SAND2013-5496C

Exceptional service in the national interest

Sandia National Laboratories

Automatic Volume-Tracking Reconstruction of Interfaces in Multi-material Elements

R. M. J. Kramer and S. J. Mosso

Sandia National Laboratories, Albuquerque, NM

July 23, 2013

U.S. DEPARTMENT OF ENERGY

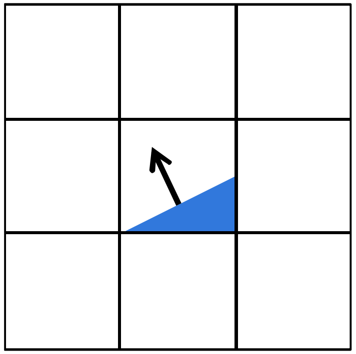
NNSA National Nuclear Security Administration

Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

Interface Reconstruction

- Young's 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

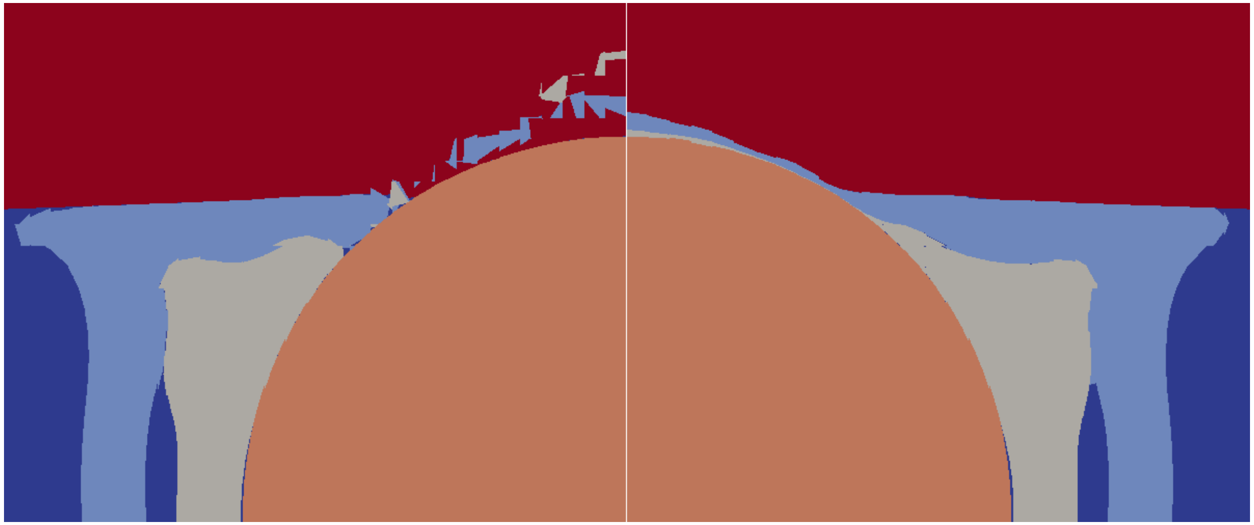


$$\mathbf{n} = -\nabla V$$

  - For more than two materials, an ordering is required
- Extended to allow intersecting and terminating interfaces by selective gradient calculation (Mosso & coworkers)
  - Pattern Interface Reconstruction (PIR)

The XFEM in ALEGRA

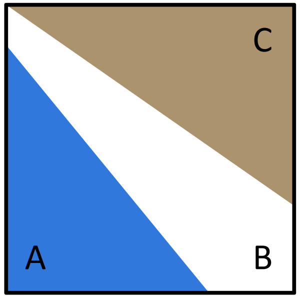
- ALEGRA: multiphysics Arbitrary Lagrangian-Eulerian simulation software developed at Sandia
- The eXtended Finite Element Method for material interfaces:
  - Enrichment of velocity field for each material
  - Effectively an adaptive refinement technique: material interfaces are resolved in multi-material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

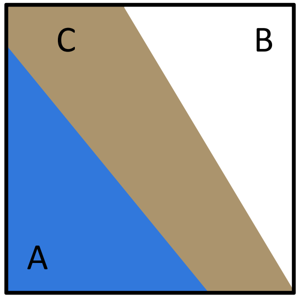


The Ordering Problem

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

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





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

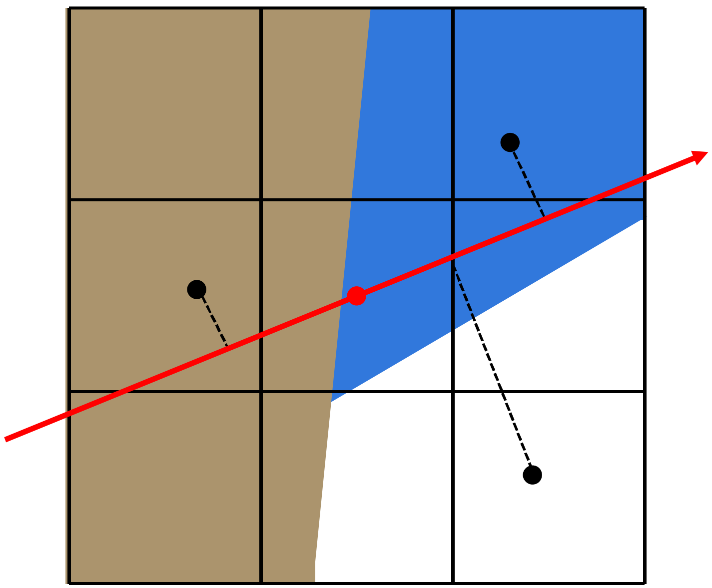
- For *N* materials, there are (*N*-2)*N*! ordering combinations
  - Quickly becomes burdensome for users running complex problems
- Automatic ordering: Mosso & Clancy (1994), Benson (1998)

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

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:

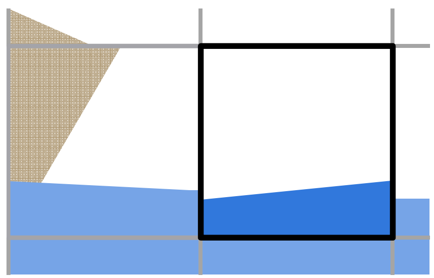
$$-\nabla V_f \quad \text{or} \quad -\nabla \left(\sum V_f\right)$$



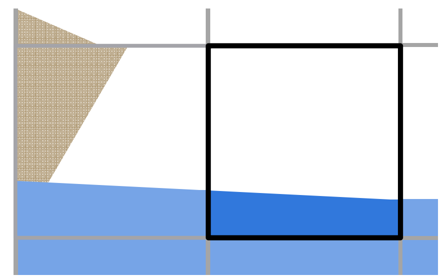
Ordering ‘Fixes’

- 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

White/(Tan)/Blue



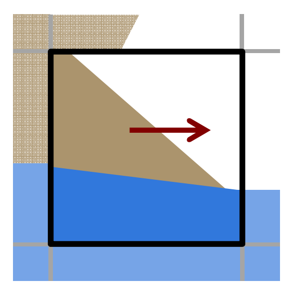
vs.



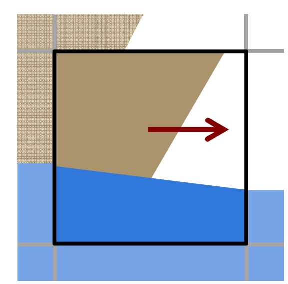
Blue/(Tan)/White

- Accumulating gradient choice at T-intersections:
  - Usually accumulation is best for the second material (e.g., layers)
  - Terminating interface may be ‘better’ without accumulation

Blue/Blue+Tan



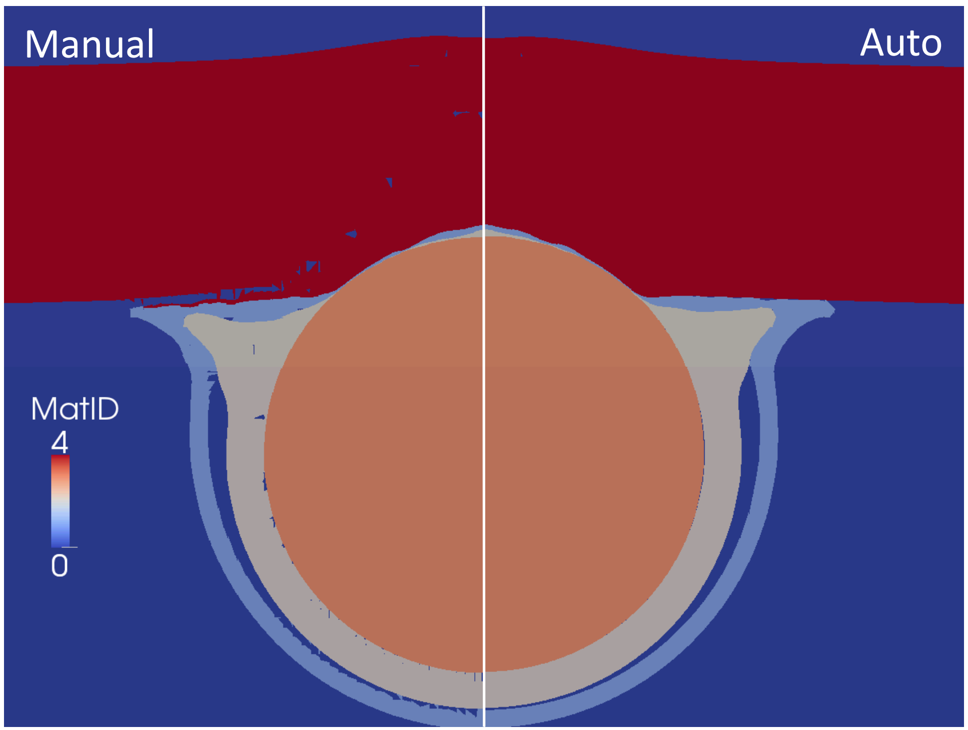
vs.



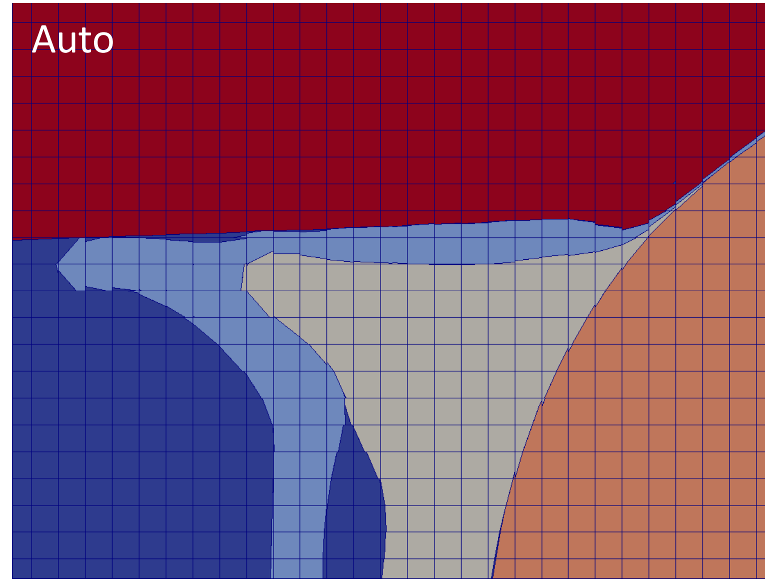
Blue/Tan

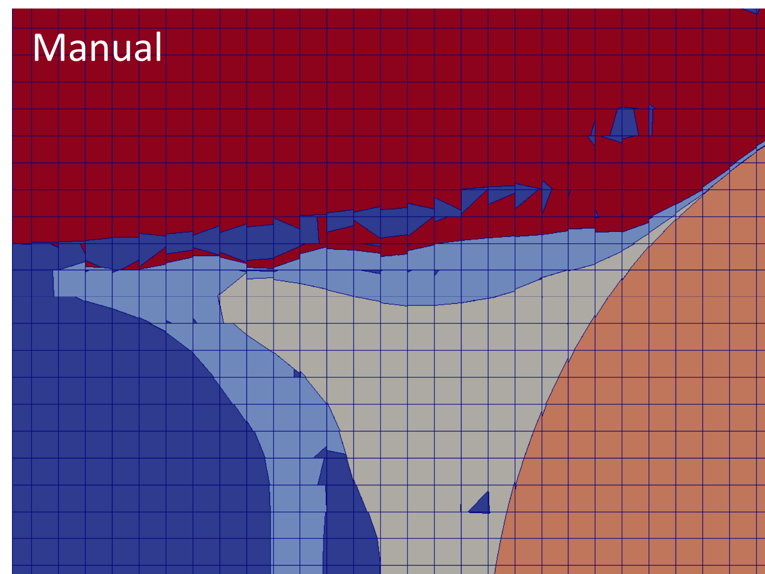
An Example

- Nested spheres striking a plate
- 4 materials + void



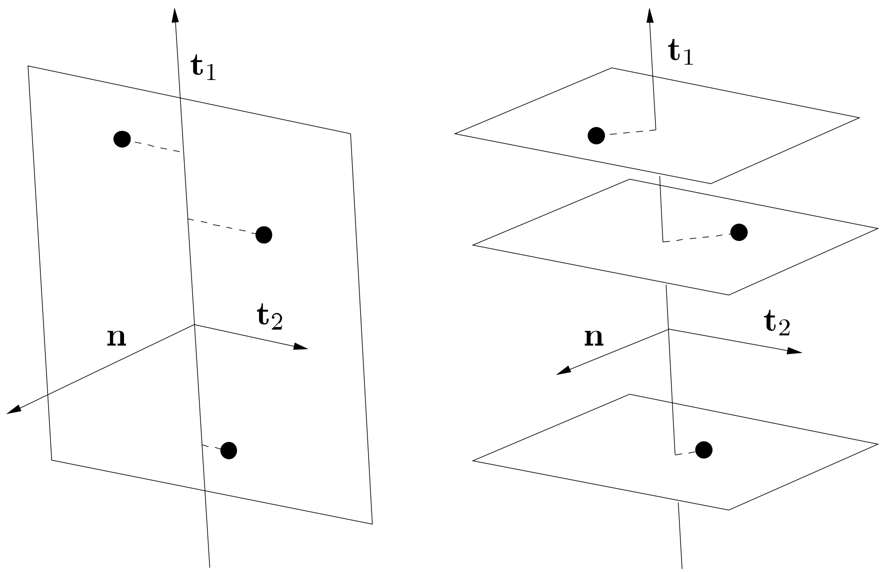
V_{impact} = 427 m/s





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

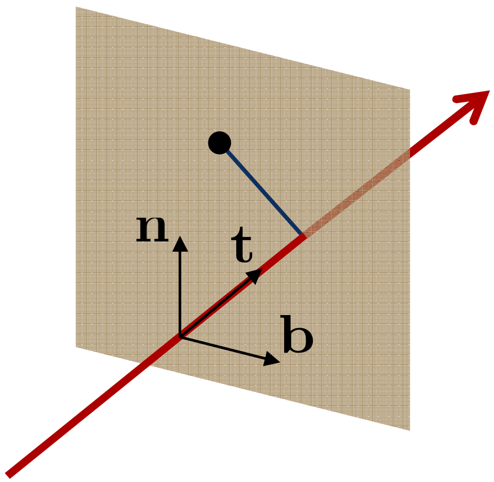


$$\mathrm{SSE} = \sum_{m=1}^{M} w_m \left[(x_m - \hat{x}_m)^2 + (y_m - \hat{y}_m)^2 + (z_m - \hat{z}_m)^2 \right] = R_{\mathbf{n}}$$

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

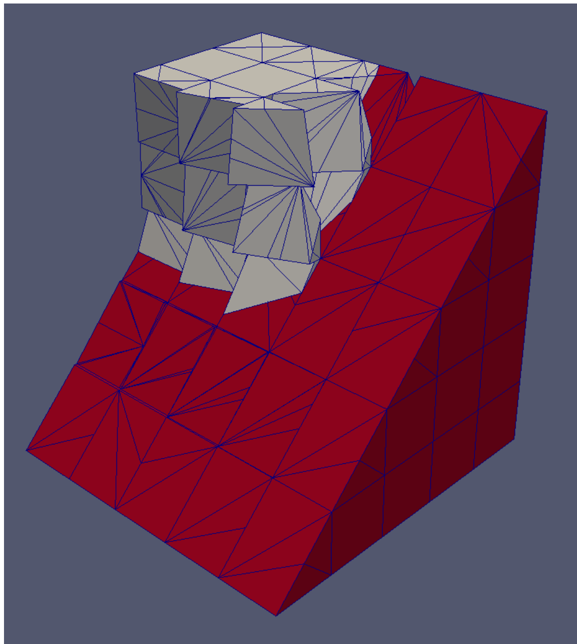
Algorithm (3-D)

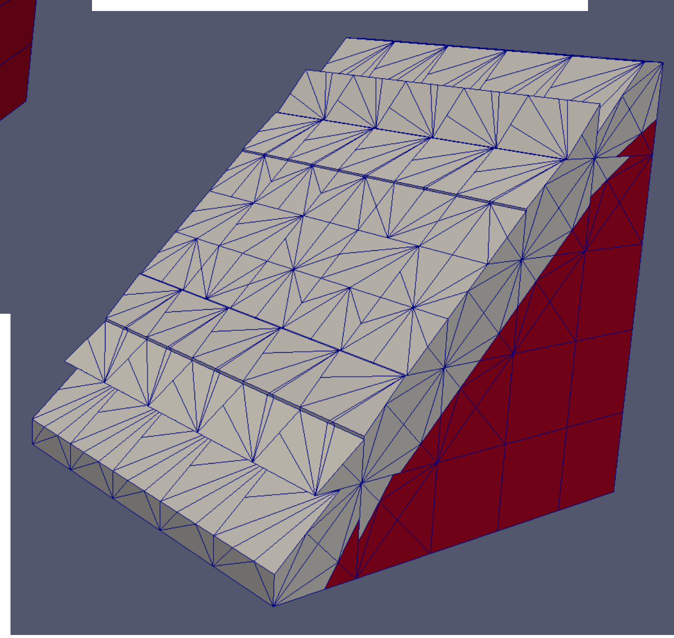
1. Calculate local material centroid approximations
2. Fit a basis to the centroids
   - Newton method for initial solution, then complete the basis
   - Fail-safe sequence to ensure a solution is found
3. Identify tangential direction (ordering line)
4. Define ordering by distances along line of projected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

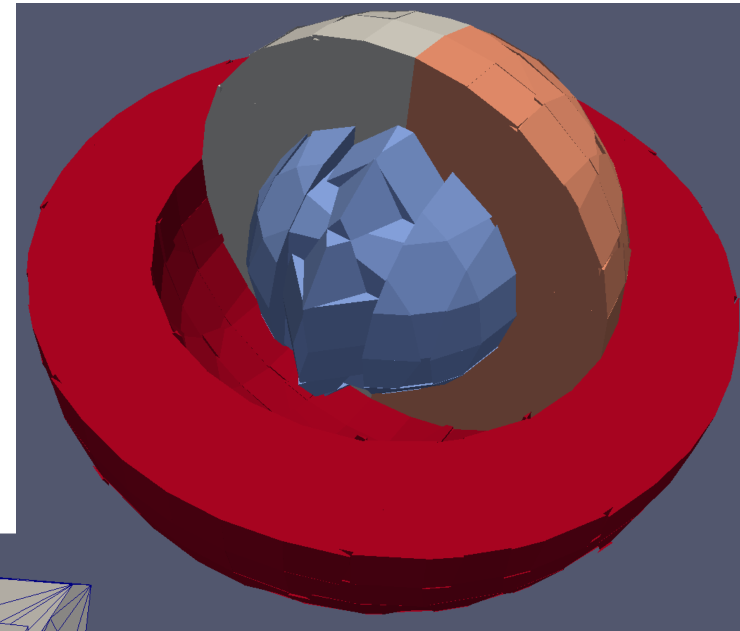


3-D Demonstrations

- Verification tests

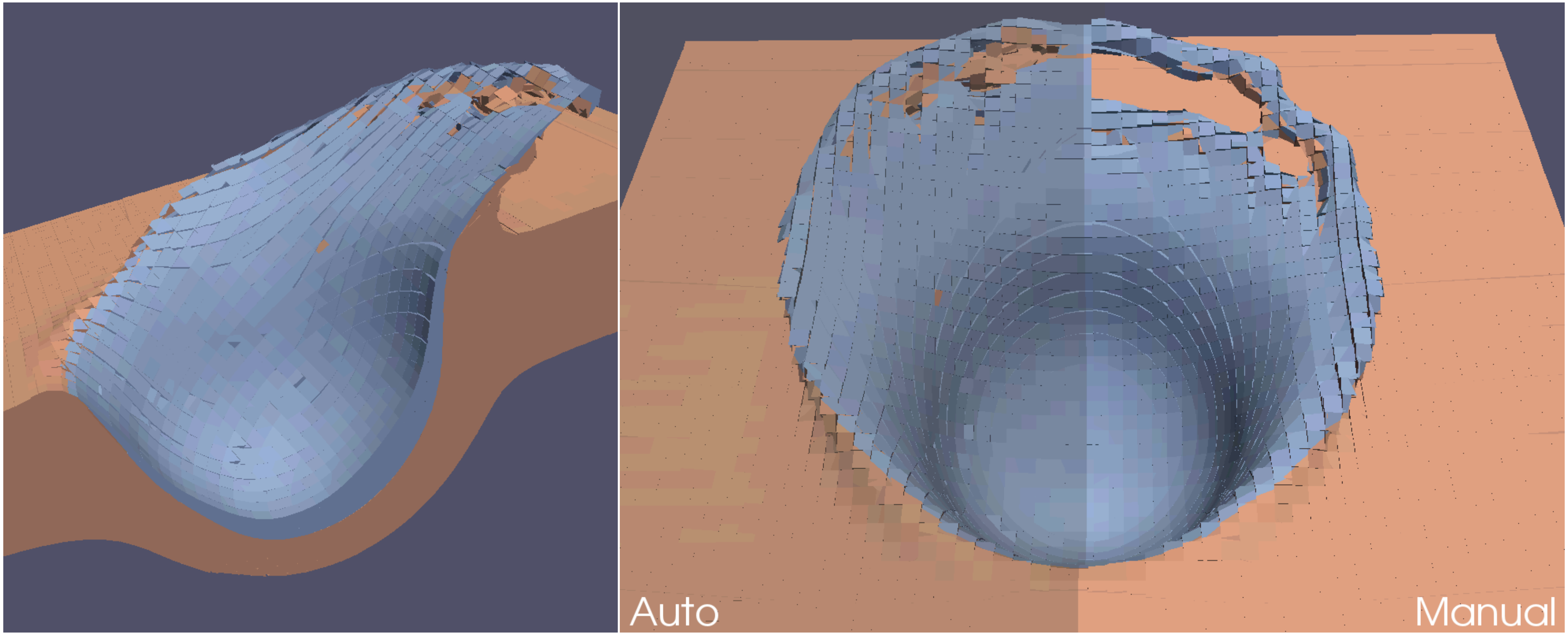






3-D Results

- Preliminary demonstration: Whipple shield



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