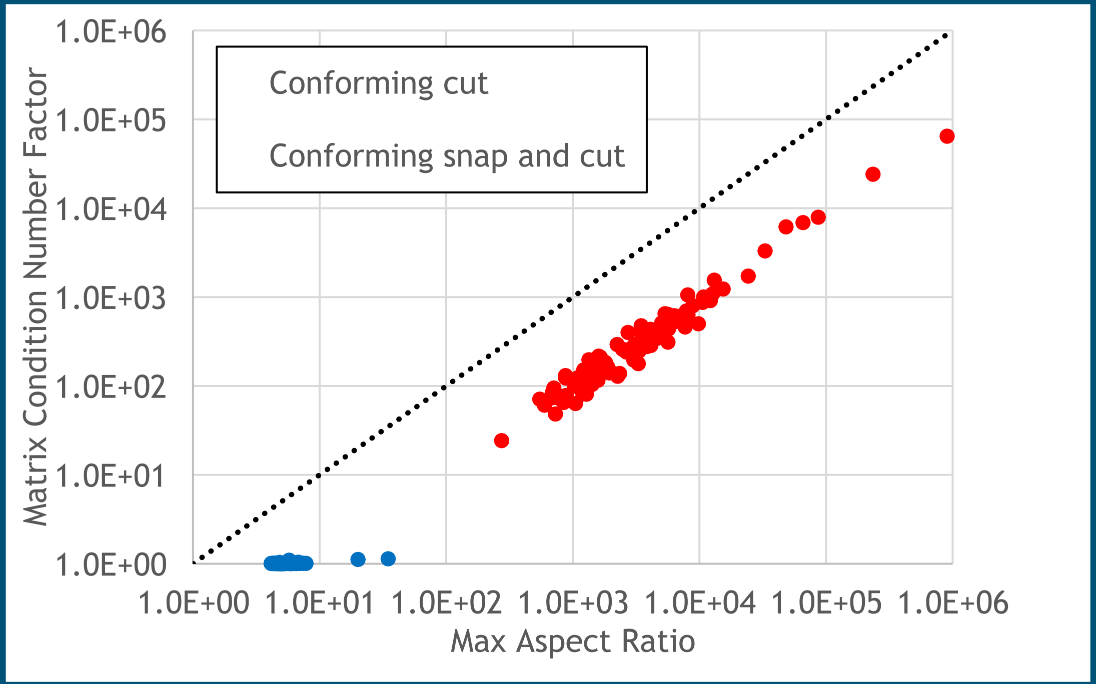
Zoom in of snap candidates



Resulting snapped and cut mesh

Performance of Simple Snapping Procedure for Randomly Place Sphere





Conforming cut mesh   Conforming snap and cut mesh

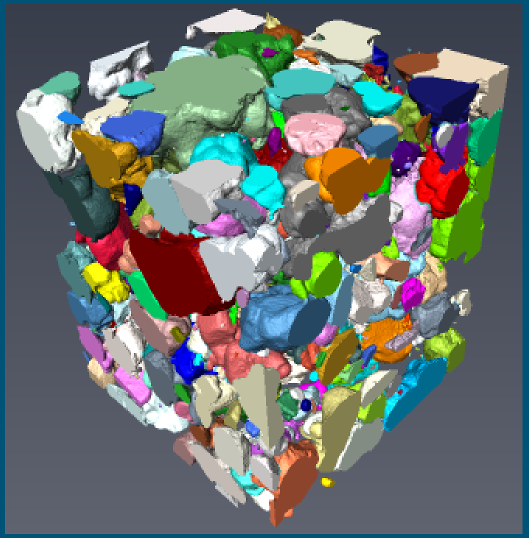
Test
- 100 cases with randomly placed sphere in box
- Calculate maximum aspect ratio and estimated condition number for Laplacian on conforming mesh

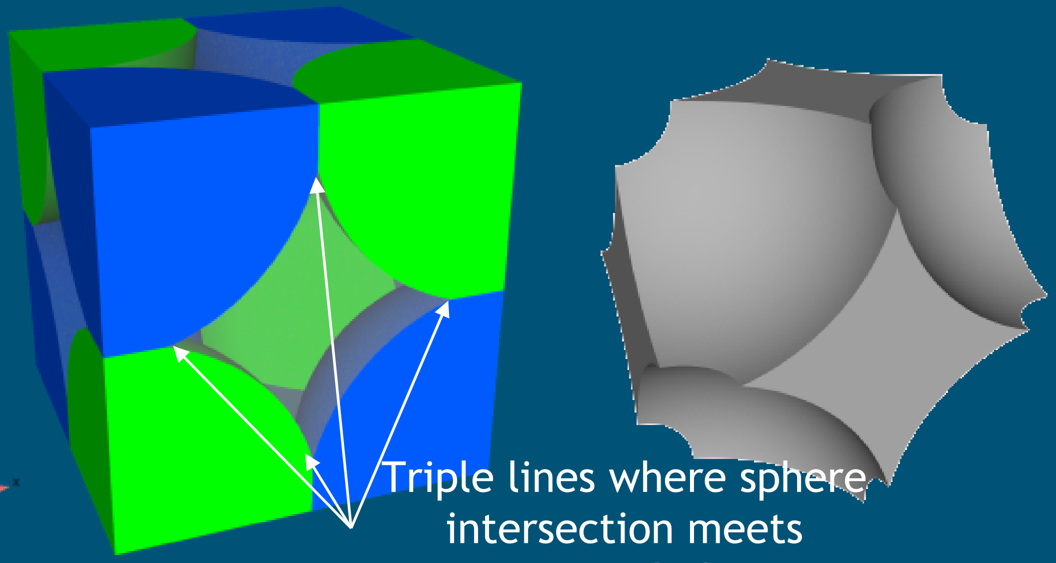
Results
- Without snapping, aspect ratio and condition number show many orders of variation. These quantities are highly correlated.
- Snapping reduces aspect ratio and condition number to small multiples of uncut mesh values

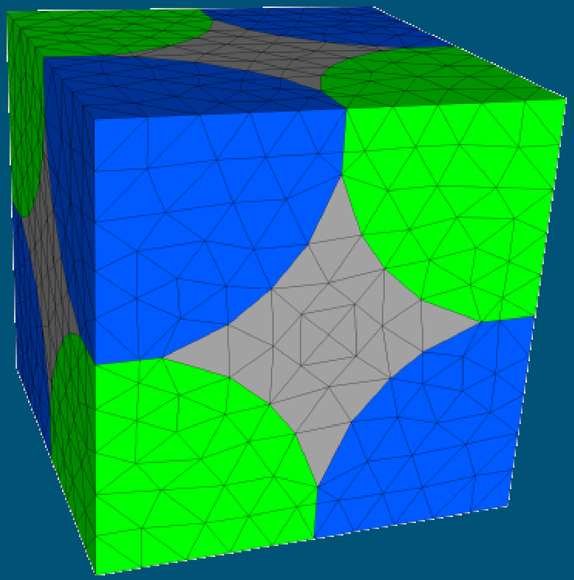
Snapping Strategy for Many Materials

Handling many materials requires capturing not only interfaces, but intersection of interfaces

- Triple lines at 3 phase intersections and quadruple points where 4 phases meet







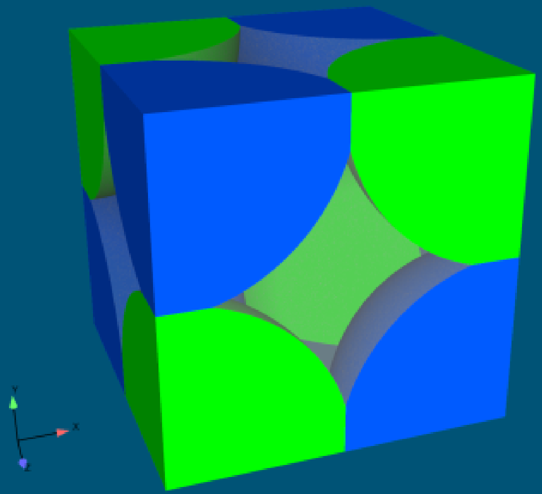
- Find intersections between triple lines and element faces and quadruple points within elements
- Prioritize capture of sharp features over interfaces

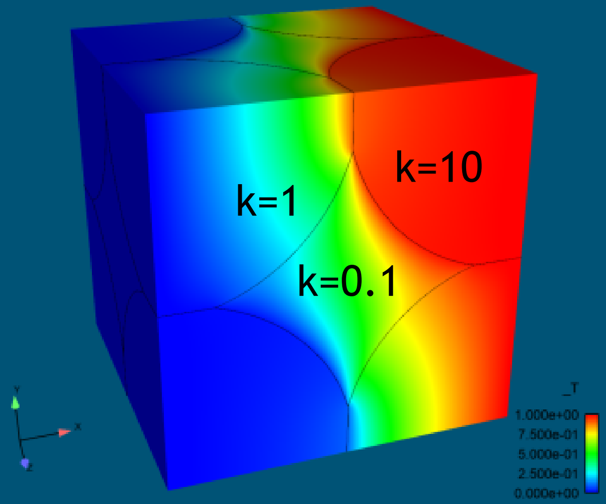
3 Phase Conduction Problem Benchmark

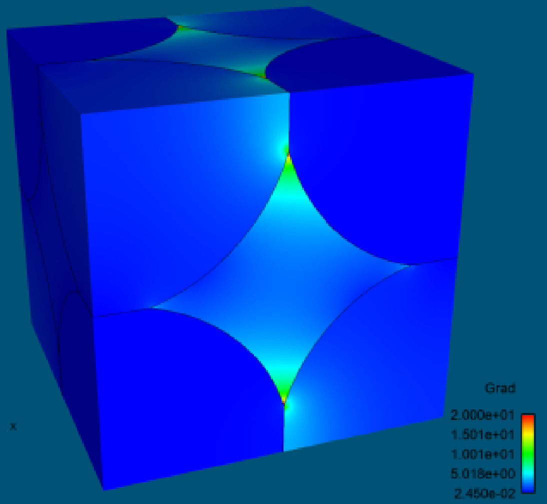
Conduction in a Simple Cubic Array of Overlapping Spheres
- Triple lines where sphere intersection meets interstitial phase
- Non-smooth temperature profile due to sharp corners and disparate conductivity

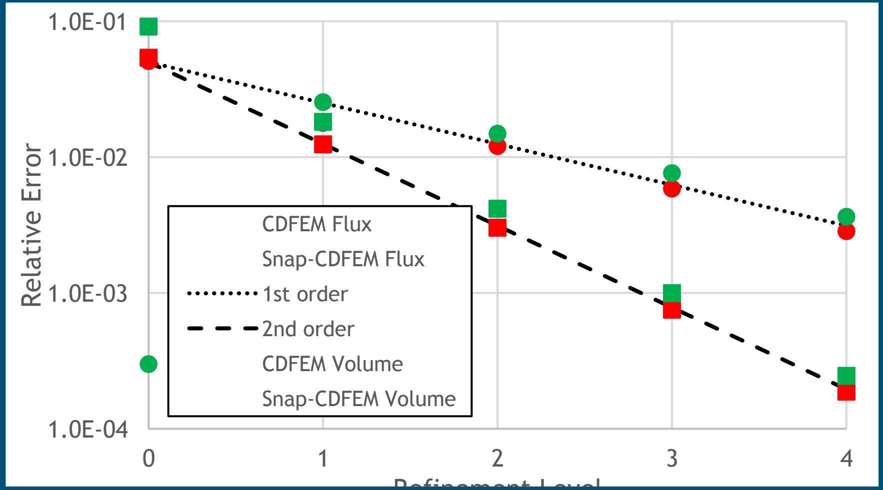
Accuracy
- Optimal convergence rate for geometric and flux quantities regardless of discretization strategy
- Snapping increases error slightly because fewer DOFs

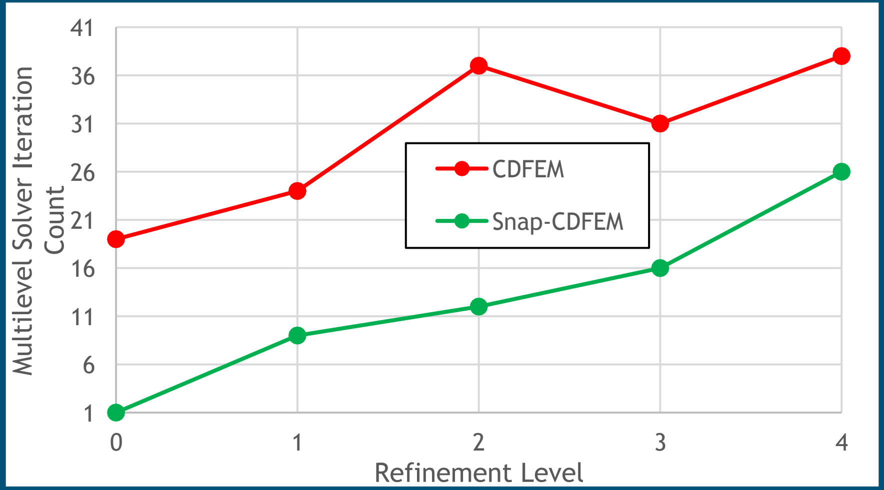
Solvability
- Multilevel solver (parallel and DOF scalable)
- Snapping reduces solver costs by 2-3x







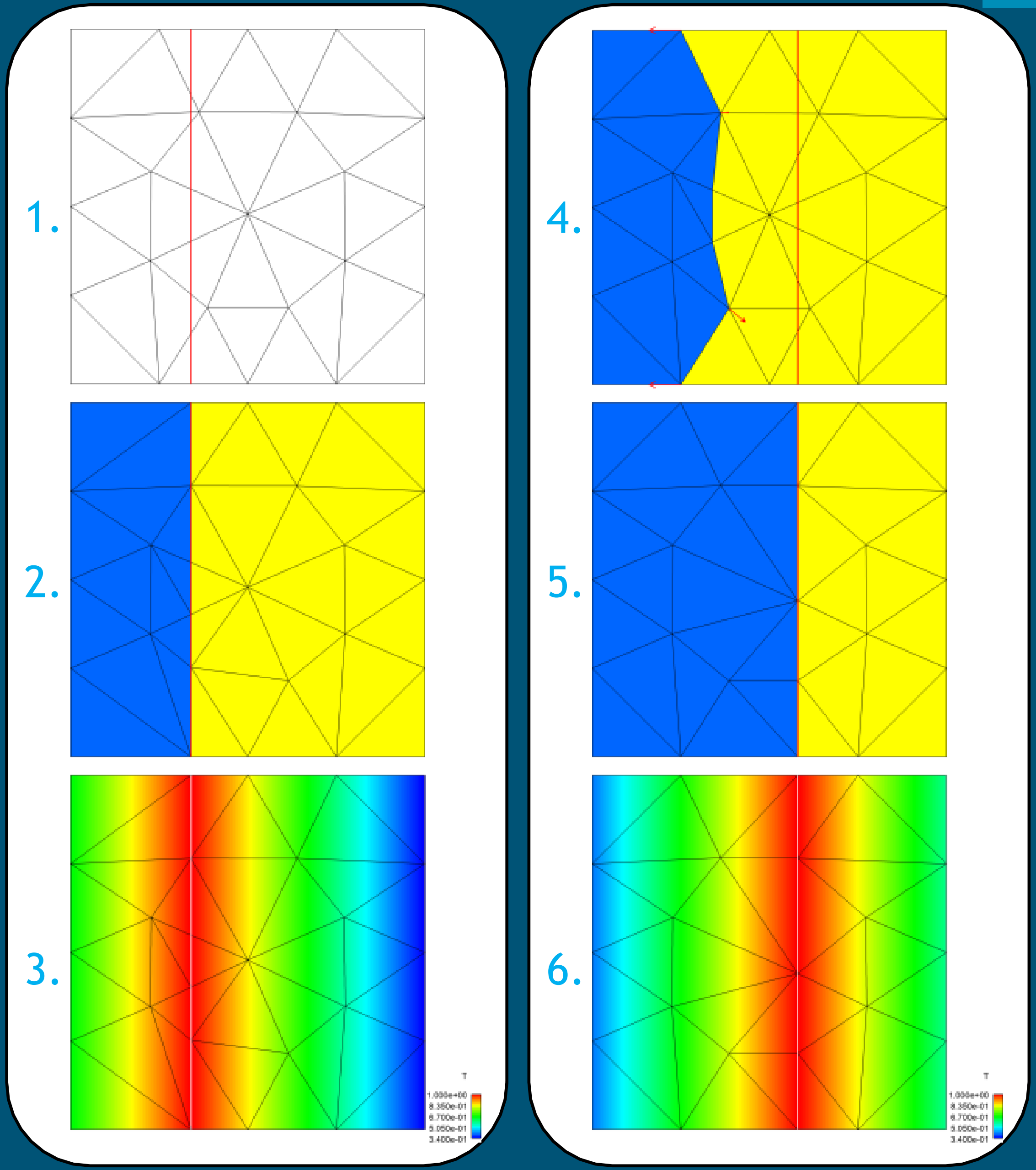




cThruAMR Algorithm

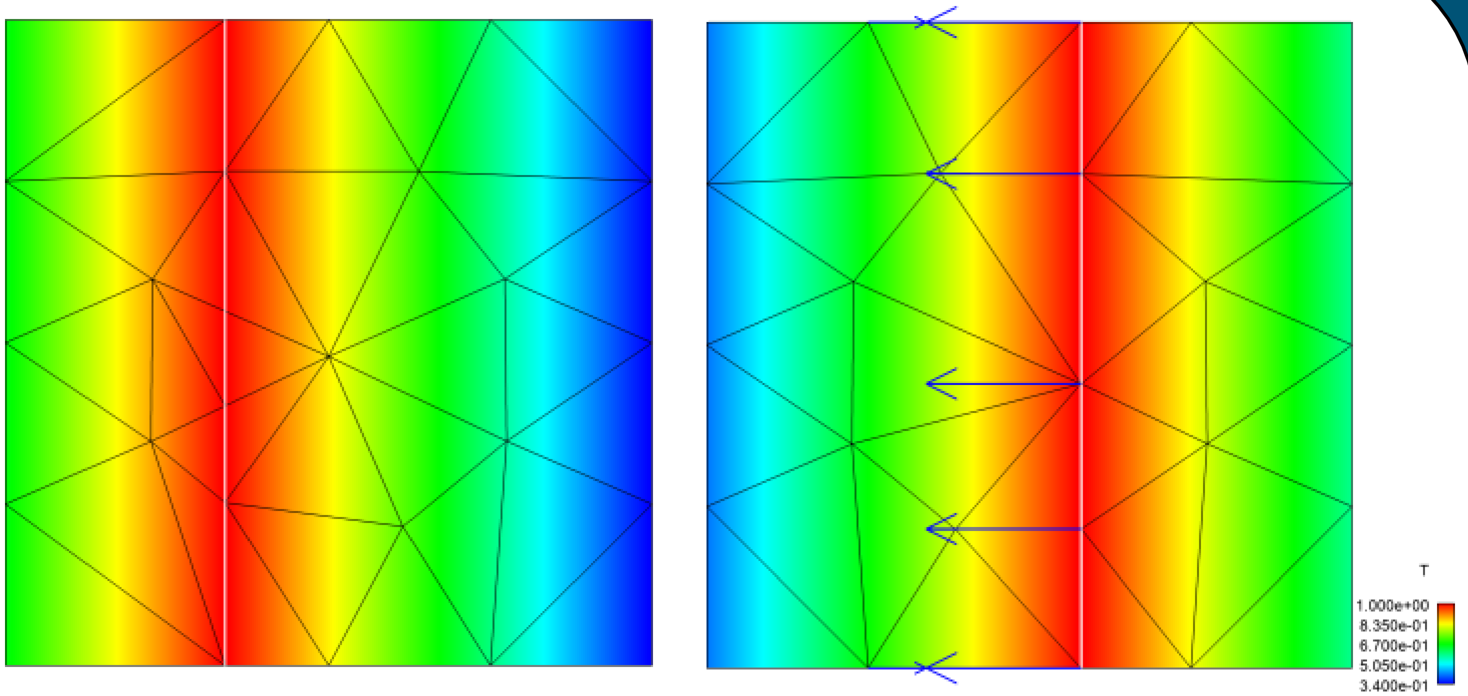
Integrate snapping and cutting for transient level set problems: conforming transient h-r unstructured adaptive mesh refinement (cThruAMR)

1. Initialize level sets on input mesh
2. Create conforming mesh by snapping and cutting
   - Snap whenever quality is higher than cutting quality
3. Initialize physics on conforming mesh
4. Advect level sets while “reversing” snap displacements
5. Create new conforming mesh by snapping and cutting
6. Solve physics on conforming mesh
   - Include moving mesh term where interface nodes and nodes that have changed material are considered to have advected from the nearest point on the old interface



cThruAMR Mesh Motion: CDFEM Mesh Displacement

- CDFEM Mesh Displacement during physics solve
  - Nodes on the interface or that change material are considered to have been originated at the closest point of the previous interface
  - Designed to exactly preserve discontinuous linear field and converge at optimal rates for nonlinear fields
    - Kramer, R. M. J. and Noble, D. R. (2014), A conformal decomposition finite element method for arbitrary discontinuities on moving interfaces, *Int. J. for Numerical Methods in Engineering*, **100**, pp. 87– 110, doi: 10.1002/nme.4717



Applying CDFEM Mesh Displacement during physics advection/solve

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

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

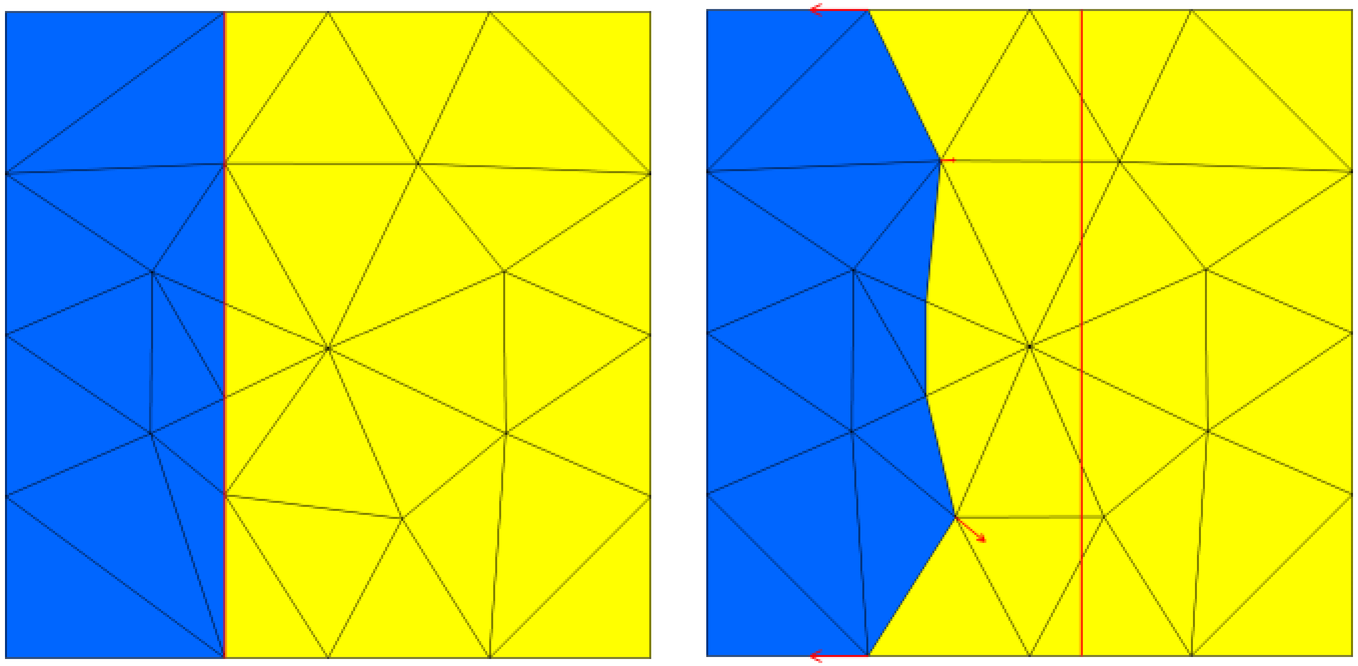
cThruAMR Mesh Motion: Snap Displacement

"Reversing" Snap Displacement during physics solve

- Nodes are advected back to their original locations while the level set is advected according to the current velocity
  - Result is original mesh with additional CDFEM nodes with level set at new location

Other option

- Advect level set on current mesh, contour level sets, unsnap, snap/cut based on intersections between level set contours and unsnapped mesh
  - Less/more diffusive for large/small interface motion?



"Reversing" Snap Displacements during level set advection/solve

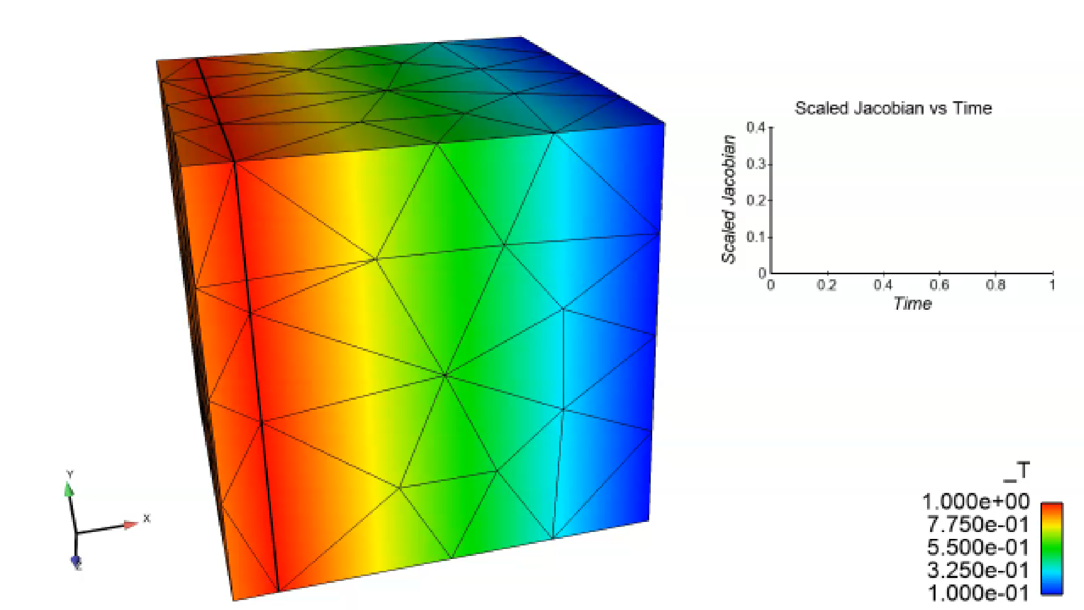
$$\int_\Omega \frac{D\psi}{Dt} w_i \, d\Omega \approx \sum_J \int_{\Omega_J^{n+1}} \left(\frac{\psi_J^{n+1}(\mathbf{x}) - \tilde{\psi}_J^n(\mathbf{x})}{\Delta t} + (\mathbf{u} - \dot{\mathbf{x}}(\mathbf{x})) \cdot \nabla \psi_J^{n+1}(\mathbf{x}) \right) w_i \, d\Omega$$

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

Demonstration Problems

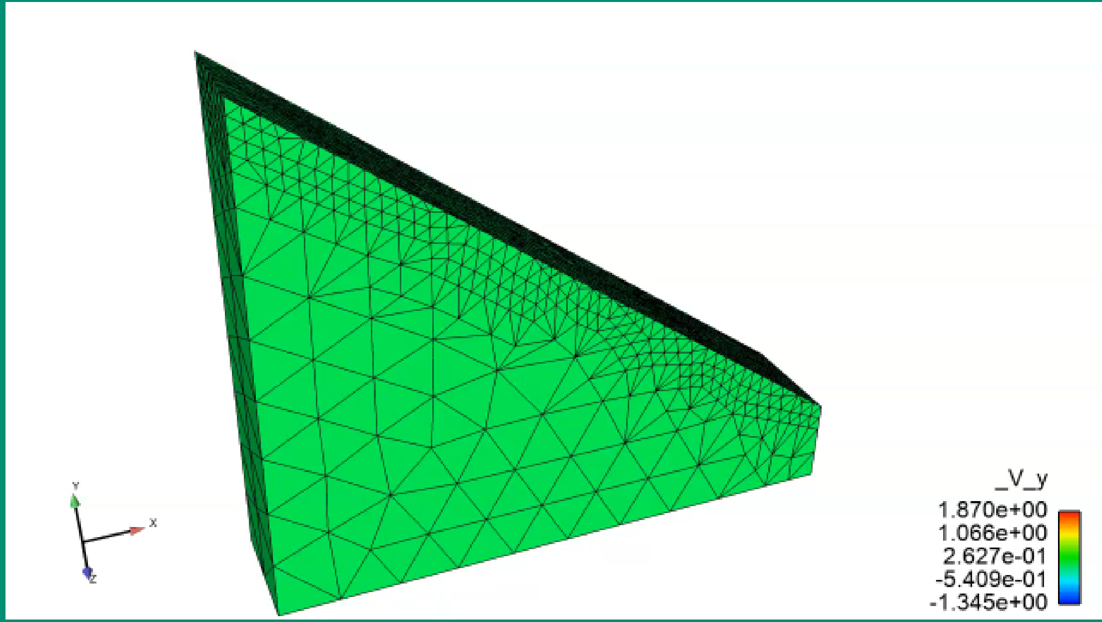
Patch Test: Pure Advection of Slope Discontinuity

- Results
  - Preserves discontinuous exact solution to machine precision
  - Quality is good for all times



Simple 3D Fluid: Gravity Wave with Non-Conformal Refinement

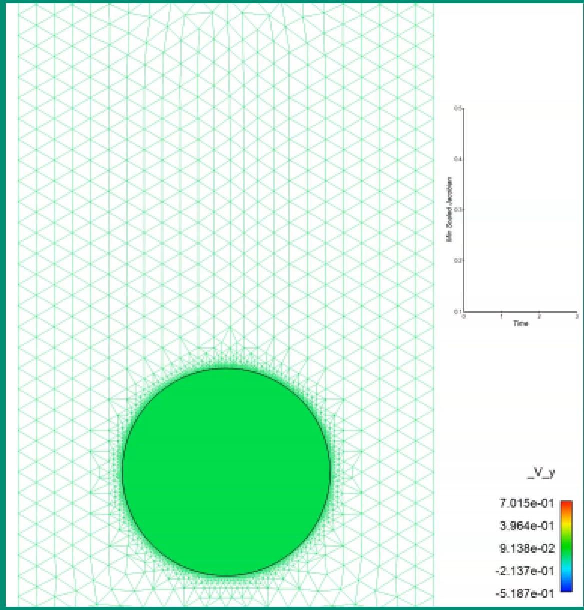
- Multiple levels of non-conformal refinement followed by h-r conformal refinement (cThruAMR)

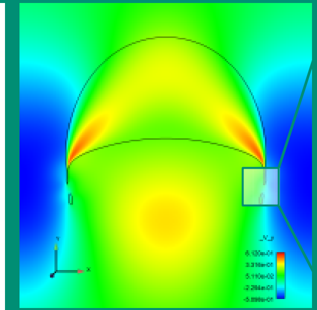


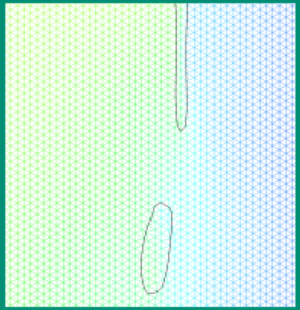
Rising Bubble Problems

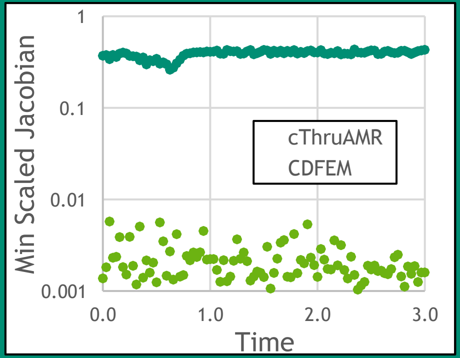
Problem: 2D Rising bubble

- Benchmark problem for level set codes with topology change
- Results
  - Quality is ~100x better than CDFEM for all times
  - Topology change handled robustly
  - Non-conformal refinement in vicinity of interface



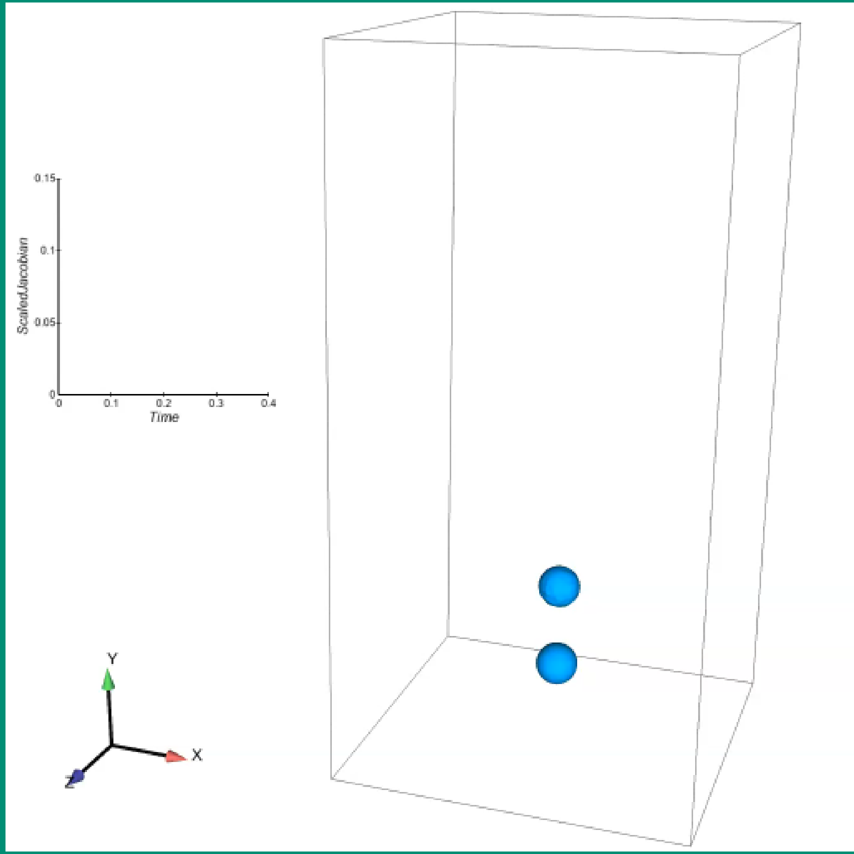




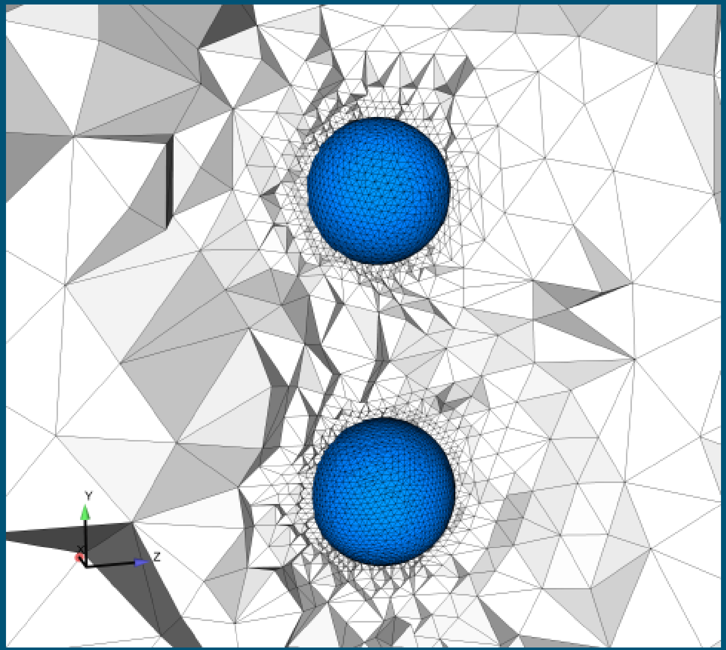


Problem: 3D Rising, merging bubbles

- Results
  - Quality worse than 2D but improved over CDFEM
  - Topology change handled robustly
  - Non-conformal refinement in vicinity of interface

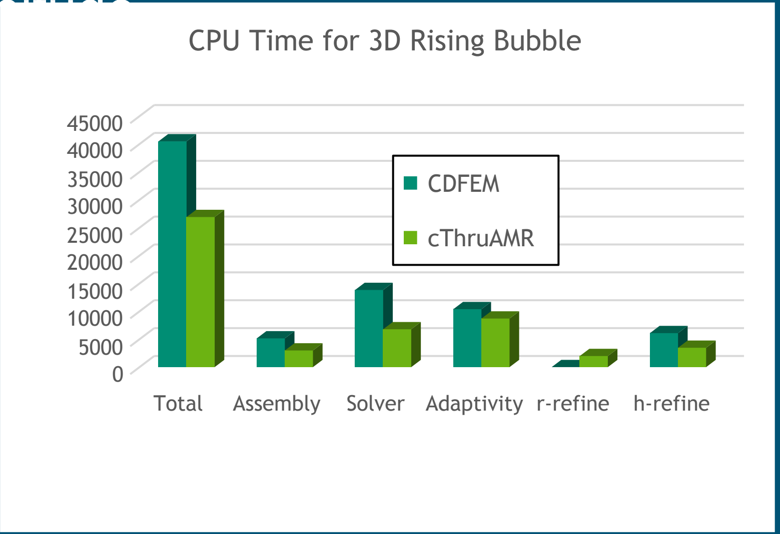


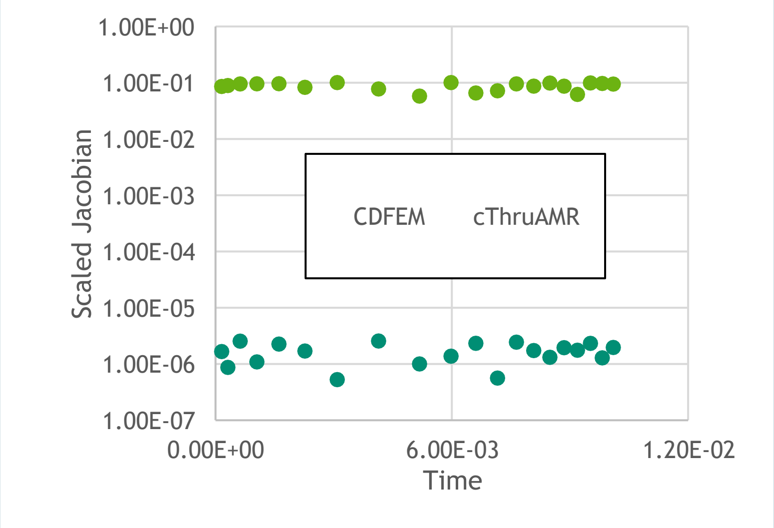
Improved cThruAMR Performance over CDFEM



Test Problem: Two Rising Bubbles

- Overall CPU time reduced by more than 33%
  - Reduced number of DOFs leads to reduced assembly and solver times
- Quality Improvement
  - The resulting scaled Jacobian improves by approximately 5 orders of magnitude





Open Source Code Krino in Trilinos: Capabilities

Signed Distance Calculations

- Capabilities
  - Compute signed distance from multiple surface types
    - Analytic surfaces: Spheres, planes, cylinders, ellipsoids
    - Faceted surfaces: STLs, meshed surfaces, level sets
- Algorithms
  - Scalable Euclidean distance calculation (exact but “sees through” mesh boundaries)
  - Fast Marching on triangle and tetrahedral elements (approximate, length of shortest path within mesh)
- Application/Usage
  - Nearest distance to wall for turbulence models
  - Level set initialization
  - Level set reinitialization/renormalization

Snapping and Conforming Decomposition

- Capabilities
  - Decomposes elements to conform to background elements and level sets passing through elements
  - Snap nodes of background mesh to intersections between the background mesh and the level sets prior to decomposition
  - Optionally uses open source code percept to refine intersected background mesh elements
- Algorithms
  - Level set per interface, “level set” per phase (interfaces defined by lower envelope of distance functions)
- Application/Usage
  - Automatic tet meshing of topologically complex domains
    - Microstructure or mesoscale transport applications

Summary/Conclusions

- Conforming (interface enriched) discretizations provide powerful tools for analyzing multiphase and multimaterial problems with dynamic interfaces
  - Particularly well-suited for manufacturing simulations
- Conforming Transient h-r Unstructured Adaptive Mesh Refinement (cThruAMR) produces good quality discretizations for dynamic level set problems
  - Combined snapping and cutting strategy produces much higher quality meshes than cutting alone
    - Impacts element quality, matrix conditioning, robustness, DOF count, and CPU costs for assembly and linear solver
- Open source code krino provides useful level set and discretization capabilities

- Future Work
    - Combination of snapping, cutting, and swapping strategy to provide higher quality discretizations