Lagrangian Models and Remapping Algorithms for 2D Multimaterial ALE Methods

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Overview

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    - Centroid tracking.
    - Artificial viscosity.
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  - III. Remapping.
    - Single Multimaterial Cell-Centered Quantity.
    - Complete Remapping of All Multimaterial Quantities.
- Numerical examples.
- Conclusion.
Introduction

- **Eulerian** methods – static mesh, mass flux through mesh edges.

- **Lagrangian** methods – mesh moving with fluid, no mass flux. Mesh can tangle.

- Combination – **ALE** – computational mesh moves with the fluid due to Lagrangian solver, Eulerian part (smoothing+remapping) keeps the mesh smooth.

- Multimaterial ALE – more than 1 materials allowed in each cell, amount defined by mass/volume fractions and position by material centroid.

- Lagrangian step and remapping step must provide new volume fractions and material centroids.

Multi-Material ALE Algorithm

Initialization

$t = 0$

$i = 0$

Main Program Loop

$t = t + \Delta t$

$i = i + 1$

LAGRANGIAN STEP
- update quantities
- update mesh
- update $\alpha_{c,(k)}$ and $\overline{z}_{c,(k)}$
- closure model

Mesh Smoothing

REMAPPING
- remap all cell quantities
- remap nodal momenta
- correct energy
- update $\alpha_{c,(k)}$ and $\overline{z}_{c,(k)}$
- closure model

Compute timestep $\Delta t$

End

if $(i > i_{\text{max}})$ or (bad_quality_mesh)

yes

no

Until $t < t_{\text{max}}$

no

End

MOMENT OF FLUID (MOF) METHOD
- Find pure material polygons
- Use information from one cell only
- Matches $\alpha_{c,(k)}$ exactly
- Matches $\overline{z}_{c,(k)}$ as accurate as possible

Single-Material Lagrangian Step

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Single-Material Lagrangian Step

\[ \frac{1}{\rho} \frac{d\rho}{dt} = -\nabla \cdot \mathbf{w}, \quad \rho \frac{d\mathbf{w}}{dt} = -\nabla \cdot \mathbf{p}, \quad \rho \frac{d\varepsilon}{dt} = -p \nabla \cdot \mathbf{w} \]

- Scalar quantities (density, pressure, internal energy) defined inside grid cells, vector quantities (positions, velocities) defined on grid nodes [Caramana, Burton, Shashkov, Whalen (JCP, 1998)], [Campbell, Shashkov (2000)].

- Based on evaluation of forces in each grid node.
  - Zonal pressure force – force from all neighboring grid cells to the node due to the pressure inside cells.
  - Viscosity force – adds artificial viscosity. Easy “bulk viscosity” based on Kuropatenko formula, or more complicated edge [Caramana, Shashkov, Whalen (JCP, 1998)] or tensor [Campbell, Shashkov (2000)] formulas.
  - Possibility to include other force sources, e. g. gravity.
Multimaterial Models

- Many models for multimaterial Lagrangian step, main difference basically in update of volume fractions.

- Model 1 – constant volume fractions $\alpha_{c,(k)}^{n+1} = \alpha_{c,(k)}^n$, simplest, allows to use material forces $F_{c,n,(k)}$ in energy update.

- Model 2 – pressure relaxation by solving system

$$\alpha_{c,(i)}^{n+1} = \alpha_{c,(i)}^n + \sum_j \alpha_{c,(i)}^{n+1} \alpha_{c,(j)}^{n+1} R(i,(j)) \frac{B(i)}{D},$$

where $R(i,(j)) = \left(p_{c,(i)}^{n+1} - p_{c,(j)}^{n+1}\right) + \left(A(j) - A(i)\right) \frac{V_{c}^{n+1} - V_{c}^n}{V_{c}^{n+1}}$, and $A(i) = \gamma(i) p_{c,(i)}^{n+1}$, $B(i) = \prod_{i\neq j} A(j)$, $D = \sum_j \alpha_{c,(j)}^{n+1} B(j)$

- Model 3 – volume fractions by movement of interface using acoustic Riemann solver $w_{c,(i),(j)} = \frac{w_{c,(i)} \alpha_{c,(i)}^n + w_{c,(j)} \alpha_{c,(j)}^n + p_{c,(i)}^n - p_{c,(j)}^n}{\rho_{c,(i)}^n s_{c,(i)} + \rho_{c,(j)}^n s_{c,(j)}}$, interface treated similarly as nodes.

- Other models – relaxation of temperature, entropy, ...
Multimaterial Lagrangian Step

- Multimaterial Lagrangian step computes all quantities and nodal positions in the next time level + new volume fractions and material centroids.

- No subzonal pressure forces for now.

- Algorithm:
  - \( P^n_{\mathcal{C},(k)} = \mathcal{P} \left( \gamma, P^n_{\mathcal{C},(k)}; \varepsilon^n_{\mathcal{C},(k)} \right), \)
  - \( P^n_{\mathcal{C}} = \sum_{(k)} \alpha^n_{\mathcal{C},(k)} P^n_{\mathcal{C},(k)} \)
  - \( F_{\mathcal{C},n}, F_{n} = \sum_{\mathcal{C} \in C(n)} F_{\mathcal{C},n}, F^q \)
  - \( w^{n+1}_n = w_n - \frac{\Delta t}{m_n} F_n, \)
  - \( w^{n+1/2}_n = (w^n_n + w^{n+1}_n)/2 \)
  - update volume fractions \( \alpha^{n+1}_{\mathcal{C},(k)} \)
  - \( z^{n+1}_n = z^n_n + \Delta t w^{n+1}_n \)
  - update cell volumes \( V^{n+1}_{\mathcal{C},(k)} = \alpha^{n+1}_{\mathcal{C},(k)} V^n_{\mathcal{C},(k)} \)
  - update material centroids \( z^{n+1}_{\mathcal{C},(k)} \)
  - \( \rho^{n+1}_{\mathcal{C}} = \frac{m_C}{V^{n+1}_{\mathcal{C}}}, \rho^{n+1}_{\mathcal{C}} = \frac{m_C}{V^{n+1}_{\mathcal{C},(k)}} \)
  - \( Q^p_{\mathcal{C}} = - \left( F_{\mathcal{C},n}, w^{n+1/2}_n \right), \)
  - \( Q^q_{\mathcal{C}} = - \left( F^q_{\mathcal{C},n}, w^{n+1/2}_n \right), \)
  - \( \varepsilon^{n+1}_{\mathcal{C},(k)} = \varepsilon^n_{\mathcal{C},(k)} - \frac{1}{m_{\mathcal{C},(k)}} \left( \frac{\Delta t Q^p_{\mathcal{C}}}{m_{\mathcal{C},(k)}} \alpha^{n+1}_{\mathcal{C},(k)} + \frac{\Delta t Q^q_{\mathcal{C}}}{m_{\mathcal{C},(k)}} \right) \left( \alpha^{n+1}_{\mathcal{C},(k)} - \alpha^n_{\mathcal{C},(k)} \right) \left( V^n_{\mathcal{C},(k)} p^{n+1/2}_{\mathcal{C}} \right) \)
  - \( \varepsilon^{n+1}_{\mathcal{C}} = \sum_{(k)} \frac{m_{\mathcal{C}}}{m_{\mathcal{C},(k)}} \varepsilon^{n+1}_{\mathcal{C},(k)} \)
Centroid Tracking

- From old and new nodal positions and volume fractions, and old material centroids, we need to compute new material centroids.

- Computing centroids in parametric space $\xi$, $\eta$ by inverting
  \[ z_{c, (k)}^n = (1 - \xi) (1 - \eta) z_{n1}^n + \xi (1 - \eta) z_{n2}^n + \xi \eta z_{n3}^n + (1 - \xi) \eta z_{n4}^n \]

- Suppose, position in parametric space does not change, find new centroid using
  \[ z_{mid, (k)}^n = (1 - \xi) (1 - \eta) z_{n1}^{n+1} + \xi (1 - \eta) z_{n2}^{n+1} + \xi \eta z_{n3}^{n+1} + (1 - \xi) \eta z_{n4}^{n+1} \]

- Use MOF algorithm [Ahn, Shashkov (JCP, 2007, In press)] to perform material reconstruction from $z_{c, (k)}^{mid}$ and $\alpha_{c, (k)}^{n+1}$.

- Find real centroids $z_{c, (k)}^{n+1}$ from reconstructed pure MOF polygons.
Artificial Viscosity

- Not clear how to compute viscosity forces for each material.
- Walk-around – compute common viscosity forces (from common quantities) and redistribute them to materials by mass fractions. Corresponding to mass weighted heating distribution.
- This approach allows to use all standard single-material viscosity approaches – bulk, edge, or tensor viscosity forces, using average common quantities in it.
- Multimaterial viscosity must be specially treated in energy equation (coming from multimaterial volume divergence):
  \[
  \varepsilon_{C,(k)}^{n+1} = \varepsilon_{C,(k)}^{n} - \frac{1}{m_c} \left( \Delta t Q_{C}^{p} \alpha_{C,(k)}^{n+1} + \Delta t Q_{C}^{q} \frac{m_{C,(k)}}{m_c} + \left( \alpha_{C,(k)}^{n+1} - \alpha_{C,(k)}^{n} \right) V_{C}^{n} p_{C}^{n+1/2} \right)
  \]
  - For single material cell it reduces to standard form.
Mesh Rezoning

Example of disturbed and smoothed meshes by RJM method
Multimaterial Remapping of Single Quantity

- **Given:** Lagrangian \( \{c\} \) and rezoned \( \{\tilde{c}\} \) meshes, volume fractions \( \alpha_{c,(k)} \) and material centroids \( z_{c,(k)} \) in Lagrangian cells.

- **Given:** Mean values \( g_{c,(k)} = \frac{G_{c,(k)}}{V_{c,(k)}} \) of unknown underlying function
  \( g = \rho \), \( g = \rho u \), \( g = \rho \left( \varepsilon + \frac{1}{2} \| w \|^2 \right) \).

- **Goal:** Find masses \( G_{\tilde{c},(k)} = \int g(z) \, dV \) and mean values
  \( g_{\tilde{c},(k)} = \frac{G_{\tilde{c},(k)}}{V_{\tilde{c},(k)}} \) in rezoned cells such that the algorithm is accurate, conservative, and linearity-preserving \((\forall (k))\).

- **Goal:** Find new volume fractions \( \alpha_{\tilde{c},(k)} \) and centroids \( z_{\tilde{c},(k)} \) for each material in new cells.

- Our method based on piecewise-linear reconstruction and exact integration (using intersections).
Single Quantity – Reconstruction

- **Piecewise-linear reconstruction**
  
  \[ g_{C,k}(x, y) = g_{C,k} + \left( \frac{\partial g}{\partial x} \right)_{C,k} (x - x_{C,k}) + \left( \frac{\partial g}{\partial y} \right)_{C,k} (y - y_{C,k}). \]

- **Slopes (explicit formulae) from minimization of functional**

  \[ F \left( \left( \frac{\partial g}{\partial \{x, y\}} \right)_{C,k}^\text{unlim} \right) = \sum_{C' \in C(C)} \left( g_{C',k} - \frac{\int_{C'} g_{C,k}(z) dV}{V_{C'}} \right)^2. \]

- **Barth-Jespersen Limiter**

  \[ \left( \frac{\partial g}{\partial \{x, y\}} \right)_{C,k}^\text{BJ} = \Phi_{C,k} \left( \frac{\partial g}{\partial \{x, y\}} \right)_{C,k}^\text{unlim}, \quad \Phi_{C,k} = \min_{n \in N(C)} \Phi_{C,k}^n, \]

  \[ \Phi_{C,k}^n = \begin{cases} 
  \min \left\{ 1, \frac{g_{C,k}(n) - g_{C,k}}{g_{C,k}^\text{unlim}(n) - g_{C,k}} \right\} & \text{for } g_{C,k}(n) - g_{C,k} > 0 \\
  \min \left\{ 1, \frac{g_{C,k}^\text{unlim}(n) - g_{C,k}}{g_{C,k}(n) - g_{C,k}} \right\} & \text{for } g_{C,k}(n) - g_{C,k} < 0 \\
  1 & \text{for } g_{C,k}(n) - g_{C,k} = 0 
\end{cases} \]

Remapping – Reconstruction

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Single Quantity – Integration

• Exact integration using intersections.
• For each cell \(c\), perform MOF material reconstruction to get polygons of pure materials \(P_{c}(k)\).
• Find intersection of pure polygon \(P_{c}(k)\) with each new neighboring cell \(\tilde{c}' \in C(\tilde{c})\), \(I(P_{c}(k), \tilde{c}')\).
• Compute mass in intersections \(G_{I(P_{c}(k), \tilde{c}')} = \int g_{c}(k)(z) \, dV = g_{c}(k) A_{1} + \left( \frac{\partial g}{\partial x} \right)_{c}(k) \left( A_{x} - x_{c}(k) A_{1} \right) + \left( \frac{\partial g}{\partial y} \right)_{c}(k) \left( A_{y} - y_{c}(k) A_{1} \right)\),
  where \(A_{f} = \int f \, dV\).
• Update mass \(G_{\tilde{c}'}(k)\) in new cell \(\tilde{c}'\) by adding the mass \(G_{I(P_{c}(k), \tilde{c}')}\), and integrals \(J^{\{1,x,y\}}_{\tilde{c}'}(k)\) by adding \(A_{1}, A_{x}, A_{y}\).
• New volume \(V_{\tilde{c}'}(k) = J^{1}_{\tilde{c}'}(k)\), volume fraction \(\alpha_{\tilde{c}'}(k)\), material centroid \(\{x, y\}_{\tilde{c}'}(k) = J^{\{x,y\}}_{\tilde{c}'}(k) / J^{1}_{\tilde{c}'}(k)\), and new density \(g_{\tilde{c}'}(k) = G_{\tilde{c}'}(k) / J^{1}_{\tilde{c}'}(k)\).
Multimaterial Remapping of Complete Set of Quantities

- Remap (using previous algorithm) to get new $\tilde{V}_c(k)$, $\tilde{z}_c(k)$, $\tilde{\alpha}_c(k)$.
- Identify cell status from $\tilde{\alpha}_c(k)$ (SM/MM cell, materials, ...).
- Remap $\rho_c(k) \Rightarrow \tilde{\rho}_c(k)$, $m_c(k)$.
- Old nodal momenta $\mu_n = m_n \mathbf{w}_n$ and nodal kinetic energy $E_k_n = \frac{1}{2} m_n (u_n^2 + v_n^2)$.

- Compute exchange mass between pure polygons $P_c(k)$ (from MOF) of each material $(k)$ of $c$ and all new neighbors $\tilde{c}' \in C(\tilde{c})$:
  $$\delta m_{c(k),\tilde{c}'} = \int_{P_c(k) \cap \tilde{c}'} \rho_{c(k)}(\mathbf{z}) \, dV - \int_{P_{c'}(k) \cap \tilde{c}} \rho_{c'}(\mathbf{z}) \, dV.$$  

- Extension of mass change among nodal regions from [Pember, Anderson (2000)]:
  $$\delta m_{\rightarrow n,c} = \frac{1}{8} \sum_{i=1}^{4} \delta m_{\rightarrow i}, \quad \delta m_{\uparrow n,c} = \frac{1}{8} \sum_{i=1}^{4} \delta m_{\uparrow i},$$  $$\delta m_{/ n,c} = \frac{1}{4} \sum_{i=1}^{2} \delta m_{/ i}.$$
Multimaterial Remapping of Complete Set of Quantities

- Nodal mass \( m_{\tilde{n}} = m_{n} + \sum_{c \in C(n)} \left( \delta m_{n,c} + \delta m_{\uparrow n,c} + \delta m_{\rightarrow n,c} \right) \).

- Reconstruct velocity in centers of nodal swept regions by interpolation from nodal values \( \Rightarrow w_{\rightarrow n,c}, w_{\uparrow n,c}, w_{\rightarrow n,c} \).

- Remap momenta \( \mu_{\tilde{n}} = \mu_{n} + \sum_{c \in C(n)} \left( \delta m_{n,c} w_{\rightarrow n,c} + \delta m_{\uparrow n,c} w_{\uparrow n,c} + \delta m_{\rightarrow n,c} w_{\rightarrow n,c} \right) \).

- New velocity \( w_{\tilde{n}} = \mu_{\tilde{n}} / m_{\tilde{n}} \).

- New kinetic energy \( \overline{Ek}_{\tilde{n}} = \frac{1}{2} m_{\tilde{n}} \left( u_{n}^{2} + v_{n}^{2} \right) \), and remapped kinetic energy \( Ek_{\tilde{n}} = Ek_{n} + \sum_{c \in C(n)} \left( \frac{1}{2} \delta m_{n,c} \left( |w_{\rightarrow n,c}|^{2} \right) + \frac{1}{2} \delta m_{\uparrow n,c} \left( |w_{\uparrow n,c}|^{2} \right) + \frac{1}{2} \delta m_{\rightarrow n,c} \left( |w_{\rightarrow n,c}|^{2} \right) \right) \).

- Kinetic energy discrepancy \( \delta Ek_{\tilde{n}} = Ek_{\tilde{n}} - \overline{Ek}_{\tilde{n}} \) in each node.
Multimaterial Remapping of Complete Set of Quantities

- Redistribute nodal kinetic energy discrepancy $\delta E k_{\tilde{n}}$ into materials $(k)$ of all adjacent cells $\tilde{c} \in C(\tilde{n})$:

$$\delta E k_{\tilde{n}, \tilde{c}, (k)} = \left( \frac{m_{\tilde{c}}}{\sum_{\tilde{c} \in C(\tilde{n})} m_{\tilde{c}}} \right) \alpha_{\tilde{c}, (k)} \delta E k_{\tilde{n}}$$

- Remap (using single quantity algorithm) old density of internal energy $e_{\tilde{c}, (k)} = \rho_{\tilde{c}, (k)} \varepsilon_{\tilde{c}, (k)}$ to get new internal energy $Ei_{\tilde{c}, (k)}$.

- Repair internal energy according to kinetic energy discrepancy

$$\widetilde{E}i_{\tilde{c}, (k)} = Ei_{\tilde{c}, (k)} + \sum_{\tilde{n} \in N(\tilde{c})} \delta E k_{\tilde{n}, \tilde{c}, (k)}$$

to ensure energy conservation.

- Specific internal energy $\varepsilon_{\tilde{c}, (k)} = \frac{\widetilde{E}i_{\tilde{c}, (k)}}{m_{\tilde{c}, (k)}}$, $\varepsilon_{\tilde{c}} = \frac{\sum_{\forall (k)} \varepsilon_{\tilde{c}, (k)} m_{\tilde{c}, (k)}}{\sum_{\forall (k)} m_{\tilde{c}, (k)}}$. 
Numerical Example – Rayleigh-Taylor Instability

- Disturbed interface of heavy on top of light one, gravity.

![Graphs showing the progression of Rayleigh-Taylor Instability over time.]

- Lagrangian fails soon, ALE continues.
Numerical Example – Sulfur Hexafluoride Cylinder


- Deposition of shock energy to vorticity.

![Numerical Example – SF6 Cylinder](image-url)
Conclusion

- Lagrangian models generalized to multimaterial case.
- Developed multimaterial remapping.
- Developed tracking of centroids and new volume fractions estimate in both Lagrangian and remapping stages.
- All methods implemented to research multimaterial ALE code.
- Code produces reasonable results for multimaterial simulations.

Future Work

- Anti-hourglass stabilization [Scovazzi, Love, Shashkov (2007)].
- More complicated EOS different for each material.
- Try more multimaterial Lagrangian models.