XFEM for Multi-Material Eulerian Solid/Hydrodynamics

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U.S. DEPARTMENT OF ENERGY

NNSA National Nuclear Security Administration

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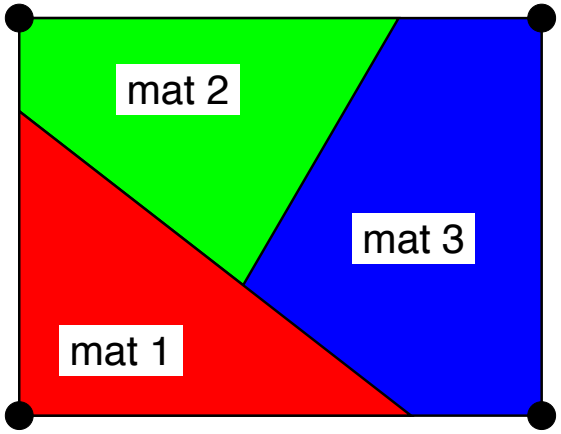
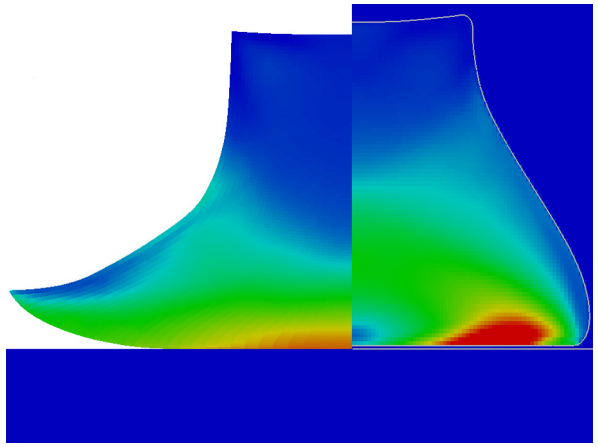
Introduction:

- 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:

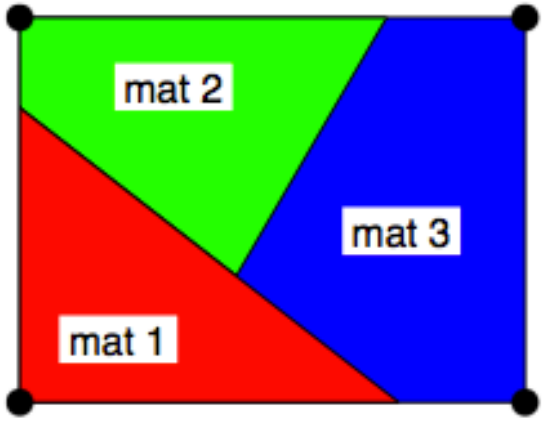
$$\mathbf{a}^n = \mathbf{M}^{-1}\left(\mathbf{f}_{ext}^n - \int \mathbf{B}^t \boldsymbol{\sigma}^n dV\right)$$

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

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

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

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

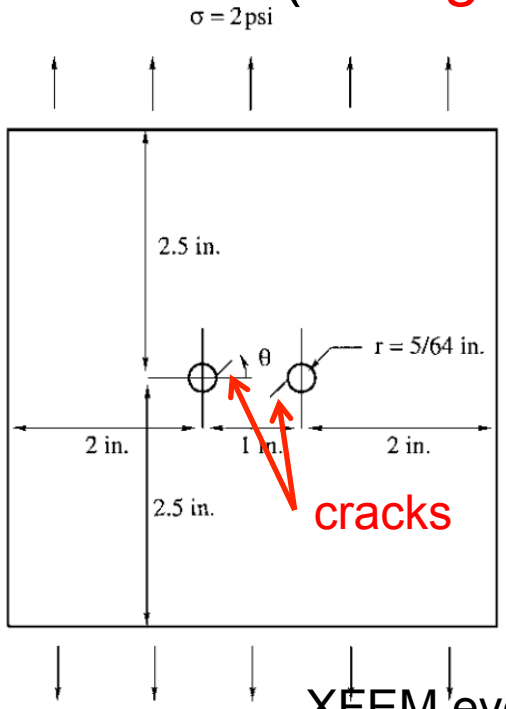


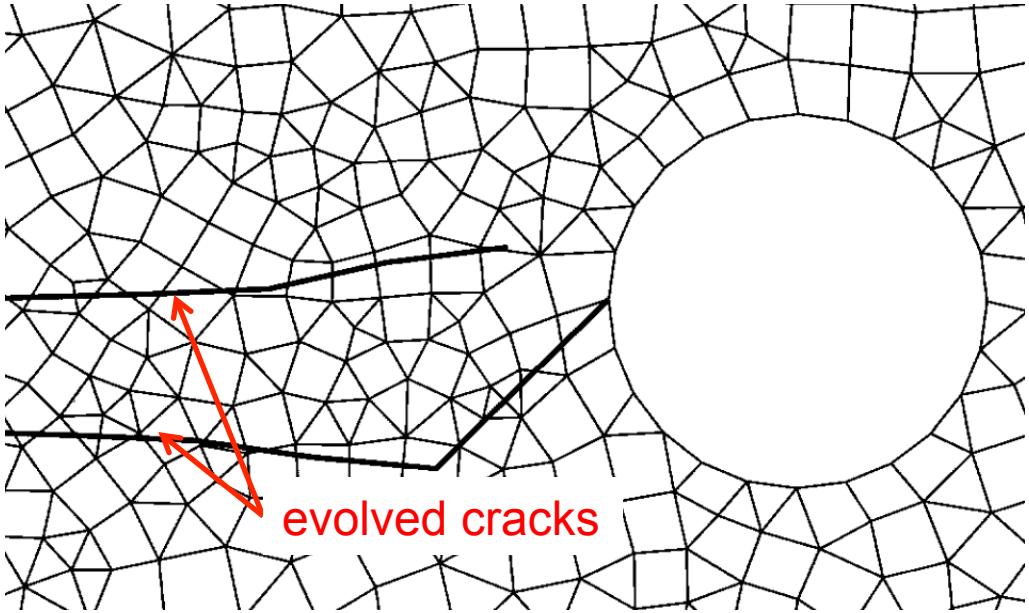
$$\mathbf{D}_m^e = \mathbf{D}^e$$

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

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)

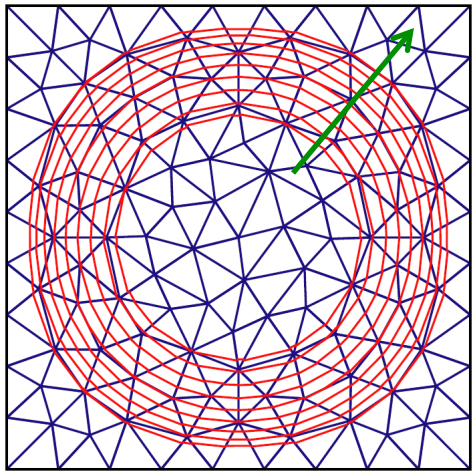




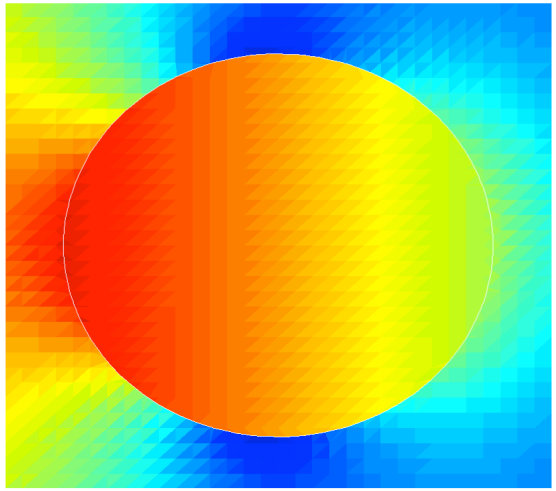
XFEM evolved cracks from MDB99

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.

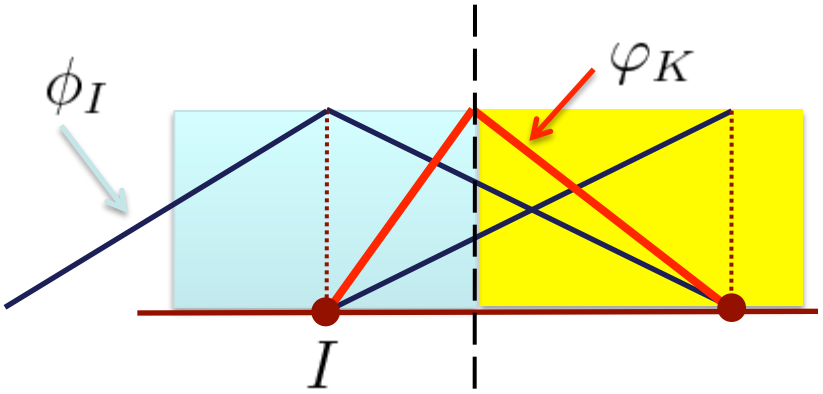
XFEM enrichments:

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

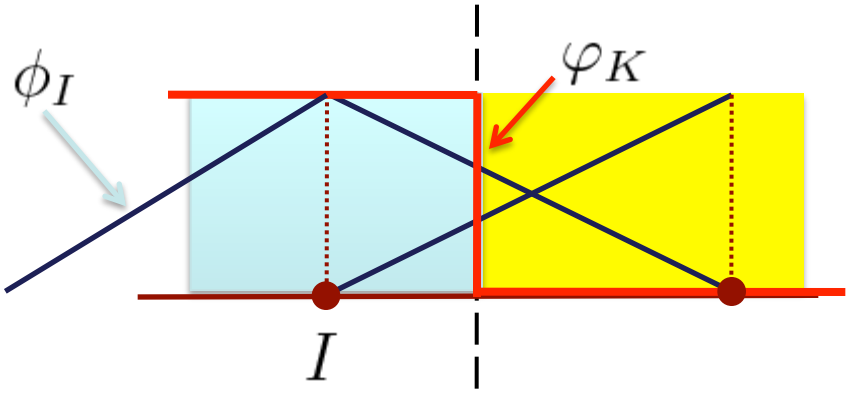
Standard FEM basis

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.

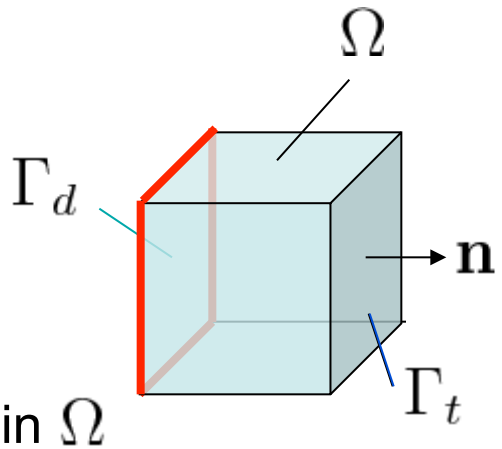
Requires discontinuity location:

- 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.

See Kramer and Mosso's talk for details.

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:

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

consider mass matrix

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

XFEM (consistent) mass matrix

For two materials we will want to use two “non-overlapping” Heaviside functions. One to “cover” the domain of each material.

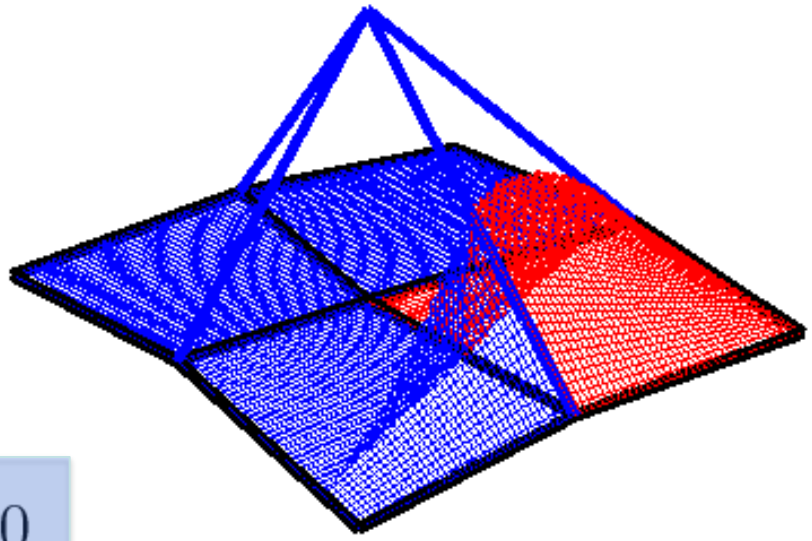
$$\mathbf{u}^h(\mathbf{x}) = \sum_I^{N_n} \left[\mathcal{H}^1(\mathbf{x}) \phi_I(\mathbf{x}) \mathbf{u}_I^1 + \mathcal{H}^2(\mathbf{x}) \phi_I(\mathbf{x}) \mathbf{u}_I^2 \right]$$

and the (consistent) Galerkin mass matrix is:

$$m^1_{I,J} = \int_\Omega \rho \phi_I \mathcal{H}^1 \phi_J \mathcal{H}^1 d\Omega$$

$$m^2_{I,J} = \int_\Omega \rho \phi_I \mathcal{H}^2 \phi_J \mathcal{H}^2 d\Omega$$

$$m^{12}_{I,J} = \int_\Omega \rho \phi_I \mathcal{H}^1 \phi_J \mathcal{H}^2 d\Omega = 0$$



No coupling between materials

Materials move independently:

Assume two materials for simplicity then the momentum equation is:

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

The element level versions of the above terms are:

internal forces:

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

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

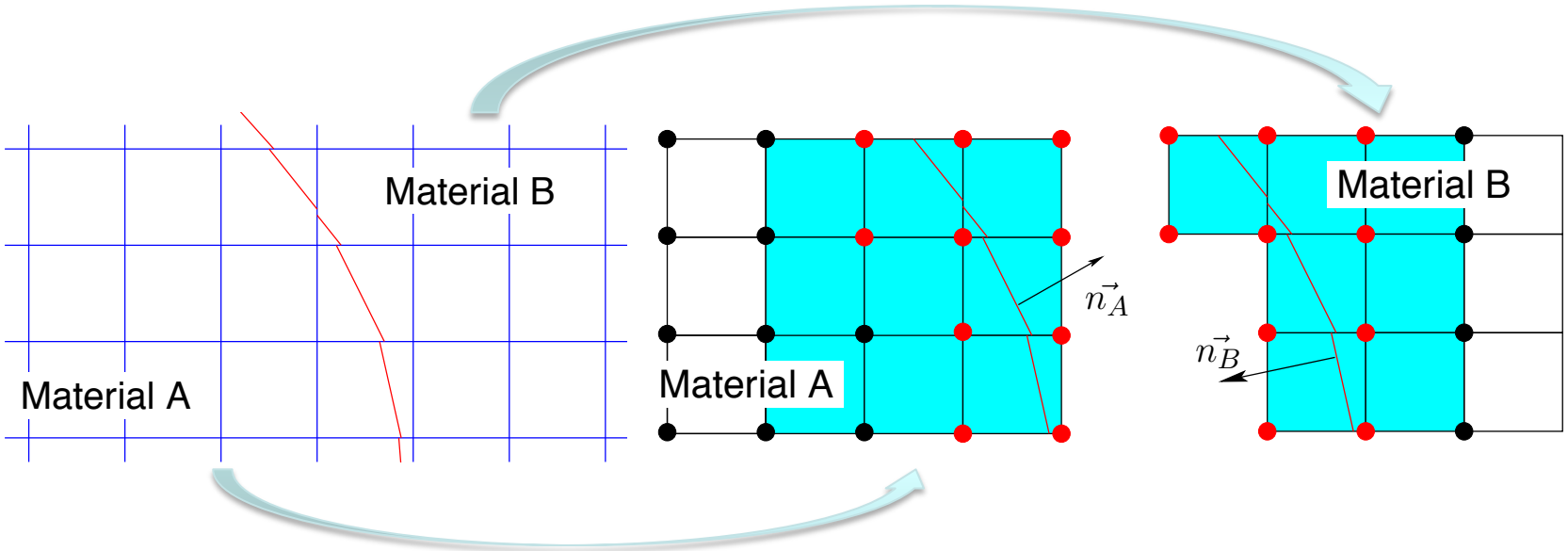
As stress for material 1 is only defined under Heaviside for material 1 (and vice-versa for material 2) we have:

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

No coupling between materials

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 (see C. Siefert's poster).

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

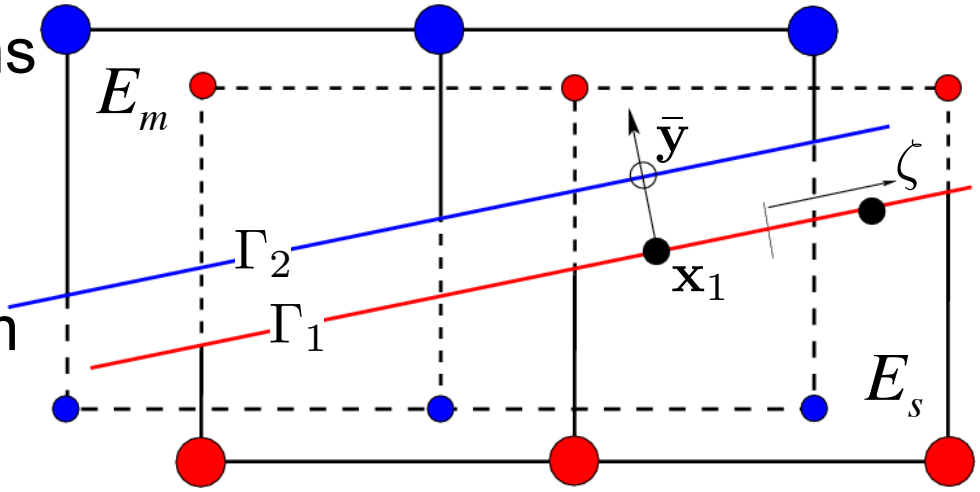
Constraint matrices

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

Velocity constraint

Lagrange Multipliers:

- Momentum residual is augmented with LM functional.
- Some essential components are:
  - Choice of basis functions
  - What to "enforce"
  - Finding interactions
  - Solving resultant system



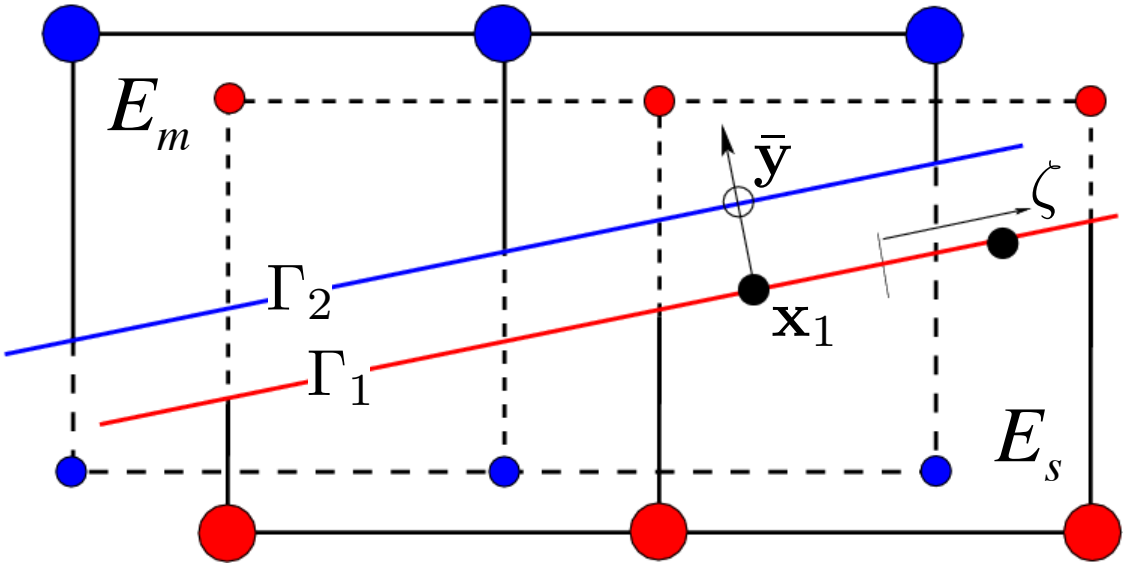
$$\Pi_c = \int_{\Gamma_c} \dot{g}\lambda d\Gamma$$

$$\delta\Pi_c = \int_{\Gamma_c} \delta\dot{g}\lambda d\Gamma + \int_{\Gamma_c} \dot{g}\delta\lambda d\Gamma = \delta\mathcal{P}_c + \delta\mathcal{C}$$

$$\dot{g}^h = \sum_I M_I(\zeta)\dot{g}_I \qquad \lambda^h = \sum_J Q_J(\zeta)\Lambda_J$$

$$\dot{g}^h(\mathbf{x}) = (\mathbf{v}_m(\bar{\mathbf{y}}) - \mathbf{v}_s(\mathbf{x})) \cdot \mathbf{n}$$

“Face-Face” strategy …



Quadrature and Lagrange Multiplier:

$$\mathcal{C} = \sum_{e \in \Gamma_1} \Lambda^e \sum_{q \in e} W_q j_q (\mathbf{v}_m(\bar{\mathbf{y}}_q) - \mathbf{v}_s(\mathbf{x}_q)) \cdot \mathbf{n}$$

$$\delta \mathcal{C}_e = (\mathbf{G}^t)_e \mathbf{v} = \sum_{q \in e} W_q j_q (\mathbf{v}_m(\bar{\mathbf{y}}_q) - \mathbf{v}_s(\mathbf{x}_q)) \cdot \mathbf{n} = \mathbf{0}$$

Enforcement phase:

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

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

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

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

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

contact forces

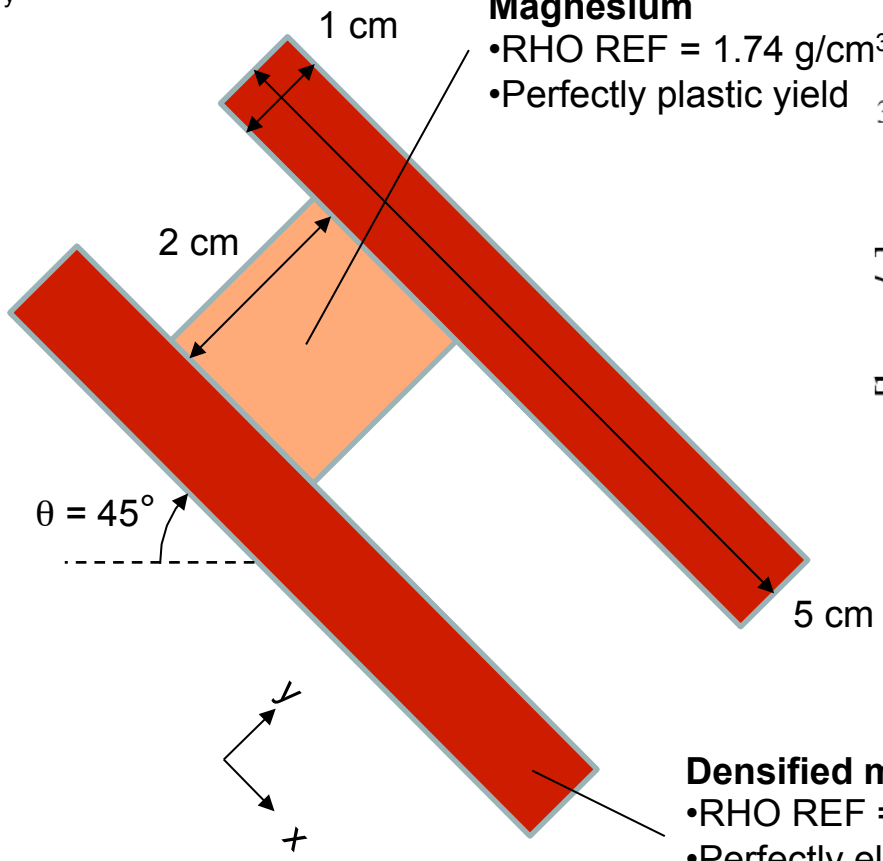
Remap Step:

- 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.

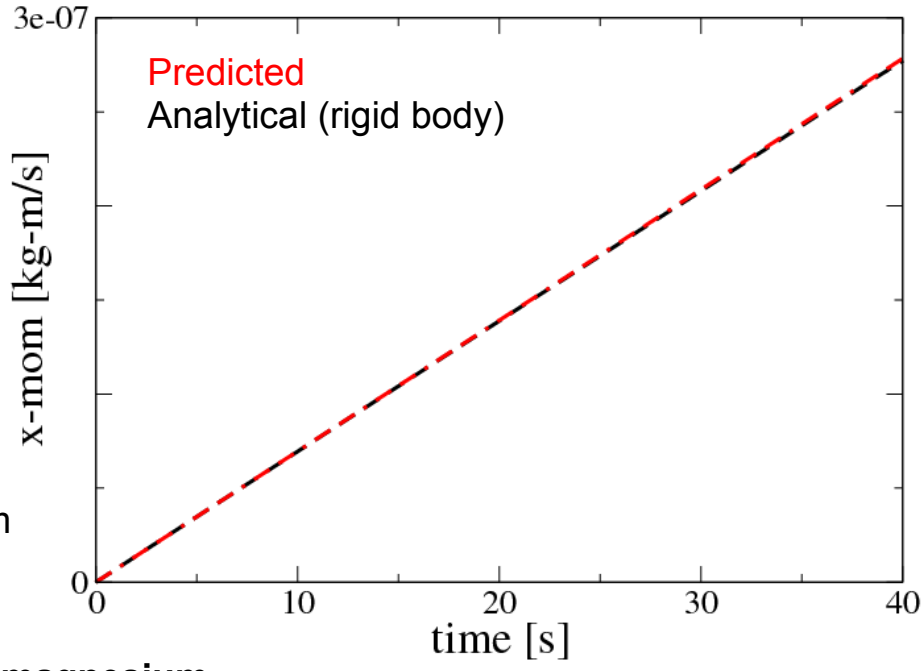
Sliding block:

body acceleration
$a_x = 1.0\times10^{-4}$ cm/s^2
$a_y = -1.0\times10^{-4}$ cm/s^2

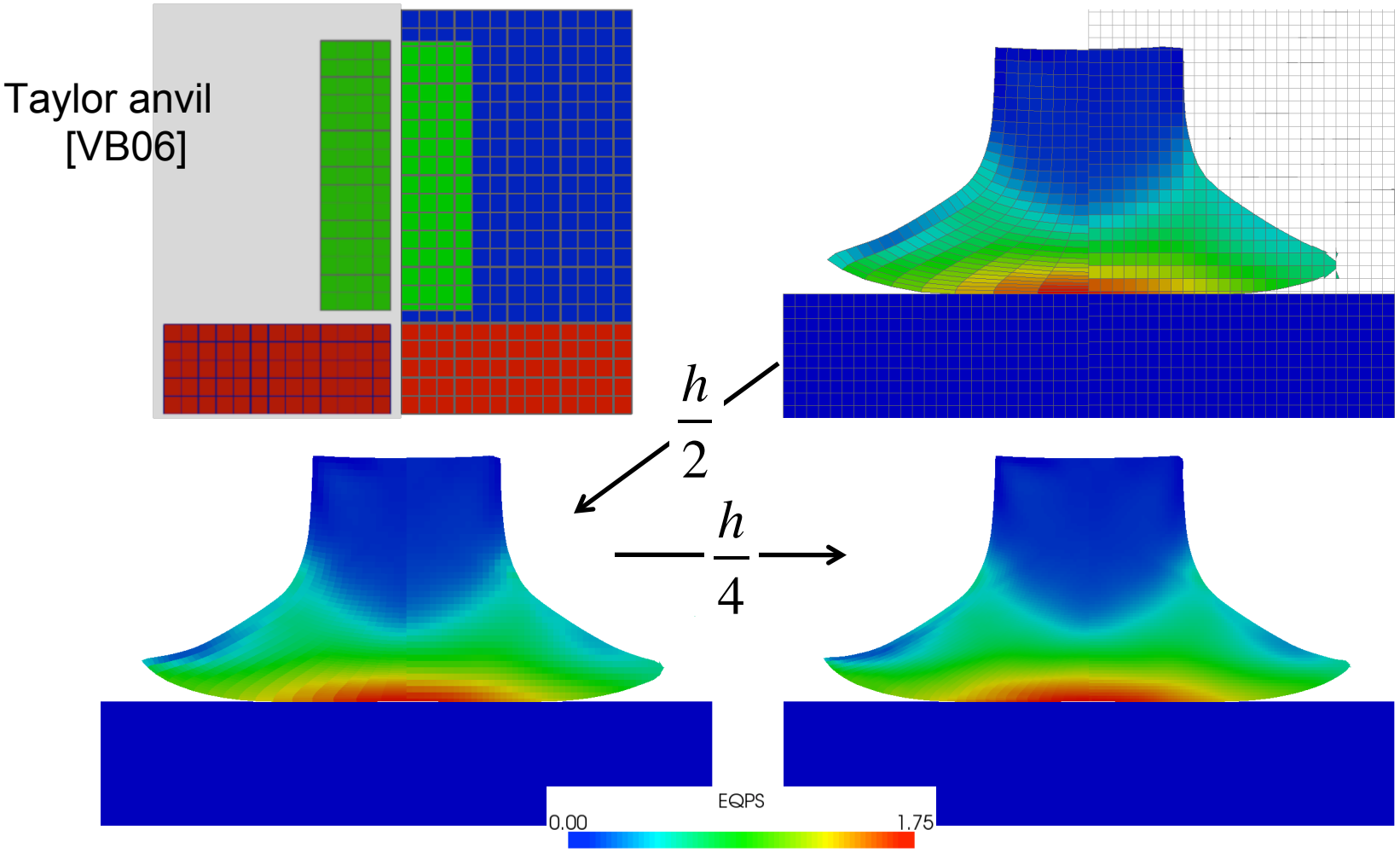


Magnesium
- RHO REF = 1.74 g/cm^3
- Perfectly plastic yield

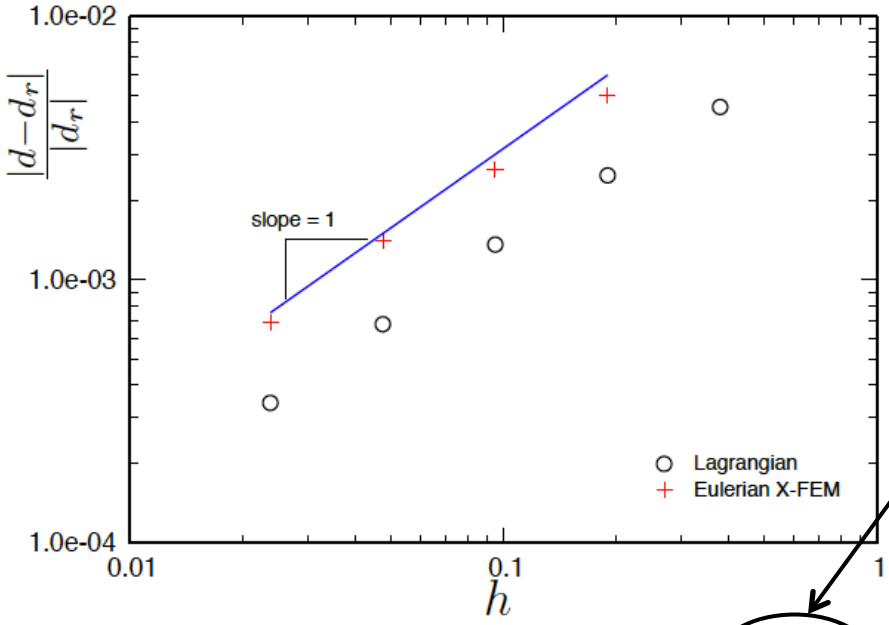
Densified magnesium
- RHO REF = 17.4 g/cm^3
- Perfectly elastic



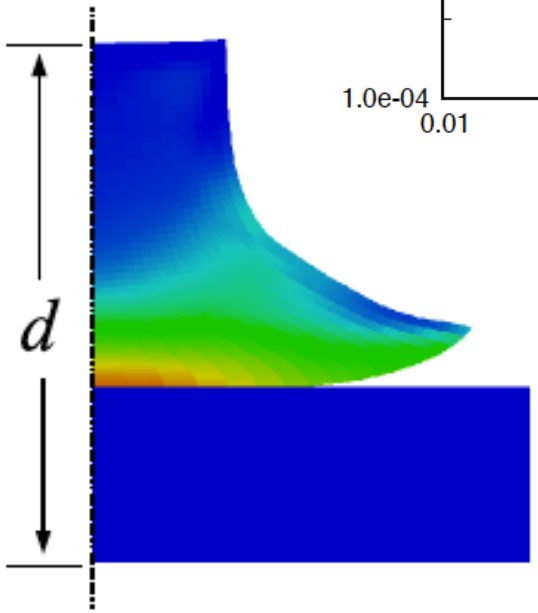
Lagrangian quality results:

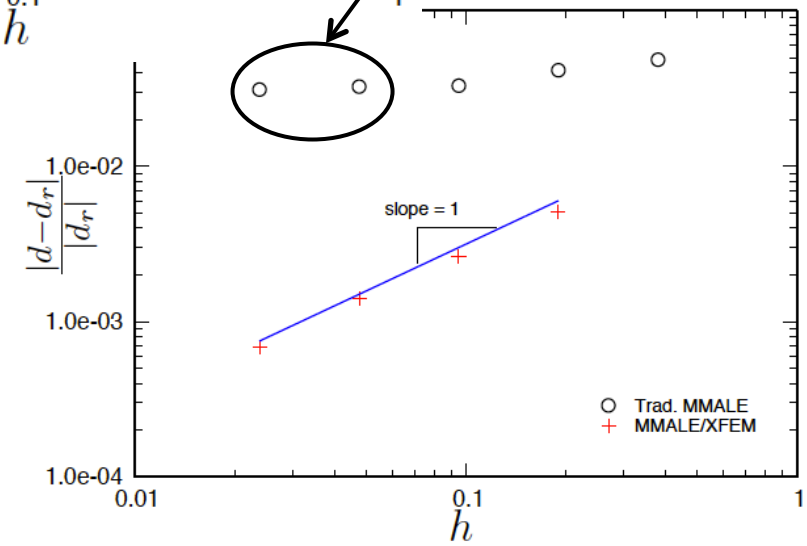


Eulerian gets wrong answer:



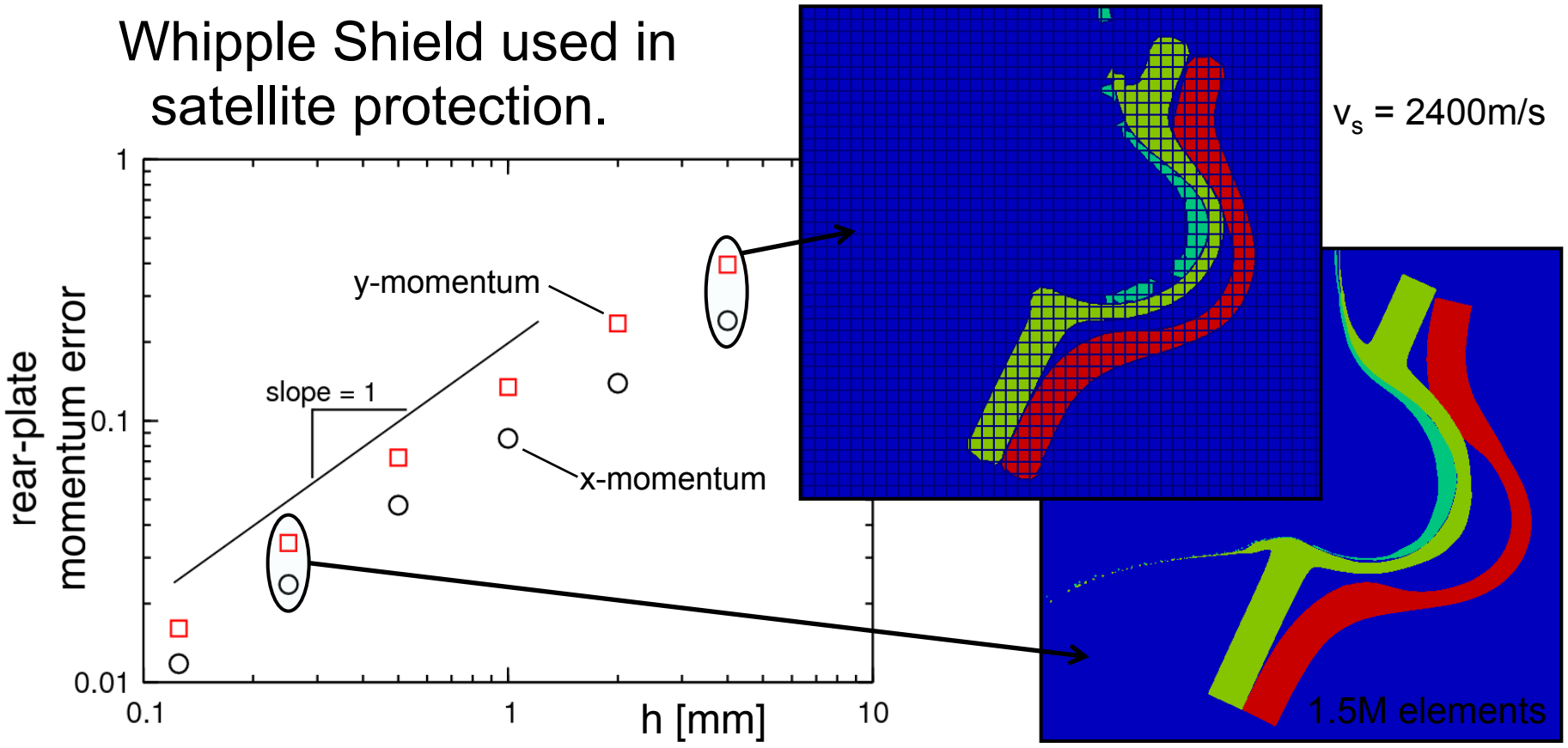
Standard Eulerian converges to a different solution.





Whipple shield example:

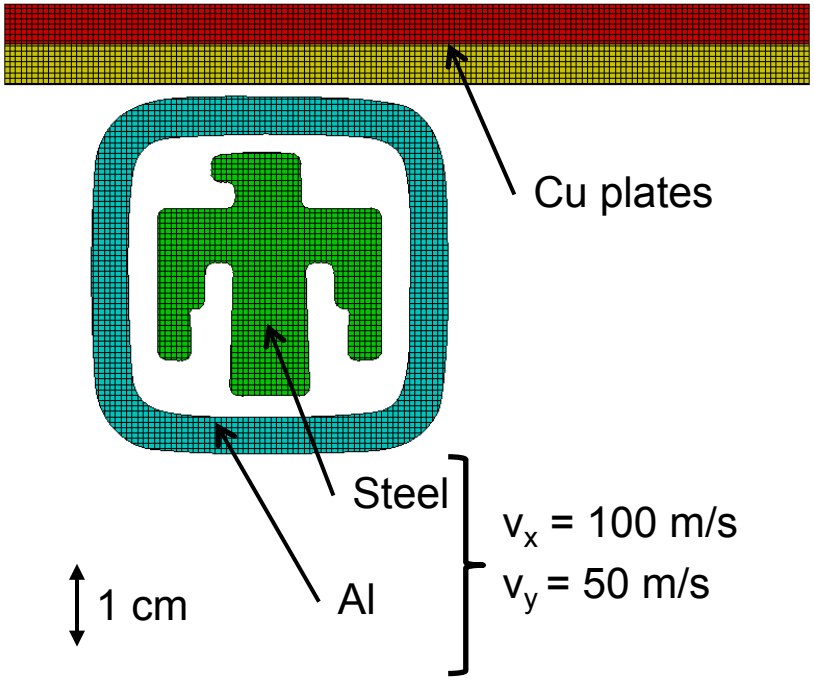
Whipple Shield used in satellite protection.

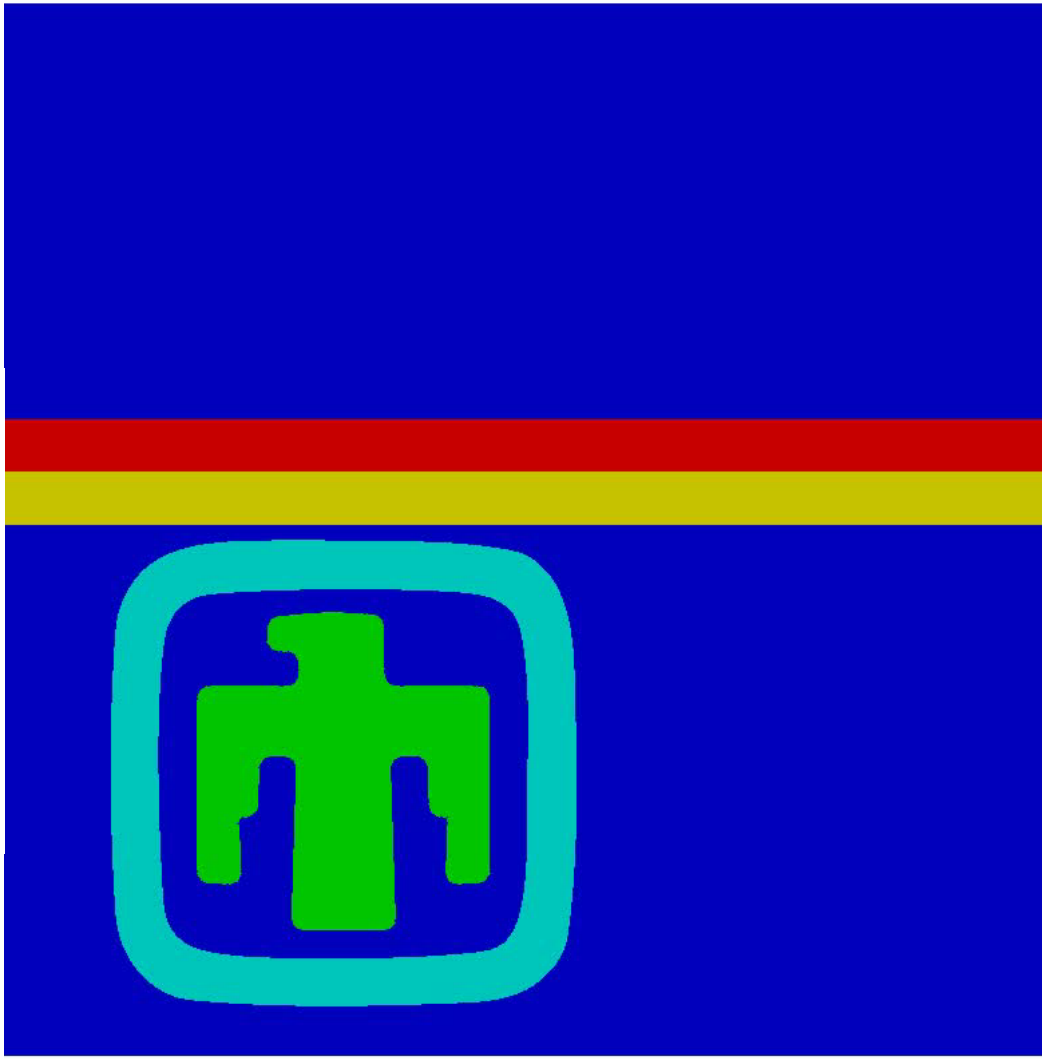


High-velocity impact difficult for Lagrangian and unrealistic for Eulerian are possible with X-FEM.

A more whimsical example:

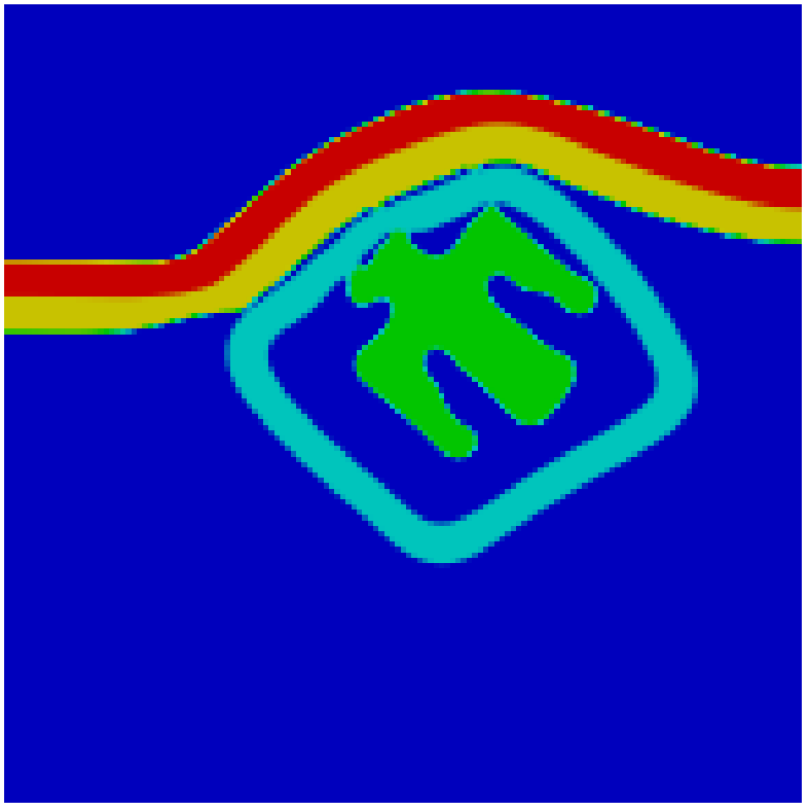
Logo with initial velocity impacts stationary, layered copper plates.



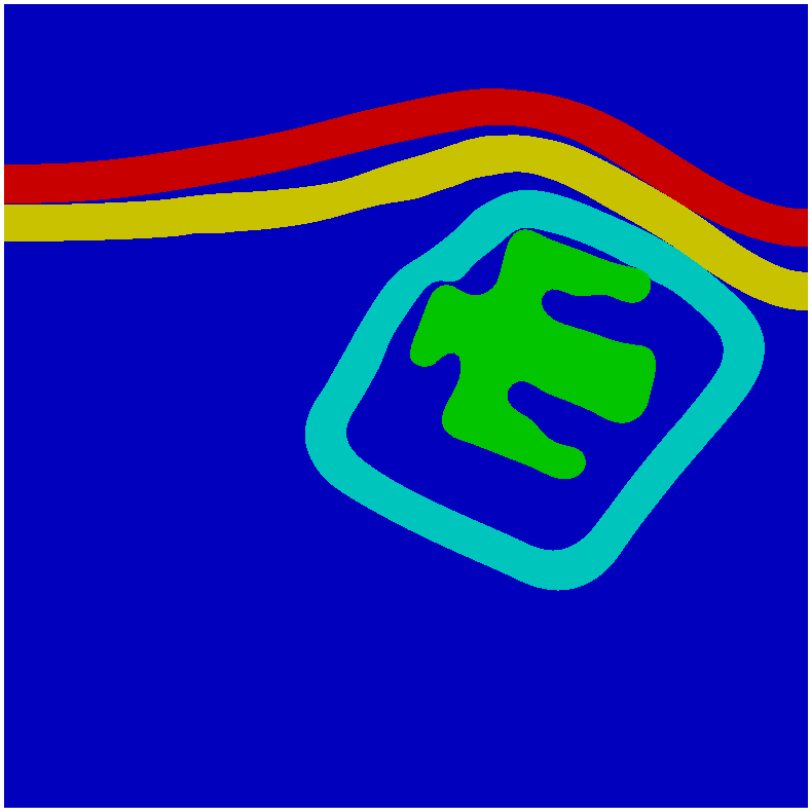


… and a comparison:

Standard approach



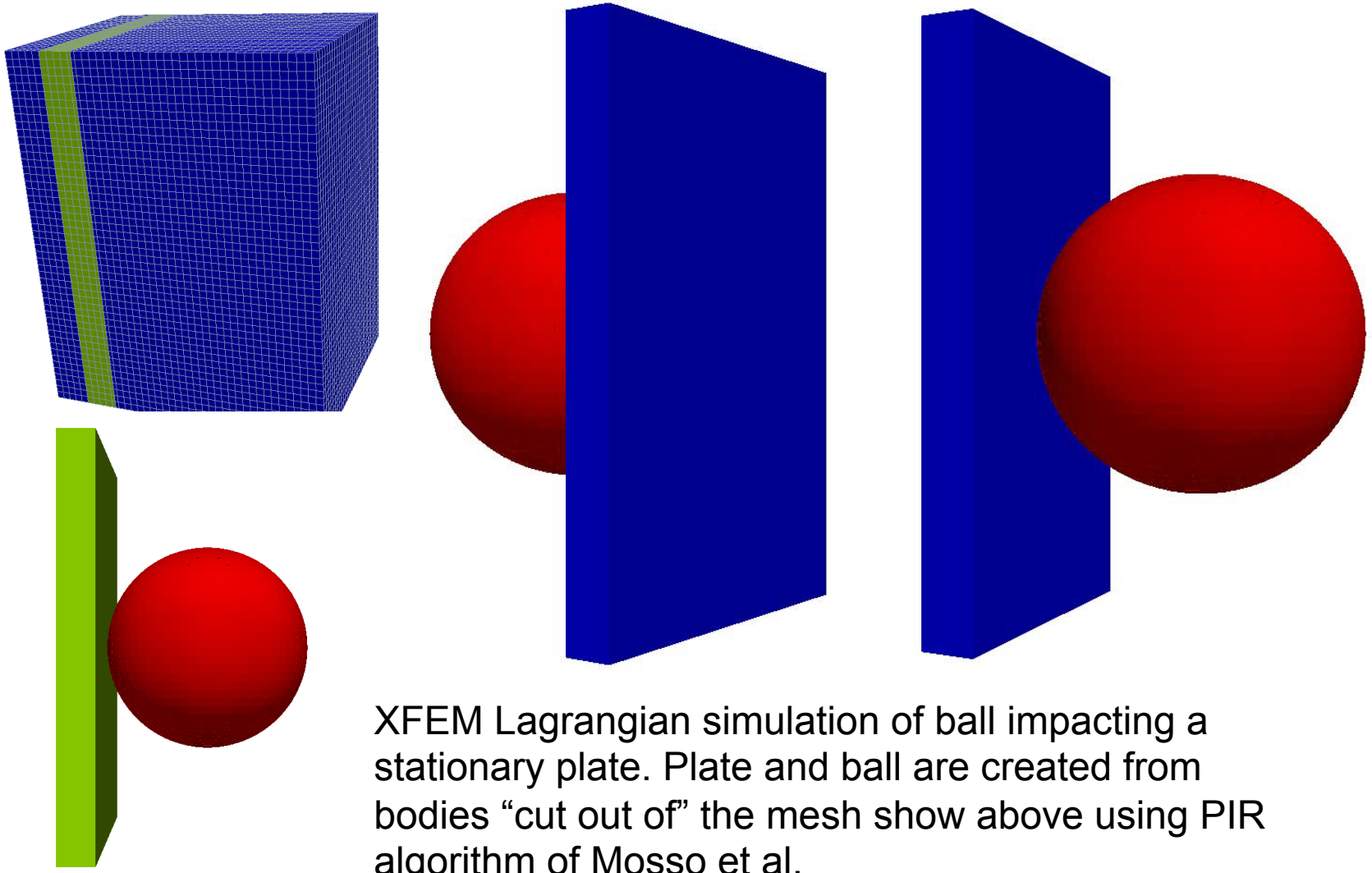
XFEM approach



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.

Hold Back Slides

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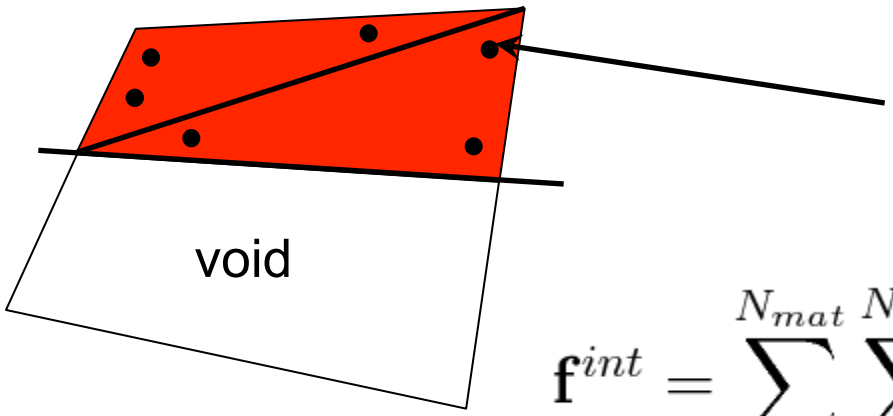
We use XFEM to …

Develop an Eulerian capability to treat intra-element interface behavior incorporating sound, realistic physics:

- as a true surface (not volumetric) phenomenon,
- with distinct velocity/displacement fields for each material in an element,
- while maintaining the advantages of ALEGRA's explicit-dynamics code-base,
- and capitalizing on our existing infrastructure.

Subdomain quadrature:

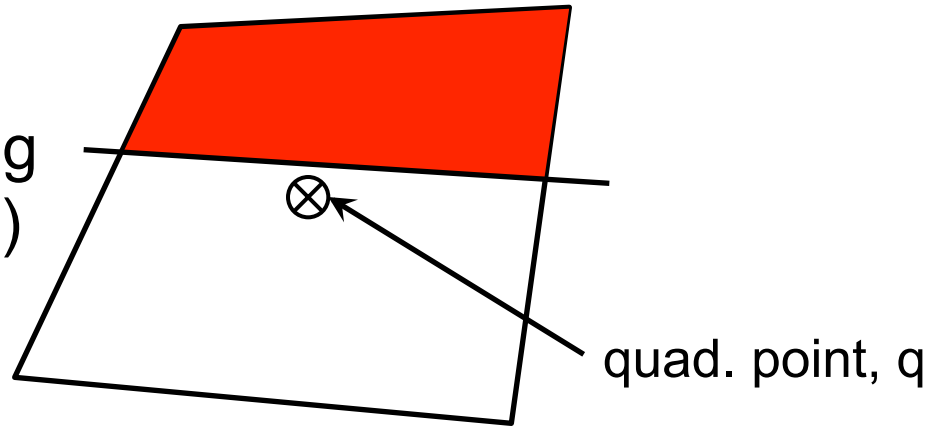


$$\mathbf{f}^{int} = \sum_{m=1}^{N_{mat}} \sum_{s=1}^{N_{sub}} \sum_{l=1}^{N_{gauss}} \left(\mathcal{H}_m \mathbf{B}^T \boldsymbol{\sigma}_m \, |J| \right)_l \cdot w_l$$

- Frequently used in literature but…
  - Overly stiff (subject to volumetric locking)
  - Requires tracking of state at many more points.
  - Many more material model evaluations (expensive).
- So, not practical in “real” code.

Using mean quadrature:

- Approach follows Song and Belytschko (2006)



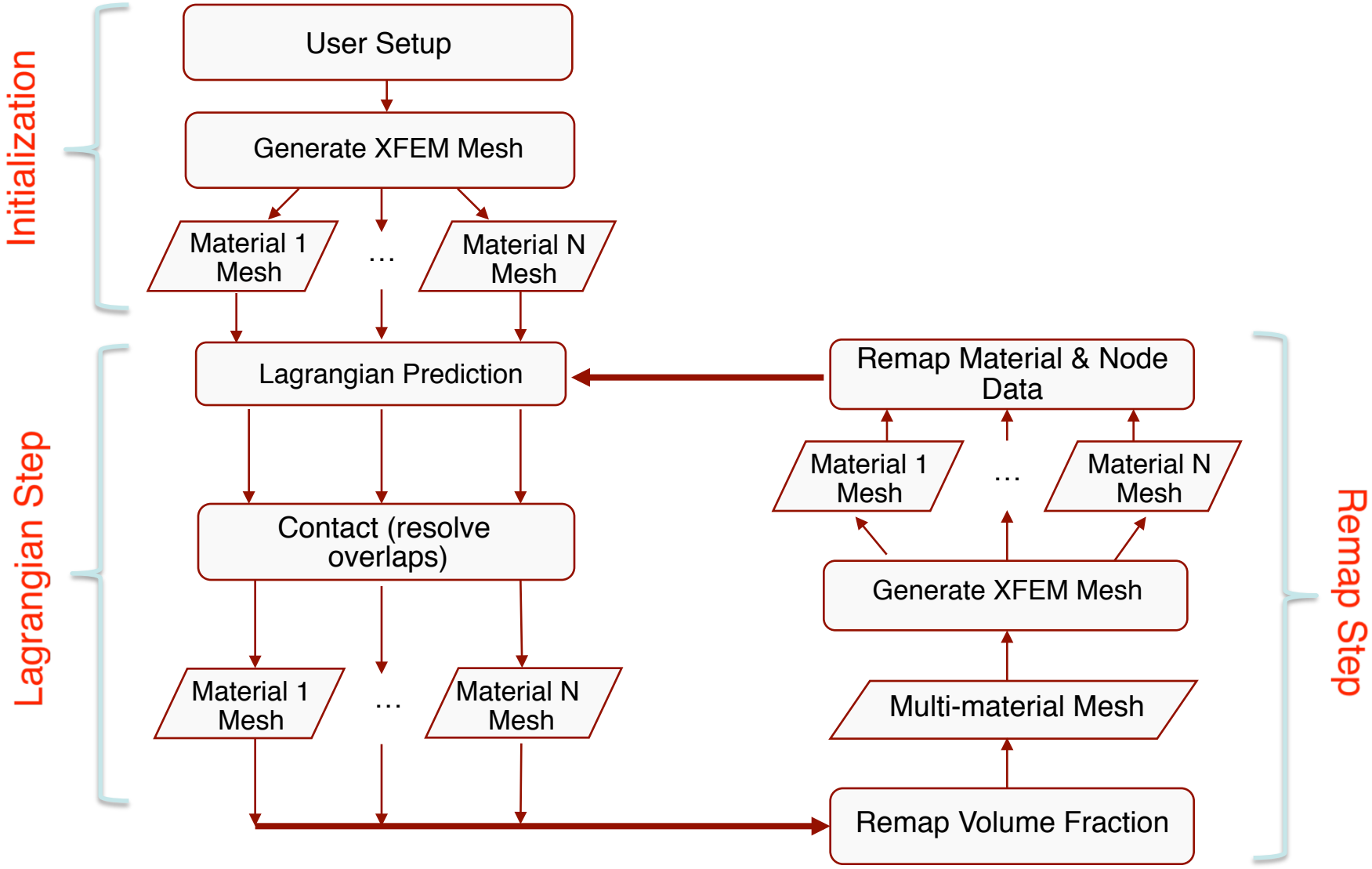
- Compute single-point result as if fully filled and scale by material volume fraction in cell/element:

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

$$\approx \frac{A_1}{A_e} \int_{\Omega^e} \mathbf{B}^T \boldsymbol{\sigma}_1 d\Omega^e$$

$$\approx \frac{A_1}{A_e} \left(\mathbf{B}^T \boldsymbol{\sigma}_1 |J| \right)_q \cdot w_q$$

Summary of algorithm flow:



Search phase:

- Search phase finds interactions between materials.
- Key to computing constraint matrices.
- Begins by solving unconstrained momentum equations to get predicted, t*, configuration.