Moment-of-Fluid Analytic Reconstruction on 2D Cartesian grids

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I2M laboratory: Mechanical institute of Bordeaux

Team incompressible CFD

PhD: Discrete Helmholtz-Hodge Decomposition
  - Polyhedral meshes
  - Structure detection (vortex, source/sink) in vector fields for CFD
  - Mimetic schemes (Compatible Discrete Operators)

Post-doc since May 15\textsuperscript{th}, 2015
  - Volume-of-Fluid (implemented in 2D & 3D)
  - **Moment-of-Fluid** in collaboration with CELIA (Jérôme Breil)
  - Notus project
Introduction: Notus

- Open-source CFD code
- Dedicated to the modelization and simulation of incompressible fluid flows
- Designed to run on massively parallel supercomputers
- Finite volumes, 2D & 3D Cartesian staggered grid
- Validated and documented
- Available for download (soon!) http://notus-cfd.org
Introduction: Notus main features

Notus

Computational Fluid Dynamics

- Multiphysic applications
  - Incompressible Navier-Stokes equations
  - Multiphase flows $\rightarrow$ breaking waves
  - Energy equation $\rightarrow$ energy storage, phase change
  - Fluid – structure interactions (elasticity)

- Numerical schemes
  - Multiphase: Level-set, Volume-of-Fluid, **Moment-of-Fluid**
  - Velocity–pressure: Goda, Timmermans

- 2$^{nd}$-order immersed boundary method to represent any boundary shapes

- External linear solvers: HYPRE, MUMPS

- Output: ADIOS library (developed at Oak Ridge National Laboratory)
1. Introduction

2. Moment-of-Fluid

3. Revisiting MOF on Cartesian grids

4. Numerical results

5. Conclusion & perspectives
VOF-PLIC formulation

Original data
- $\Omega$ polygonal cell of vertices $\{p_1, \cdots, p_n\}$
- $\omega_1^*$ portion of fluid 1 in the cell $\Omega$
- Exponent $* \rightarrow$ reference data

VOF representation
- $|\omega_1^*|$ volume of fluid 1

PLIC reconstruction
- Constraint: $|\omega_1^\ell(\phi)| = |\omega_1^*|$
- $\omega_1^\ell(\phi)$ polygonal approximation of $\omega_1^*$
- Exponent $\ell \rightarrow$ reconstructed data

Find 2 parameters:
- $n$ interface normal
- $d$ distance to the origin
Limitations of VOF-PLIC methods

**Problem**

The volume fraction is insufficient to make a cell-wise reconstruction

→ We need the neighboring cells (gradient of the volume fraction)

**Idea**

Add information to have a *local* (cell-wise) reconstruction → Moment of Fluid
Moment-of-fluid: Moment?

Momentum of order 0 (volume)

\[ M_0(\omega) = \int \omega \, dx = |\omega| \]

Volume fraction (relative to a cell $\Omega$)

\[ \mu(\omega) = \frac{M_0(\omega)}{M_0(\Omega)} \]

Momentum of order 1

\[ M_1(\omega) = \int \omega \, x \, dx \]

Centroid

\[ x_c(\omega) = \frac{M_1(\omega)}{M_0(\omega)} \]
Moment-of-fluid: Moment?

Momentum of order 0 (volume)

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Volume fraction (relative to a cell \( \Omega \))

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Momentum of order 1

\[ M_1(\omega) = \int_{\omega} x \, dx \]

Centroid

\[ x_c(\omega) = \frac{M_1(\omega)}{M_0(\omega)} \]

- \( M_0(\Omega) = 4 \)
- \( M_0(\omega) = 0.9 \)
- \( \mu(\omega) = 0.225 \)

- \( M_1(\omega) = (0.45, 0.36) \)
- \( x_c(\omega) = (0.5, 0.4) \)
Moment-of-fluid: Formulation

Data:
- Volume fraction of any portions of fluid $\mu$ in each cells
- Centroid of any portions of fluid $x_c$ in each cells

Reconstruction method:
- VOF-PLIC: $|\omega^\ell| = |\omega^*|$ for each cell
  $\rightarrow$ under-determined problem!
- MOF: $|\omega^\ell| = |\omega^*|$ and $x_c(\omega^\ell) = x_c(\omega^*)$ for each cell
  $\rightarrow$ over-determined problem!

Minimization problem:
- Find $\omega^\ell = \arg\min_{\omega^\ell} |x_c(\omega^\ell) - x_c(\omega^*)|^2$
- Under constraint $|\omega^\ell| = |\omega^*|$

Moment-of-fluid: Formulation

Data:

- Volume fraction of any portions of fluid $\mu$ in each cells
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Reconstruction method:

- **VOF-PLIC:** $|\omega^\ell| = |\omega^*|$ for each cell
  $\rightarrow$ *under-determined* problem!

- **MOF:** $|\omega^\ell| = |\omega^*|$ and $x_c(\omega^\ell) = x_c(\omega^*)$ for each cell
  $\rightarrow$ *over-determined* problem!

Minimization problem:

- Find $\omega^\ell = \arg\min_{\omega^\ell} |x_c(\omega^\ell) - x_c(\omega^*)|^2$
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Moment-of-fluid: Formulation

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- Volume fraction of any portions of fluid \( \mu \) in each cells
- Centroid of any portions of fluid \( x_c \) in each cells

Reconstruction method:

- VOF-PLIC: \(|\omega^\ell| = |\omega^*|\) for each cell
  \(\rightarrow\) under-determined problem!

- MOF: \(|\omega^\ell| = |\omega^*|\) and \(x_c(\omega^\ell) = x_c(\omega^*)\) for each cell
  \(\rightarrow\) over-determined problem!

Minimization problem:

- Find \( \omega^\ell = \arg\min_{\omega^\ell} |x_c(\omega^\ell) - x_c(\omega^*)|^2 \)
- Under constraint \(|\omega^\ell| = |\omega^*|\)

Minimization: Example

- $\mu(\omega^*) = 0.3$
- $x_c(\omega^*) = (-0.3, -0.3)$

Objective function: \( \Delta \) possible local minima

Solution: \( \phi \approx 0.841 \)

Remark

One interface reconstruction per minimization iteration: highly time consuming.
Minimization: Example

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Examples of static reconstructions

Backward advection: Compute the pre-image $\Omega^{n-1}$ of $\Omega^n$ with a Runge-Kutta 2 method.

We can show that the centroids almost follow an advection equation:

$$\frac{d}{dt} x_c(\omega) = v(x_c(\omega)) + O(h^2)$$

→ Forward advection of the centroids (RK2)

Remark

Requires a polygon/polygon intersection algorithm
Multimaterial reconstruction: Remark on B-tree dissection

Without B-tree dissection

With B-tree dissection
1 Introduction

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4 Numerical results

5 Conclusion & perspectives
How to improve MOF on Cartesian grids?

- All the cells are convex
  - Sub-polygons remains convex too! → All the polygons are convex
  - Improve the Flood Algorithm
  - Fast convex polygon/polygon intersection (O’Rourke et al. (1982))

- All the cells are rectangles
  → Analytic solution to the minimization problem
Revisiting MOF on Cartesian grids

Improve Flood Algorithm

Flood algorithm on convex cells

Initial condition
- Flood direction $\mathbf{n}$
- Volume of fluid $V^* = |\Omega|/2$

Algorithm (find $\xi^*$)
1. Project vertices
2. Start from the first point ($p_4$)
3. Find the closest neighbor point
4. Generate the section
5. If $V_{total} > V^*$ exit
6. Repeat 3

Result
- $\xi^*$ given by quadratic interpolation

$\rightarrow$ Convexity: no need to sort the $\xi_n$

$$\alpha = \frac{V - V_{tot}}{V_{trapezoid}} \quad \beta = \sqrt{\left(\frac{|\Gamma|}{|\Gamma_{next}| + |\Gamma|}\right)^2 + \alpha \frac{|\Gamma_{next}| - |\Gamma|}{|\Gamma_{next}| + |\Gamma|} + \frac{|\Gamma|}{|\Gamma_{next}| + |\Gamma|}}$$

$$\xi^* = \xi + (\xi_{next} - \xi) \frac{\alpha}{\beta}$$

Analytic reconstruction: Motivations & proposal

Idea:
- On Cartesian grids, cells are rectangles
- Symmetry: locus of centroids very regular
- Possible parametrization
- Analytic solution to minimization problem

Bonus:
- No problem with local minima
- Upgrade a VOF-PLIC algorithm
- Easier to implement
- Faster for equivalent result
Analytic reconstruction: possible configurations ($\mu \leq 0.5$)

- 8 configurations
- Reduced to 2 by symmetry
- Triangle $\rightarrow$ Hyperbola
- Trapezoid $\rightarrow$ Parabola

triangle

trapezoid
Analytic solution: Parametrization of the hyperbola

\[ \sqrt{2V \frac{n_x}{n_y}} \]

\[ g_x = \frac{1}{3} \sqrt{2V \frac{n_y}{n_x}} \]
\[ g_y = \frac{1}{3} \sqrt{2V \frac{n_x}{n_y}} \]
\[ \Rightarrow g_y = \frac{9V}{2g_x} \]

Parameters

- Normal \( \mathbf{n} = (n_x, n_y) \)
- Volume \( V \)
Problem

- Let \( p = (p_x, p_y) \) any point of \( \mathbb{R}^2 \) (e.g. the reference centroid)
- Find the closest point of \( p \) to the hyperbola \( H \)
- For all \( x \in \left[ \frac{2V}{3c_x}, \frac{c_x}{3} \right] \), \( H(x) = \frac{9V}{2x} \)

Solution

- The closest point of \( p \) to the hyperbola is its orthogonal projection
- Tangent to the curve for the coordinate \( g_x \): \( (1, H'(g_x)) \)
- Orthogonal projection: \( (g_x - p_x, H(g_x) - p_y) \cdot (1, H'(g_x)) = 0 \)

The coordinate \( x \) of \( x_c(\omega^\ell) = (x, H(x)) \) is one of the solution of

\[
x^4 - p_x x^3 + \frac{2}{9} V p_y x - \left( \frac{2V}{9} \right)^2 = 0
\]
Analytic solution: Parabola

For all \( x \in \left[ \frac{c_x}{3}, \frac{2c_x}{3} \right] \)

\[
P(x) = \frac{V}{2c_x} + \frac{6V}{c_x} \left( \frac{1}{2} - \frac{x}{c_x} \right)^2
\]

Let \( p = (p_x, p_y) \) any point of \( \mathbb{R}^2 \)

The closest point of \( p \) to the parabola \( P \) is its orthogonal projection

The coordinate \( x \) of \( x_c(\omega^\ell) = (x, P(x)) \) is one of the solution of

\[
x - p_x - \frac{12V}{c_x^2} \left( \frac{1}{2} - \frac{x}{c_x} \right) \left( \frac{V}{2c_x} - p_y \right) - \frac{72V^2}{c_x^3} \left( \frac{1}{2} - \frac{x}{c_x} \right)^3 = 0
\]
Analytic reconstruction: Algorithm

- Multiple solutions inside one configuration
  → Maybe outside their definition domain
- Solutions found in many configurations
- Limit the search of solution in one quadrant

Obviously too far

Outside of definition domain
Analytic solution: Algorithm

1. If $\mu > 0.5$ solve the dual problem
2. Locate the quadrant where $x_c(\omega^*)$ is
   - $x_c(\omega^*) \in Q_1$ try $\{1, 2, 4\}$
   - $x_c(\omega^*) \in Q_2$ try $\{2, 3, 6\}$
   - $x_c(\omega^*) \in Q_3$ try $\{6, 8, 9\}$
   - $x_c(\omega^*) \in Q_4$ try $\{4, 7, 8\}$
3. Solve 2 cubic and 1 quartic
   → Strobach, Fast quartic solver (2010)
   → Strobach, Solving cubics by polynomial fitting (2011)
4. Eliminate wrong solutions
5. Find the closest solution
6. Compute $n$ and $d$ from the solution

Results

About 30% to 300% faster than minimization
2nd order verified in time and space
Numerical results: Error computation

Local errors
- Distance error
  \[ \Delta \Gamma = \max_{x^* \in \Gamma^*} \min_{x \in \Gamma^e} |x - x^*| \]
- Area of symmetric difference
  \[ \Delta \omega = |\omega^e \Delta \omega^*| \]
  \[ A \Delta B = (A \setminus B) \cup (B \setminus A) \]

Global error
- Average deviation (equivalent to \( \Delta \Gamma \))
  \[ \Delta \Gamma_{avg} = \frac{1}{|\partial \omega^*|} \sum_{i=1}^{N} |\omega^e_i \Delta \omega^*_i| \]

Numerical results: Sheared flow spatial convergence

**Parameters**
- Iterations: 1000
- Time step: $10^{-4}$ s
- Mesh: $N \times N$, $N \in \{16, 32, \ldots, 4096\}$

**Vector field**
$$u(x, y, t) = \begin{bmatrix} -2 \sin^2(\pi x) \sin(\pi y) \cos(\pi y) \\ 2 \sin^2(\pi y) \sin(\pi x) \cos(\pi x) \end{bmatrix} \cos\left(\pi \frac{t}{T}\right)$$

**Spatial convergence**

<table>
<thead>
<tr>
<th>$N$</th>
<th>$\Delta \Gamma_{avg}$</th>
<th>order</th>
</tr>
</thead>
<tbody>
<tr>
<td>512</td>
<td>$1.34 \cdot 10^{-6}$</td>
<td>2.03</td>
</tr>
<tr>
<td>1024</td>
<td>$3.09 \cdot 10^{-7}$</td>
<td>2.11</td>
</tr>
<tr>
<td>2048</td>
<td>$7.19 \cdot 10^{-8}$</td>
<td>2.10</td>
</tr>
<tr>
<td>4096</td>
<td>$1.60 \cdot 10^{-8}$</td>
<td>2.17</td>
</tr>
</tbody>
</table>
# Numerical results: Sheared flow time convergence

## Convergence with RK2

<table>
<thead>
<tr>
<th>Time step</th>
<th>$\Delta \Gamma_{\text{avg}}$</th>
<th>order</th>
</tr>
</thead>
<tbody>
<tr>
<td>$5 \cdot 10^{-4}$</td>
<td>$2.48 \cdot 10^{-7}$</td>
<td>$-0.21$</td>
</tr>
<tr>
<td>$2.5 \cdot 10^{-4}$</td>
<td>$2.86 \cdot 10^{-7}$</td>
<td>$-0.12$</td>
</tr>
<tr>
<td>$1.25 \cdot 10^{-4}$</td>
<td>$3.11 \cdot 10^{-7}$</td>
<td>$-0.12$</td>
</tr>
</tbody>
</table>

→ Does not converge! (even with a thinner grid)

## Convergence with Euler

<table>
<thead>
<tr>
<th>Time step</th>
<th>$\Delta \Gamma_{\text{avg}}$</th>
<th>order</th>
</tr>
</thead>
<tbody>
<tr>
<td>$5 \cdot 10^{-4}$</td>
<td>$2.93 \cdot 10^{-4}$</td>
<td>$-0.25$</td>
</tr>
<tr>
<td>$2.5 \cdot 10^{-4}$</td>
<td>$1.46 \cdot 10^{-4}$</td>
<td>$1.00$</td>
</tr>
<tr>
<td>$1.25 \cdot 10^{-4}$</td>
<td>$7.32 \cdot 10^{-5}$</td>
<td>$1.00$</td>
</tr>
</tbody>
</table>

→ $1^{\text{st}}$ order verified with Euler

## Parameters
- Total time: 0.5 s
- Mesh: $1024 \times 1024$
- Time step: $\{5 \cdot 10^{-4}, \ldots, 1.25 \cdot 10^{-4}\}$ s

→ Error RK2 < Error Euler

## Conclusion
Spatial error dominates
→ Try a case without spatial error
Convergence with RK2

<table>
<thead>
<tr>
<th>Time step</th>
<th>$\Delta \Gamma_{\text{avg}}$</th>
<th>order</th>
</tr>
</thead>
<tbody>
<tr>
<td>$1 \cdot 10^{-2}$</td>
<td>$4.93 \cdot 10^{-5}$</td>
<td>$-2.93 \cdot 10^{-5}$</td>
</tr>
<tr>
<td>$5 \cdot 10^{-3}$</td>
<td>$1.23 \cdot 10^{-5}$</td>
<td>$2.00$</td>
</tr>
<tr>
<td>$2.5 \cdot 10^{-3}$</td>
<td>$3.08 \cdot 10^{-6}$</td>
<td>$2.00$</td>
</tr>
<tr>
<td>$1.25 \cdot 10^{-3}$</td>
<td>$7.71 \cdot 10^{-7}$</td>
<td>$2.00$</td>
</tr>
<tr>
<td>$6.25 \cdot 10^{-4}$</td>
<td>$1.93 \cdot 10^{-7}$</td>
<td>$2.00$</td>
</tr>
</tbody>
</table>

Vector field

$$u_x(x, y, t) = 0.3\pi \sin(\pi t)$$

Conclusion

$2^{\text{nd}}$ order with RK2
Minimization vs Analytic: Static reconstruction

Static reconstruction (2 materials)

Mesh: $2048^2$

Time ratio minimization / analytic:

<table>
<thead>
<tr>
<th></th>
<th>Min. $10^{-15}$</th>
<th>Min. $10^{-8}$</th>
<th>Min. $10^{-6}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ana.</td>
<td>2.80</td>
<td>2.05</td>
<td>1.80</td>
</tr>
</tbody>
</table>
Minimization vs Analytic: Dynamic reconstruction

Advection of 5 materials in a sheared flow

For mixed cells:
→ First material uses analytic reconstruction
→ Use minimization in remaining space

Mesh: $128^2$

Time ratio minimization / analytic :

<table>
<thead>
<tr>
<th></th>
<th>Min. $10^{-15}$</th>
<th>Min. $10^{-8}$</th>
<th>Min. $10^{-6}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ana. &amp; Min. $10^{-15}$</td>
<td>2.54</td>
<td>1.70</td>
<td>1.41</td>
</tr>
<tr>
<td>Ana. &amp; Min. $10^{-8}$</td>
<td>3.10</td>
<td>2.08</td>
<td>1.72</td>
</tr>
<tr>
<td>Ana. &amp; Min. $10^{-6}$</td>
<td>2.92</td>
<td>1.97</td>
<td>1.62</td>
</tr>
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</table>
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Conclusion & perspectives

Conclusion

- MoF has been revisited on Cartesian grids (only in 2D yet)
- Proposition of an analytic reconstruction algorithm

Perspectives

- Symmetric reconstruction (Hill, R. N. and Shashkov, M. (2013))
- Filament capturing (Jemison, M., Sussman, M., Shashkov, M. (2015))
- MOF 3D
  - Intersection of polyhedron
  - Initialization from surface meshes
  - Analytic solution on Cartesian grid?
  - Advection
- Coupling of MOF with level-set (Jemison et al. (2013))
Thank you
Mesh $400 \times 200$, domain dimensions $(0.993, 0.5)$
Centroid advection

Fluid domain $\omega(t)$. Eulerian velocity $u(x, t)$. $\text{div } u = 0$.

\[
\frac{d}{dt} \int_{\omega(t)} x \, dx = \int_{\omega(t)} \left( \frac{\partial}{\partial t} \text{Id}(x) + u(x, t) \cdot \nabla \text{Id}(x) + \text{Id}(x) \text{div } u(x, t) \right) \, dx
\]

\[
= \int_{\omega(t)} u(x, t) \, dx
\]

\[
= \int_{\omega(t)} \left( u(x_c, t) + [\nabla u(x_c, t)] (x - x_c) + O(|x - x_c|^2) \right) \, dx
\]

\[
= |\omega(t)| u(x_c, t) + \nabla u(x_c, t) \int_{\omega(t)} (x - x_c) \, dx + O(h^2)
\]

Thus

\[
\frac{d}{dt} x_c = u(x_c) + O(h^2)
\]
Advection: 5 fluids on a sheared flow
**Limitations of MOF: Filaments**

- The filament does not move if the time step is too small!
Limitations of MOF: Possible solution

- Detection of filament at the advection step
- Introduction of a virtual fluid A’
- 3-fluid reconstruction