Moment of Fluid Interface Reconstruction

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Outline

1. Introduction
   - Interface Capturing
   - VOF overview

2. Moment of Fluid (MOF) Formulation
   - Problem Formulation
   - Analysis of MOF optimization problem

3. Implementation of MOF Algorithm

4. MOF vs. VOF comparisons
   - Static Tests
   - Dynamic Tests
   - Multi-material interfaces

5. Summary
Why do we care about interfaces?

- When modeling multiple fluids, we want to know where one fluid stops and the other begins.
- May want to use different EOS models/model equations.
- Need the interface to properly calculate physical properties (i.e., surface tension, etc...).
- Want to limit non-physical behaviors.
Current Interface Capturing Techniques

Current Popular Interface Capturing Methods:
- Level Set Method
- Volume of Fluids (VOF)
- Front-Tracking
VOF Main Ideas

- High level overview of VOF
  - Reconstruct interface every timestep
  - Track the volume fraction of the primary fluid (assuming only 2 fluids)
  - Identify a PLIC (Piecewise-Linear Interface Construction) for each cell
VOF PLIC Methods

- Some ways to generate the PLIC for a cell using VOF
  - Gradient of volume fraction function
  - Common linear interface for a cluster of cells
  - Average normals of surrounding cells
VOF Drawback

So what is the major drawback of the described methods?
- Need surrounding cells data to construct the interface in the current cell

![Figure: 3 current VOF algorithms attempting to reconstruct zigzags of varying sizes](image)

*Figure:* 3 current VOF algorithms attempting to reconstruct zigzags of varying sizes
So how do we improve on this drawback?
- Track both the volume fractions and the centroids of the primary fluid

Benefits:
- Resolve interface details as small as grid
- Only require current cell data, so grid structure not important
- Identical treatment for interior or boundary cell

Figure: MOF algorithm reconstructing zigzags of varying sizes
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5. Summary
∑ ⊂ ℝ² is a mixed cell
ω ⊂ ∑ is a non-trivial cell fraction occupied by a single component
F∑ is the family of all non-trivial open subsets of ∑
∑c(ω) is the centroid of ω
µ(ω) is the volume fraction of the component in ω
Γ(ω) is the interface between ω and ω'
Fh∑ is the class of F∑ where the interface is linear
ωh ∈ Fh∑ is a cell fraction represented by a linear interface
Ideal Formulation

- Let $\Omega$ contain only two fluid components
- Let $\omega^*$ be the true cell fraction occupied by the tracked component
- Goal: Find a $\omega_h^* \in F^h_{\Omega}$ which matches $\mu^*$ and $\vec{x}_c(\omega^*)$
- However, it is unrealistic to match both exact properties with a PLIC
Matching centroids exactly

- What if we decide to match the centroids exactly?
- Cannot guarantee we preserve the volume

- We observe this will force $\omega_h$ to be determined

- Each truncation volume is uniquely identified by its centroid
  - Reconstruct linear interfaces exactly
We care most about mass conservation
Need to match volume fractions exactly

**Goal:** Match the volume fraction exactly and minimize the error of the centroid with a cutoff $\omega_h$

We can then formulate this as an optimization problem
Optimization Problem

Find a cut-off \( \omega^*_h \in F_{\Omega}^{h,\mu^*} \) such that

\[
\omega^*_h = \min_{\omega_h \in F_{\Omega}^{h,\mu^*}} \| \vec{x}_c(\omega_h) - \vec{x}^* \|^2_2
\]

This is equivalent to

Find a point \( \vec{x}^*_h \in X_{\Omega}^{h,\mu^*} \) such that

\[
\vec{x}^*_h = \min_{\vec{x}_h \in X_{\Omega}^{h,\mu^*}} \| \vec{x}_h - \vec{x}^* \|^2_2
\]
We will use the following version of the optimization problem

\[
\bar{x}_h^* \in X_{\Omega}^{h,\mu*}\quad \text{such that}
\bar{x}_h^* = \arg \min_{\bar{x}_h \in X_{\Omega}^{h,\mu*}} \| \bar{x}_h - \bar{x}^* \|^2_2
\]

to analyze the following with respect to initial data perturbation:

1. Existence
2. Uniqueness
3. Stability
Existence

To analyze the Existence of the MOF reconstruction optimization problem let’s consider the following figures.

Figure: Locations for potential $X^{h,\mu^*}$ and $X^{h,\mu^*}$ where $\mu^* = 0.25$
To analyze the Uniqueness of the MOF reconstruction optimization problem let’s consider the following figures.
Stability

To analyze the Stability of the MOF reconstruction optimization problem let’s consider the following figure.

Figure: Locations for minimal error centroid locations for true centroid perturbation
Analysis of Errors

- Errors with our reconstruction are calculated 3 ways
  - \( \Delta M_1 \): Distance between centroids (Defect of 1st moment)
  - \( \Delta \omega \): Area of \((\cup - \cap)\) (Symmetric Difference)
  - \( \Delta \Gamma \): Max Deviation of the Interface (Hausdorff Distance)

- The following bounds are obtained:
  \( d = \) diameter of cell, \( R = \) curvature of \( C^2 \) curve

- \( \Delta M_1 = O\left(\frac{d^5}{R^2}\right) \)
- \( \Delta \omega = O\left(\frac{d^3}{R}\right) \)
- \( \Delta \Gamma = O\left(\frac{d^2}{R}\right) \)

- \( \Delta M_1 = O\left(d^3\right) \)
- \( \Delta \omega = O\left(d^2\right) \)
- \( \Delta \Gamma = O\left(d\right) \)

Top Row: interface \( \in C^2 \)
Bottom Row: non-smooth interface
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5 Summary
Areas and Centroids

- We calculate areas of a n-sided polygon via the formula:

\[ |\omega| = \frac{1}{2} \sum_{i=1}^{n} \vec{x}_i \times \vec{x}_{i+1} \]

- We calculate centroids of a n-sided polygon via the formula:

\[ \vec{x}_c(\Omega) = \frac{1}{6|\Omega|} \sum_{i=1}^{n} (\vec{x}_i \times \vec{x}_{i+1})(x_i + x_{i+1}) \]

- Where \( \vec{x} \times \vec{y} = x_1 y_2 - x_2 y_1 \)
Numerical Optimization

- Goal: To parameterize the set of all possible centroids for a given optimal volume fraction
- Think of it as $\vec{x}_h \in X_{h,\mu^*}^\Omega$ characterized by $\vec{x}_h(\phi)$ where $\phi = \text{local inward normal}$
- This leads to an objective function of $f(\phi) = \|\vec{x}_h(\phi) - \vec{x}^*\|_2^2$
Numerical Optimization

Figure: Parametrization of the search space
 Numerical Optimization

- To complete the numerical optimization, any line search algorithm available can be used.
- You will encounter normal drawbacks of a line search algorithm.
  - Need a good initial guess and trial step selection.

- Initial Guess: angle of $\vec{x}_c(\Omega) - \vec{x}^*$
  - Claim: Specifies the point on the slope of a global min or top of hill dividing two global minima.
  - Claim: Conservative trail step will reach the global min.
Optimal Function Derivative

To complete the derivative of the objective function

\[ f'(\phi) = 2((\bar{x}_h(\phi) - \bar{x}^*) \cdot \bar{x}'_h(\phi)) \]

consider two cases:

1. **Case 1: Convex Cell → interface is a single segment**

   \[ \bar{x}'_h(\phi) = \frac{|\Gamma(\phi)|^3}{12\mu*|\Omega|} \tilde{t}(\phi) \text{ where } \tilde{t}(\phi) = [-\sin\phi, \cos\phi]^T \]

2. **Case 2: Non-Convex Cell and interface is several segments of the cut-line**

   \[ \bar{x}'_h(\phi) = \frac{M_2(\Gamma(\phi))}{\mu*|\Omega|} \tilde{t}(\phi) \text{ where } M_2(\Gamma) = \int_{\Gamma} \|ar{x} - \bar{x}_h(\Gamma)\|^2 \]
Recovering the centroid from $\phi$

- The optimization gives us the value for $\phi$ which minimizes the objective function.
- We care about $\bar{x}_h(\phi)$ but may not know this direct relationship.
- We can recover the centroid in 3 steps:
  1. calculate the unit vector $\bar{n}(\phi)$
  2. find $\omega_h(\phi) \in F^h_{\Omega,\mu^*}$ associated with $\bar{n}(\phi)$
  3. calculate $\bar{x}_h(\phi)$ of $\omega_h(\phi)$ using centroid formula
- We focus our attention on item 2 above.
Instead let us choose to find $\omega_h \in F^{h,\bar{n}(\phi)}_\Omega$ which matches $\mu^*$

We wish to solve $\mu(\xi^*) = \mu^*$

The Flood Algorithm can be used to solve this by making the following observations:

1. $\mu(\xi)$ is a continuous monotone function
2. $\mu(\xi)''$ is a piecewise-constant function with discontinuous points at the vertex heights
3. $\mu(\xi)$ is either quadratic or linear over each interval between vertex heights in non-descending order
Flood Algorithm

Figure: Geometric interpretation of flood algorithm for convex and non-convex cells
**Flood Algorithm**

1. Permute the vertices into a non-descending order $(i_1, i_2, \ldots, i_n)$
2. Start from vertex $i_1$ where $\mu_1 = 0$ and $|\Gamma_1| = 0$
3. Move "up" using the trapezoid rule:
   \[
   \mu_{i_k} = \mu_{i_{k-1}} + \frac{(\xi_{i_k} - \xi_{i_{k-1}})(|\Gamma_k| + |\Gamma_{k-1}|)}{2|\Omega|}
   \]
   until $\mu^*$ has been framed
4. Interpolate over the interval via:
   - Linear: $\xi^* = \xi_{i_k^*} + \frac{\mu^* - \mu_{k^*}}{\mu_{k^*+1} - \mu_{k^*}} (\xi_{i_{k^*+1}} - \xi_{i_k^*})$
   - Quadratic: $\xi^* = \sqrt{\xi_{i_k^*}^2 + \frac{\mu^* - \mu_{k^*}}{\mu_{k^*+1} - \mu_{k^*}} (\xi_{i_{k^*+1}}^2 - \xi_{i_k^*}^2)}$
Comparing MOF with the following VOF algorithms:

- LSGQ → Least Square Gradient with reciprocal quadratic weights (1st order)
- LVIRA → Least Square Volume Interface Reconstruction Algorithm (2nd order)
- Swartz (2nd order)
Figure: From Right to Left: LSGQ, LVIRA, Swartz, MOF
Letter "A"

Figure: From Right to Left: LSGQ, LVIRA, Swartz, MOF
Error Analysis

Figure: Interface Reconstruction Errors
In order to do time advanced simulations, a method for time-advance of volume fractions and of centroids is needed.

Any algorithm for this method will suffice here.

Authors used a Lagrangian/Remap method which is mass conservative.
Reversible Vortex

Figure: From Right to Left: LSGQ, LVIRA, Swartz, MOF
Extension to multiple \( \geq 3 \) fluids

- Looking for a polygonal approximation to the multi-material cell
- Method is extended to multi-material interfaces in 2 ways:
  1. Serial Dissection (SD) approach
  2. B-Tree Dissection (BTD) approach
Advantages of MOF in multi-materials

- Don’t need to specify the ordering of fluids (a drawback of VOF)
- More accurate reconstructions than VOF
- 2nd order accurate for $C^2$ interfaces
2nd order tests

Figure: Test partitions used to analyze order of reconstruction algorithm. Y-junction is not $C^2$
2nd order tests

**Figure**: Test partitions used to analyze order of reconstruction algorithm. Y-junction is not $C^2$
MOF-BTD vs. MOF-SD

Figure: Comparison of BTD (middle) with SD (bottom) MOF
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Summary

- MOF is an extension of VOF interface reconstruction method that tracks centroids and volume fractions.
- MOF is 2nd order in that it reconstructs linear interfaces exactly.
- MOF only uses local data within the cell, does not require neighbor information (2 materials).
- MOF performs much better than current VOF direct and iterative methods currently available as 2nd order.
References
