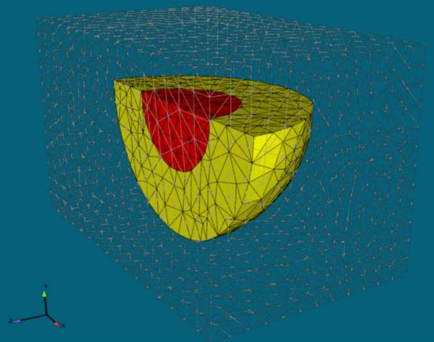
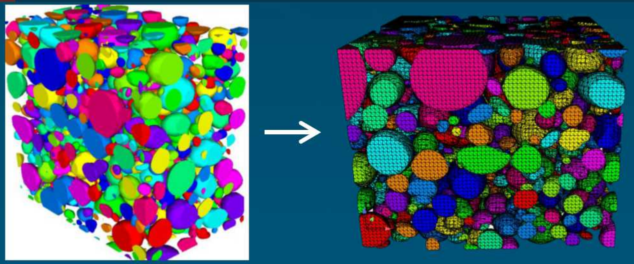
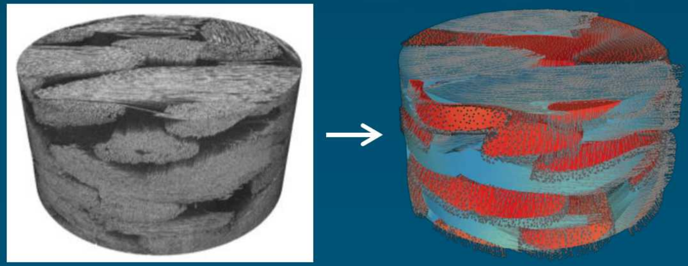
Sandia National Laboratories

SAND2019-8685C

Producing Credible Discretizations by Combining Conformal Decomposition and Incremental Mesh Improvement







PRESENTED BY

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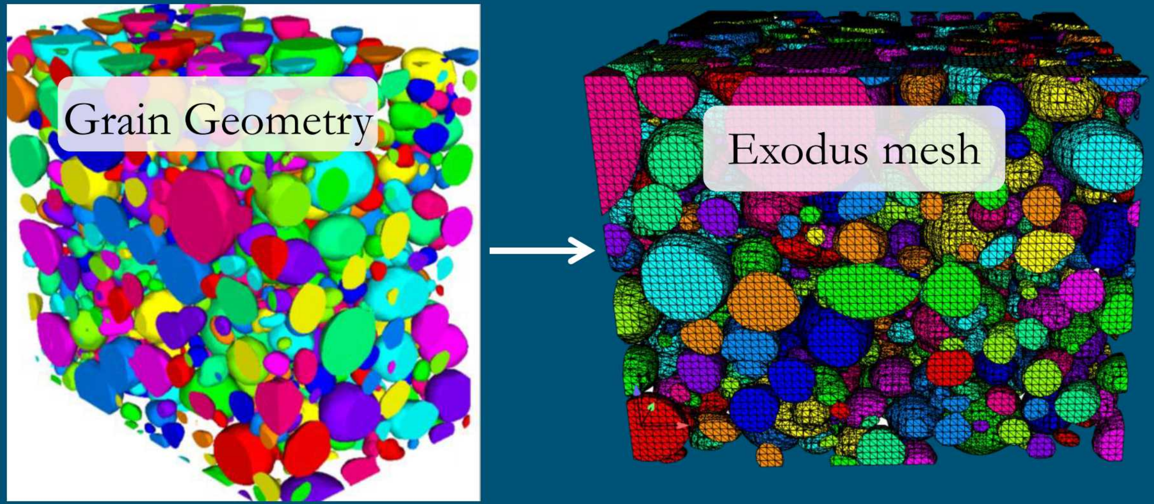
Motivation: Microstructure Modeling

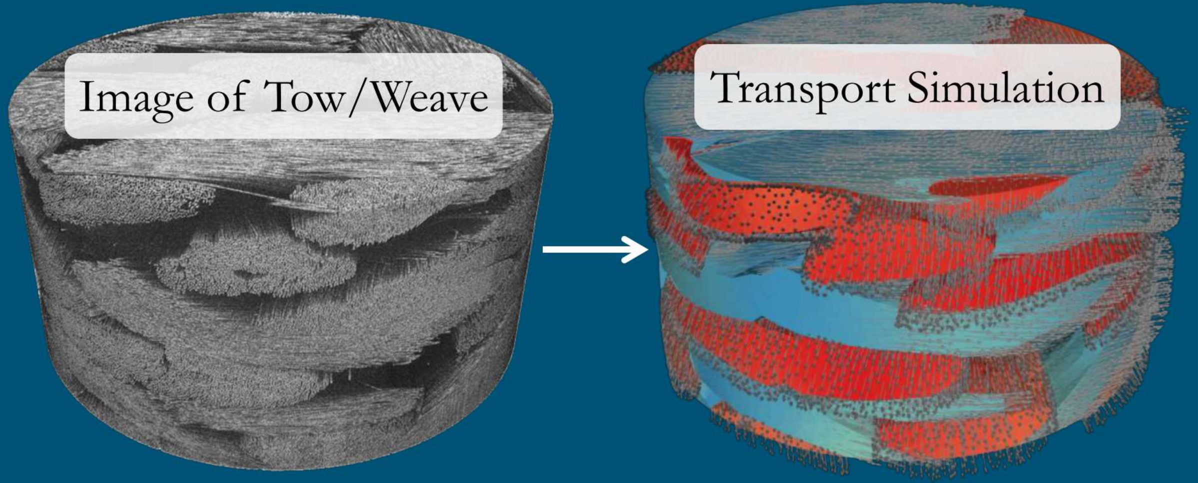


Electrode Geometry

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

Physics

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



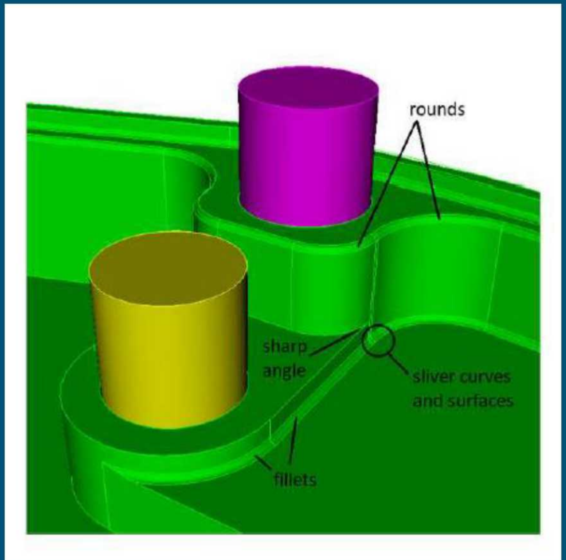
Thermal Protection System Geometry

- 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

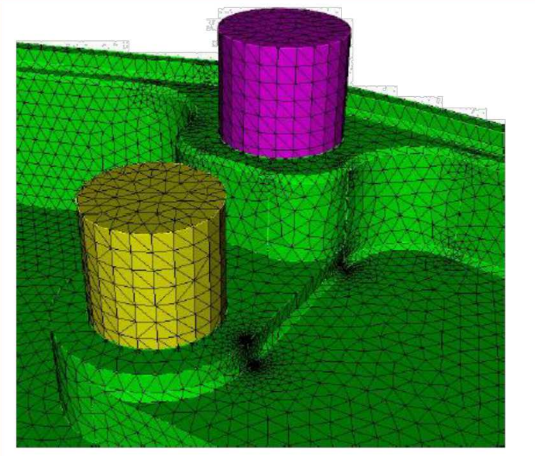
Physics

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

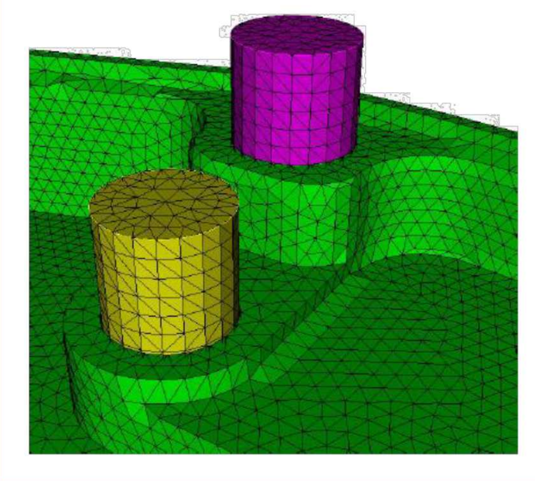
Motivation: As-built Models Instead of CAD-feature-based Models



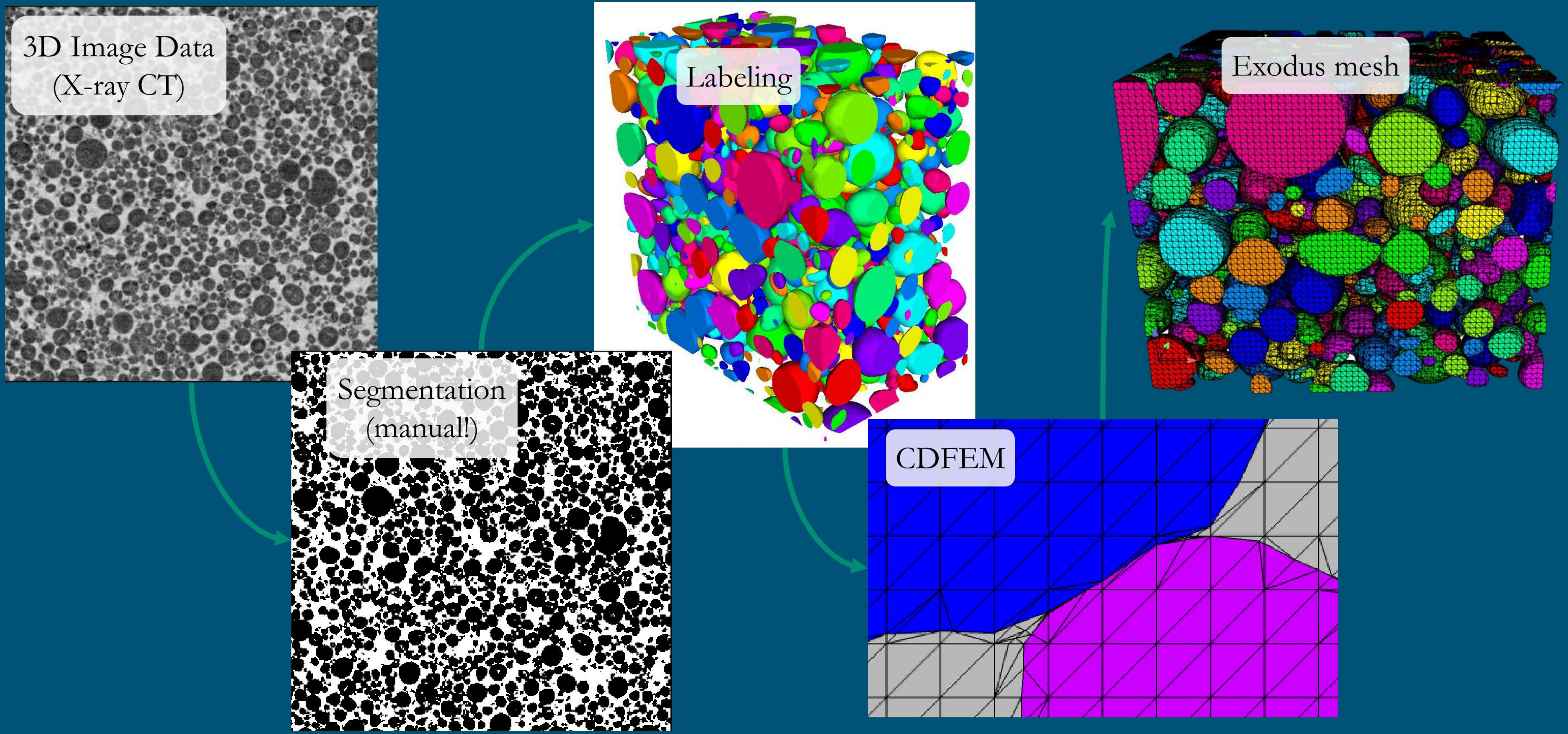
Mesh fine CAD features



Mesh as-built coarse features



Mesoscale geometry from CT data using CDFEM



Roberts et al JES 2014, Roberts et al JEECS 2016

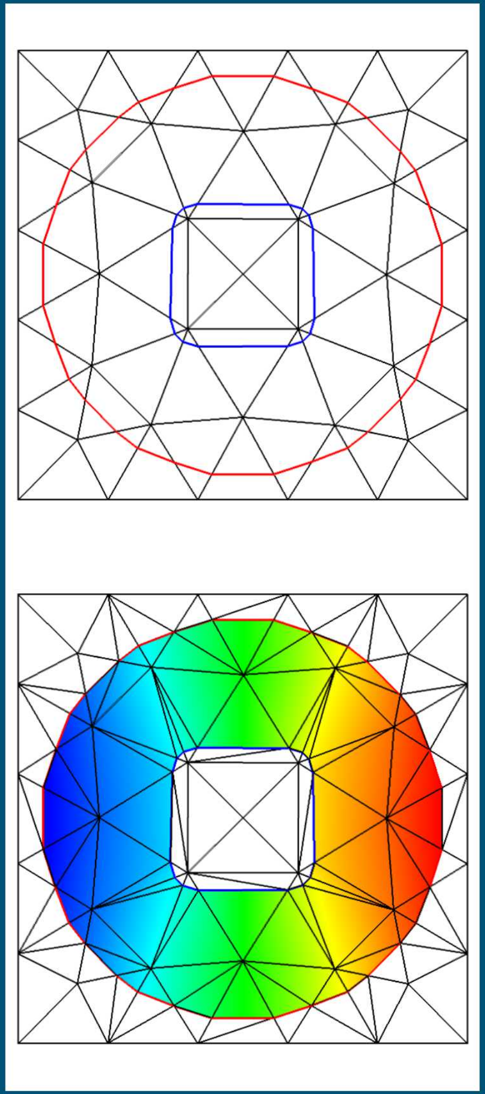
Conformal Decomposition Finite Element Method (CDFEM)

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

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

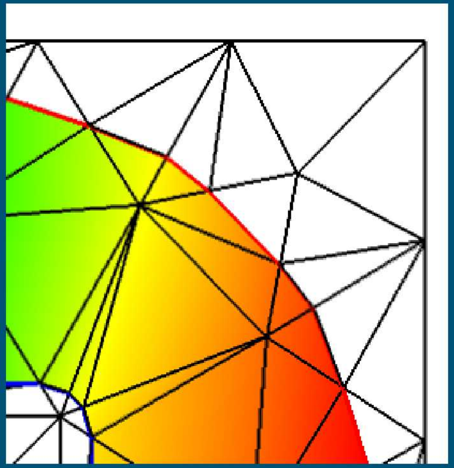
- ❌ Infinitesimal edge lengths
- ❌ Arbitrarily high aspect ratios (small angles)
- ✓ Can introduces large angles. Can be controlled by cutting largest angle.

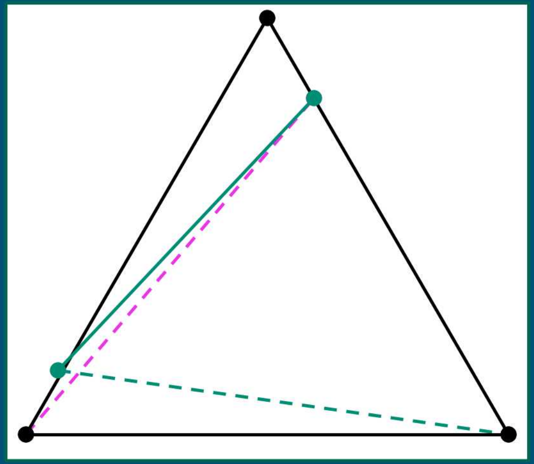
Consequences

- ✓ 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 incrementally improve the quality of a CDFEM mesh to produce a credible discretization?

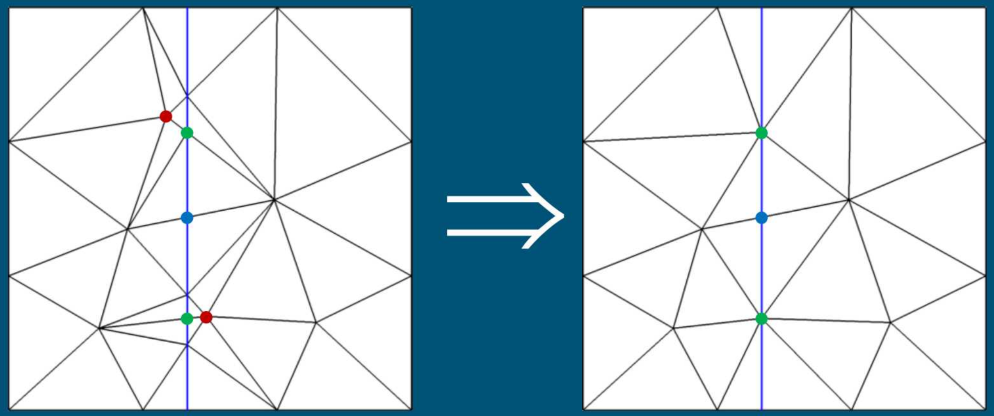




Strategies to Circumvent Poor CDFEM Conditioning

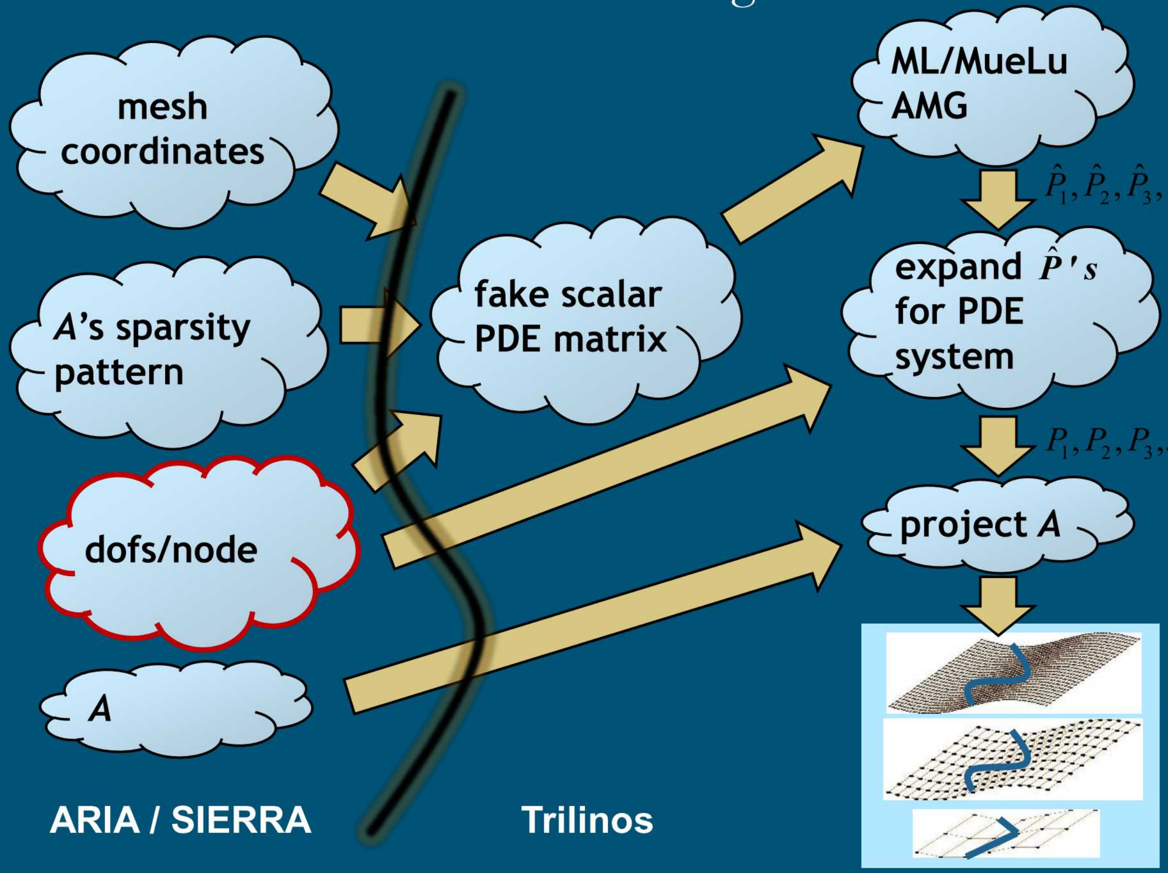
Coarsen by Snapping "bad" nodes

- 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, •→•)



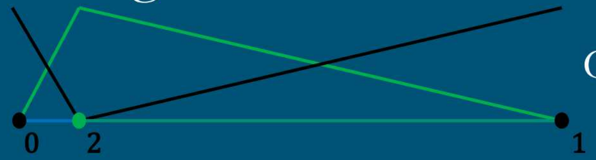
Specialized Preconditioners

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

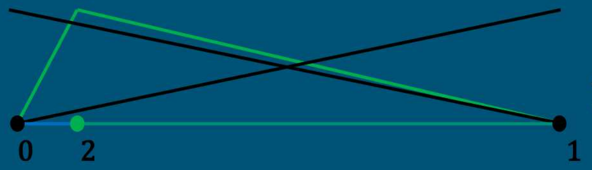


Strategies to Circumvent Poor CDFEM Conditioning

Change to hierarchical interface DOFs



CDFEM Basis in 1-D



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

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

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

Can be posed as preconditioner of original system

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

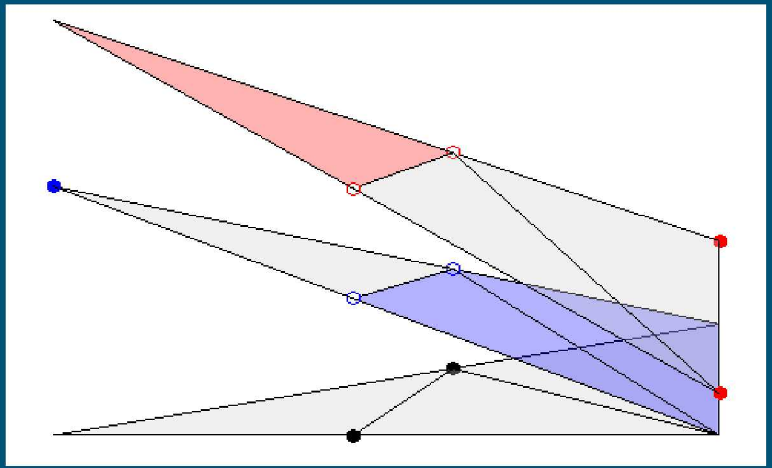
Coarsen the interface enrichment

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

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

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

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



Incremental Mesh Improvement

Perform Incremental Mesh Improvements to Improve Quality

- Edge swaps
- Edge collapses

Software Capability

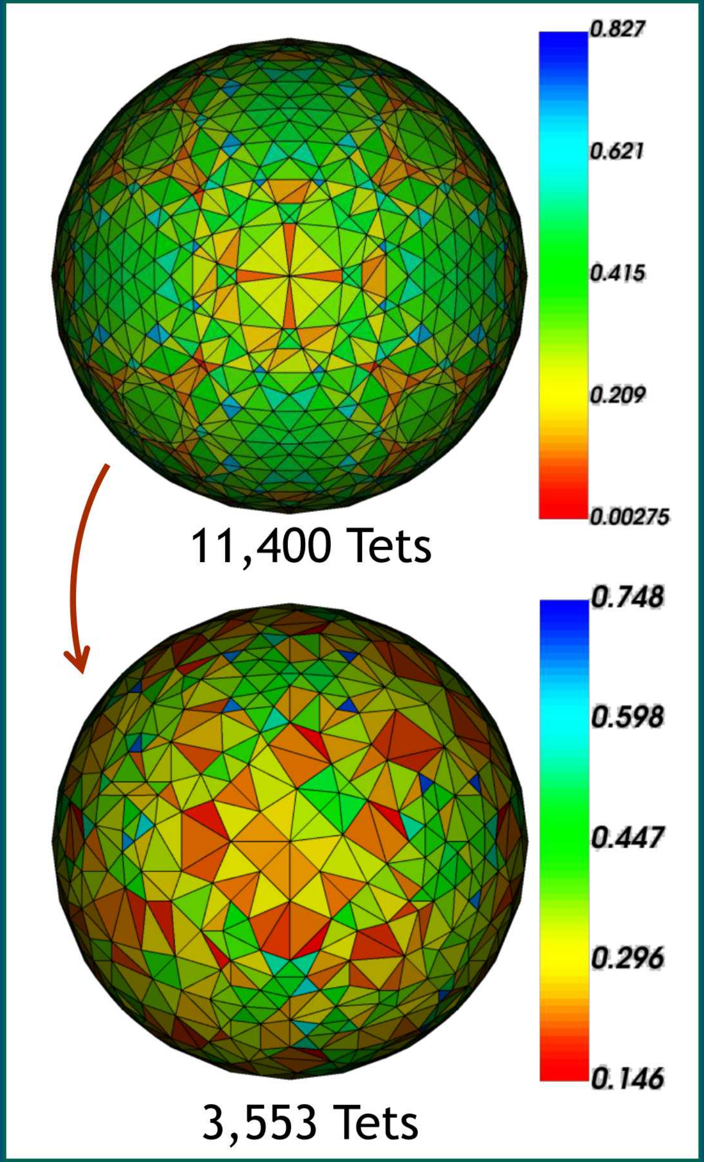
- Software library named Emend
- Distributed memory support via Sierra toolkit (stk)

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

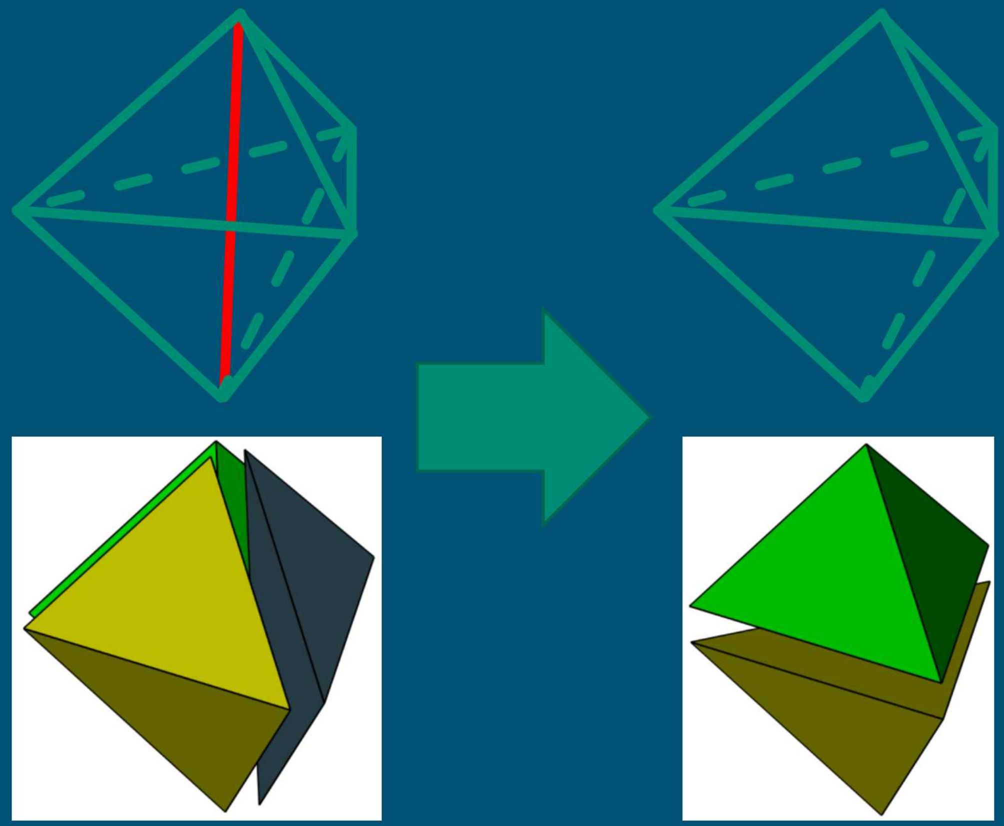
- After conformal decomposition, improve quality with topology-preserving incremental mesh improvements



Incremental Mesh Improvement: Edge Swapping

n tets surround each edge. The tets around the edge can be removed and replaced with alternate connectivity to optimize element quality.

For $n = 3$, the 3 tets are replaced with 2. There is only 1 configuration possible for the 2 tets.



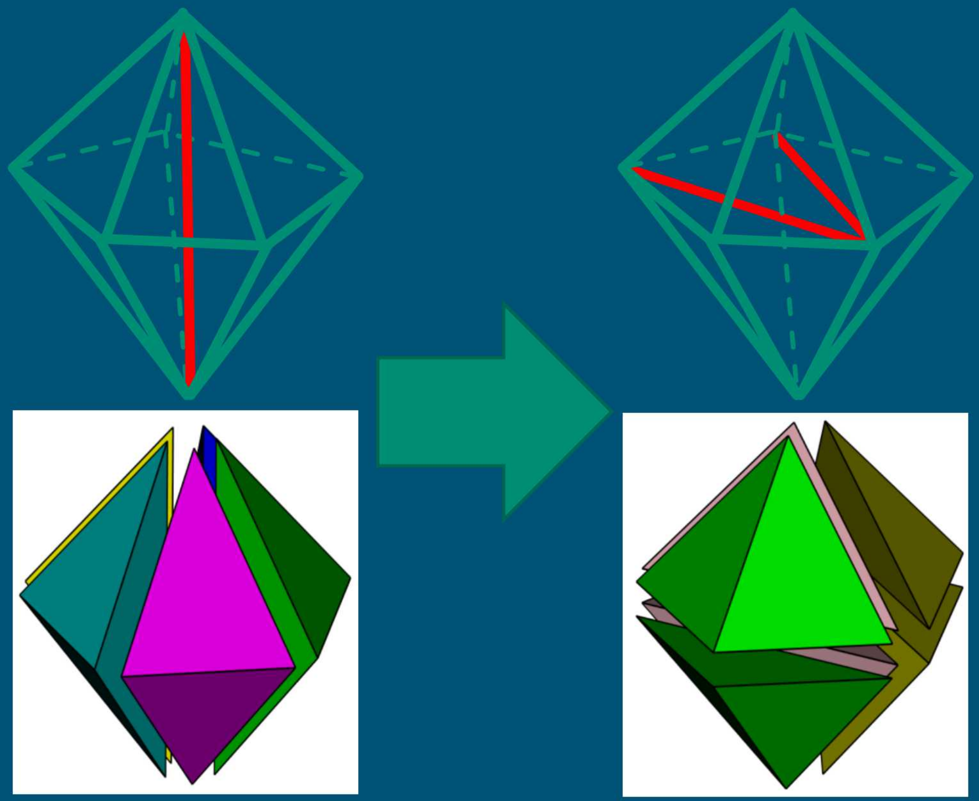
Edge Swapping: Possible Configurations

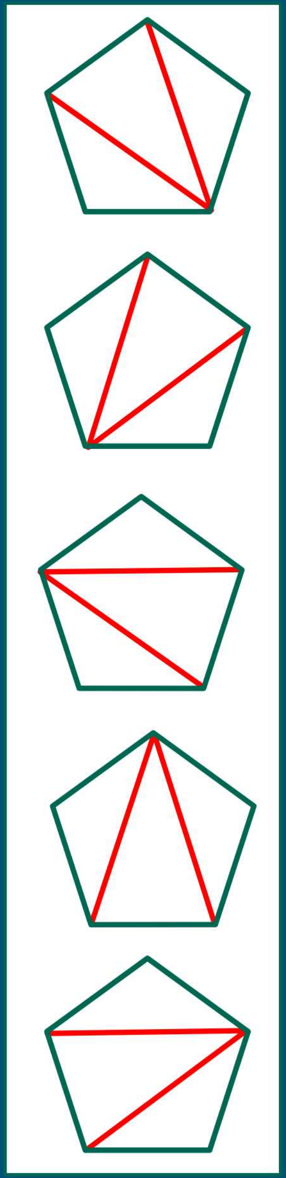
For $n = 5$, the 3 tets are replaced with 6 tets.

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

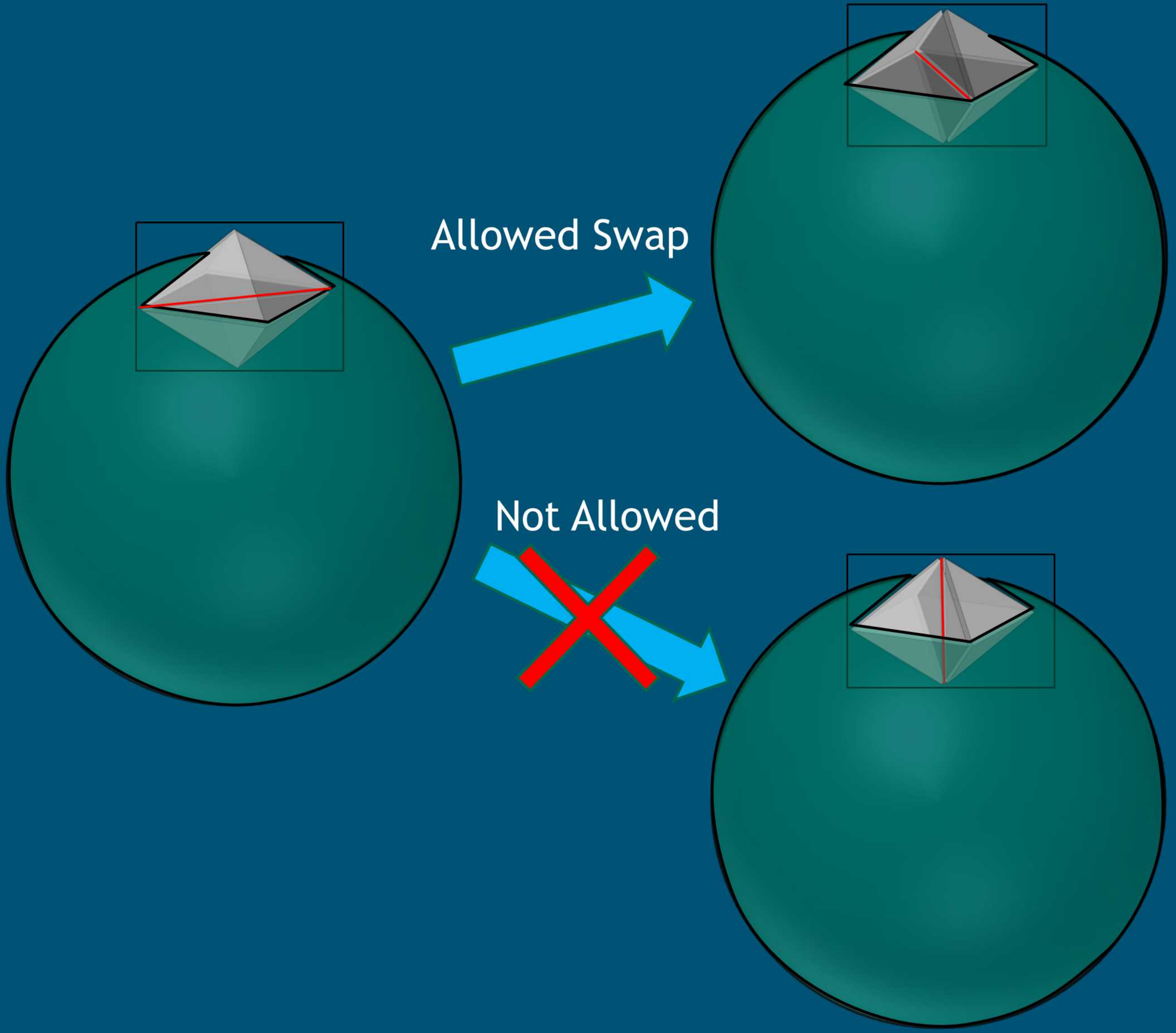
Currently handling cases with 3, 4, 5, 6, or 7 tets around an edge

Developed in collaboration with Dan Ibanez

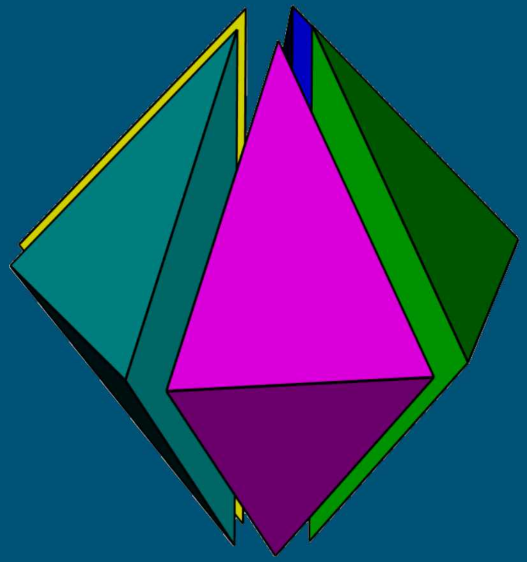




Preserving Topology During Edge Swaps

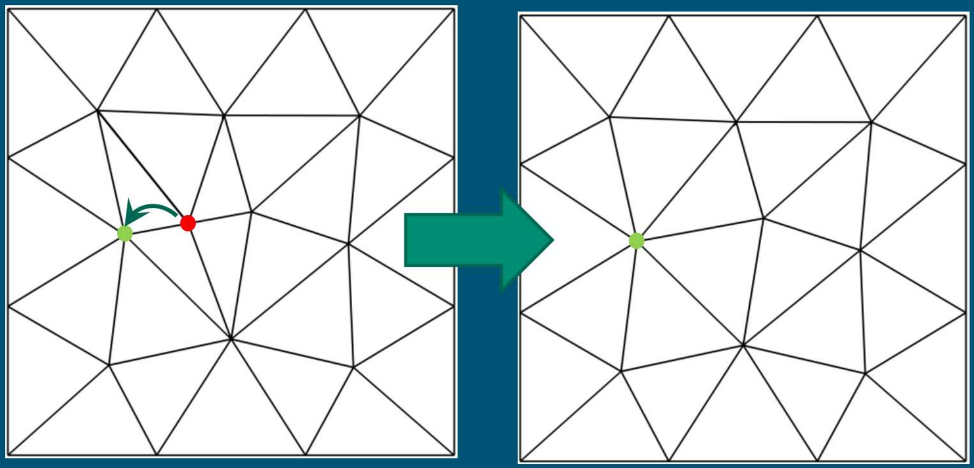


Volume association of each node of the elements surrounding the edge must be unchanged, and all elements must have a unique volume association determined by the intersection of the volume associations of the nodes of the element

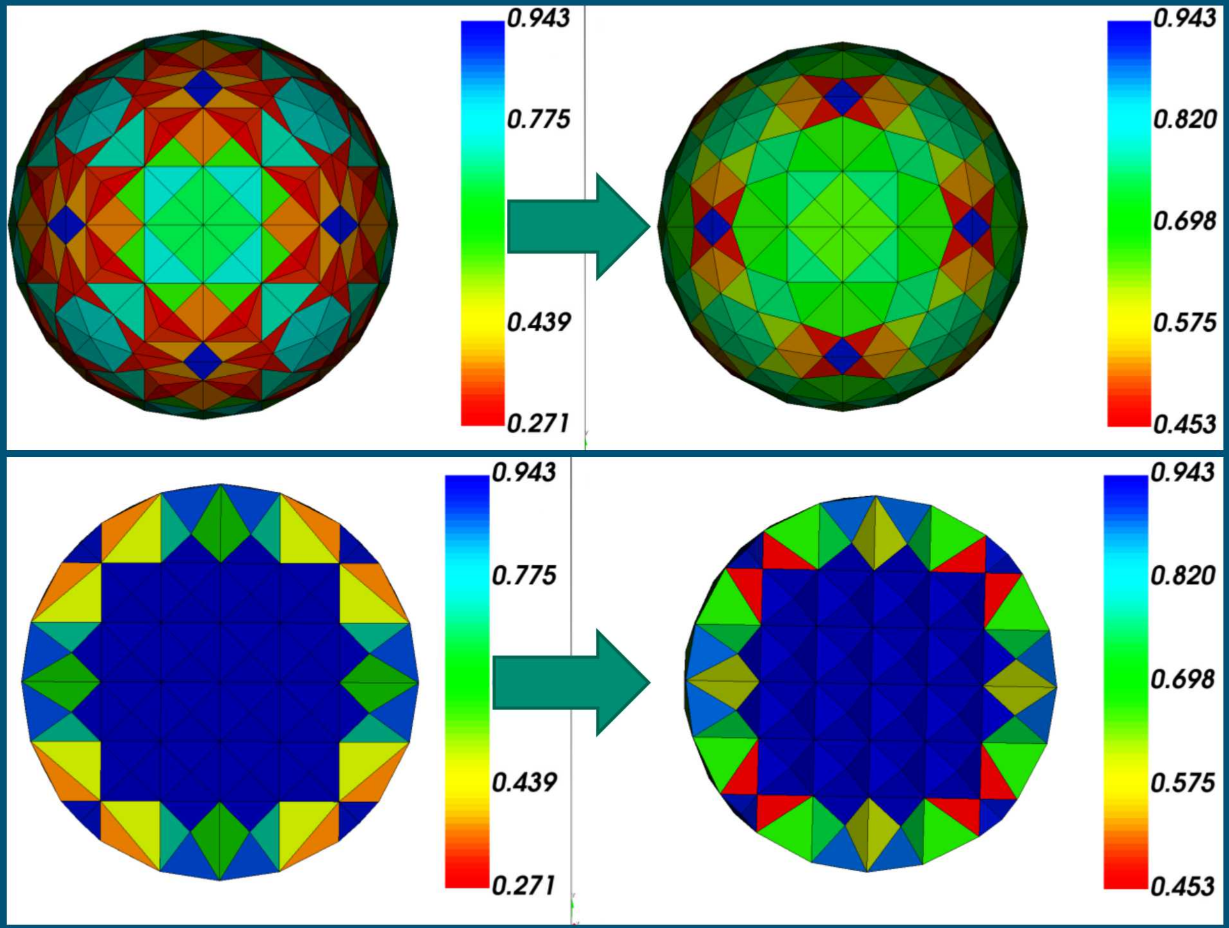


Edge Collapses to Improve Quality

Without Collapse With Collapse

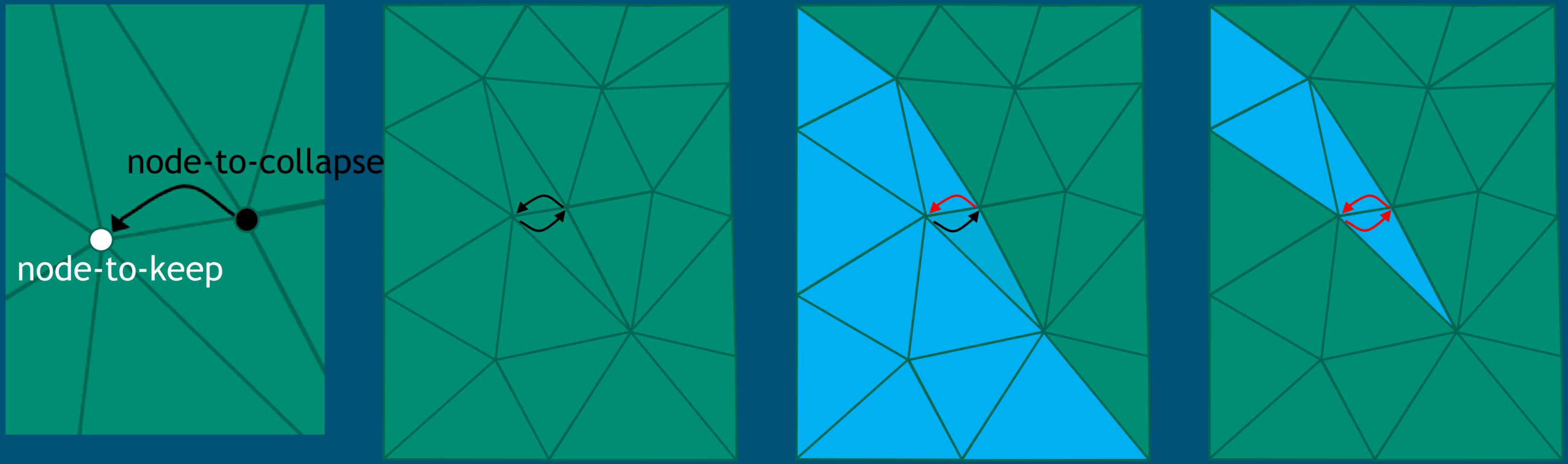


Without Collapse With Collapse



- Collapses remove superfluous edges, significantly improving the quality

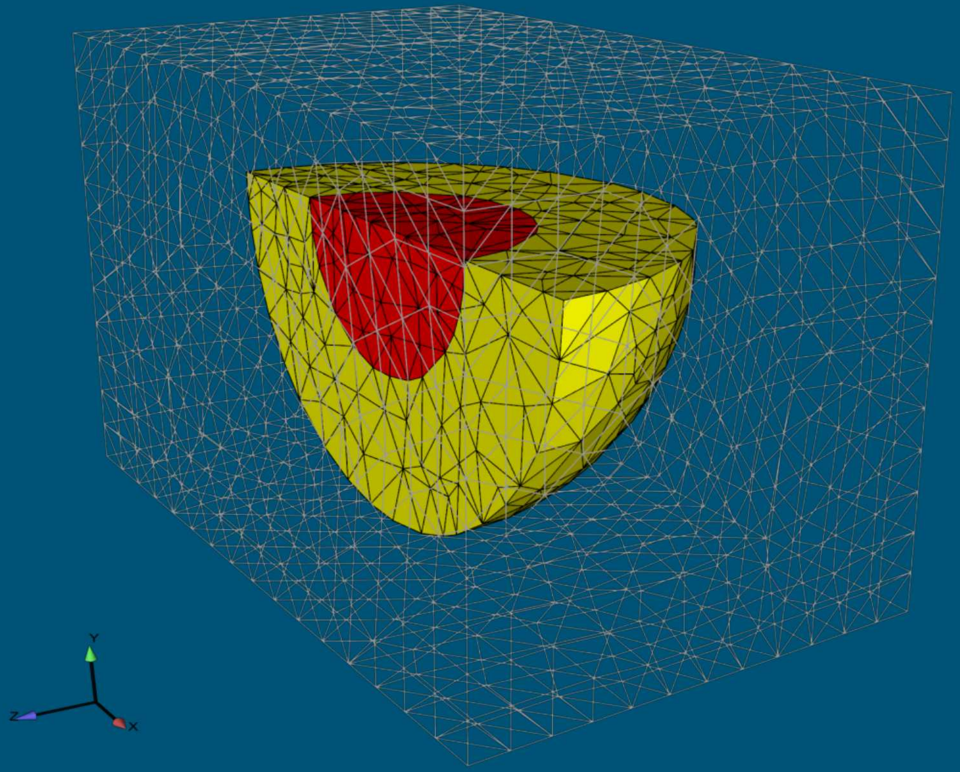
Preserving Topology During Edge Collapse



- 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

Test Problem



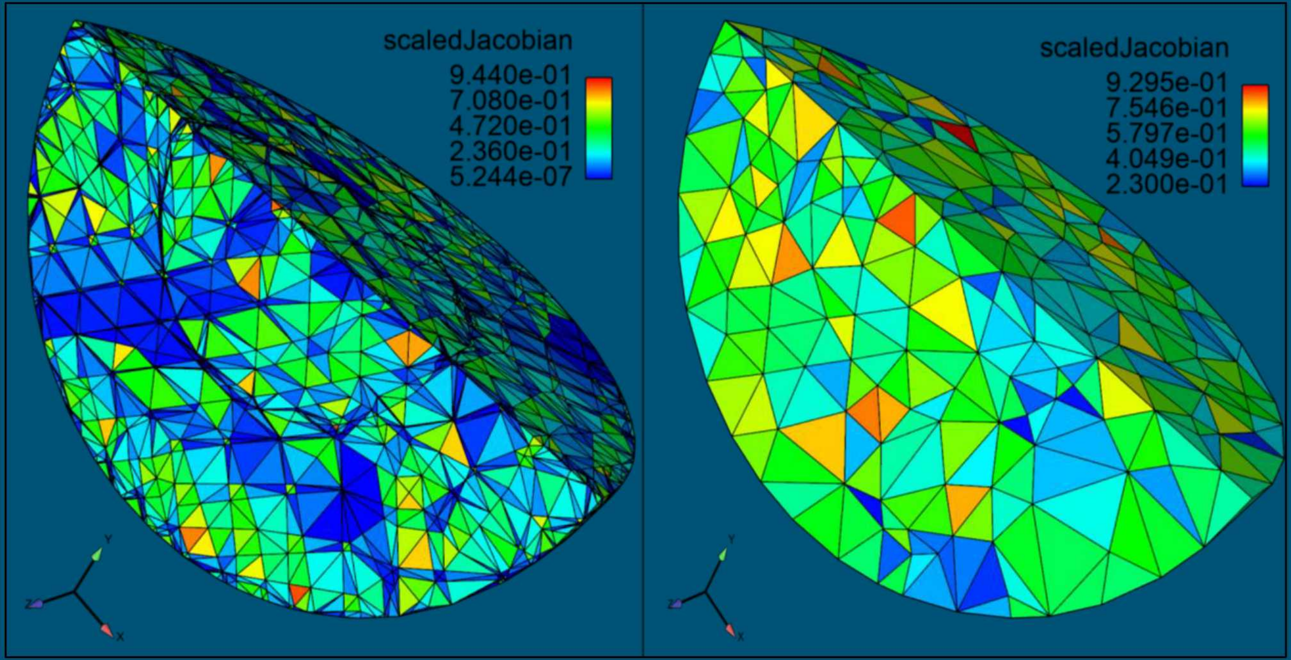
Sphere Wedge – Geometry with bounding surfaces, curves, and vertices, assembly of two touching volumes

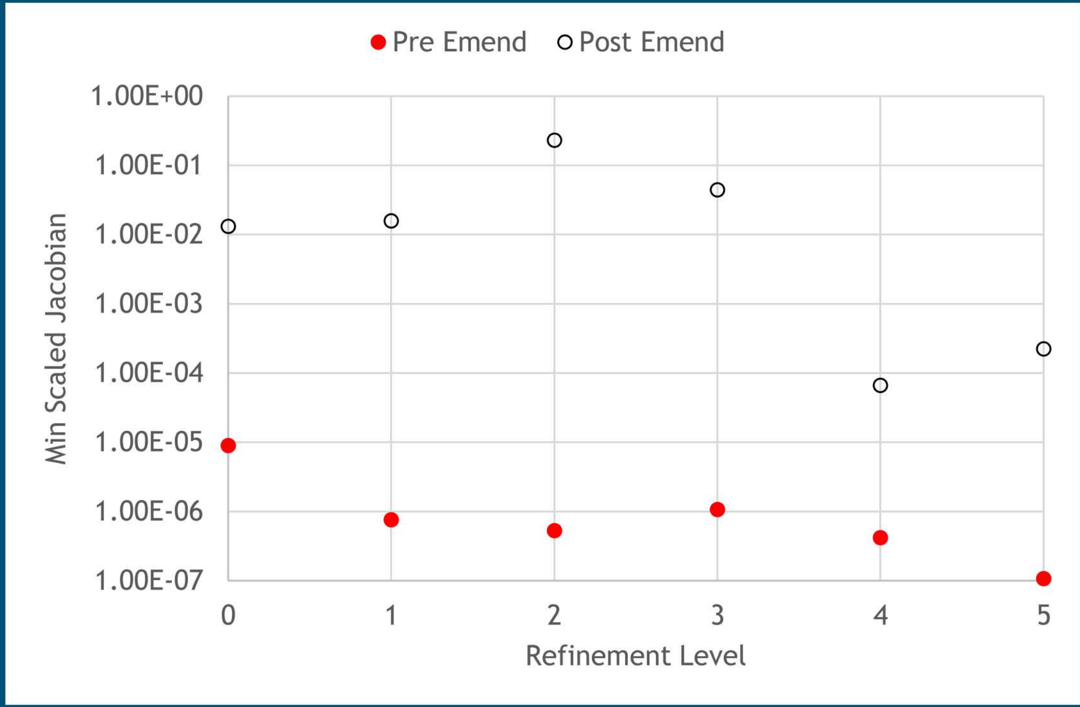
Workflow

- Collapse short edges while maintaining global worst quality (without creating edges that are too long. Local quality allowed to degrade.)
- Swap edges that locally improve quality
- Collapse edges that locally improve quality (without creating edges that are too long)

Credit to Dan Ibanez

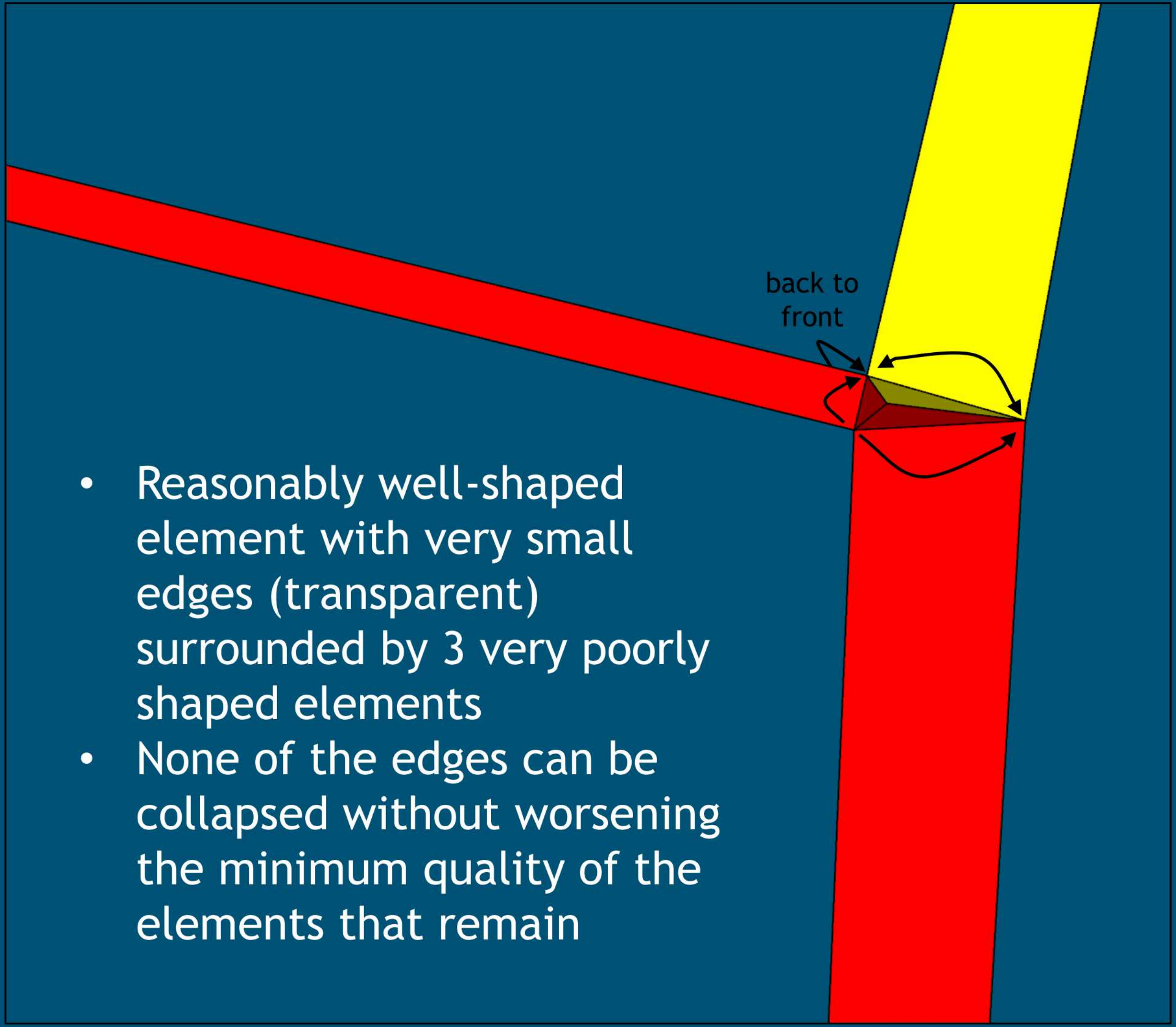
Results: Incremental Mesh Improvement





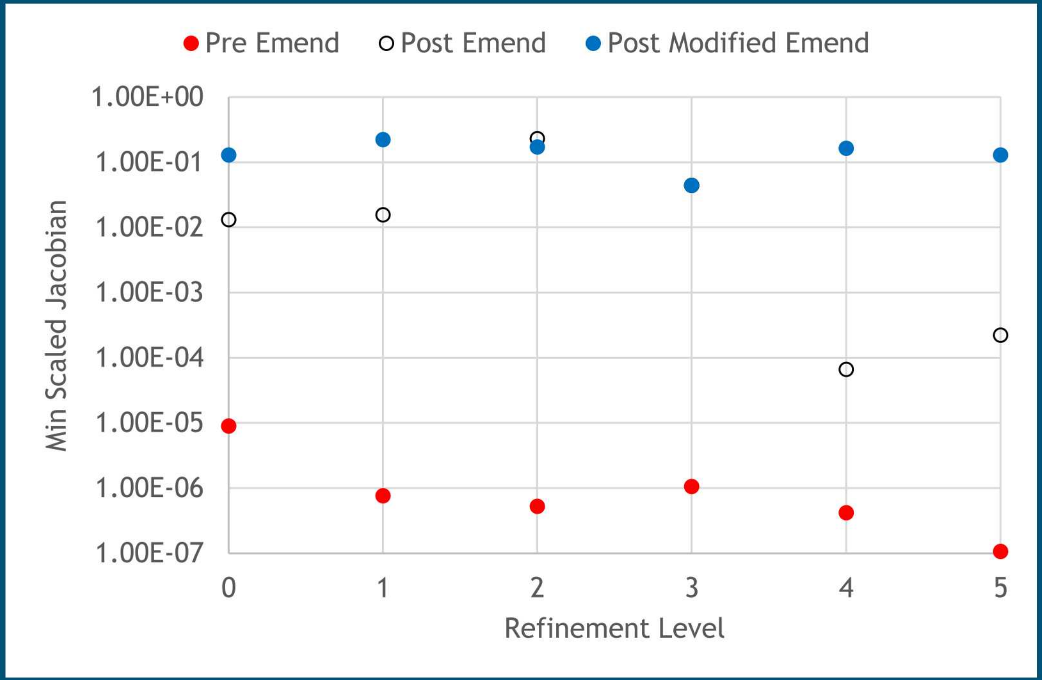
	After Krino	After Emend
Max Aspect Ratio	1.94E+03	3.38E+00
Min Element Volume	9.52E-11	4.79E-03
Max Condition No.	1.88E+03	2.88E+00
Min Scaled Jacobian	5.24E-07	2.30E-01
#Tets	11039	2856

Bad Elements That Cannot Be Eliminated by Edge Swap or Single Edge Collapse

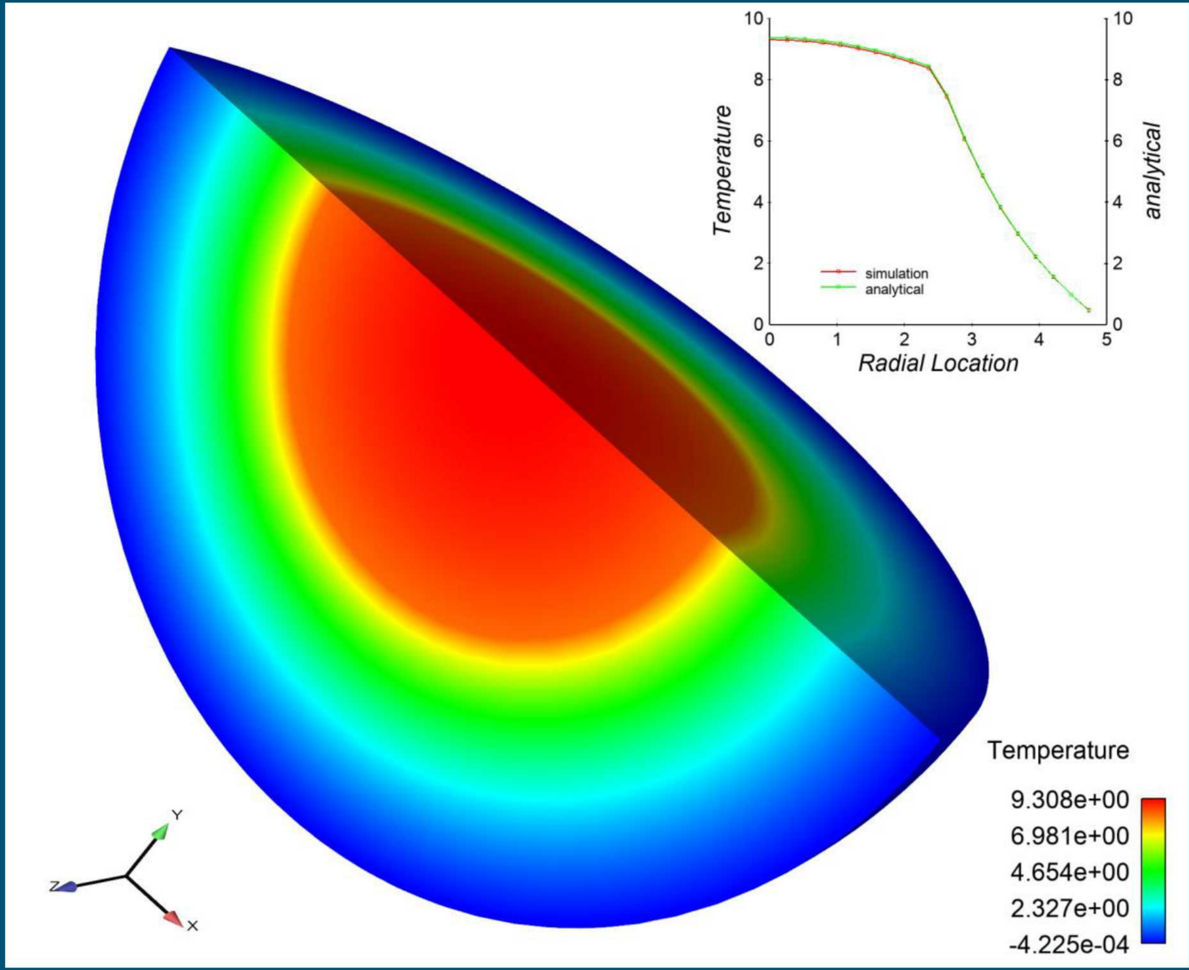


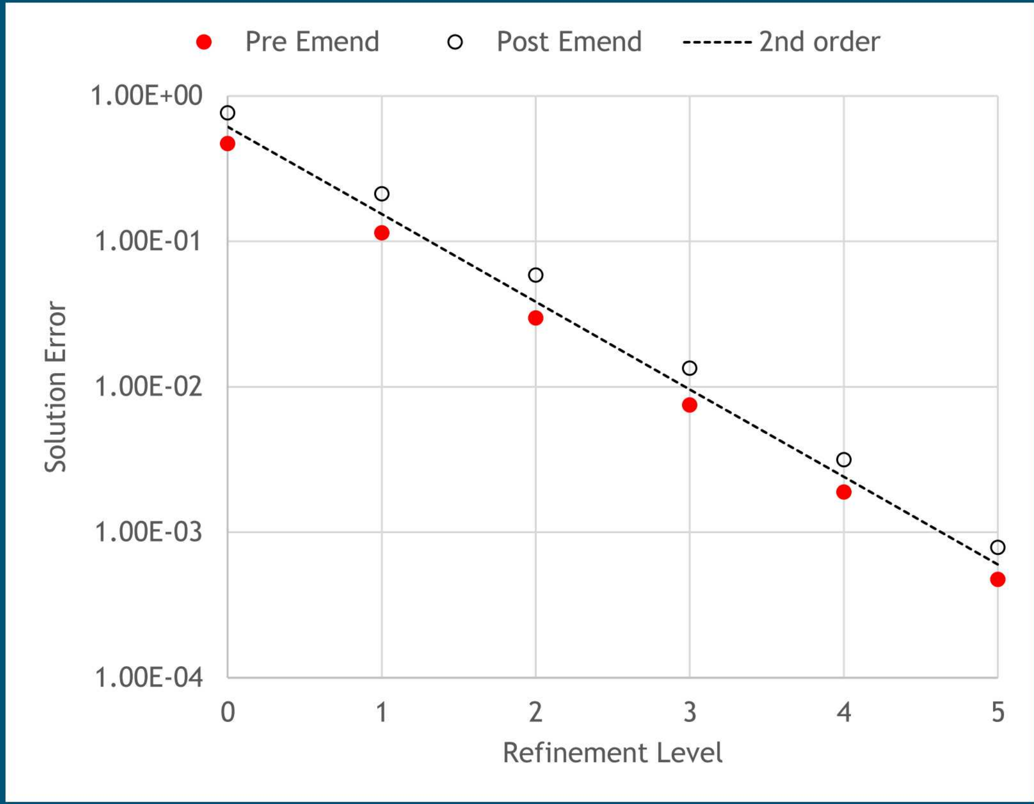
- Reasonably well-shaped element with very small edges (transparent) surrounded by 3 very poorly shaped elements
- None of the edges can be collapsed without worsening the minimum quality of the elements that remain

- Work-around is to allow quality to degrade moderately for a single collapse
- Long term solution?: Consider multiple simultaneous collapses, i.e. face collapses with two nodes collapsing to the 3rd node of face



Results: Solution Accuracy

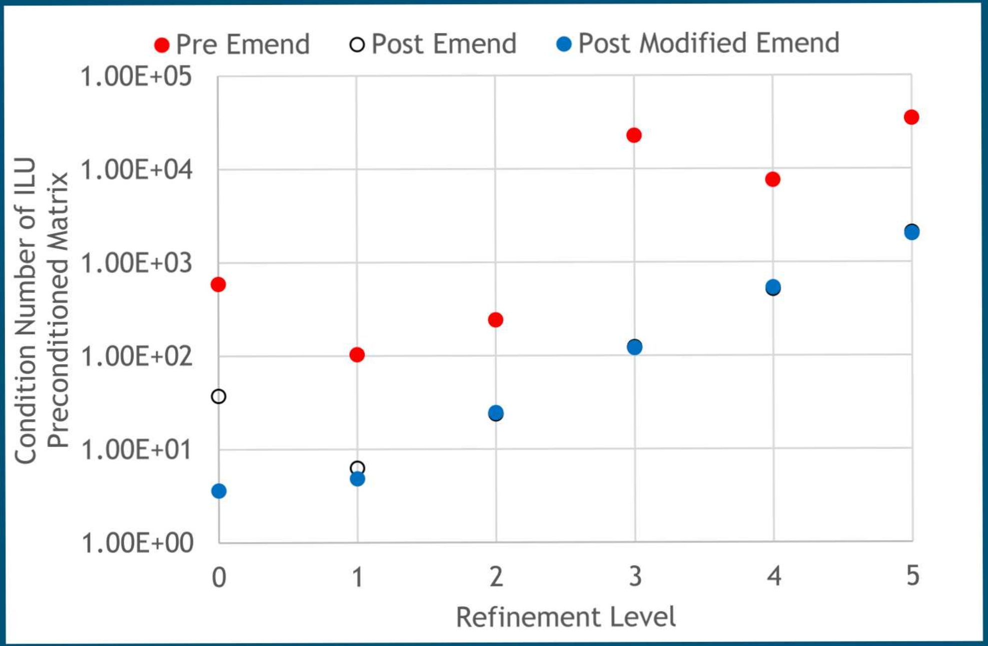


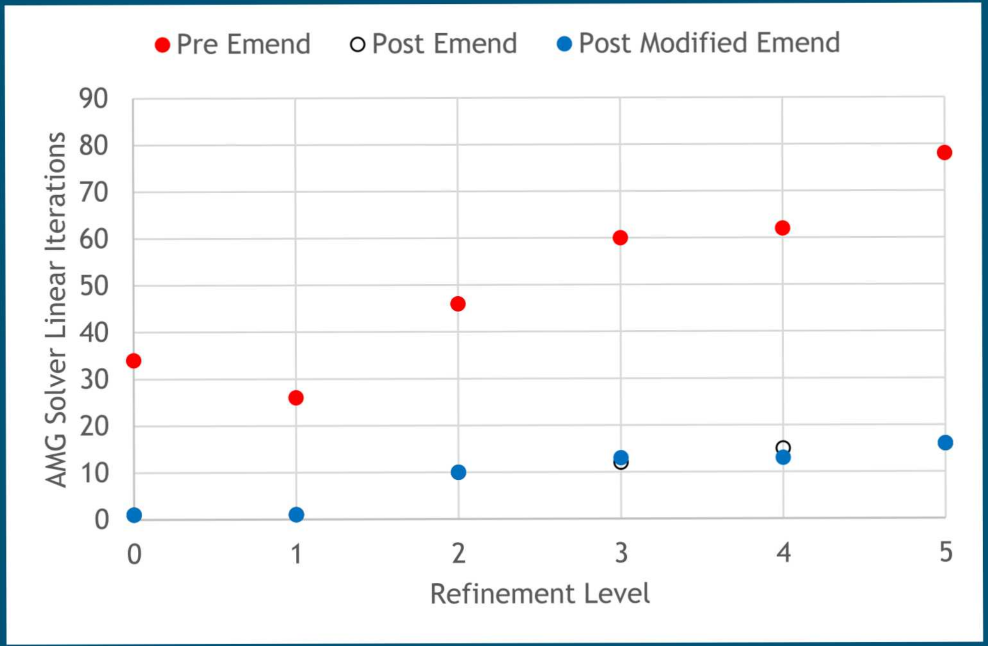


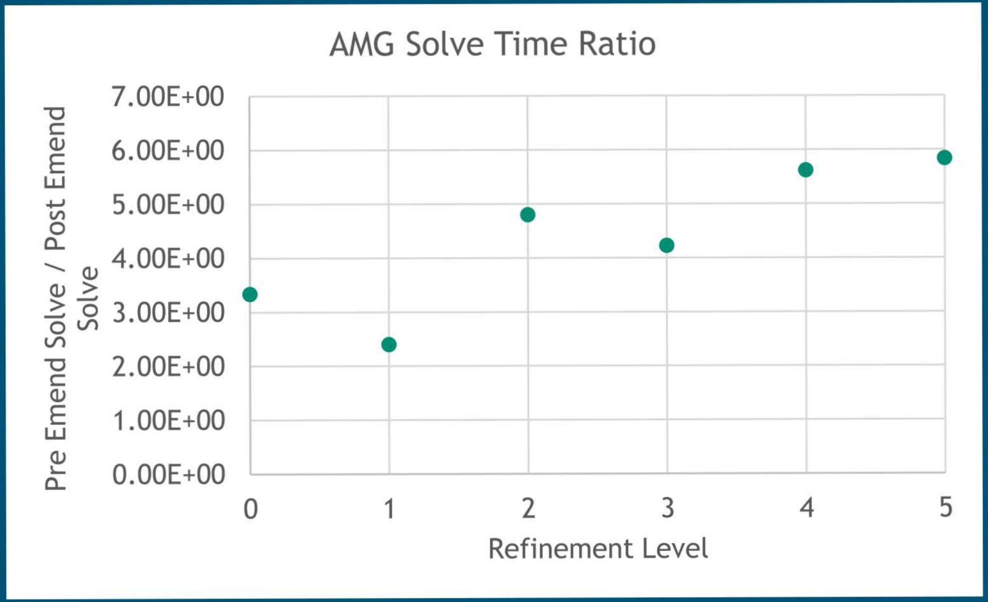
$$T(r) = \begin{matrix} A_i r^2 + C_i & r \leq R \\ A_o r^2 + B_o/r + C_o & r > R \end{matrix}$$

- Optimal rates of convergence obtained with original or improved mesh
- More accurate with original mesh despite low quality elements

Results: Solver Performance







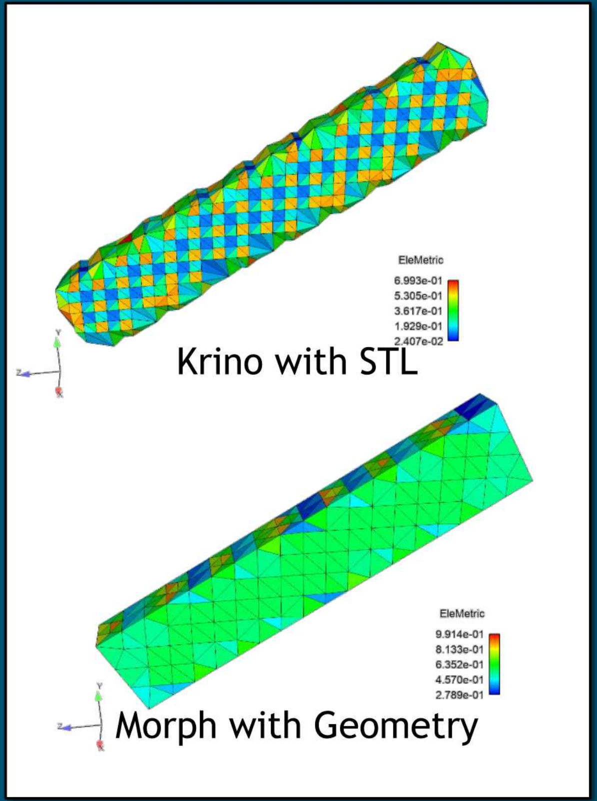
- Consistent with findings for other interface enriched methods, condition number scales as expected, only moderately higher than that for well-shaped mesh
- Nonetheless, well-shaped post Emend mesh significantly lowers solver iterations and time

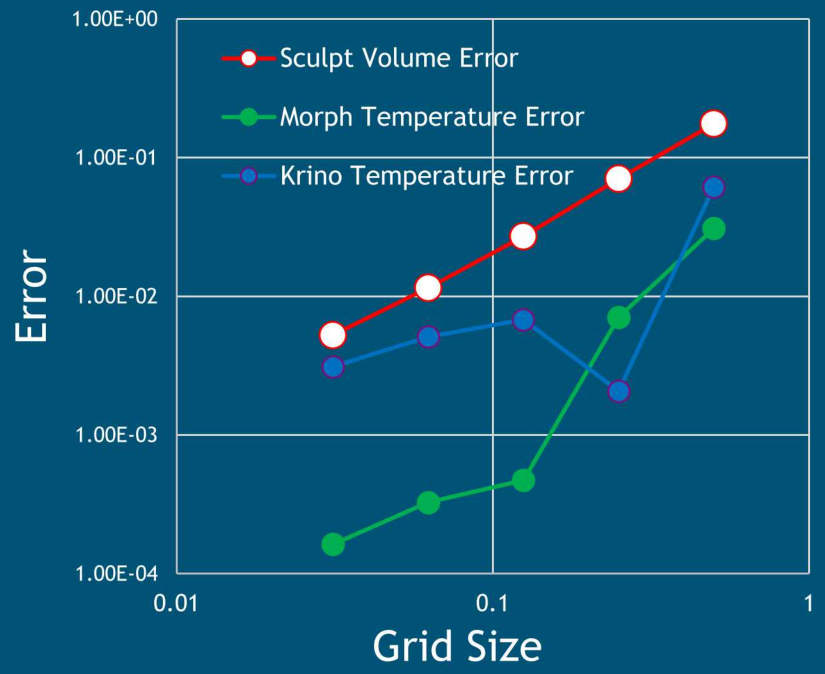
Summary/Conclusions

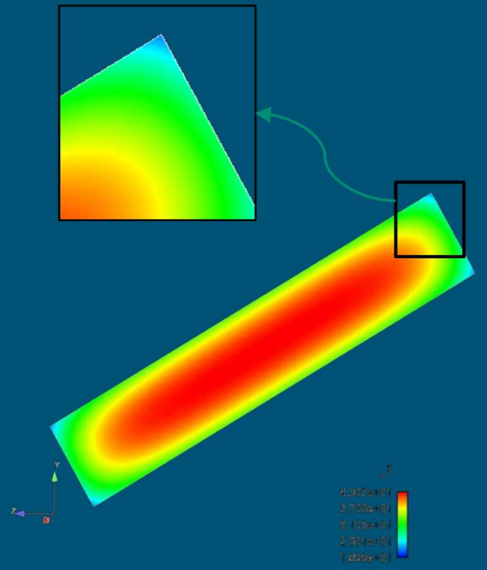
- Recursive cutting procedure in CDFEM produces elements with vanishing quality
- Emend tool highly successful at improving quality while preserving topology
- While condition number only moderately impacted, solve times improve by ~5x with only mild degradation in accuracy
- Future Work
  - Additional transformations to further improve quality (face collapses?)
  - Allow transformations that change topology when "small enough"

Issue with Surface-Based Geometry Definition: Sharp Feature Capture

- Are sharp features like curves and vertices captured?





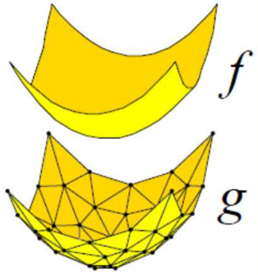


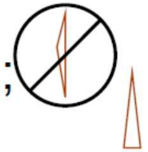
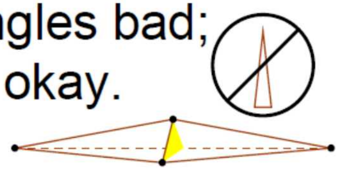
Temperature Profile within Beam

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