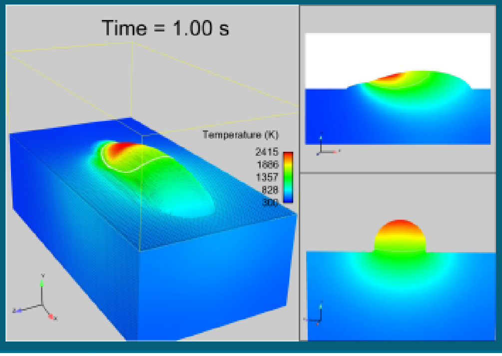
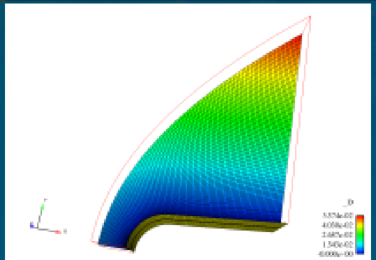
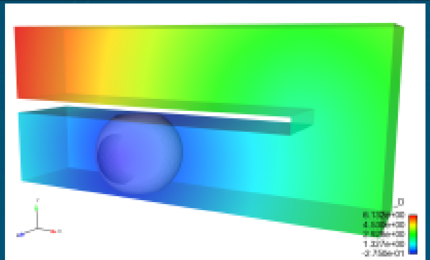
SAND2021-14881C

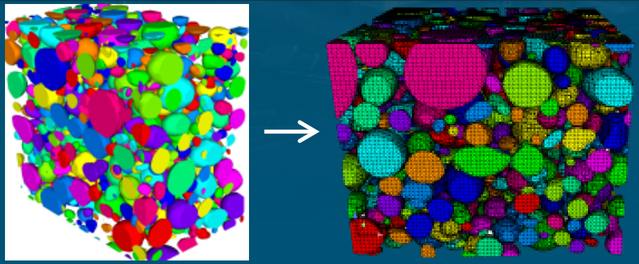
Sandia National Laboratories

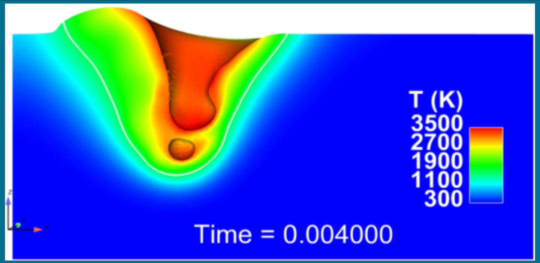
Introduction to Krino











PRESENTED BY

David R. Noble

Package Description

Level Set Toolkit

- Krino (pronunciation KREE-noe)
- Pertinent Greek definitions:
  - To separate, select, choose; To determine, resolve, decree

Authors

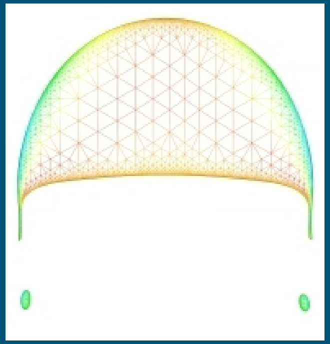
- Sandia: David Noble, Steve Bova, Victor Brunini, Alec Kucala
- External: Brad Trembacki

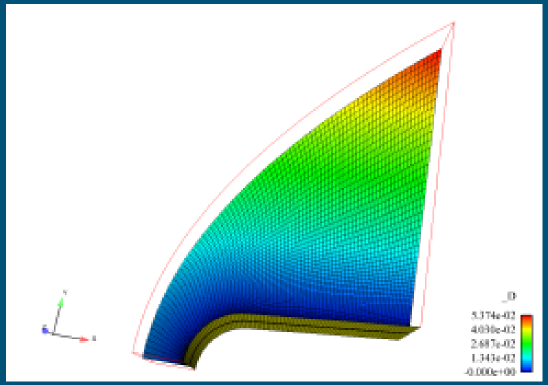
History

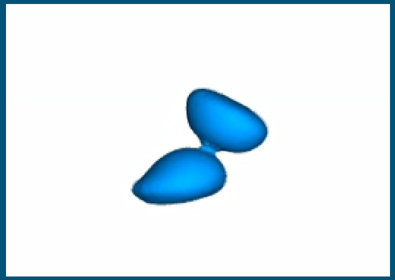
- Developed in SIERRA for more than 10 years. Like STK and Percept, primary repository remains in SIERRA
- Open sourced and added to Trilinos this year

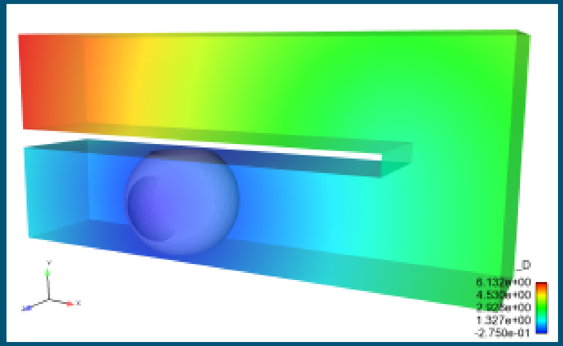
Dependencies

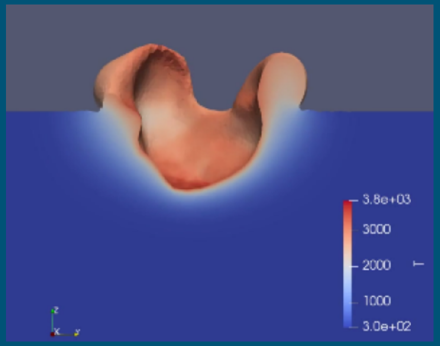
- Trilinos: STK, Percept, Intrepid, Kokkos
- TPLs: Boost, MPI, YAML (for executable)

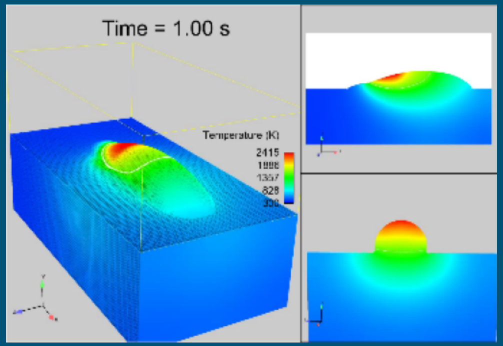












Package Components

Signed Distance Initialization

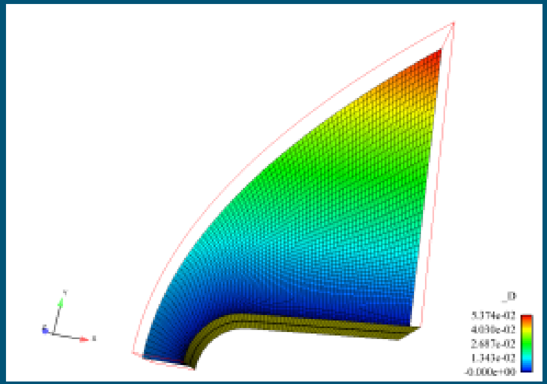
- From analytic bodies including spheres, cylinders, planes, ellipsoids
- From faceted surfaces including mesh surfaces, STLs, and level set isosurfaces

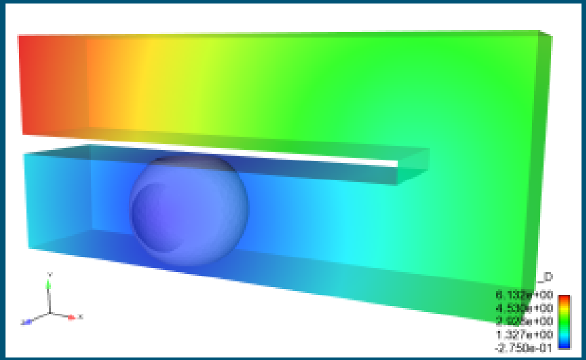
Signed Distance Reinitialization

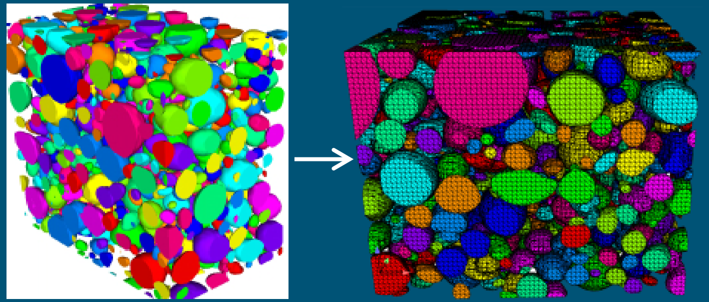
- Euclidean distance to nearest point on isosurface
- Fast marching for shortest path through the mesh (Eikonal equation solver)
  - Also supports time-of-arrival calculations for fronts that move with a speed that is only a function of location

Interface Conforming Discretizations

- Conforming decomposition finite element method (CDFEM)
- Conforming transient h-r unstructured adaptive mesh refinement (cThruAMR)







Signed Distance Initialization

Signed Distance

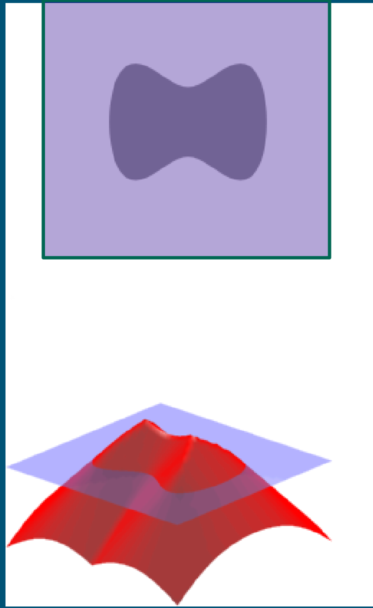
- Distance to nearest point on interface with sign convention
- Optional narrow band support for computing distance only near interfaces

Analytic Bodies

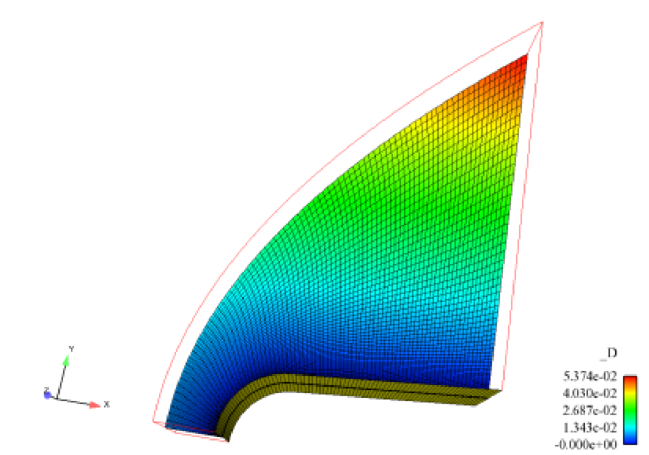
- Spheres, cylinders, planes, ellipsoids

Faceted Surfaces

- Input STL or mesh surface (sideset)
- Signed Euclidean distance to nearest point on faceted surface
- Balanced, distributed memory facet search tree used for efficiency
  - Cost O(N log(M)/p) where N is number of nodes in mesh, M is number of facets, and p is number of MPI processes
  - In worst case, all facets present on all processors
  - Narrow band limits both memory and cost



Signed distance (from Wikipedia)

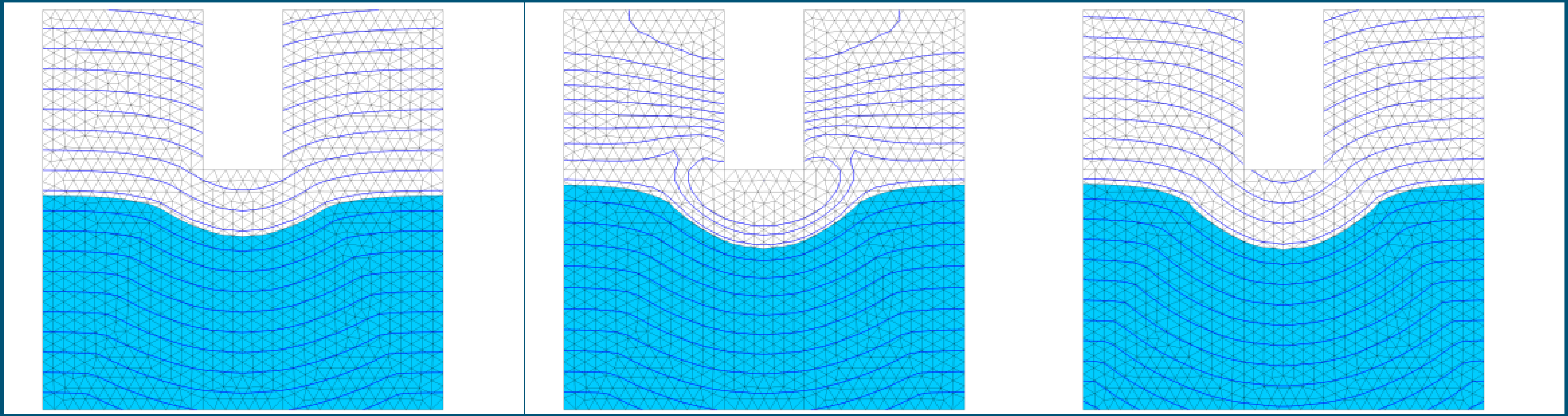


Nearest distance to wall

Signed Distance Reinitialization: Euclidean Signed Distance

Euclidean distance to nearest point on isosurface

- Isosurface is contoured into piecewise linear facets (2D or 3D)
  - Nonlinear elements are recursively decomposed into linear triangles and tetrahedra until error measure is satisfied
- Signed distance is calculated using facet tree



Level set is initialized to signed distance

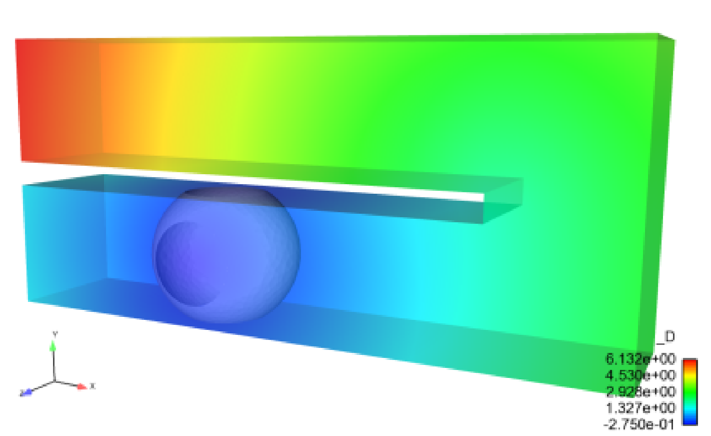
Level set is no longer signed distance due to advection

Reinitialization restores level set to signed distance

Signed Distance Reinitialization: Fast Marching

Fast Algorithm for Solving Eikonal equation, $|\nabla\varphi| = 1$

- Initialize signed distance in elements crossed by level set by scaling level set values to obtain unit gradient
- Sequential evaluation of neighboring elements with lowest signed distance
- Low O(N) cost



General form used for computing time-of-arrival, $|\nabla\varphi| = 1/f(x)$

- Front speed $f(x)$

Supported elements

- Triangles and Tetrahedra
- Anticipate Quadrilateral and Hexahedral support in FY22

Platform support

- Distributed memory via MPI (poor parallel scalability due to sequential algorithm)
- Possible Fast Iterative Method for better scalability and GPU support in FY22?

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

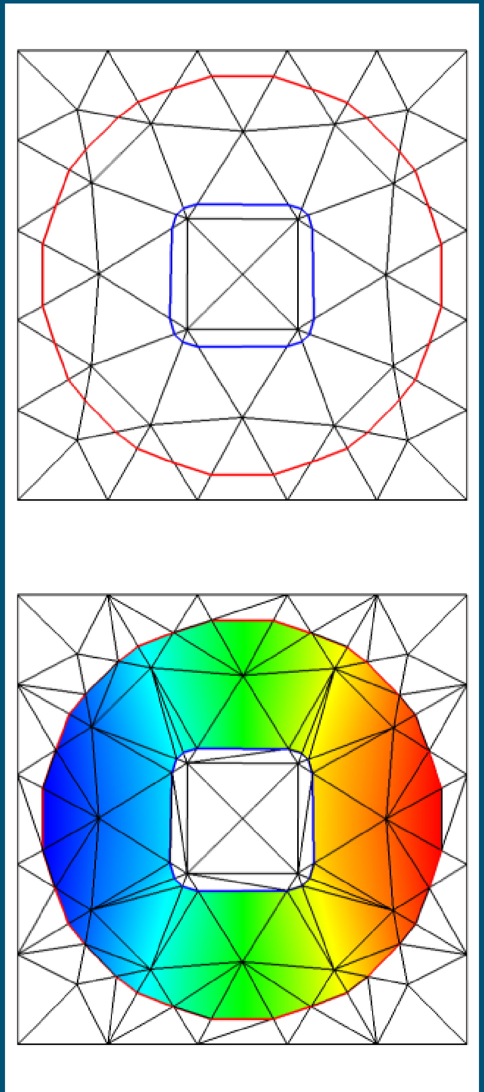
- Li et al. (2003) FEM on Cartesian Grid with Added Nodes
- Interface enriched finite element methods: IGFEM, HIFEM (Soghrati, et al. 2012), DE-FEM (Aragon and Simone, 2017)
- XFEM toolkit (XTK), Maute et al. CU Boulder – Generate conformal sub-elements for XFEM integration

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

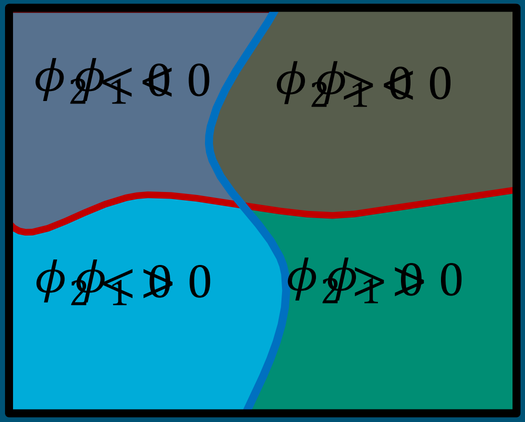
- Similar to finite element adaptivity
- Uses standard finite element assembly including data structures, interpolation, quadrature
- **CDFEM is Conformal Transient Unstructured h-adaptivity**

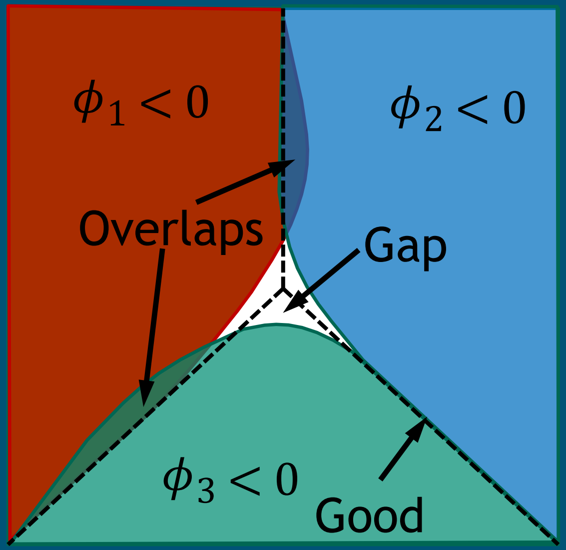


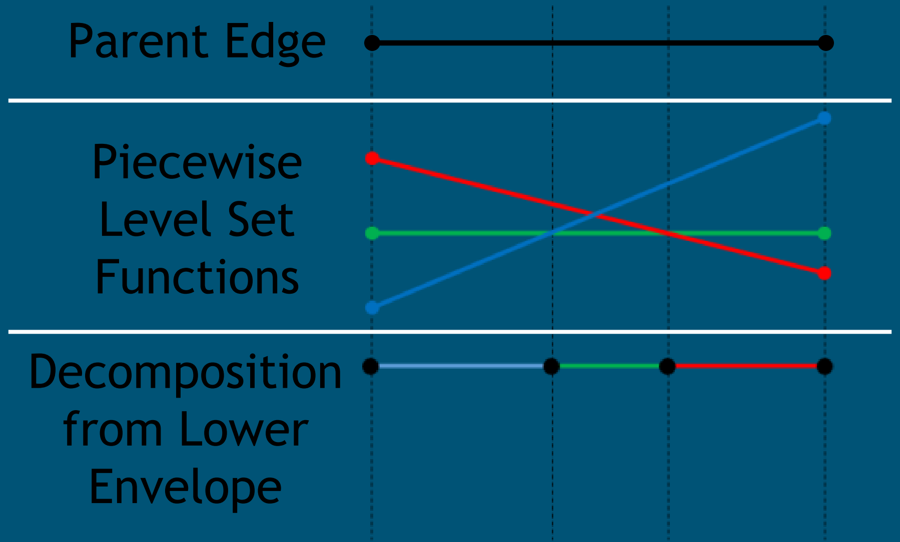
Interface Conforming Discretizations: Interface Definition for Many Materials

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
- One 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
  - Remedy: Use lower envelope to uniquely define behavior in gaps and overlaps
    - A point is material i if $\phi_i < \phi_j \; \forall \, j \neq i$



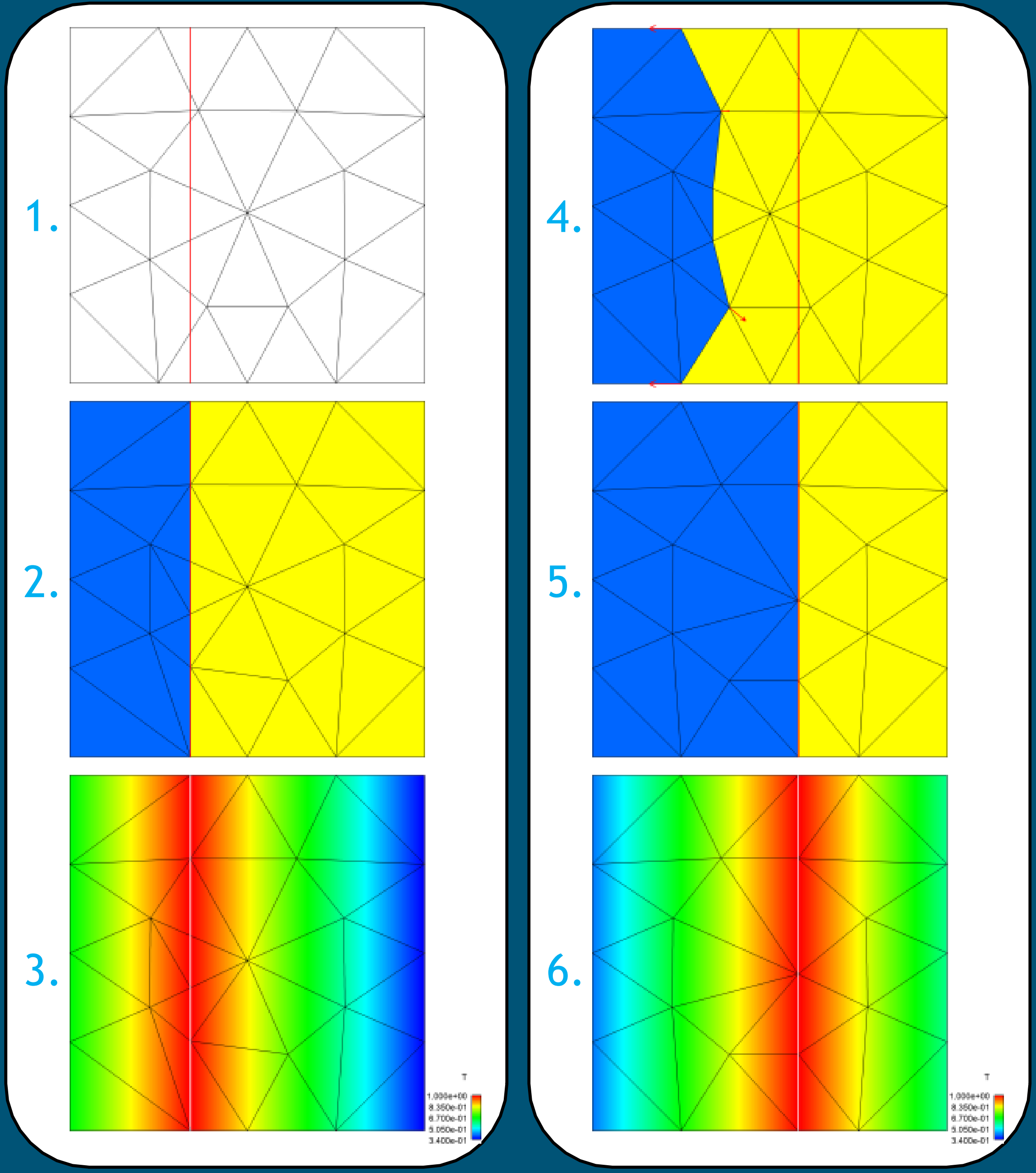




Interface Conforming Discretizations: cThruAMR

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

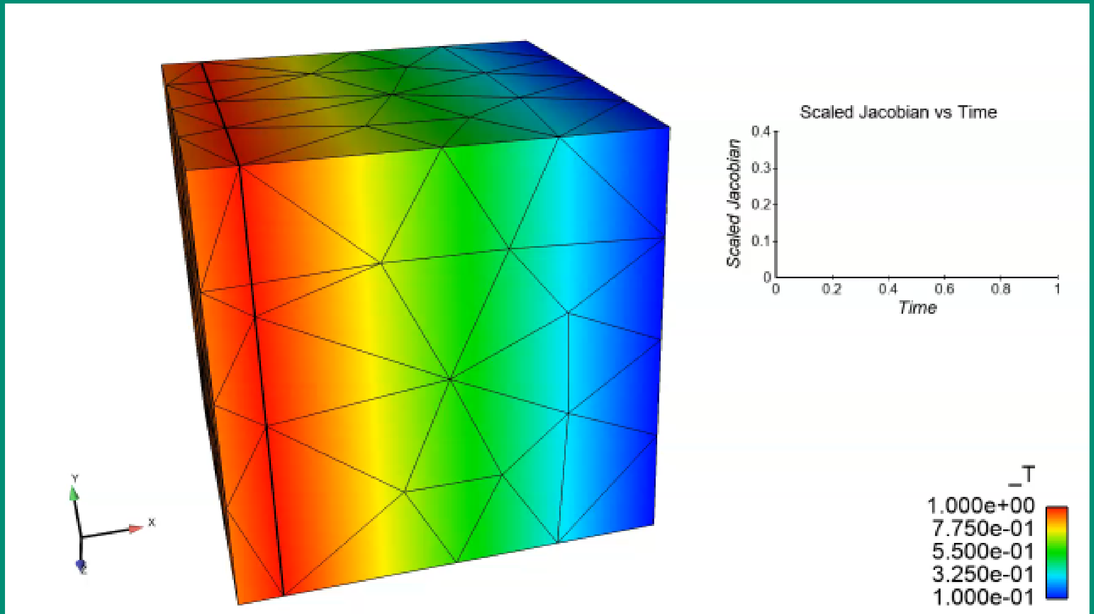
1. Initialize level sets on input mesh (Krino)
2. Create conforming mesh by snapping and cutting (Krino)
   - Snap whenever quality is higher than cutting quality
3. Initialize physics on conforming mesh (Aria)
4. Advect level sets while "reversing" snap displacements (Aria)
5. Create new conforming mesh by snapping and cutting (Krino)
   - Physical variables and mesh velocity calculated for interface nodes and nodes that have changed material by finding the nearest point on the old interface
6. Solve physics on conforming mesh (Aria)
   - Includes moving mesh velocity term



Development and Verification of cThruAMR

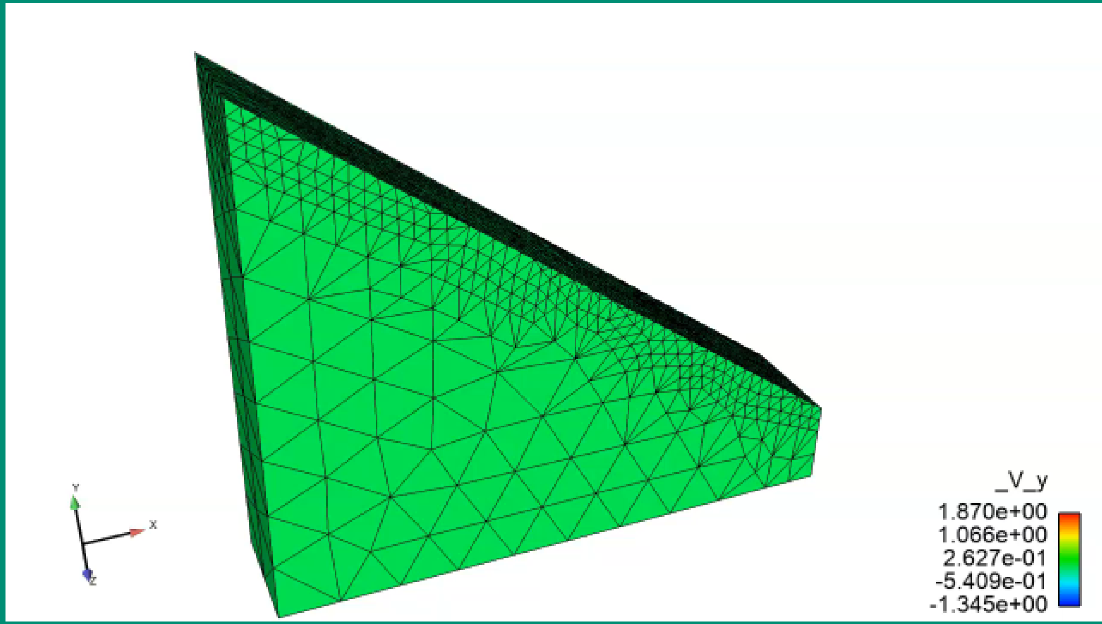
Patch Test: Pure Advection of Slope Discontinuity

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



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

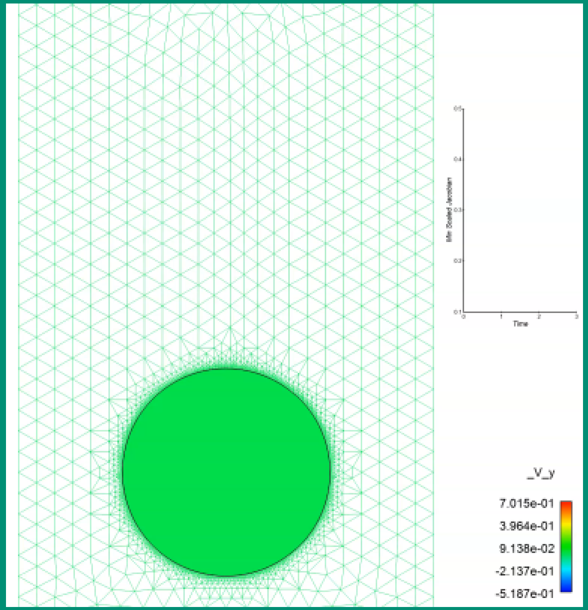
- Multiple levels of non-conformal refinement followed by h-r conformal refinement (cThruAMR)

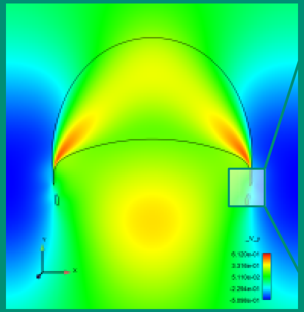


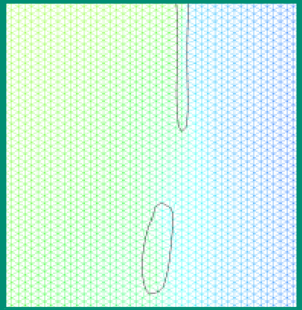
Rising Bubble Problems

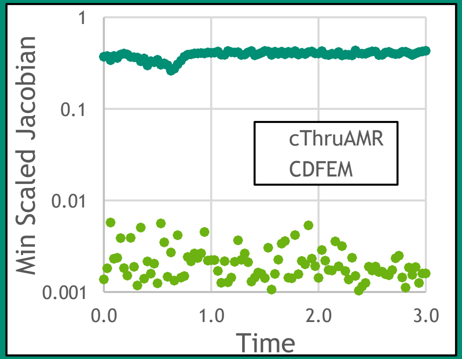
Problem: 2D Rising bubble

- 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



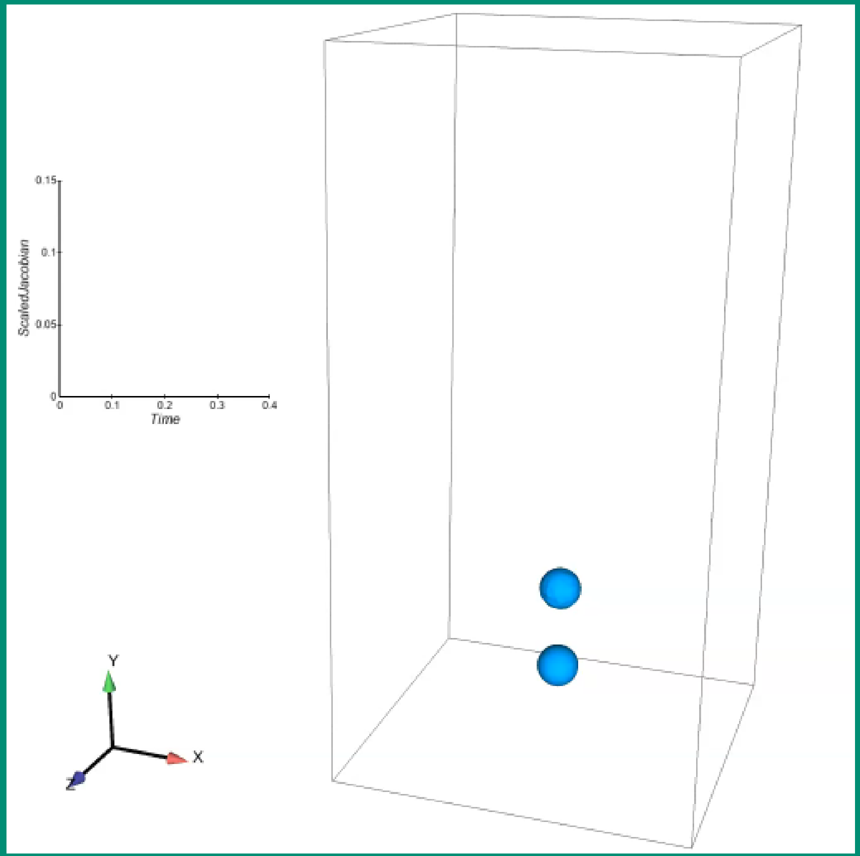






Problem: 3D Rising, merging bubbles

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



Conclusions

- New package Krino for signed distance initialization/reinitialization and interface conforming discretizations

- Ongoing work
  - Additional element support for fast marching methods
  - GPU-friendly algorithms including Fast Iterative Methods?
  - Improved quality interface conforming discretizations

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