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

Antoine Lemoine [1] Stéphane Glockner [2] Jérôme Breil [3]

[1] Univ. Bordeaux, I2M, UMR 5295, F-33400 Talence, France.

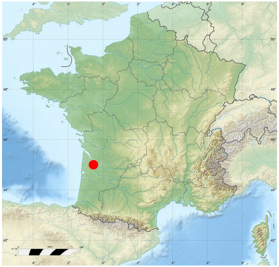
[2] Bordeaux INP, I2M, UMR 5295, F-33400 Talence, France.

[3] CEA CESTA, 15 Avenue des Sablières, CS 60001, 33116 Le Barp Cedex, France.

January 25th, 2016

Introduction: I2M

- 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 15th, 2015
  - Volume-of-Fluid (implemented in 2D & 3D)
  - **Moment-of-Fluid** in collaboration with CELIA (Jérôme Breil)
  - Notus project



Source: Eric Gaba – Wikimedia Commons

Introduction: Notus

notus
Computational Fluid Dynamics

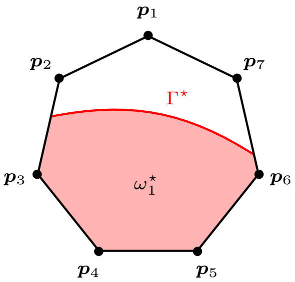
- Open-source CFD code
- Dedicated to the modelization and simulation of incompressible fluid flows
- Designed to run on massively parallel supercomputers
- Finite volumes, 2D & 3D Cartesian staggered grid
- Validated and documented
- Available for download (soon!) `http://notus-cfd.org`

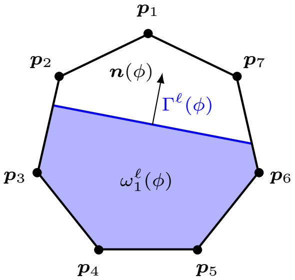
Introduction: Notus main features

notus
Computational Fluid Dynamics

- Multiphysic applications
  - Incompressible Navier-Stokes equations
  - Multiphase flows → breaking waves
  - Energy equation → 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)

VOF-PLIC formulation





Original data

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

VOF representation

- $|\omega_1^\star|$ volume of fluid 1

PLIC reconstruction

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

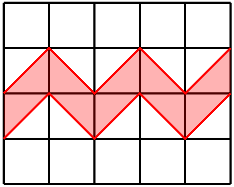
Find 2 parameters:

- $\boldsymbol{n}$ interface normal
- d distance to the origin

Limitations of VOF-PLIC methods

Problem

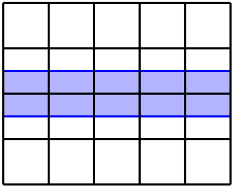
The volume fraction is insufficient to make a cell-wise reconstruction
$\rightarrow$ We need the neighboring cells (gradient of the volume fraction)



Original interface

0	0	0	0	0
0.5	0.5	0.5	0.5	0.5
0.5	0.5	0.5	0.5	0.5
0	0	0	0	0

VOF representation



PLIC reconstruction

Idea

Add information to have a *local* (cell-wise) reconstruction $\longrightarrow$ Moment of Fluid

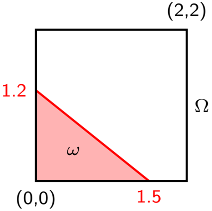
Moment-of-fluid: Moment?

Momentum of order 0 (volume)

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

Volume fraction (relative to a cell Ω)

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



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

Momentum of order 1

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

Centroid

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

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

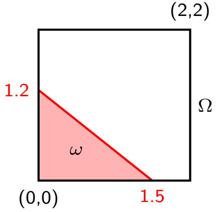
Moment-of-fluid: Moment?

Momentum of order 0 (volume)

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

Volume fraction (relative to a cell Ω)

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



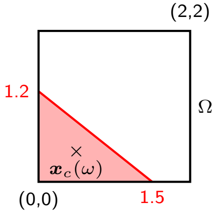
- $M_0(\Omega) = 4$
- $M_0(\omega) = 0.9$
- $\mu(\omega) = 0.225$

Momentum of order 1

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

Centroid

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



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

Moment-of-fluid: Formulation

Data:

- 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 $\omega^\ell = \underset{\omega^\ell}{\operatorname{argmin}} \, |\boldsymbol{x}_c(\omega^\ell) - \boldsymbol{x}_c(\omega^\star)|^2$
- Under constraint $|\omega^\ell| = |\omega^\star|$

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

Moment-of-fluid: Formulation

Data:

- 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 $\omega^\ell = \underset{\omega^\ell}{\operatorname{argmin}} \, |\boldsymbol{x}_c(\omega^\ell) - \boldsymbol{x}_c(\omega^\star)|^2$
- Under constraint $|\omega^\ell| = |\omega^\star|$

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

Moment-of-fluid: Formulation

Data:

- 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!

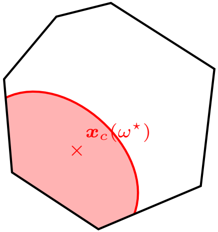
Minimization problem:

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

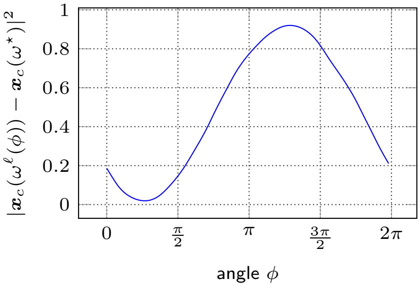
Reference: Dyadechko, V., Shashkov, M. (2007)

Minimization: Example

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



Objective function: ⚠ possible local minima



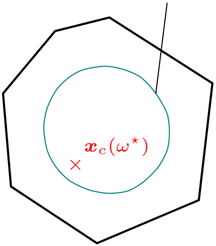
Solution: $\phi \approx 0.841$

Remark

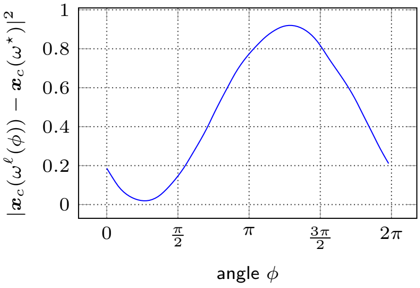
One interface reconstruction per minimization iteration: highly time consuming

Minimization: Example

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



Objective function: ⚠ possible local minima



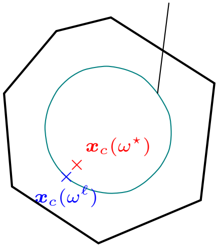
Solution: $\phi \approx 0.841$

Remark

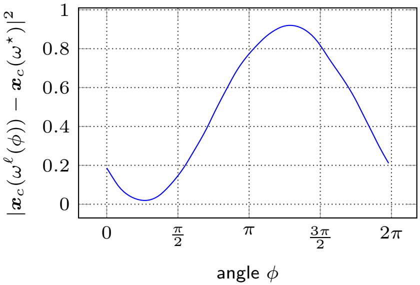
One interface reconstruction per minimization iteration: highly time consuming

Minimization: Example

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



Objective function: ⚠ possible local minima



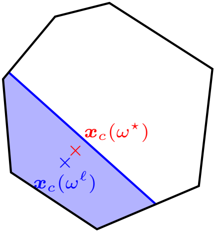
Solution: $\phi \approx 0.841$

Remark

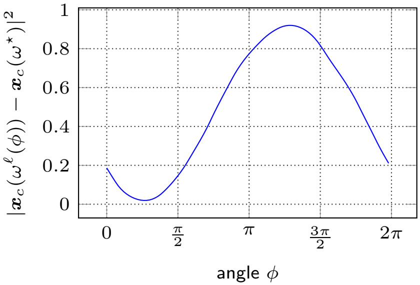
One interface reconstruction per minimization iteration: highly time consuming

Minimization: Example

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



Objective function: ⚠ possible local minima



Solution: $\phi \approx 0.841$

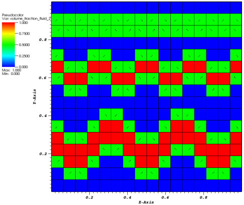
Remark

One interface reconstruction per minimization iteration: highly time consuming

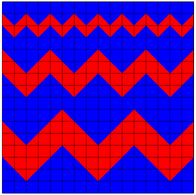
Examples of static reconstructions

Zigzags

Volume fraction

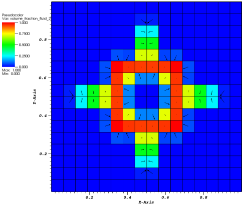


MoF reconstruction

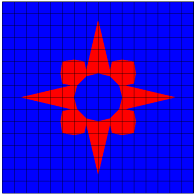


Compass

Volume fraction

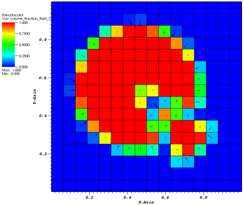


MoF reconstruction

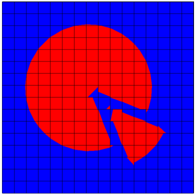


Pie

Volume fraction

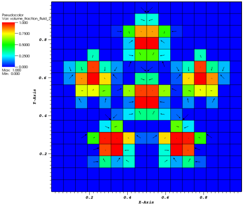


MoF reconstruction

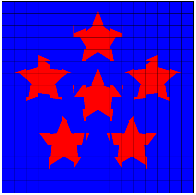


Stars

Volume fraction



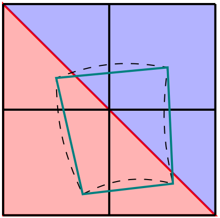
MoF reconstruction



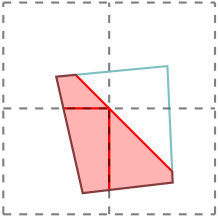
Volume fraction and centroids data from: Dyadechko, V., Shashkov, M. (2007)

Backward advection: Lagrangian remap

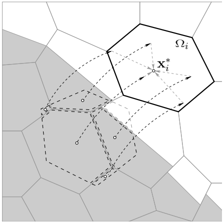
Backward advection: Compute the pre-image Ω^{n-1} of Ω^n with a Runge-Kutta 2 method.



Backward advection



Polygonal intersection
red fluid



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

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

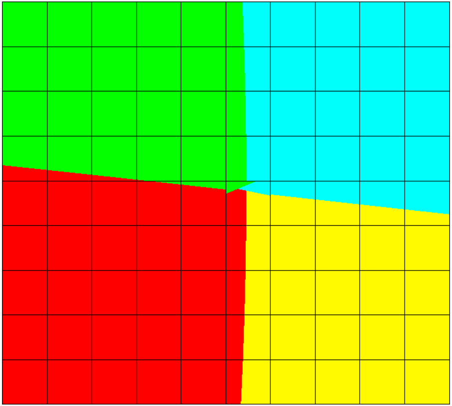
$$\frac{d}{dt}\boldsymbol{x}_c(\omega) = \boldsymbol{v}(\boldsymbol{x}_c(\omega)) + \mathcal{O}(h^2)$$

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

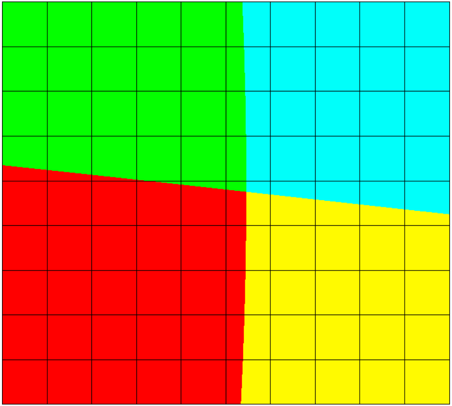
Remark

Requires a polygon/polygon intersection algorithm

Multimaterial reconstruction: Remark on B-tree dissection



Without B-tree dissection

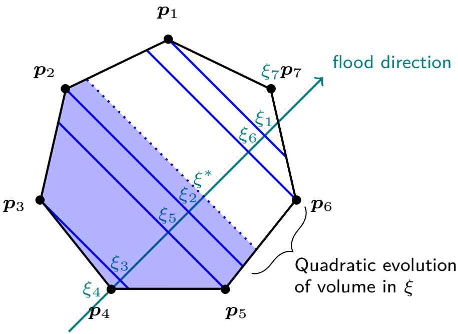


With B-tree dissection

How to improve MOF on Cartesian grids?

- All the cells are convex
  - Sub-polygons remains convex too! $\rightarrow$ All the polygons are convex
  - Improve the Flood Algorithm
  - Fast convex polygon/polygon intersection (O'Rourke *et al.* (1982))
- All the cells are rectangles
  $\rightarrow$ Analytic solution to the minimization problem

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

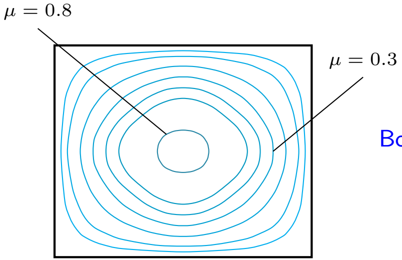
→ Convexity: no need to sort the ξ_n

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

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

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

Analytic reconstruction: Motivations & proposal



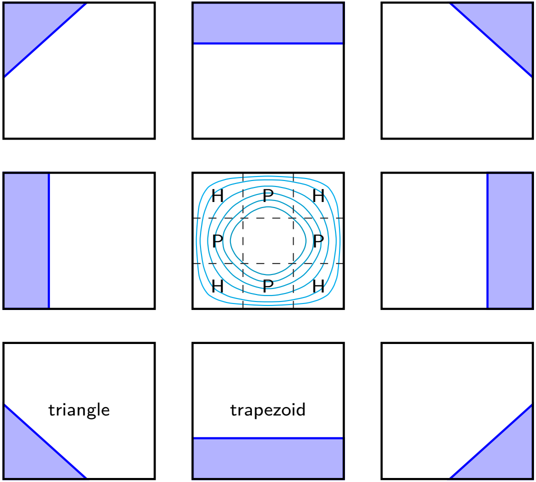
Idea:

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

Bonus:

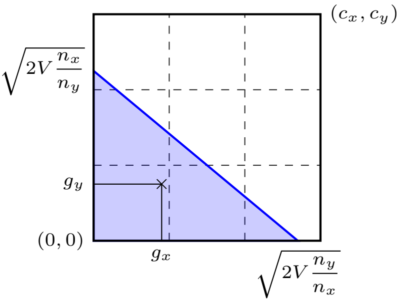
- No problem with local minima
- Upgrade a VOF-PLIC algorithm
- Easier to implement
- Faster for equivalent result

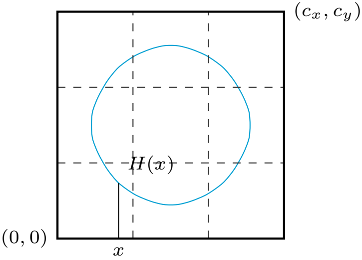
Analytic reconstruction: possible configurations ($\mu \leq 0.5$)



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

Analytic solution: Parametrization of the hyperbola





Parameters

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

Parametrization

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

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 $x \in \left[\frac{2V}{3c_x}, \frac{c_x}{3}\right]$ $\qquad H(x) = \frac{9V}{2x}$

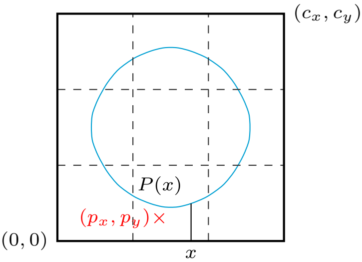
Solution

- 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 coordinate x of $\boldsymbol{x}_c(\omega^\ell) = (x, H(x))$ 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



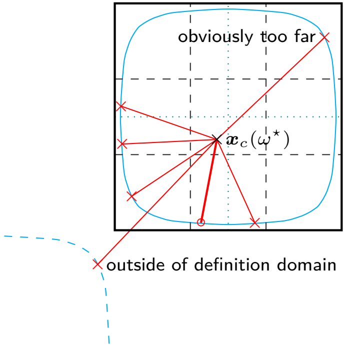
For all $x \in \left[\frac{c_x}{3}, \frac{2c_x}{3}\right]$

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

Let $\boldsymbol{p} = (p_x, p_y)$ any point of $\mathbb{R}^2$
The closest point of $\boldsymbol{p}$ to the parabola P is its orthogonal projection
The coordinate x of $\boldsymbol{x}_c(\omega^\ell) = (x, P(x))$ is one of the solution of

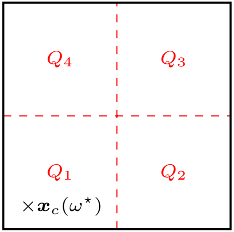
$$x - p_x - \frac{12V}{c_x^2}\left(\frac{1}{2} - \frac{x}{c_x}\right)\left(\frac{V}{2c_x} - p_y\right) - \frac{72V^2}{c_x^3}\left(\frac{1}{2} - \frac{x}{c_x}\right)^3 = 0$$

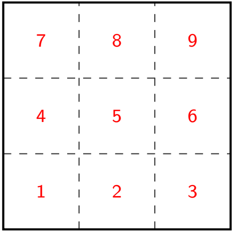
Analytic reconstruction: Algorithm



- Multiple solutions inside one configuration
  $\rightarrow$ 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

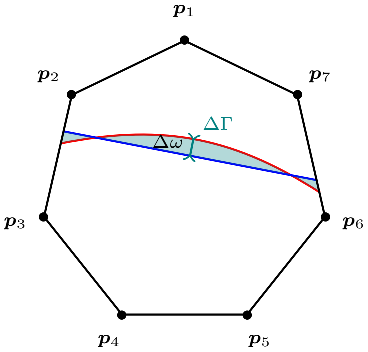
   $\rightarrow$ Strobach, Fast quartic solver (2010)

   $\rightarrow$ 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^{nd} order verified in time and space

Numerical results: Error computation



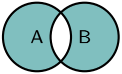
Local errors

- Distance error

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

- Area of symmetric difference

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



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

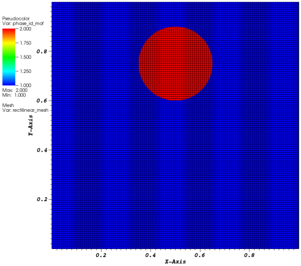
Global error

- 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)

Numerical results: Sheared flow spatial convergence



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

$\rightarrow$ 1^{st} 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

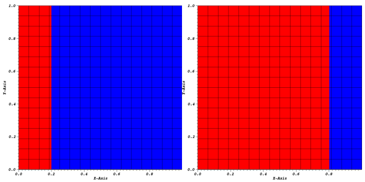
$\rightarrow$ Error RK2 $<$ Error Euler

Conclusion

Spatial error dominates

$\rightarrow$ Try a case without spatial error

Numerical results: Accelerated front flow time convergence



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

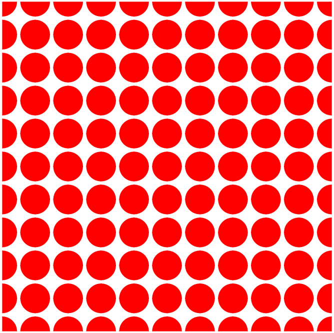
2^{nd} order with RK2

Minimization vs Analytic: Static reconstruction

Static reconstruction (2 materials)

Mesh: 2048^2
Time ratio minimization / analytic:

	Min. 10^{-15}	Min. 10^{-8}	Min. 10^{-6}
Ana.	2.80	2.05	1.80



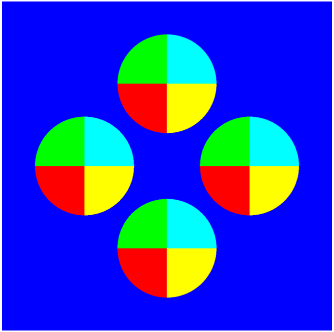
Minimization vs Analytic: Dynamic reconstruction

Advection of 5 materials in a sheared flow

For mixed cells:
$\rightarrow$ First material uses analytic reconstruction
$\rightarrow$ Use minimization in remaining space

Mesh: 128^2
Time ratio minimization / analytic :

	Min. 10^{-15}	Min. 10^{-8}	Min. 10^{-6}
Ana. & Min. 10^{-15}	2.54	1.70	1.41
Ana. & Min. 10^{-8}	3.10	2.08	1.72
Ana. & Min. 10^{-6}	2.92	1.97	1.62



Conclusion & perspectives

Conclusion

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

Perspectives

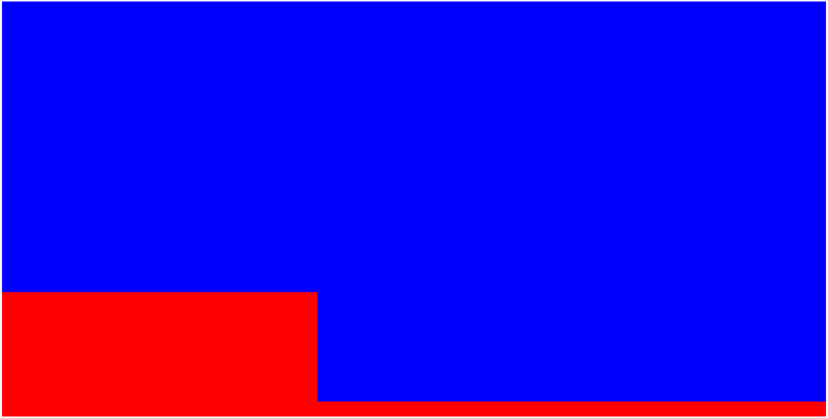
- Symmetric reconstruction (Hill, R. N. and Shashkov, M. (2013))
- Filament capturing (Jemison, M., Sussman, M., Shashkov, M. (2015))
- MOF 3D
  - Intersection of polyhedron
  - Initialization from surface meshes
  - Analytic solution on Cartesian grid?
  - Advection
- Coupling of MOF with level-set (Jemison *et al.* (2013))

Thank you

Appendix

Dam break – Air / Water

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



Centroid advection

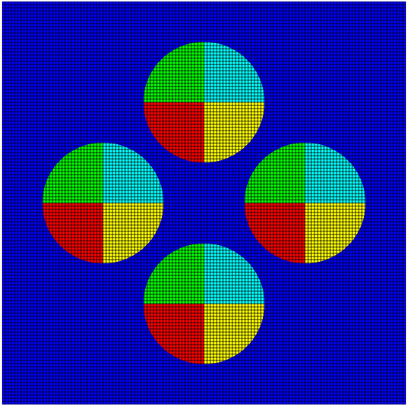
Fluid domain $\omega(t)$. Eulerian velocity $\boldsymbol{u}(\boldsymbol{x},t)$. $\operatorname{div}\boldsymbol{u}=0$.

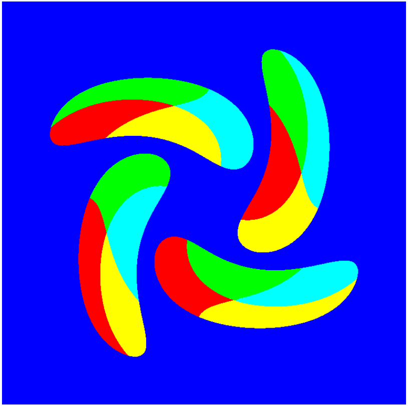
$$\begin{aligned}
\frac{d}{dt}\int_{\omega(t)} \boldsymbol{x}d\boldsymbol{x} &= \int_{\omega(t)} \left(\frac{\partial}{\partial t}\mathrm{Id}(\boldsymbol{x}) + \boldsymbol{u}(\boldsymbol{x},t)\cdot\nabla\mathrm{Id}(\boldsymbol{x}) + \mathrm{Id}(\boldsymbol{x})\operatorname{div}\boldsymbol{u}(\boldsymbol{x},t)\right)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

Thus

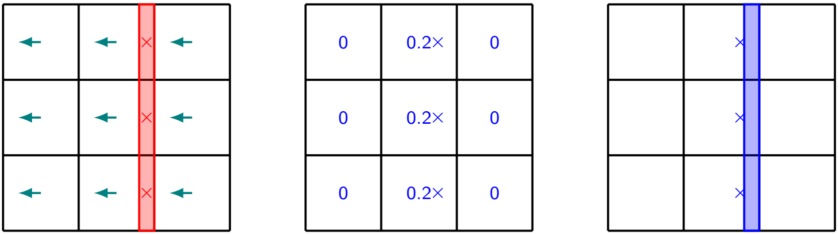
$$\frac{d}{dt}\boldsymbol{x}_c = \boldsymbol{u}(\boldsymbol{x}_c) + \mathcal{O}(h^2)$$

Advection: 5 fluids on a sheared flow





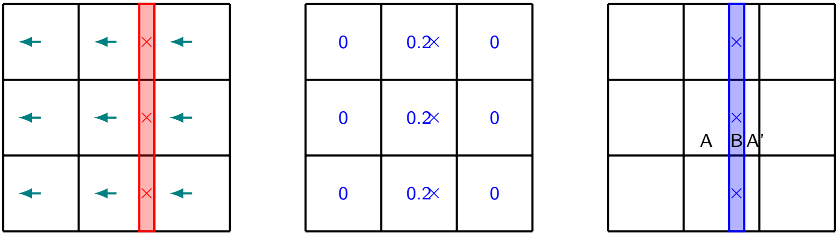
Limitations of MOF: Filaments



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)