Lagrangian / Eulerian Numerical Methods for Fluid Interface Advection on Unstructured Meshes

Dr.-Ing. Tomislav Marić

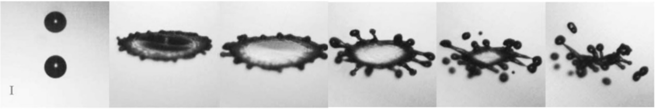
Dr.-Ing. Holger Marschall
Prof. Dr. rer. nat. Dieter Bothe

Mathematical modeling and analysis, TU Darmstadt

PRACE IHPCSS Ostrava, Czech Republic, July 08-13, 2018

Introduction

Modeling the flow of immiscible fluids



Binary droplet collisions researched by Liu and Bothe 2016.

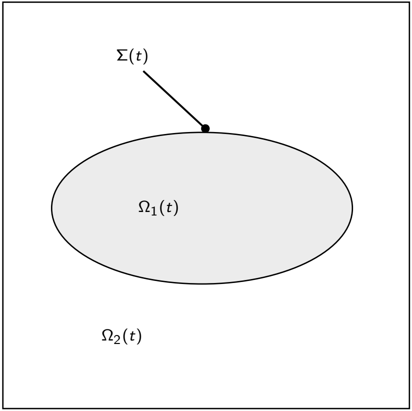
Modeling assumptions

- A sharp interface forms between immiscible phases.
- The interface stays sharp as it evolves.
- The interface can topologically change.
- The phases are considered as incompressible.

Introduction

Goal definition

- The solution domain Ω is split into two sub-domains $\Omega_1(t)$ and $\Omega_2(t)$, such that $\Omega = \Omega_1(t) \cup \Omega_2(t)$.
- The evolving interface is the boundary between $\Omega_1(t)$ and $\Omega_2(t)$: $\Sigma(t)$.
- $\Sigma(t)$ evolves with a velocity $\mathbf{u}_\Sigma(\mathbf{x}, t)$.
- **Goal**: numerically track $\Sigma(t)$ as accurately as possible.

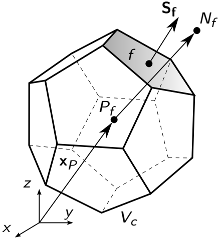


Interface $\Sigma(t)$ separating the solution domain Ω.

The geometrical Volume of Fluid Method

Domain and phase indicator discretization

Domain is discretized as $\Omega_h = \cup_c V_c$, V_c are polyhedra with volume $|V_c|$.



- **Step 1 (Interface reconstruction):** $I_1(x,t)$ **approximated by a sharp piecewise-planar indicator**

$$I_{1,c}(\mathbf{x},t) = \begin{cases} 1, \mathbf{n}_c \cdot (\mathbf{x} - \mathbf{p}_c) > 0, \\ 0, \text{otherwise.} \end{cases} \tag{1}$$

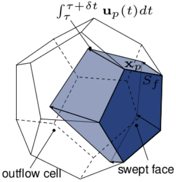
- VoF equation:

$$\alpha_1^{n+1} = \alpha_1^n - \frac{1}{|V_c|} \sum_f \int_\tau^{\tau+\delta t} \int_{S_f} I_{1,c}(x,t) \mathbf{u} \cdot \mathbf{n} dodt + O(\delta x^2) \tag{2}$$

The geometrical Volume-of-Fluid Method

Dimensionally un-split volumetric flux calculation

Step 2: volume fraction advection



Flux volume calculation.

- **Lagrangian backward tracing**
  - Sweep S_f backward in time.
- Unique cell corner point velocities.
- Explicit third order accurate cell center displacement integration:

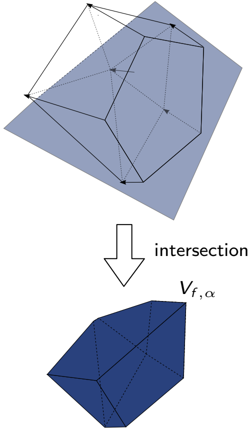
$$\delta \mathbf{x}(t + \delta t) = \mathbf{u}(\mathbf{x}, t)\delta t + \frac{d\mathbf{u}}{dt}(\mathbf{x}, t)\delta t^2 + O(\delta t^3) \quad (3)$$

- Second order accurate cell center to cell corner interpolation:

$$\phi_p = \frac{1}{|N_{pc}|}\sum_{pc \in N_{pc}} \phi_{pc} + \nabla \phi_{pc} \cdot (\mathbf{x}_p - \mathbf{x}_c) + O(\delta x^2) \quad (4)$$

The geometrical Volume-of-Fluid Method

Intersection of the fluxed phase volume



Final approximation step:

$$\alpha_c^{n+1} = \alpha_c^n - \frac{1}{|V_c|} \sum_f |V_f^\alpha| \quad (5)$$

$$V_f^\alpha = V_f^\alpha \cap V_i \cap I_i(\mathbf{x}, t) \quad (6)$$

$$i \in \{n : |V_f^\alpha \cap V_n| \geq 0, \alpha_j > \epsilon_r\} \quad (7)$$

Highlights

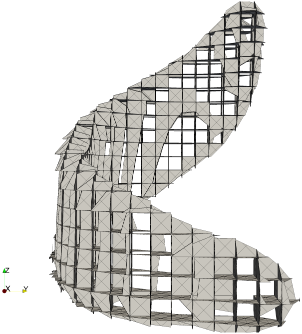
- Collision detection tests are used to reduce the number of required intersections.
- **Execution time $\leq$ execution time on Cartesian structured meshes.**
- The geometrical library relies on function overloading based on arbitrary properties of types, in the C++ programming language (Järvi, Marcus, and Smith 2010).

The geometrical Volume of Fluid Method

Results : fulfilled requirements

Requirements of an accurate interface advection method[1]

- ✓ **Volume conservation near machine tolerance.**
- ✓ **Exact numerical boundedness.**
- ✓ **Second order convergent in time and space.**
- ✓ **Topologically robust and stable for $CFL = 1$.**
- ✓ **No residual wisps, even at $\alpha_w < \epsilon_r = 1e - 09$.**
- ✓ **No numerical diffusion.**
- ✗ **Computationally efficient.**
  - ✓ : Partial specializations for `std::vector`.
  - ✓ : Reconstruction algorithm enhancements.
  - ✐ : More serial optimizations.
  - ✐ : MPI 3.0 RMA?
  - **High accuracy demand: HPC a critical topic.**
- ✓ **'Easily' parallelizable**.
- ✓ **Geometrically complex solution domains.**



Fluxed phase volumes, 3D shear case, $CFL = 0.5$, $T = 3s$, $N = 32$.

[1] D. B. Kothe et al. (1999). "A second-order accurate, linearity-preserving volume tracking algorithm for free surface flows on 3-D unstructured meshes". In: Proceedings of the 3rd ASME/JSME Joint Fluids Engineering Conference, San Francisco, CA, pp. 1–6

The geometrical Volume of Fluid Method

Impact and publications

Impact: increased accuracy of two-phase flow simulations

- spray coating/cooling,
- ink-jet printing,
- bubble column reactions,
- metal casting,
- ship/offshore hydrodynamics,
- ...

Relevant publications:

Tomislav Marić, Holger Marschall, and Dieter Bothe (2013). “voFoam-a geometrical volume of fluid algorithm on arbitrary unstructured meshes with local dynamic adaptive mesh refinement using OpenFOAM”. In: arXiv preprint arXiv:1305.3417

Tomislav Marić, Holger Marschall, and Dieter Bothe (2015). “lentFoam–A hybrid Level Set/Front Tracking method on unstructured meshes”. In: Computers & Fluids 113, pp. 20–31

Tomislav Marić, Holger Marschall, and Dieter Bothe (2018). “An enhanced un-split face-vertex flux-based VoF method”. In: Journal of Computational Physics