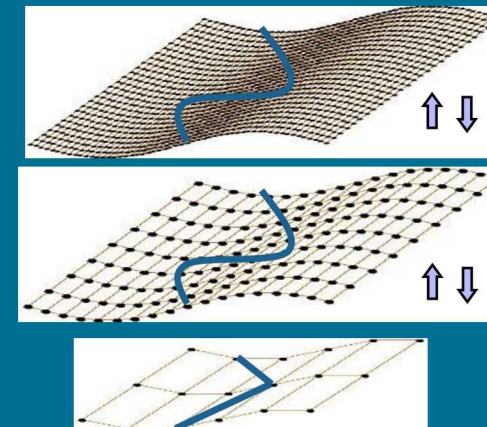
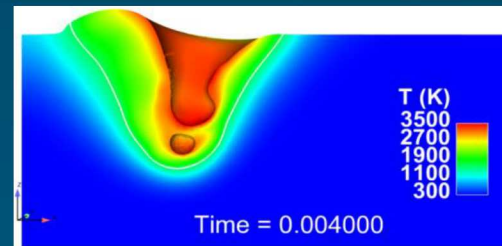
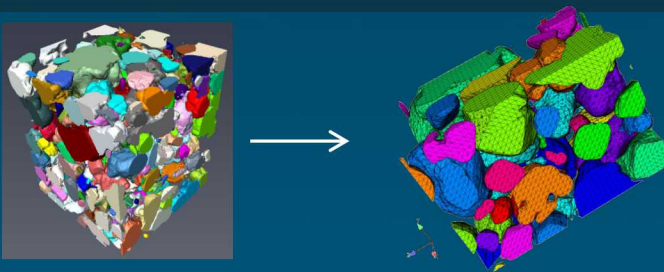
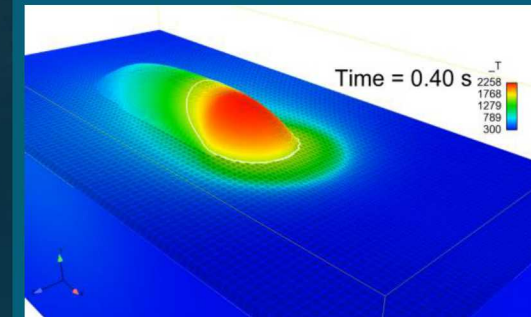




# Approaches for Obtaining Accurate and Well-Conditioned Enriched Methods for Many Materials



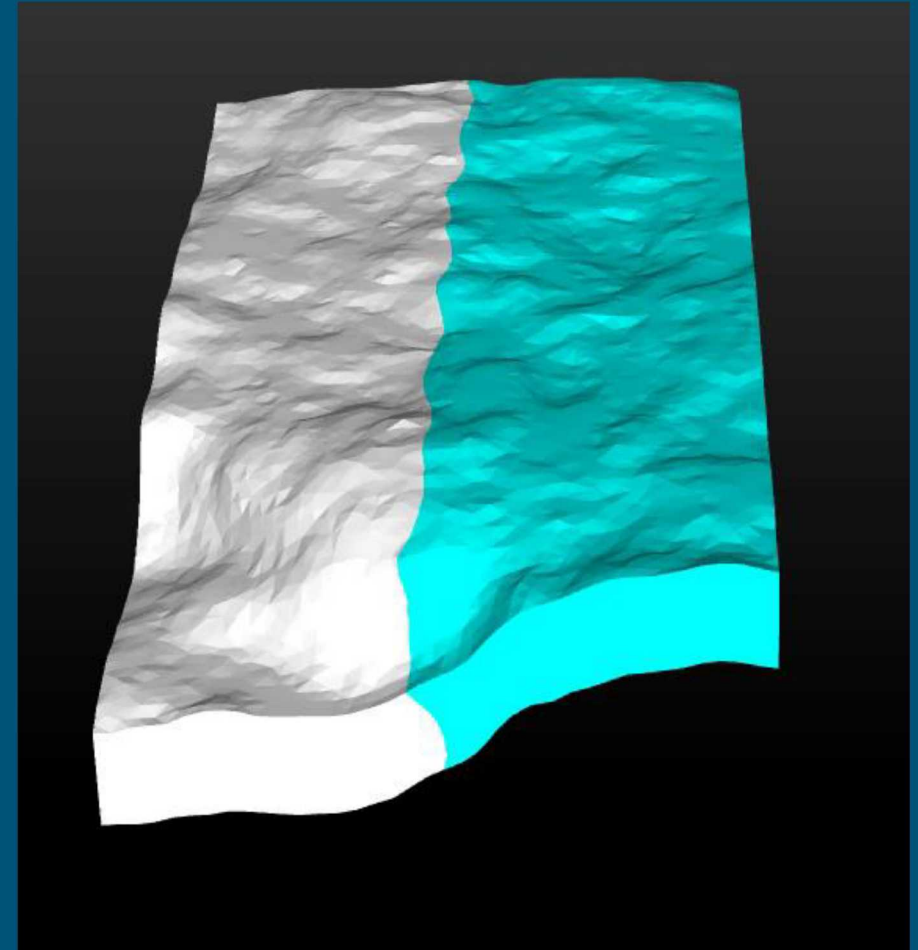
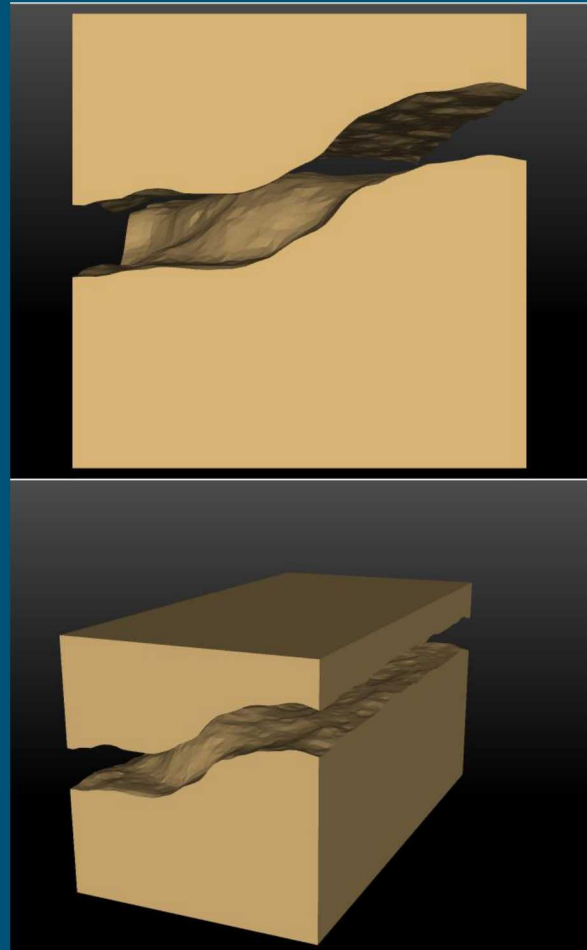
PRESENTED BY

David R. Noble

# Use Case: Flow Through a Scan of a Real 3D Fracture



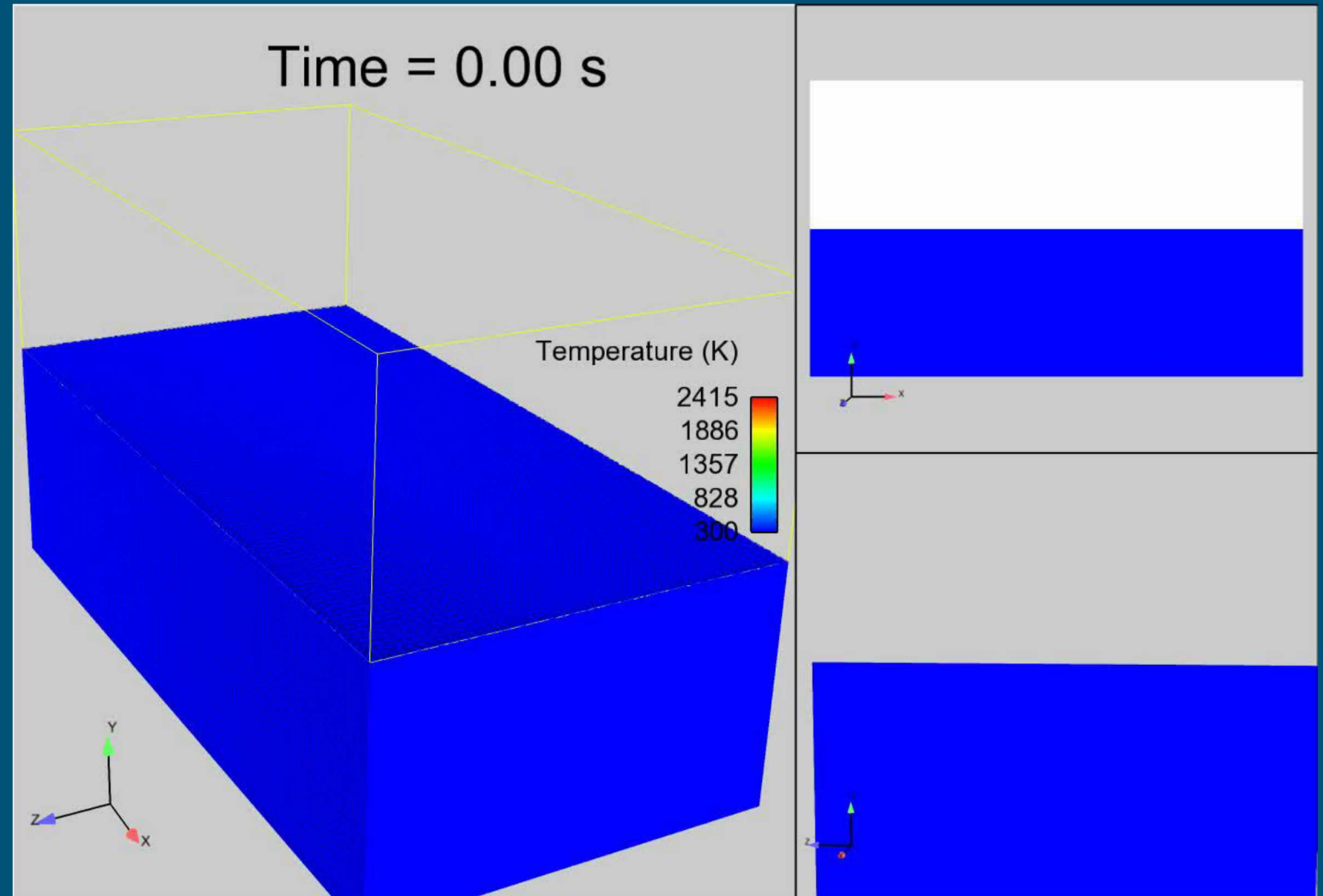
- Flow through fracture using Micro-CT scan of actual sandstone fracture
- Interfacial conditions include capillarity and wetting conditions along triple line
- Currently sequential conformal decompositions
  - Decompose with respect to fracture
  - Solve multiphase flow with decomposition with respect to moving interface
- For soluble material or deforming fracture, would like to use multiple dynamic interfaces



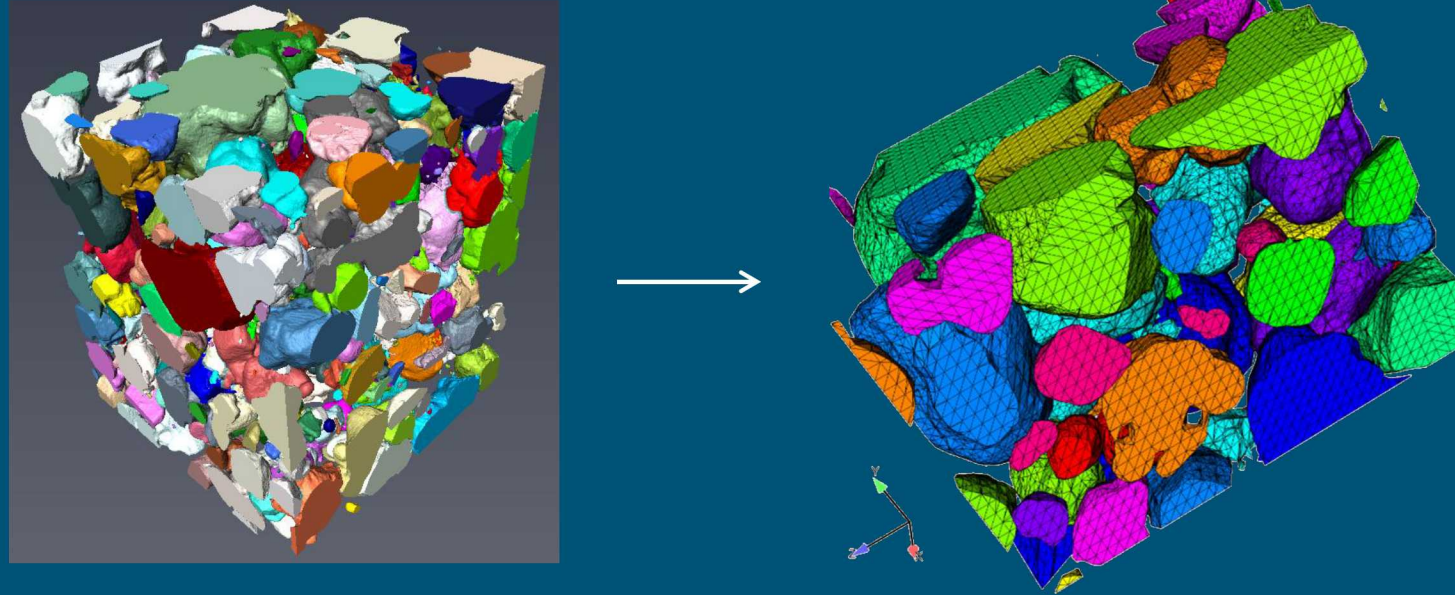
# Use Case: Additive Manufacturing



- Additive manufacturing via selective laser melting involves using a laser to apply intense heating
- Complex interfacial transport involving capillarity, laser heating, non-equilibrium vaporization, gives rise to dynamic, discontinuous physics and fields
- Currently modeled using conformal decomposition using level set for vapor-fluid interface
- Solid-fluid interface is modeled using temperature-dependent viscosity
  - Does not allow for solving for solid deformation during solidification
  - Would like to use separate sharp interface for solid-fluid interface allowing coupled solid-fluid-gas transport



# Use Case: Battery Performance



Numerous materials in contact

- Distinct anisotropic properties from grain to grain

Complex volumetric and interfacial physics

- Electrochemistry, possibly with contact resistance at grain boundaries

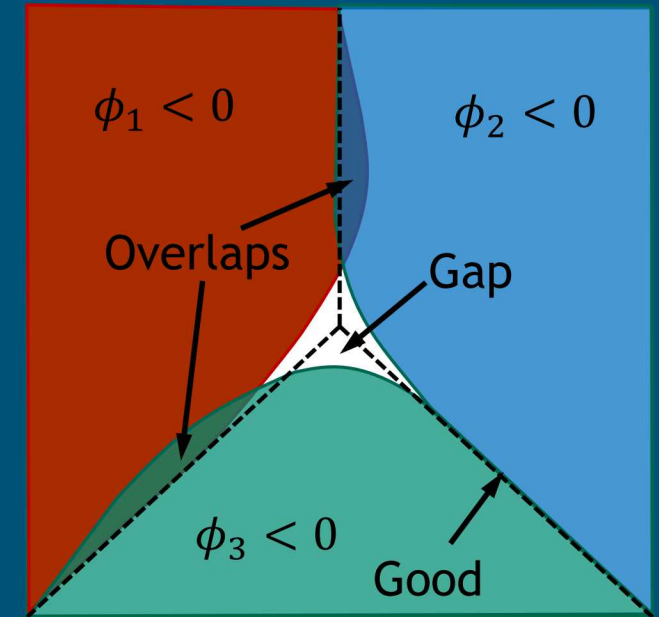
Static, but complex topology

- Obtained from experimental image reconstruction

# Level Sets for Many Materials

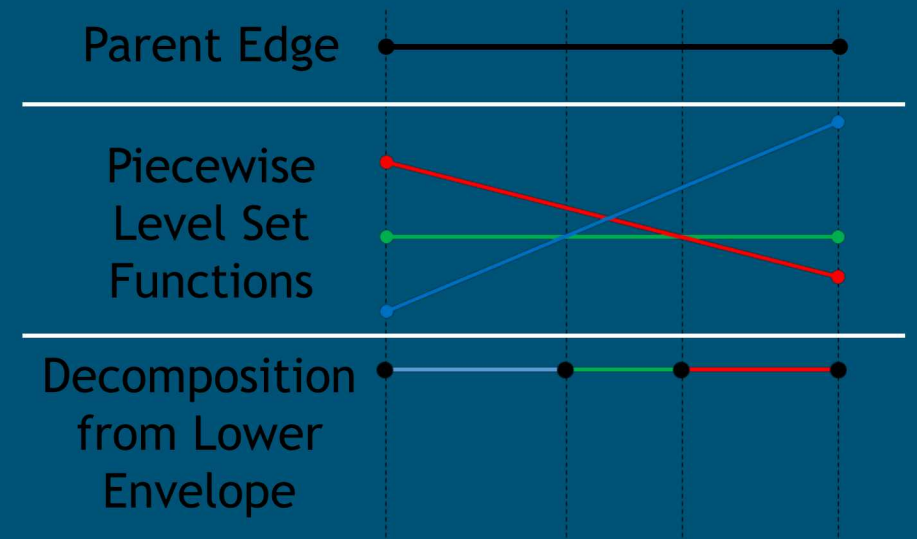
## Level Set Description for Many Materials ( $>2$ )

- One level set per interface
  - Strictly defines  $2^n$  materials (or phases)
  - Not trivial to initialize level sets knowing location of materials
- Level set per material
  - Trivial to initialize level set knowing location of materials (signed distance)
  - Subject to overlaps and/or gaps
  - Interpolant may have overlaps and/or gaps even if nodal field is exact



## Selected Strategy

- One level set per material
- Use lower envelope to uniquely define behavior in gaps and overlaps
  - A point is material  $i$  if  $\phi_i < \phi_j \forall j \neq i$



# 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

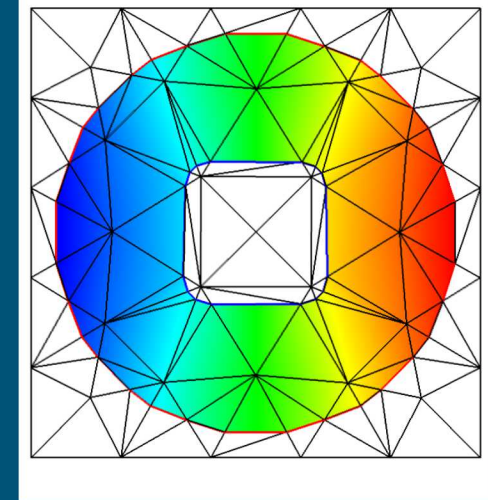
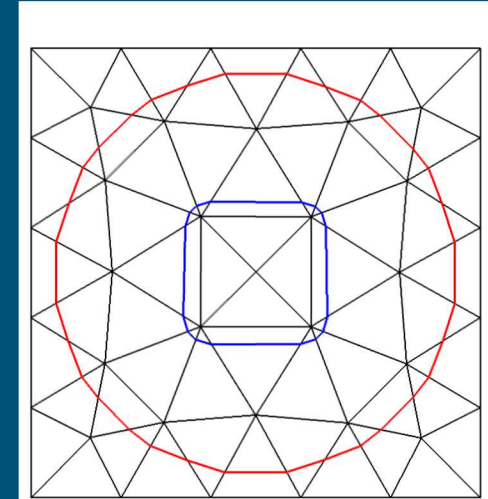
- Extension to higher order (Fries)
- Approximation space equivalent to that in DE-FEM for linear elements (Aragon)

## 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



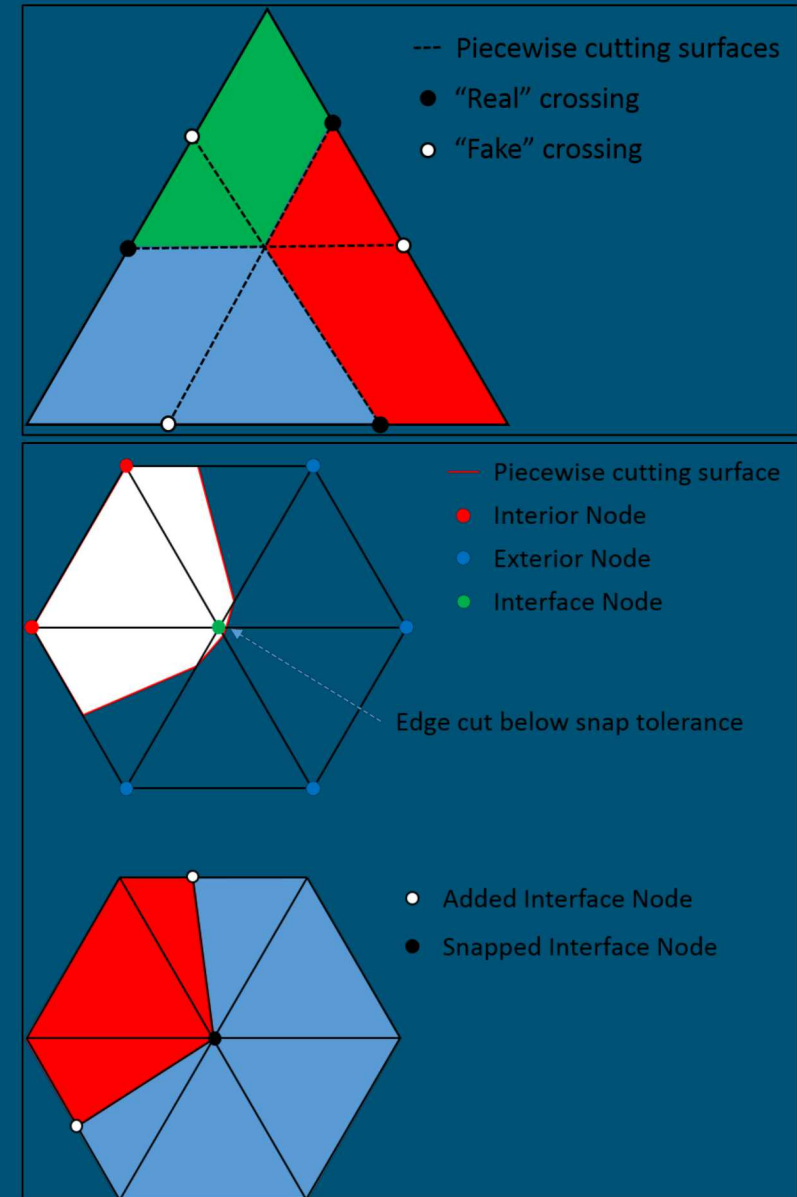
# CDFEM for Many Materials

## Recursive Conformal Decomposition

- Determine lower envelope on each edge
- Create piecewise-planar cutting surfaces for each level set transition
- For elements with triple points, cutting surfaces terminate at “fake” crossings (transition between level sets that are not lowest level set)

## Simple Snapping Procedure

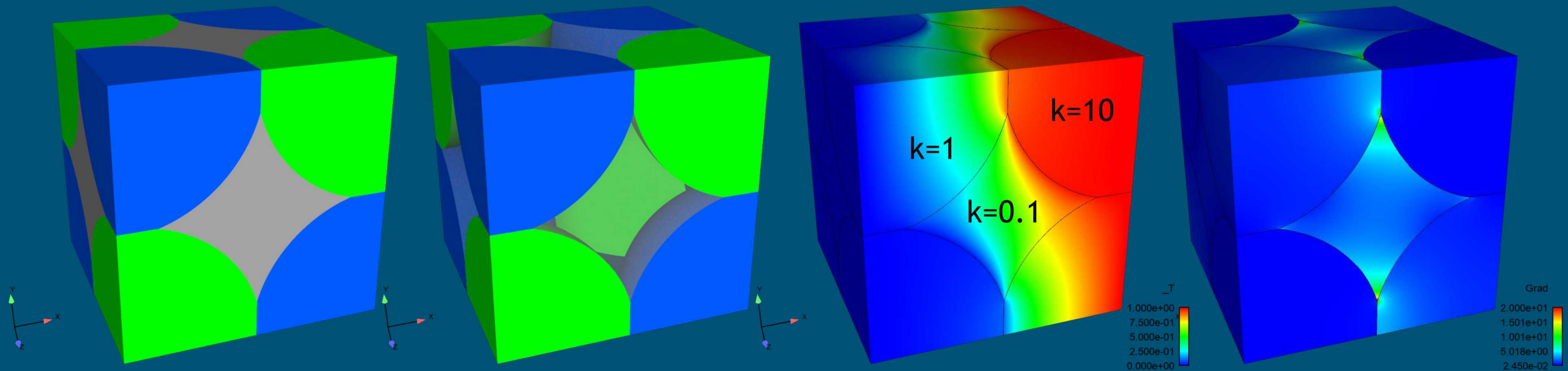
- If any edge cut below tolerance, move interface to nearest node on all edges supported by that node
- Introduces error in interface location
  - Only appropriate for infinitesimal snap tolerance



# 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

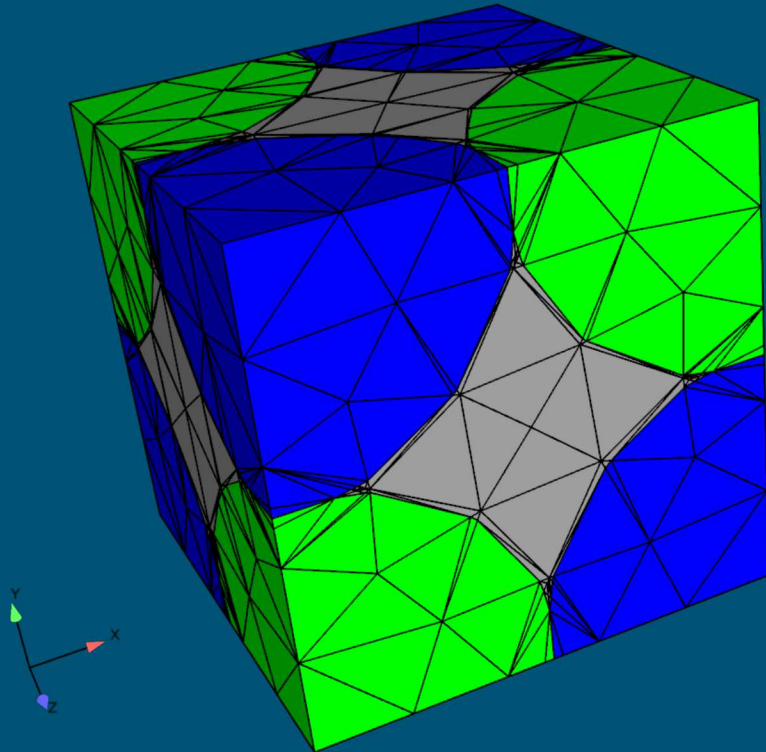




# Many Phase CDFEM Results

## Many-Phase CDFEM for Conduction Problem

- Very poor quality
- Optimal accuracy
- Little to no impact on GMRES-Jacobi Solves on refined meshes



### Scaled Jacobian

Average: 2.339160e-01

Minimum: 2.679434e-06

Maximum: 9.312074e-01

### Condition Number

Average: 1.612178e+01

Minimum: 1.007120e+00

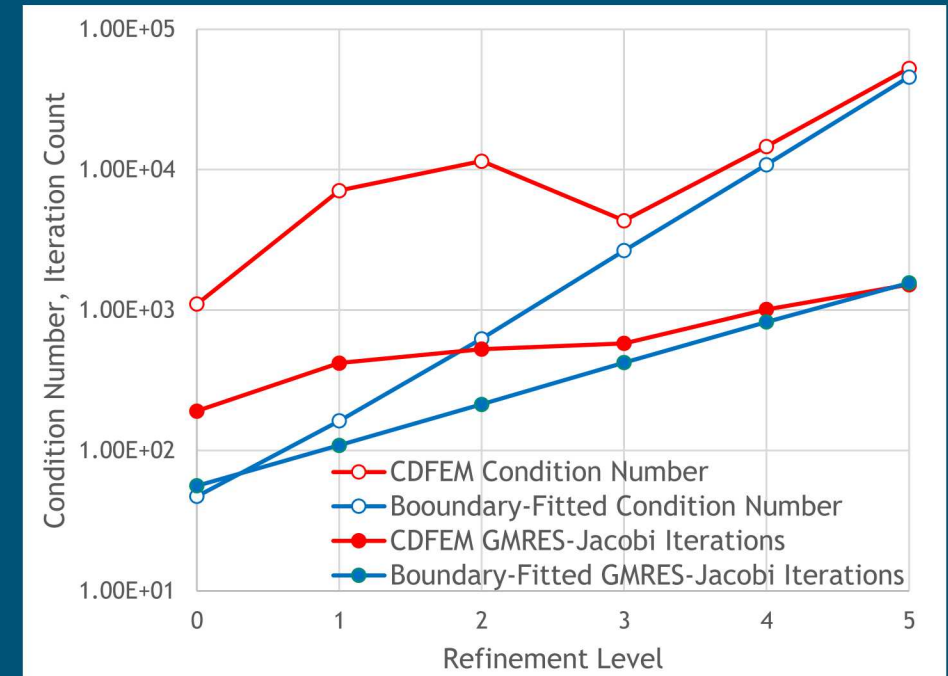
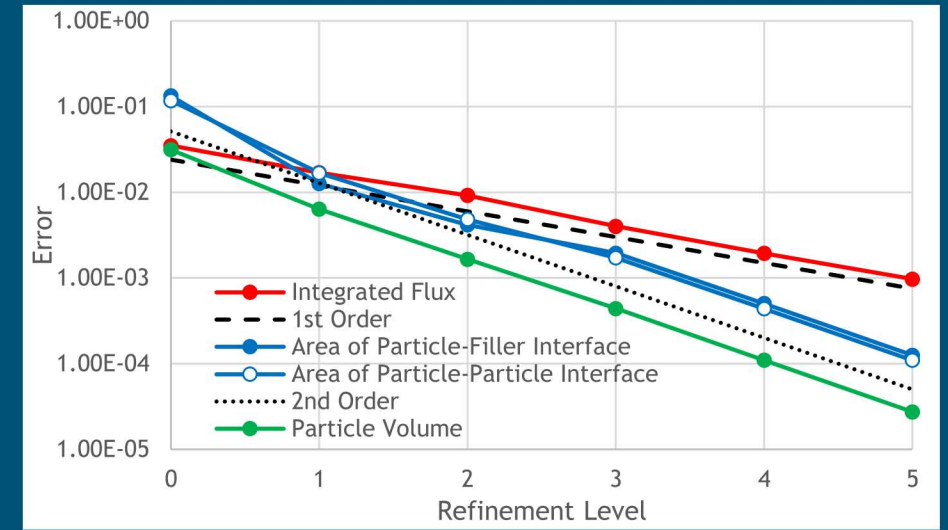
Maximum: 5.724501e+03

### Aspect Ratio

Average: 1.740721e+01

Minimum: 1.060456e+00

Maximum: 5.362165e+03

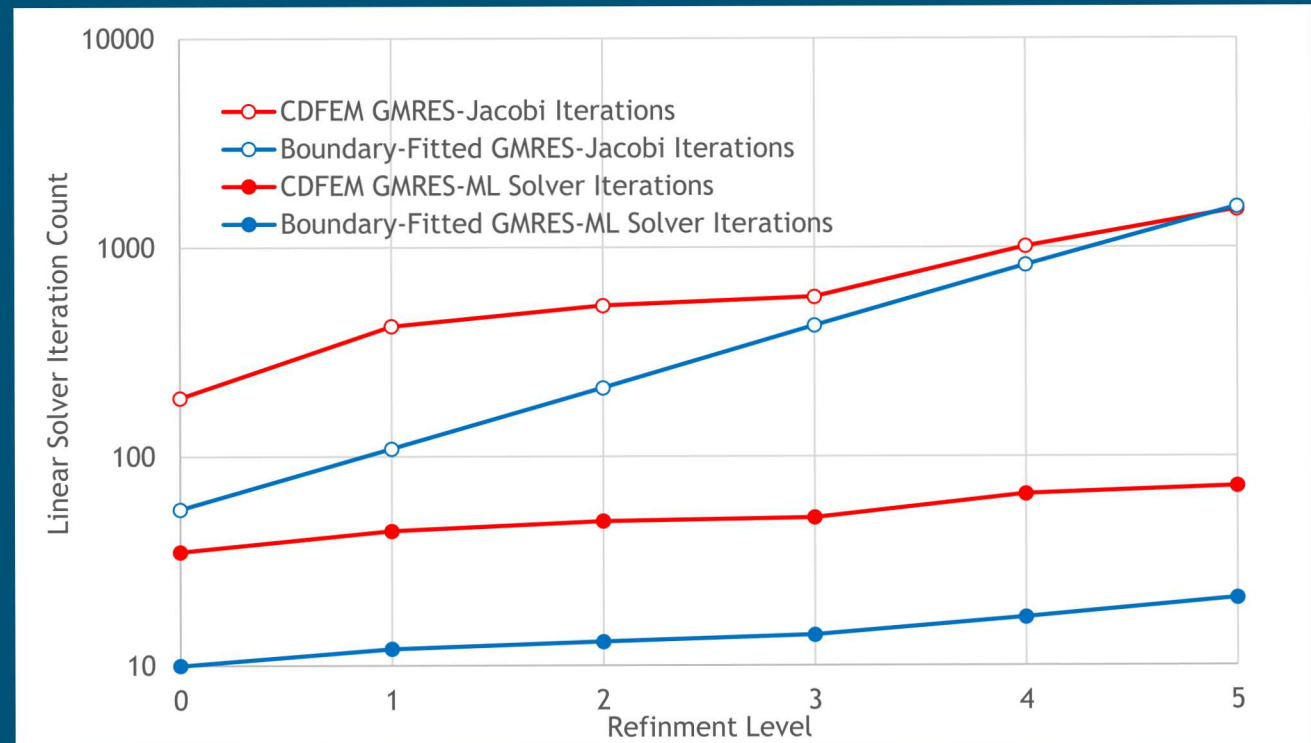
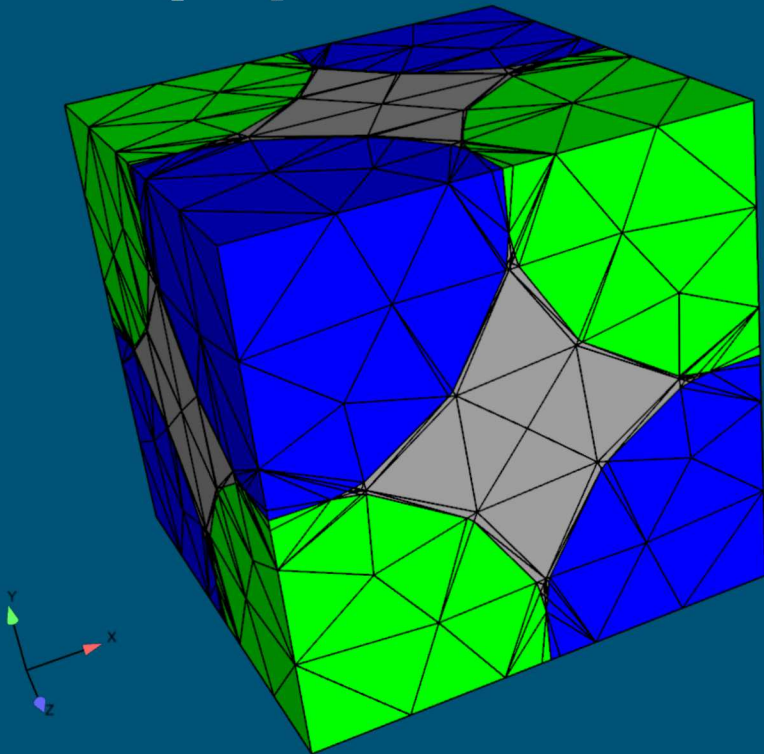


# Many Phase CDFEM Algebraic Multigrid Results



## Many-Phase CDFEM for Conduction Problem

- Little to no impact on GMRES-Jacobi Solves on refined meshes
- Factor of 3 to 4 increase in cost of GMRES-ML Solves (Algebraic Multigrid)
- Consistent with customer issues with poor performance and long solve times on complex problems



# Methods for Handling the Poorly Conditioned Matrices Produced by Enriched Methods



## Ghost Stabilization

- Least experienced in this area, may not be appropriate for CDFEM
- Shown to successfully control condition number for CutFEM
- Convergent, but possibly excessive diffusion

## Space “Coarsening”

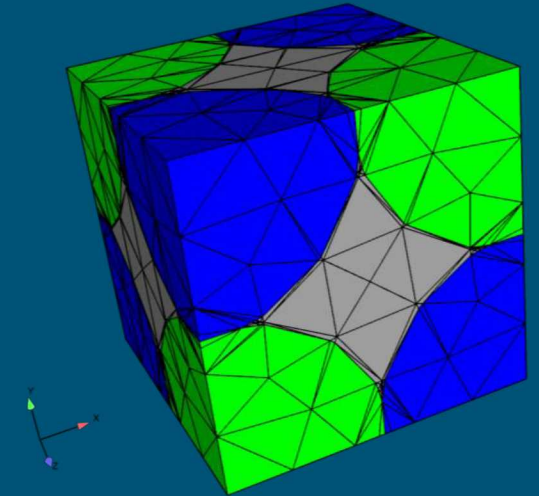
- Project CDFEM or CutFEM solution to coarser space to improve conditioning
- Allows separation of geometric resolution and solution resolution
- Basis function removal (Badia)

## “Specialized” Solvers/Preconditioners

- Only method for dealing with condition number with problem size
- Specialized preconditioners for XFEM/CutFEM/CDFEM have shown great results
- Strategies may be problem-dependent

## Background Grid Snapping

- Manipulate background grid to eliminate sliver elements
- “Partial” Snap to Interface (Kramer, Duarte), Snap from Interface (Fries)
- “Full” Snap to Interface: CISAMR (Soghrati), Morph (Staten)

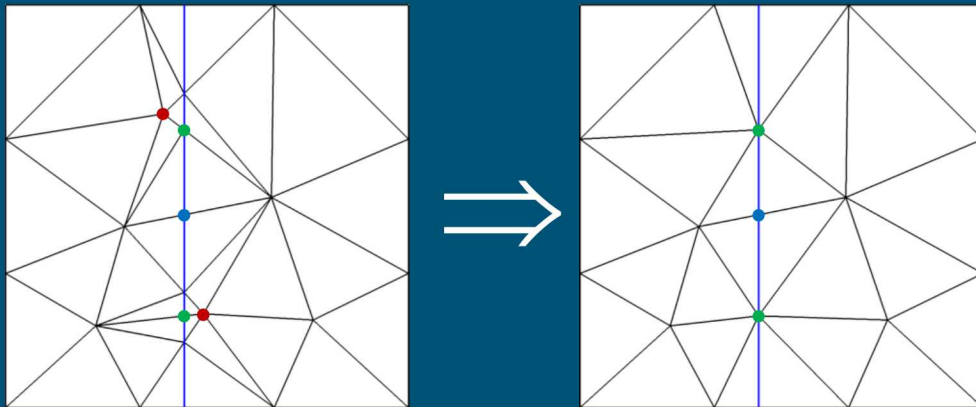


# “Partial” Snap to Interface for Improving Discretization Quality



## Snap “bad” nodes

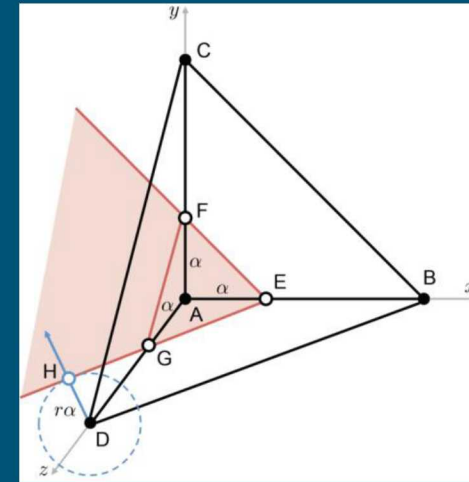
- Determine edge cut locations using level set
- When any edges of a node are cut below a specified ratio, move the node to the closest edge cut location (snap background mesh nodes to interface,  $\bullet \rightarrow \bullet$ )



## Maximum snap tolerance for non-degenerate mesh

- Cannot allow all nodes of an element to snap to the interface
- Maximum snap tolerance,  $\alpha$ , in terms of maximum to minimum edge length ratio,  $r$

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



- Maximum snap tolerance of 0.37 for equilateral tetrahedron mesh and 0.29 for structured mesh

# 3D Weak Discontinuity Test Problem With Partial Snapping

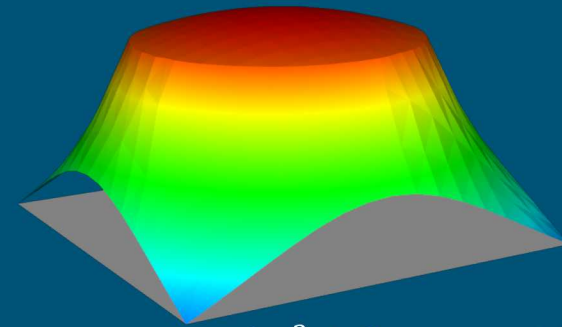
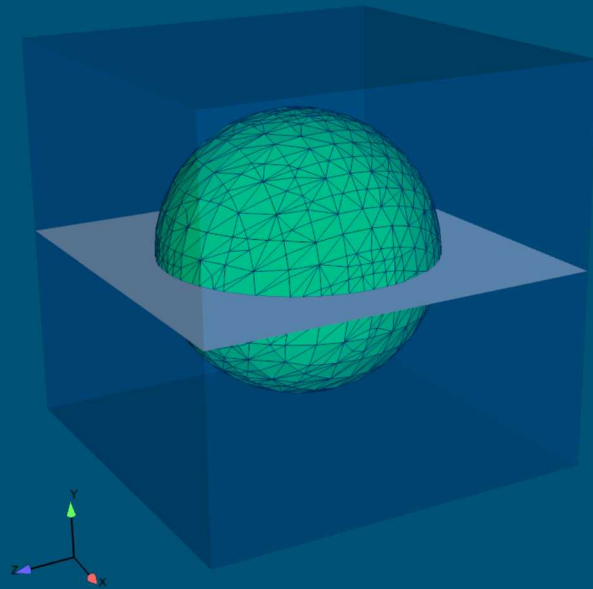
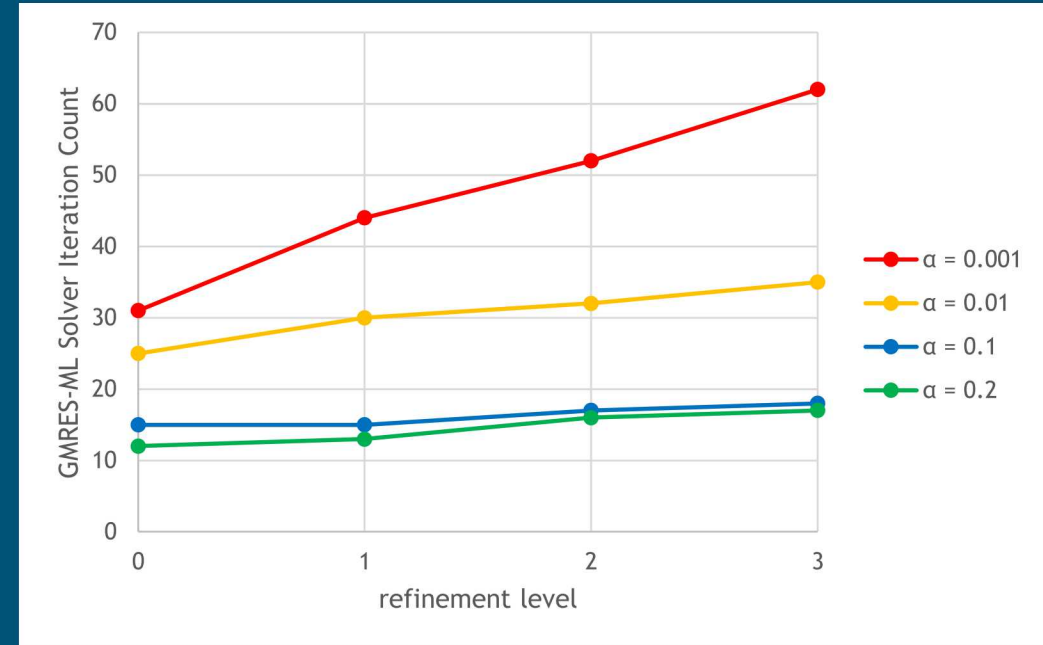


## Scalar Diffusion Problem with Weak Discontinuity

- Mimics conduction in solid with imperfect contact
- 50 realizations of randomly placed sphere to explore impact of subelement quality
- Vary edge snap tolerance from 0.001 to 0.2
- Examine maximum linear system iteration count over 50 cases

## Conclusions

- Most of improvement from snapping obtained with tolerance of 0.1



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

Temperature

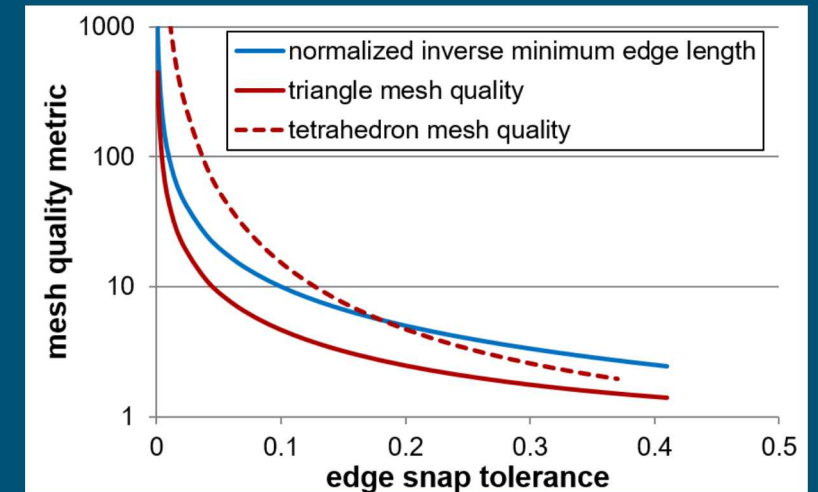
3.692e-01

2.616e-01

1.540e-01

4.643e-02

-6.117e-02



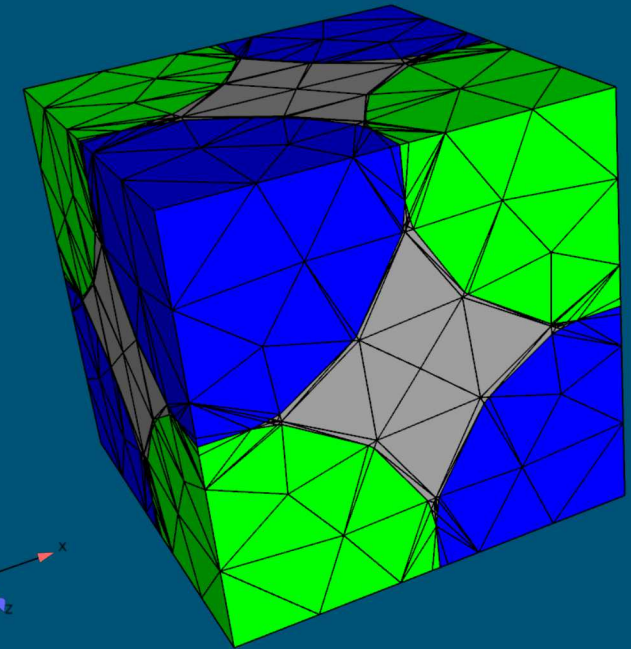
# Snap to Interface for Many Materials

## “Partial” snap methods

- Most of benefit for implicit problems even for relatively small snap tolerance ( $\sim 0.1$ )
- Naïve implementation of same strategy to multiple interfaces will create degenerate elements because edge length ratio grows with each cut

## New methods developed for “Full” snap

- CISAMR (Soghrati) showed it was possible to always snap by only considering cut location along Cartesian edges
  - For each Cartesian edge that is crossed by an interface, move the nearest node to the crossing location
- Morph (Staten) extended this concept to any geometry by snapping nodes to vertices, then to intersections between Cartesian faces and curves, then intersections between surfaces and Cartesian edges
  - Readily applicable to level set intersection points, curves, and surfaces

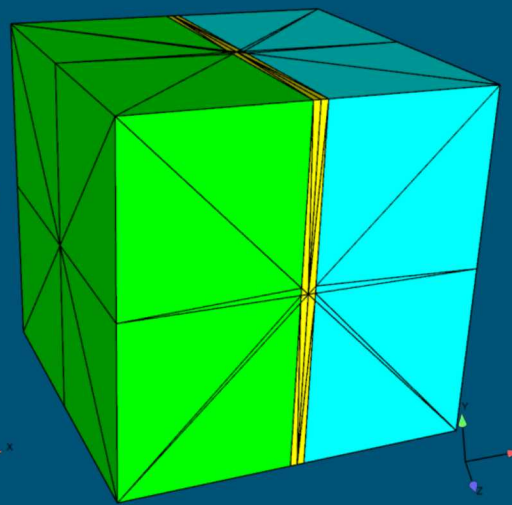




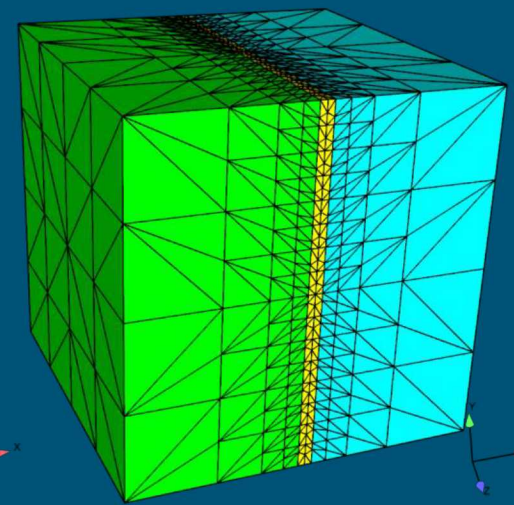
# Possible Issue With “Full” Snapping: High Aspect Ratio Elements Aren’t Always Bad

Pathology handling for “Full” snapping (interfaces too close)

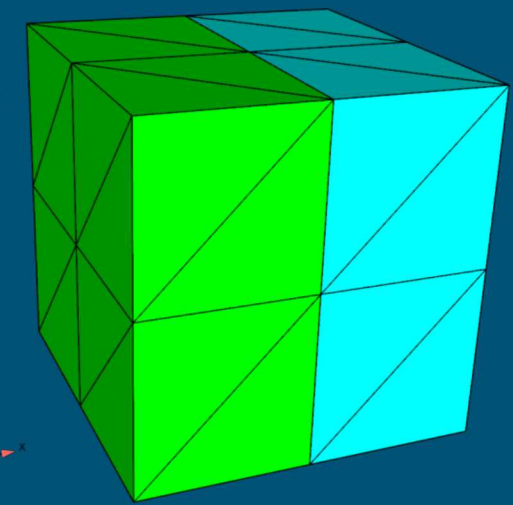
- CISAMR – adapt until unacceptable cases are resolved
- Morph – Filter intersections between geometry and background mesh such that no intersection points are within  $h/2$  of one another



CDFEM



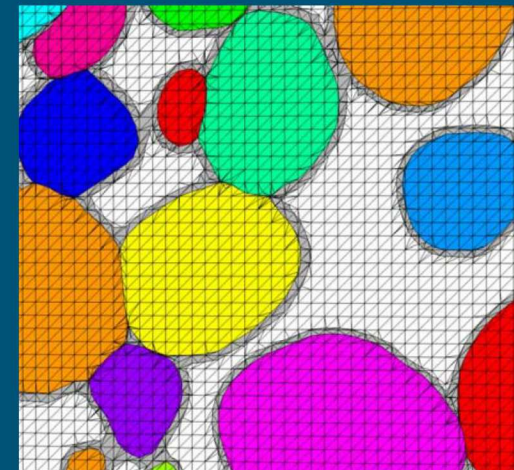
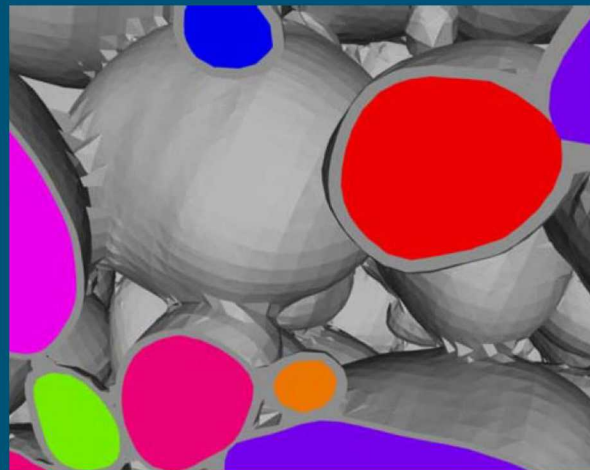
Adapt Until Resolved



Remove Unresolved Features

Resulting meshes are high quality with bounded aspect ratio

- Generally very desirable property
- Not universally desirable



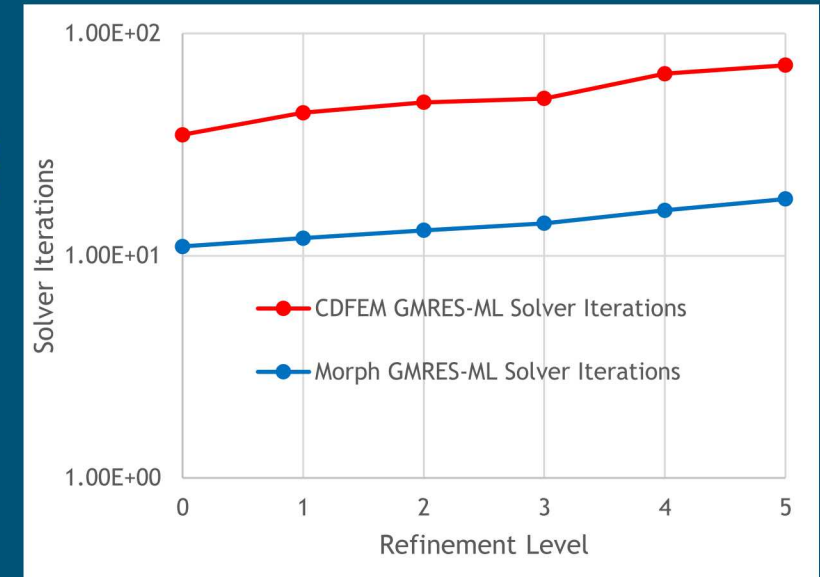
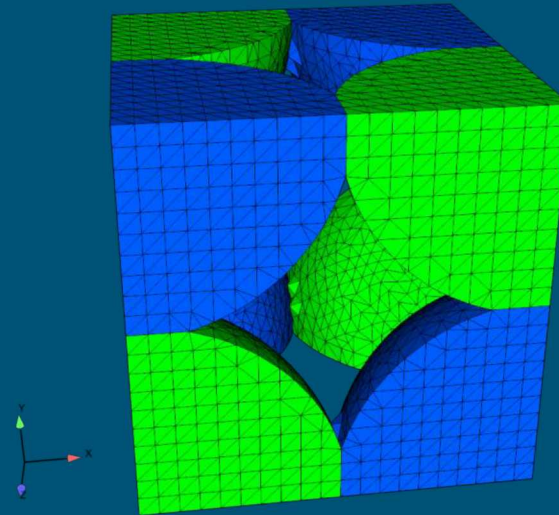
Features

# Morph for Many Materials



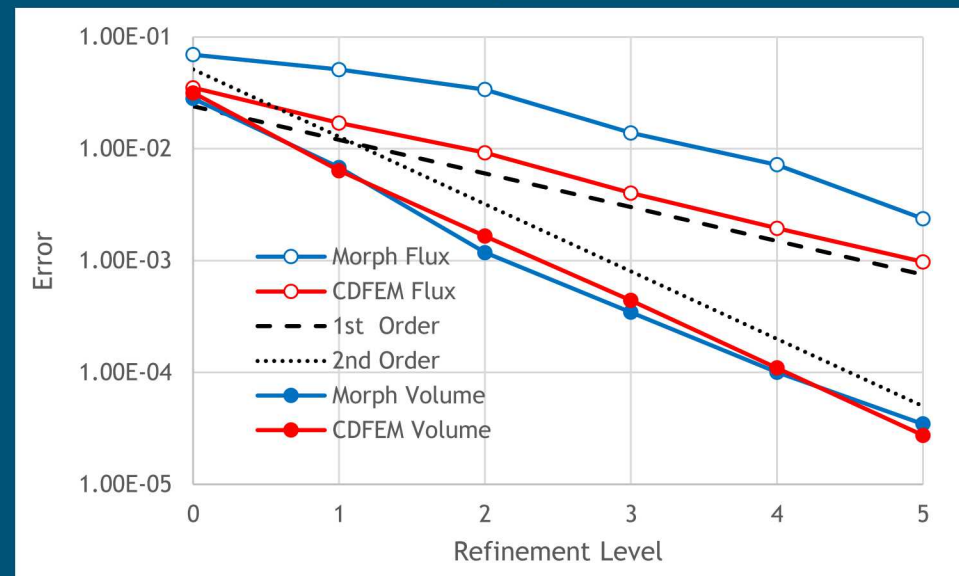
## Morph

- Presented earlier today by Matt Staten, “Parallel and Dirty CAD Tolerant Tetrahedral Mesh Generation with Feature Capture”, 14:00 - 14:20, Symposium on Trends in Unstructured Mesh Generation
- Developed for single part meshing with plans to extend to multiple parts
- Modified to handle multiple volumes with triple lines
- Produces high quality mesh
- Some additional development needed to fully support this use-case



## Results

- Good conditioning and solver iteration count obtained



# Summary/Conclusions

- Many-material problems readily described using one level set per material or phase
  - Interfaces defined by lower envelope
- CDFEM for many-material problems leads to infinitesimal edge lengths, vanishing quality, and unbounded aspect ratios
- Poor quality discretizations lead to large condition numbers and poor linear solver performance
- Snap-to-interface algorithms successfully control condition numbers and restore good linear solver performance
- Other interesting alternatives include specialized preconditioners and basis function removal
- Snap-to-interface methods produce high quality elements with low aspect ratios
  - Generally advantageous but can be highly inefficient for resolving high aspect ratio features
- Newly developed Morph capability appears amenable to many-material problems
  - Good quality, convergent, good linear solver performance

# CDFEM Discretization “Coarsening” via Linear Constraints

Coarsen the interface enrichment

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

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

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

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

