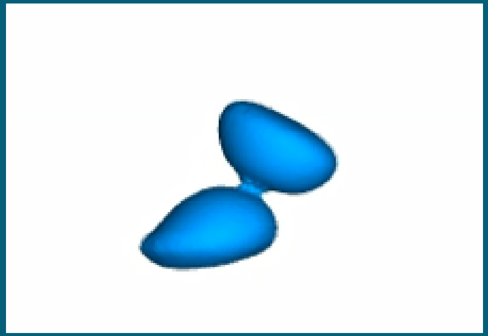
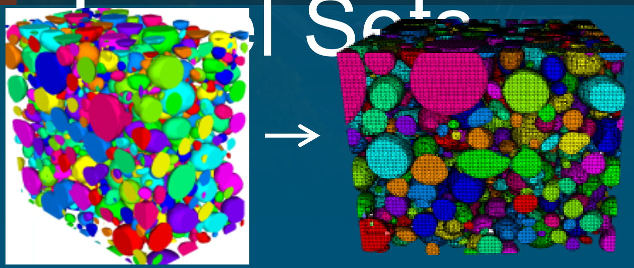
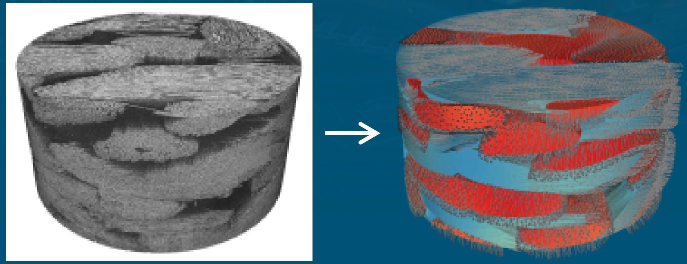
SAND2021-8909C

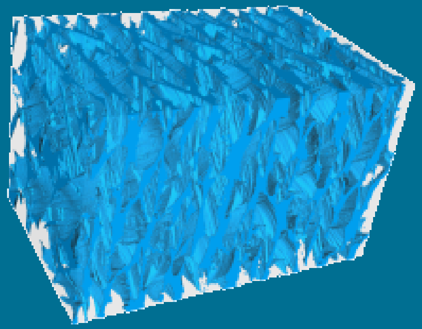
Sandia National Laboratories

New Strategies for Automated Tetrahedral Mesh Generation for Producing Credible Discretizations from 3D Image Data and Transient Level Sets









PRESENTED BY

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U.S. DEPARTMENT OF ENERGY NNSA

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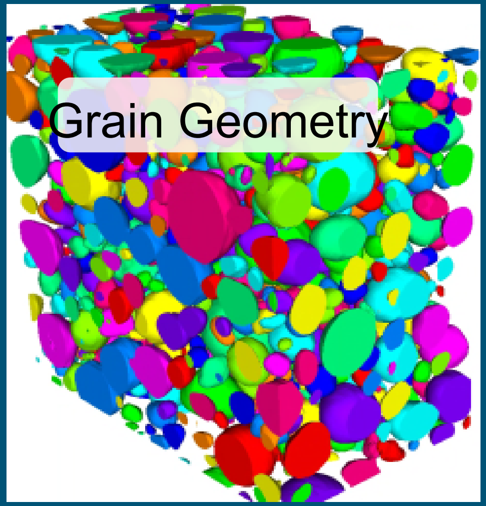
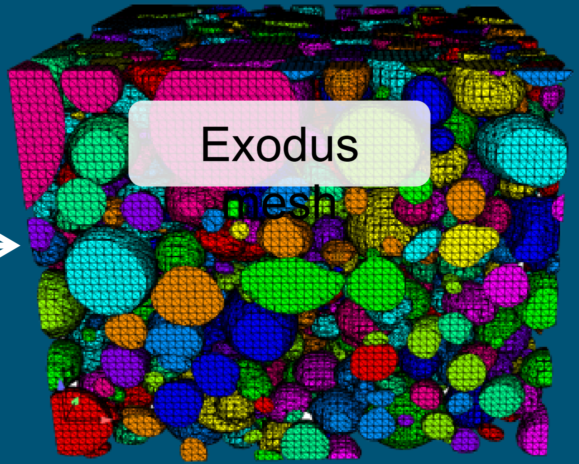
Motivation: Mesoscale Modeling



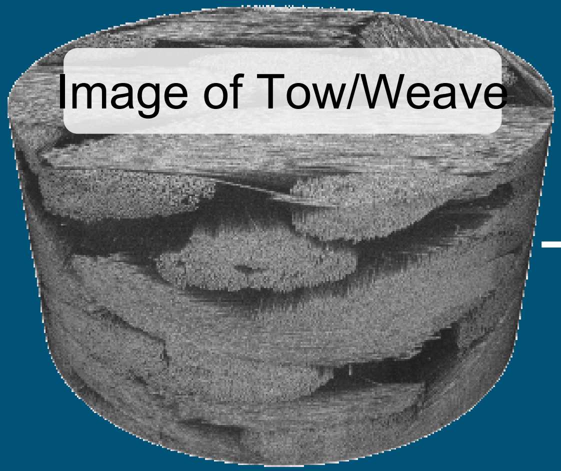


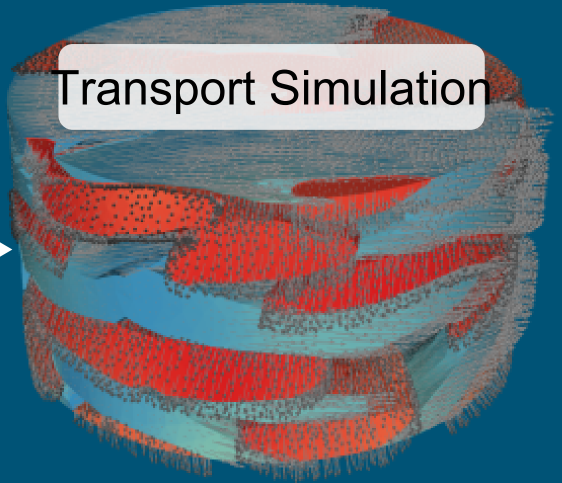
Electrode Geometry

- Numerous materials in contact, distinct anisotropic properties from grain to grain
- Obtained from image reconstruction

Physics

- Electrochemistry, possibly with contact resistance at grain boundaries
- Current simulation for static geometry, but generally dynamic due to swelling





Thermal Protection System Geometry

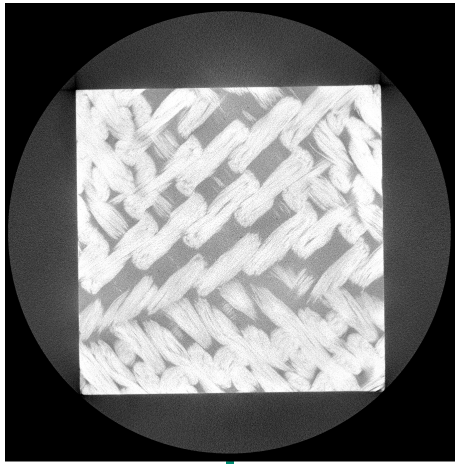
- Microscale: Individual fiber filaments spun into tow of 1,000+ fibers, impregnated with resin. Fiber arrangement affects tow properties.
- Mesoscale: Woven carbon fiber surrounded by phenolic resin. Governed by weave geometry, resin/tow properties
- Macroscale: Typical performance assessments and modeling (e.g. CMA). Composite properties required

Physics

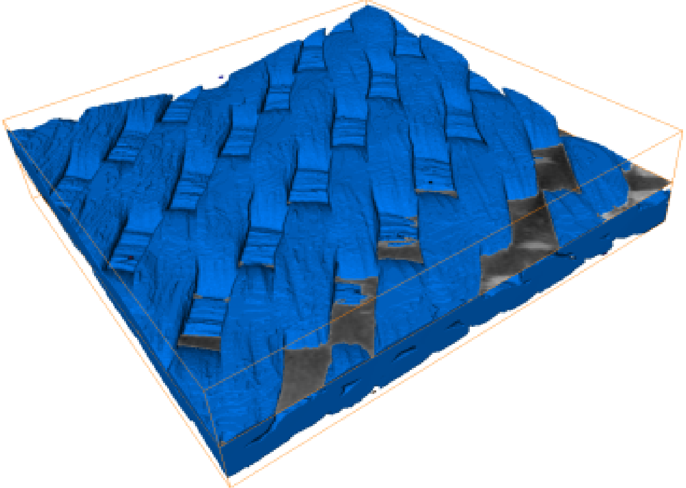
- Porous media flow, thermal transport, chemistry and mechanics (pressurization) at mesoscale
- Current simulation for static geometry, but generally dynamic due to chemistry/ablation

Motivation: Credible, Automated Meshing of Images (CAMI)

Raw greyscale image (XCT)

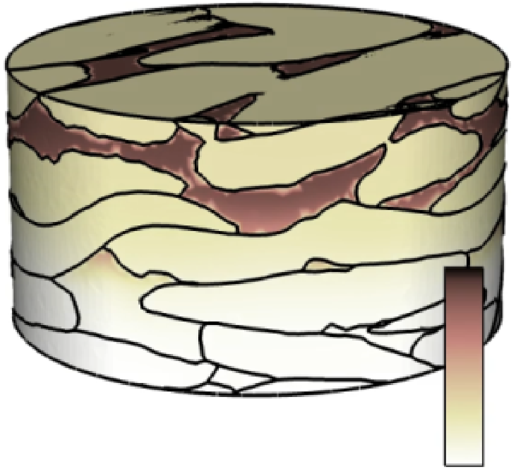


Surface mesh (STL)



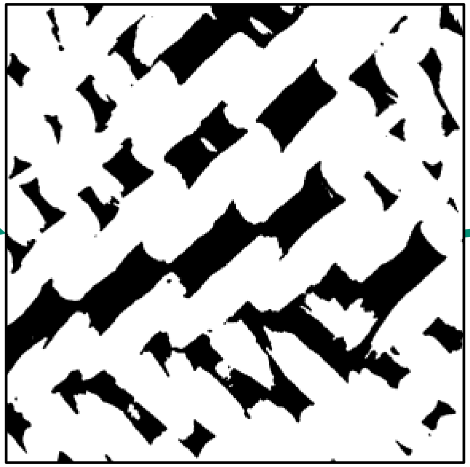
Meshing:
- Cubit
- CDFEM
- Poor quality
- CDFEM+Snap+Emend
- High quality

Physics simulation



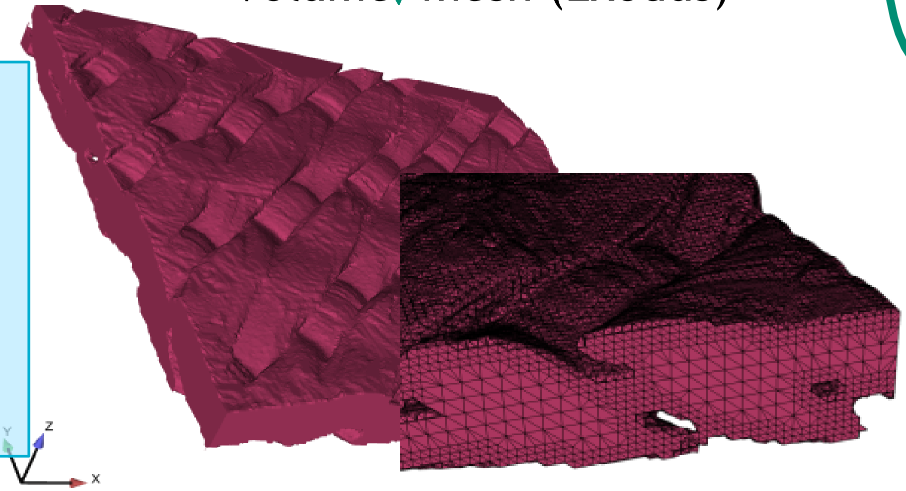
Segmentation:
- Manual thresholds
- SME-dependent
- Non-repeatable
- Deep learning
- Automatic
- Repeatable

Binarized image



Interface Identification:
- Avizo stair mesh
- Arbitrary smooth
- Manual
- Marching cubes
- Occupancy Networks?

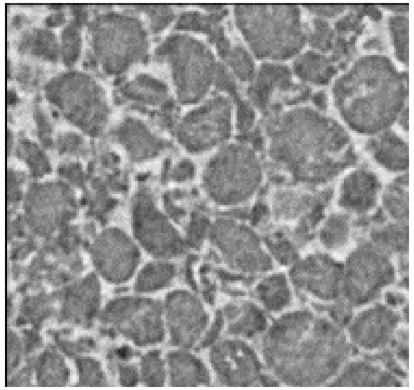
Volume mesh (Exodus)



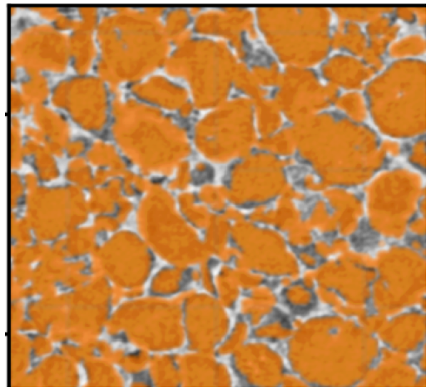
Credible, automated image-to-mesh with uncertainty will revolutionize engineering analysis of as-built parts!

Deep learning produces accurate segmentations with per-voxel UQ

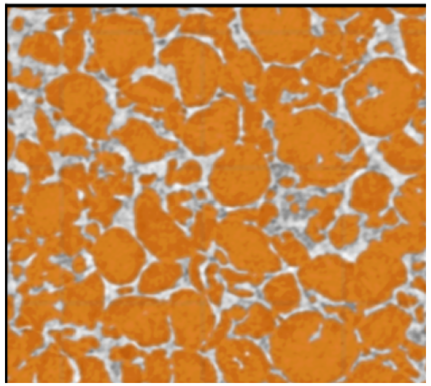
Slice from CT image of graphite electrode



Human label (orange) overlaid on CT scan of battery

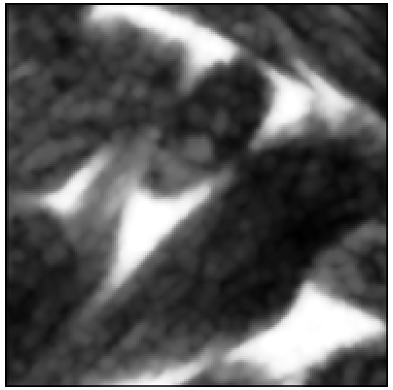


Deep learning label (orange) overlaid on CT scan of battery

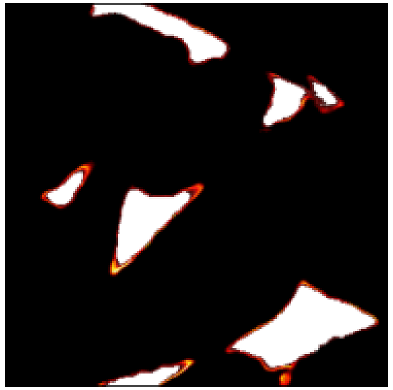


LIB: Incrementally trained DL model segments to high accuracy, higher than human labels in some cases

Slice from CT scan of TPS



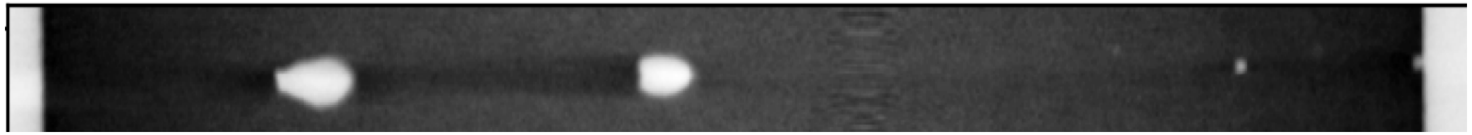
Deep learning segmentation with uncertainty map



TPS: Accurate segmentations on held-out sub-volumes, with per-voxel UQ

Laser welds: 99.2% accuracy to manual labels with uncertainty maps on ambiguous features.

CT scan of laser welded material

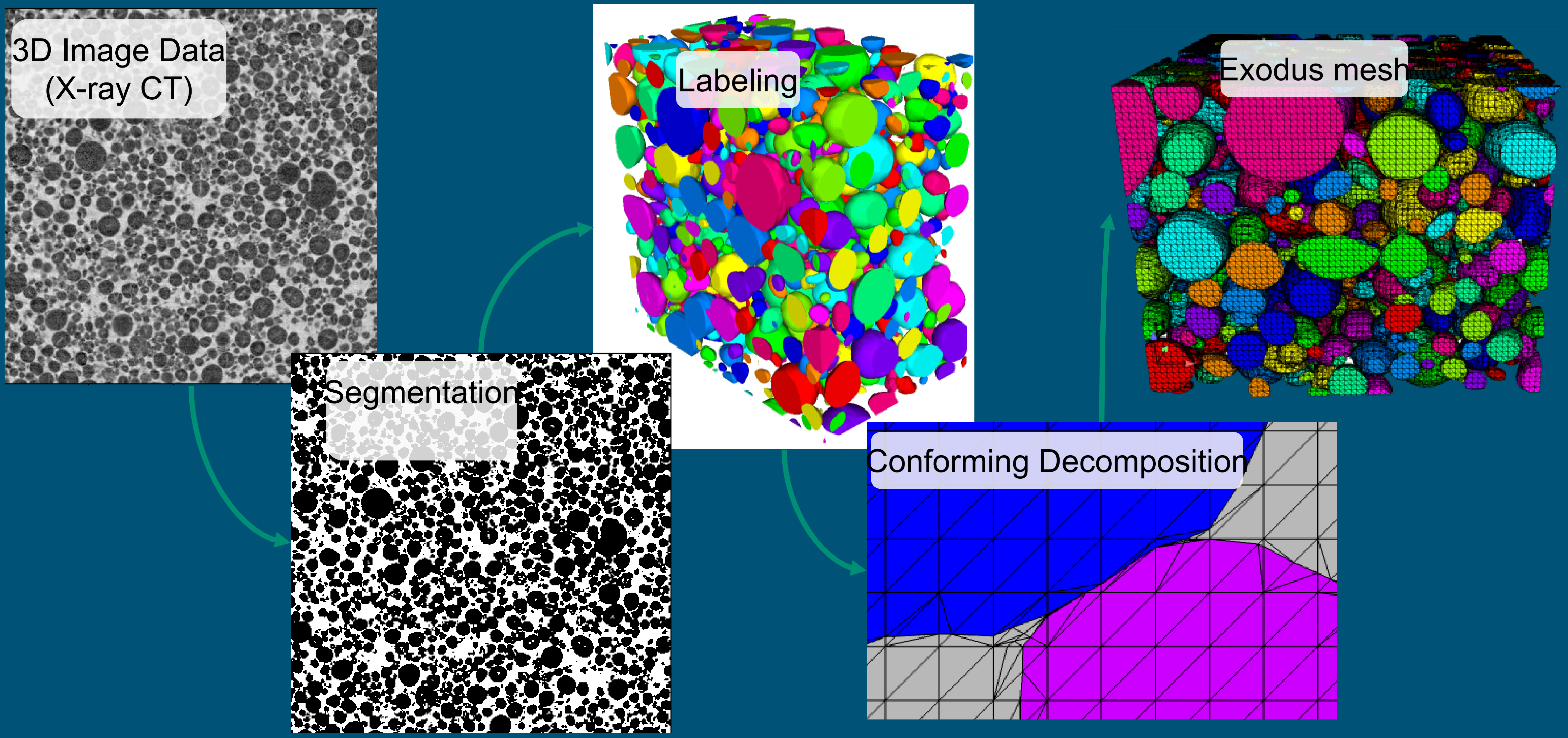


Accurate deep learning segmentation

DL inferences takes minutes on GPU vs. hours to days manually!

We have proven DL models capable of flexible and accurate image segmentation with rigorous per-voxel UQ estimates

Mesoscale geometry from CT data using CDFEM



Roberts et al JES 2014, Roberts et al JEECS 2016

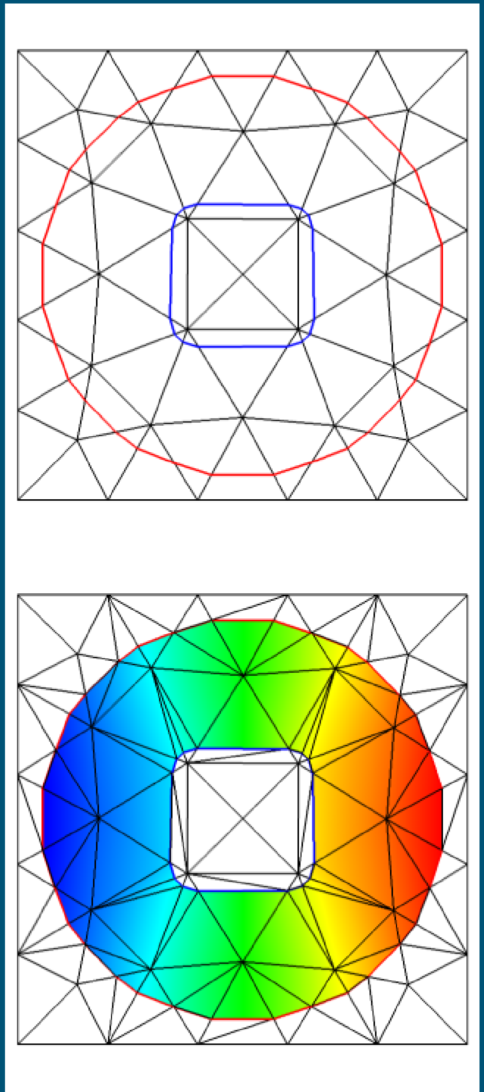
Conforming Decomposition Finite Element Method (CDFEM)

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 conformal 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



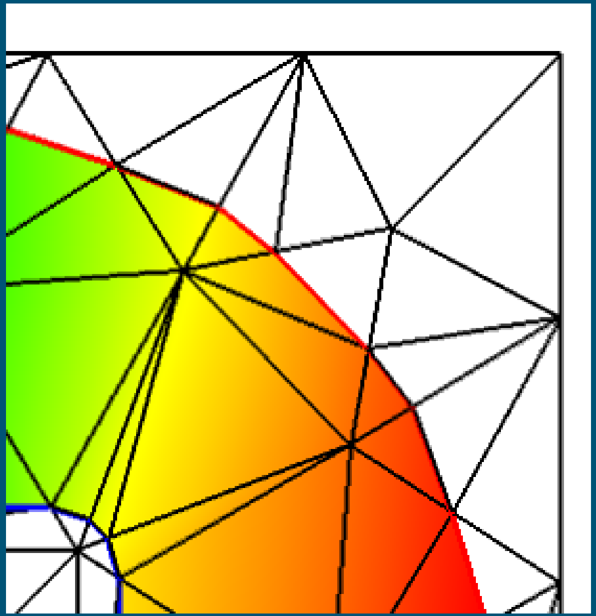
But What About the Low Quality Elements?

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

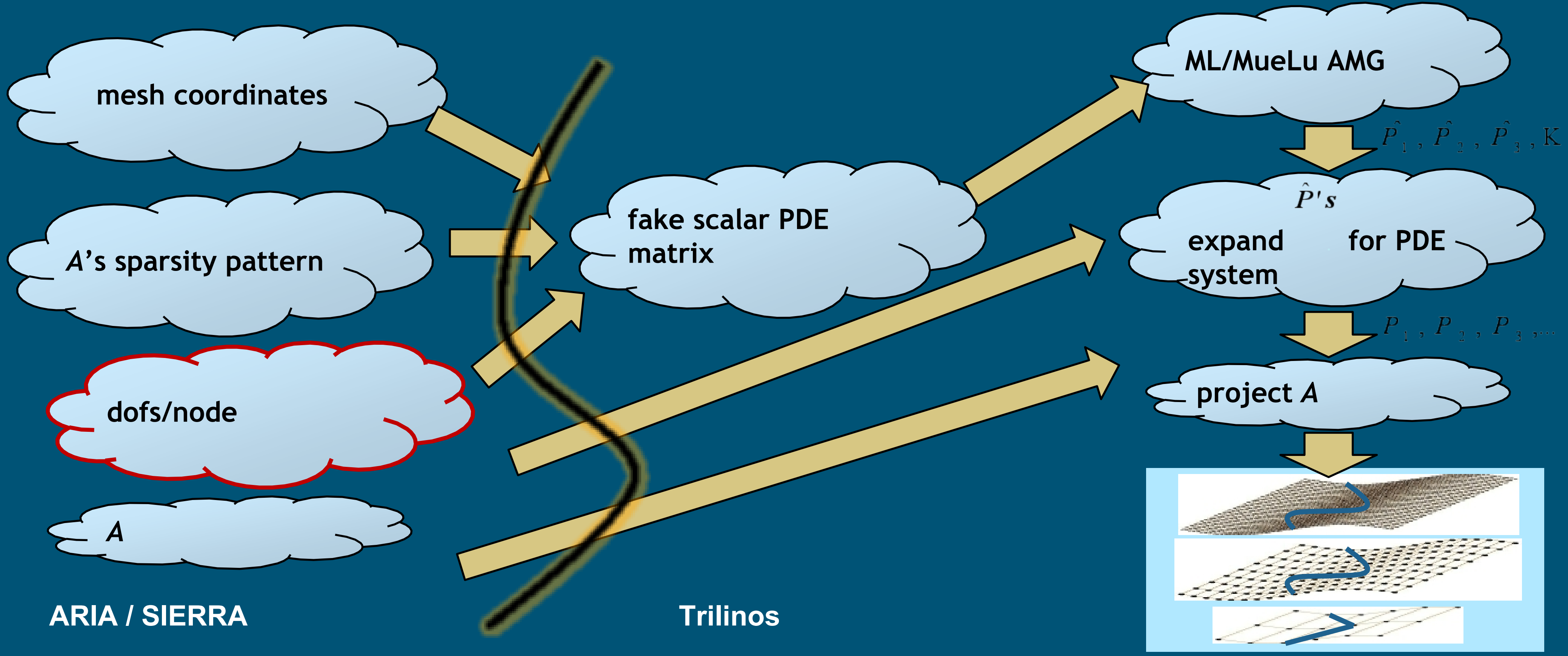
- Can we use a combination of snapping, cutting, and incremental mesh improvement to provide good quality discretizations for topologically complex and/or moving interfaces?

Solver Strategies to Circumvent Poor CDFEM Conditioning

mesh → discretization → assembly → solve

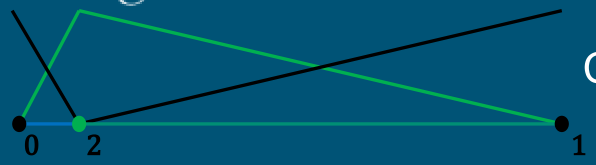
Specialized Preconditioners

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

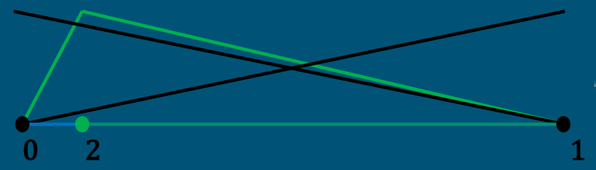


Change of Variables for Improving Discretization Quality

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

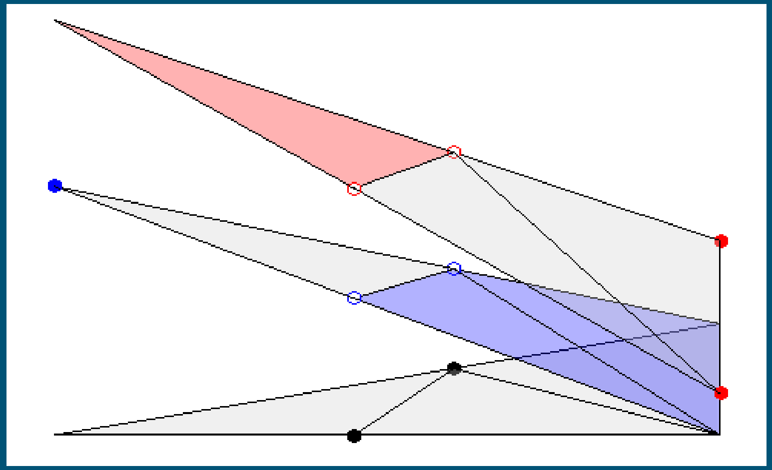
$$M^{-1} = c\hat{M}^{-1}c^t \quad \hat{M}^{-1} = \hat{L}\hat{L}^t \quad \hat{L}^t\hat{A}\hat{L} = L^t A L \text{ if } L = c\hat{L}$$

Coarsen the interface enrichment

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

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

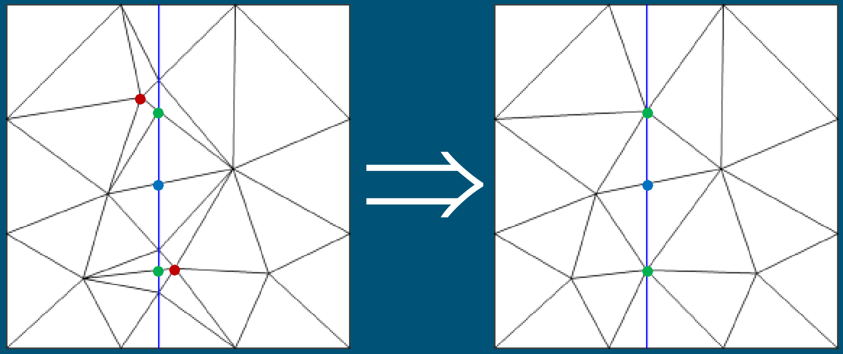
$$A_{XFEM}\begin{bmatrix} u^P \\ u^{XFEM} \end{bmatrix} = b^{XFEM},\ M = \begin{bmatrix} I & 0 \\ C_P & C_{XFEM} \end{bmatrix}$$



Mesh-based Strategy for Improving Discretization Quality: Snapping

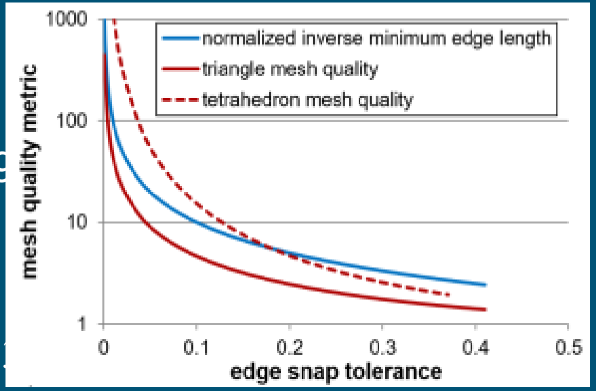
Snap "bad" nodes

- Related work:
  - Labelle and Shewchuk (2007) on Isosurface Stuffing
  - Soghrati et al (2017) on CISAMR
  - Sanchez-Rivadeneira et al (2020) on stable GFEM with snapping
- 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, •→•)

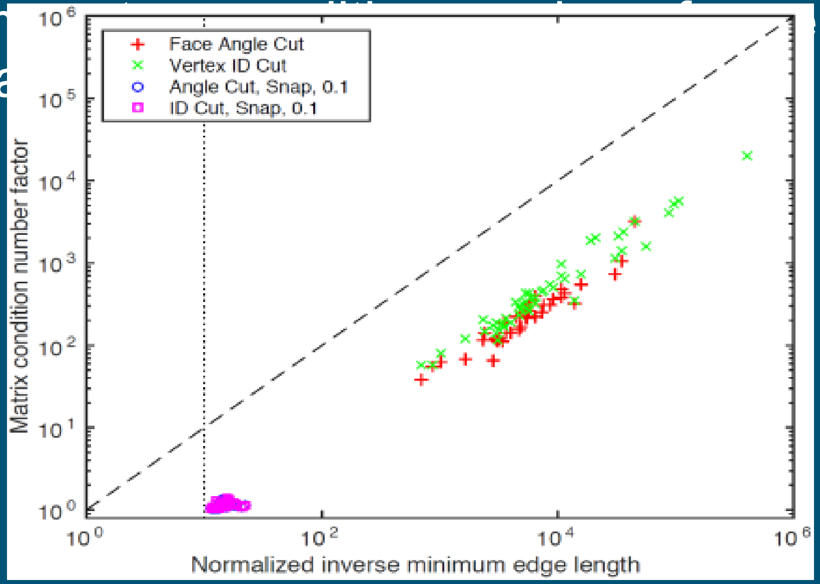


Even small snap tolerance effective at improving quality

- Provable element quality
  - $$Q_w = \frac{1}{1296\sqrt{2}V}\left(\sum_e h_e\right)^3$$ (Berzins 199
  - For snap tolerance of 0.1, Q_w=15.



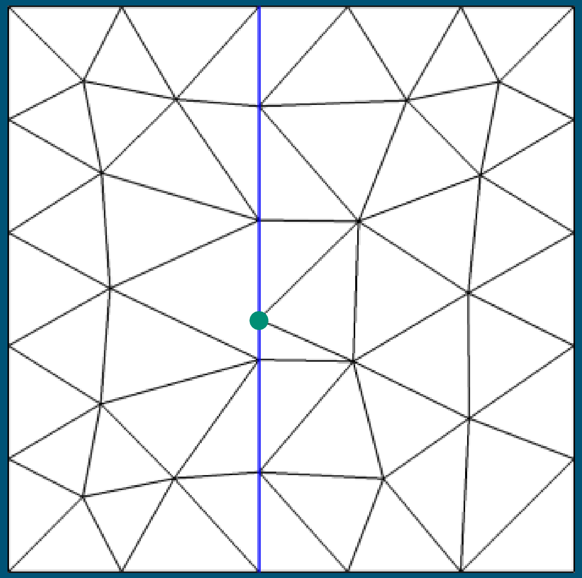
- Large in … mbled Laplacia



Selection of Snap Tolerance

Too large of snap tolerance leads to degenerate mesh

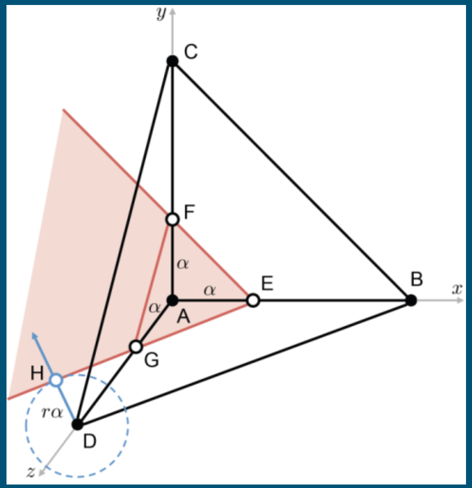
- Cannot allow all nodes of an element to snap to the interface



Maximum snap tolerance for non-degenerate mesh

- Maximum snap tolerance, α, in terms of maximum to minimum edge length ratio, r

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

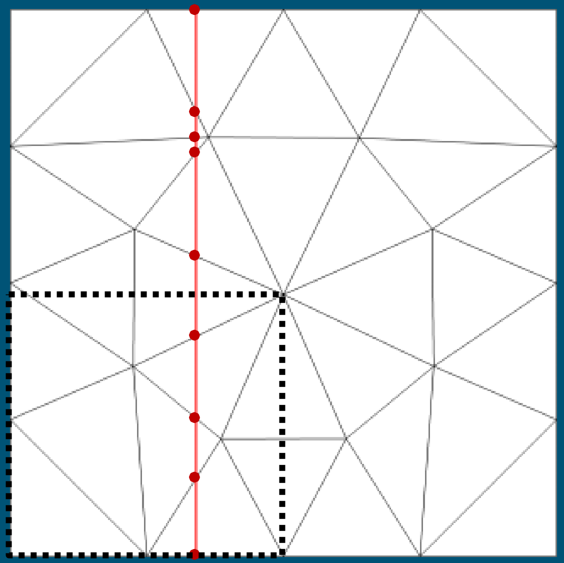


- Maximum snap tolerance of 0.37 for equilateral tetrahedron mesh (theoretical, lengths of 1) and 0.29 for right angle structured mesh (lengths of 1 and $\sqrt{2}$)
- Maximum $\alpha \to 0$ as $r \to \infty$

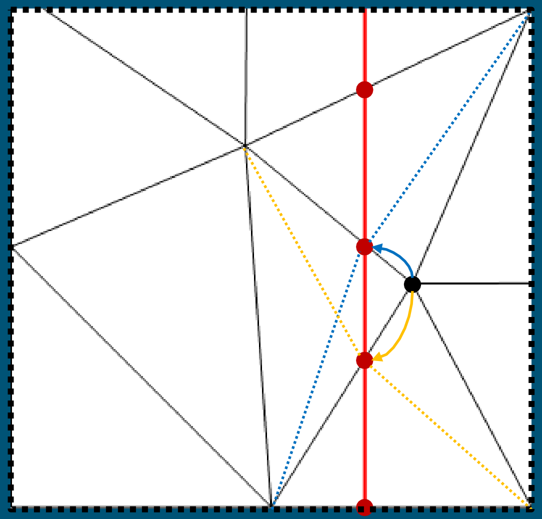
Simpler Snapping Algorithm: Snap When Quality is Better than Cutting

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

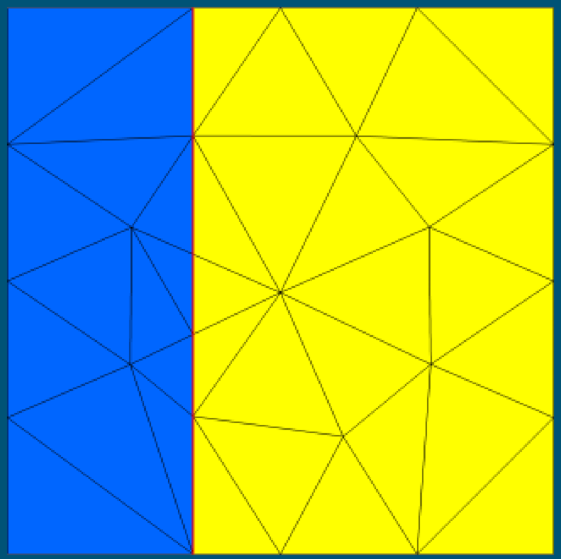
- The estimated cutting quality for a node is the minimum quality of the elements that would be produced by cutting each edge using the node at its intersection point
- The snapping quality for a node and intersection point is the minimum quality of the elements if the node is moved to that intersection 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

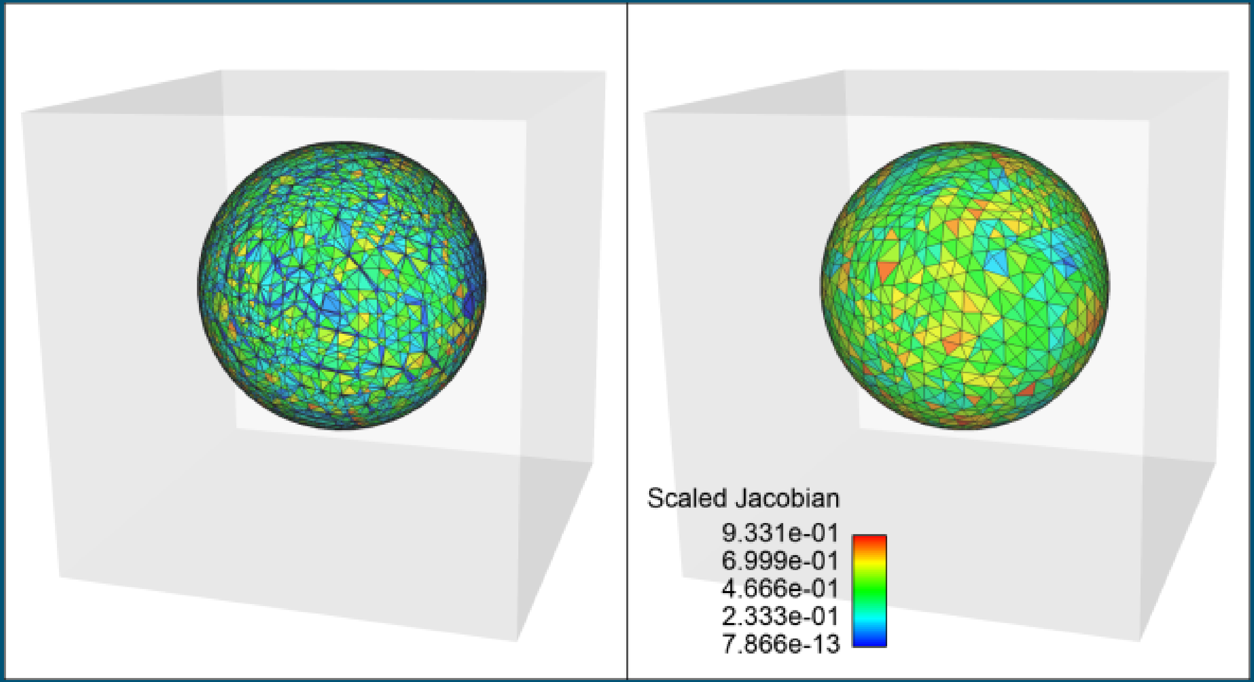


Zoom in of snap candidates

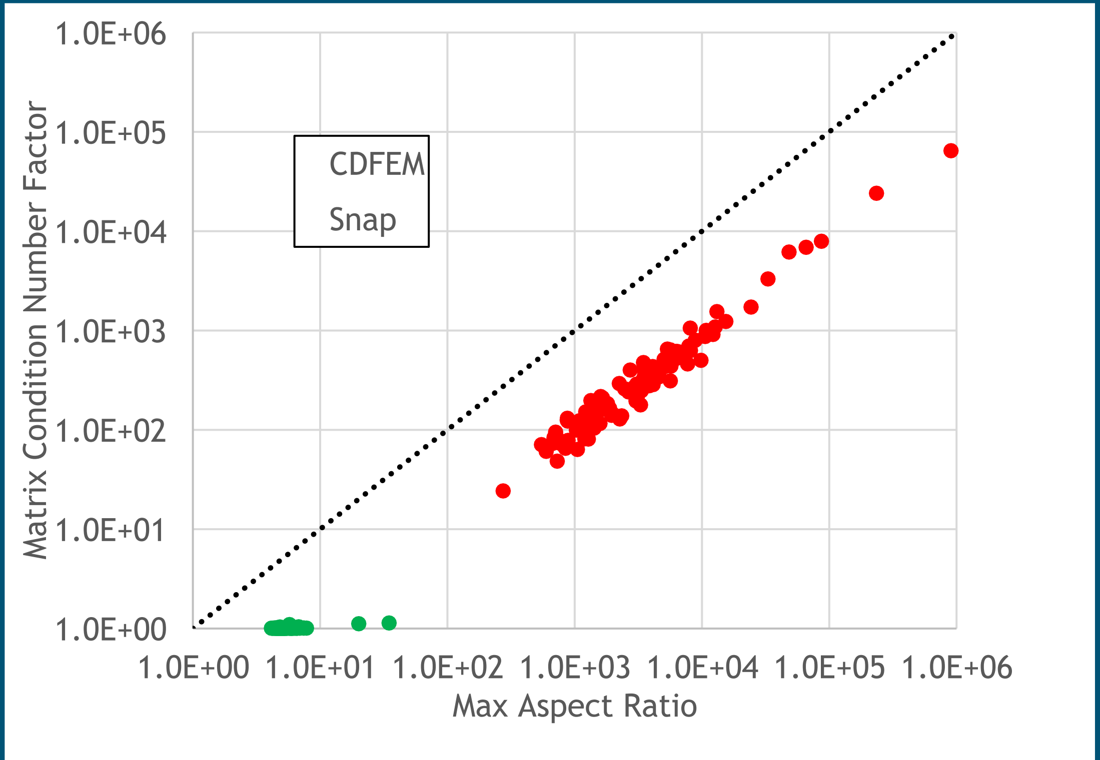


Resulting snapped and cut mesh

Performance of Simple Snapping Procedure for Randomly Place Sphere



Cut mesh | 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

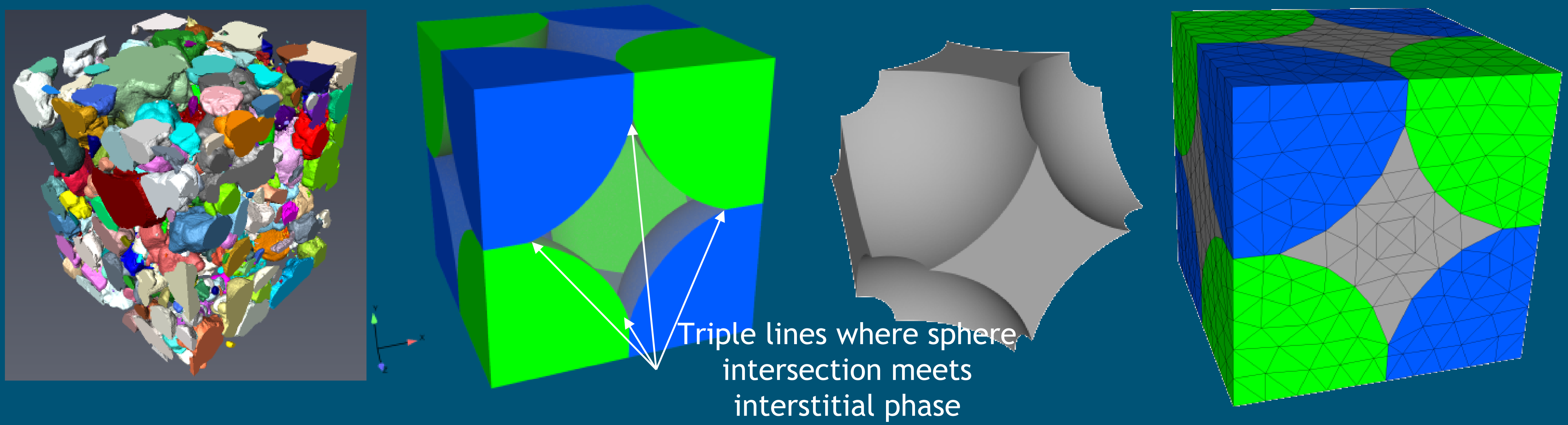
Results

- 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

Extension of 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

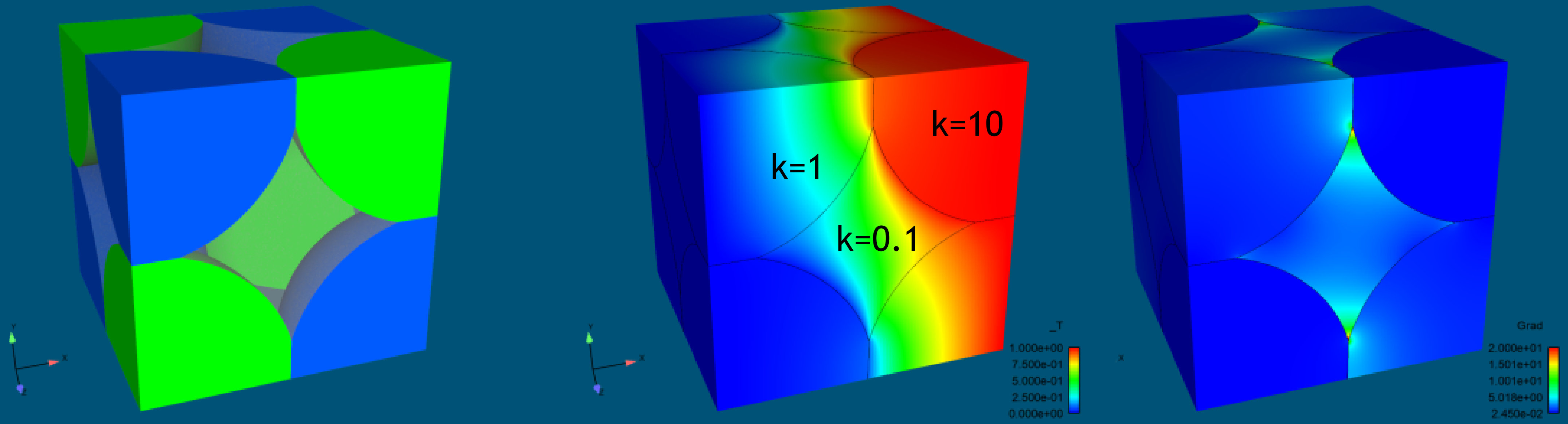


- Find intersections between triple lines and element faces and quadruple points within elements
- Prioritize capture of sharp features over interfaces

3 Phase Conduction Problem

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



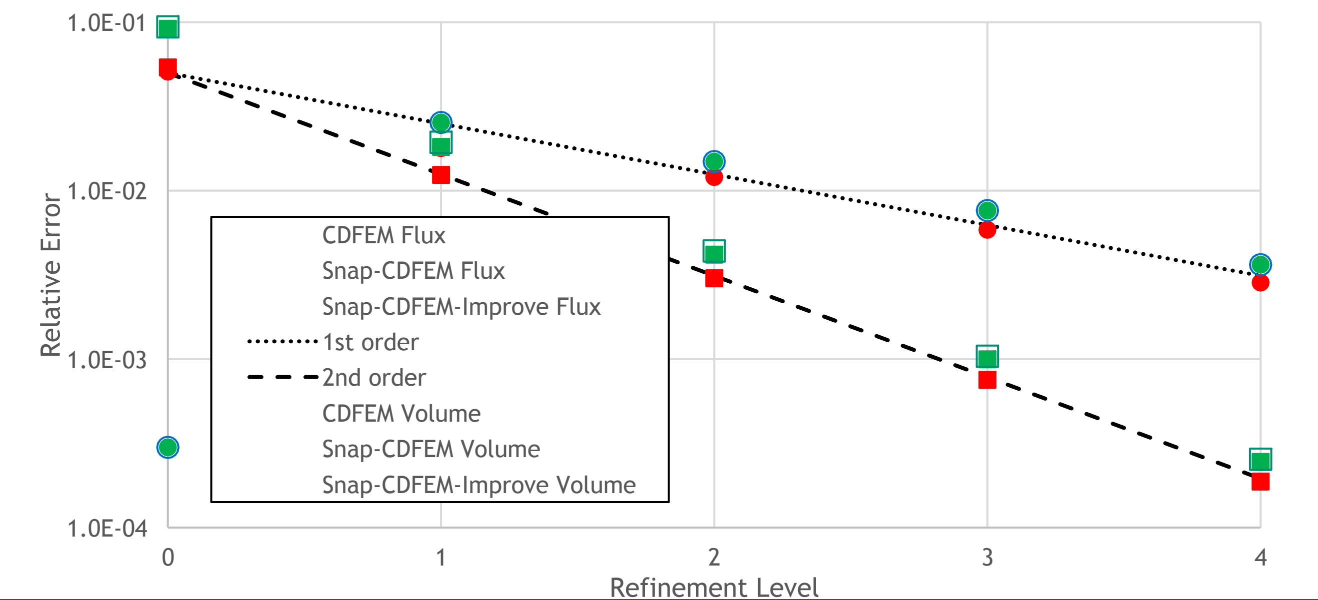
3 Phase Conduction Problem Results

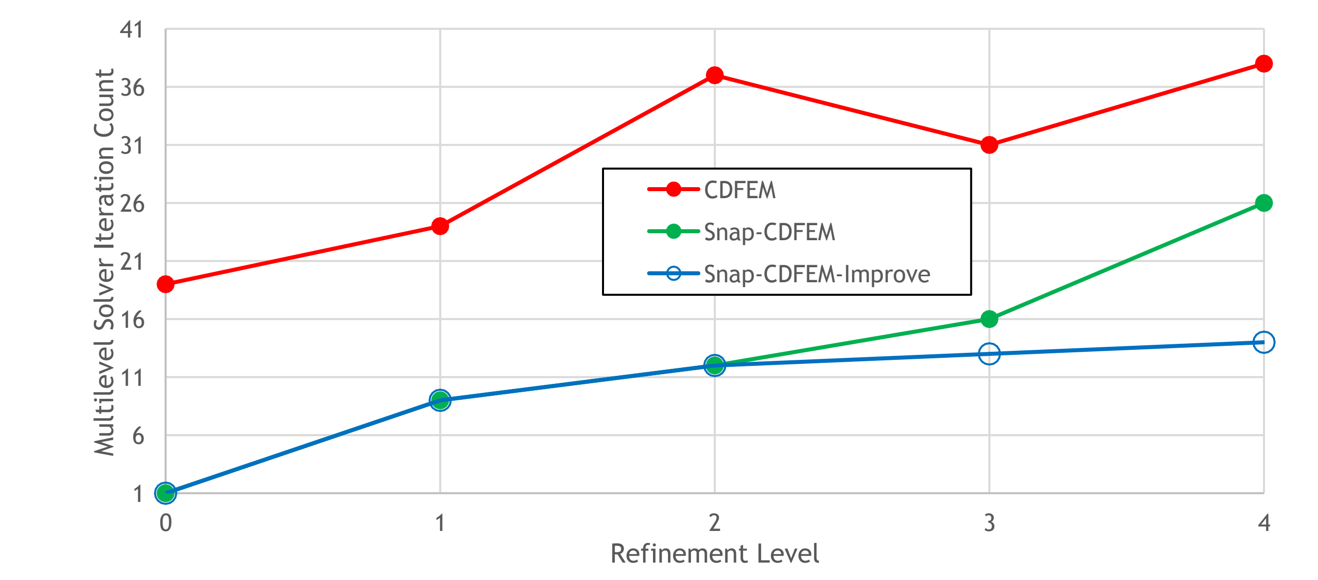
Accuracy

- 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
- On finest meshes, snapped meshes still show issue with scalability





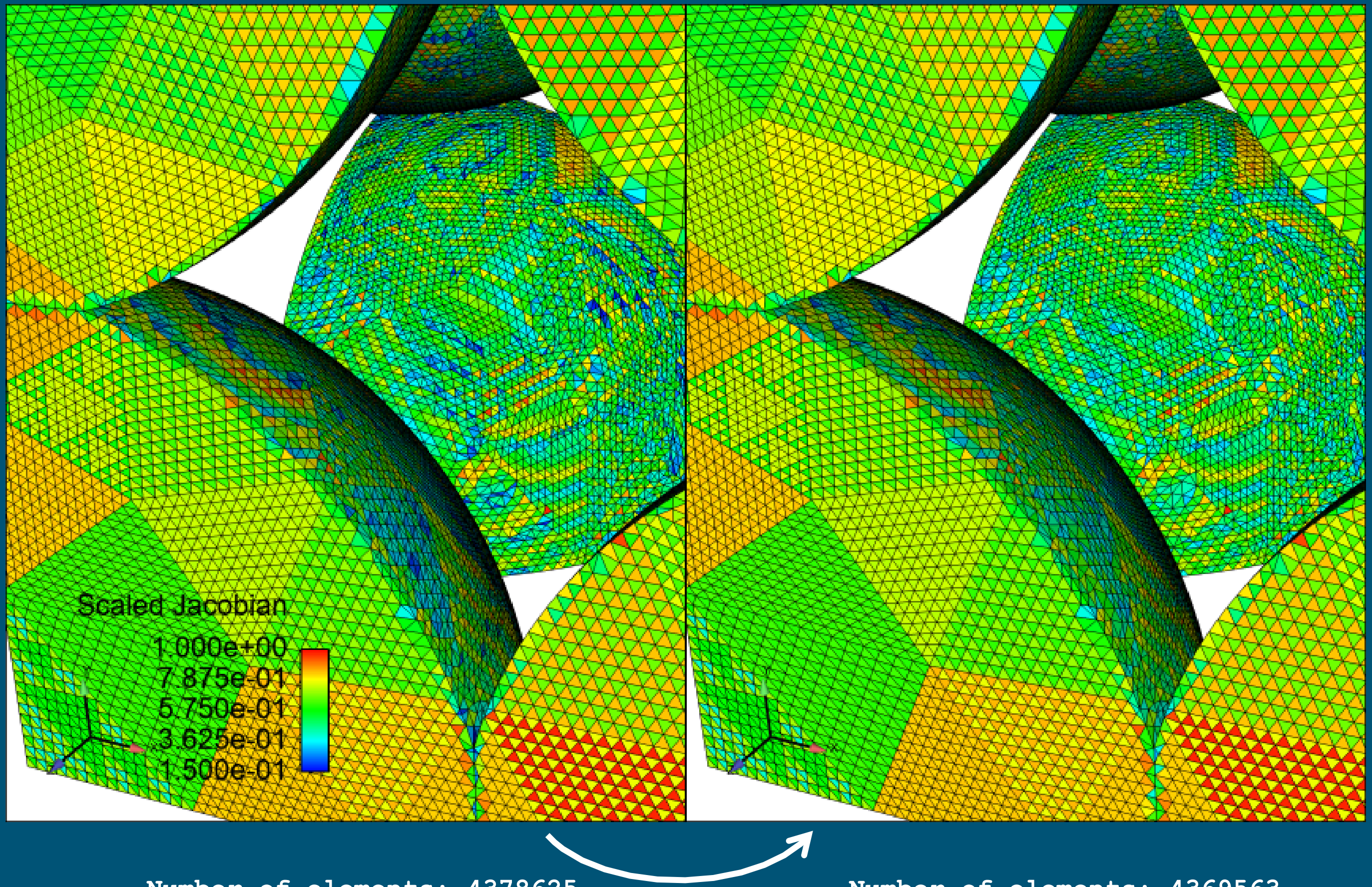
Incremental Mesh Improvement for Further Improving Discretization Quality

Perform Incremental Mesh Improvements to Improve Quality
- Edge swaps
- Edge collapses

Software Capability
- Software library named Emend
- Distributed memory support via Sierra toolkit (stk)

Related Work
- OmegaH –Ibanez, Topology preserving transformations for multi-part meshes
- TetWild – Panozzo, Able to perform non-topology preserving transformations using user prescribed length scale for single part meshes

Workflow
- After snapping and conformal decomposition,



Number of elements: 4378625

Quality Metric	Min	Max
Scaled Jacobian	0.00824	0.985
Aspect Ratio	1.01	64.9
Mean Ratio	0.0567	0.999

Number of elements: 4369563

Quality Metric	Min	Max
Scaled Jacobian	0.146	0.985
Aspect Ratio	1.01	5.02
Mean Ratio	0.358	0.999

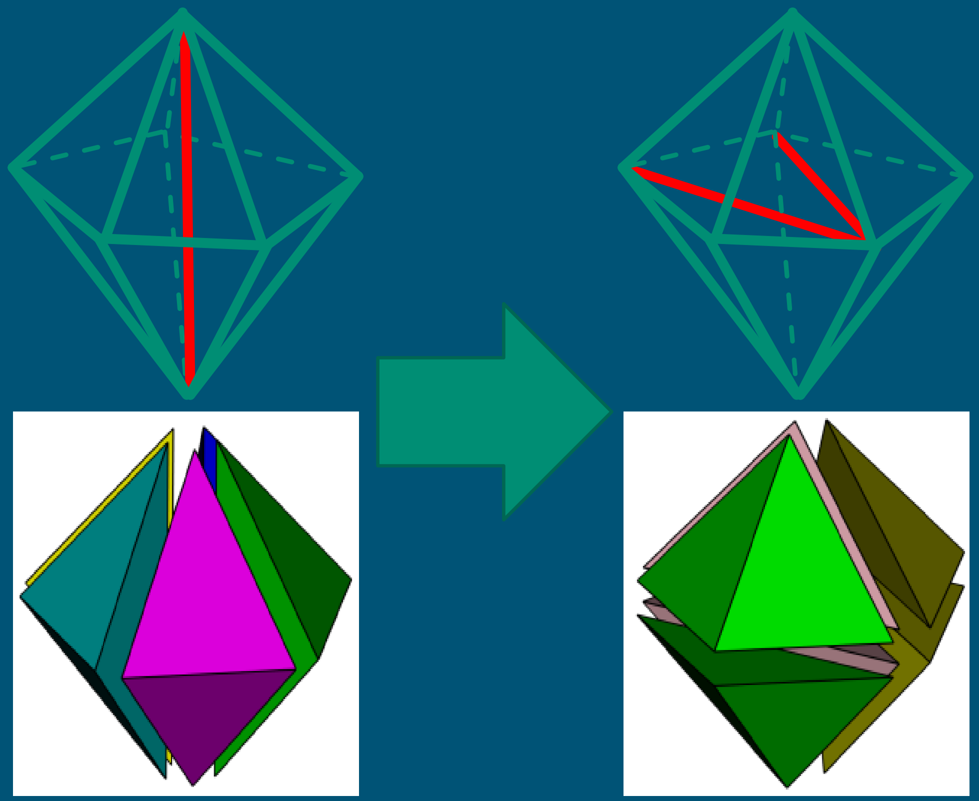
Incremental Mesh Improvement: Edge Swapping

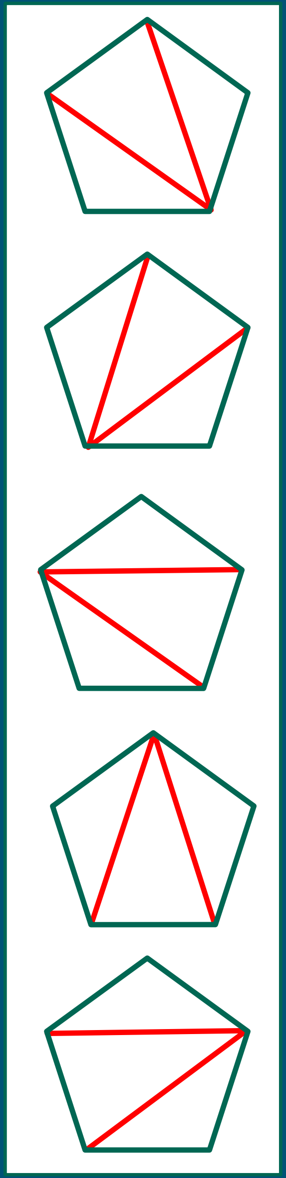
For *n* = *5*, the 3 tets are replaced with 6 tets.

There are 5 possible configurations for the 6 tets. Choose the one with best quality.

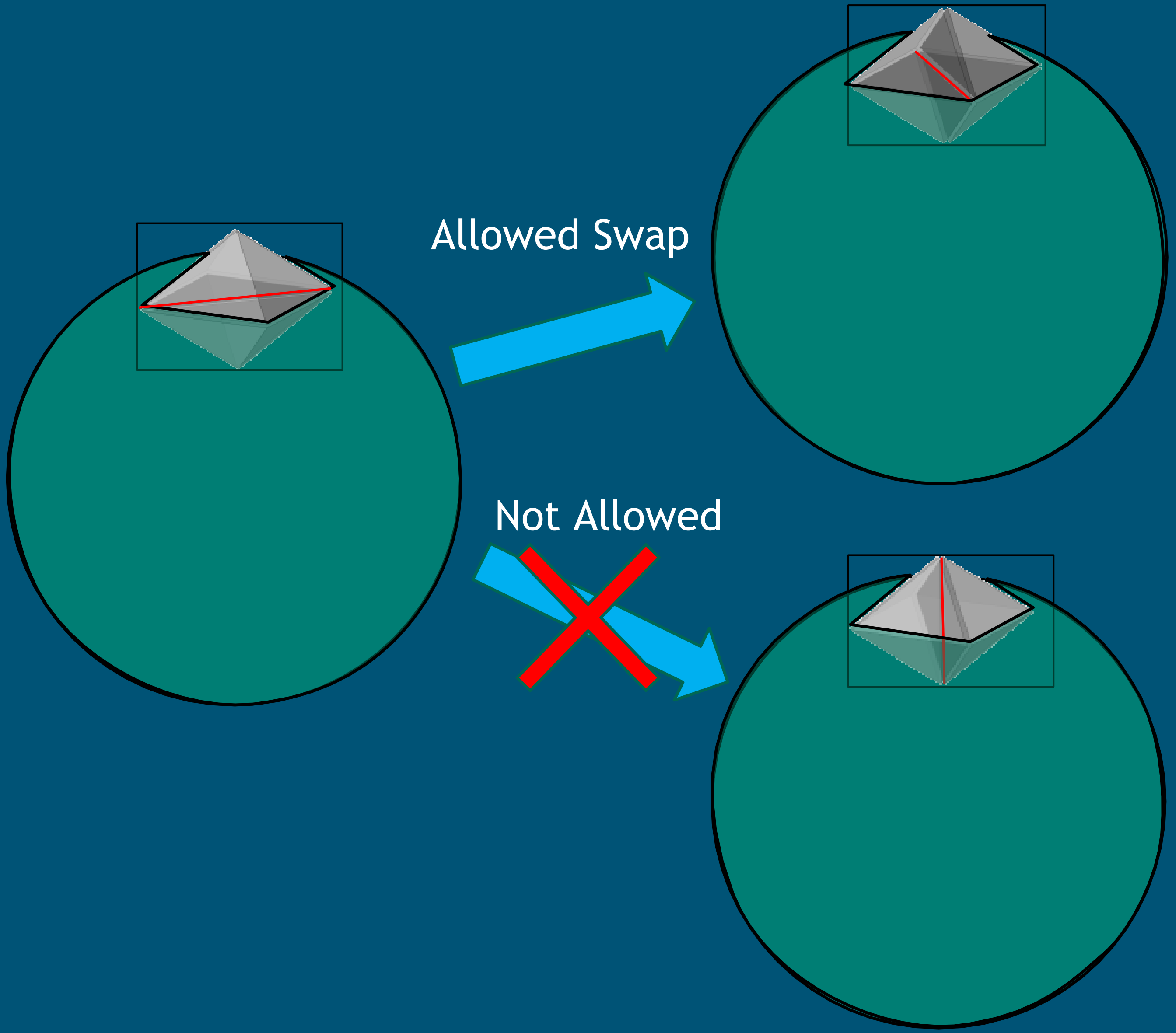
Currently handling cases with 3, 4, 5, 6, or 7 tets around an edge

Developed in collaboration with Dan Ibanez

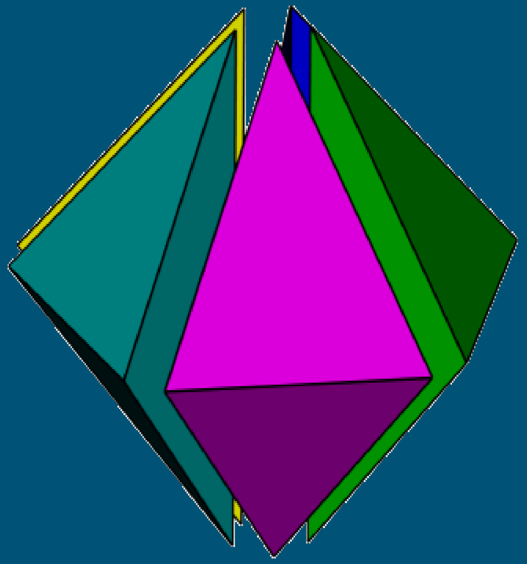




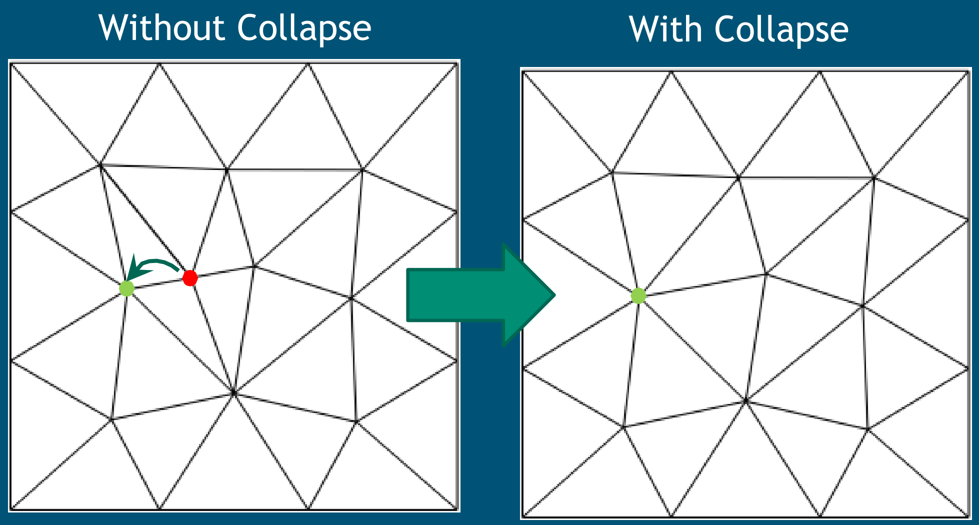
Preserving Topology During Edge Swaps

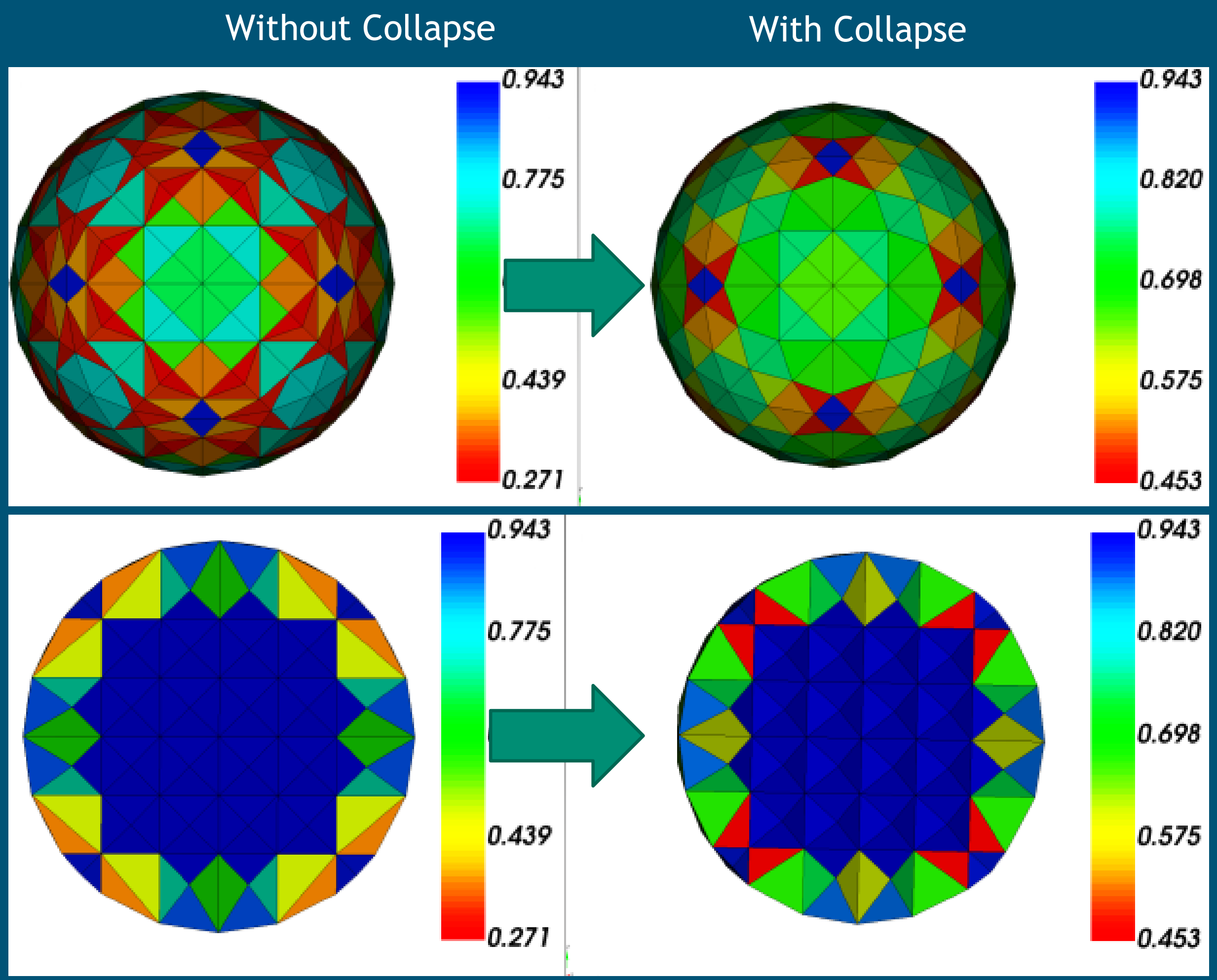


Volume association of each node of the elements surrounding the edge must be unchanged, and all elements must have a unique volume association determined by the intersection of the volume associations of the nodes of the element



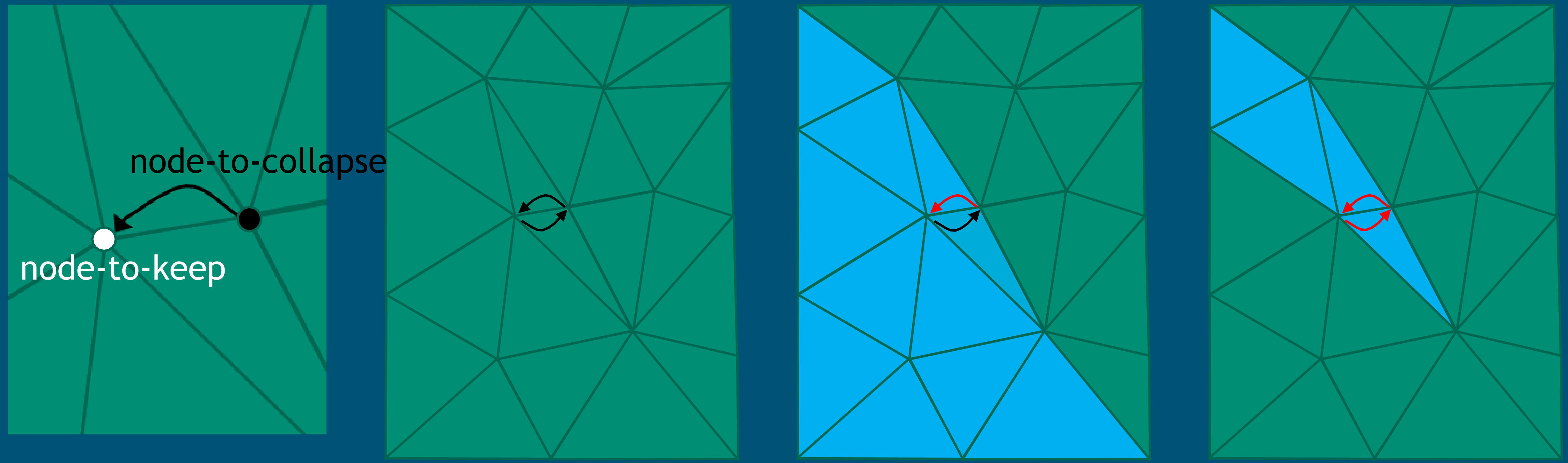
Edge Collapses to Improve Quality





- Collapses remove superfluous edges, significantly improving the quality

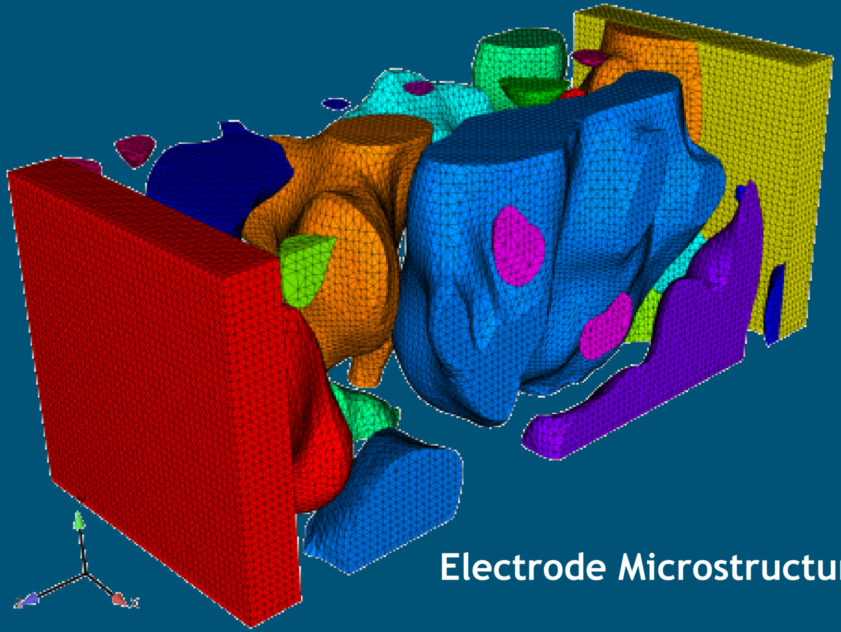
Preserving Topology During Edge Collapse



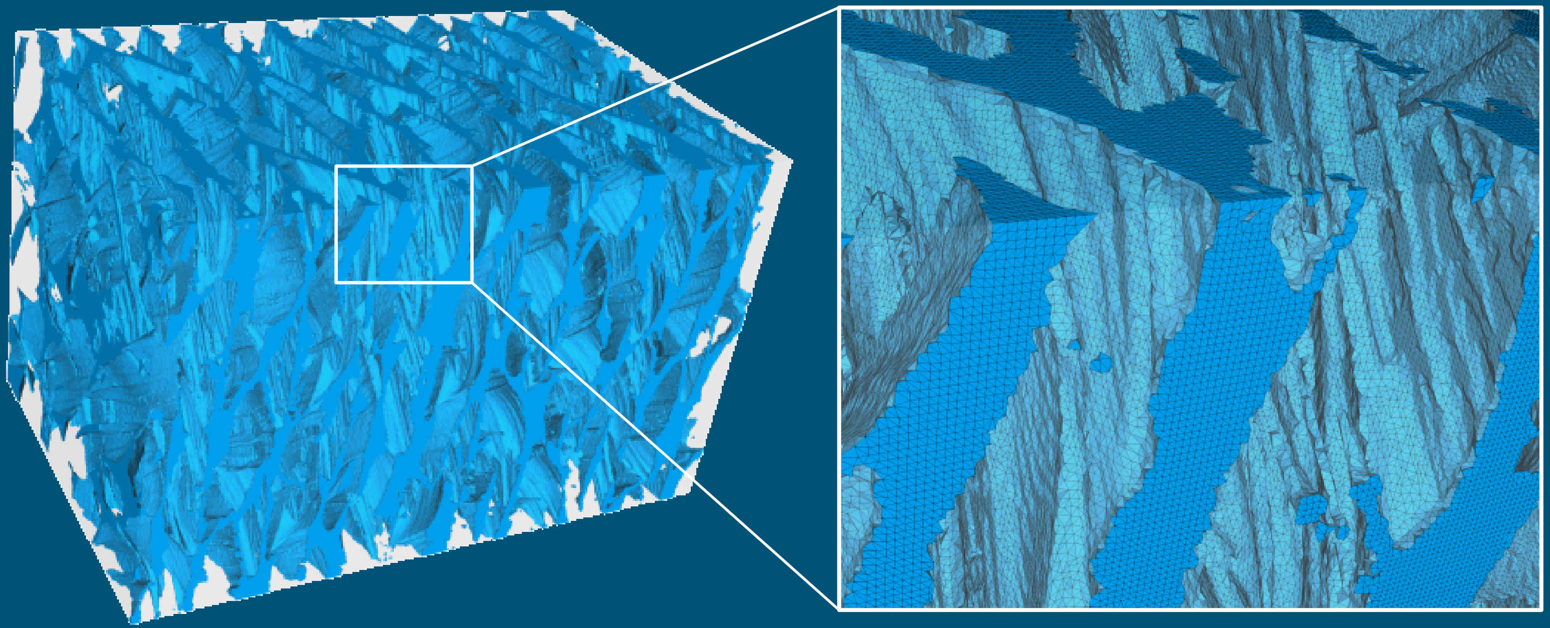
- Current topology-based strategy thanks to Dan Ibanez
- TetWild instead uses distance from boundary triangle to input geometry to filter transformations

- Geometric associations of node-to-keep must contain associations of node-to-collapse
- In 2D and 3D, non-collapsing side attached to node-to-collapse must have same associations as element to collapse
- In 3D, non-collapsing edge attached to node-to-collapse must have same associations as face to collapse

Credible Discretizations from 3D Image Data



Electrode Microstructure



Fibrous Microstructure

Quality Discretizations for Dynamic Level Sets

Motivation

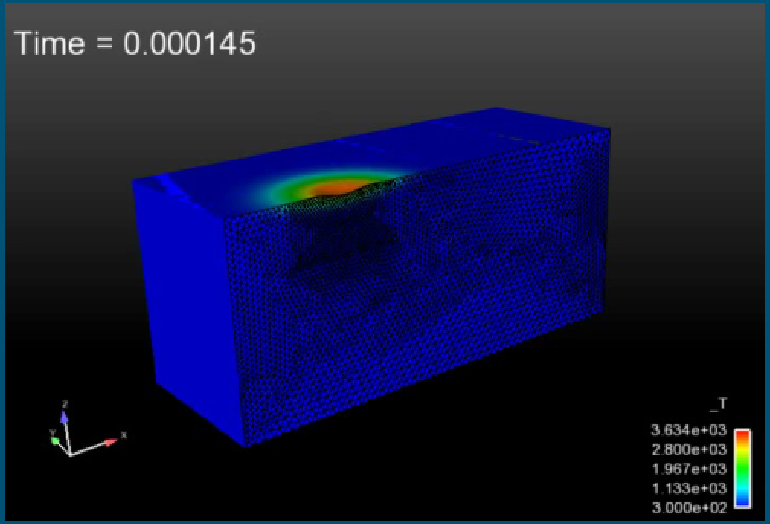
- Numerous transport problems with moving interfaces with discontinuous physics and fields

Solution

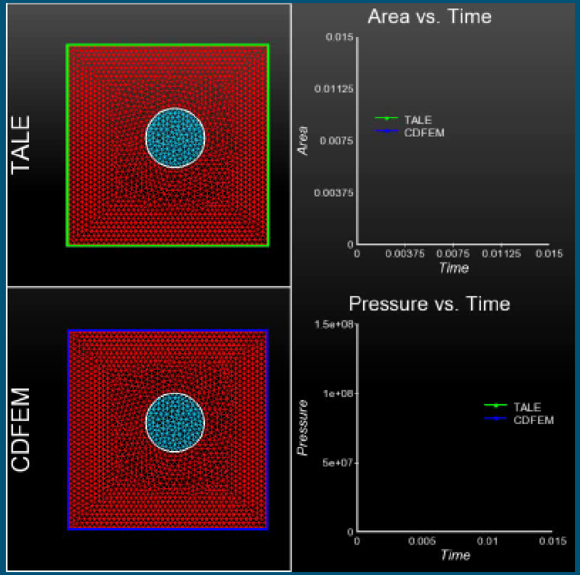
- cThruAMR - Conforming, transient, h-r unstructured adaptive mesh refinement

Related Work

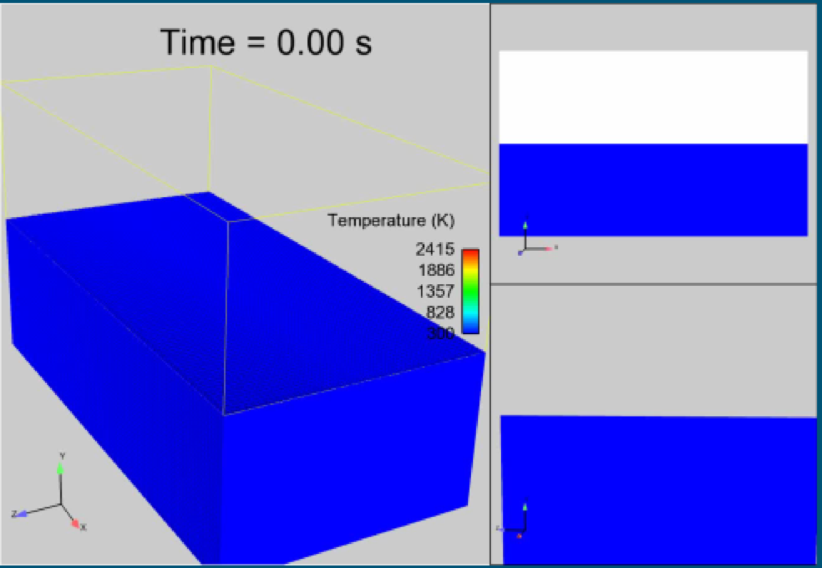
- CISAMR – Conforming to Interface Structured Adaptive Mesh Refinement (Soghrati)



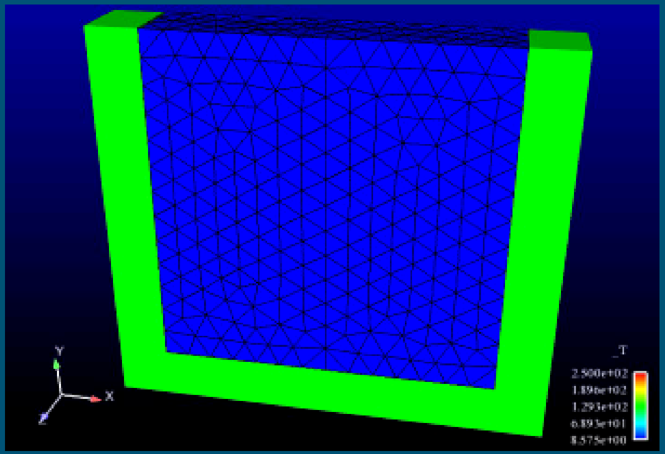
Laser welding



Conductive burn of energetic materials



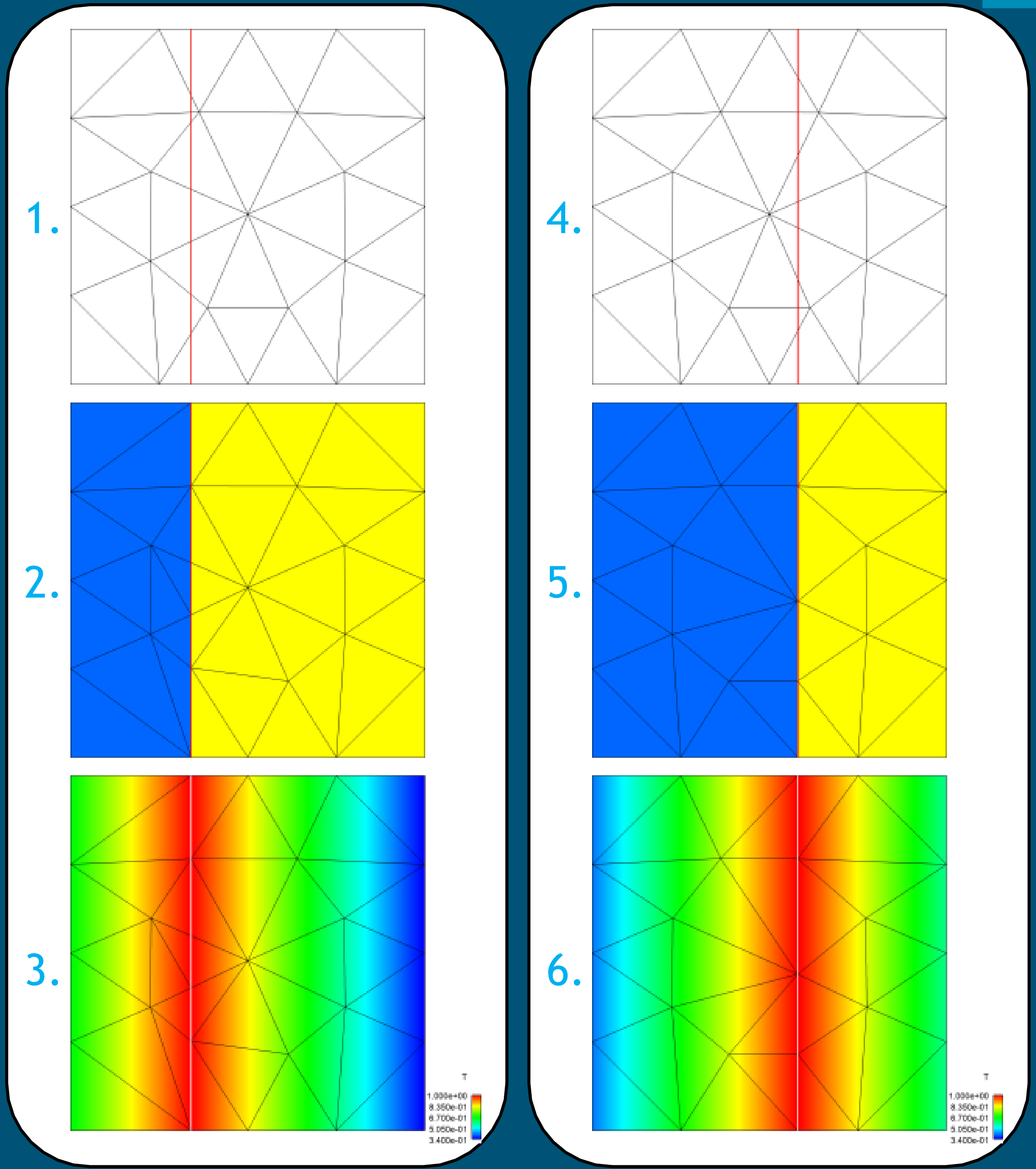
Additive Manufacturing



Material Death

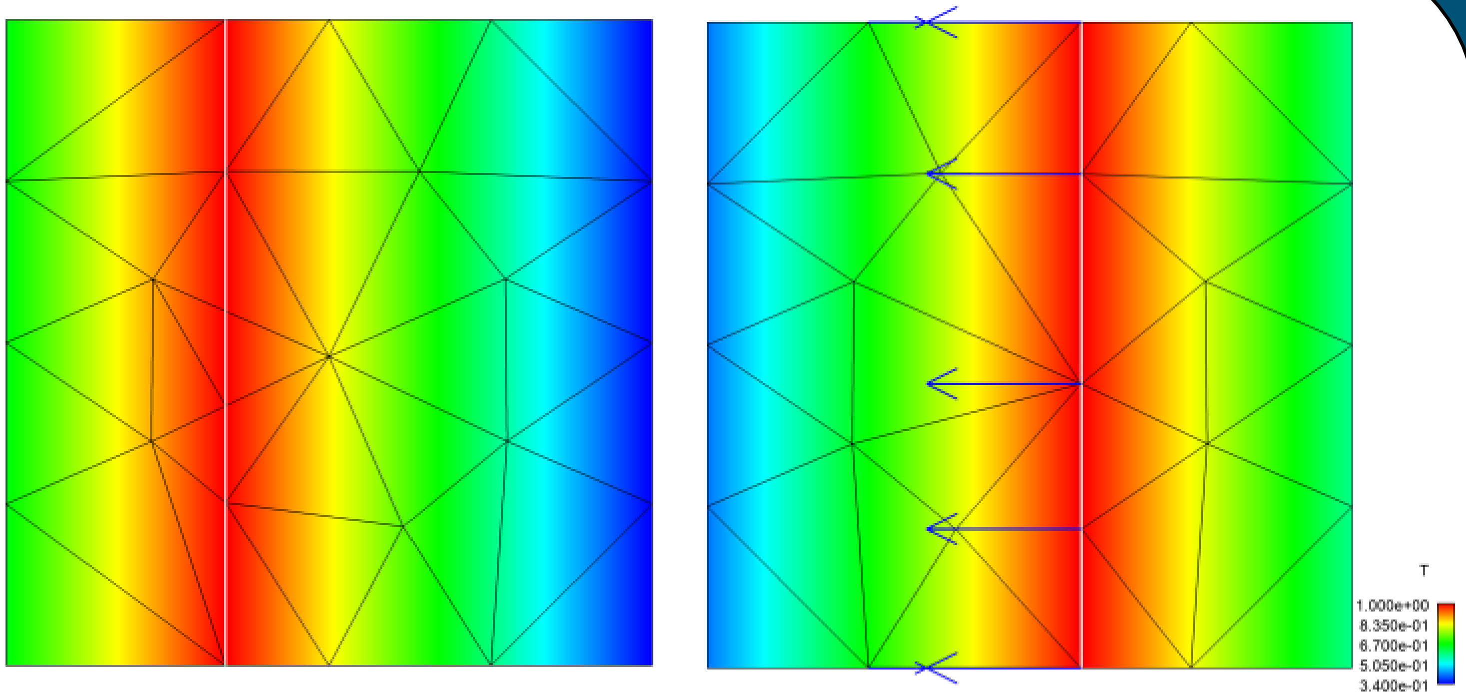
cThruAMR Algorithm

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

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

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

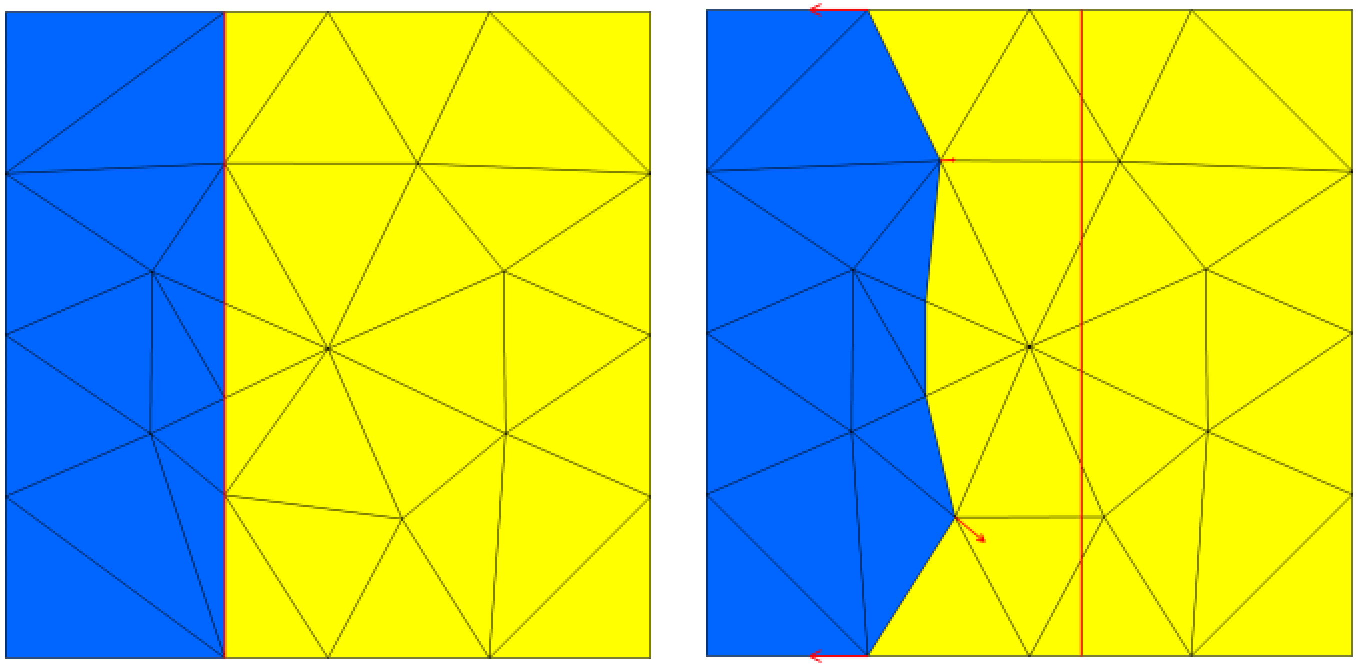
cThruAMR Mesh Motion: Snap Displacement

"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

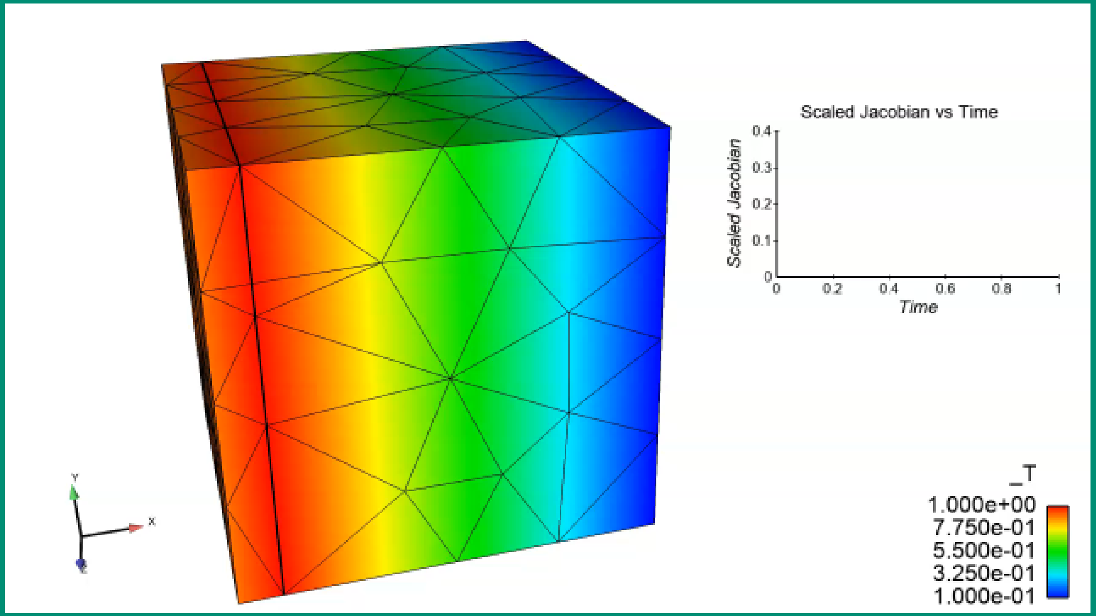
$$\int_\Omega \frac{D\psi}{Dt} w_i \, d\Omega \approx \sum_J \int_{\Omega_J^{n+1}} \left(\frac{\psi_J^{n+1}(\mathbf{x}) - \tilde{\psi}_J^n(\mathbf{x})}{\Delta t} + (\mathbf{u} - \dot{\mathbf{x}}(\mathbf{x})) \cdot \nabla \psi_J^{n+1}(\mathbf{x}) \right) w_i \, d\Omega$$

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

Demonstration Problems

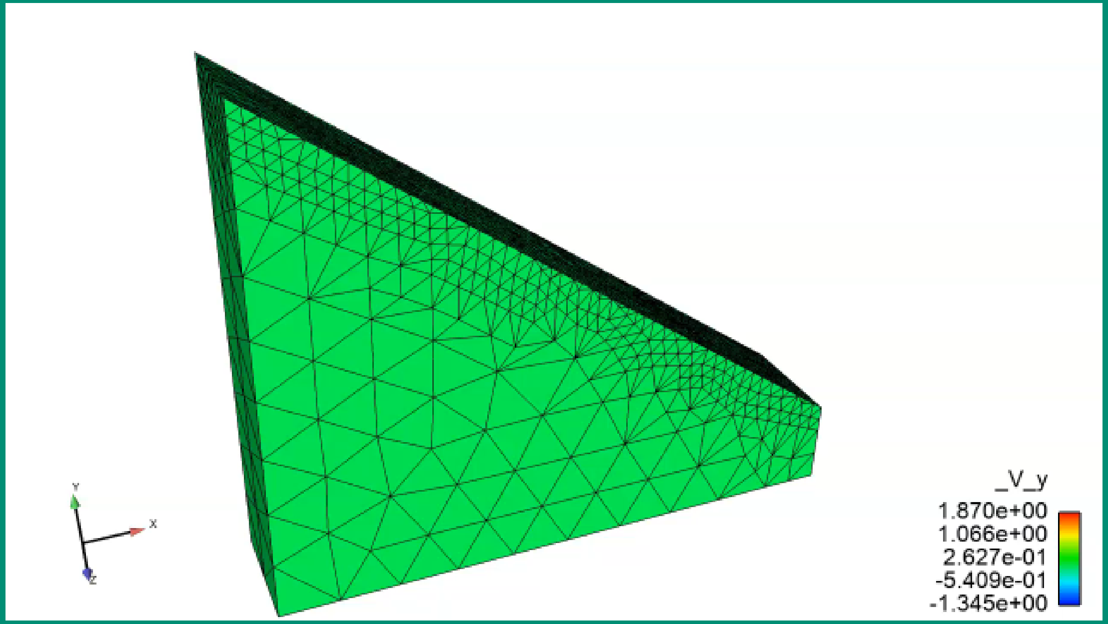
Patch Test: Pure Advection of Slope Discontinuity

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



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

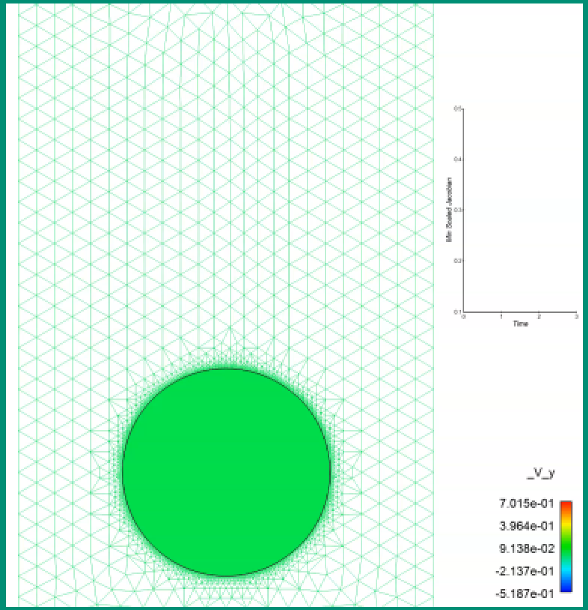
- Multiple levels of non-conformal refinement followed by h-r conformal refinement (cThruAMR)

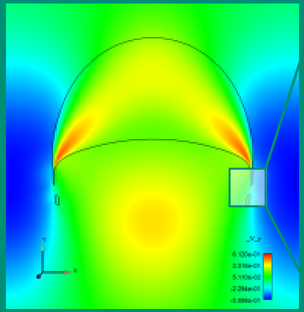


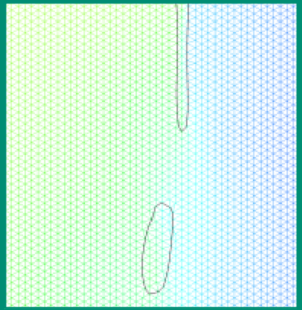
Rising Bubble Problems

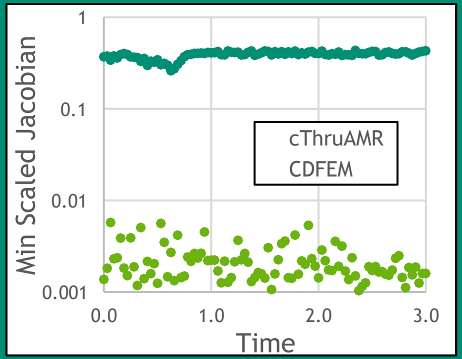
Problem: 2D Rising bubble

- 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



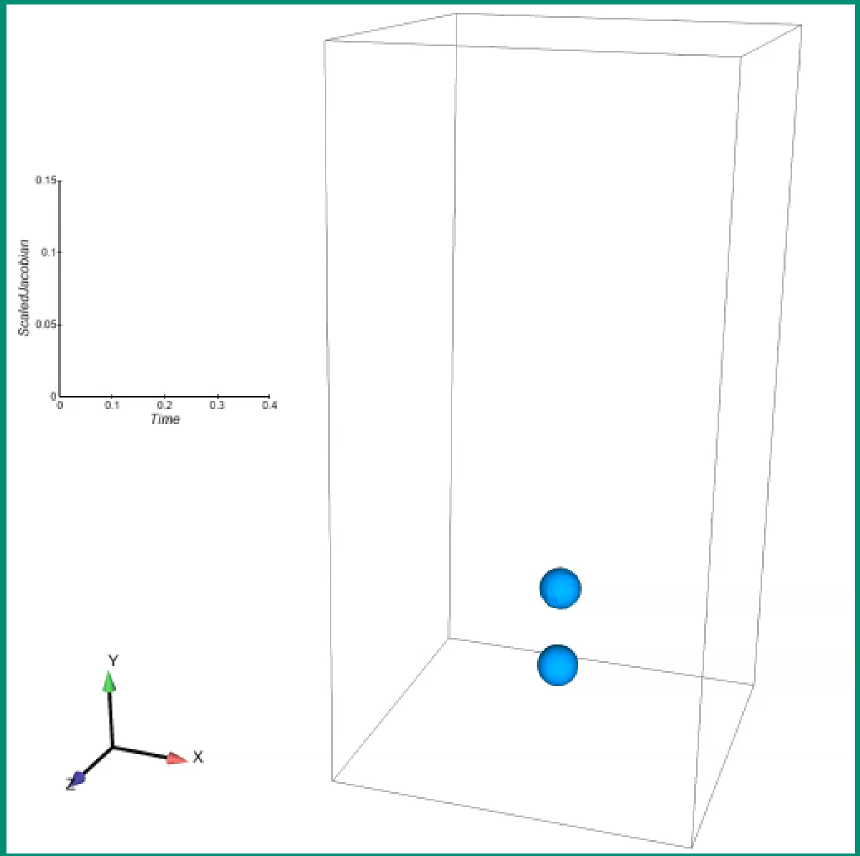






Problem: 3D Rising, merging bubbles

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



Open Source Code Krino: 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

- Realizing our goal for Credible, Automated Meshing of Images (CAMI)
- Combined snapping and cutting strategy produces much higher quality meshes than cutting alone
    - Impacts element quality, matrix conditioning, robustness, and linear solver costs
  - Quality is still further improved by incremental mesh improvement
  - Overall performant and robust strategy for automated tet mesh generation for image-based geometry
- conforming Transient h-r unstructured Adaptive Mesh Refinement (cThruAMR) producing good quality discretizations for dynamic level set problems
- Future Work
    - Combination of snapping, cutting, and swapping strategies that won't require incremental mesh improvement