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Automatic Ordering for Volume-of-Fluid Interface Reconstruction in Multi-material Elements

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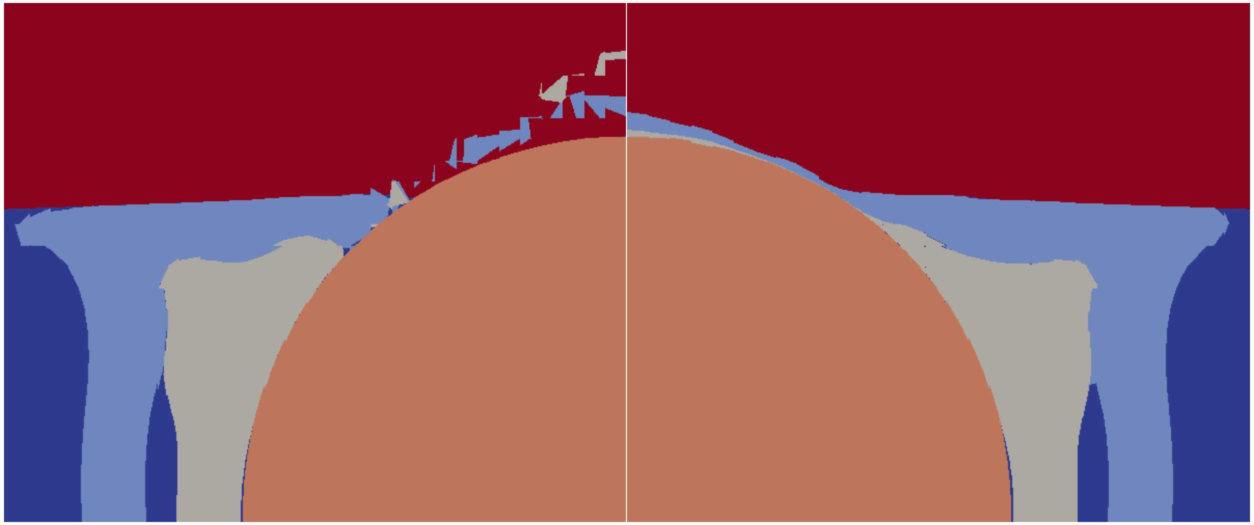
The XFEM in ALEGRA

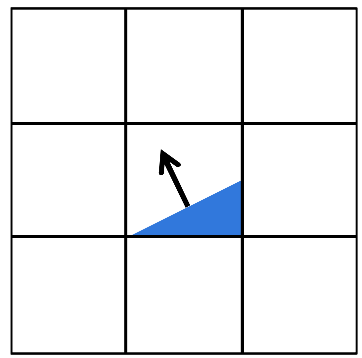
- ALEGRA: multiphysics Arbitrary Lagrangian-Eulerian simulation software developed at Sandia
- The eXtended Finite Element Method for material interfaces:
  - Enrichment of velocity field for each material
  - Effectively an adaptive refinement technique: material interfaces are resolved in multi-material elements, avoiding mixed-material models
- XFEM demands accurate interface reconstruction



Interface Reconstruction

- Youngs' Method for interface reconstruction (1982):
  - Volume-of-fluid method: discretely mass conserving
  - *Only data available for reconstruction are the volume fractions*
  - Interface normal computed from gradient of volume fraction

0.0	0.0	0.0
0.0	0.4	0.8
0.8	1.0	1.0

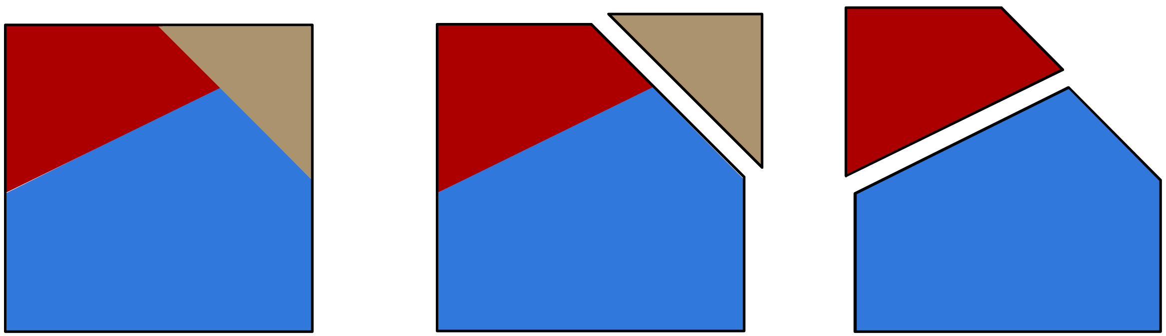


$$\mathbf{n} = -\nabla V$$

  - For more than two materials, an ordering is required
- ALEGRA has no infrastructure for tracking local (sub-element) material centroids

Pattern Interface Reconstruction

- Youngs' method extended to allow intersecting and terminating interfaces by selective gradient calculation (Mosso & coworkers)
- Interfaces cut from arbitrary polygons/polyhedra



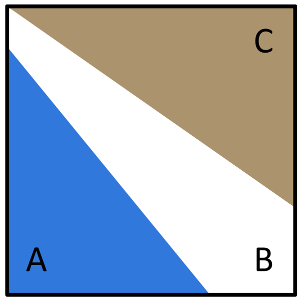
Mixed Element   Tan/(Red+Blue)   Red/Blue

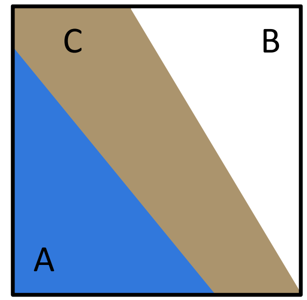
- Second-order accurate with smoothing
- Enables XFEM in ALEGRA, but not exclusive to it

The Ordering Problem

- A-B-C or A-C-B? Accumulate volume fractions?
  - Each interface is computed from an A | not A proposition

$$\mathbf{n}_A = -\nabla V_A$$
$$\mathbf{n}_B = -\nabla (V_A + V_B) = \nabla V_C$$





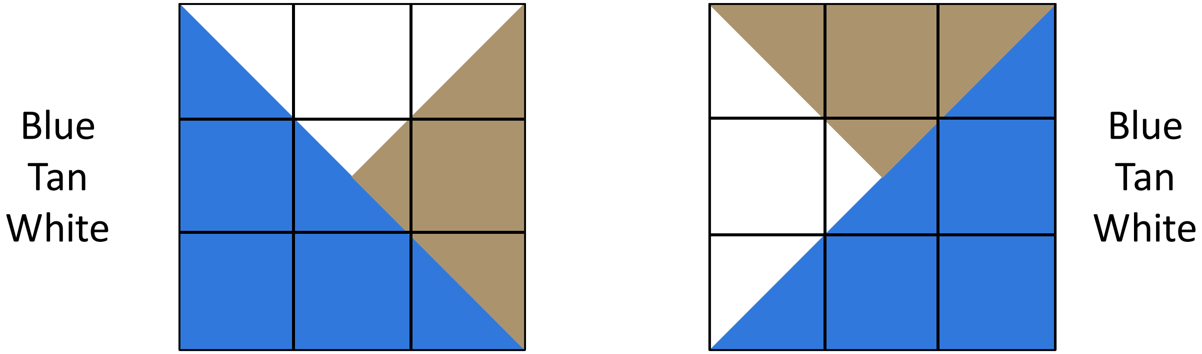
$$\mathbf{n}_A = -\nabla V_A$$
$$\mathbf{n}_C = -\nabla (V_A + V_C) = \nabla V_B$$

- For *N* materials, there are (*N*-2)*N*! ordering combinations
  - Quickly becomes burdensome for users running complex problems

Manual Ordering	Automatic Ordering
Specified by user	No *a priori* input required
Global material ordering	Local material ordering
Static	Dynamic

Ordering Algorithm

- Automatic ordering: Mosso & Clancy (1994), Benson (1998)
  - Sijoy & Chaturvedi (2010) combined these for similar approach
  - Our method handles PIR interfaces, extended to 3-D
- Critical that ordering should be grid-independent
  - Given interface should yield the same ordering regardless of frame

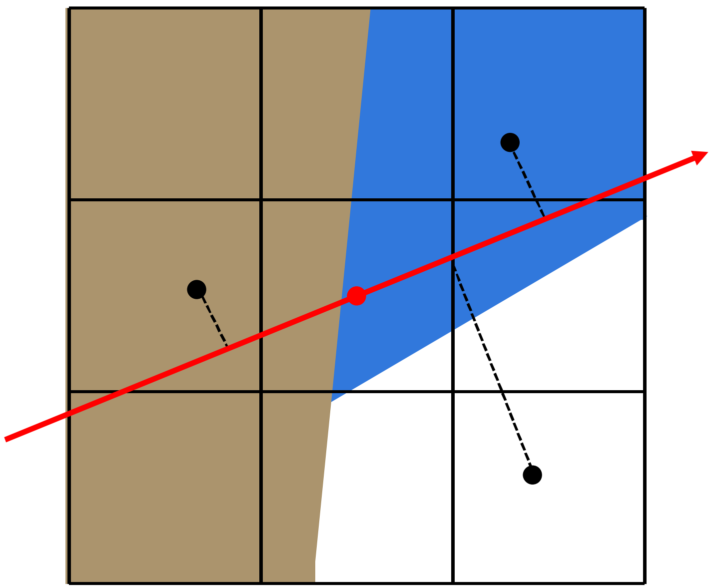


- Requires perpendicular-distance least squares regression
- Use local material position approximation

Algorithm (2-D)

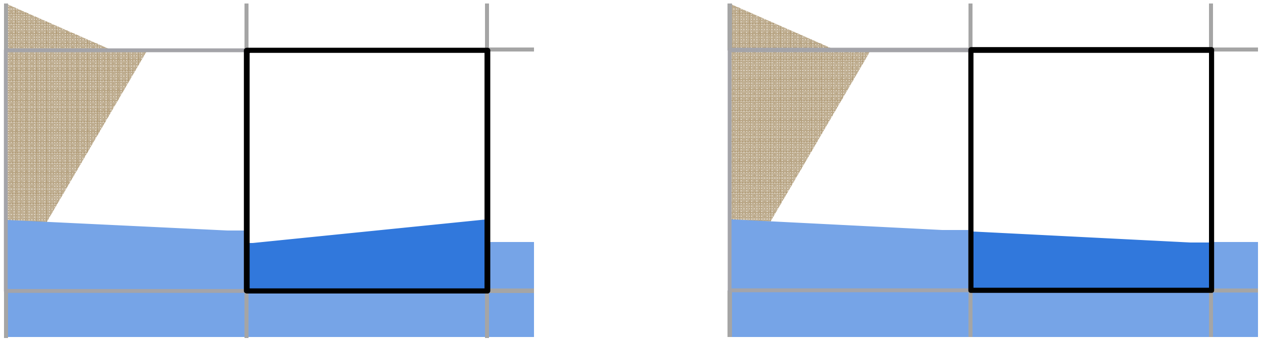
1. Calculate local material centroid approximations
   - Approximate materials as located at centroid of each neighbor
2. Fit a line to the centroids
   - Volume-fraction weighted least squares fit
   - Perpendicular distance regression for grid independence
3. Define ordering by distances along line of projected material centroids
   - Choice of ordering direction: material closest to the line determines direction
4. For certain cases, modify ordering or gradient to improve interfaces
   - Choice of gradient approximation:

     $-\nabla V_f$ or $-\nabla\left(\sum V_f\right)$



Ordering ‘Fixes’ (1)

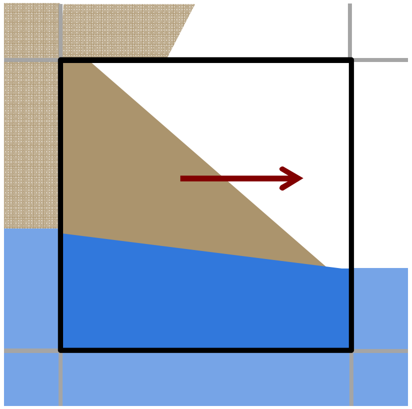
- Identify candidates by regression quality indicator
- Effectively a low-order smoothing: improving gradients
- Ordering direction choice:
  - Largest volume material usually closest to the line, ordered first
  - Can be distorted by appearance of another material in neighborhood
  - Compute centroid of the complement of each candidate material and compare distances from original regression line



White/(Tan)/Blue vs. Blue/(Tan)/White

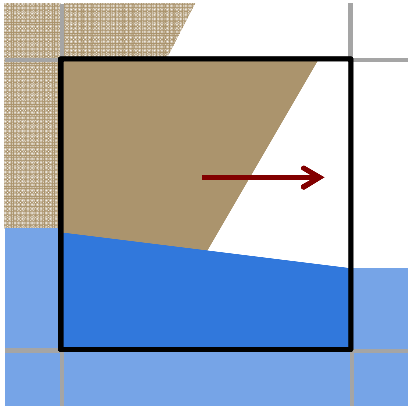
Ordering 'Fixes' (2)

- PIR allows for intersecting interfaces: T-intersections
  - Angle of intersection depends on gradient calculation choice
- Gradient choice at T-intersections:
  - Usually accumulation is best for the second material (e.g., layers)
  - Terminating interface may be 'better' without accumulation: when T-intersection is identified, compute both interfaces
  - Choose the interface that better suits the neighborhood



Blue/Blue+Tan

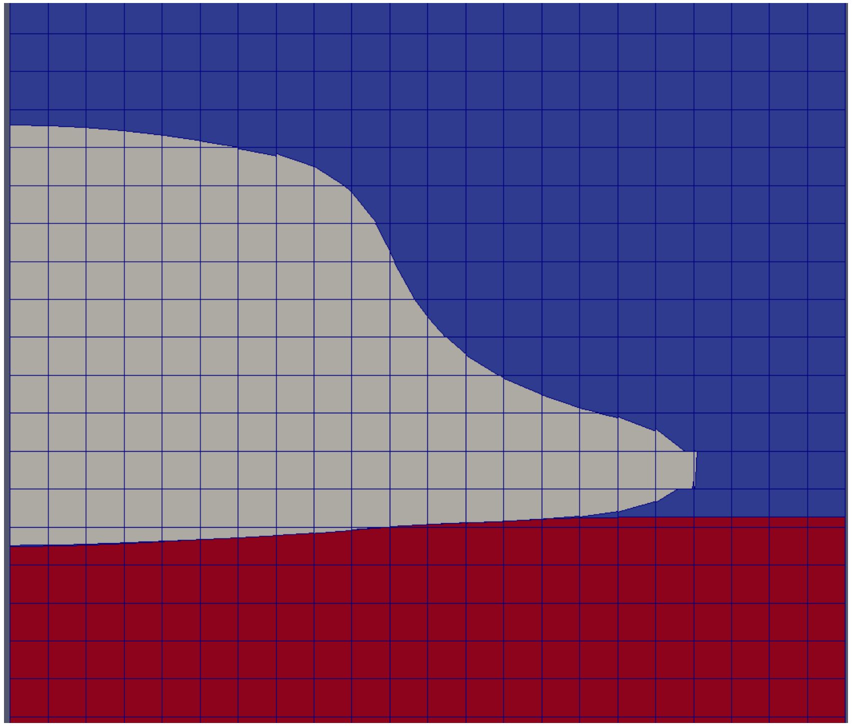
vs.



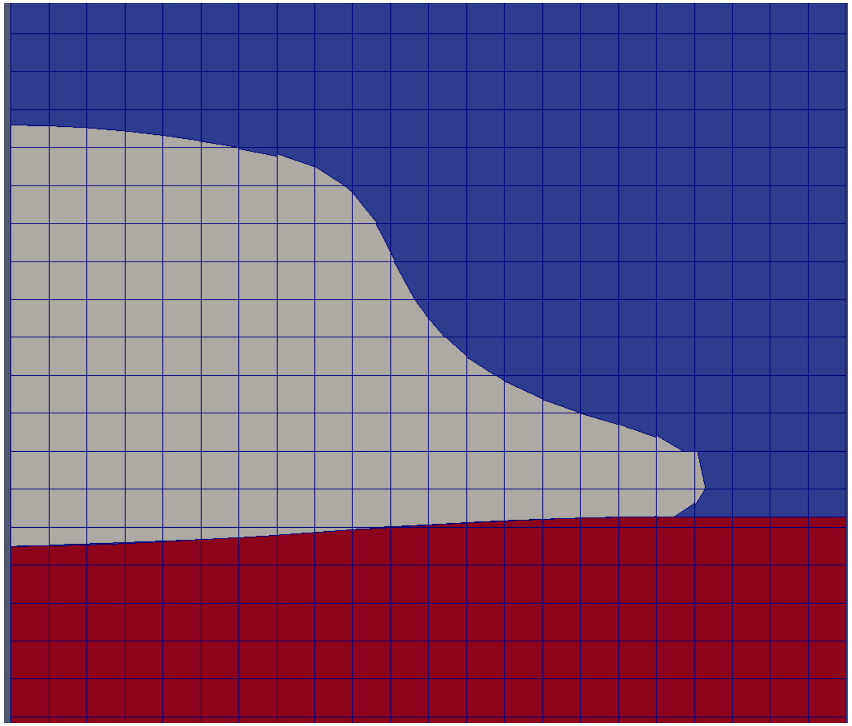
Blue/Tan

Demonstration Problem

- Low-resolution block impacting a wall, Eulerian XFEM
  - Manual ordering gives ‘reference’ solution [not converged]



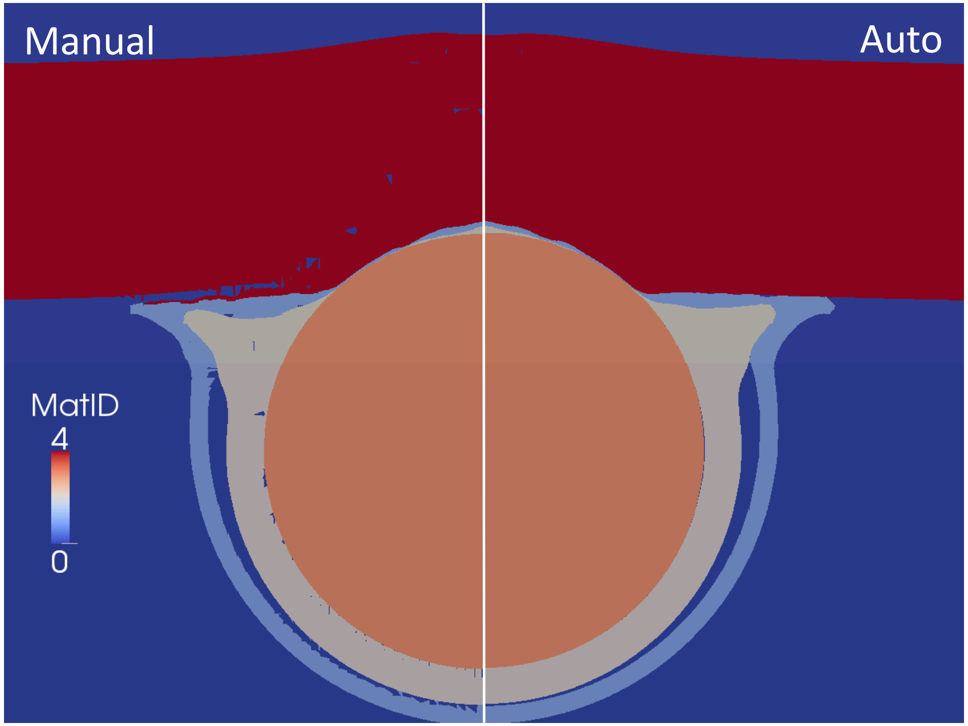
Automatic Ordering



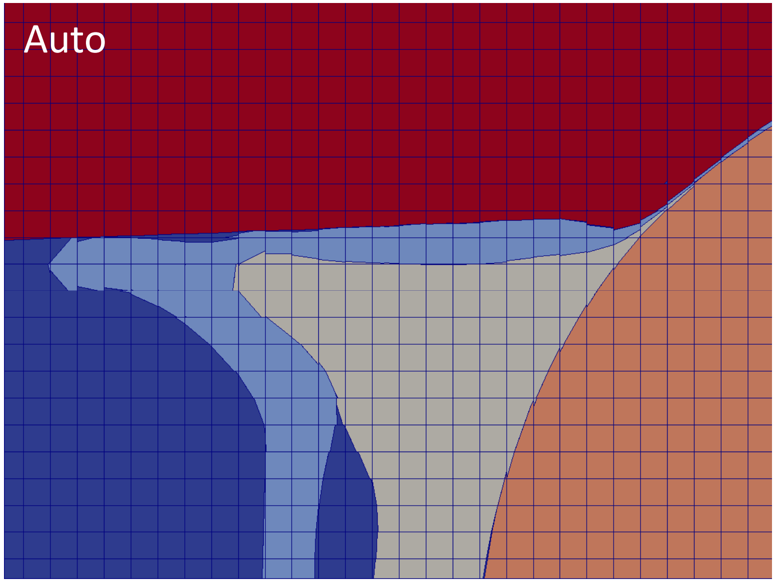
Manual Ordering

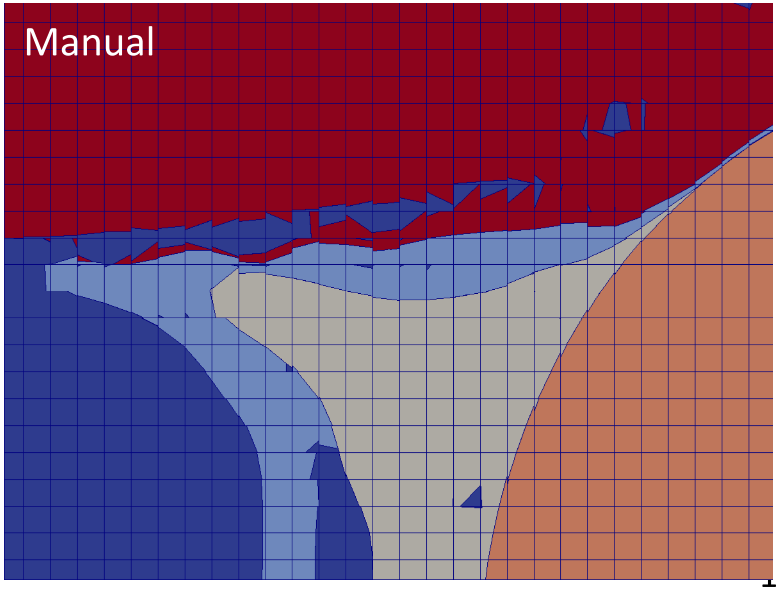
A Contrived Example

- Nested spheres striking a plate
- 4 materials + void



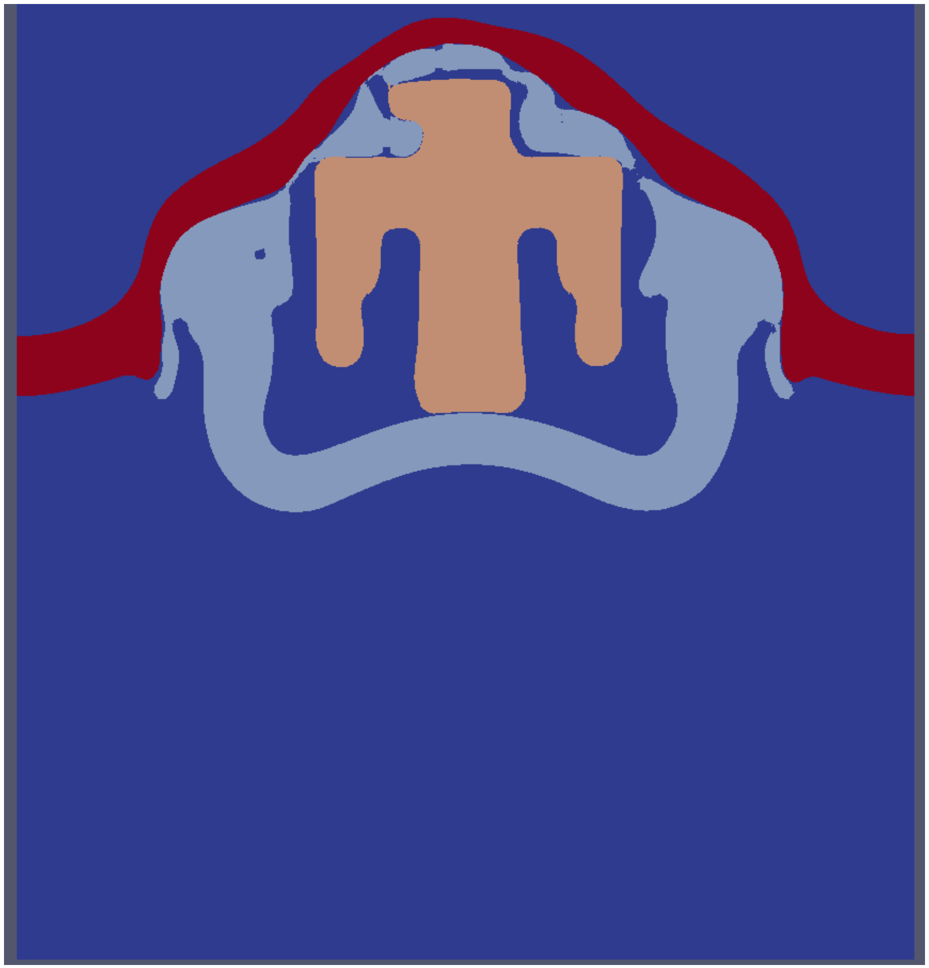
V_{impact} = 427 m/s

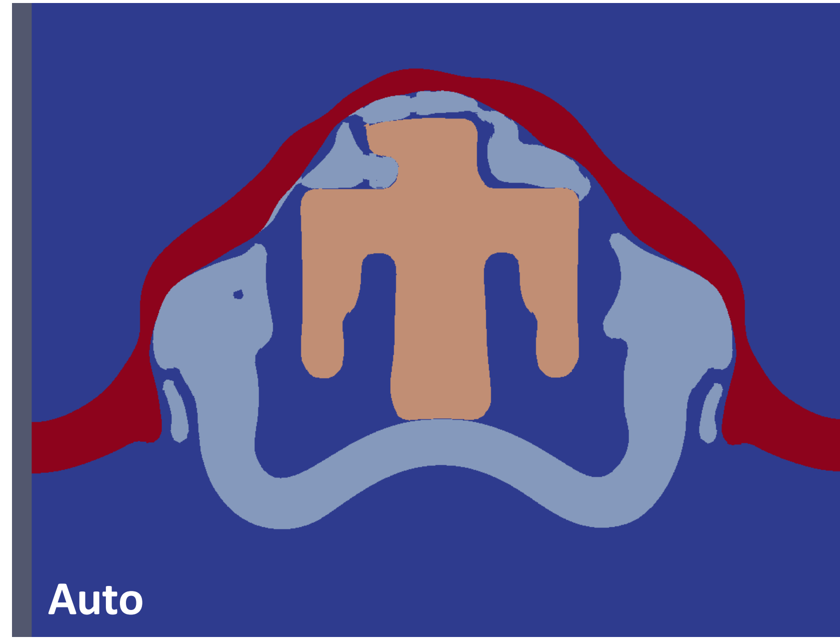


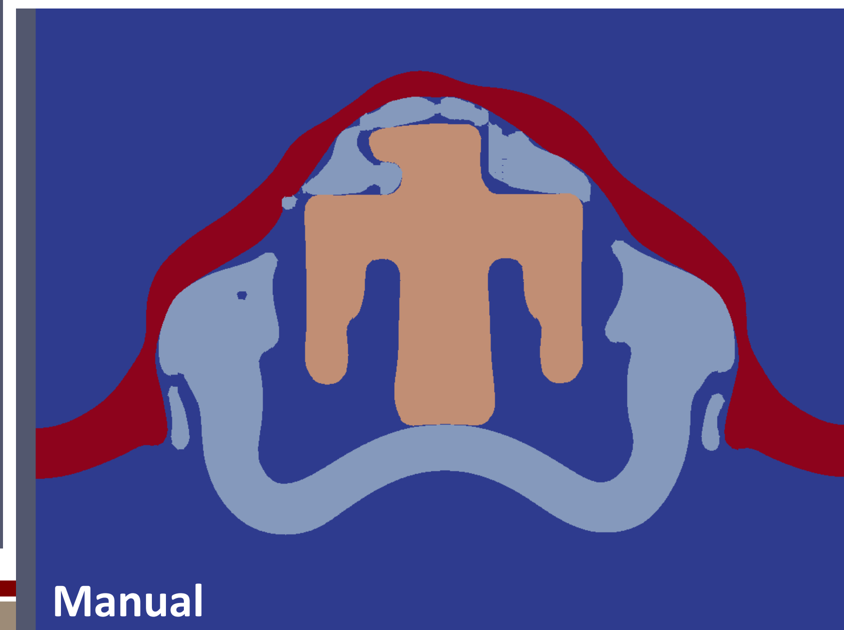


Another Example

- Plate impact at 800 m/s

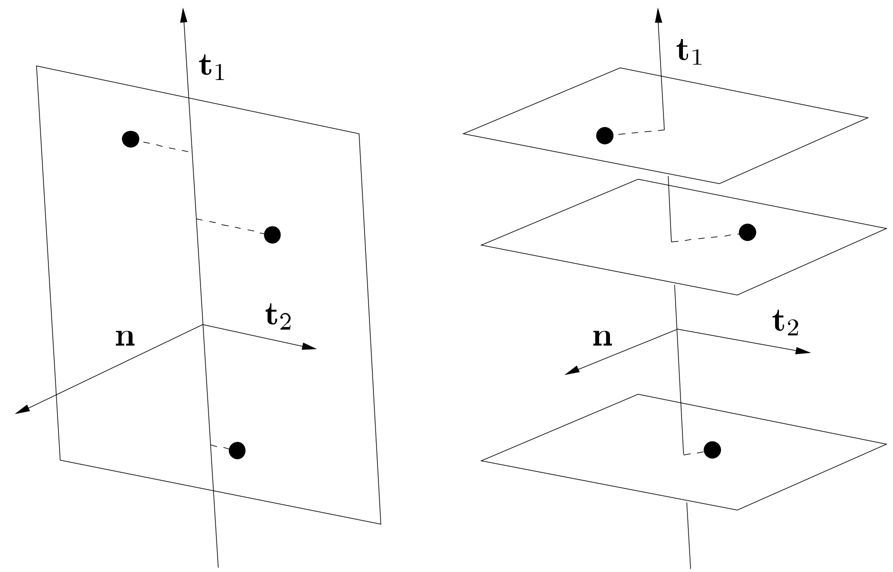






Extension to 3-D

- Need an ordering direction: start by fitting a basis
  - Error equation: normal of the plane
  - Residual equation: tangential direction
- Extreme points coincide to define the basis directions

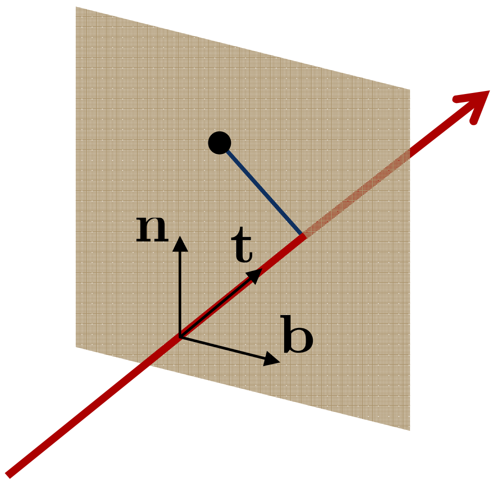


$$\mathrm{SSE} = \sum_{m=1}^{M} w_m \left[(x_m - \hat{x}_m)^2 + (y_m - \hat{y}_m)^2 + (z_m - \hat{z}_m)^2 \right] = R_{\mathbf{n}}$$

$$\mathrm{SSR} = \sum_{m=1}^{M} w_m \left[(\hat{x}_m - \bar{x})^2 + (\hat{y}_m - \bar{y})^2 + (\hat{z}_m - \bar{z})^2 \right] = R_{\mathbf{t}}$$

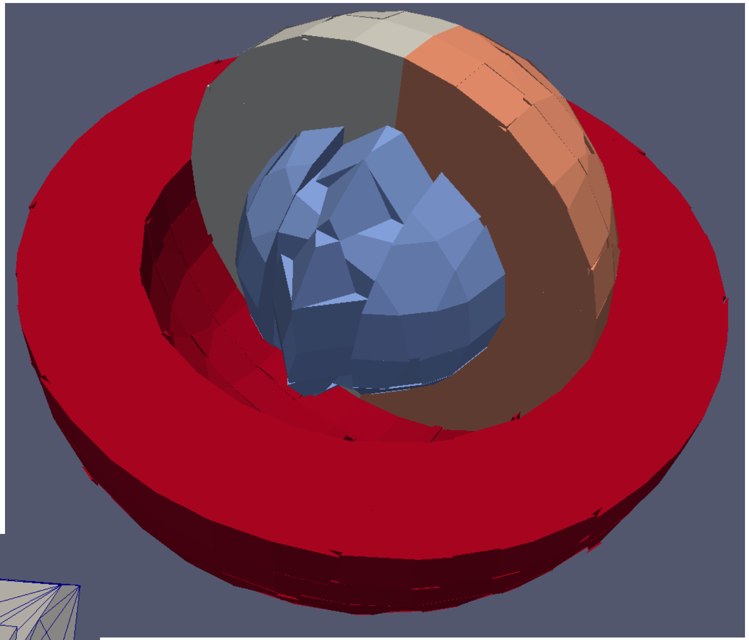
Algorithm (3-D)

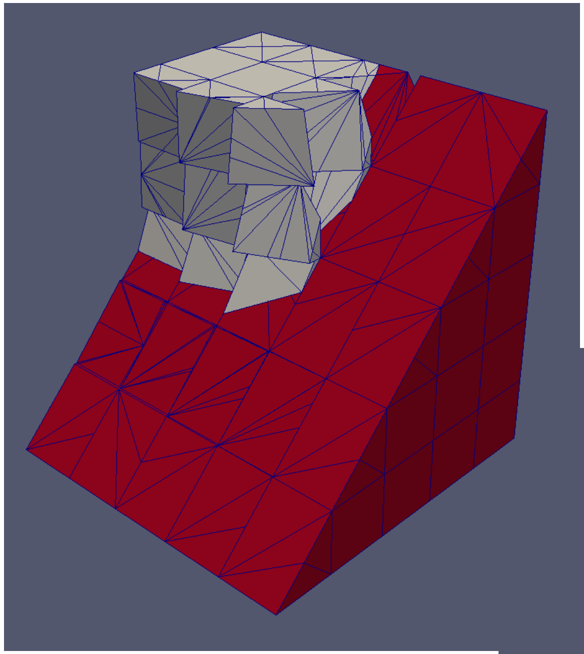
1. Calculate local material centroid approximations
2. Fit a basis to the centroids
   - Newton method for initial solution, then complete the basis
   - Fail-safe sequence to ensure a solution is found
3. Identify tangential direction (ordering line)
4. Define ordering by distances along line of projected material centroids
   - Same logic as 2-D, based on distance projected on the intersection plane
5. Check for ordering overrides (as in 2-D)
   - Switch ordering if necessary
   - Check gradients at T-intersections

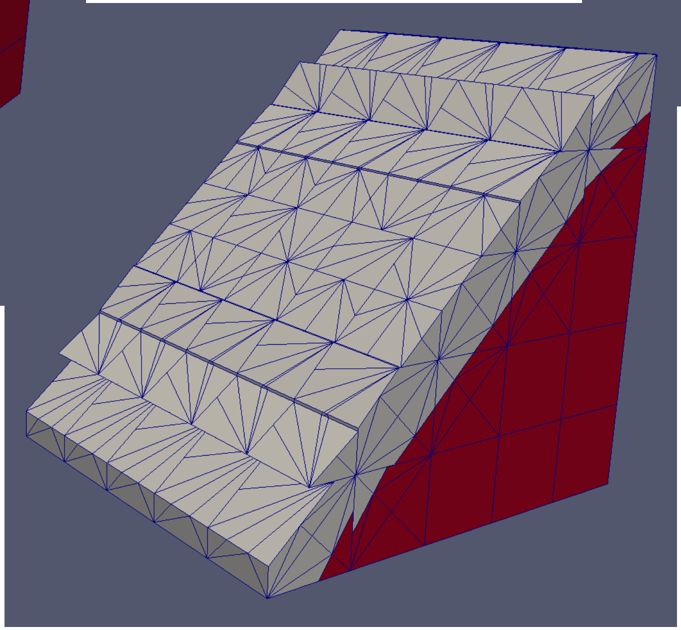


3-D Demonstrations

- Verification tests

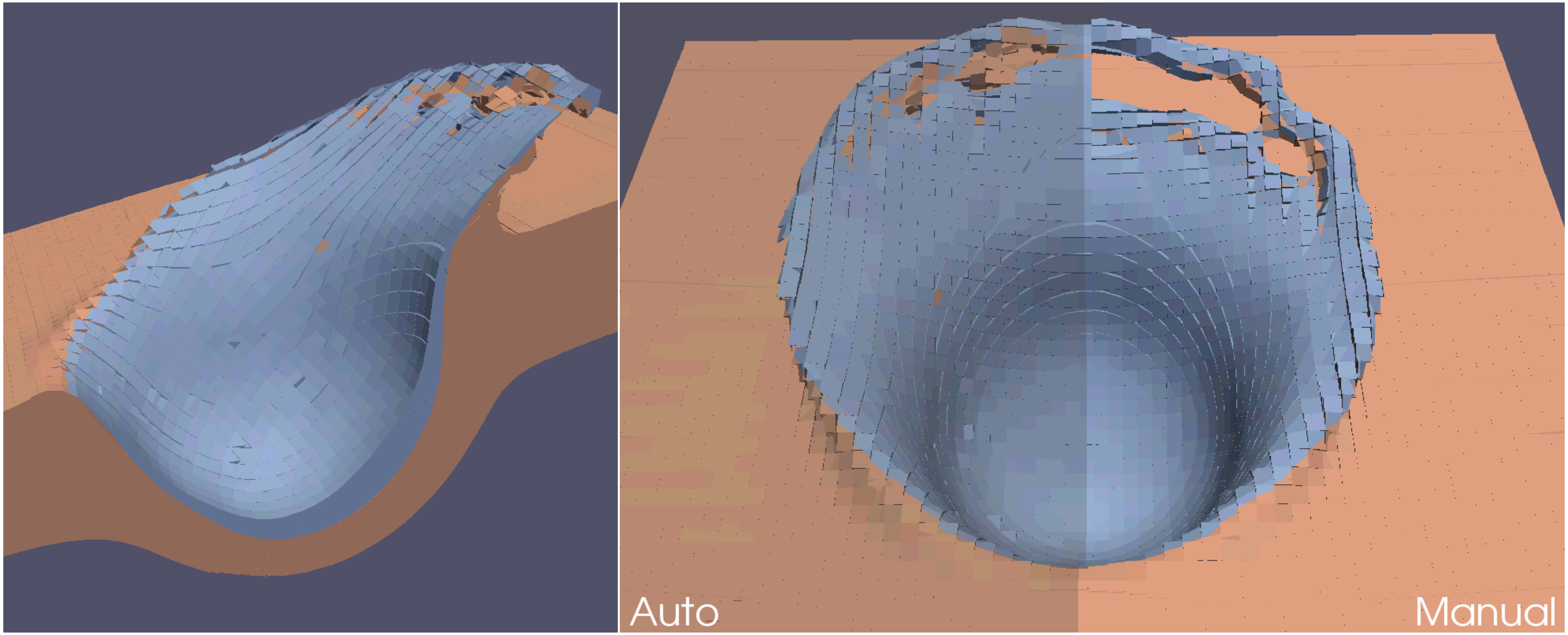






3-D Examples

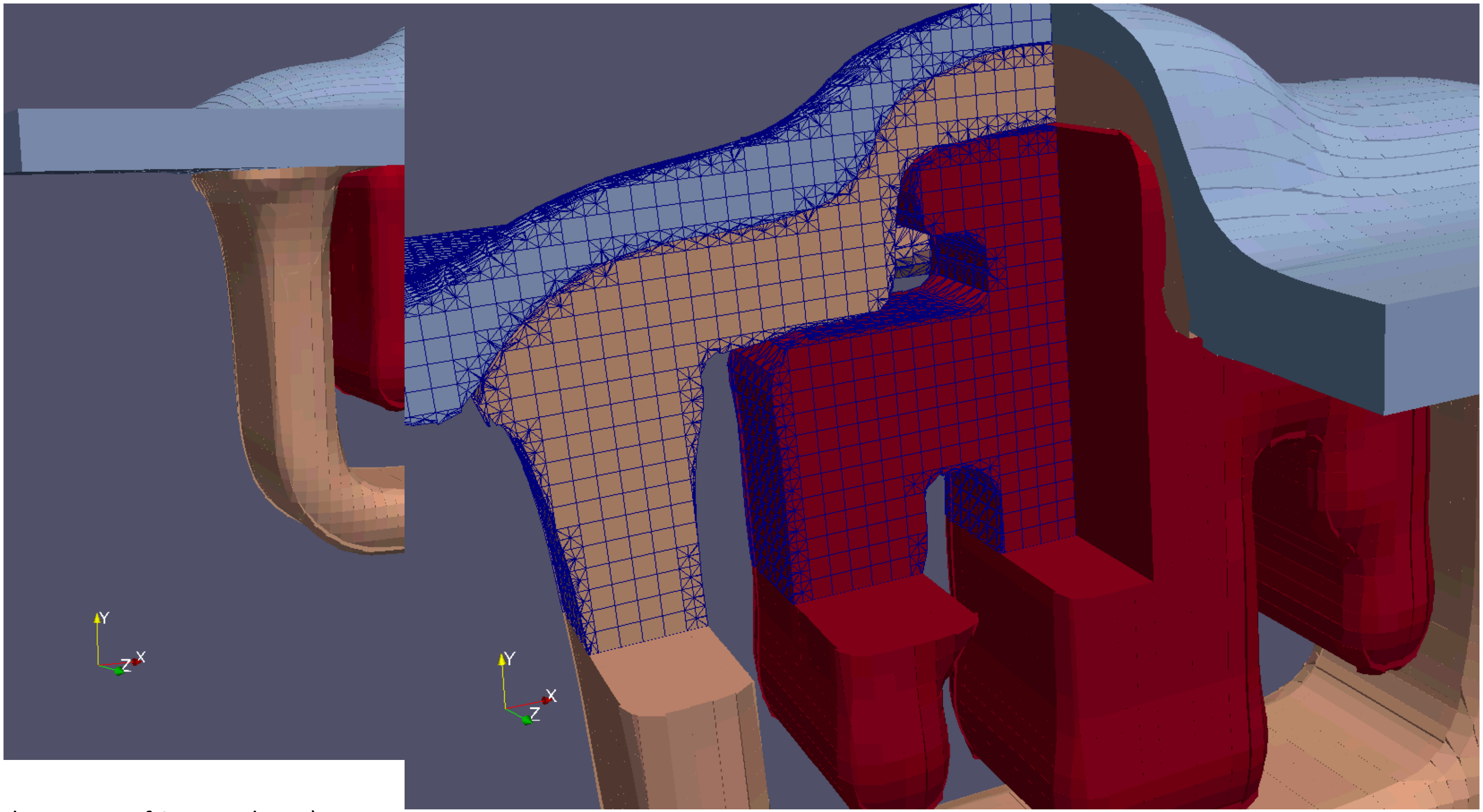
- Whipple shield: sphere impacting plate in air



- An enabling feature for 3-D Eulerian XFEM in ALEGRA

3-D Examples

- Plate impact at 750 m/s (3-D Eulerian, without XFEM)



(Model courtesy of Scott Roberts)