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Sandia National Laboratories

XFEM for Multi-Material Eulerian Solid/Hydrodynamics

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U.S. DEPARTMENT OF ENERGY

National Nuclear Security Administration

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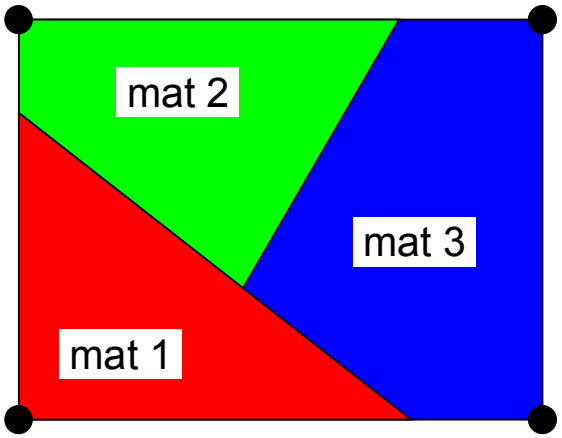
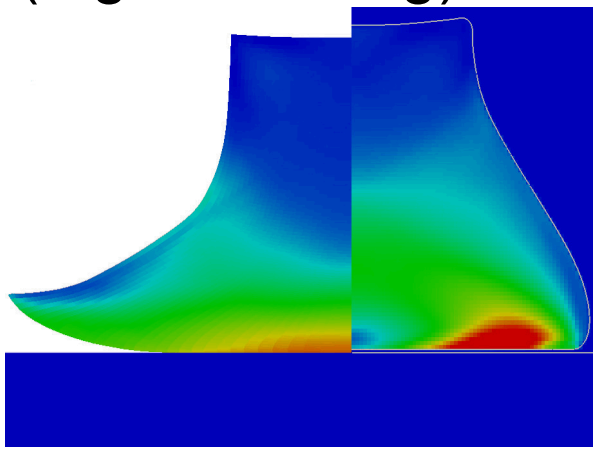
Introduction:

- Our problems frequently require an Eulerian approach.
- Traditional treatment of multi-material cells (with unmixed materials and strength) are arguably deficient:
  - Single velocity/displacement field per element.
  - Ignore interface mechanics (e.g. for sliding).



A multi-material cell …



… and it's effect with ad-hoc treatment.

- We are NOT attempting to address models for well mixed materials (e.g. gases).

Our problem:

- Solve model equations:

mass: $$\frac{d}{dt}(\rho dv) = \frac{d}{dt}(dm) = 0$$

momentum: $$\rho\frac{d}{dt}\dot{\mathbf{u}} = \rho\ddot{\mathbf{u}} = \nabla\cdot\boldsymbol{\sigma} + \mathbf{f}$$

energy: $$\rho\frac{d}{dt}e = \boldsymbol{\sigma} : \mathbf{D}$$

- Use traditional “Operator-Split” approach:
  - Lagrangian step solve of above equations.
  - Generate new mesh (Eulerian)
  - Perform remap (See Mosso et al. presentation)

Closure needed for mixed cells:

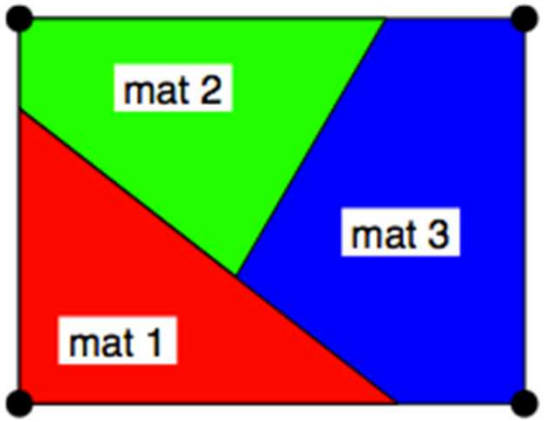
$$\mathbf{a}^n = \mathbf{M}^{-1}\left(\mathbf{f}_{ext}^n - \int \mathbf{B}^t \boldsymbol{\sigma}^n dV\right)$$

$$\mathbf{v}^{n+\frac{1}{2}} = \mathbf{v}^{n-\frac{1}{2}} + \Delta t \mathbf{a}^n$$

$$\mathbf{D}^{n+1/2} = \frac{1}{2}\left(\mathbf{L}^t + \mathbf{L}\right)^{n+\frac{1}{2}}$$

$$\boldsymbol{\sigma}_m^{n+1} = \mathcal{M}_m\left(\boldsymbol{\sigma}_m, \mathbf{D}_m^{n+\frac{1}{2}}, \ldots\right)$$

$$e_m^{n+1} = e_m^n + \Delta t \int \boldsymbol{\sigma}_m^n : \mathbf{D}_m^{n+\frac{1}{2}} dV$$

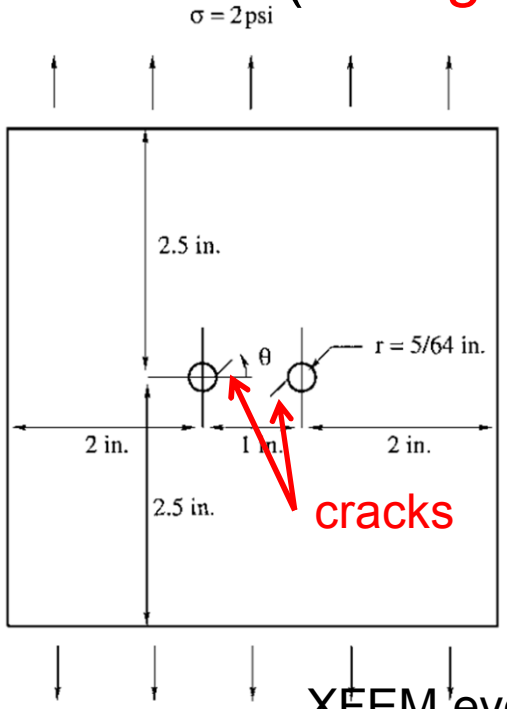


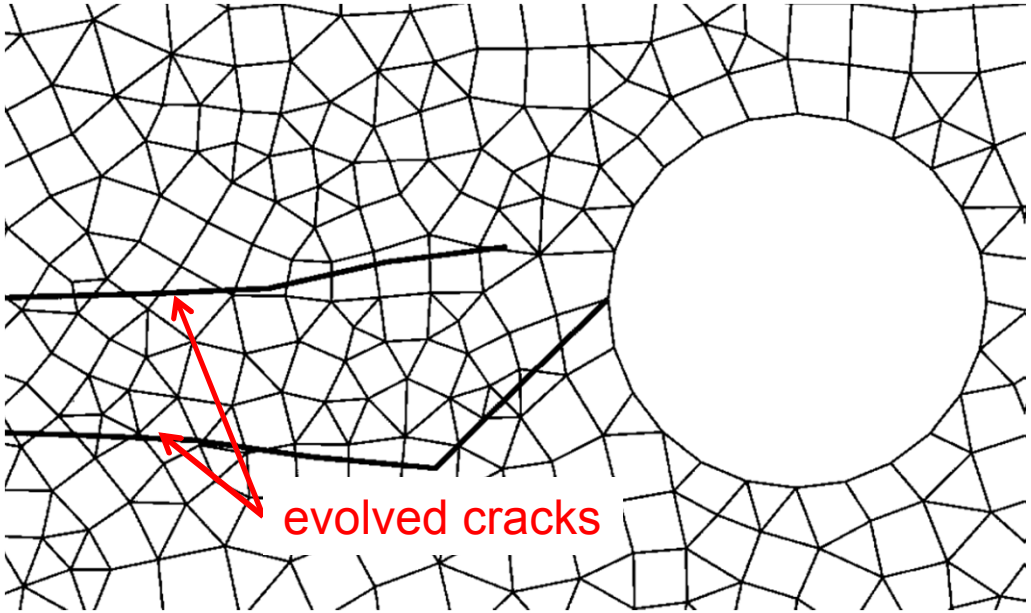
$$\mathbf{D}_m^e = \mathbf{D}^e$$

$$\boldsymbol{\sigma} = \sum_m \frac{V_m}{V}\boldsymbol{\sigma}_m$$

The XFEM:

- XFEM is the eXtended Finite Element Method
- Originated in the late 1990s at Northwestern University to model crack growth.
- Cracks are discontinuities in the displacement field variables (strong discontinuity)

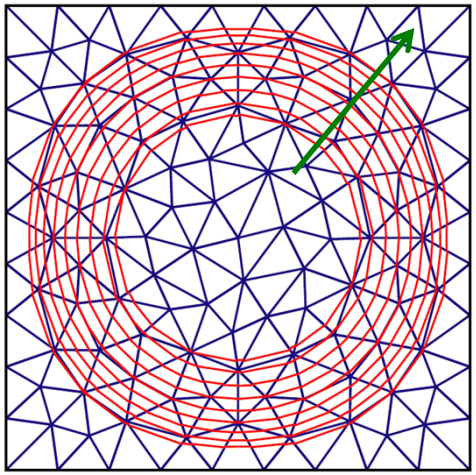




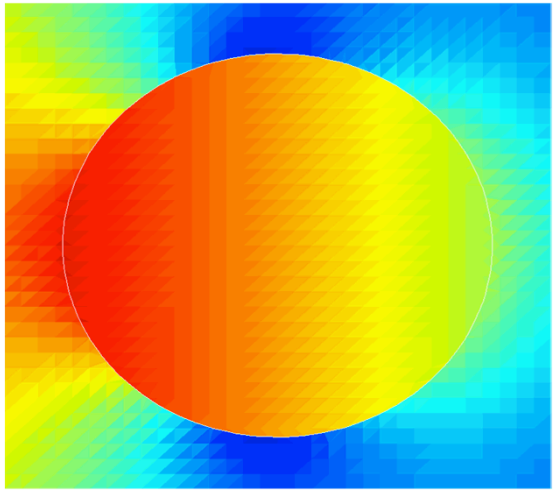
XFEM evolved cracks from MDB99

Extended to other physics:

- Further developed to model other problems with important evolving “features.”
- Often characterized by discontinuities in field variable derivatives (temperature gradient; weak discontinuity).
- Less cumbersome than adaptively body-fitted mesh.



XFEM/VOF evolved phase-change interface (DMRV08).



XFEM for magnetics with edge-based elements (SBKV13).

Partition of Unity Framework:

- Partition-of-unity (POU) approach constructs basis functions as products of standard FEM bases and local, enriched bases.

$$\mathbf{u}^h(\mathbf{x}) = \sum_I \phi_I(\mathbf{x})\mathbf{u}_I + \sum_K \sum_J \phi_J(\mathbf{x})\varphi_K(\mathbf{x})\mathbf{u}_J^K$$

Standard FEM basis

enrichment(s)

- XFEM seeks to capture discontinuities, hence enrichment functions are generally strongly or weakly discontinuous.
- Aside: The Generalized Finite Element Method (GFEM) is essentially XFEM. Developed in parallel at different Universities.

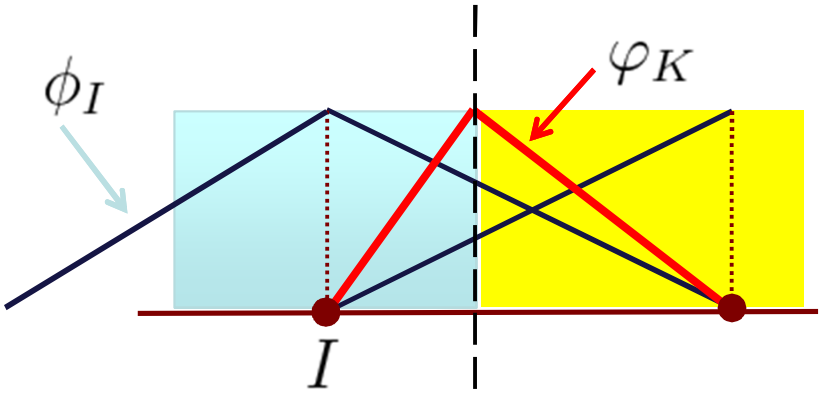
XFEM enrichments:

$$\mathbf{u}^h(\mathbf{x}) = \sum_I \phi_I(\mathbf{x})\mathbf{u}_I + \sum_K \sum_J \phi_J(\mathbf{x})\varphi_K(\mathbf{x})\mathbf{u}_J^K$$

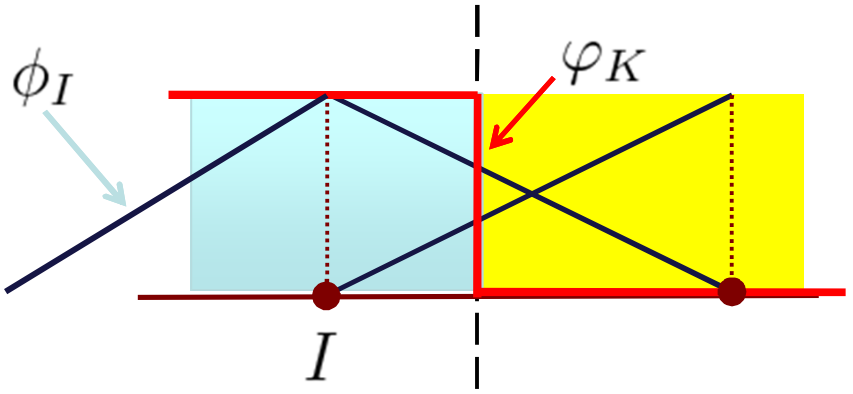
Standard FEM basis

enrichment(s)

- Ridge (weak)
  - parasitic high order terms
  - complex multi-interface treatment
  - Some forms require blending



- Heaviside (weak & strong)
  - re-tie weak discontinuities
  - simple multi-interface treatment
  - nice implementation “tricks”



XFEM Heaviside enrichments:

- Enrichment term of the Heaviside enriched basis contains the space of the classical term (can represent a constant and linear). Hence the classical term is dropped [SB05].

$$\mathbf{u}^h(\mathbf{x}) = \sum_I \phi_I(\mathbf{x})\mathbf{u}_I + \sum_K \sum_J \phi_J(\mathbf{x})\varphi_K(\mathbf{x})\mathbf{u}_J^K$$

Standard FEM basis

enrichment(s)

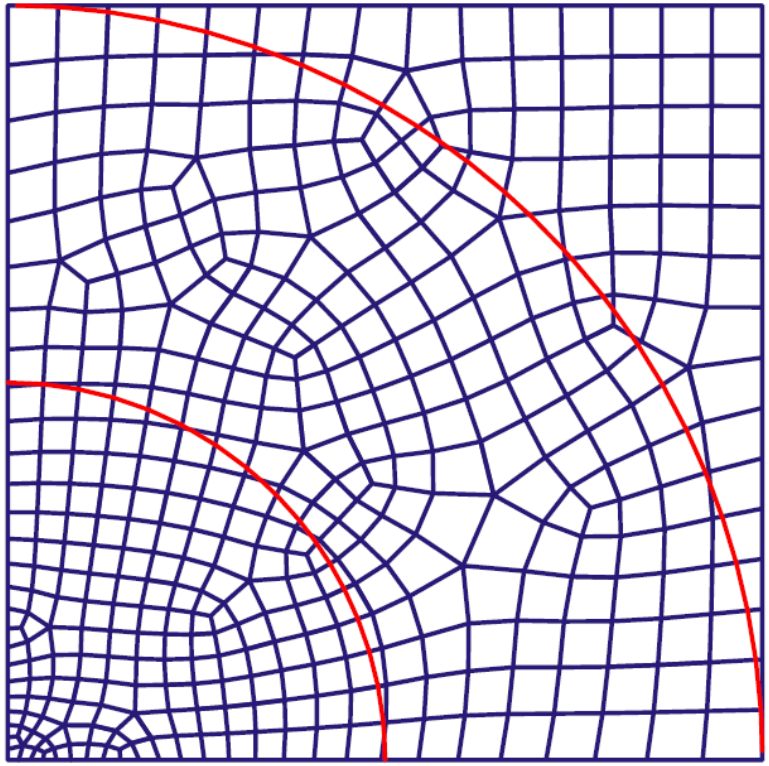
- This reduced basis is an important component of our ALEGRA implementation as we will see later.
- From this point on XFEM implies Heaviside XFEM.

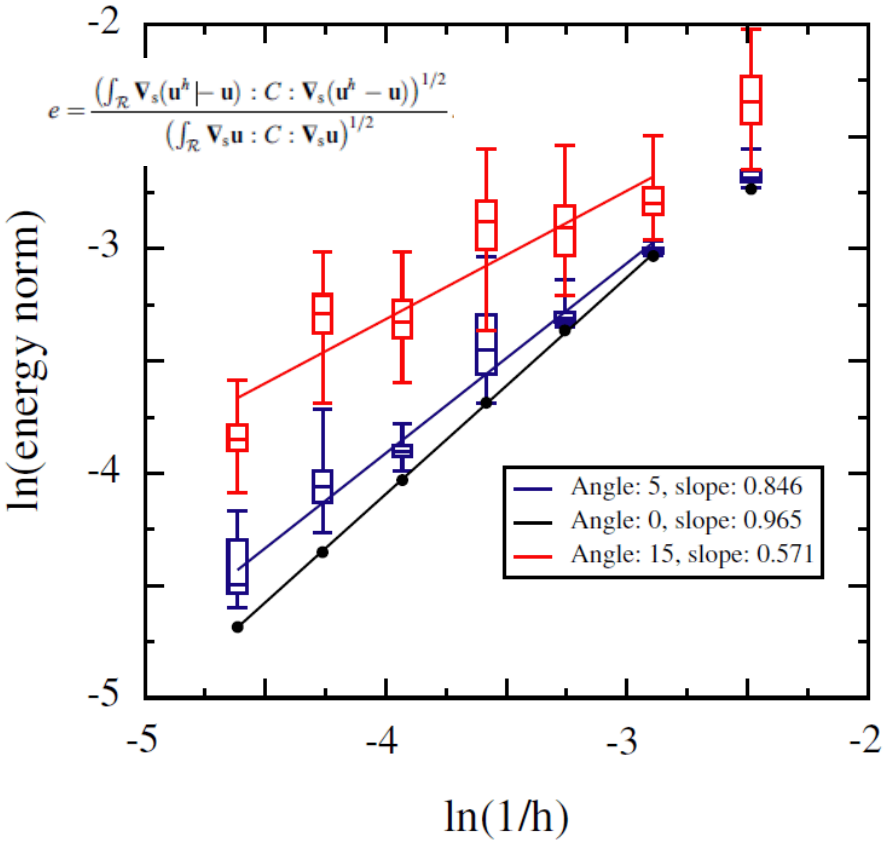
Requires discontinuity location:

- Requires knowledge of the interface/discontinuity location (strong or weak).
- Traditionally uses Level-Set approach …
  - Interface is located by evolving a level-set function.
  - Typically requires frequent fix-ups.
  - Confounded by complex interface intersections.
  - Doesn't conserve mass.
- We use Interface Reconstruction …
  - Material volume fractions are advected with flow.
  - Interface is reconstructed from volume fraction field.
  - Allows evolving, complex interface intersections.
  - Conserves mass.

Accuracy Depends on Interface:

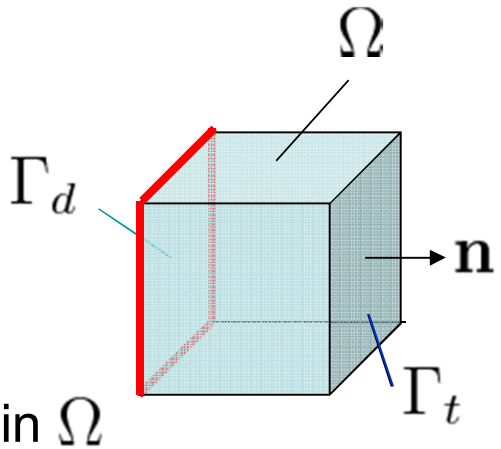
- XFEM depends on good material interface description:
  - Need to locate the interface in an element from volume fractions
  - Interface reconstruction guarantees mass conservation (cf. level sets)





XFEM discretization:

Illustrate with the momentum balance equation:



PDE: $$\rho \frac{d}{dt}\dot{\mathbf{u}} = \rho\ddot{\mathbf{u}} = \nabla \cdot \boldsymbol{\sigma} + \mathbf{f} \quad \text{in } \Omega$$

ICs: $\mathbf{u}(\mathbf{x},0) = \mathbf{u}_0(\mathbf{x})$ and $\dot{\mathbf{u}}(\mathbf{x},0) = \mathbf{v}_0(\mathbf{x})$ in Ω

BCs: traction: $\boldsymbol{\sigma} \cdot \mathbf{n} = \mathbf{t}$ on Γ_t

dirichlet: $\mathbf{u} = \mathbf{u}_d$ on Γ_d

Or in weak form:

$$\int_\Omega \left[\rho\delta\mathbf{w} \cdot \ddot{\mathbf{u}} + \boldsymbol{\sigma} : \nabla\delta\mathbf{w}\right] d\Omega = \int_\Omega (\delta\mathbf{w} \cdot \mathbf{f})\, d\Omega + \int_{\Gamma_t} (\delta\mathbf{w} \cdot \mathbf{t})\, d\Gamma_t$$

ICs: $\mathbf{u}(\mathbf{x},0) = \mathbf{u}_0(\mathbf{x})$ and $\dot{\mathbf{u}}(\mathbf{x},0) = \mathbf{v}_0(\mathbf{x})$ in Ω

BC: $\mathbf{u} = \mathbf{u}_d$ on Γ_d

Materials move independently:

Assume two materials for simplicity then the momentum equation is:

$$\mathbf{u}^h(\mathbf{x}) = \sum_I^{N_n} \left[\mathcal{H}^1(\mathbf{x})\phi_I(\mathbf{x})\mathbf{u}_I^1 + \mathcal{H}^2(\mathbf{x})\phi_I(\mathbf{x})\mathbf{u}_I^2\right]$$

$$\begin{bmatrix} \mathbf{M}_1 & \mathbf{0} \\ \mathbf{0} & \mathbf{M}_2 \end{bmatrix} \begin{bmatrix} \mathbf{v}_1^{new} \\ \mathbf{v}_2^{new} \end{bmatrix} = \Delta t \begin{bmatrix} \mathbf{f}_1^{int} + \mathbf{f}_1^{ext} \\ \mathbf{f}_2^{int} + \mathbf{f}_2^{ext} \end{bmatrix} + \begin{bmatrix} \mathbf{M}_1\mathbf{v}_1^{old} \\ \mathbf{M}_2\mathbf{v}_2^{old} \end{bmatrix}$$

The element level versions of the above terms are:

internal forces:

$$\mathbf{f}_{1,e}^{int} = \int_{\Omega_e} \mathcal{H}_1 \mathbf{B}^T \boldsymbol{\sigma}_1 d\Omega_e$$

$$\mathbf{f}_{2,e}^{int} = \int_{\Omega_e} \mathcal{H}_2 \mathbf{B}^T \boldsymbol{\sigma}_2 d\Omega_e$$

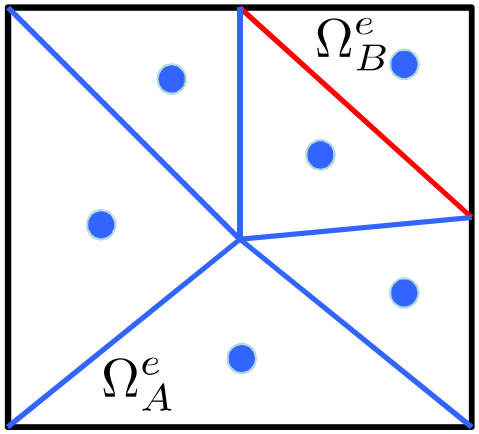
As stress for material 1 is only defined under Heaviside for material 1 (and vice-versa for material 2) we have:

$$\mathbf{f}_{12,e}^{int} = \int_{\Omega_e} \mathcal{H}_1 \mathbf{B}^T \boldsymbol{\sigma}_2 d\Omega_e = 0$$

No coupling between materials

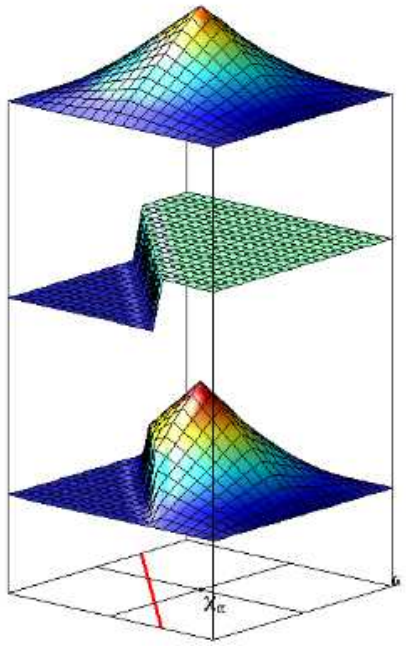
Internal Force Quadrature:

Sub-domain quadrature



$$\int_{\Omega^e} f(\mathbf{x})dv \approx \sum_s \sum_{q_s} w_{q_s} f(\mathbf{x}_{q_s})$$

$$f^e(\mathbf{x}) = \begin{cases} \mathbf{B}^T \boldsymbol{\sigma}_A \text{ in } \Omega_A \\ 0 \text{ in } \Omega_B \end{cases}$$

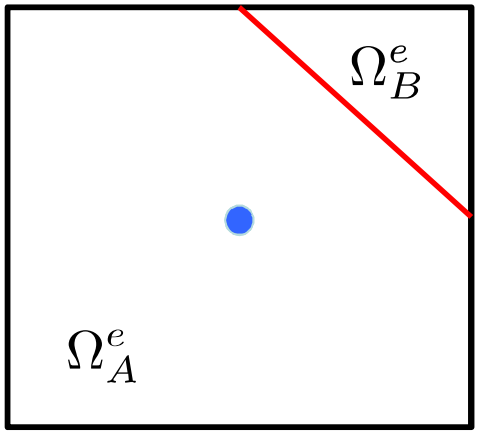


$$\mathbf{f}_{1,e}^{int} = \int_{\Omega_e} \mathcal{H}_1 \mathbb{B}^T \boldsymbol{\sigma}_1 d\Omega_e$$

- Extends to three-dimensions.
- Material state required at each (additional) quad point.
- Mappings can get complicated for iso-parametric elements.
- Exact (full) integration can actually be a problem.

Internal Force Quadrature:

Averaged Stress Approach (Song et al. 2006)



$$\boldsymbol{\sigma}_e = \frac{V_A^e \boldsymbol{\sigma}_A}{(V_A^e + V_B^e)}$$

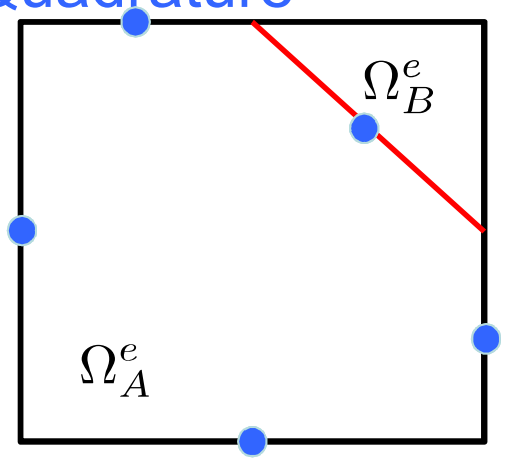
$$\mathbf{f}_e^{int} = \boldsymbol{\sigma}_e \frac{V_A^e}{V^e} \int_{\Omega_e} \mathbf{B}^T dv$$

$$\approx \boldsymbol{\sigma}_e \frac{V_A^e}{V^e} \mathbf{B}_0^T w_0$$

- Time-step is unchanged from standard mixed cell approach.
- Simple to implement.
- No locking though requires (standard) hourglass stabilization.
- Assumes constant volume fraction through Lagrangian step.
- Independent of interface orientation.

Internal force Quadrature:

Material Mean Quadrature



$$\mathbf{f}_e^{int} = \int_{\Omega_e} \mathcal{H}_A \mathbf{B}^T \boldsymbol{\sigma}_A dv$$
$$= \int_{\Omega_{A\,e}} \mathbf{B}^T dv \boldsymbol{\sigma}_A = \overline{\mathbf{B}}_A^T \boldsymbol{\sigma}_A$$

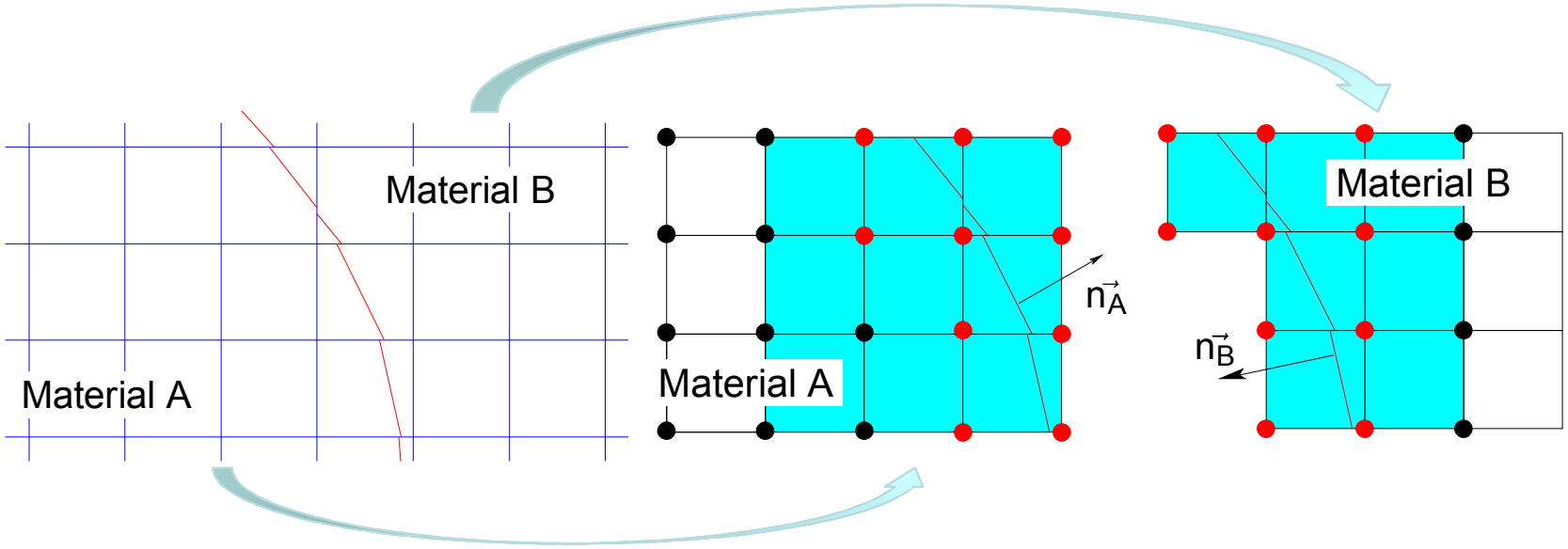
using Green-Gauss theorem:

$$\overline{\mathbf{B}}_A = \begin{bmatrix} \int_{\Gamma_A} \mathbf{N} n_x & \mathbf{0} \\ \mathbf{0} & \int_{\Gamma_A} \mathbf{N} n_y \\ \int_{\Gamma_A} \mathbf{N} n_x & \int_{\Gamma_A} \mathbf{N} n_y \end{bmatrix}$$

- Does not assume constant volume fraction.
- Sensitive to interface orientation.
- Does not demonstrate locking.
- Time-step slightly reduced relative to averaged stress approach.

Construct hierarchy of entities:

- Parents are original elements / nodes.
- Parent elements are enriched (e.g. have Children) if they have more than one material (including void).
- Parent nodes are enriched if they are attached to an enriched element.
- Parents have as many Children as they do materials.
- Children have one material.



Recoupling material responses:

- Materials in a mixed cell now have unique velocity fields and hence deformation rates.
- Hence, individual material responses are decoupled from one-another.
- Without modification, materials move without regard to one another's deformation.
- Significant/active area of research to "recouple" material responses at their interfaces.

Interaction enforced with LMs:

- Recouple materials via “Lagrange multipliers.”
- Lagrange multipliers applied to “constrain” materials such that they do not penetrate one another.
- We actually constrain materials to share normal component of velocity at shared interfaces.

$$\begin{bmatrix} \mathbf{M}_1 & \mathbf{0} & \mathbf{G}_1 \\ \mathbf{0} & \mathbf{M}_2 & \mathbf{G}_2 \\ \mathbf{G}_1^T & \mathbf{G}_2^T & \mathbf{0} \end{bmatrix} \begin{bmatrix} \mathbf{v}_1^{new} \\ \mathbf{v}_2^{new} \\ \boldsymbol{\lambda} \end{bmatrix} = \begin{bmatrix} \Delta t \left(\mathbf{f}_1^{int} + \mathbf{f}_1^{ext} \right) + \mathbf{M}_1 \mathbf{v}_1^{old} \\ \Delta t \left(\mathbf{f}_2^{int} + \mathbf{f}_2^{ext} \right) + \mathbf{M}_2 \mathbf{v}_2^{old} \\ \mathbf{0} \end{bmatrix}$$

Lagrange multipliers

Constraint matrices

$$\mathbf{G}_1^T \mathbf{v}_1^{new} + \mathbf{G}_2^T \mathbf{v}_2^{new} = \mathbf{0}$$ Velocity constraint

Enforcement phase:

- Solve resulting system for Lagrange multipliers.
- Compute contact forces.
- Update “new” velocities.

$$\begin{bmatrix} \mathbf{M} & \mathbf{G} \\ \mathbf{G}^T & \mathbf{0} \end{bmatrix} \begin{bmatrix} \mathbf{v}^{new} \\ \lambda \end{bmatrix} = \begin{bmatrix} \Delta t \mathbf{f}^{int} + \mathbf{M}\mathbf{v}^{old} \\ \mathbf{0} \end{bmatrix}$$

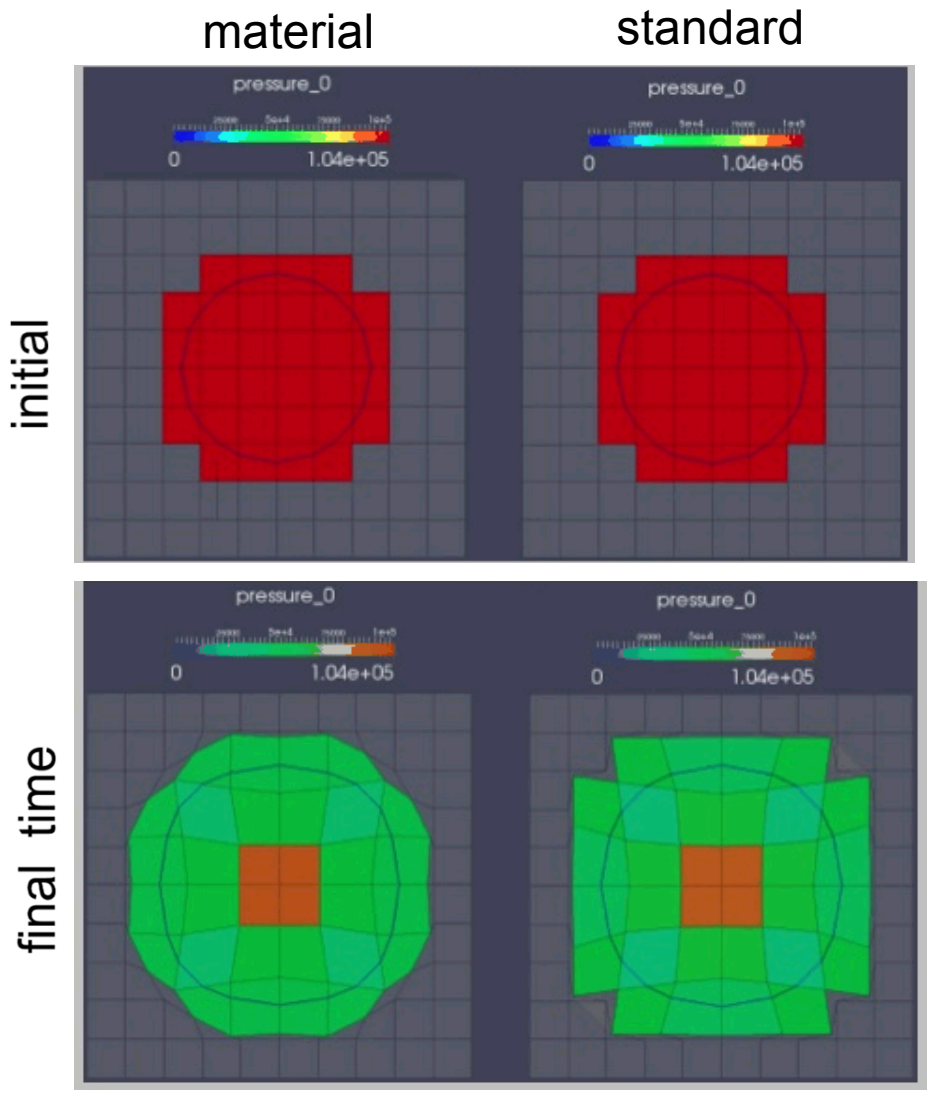
$$\mathbf{G}^T \mathbf{v}^{new} = \mathbf{G}^T \mathbf{M}^{-1} \mathbf{G} \boldsymbol{\lambda} - \mathbf{G}^T \left(\mathbf{v}^{old} + \mathbf{M}^{-1} \mathbf{f}^{int} \right) = \mathbf{0}$$

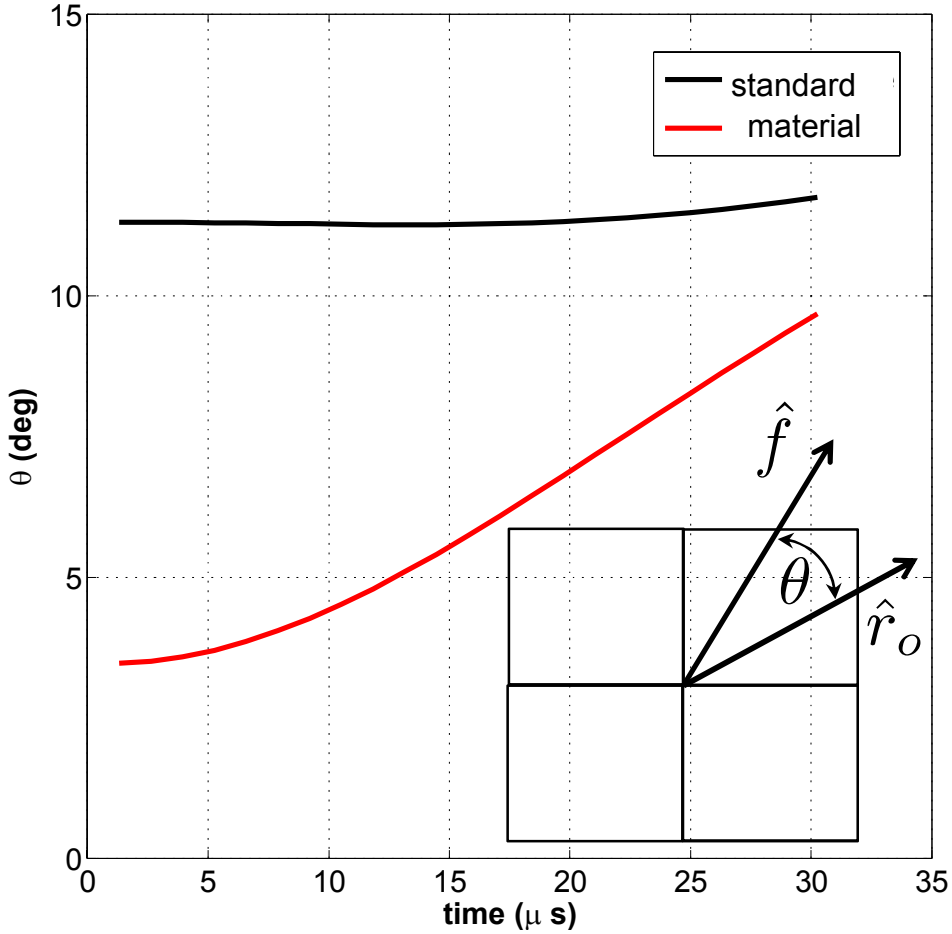
$$\mathbf{A}\boldsymbol{\lambda} = \mathbf{b}$$

$$\mathbf{v}^{new} = \mathbf{M}^{-1} \mathbf{G} \boldsymbol{\lambda} - \left(\mathbf{v}^{old} + \mathbf{M}^{-1} \mathbf{f}^{int} \right)$$

contact forces

Material B-Matrix:

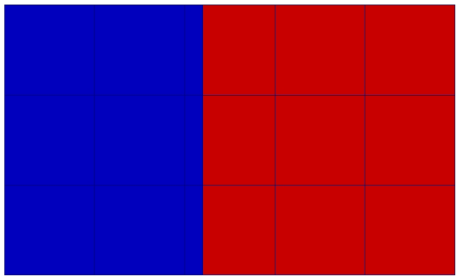




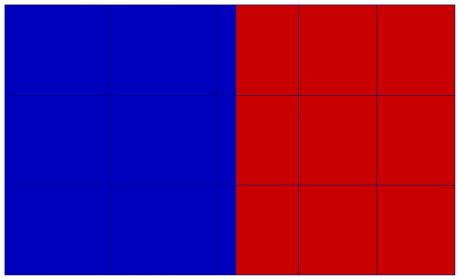
Material B-Matrix:

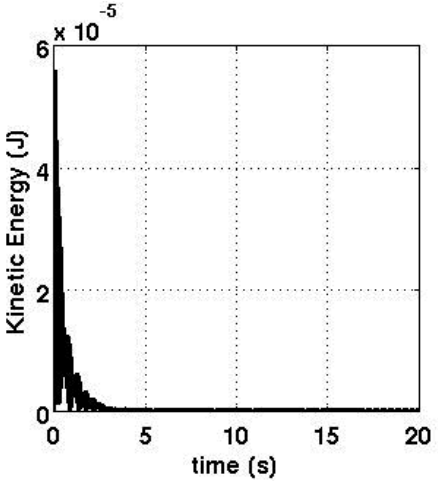
Material B-matrix

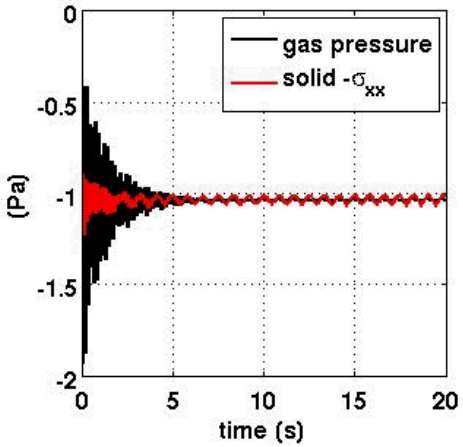
t = 0



t = 20 s

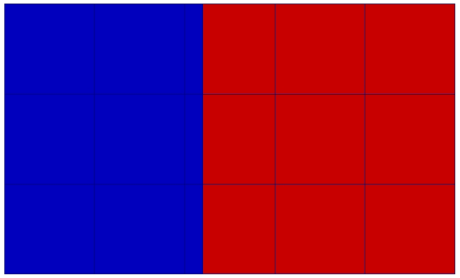




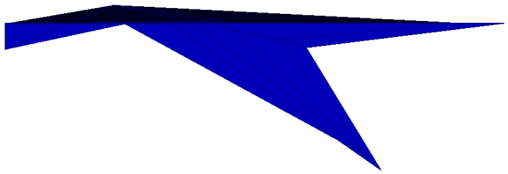


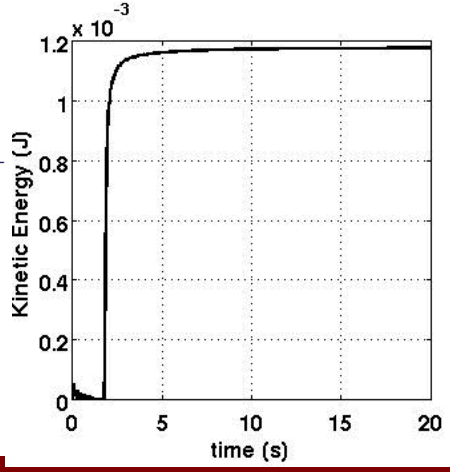
Old B-matrix

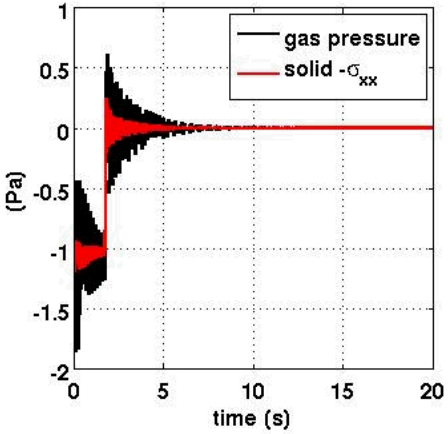
t = 0



t = 20 s



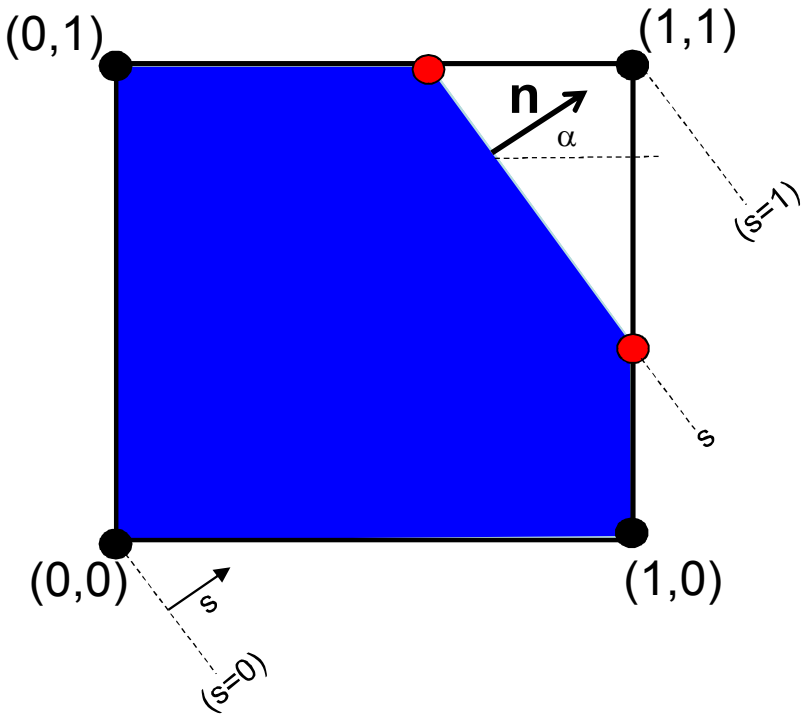


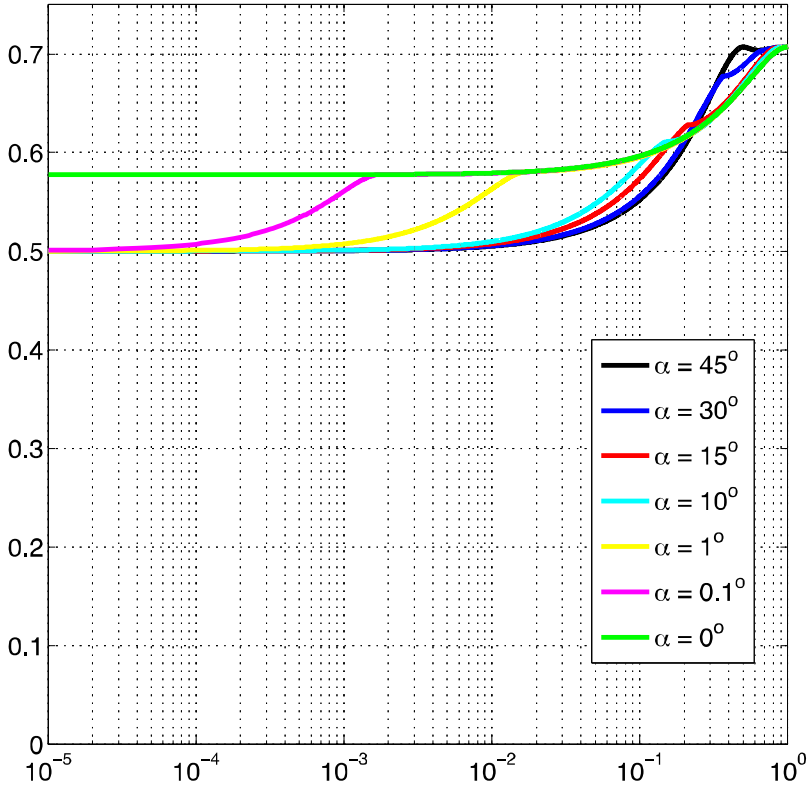


Material B-Matrix / Stable dt:

$$\Delta t = \frac{\ell}{c}$$

$$\ell = \frac{A}{\sqrt{tr(\mathbf{B}_e^T \cdot \mathbf{B}_e)}}$$





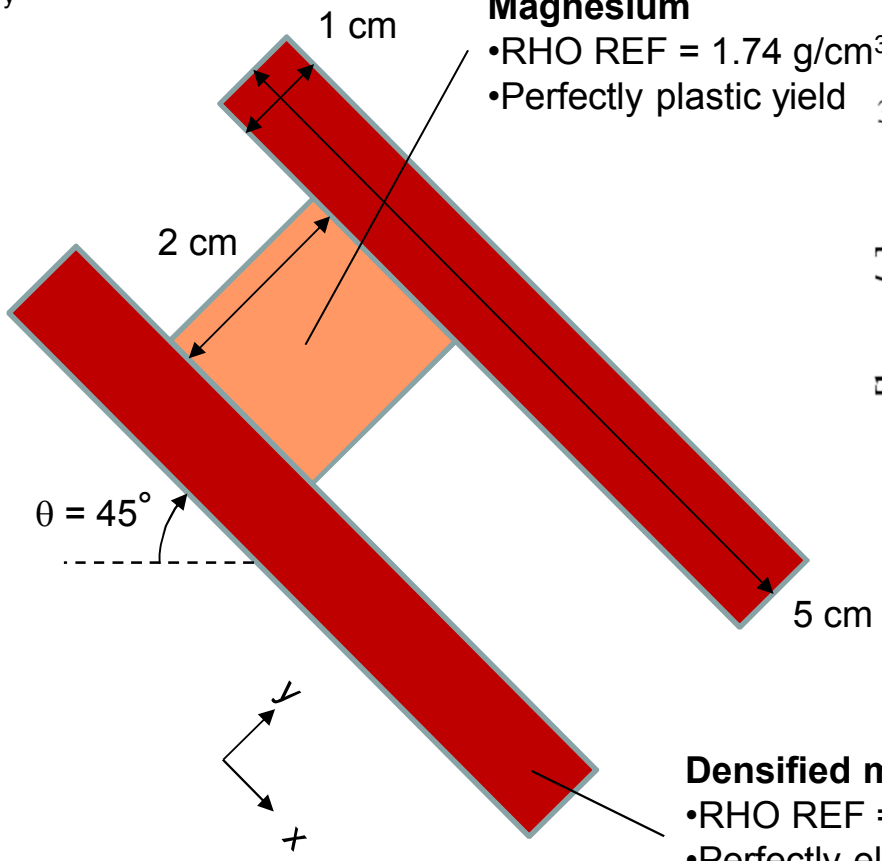
Remap Step:

- Transfer volume fractions from end of previous Lagrangian step to start of next step.
- Construct new parent-child hierarchy.
- Transfer velocities and material state from mesh at end of Lagrangian step to start of next step.
  - Conserve mass, momentum and internal energy.
- Construct interfaces for next Lagrangian step.

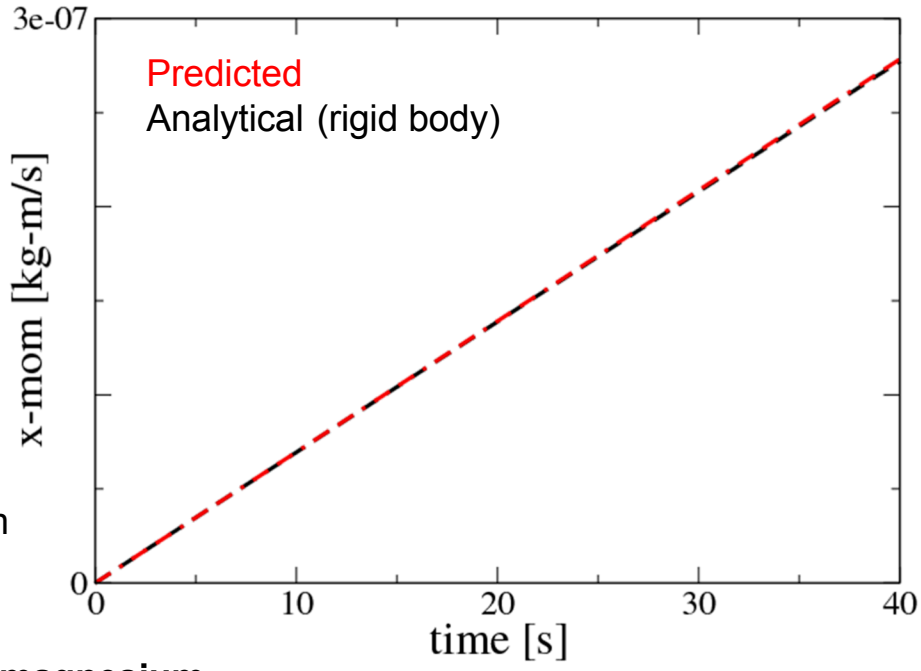
See S. J. Mosso's talk for details.

Sliding block:

body acceleration
$a_x = 1.0 \times 10^{-4}$ cm/s^2
$a_y = -1.0 \times 10^{-4}$ cm/s^2

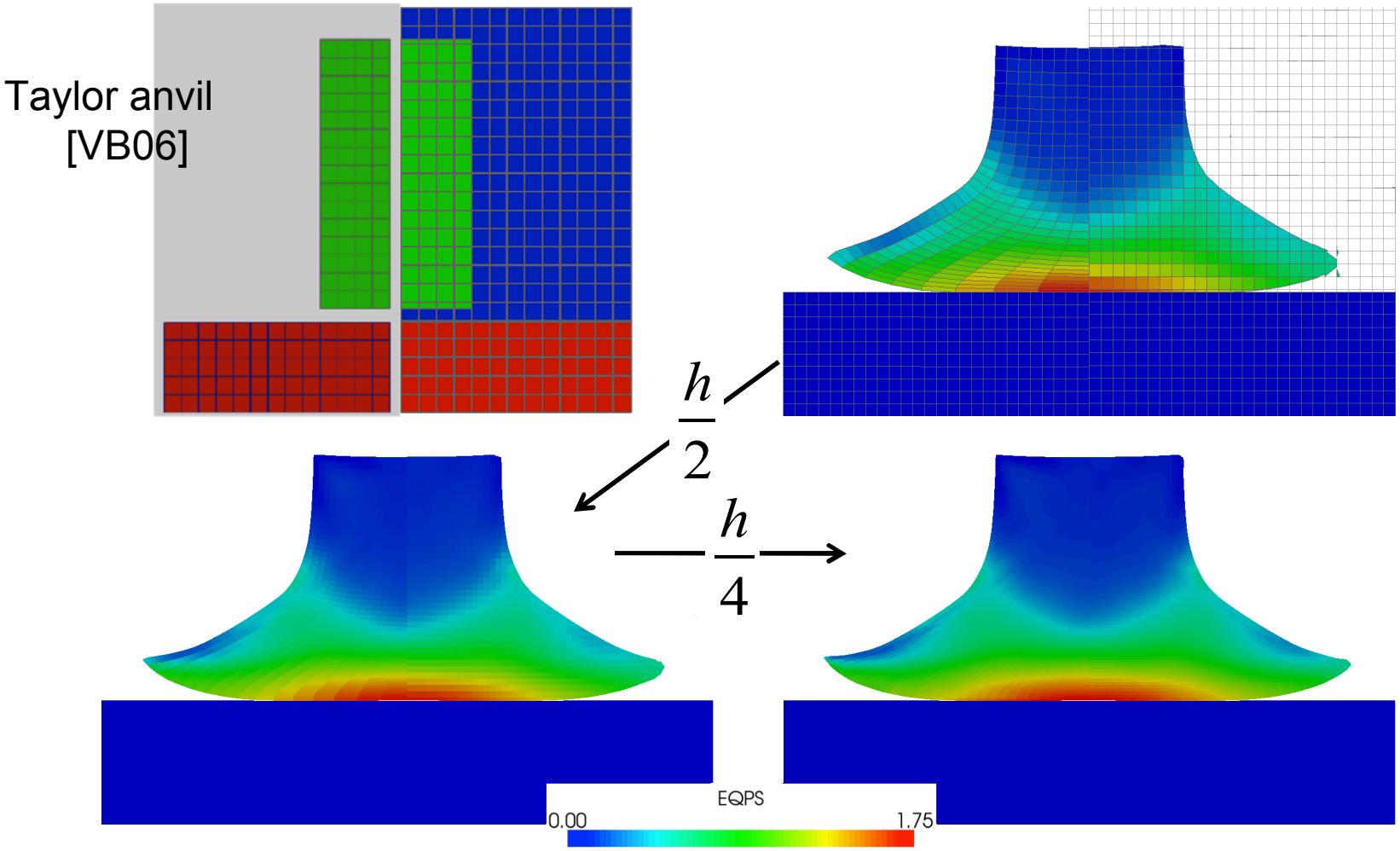


Magnesium
•RHO REF = 1.74 g/cm^3
•Perfectly plastic yield

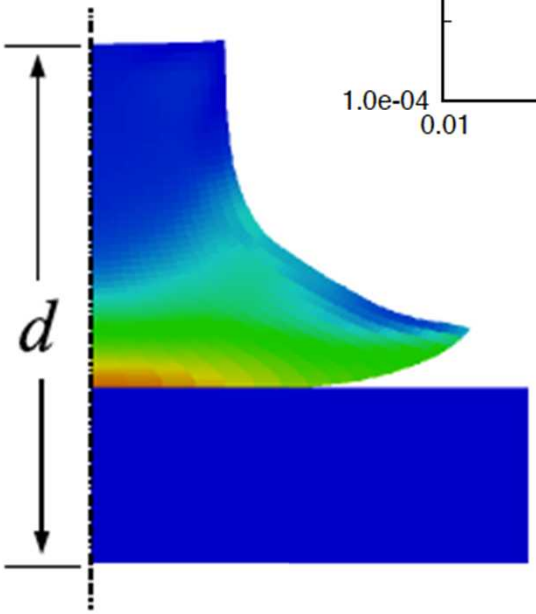


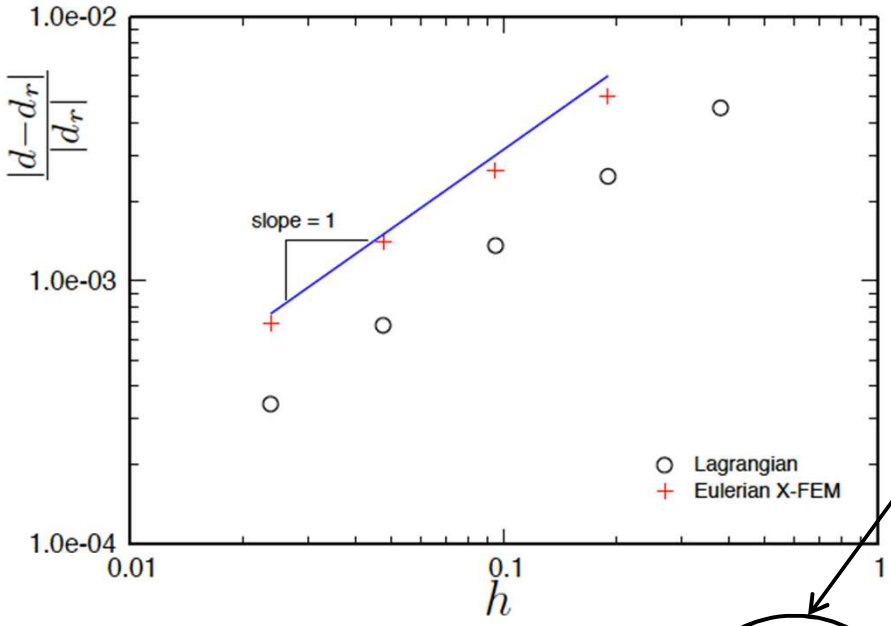
Densified magnesium
•RHO REF = 17.4 g/cm^3
•Perfectly elastic

Lagrangian quality results:

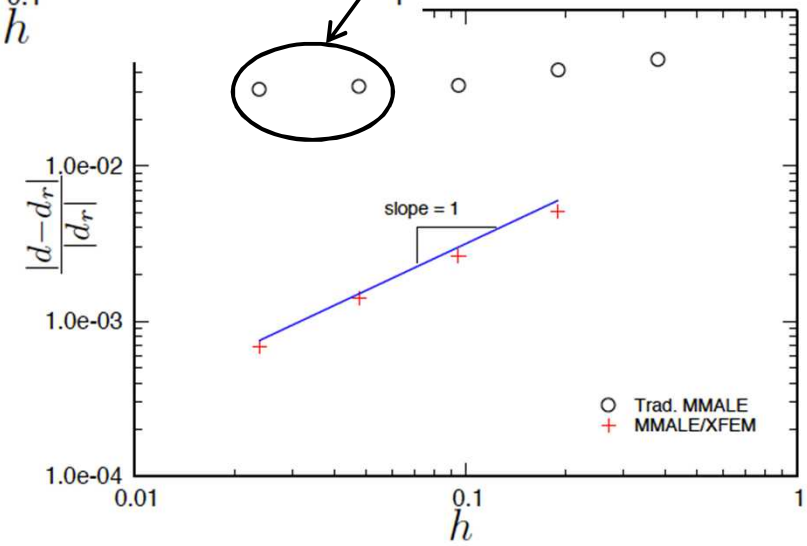


Eulerian gets wrong answer:



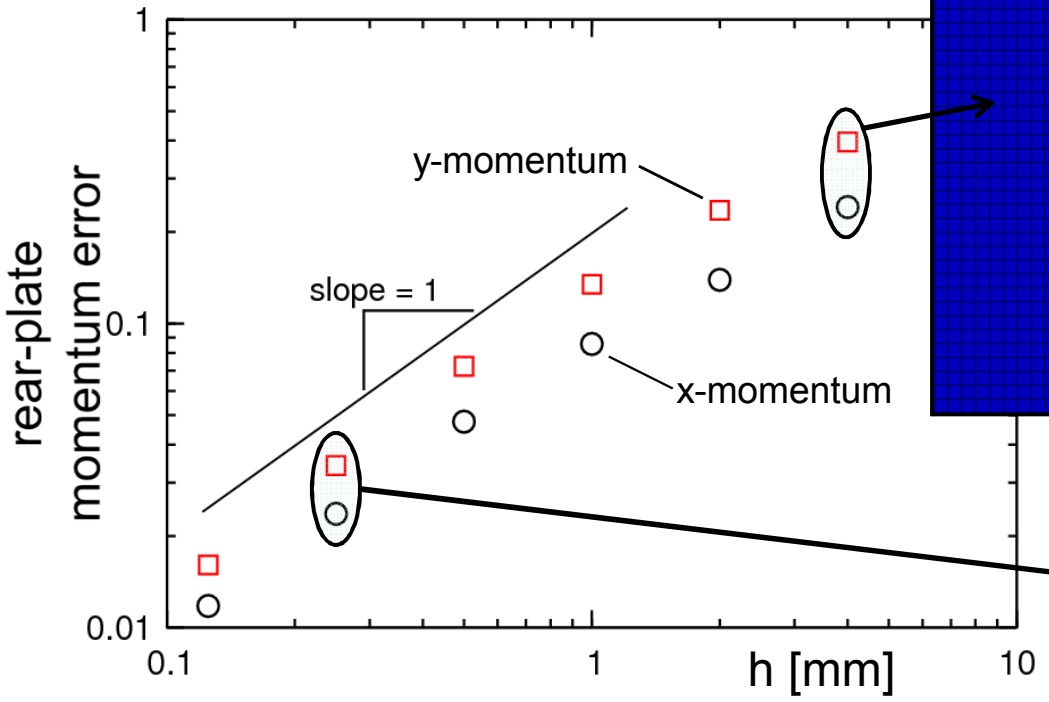


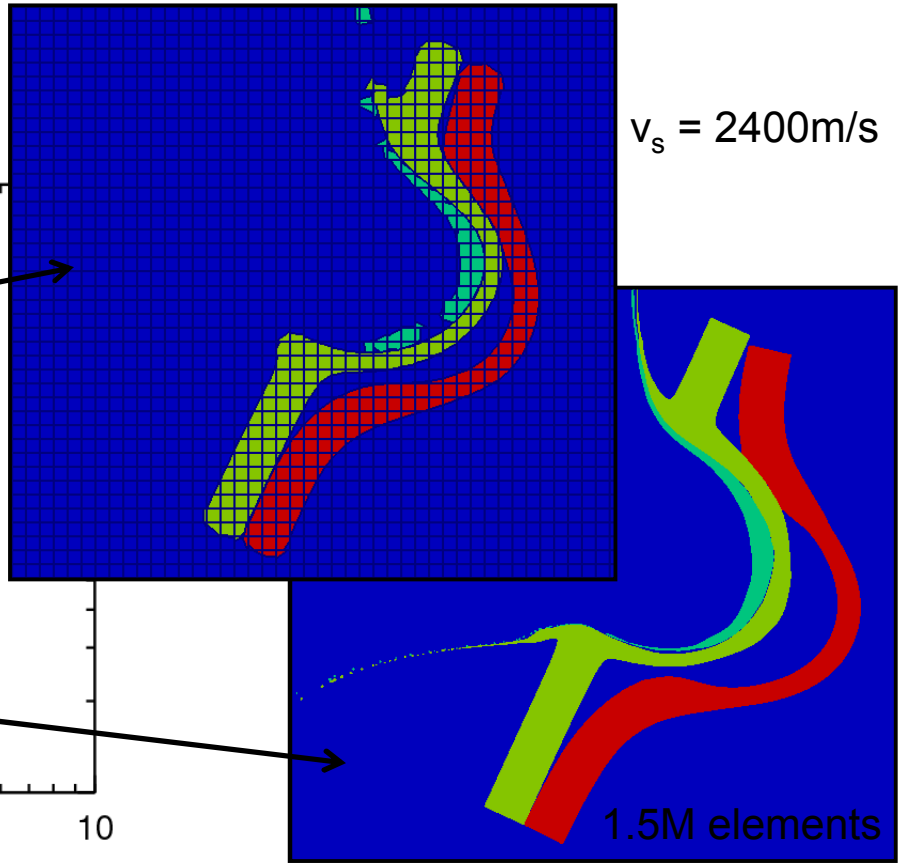
Standard Eulerian converges to a different solution.



Whipple shield example:

Whipple Shield used in satellite protection.

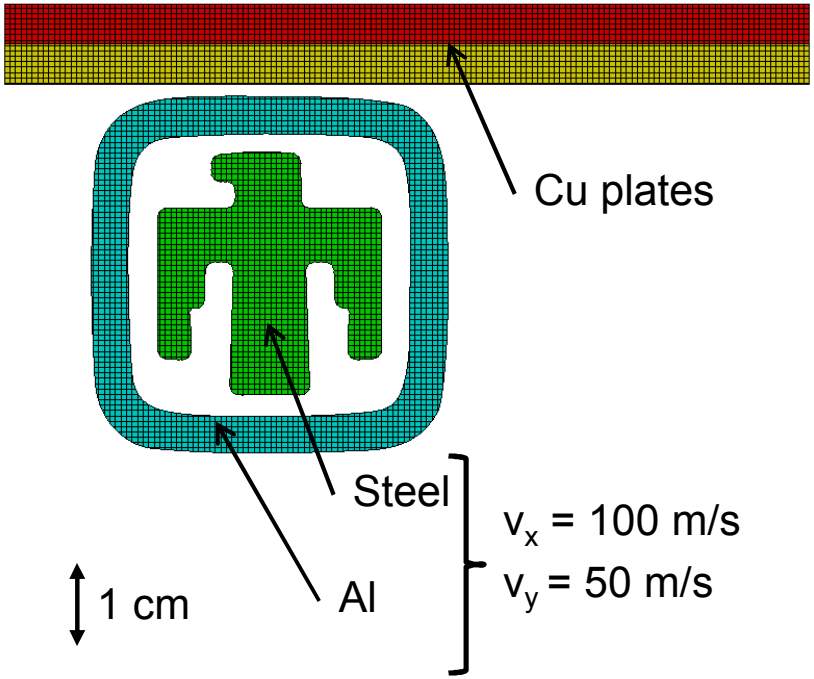


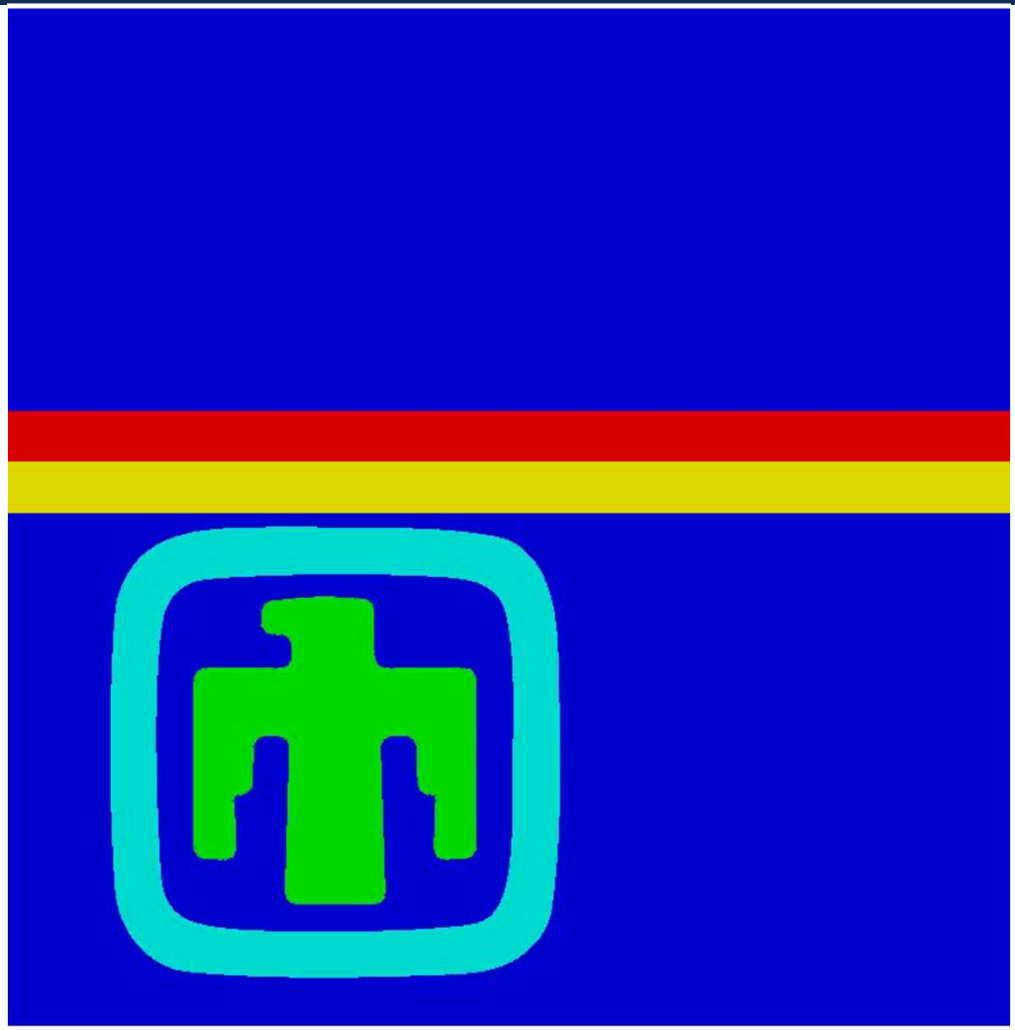


High-velocity impact difficult for Lagrangian and unrealistic for Eulerian are possible with X-FEM.

A more whimsical example:

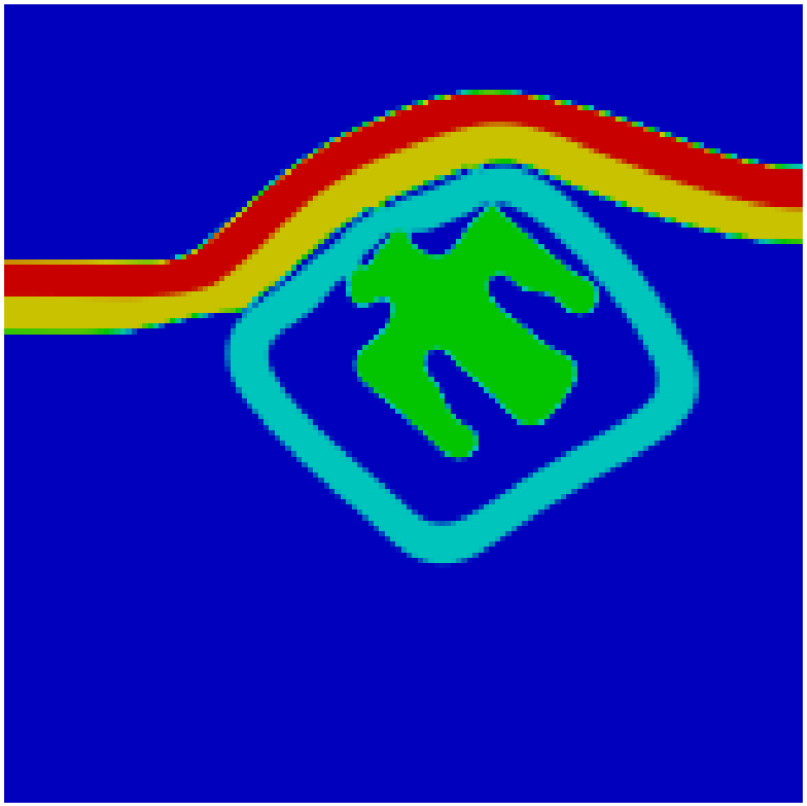
Logo with initial velocity impacts stationary, layered copper plates.



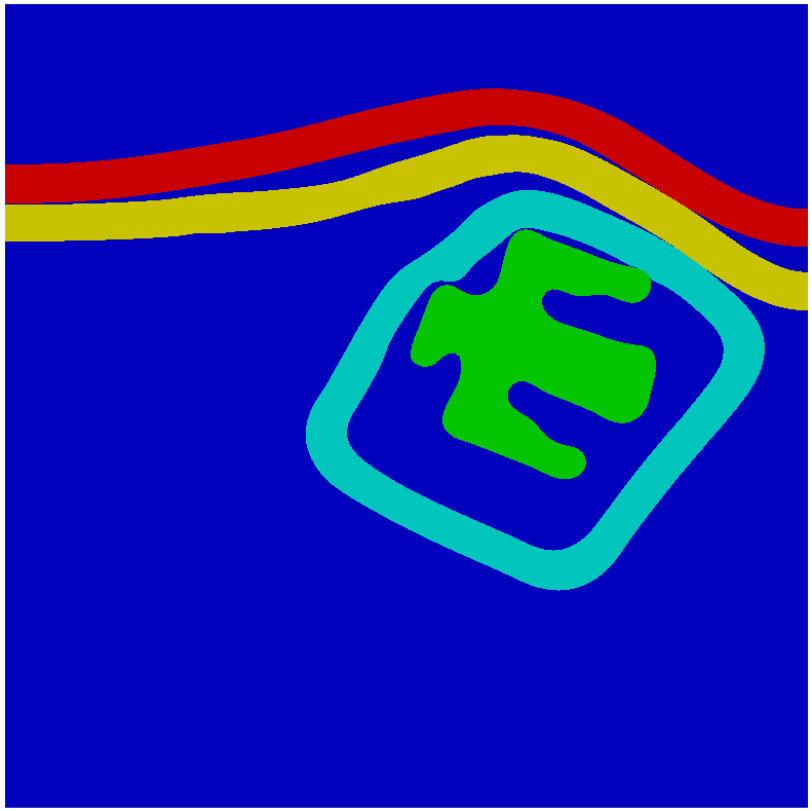


… and a comparison:

Standard approach



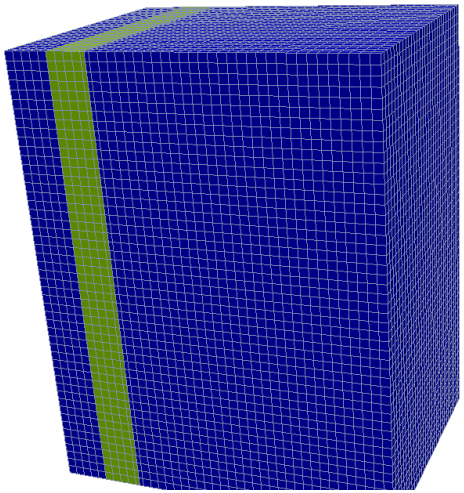
XFEM approach

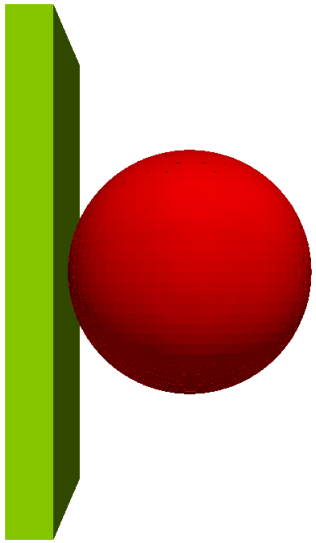


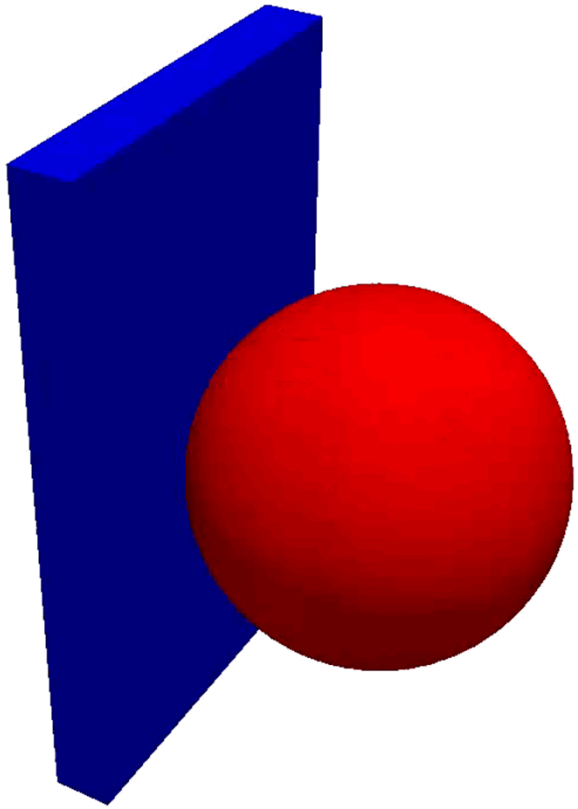
Geometry at time = 1.0e-2 s.

As expected, standard approach with shared velocity fields between materials shows bonding while XFEM allows material impact and separation.

3D work is ongoing:







XFEM Lagrangian simulation of ball impacting a stationary plate. Plate and ball are created from bodies “cut out of” the mesh show above using PIR algorithm of Mosso et al.

Conclusions:

- Developing capability to more accurately treat multi-material cells in an “operator-split” ALE context.
- Capability builds on existing ALE infrastructure.
- Uses X-FEM ideas to provide unique kinematics for each material in a cell.
- Uses interface reconstruction rather than level-set ideas to address conservation and complex interface intersections.
- Demonstrates good convergence/accuracy for problems investigated here.