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XFEM for Multi-Material Eulerian Solid/Hydrodynamics in ALEGRA

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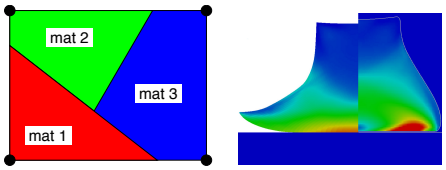
Motivation:

- Our Problems frequently require an Eulerian approach due to large vorticity.
- Traditional treatment of multi-material cells with unmixed materials and strength are arguably deficient for reasons that include:
  - They allow only a single velocity/displacement field per element.
  - They ignore interface mechanics such as sliding.



A multi-material cell and it's effect with ad-hoc treatment.

The Equations:

- ALEGRA is a Arbitrary Eulerian Lagrangian (ALE) code that can be used to solve for a range of coupled physics.
- Of interest here is the solution to the coupled conservation of mass, momentum and energy equations:

$$\frac{d}{dt}(\rho dv) = \frac{d}{dt}(dm) = 0 \qquad \rho\frac{d}{dt}\dot{\mathbf{u}} = \rho\ddot{\mathbf{u}} = \nabla\cdot\boldsymbol{\sigma} + \mathbf{f} \qquad \rho\frac{d}{dt}e = \boldsymbol{\sigma} : \mathbf{D}$$

- Specifically, ALEGRA uses the traditional "Operator-Split" approach:
  - First, take a Lagrangian step to solve the above equations.
  - Next, generate a new mesh. This is often call the "remesh step".
  - Finally, perform a data transfer step from the Lagrangian mesh to the new mesh. This is the "remap step" and generally imposes constraints that i) preserve energy and momentum and ii) enforce monotonicity in the data on the target mesh.

The Problem:

- The result of the remap step noted above is that more than one material may be present in an element (or computational cell). The result is that a closure model must be introduced as illustrated in the ALEGRA Lagrangian step as show:

Update acceleration with internal and external forces:

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

Integrate acceleration to get new velocity field:

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

Given the velocity field compute deformation measures:

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

Update (integrate in time) stress to new time given a material model, deformation measure and old stress:

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

Update (integrate in time) the internal energy:

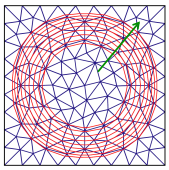
$$\epsilon_m^{n+1} = \epsilon_m^n + \Delta t \int \boldsymbol{\sigma}_m^n : \mathbf{D}_m^{n+\frac{1}{2}} dV$$

Some closure model is needed to compute mixed material deformation measures and stresses:

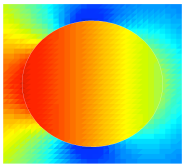
$$\mathbf{D}^e_m = \mathbf{D}^e$$
$$\boldsymbol{\sigma} = \sum_m \frac{V_m}{V}\boldsymbol{\sigma}_m$$

Solution --- The XFEM:

- Origins:
  - 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 and are often called strong discontinuities.
  - SIERRA/SM has implemented a robust XFEM crack mechanics treatment.
- Multi-material and moving interfaces:
  - The method was further developed to model other problems with evolving features.
  - These problems are often characterized by discontinuities in the field derivatives (e.g. temperature) and are referred to as weak discontinuities.
  - For moving interfaces (and particularly for explicit dynamics) the method has advantages over adaptively body-fitted meshes.



XFEM/VOF evolved phase-change interface (DMRV08)



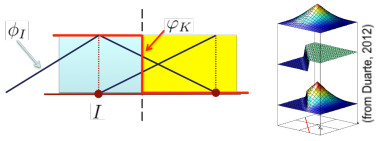
XFEM for magnetics with edge-based elements (SBKV13).

- The XFEM is a Partition-of-unity (POU) approach that constructs basis functions as products of standard FEM bases functions and local, enriched bases:

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

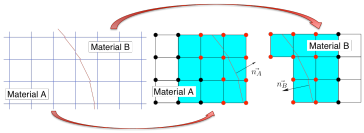
Standard FEM basis — enrichment(s)

- The XFEM seeks to capture discontinuities, hence enrichment functions are generally strongly or weakly discontinuous (often depending on the interface physics at hand).
- In our application it is convenient to use as an enrichment basis an Heaviside (or Indicator) function. Advantages include that it provides for a simple way of dealing with multiple interfaces in a cell and strong discontinuities at material interfaces.



(from Duarte, 2012)

- An advantage of Heaviside enrichment is that its application to our FEM physics discretization result in a single (partially filled) element for each material occupying a parent element as illustrated below:



- The result of this decomposition, in terms of the momentum equation and for a two material problem is two uncoupled momentum equations. Specifically, we have one momentum balance for each material.
- To ensure that the materials respond to one-another we add a contact constraint at the interfaces between materials:

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

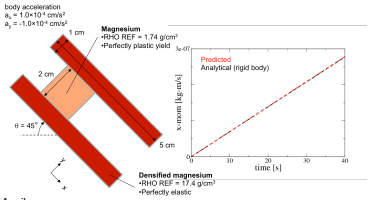
Lagrange multipliers

Constraint matrices

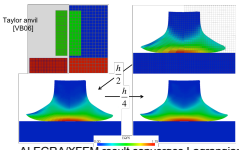
$\mathbf{G}_1^T\mathbf{v}_1^{new} + \mathbf{G}_2^T\mathbf{v}_2^{new} = 0$ Velocity constraint

Results

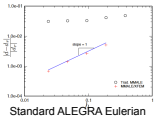
- Sliding Block:
  A problem with standard ad-hoc models for mixed cells in Eulerian calculations is that different materials in a cell will stick together. An example of the issue can be demonstrated with a block situated in a channel between two stationary blocks as illustrated below. Assuming the interface is frictionless the block should slide under the action of a gravitational field. A plot of ALEGRA/XFEM predicted versus analytical momentum is shown and clearly demonstrating the efficacy of the method.



- Taylor Anvil:
  A more complicated test problem is shown here. A deformable body strikes a rigid plate where the interface is assumed to be frictionless. Here we compare a body-fit Lagrangian calculation to an ALEGRA/XFEM simulation under several mesh refinements, again demonstrating the efficacy of the method. Note that while the ALEGRA/XFEM converges to the Lagrangian result, a standard ad-hoc mixed cell approach does not.

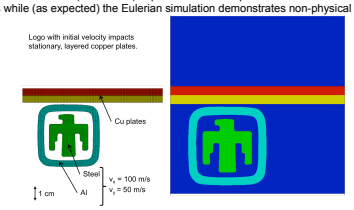


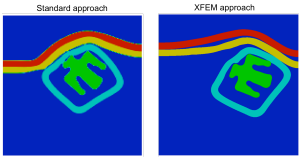
ALEGRA/XFEM result converges Lagrangian solution.



Standard ALEGRA Eulerian converges to a wrong solution.

- A more whimsical example:
  Here the ALEGRA/XFEM is compared to our standard ALEGRA Eulerian for a problem illustrated below. Specifically, the Sandia Thunderbird impacts a set of layered plates. Both simulations are performed for unfitted, Eulerian meshes. The ALEGRA/XFEM demonstrates clean (frictionless) separation between plates and thunderbird component parts while (as expected) the Eulerian simulation demonstrates non-physical "sticking."





Conclusion

A high-fidelity treatment of multi-material cells has been implemented in the ALEGRA shock hydrodynamics code. The capability builds on existing ALE infrastructure and uses XFEM ideas to provide unique kinematics for each material in a cell. The method uses interface reconstruction rather than level-set ideas to address conservation and complex interfaces intersections. Finally, the method demonstrates near Lagrangian accuracy for Eulerian calculations when interface physics are important.

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NNSA National Nuclear Security Administration