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

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Introduction: Notus

notus
Computational Fluid Dynamics

Overview:

- Open-source CFD code http://notus-cfd.org
- Dedicated to modeling and simulation of incompressible fluid flows
- Designed to run on massively parallel supercomputers
- Finite volumes, 2D & 3D Cartesian staggered grid

Multiphysic applications:

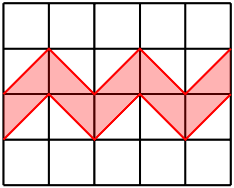
- Incompressible Navier-Stokes equations
- Multiphase flows $\rightarrow$ breaking waves
- Energy equation $\rightarrow$ energy storage, phase change
- Fluid – structure interactions (elasticity)

Many applications require interface **representation** and **reconstruction**

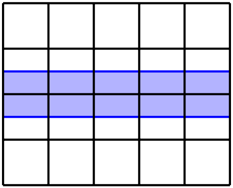
Introduction: objective

Objective: sharp interface reconstruction → Piecewise LInear Construction (PLIC)

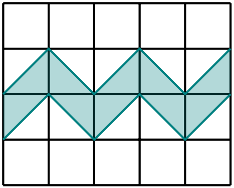
VOF-PLIC *vs* MOF:



Original interface



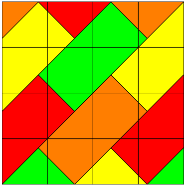
VOF-PLIC reconstruction



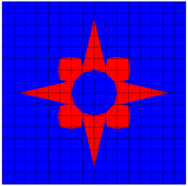
MOF reconstruction

Moment-of-Fluid (MOF) :

- Uses volume fraction + **centroids**
- Stencil reduced to only 1 cell
- 2^{nd} order of convergence
- Multimaterial reconstruction



Dyadechko & Shashkov (2006)



Example: compass

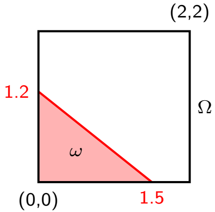
Moment-of-fluid: Moment?

0^{th} order momentum (volume)

$$M_0(\omega) = \int_\omega d\boldsymbol{x} = |\omega|$$

Volume fraction (relative to a cell Ω)

$$\mu(\omega) = \frac{M_0(\omega)}{M_0(\Omega)}$$



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

1^{st} order momentum

$$\boldsymbol{M_1}(\omega) = \int_\omega \boldsymbol{x} d\boldsymbol{x}$$

Centroid

$$\boldsymbol{x}_c(\omega) = \frac{\boldsymbol{M_1}(\omega)}{M_0(\omega)}$$

- $M_0(\omega) = 0.9$
- $\boldsymbol{M_1}(\omega) = (0.45, 0.36)$
- $\boldsymbol{x}_c(\omega) = (0.5, 0.4)$

MOF uses volume fraction **and centroids** to reconstruct interfaces

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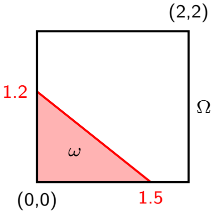

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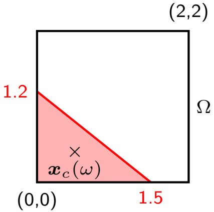

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Moment-of-fluid: formulation

Two unknowns to reconstruct the interface: **angle** and **distance**

Available information:

- **Volume fraction** of any portions of fluid μ in each cells
- **Centroid** of any portions of fluid $\boldsymbol{x}_c$ in each cells

Reconstruction method:

- VOF-PLIC: $|\omega^\ell| = |\omega^\star|$ for each cell
  $\longrightarrow$ *under-determined* problem!
- MOF: $|\omega^\ell| = |\omega^\star|$ and $\boldsymbol{x}_c(\omega^\ell) = \boldsymbol{x}_c(\omega^\star)$ for each cell
  $\longrightarrow$ *over-determined* problem!

Minimization problem:

- Find $\omega^\ell = \underset{\omega^\ell}{\operatorname{argmin}} \, |\boldsymbol{x}_c(\omega^\ell) - \boldsymbol{x}_c(\omega^\star)|^2$ $\rightarrow$ Minimize centroid distance
- Under constraint $|\omega^\ell| = |\omega^\star|$ $\rightarrow$ Preserve volume

Reference: Dyadechko, V., Shashkov, M. (2007)

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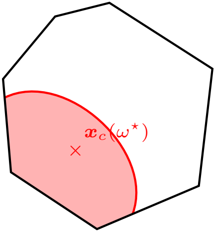
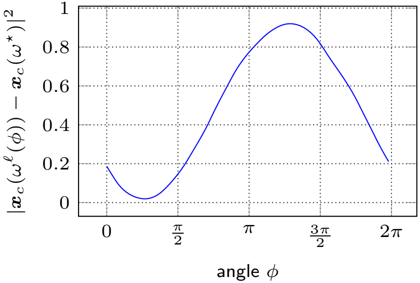
Minimization: example

Example parameters:

- $\mu(\omega^\star) = 0.3$
- $\boldsymbol{x}_c(\omega^\star) = (-0.3, -0.3)$



Objective function: ⚠ possible local minima



Solution: $\phi \approx 0.841$

Portion of fluid with curved interface and its centroid $\boldsymbol{x}_c(\omega^\star)$

Minimization: example

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- $\mu(\omega^\star) = 0.3$
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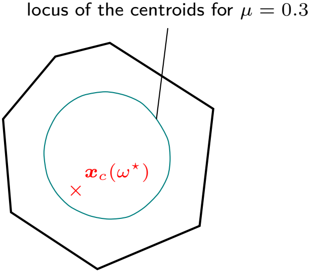
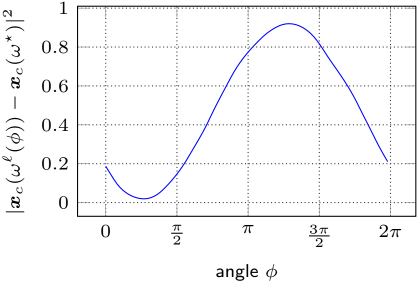


Objective function: ⚠ possible local minima



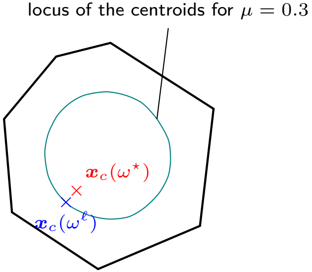
Solution: $\phi \approx 0.841$

Locus of all possible centroids for piecewise linear reconstructions for $\mu = 0.3$

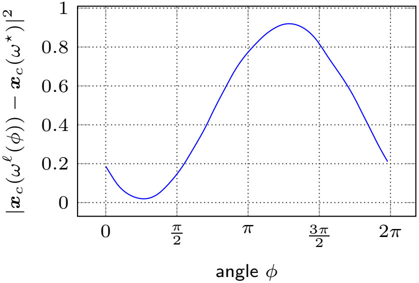
Minimization: example

Example parameters:

- $\mu(\omega^\star) = 0.3$
- $\boldsymbol{x}_c(\omega^\star) = (-0.3, -0.3)$



Objective function: ⚠ possible local minima



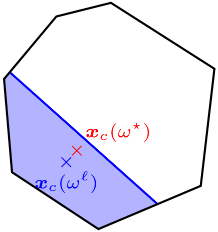
Solution: $\phi \approx 0.841$

Find the closest point $\boldsymbol{x}_c(\omega^\ell)$ on the curve to the reference centroid $\rightarrow$ **minimization**
$\longrightarrow$ The minimization algorithm stops when the **error on the angle** is small enough

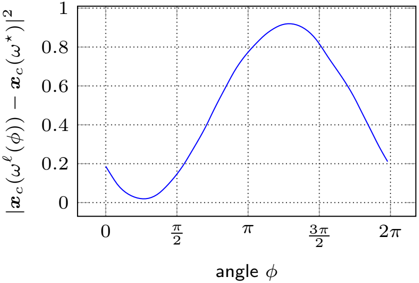
Minimization: example

Example parameters:

- $\mu(\omega^\star) = 0.3$
- $\boldsymbol{x}_c(\omega^\star) = (-0.3, -0.3)$



Objective function: ⚠ possible local minima



Solution: $\phi \approx 0.841$

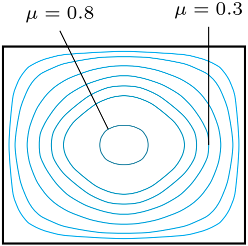
Compute the position of the interface with a **flood algorithm** (I used Breil *et al.* (2011))

Remark

One interface reconstruction per minimization iteration: highly time consuming

Analytic reconstruction: motivations & proposal

Objective: optimize the reconstruction on Cartesian grids



Locus of centroids for various volume fractions

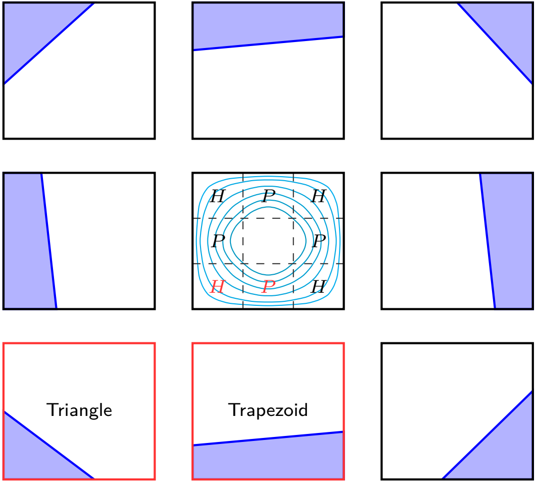
Idea:

- On Cartesian grids, cells are **rectangles**
- Use **symmetry** to reduce the number of configurations
- Possible **parametrization**
- **Analytic solution** to minimization problem

Bonus:

- Upgrade a VOF-PLIC algorithm
- Easier to implement than original method
- Faster for equivalent result
- Compatible with any rectangular meshes (*e.g.* AMR)

Analytic reconstruction: possible configurations ($\mu \leq 0.5$)

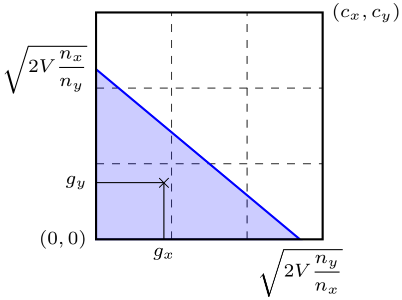


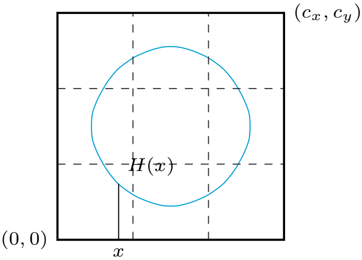
- Consider $\mu \leq 0.5$
- 8 configurations
- Reduced to 2 by symmetry
- Triangle $\rightarrow$ **Hyperbola** H
- Trapezoid $\rightarrow$ **Parabola** P

Find a **parametrization** of the parabola and the hyperbola

Analytic solution: parametrization of the hyperbola

Corner configuration → shape: triangle → centroid locus: hyperbola





Parameters

- Normal $\boldsymbol{n} = (n_x, n_y)$
- Volume V

Parametrization

$$\begin{cases} g_x = \frac{1}{3}\sqrt{2V\frac{n_y}{n_x}} \\ g_y = \frac{1}{3}\sqrt{2V\frac{n_x}{n_y}} \end{cases} \Rightarrow g_y = \frac{9V}{2g_x}$$

Analytic solution: closest point to the hyperbola

Problem

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

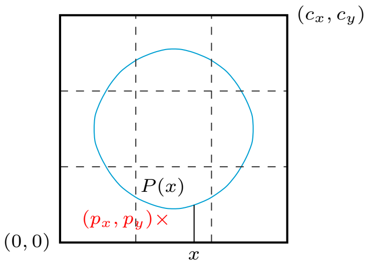
Solution

- The closest point of $\boldsymbol{p}$ 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 x coordinate of $\boldsymbol{x}_c(\omega^\ell) = (x, H(x))$ is one of the solution of a **quartic** equation:

$$x^4 - p_x x^3 + \frac{2}{9} V p_y x - \left(\frac{2V}{9}\right)^2 = 0$$

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

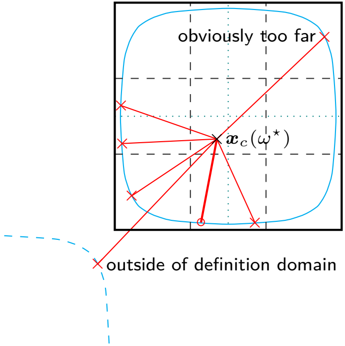
The closest point of $\boldsymbol{p}$ to the parabola P is its orthogonal projection

The x coordinate of $\boldsymbol{x}_c(\omega^\ell) = (x, P(x))$ is one of the solution of a **cubic** equation:

$$x - p_x - \frac{12V}{c_x^2}\left(\frac{1}{2} - \frac{x}{c_x}\right)\left(\frac{V}{2c_x} - p_y\right) - \frac{72V^2}{c_x^3}\left(\frac{1}{2} - \frac{x}{c_x}\right)^3 = 0$$

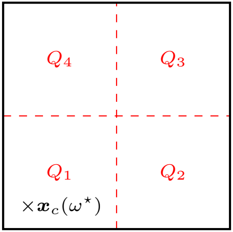
Analytic reconstruction: algorithm

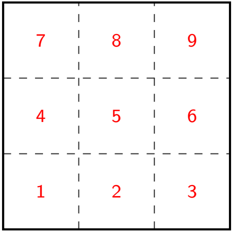
Cubic and **quartic** equations ⇒ possible analytic solution



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

Analytic solution: algorithm





1. If $\mu > 0.5$ solve the dual problem
2. Locate the quadrant where $\boldsymbol{x}_c(\omega^\star)$ is
   - $\boldsymbol{x}_c(\omega^\star) \in Q_1$ try $\{1, 2, 4\}$
   - $\boldsymbol{x}_c(\omega^\star) \in Q_2$ try $\{2, 3, 6\}$
   - $\boldsymbol{x}_c(\omega^\star) \in Q_3$ try $\{6, 8, 9\}$
   - $\boldsymbol{x}_c(\omega^\star) \in Q_4$ 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 $\boldsymbol{n}$ and d from the solution

Results

About 30% to 300% faster than minimization
2$^{\text{nd}}$ order verified in time and space

Minimization *vs* Analytic: static reconstruction

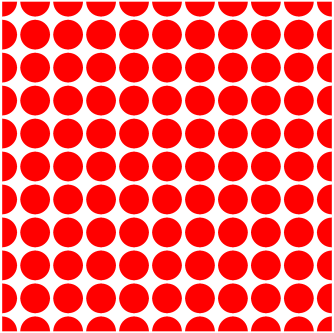
Static reconstruction (2 materials)

Mesh cells number: 2048^2

The minimization error is relative to the **angle**

Time ratio minimization / analytic:

	Min. 10^{-15}	Min. 10^{-11}	Min. 10^{-6}
Ana.	2.59	2.10	1.44



44 % to 159 % faster than minimization for static reconstruction

Minimization *vs* Analytic: dynamic reconstruction

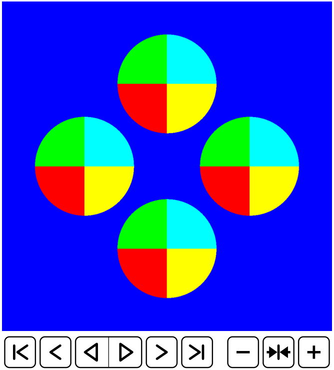
Advection of 5 materials in a sheared flow

For mixed cells:
→ First material uses **analytic reconstruction**
→ Use **minimization** for remaining materials

Mesh: 128^2

Time ratio minimization / analytic :

	Min. 10^{-15}	Min. 10^{-11}	Min. 10^{-6}
Ana. & Min. 10^{-15}	2.27	1.84	1.33
Ana. & Min. 10^{-11}	2.43	1.96	1.42
Ana. & Min. 10^{-6}	2.67	2.16	1.56



Time ratio increases when mesh size increases

Conclusion & perspectives

Conclusion

- Faster than minimization
- Can be applied to any rectangular meshes (not only Cartesian grids)

Perspectives

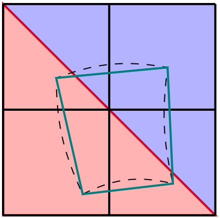
- Extension to 3D
  $\longrightarrow$ No analytic solution (yet), but a parametrization
- Coupling with other methods: level-set for surface tensions computation

Thank you

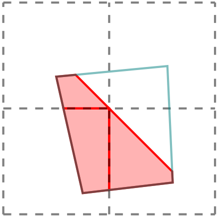
Appendix

Backward advection: Lagrangian remap

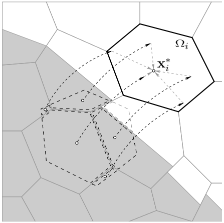
Backward advection: Compute the pre-image Ω^{n-1} of Ω^n with a Runge-Kutta 2 method.



Backward advection



Polygonal intersection
red fluid



Source: Dyadechko, V., Shashkov, M. (2007)

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

$$\frac{d}{dt}\boldsymbol{x}_c(\omega) = \boldsymbol{v}(\boldsymbol{x}_c(\omega)) + \mathcal{O}(h^2)$$

$\rightarrow$ Forward advection of the centroids (RK2)

Remark

Requires a polygon/polygon intersection algorithm

Centroid advection

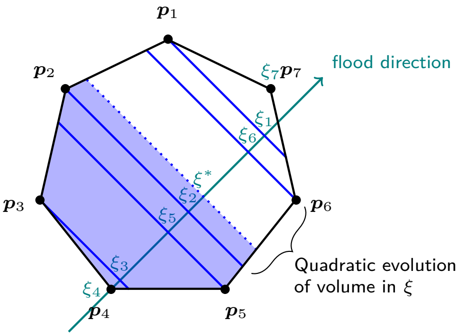
Fluid domain $\omega(t)$. Eulerian velocity $\boldsymbol{u}(\boldsymbol{x}, t)$. $\operatorname{div} \boldsymbol{u} = 0$.

$$\begin{aligned}
\frac{d}{dt} \int_{\omega(t)} \boldsymbol{x} d\boldsymbol{x} &= \int_{\omega(t)} \left(\frac{\partial}{\partial t} \mathrm{Id}(\boldsymbol{x}) + \boldsymbol{u}(\boldsymbol{x}, t) \cdot \nabla \mathrm{Id}(\boldsymbol{x}) + \mathrm{Id}(\boldsymbol{x}) \operatorname{div} \boldsymbol{u}(\boldsymbol{x}, t) \right) d\boldsymbol{x} \\
&= \int_{\omega(t)} \boldsymbol{u}(\boldsymbol{x}, t) d\boldsymbol{x} \\
&= \int_{\omega(t)} \left(\boldsymbol{u}(\boldsymbol{x}_c, t) + \left[\nabla \boldsymbol{u}(\boldsymbol{x}_c, t) \right] (\boldsymbol{x} - \boldsymbol{x}_c) + \mathcal{O}(|\boldsymbol{x} - \boldsymbol{x}_c|^2) \right) d\boldsymbol{x} \\
&= |\omega(t)| \boldsymbol{u}(\boldsymbol{x}_c, t) + \nabla \boldsymbol{u}(\boldsymbol{x}_c, t) \underbrace{\int_{\omega(t)} (\boldsymbol{x} - \boldsymbol{x}_c) d\boldsymbol{x}}_{=\mathbf{0}} + \mathcal{O}(h^2)
\end{aligned}$$

Thus

$$\frac{d}{dt} \boldsymbol{x}_c = \boldsymbol{u}(\boldsymbol{x}_c) + \mathcal{O}(h^2)$$

Flood algorithm on convex cells



Initial condition

- Flood direction $\boldsymbol{n}$
- Volume of fluid $V^\star = |\Omega|/2$

Algorithm (find ξ^*)

1. Project vertices
2. Start from the first point ($\boldsymbol{p}_4$)
3. Find the closest neighbor point
4. Generate the section
5. If $V_{\text{total}} > V^\star$ exit
6. Repeat 3

Result

- ξ^* given by quadratic interpolation

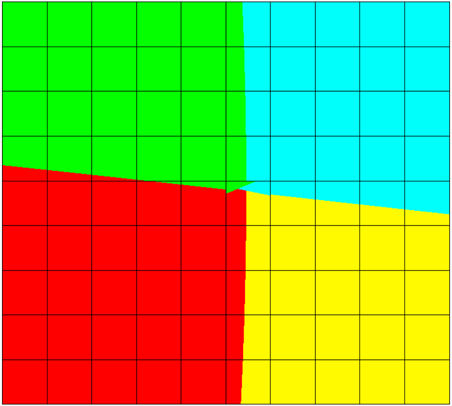
$\rightarrow$ Convexity: no need to sort the ξ_n

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

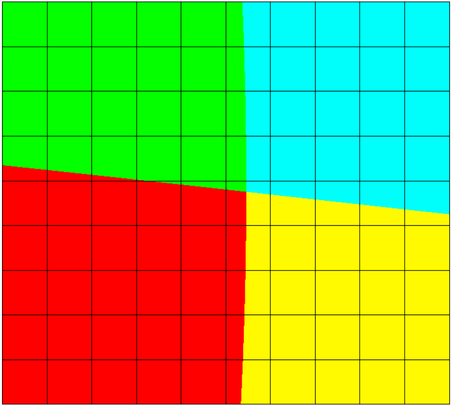
$$\xi^\star = \xi + (\xi_{\text{next}} - \xi)\frac{\alpha}{\beta}$$

Reference: Breil, J., Gelera, S., & Maire, P. H. (2011).

Multimaterial reconstruction: Remark on B-tree dissection

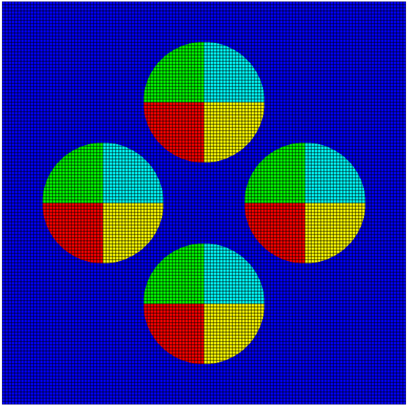


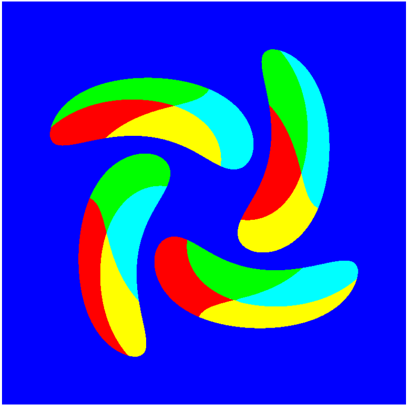
Without B-tree dissection



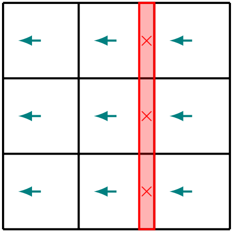
With B-tree dissection

Advection: 5 fluids on a sheared flow

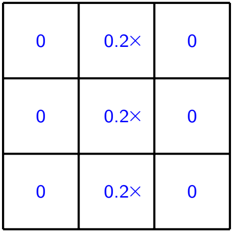




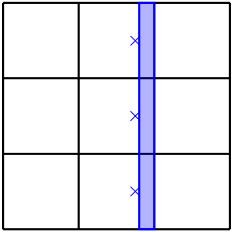
Limitations of MOF: Filaments



Initial configuration



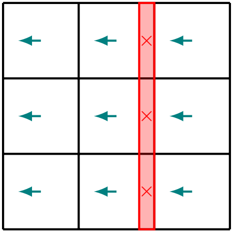
MOF representation after advection



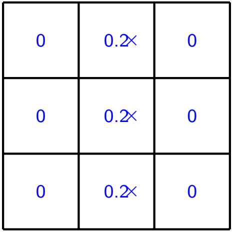
MOF reconstruction

- The filament does not move if the time step is too small!

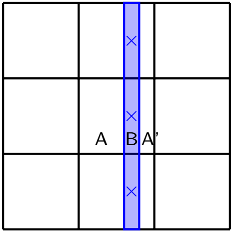
Limitations of MOF: Possible solution



Initial configuration



MOF representation after advection



MOF reconstruction

Virtual fluid A'

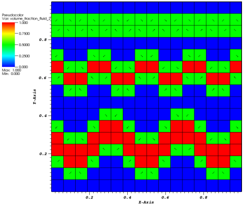
- Detection of filament at the advection step
- Introduction of a virtual fluid A'
- 3-fluid reconstruction

Reference: Jemison, M., Sussman, M., Shashkov, M. (2015)

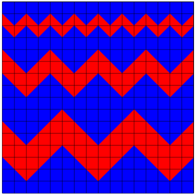
Examples of static reconstructions

Zigzags

Volume fraction

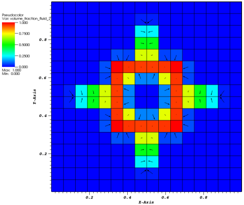


MoF reconstruction

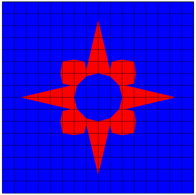


Compass

Volume fraction

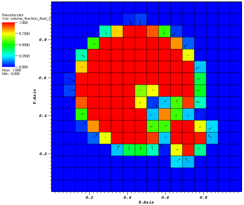


MoF reconstruction

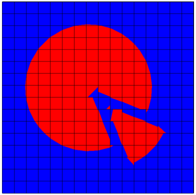


Pie

Volume fraction

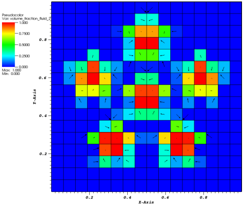


MoF reconstruction

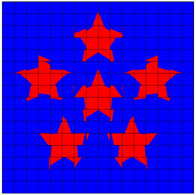


Stars

Volume fraction



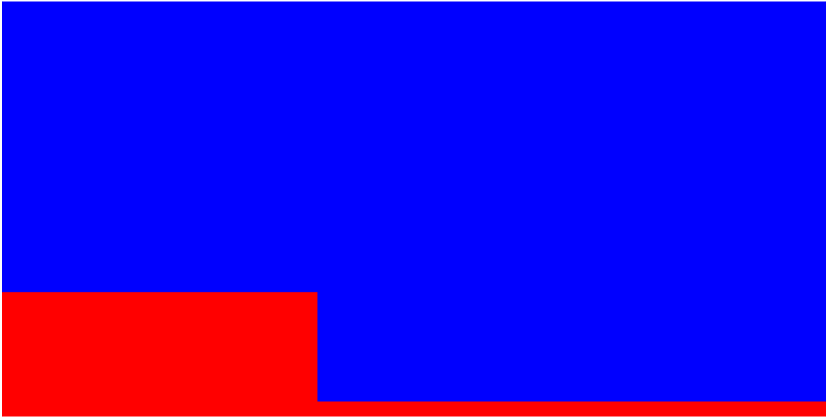
MoF reconstruction



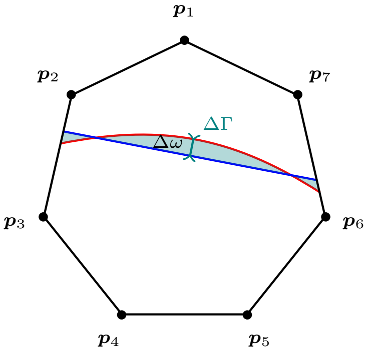
Volume fraction and centroids data from: Dyadechko, V., Shashkov, M. (2007)

Dam break – Air / Water

Mesh 400×200, domain dimensions $(0.993, 0.5)$



Numerical results: Error computation



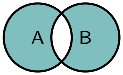
Local errors

- Distance error

$$\Delta\Gamma = \max_{x^\star \in \Gamma^\star} \min_{x \in \Gamma^\ell} |x - x^\star|$$

- Area of symmetric difference

$$\Delta\omega = |\omega^\ell \triangle \omega^\star|$$



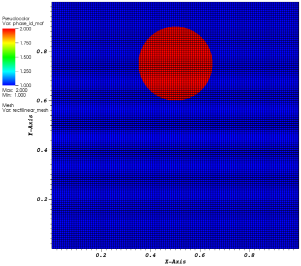
$$A \triangle B = (A \setminus B) \cup (B \setminus A)$$

Global error

- Average deviation (equivalent to $\Delta\Gamma$)

$$\Delta\Gamma_{avg} = \frac{1}{|\partial\omega^\star|} \sum_{i=1}^{N} |\omega_i^\ell \triangle \omega_i^\star|$$

Reference: Dyadechko, V., Shashkov, M. (2007)



Parameters

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

Vector field

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

Spatial convergence

N	$\Delta\Gamma_{\text{avg}}$	order
512	$1.34 \cdot 10^{-6}$	2.03
$1\,024$	$3.09 \cdot 10^{-7}$	2.11
$2\,048$	$7.19 \cdot 10^{-8}$	2.10
$4\,096$	$1.60 \cdot 10^{-8}$	2.17

Numerical results: Sheared flow time convergence

Convergence with RK2

Time step	$\Delta\Gamma_{\text{avg}}$	order
$5 \cdot 10^{-4}$	$2.48 \cdot 10^{-7}$	–
$2.5 \cdot 10^{-4}$	$2.86 \cdot 10^{-7}$	-0.21
$1.25 \cdot 10^{-4}$	$3.11 \cdot 10^{-7}$	-0.12

$\rightarrow$ Does not converge! (even with a thinner grid)

Convergence with Euler

Time step	$\Delta\Gamma_{\text{avg}}$	order
$5 \cdot 10^{-4}$	$2.93 \cdot 10^{-4}$	–
$2.5 \cdot 10^{-4}$	$1.46 \cdot 10^{-4}$	1.00
$1.25 \cdot 10^{-4}$	$7.32 \cdot 10^{-5}$	1.00

$\rightarrow$ 1st order verified with Euler

Parameters

- Total time: 0.5 s
- Mesh: 1024×1024
- Time step: $\{5 \cdot 10^{-4}, \cdots, 1.25 \cdot 10^{-4}\}$ s

$\rightarrow$ Error RK2 $<$ Error Euler

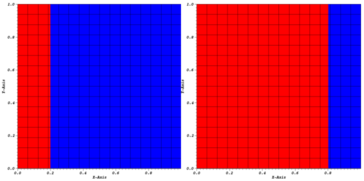
Conclusion

Spatial error dominates

$\rightarrow$ Try a case without spatial error

Convergence with RK2

Time step	$\Delta\Gamma_{\text{avg}}$	order
$1 \cdot 10^{-2}$	$4.93 \cdot 10^{-5}$	–
$5 \cdot 10^{-3}$	$1.23 \cdot 10^{-5}$	2.00
$2.5 \cdot 10^{-3}$	$3.08 \cdot 10^{-6}$	2.00
$1.25 \cdot 10^{-3}$	$7.71 \cdot 10^{-7}$	2.00
$6.25 \cdot 10^{-4}$	$1.93 \cdot 10^{-7}$	2.00



Vector field

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

Conclusion

2nd order with RK2