Breaking, merging and splashing bubbles: the art of fluid interface CFD

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The fascination of multiphase flow
GOVERNING EQUATIONS: NAVIER-STOKES

\[ \partial_t (\rho u) + \nabla \cdot (\rho u \otimes u) = -\nabla p + \nabla \cdot (2\mu D) + \sigma \kappa \delta_s n + \left( \nabla \sigma \right) \delta_s + \rho g, \]

where the strain-rate tensor \( D \) is

\[ D_{ij} = \frac{1}{2} \left( \frac{\partial u_j}{\partial x_i} + \frac{\partial u_i}{\partial x_j} \right). \]

Notice new term with surface tension \( \sigma \). Both fluids are considered incompressible

\[ \nabla \cdot u = 0. \]
Incompressibility is chosen because

- Most applications involve low Ma number flow
- Even at $Ma = 0.3$ compressibility effects are not the most important issue (e.g. in atomization problems)
- Simulation of compressible flows is technically much more difficult.
GOVERNING EQUATIONS: JUMP CONDITIONS

Another way to formulate the equations is to introduce jump conditions

\[ [X] \] Is the jump of X between fluids 1 and 2.

\[ [X] = X_1 - X_2 \]

Jump conditions:

a) velocity \[ [u] = 0 \]

b) Momentum flux: \[ \left[ \left( pI + 2\mu D \right) \cdot \mathbf{n} \right] = \sigma \mathbf{n} + \nabla \sigma \]
GOVERNING EQUATIONS: KINEMATICS

The interface $S$ follows the flow. Its normal velocity is

$$V_S = \mathbf{u} \cdot \mathbf{n}.$$ 

Another useful formulation involves the characteristic function $\chi$.

$$\partial_t \chi + \mathbf{u} \cdot \nabla \chi = 0$$

This equation inspires both VOF and level-set methods.

If $\chi = 1$ in phase 1 and $\chi = 0$ in phase 2: VOF, if $\chi = \text{distance}$, Level Set. VOF and level set share a lot of characteristics.
DEFINITION OF THE VOF METHOD

$C_{ij} = \text{Volume of « fluid » in cell } ij$
THE SIMPLEST VOF METHOD

Let \( \chi = 1 \) in phase 1 and \( \chi = 0 \) in phase 2. Then solve

\[
\partial_t \chi + \mathbf{u} \cdot \nabla \chi = 0
\]

using standard hyperbolic equations methods (e.g. TVD, FCT, ENO, Artificially compressible).

References: JADIM code (Toulouse), Issa and Ubbink.

Advantage: easy to program. Problems: interface thickens in time, lack of accuracy.
POSSIBLE GRIDS

VOF methods are not limited to regular grids, although treatment is much simpler and more accurate on regular grids.
RECONSTRUCTION

Standard VOF methods proceed in two steps: reconstruction and propagation.

(a) is a « first order », Simple Line Interface Construction, (SLIC). Its accuracy is similar to that obtained on unstructured grids.
(b) is a « second order » Piecewise Linear Interface Construction (PLIC)
The « VOF bag problem » (after Markus Meier).
All that is known is how much mass there is in each cell.
In case (a) the interface is easier to reconstruct than in case (b)
RECONSTRUCTION

Steps in reconstruction:
1. Determination of $n$.
   - Parker and Young (P.-.Y.) or « finite difference » method.
   - Puckett and Pilliod or ELVIRA least-squares method.
   - Scardovelli ’s linear fit method.

2. Position the interface once $n$ is found and $C_{ij}$ given.
DETERMINATION OF N: P.-Y. METHOD

Finite difference method: corner values

\[
n_{x,i+1/2,j+1/2} = \frac{1}{4} \left( C_{i+1,j} + C_{i+1,j+1} - C_{i,j} - C_{i,j+1} \right)
\]

\[
n_{y,i+1/2,j+1/2} = \frac{1}{4} \left( C_{i,j+1} + C_{i+1,j+1} - C_{i,j} - C_{i+1,j} \right)
\]

Finite difference method: cell center values

\[
n_{i,j} = \frac{1}{4} \left( n_{i+1/2,j+1/2} + n_{i-1/2,j+1/2} + n_{i+1/2,j-1/2} + n_{i-1/2,j-1/2} \right)
\]
DETERMINATION OF N: P.-Y. METHOD

Finite differences fail to obtain \( n \) exactly for a straight line in some cases such as the straight line below.
DETERMINATION OF N: ELVIRA

ELVIRA is interesting because it is the first truly second-order method: it approximates straight lines exactly.

It works by a *least-squares fit* to the interface normal.
Three cases exist for an interface in a 2D cell. Once interface orientation $\mathbf{n}$ is found, the interface position may be found. The equation of the interface is $\mathbf{m} \cdot \mathbf{x} = \alpha$. 
RECONSTRUCTION

(a)  (b)  (c)

(d)  (e)  (f)

(patented ?)
PROPAGATION

First manipulate the continuous form of the equations

\[
\frac{C^{n+1} - C^n}{\tau} = -\partial_x (u_x C) - \partial_y (u_y C) + (\partial_x u_x)C + (\partial_y u_y)C
\]

Discretize -> Naive split discrete form:

\[
\frac{C_{ij}^{n+1/2} - C_{ij}^n}{\tau} = -D_x (u_x C^n) = -D_x \phi_x^n
\]

\[
\frac{C_{ij}^{n+1} - C_{ij}^{n+1/2}}{\tau} = -D_y (u_y C^n) = -D_y \phi_y^n
\]
Naive method
Naive method

Geometrical definition of the discrete flux $\phi_x^n$

This is the « Eulerian » method. (as opposed to « Lagrangian »)
Naive method

Problems:

• There is no propagation into the diagonal cell: the method fails trivially for a uniform velocity field and straight interface.

• There is no guarantee that after the two steps the result is bracketed between 0 and 1 (0 < C < 1). Without this, when C > 1, one has to resort to arbitrary removal of mass.
ALTERNATING DIRECTIONS METHOD

The new method alternates directions. Here, first x-propagation the y-propagation.
ALTERNATING DIRECTIONS METHOD

1) \[
\frac{C_{ij}^{n+1/2} - C_{ij}^n}{\tau} = -D_x (u_x C^n)
\]

2) \[
\frac{C_{ij}^{n+1} - C_{ij}^{n+1/2}}{\tau} = -D_y (u_y C^{n+1/2})
\]

Does not preserve $0 < C < 1$. 
Kothe/Rider propagation method

1) Eulerian Implicit step

\[
\frac{C_{ij}^{n+1/2} - C_{ij}^n}{\tau} = -D_x (u_x C^n) - (D_x u_x)C_{ij}^{n+1/2}
\]

2) Explicit step

\[
\frac{C_{ij}^{n+1} - C_{ij}^{n+1/2}}{\tau} = -D_y^* (u_y C^{n+1/2}) - (D_y u_y)C_{ij}^{n+1/2}
\]

Leads to better mass conservation Does not preserve \( 0 < C < 1 \).
AREA PRESERVING MAPPING

Lagrangian explicit + eulerian implicit is an *area-preserving* linear mapping of the plane!

\[ x \rightarrow ax + b \]
\[ y \rightarrow cy + d \]

where the Jacobian of the transformation is \( J = ac = 1 \).
The first transform maps the top red rectangle on the bottom red rectangle. The velocities of the edges are node velocities.
Lagrangian explicit propagation transforms the central square into the red rectangle. The original figure is stretched like Arnold’s cat, but its area is preserved. Moreover, the volume fraction remains $0 < C < 1$ since all steps are now geometrical transformations, and all areas may be computed explicitly.
Defects of VOF methods:

-- flotsam and jetsam (1960)
-- wisps (1990)
-- no defect (2003)
Zalesak’s test after ten solid body rotations. 100 x 100 grid
(a) ELVIRA (solid) and linear fit (dashed) reconstructions
(b) quadratic (solid) and quadratic with continuity (dashed). Rotation is divergence-free, so all propagation methods give similar results.
TESTS

Kothe and Rider’s spiralling, stretching and reversing flow. Stream function:

$$\Psi = \sin^2(\pi x) \sin^2(\pi y) \cos\left(\frac{\pi t}{T}\right)$$
Naive propagation method

New method with various reconstructions


See wisps
Method by Aulisa, Manservisi, Scardovelli (markers+VOF)
SURFACE TENSION

Treatment of surface tension by Continuous Surface Force (« CSF » method, Brackbill, Kothe and Zemach JCP 1993)

\[ \sigma \kappa \mathbf{n} \delta_S \approx \sigma \kappa^h \nabla^h C \]

Many methods for \( \kappa \). Simplest:

\[ \kappa = -\nabla \cdot \mathbf{n} \approx -\nabla^h \cdot \left( \frac{\nabla^h C}{|\nabla^h C|} \right) \]
SURFACE TENSION

It is necessary to smooth the C function

Raw C function

Filtered C function
SURFACE TENSION

Elementary smoothing:

\[ \tilde{C}_{ij} = \frac{1}{2} C_{ij} + \frac{1}{8} \left( C_{i+1,j} + C_{i-1,j} + C_{i,j+1} + C_{i,j-1} \right) \]

Kernel smoothing:

\[ \tilde{C}(x) = \int C(y) K_{\varepsilon}(\|x - y\|) dy \]
SURFACE TENSION

Typical kernel

\[ K_{\varepsilon}(r) = A(\varepsilon) \left( 1 - \frac{r^2}{\varepsilon^2} \right)^4 \quad \text{for } r < \varepsilon \]

The constant A is chosen to normalize the discrete approximation.
SURFACE TENSION

Discrete Kernel implementation

\[ \tilde{C}_{ij} = \sum_{lm} K_{\varepsilon} (x_{ij} - x_{lm}) C_{lm} \]
SURFACE TENSION

Verification of Laplace’s law for a static bubble:

\[ R \frac{\Delta P}{\sigma} = 1. \]
SURFACE TENSION

Spurious currents around a static bubble.

Leads to difficulties when there is both a large density ratio and a large surface tension as it is the case for air-water interfaces.
SURFACE TENSION

The spurious current problem arises because of the discontinuity of $p$. Similar problems arise because of the discontinuity of $\rho g$ (when a free surface with gravity is not aligned with the grid), and also because of the discontinuity of $\mu D$.

Cut cell methods attempt better approximation of the various balances inside the cell.

This requires the accurate knowledge of the position of B and E, which may be done by abandoning VOF and reverting to marker particles.
SURFACE TENSION

markers chain : advect each marker.
SURFACE TENSION

An elementary way to distribute the surface tension force on the grid (Tryggvason’s method)
CUT CELL/MARKER METHODS

Another point of view involves looking at the momentum balance:

\[
\begin{align*}
0 &= \int \int (\mathbf{F} \cdot \mathbf{n} + \rho \mathbf{u} \cdot \nabla \mathbf{u}) \, dV \\
\end{align*}
\]

Exact balance equations:

\[
\begin{align*}
p_1 - p_2 &= \sigma / R \\
F_{\text{cap}} \cdot \mathbf{x} + \int_{C}^{F} p \, dl - \int_{A}^{D} p \, dl &= 0
\end{align*}
\]

But if \( p_i = p_{i-1} \) on figure then the discrete balance equation is not satisfied:

\[
F_{\text{cap}} \cdot \mathbf{x} + p_i - p_{i-1} \neq 0
\]
CUT CELL/MARKER METHODS

Cut cell methods try to improve the approximation of the momentum balance:

\[
F_{\text{cap}} \cdot \mathbf{x} + \int_{A}^{C} p \ dl - \int_{D}^{E} p \ dl \approx F_{\text{cap}} \cdot \mathbf{x} + p_{i-1,j} AB + p_{i-1,j+1} BC + p_{i,j} DE + p_{i,j+1} EF
\]
CUT CELL/MARKER METHODS vs Level Set/VOF

Advantages:

• great accuracy
• control when reconnection occurs

Drawbacks

• complex to code in 3D (use computational geometry?).
• no automatic reconnection
• no exact mass conservation.
VISCOSITY AND DENSITY

Viscosity and density jumps are treated by averaging in mixed cells of volume fraction 0 < C < 1. The arithmetic mean is

\[ \mu = C \mu_1 + (1 - C) \mu_2 \]

The harmonic mean is

\[ \frac{1}{\mu} = \frac{C}{\mu_1} + \frac{1 - C}{\mu_2} \]

Which mean is better depends on flow geometry.
VALIDATION OF VOF/MARKER METHODS

Comparison of analytical and numerical solutions for capillary waves, box size 64 x 64 VOF method.
VALIDATION

Mode 2 oscillation of a bubble (marker cut-cell method)
VALIDATION

Reconnection (VOF, by Denis Gueyffier)
VALIDATION

Experiment by Peregrine.

Simulation: VOF method, D. Gueyffier
VALIDATION

Right: rising bubble in oil, experiment.

Left: Simulation using the VOF method
VALIDATION

Kelvin-Helmholtz instability

Code/linear theory comparison

Better to use harmonic mean of viscosity in mixed cells (green curve)
WHAT CAN THIS BE USED FOR?

• Atomization
• Droplet impact
• Cavitation bubbles
• Bursting bubbles
ATOMIZATION

Coflowing jet atomization. Standard representation.
ATOMIZATION

Lasheras, Hopfinger, Villermaux, Raynal, Cartellier
…, (San Diego, Grenoble and Marseille)
ATOMISATION

Droplet deformation in a 2D shear layer.
Diesel engine (no coaxial gas flow)

Entry and exit conditions.

\[ \text{V}_{\text{inj}} = 300 \text{ m.s}^{-1} \]
\[ r_{\text{inj}} = 0.1 \text{ mm} \]
\[ \rho_{\text{gaz}} = 20 \text{ kg.m}^{-3} \]

2 x 8 mm

(1024 x 4096)
Laminar flow upstream

With upstream “turbulence”
ATOMISATION

Co-flowing atomizer

Parameters:
- 512 x 1024 grid
- \( r_L = 20 \text{ kg/m}^3 \)
- \( r_G = 2 \text{ kg/m}^3 \)
- \( U_G = 100 \text{ m/s} \)
- \( M = 2.5 \)
- \( R = 400 \text{ microns} \)
- \( \mu_L = 0.002 \text{ kg/m/s} \)
- \( \mu_G = 0.0001 \text{ kg/m/s} \)
- \( U_L = 20 \text{ m/s} \)
- \( \sigma = 0.030 \text{ kg/s}^2 \)
ATOMISATION
Same with turbulent entry (Enrique Lopes-Pages)
Droplets’ distribution function in coaxial jets

Laminar

Turbulent

\[ d(10^{-6} \text{m}) \]

\[ N_d \]

\[ d(10^{-6} \text{m}) \]

\[ N_d \]
128^3 simulations

3D VOF code, space periodic simulation. Diesel engine conditions.
A rare event: 
Breakup after sheet puncturing

Show movie
- 256x128x128 (2x1x1 mm) (16 procs 16x128x128 - 1 week)
- injection : 200 m/s
- t step : 0.25 ns
- density ratio diesel/air : 8.5
3D
(Anthony Leboissetier)
Conclusions

Comparaison with linear theory validates the code.

• The turbulence level on entry is important.
• Droplet sizes are exponentially distributed.
• A 2D mechanism for filament formation was found.
• Still debate on the 3D mechanism
Forecast

Present simulations in spatial 2D are resolved up to 512 x 2048. An equivalent resolution in 3D requires 512 x 512 x 2048 simulations. One can perform 128 x 128 x 256 on a 16-proc. PIII cluster. An additional factor of about 128 in CPU is necessary.

- It is likely that the 3D problem will be sufficiently resolved circa 2010.

- This forecast was published in 2001 (Scardovelli and SZ) and at the same time it was predicted that the droplet splashing problem would be solved in 2005 … well let us see.
DROPLET IMPACT

Simulation setup

Liquid

D

gas

U

Same liquid

h
DROPLET IMPACT

Early-forming jets are thin.

Perhaps an explanation to the prompt splash: (droplets break early on rough surfaces) phenomenon?
Navier-Stokes equations, two phases.

Both liquid and gas are simulated.

Example: 2 mm glycerine droplet at 6m/s

Liquid and gas are incompressible.
DROPLET IMPACT

Pressure field
DROPLET IMPACT

Axisymmetric.

Low Re Case

Re=100
We=8000
High Re Case

Re=1000
We=8000
DROPLET IMPACT

What happens in 3D?

Look from above
Why are perturbations amplified?
DROPLET IMPACT

Standing in elevator
accelerated up
Feel « normal » gravity down
Stable

Standing in elevator
Accelerated down
Feel attracted to roof
Effective gravity up: Unstable

Conclusion: Interface unstable when acceleration from light to heavy.
DROPLET IMPACT

Select a numerically « nice » case:

Not too viscous (no splashing)
Not too large Re (too unstable)

A glycerine, 4 mm droplet falling at 2 m/s

256² Simulation (128 grid points/diameter)

Repeat at 128²: same result
Re = 450,
We = 533,
D/e = 4,

last frame
Ut/D = 1.81
DROPLET IMPACT

Low resolution

Re = 450,
We = 533,
D/e = 4,
High resolution

Low resolution
DROPLET IMPACT
DROPLET IMPACT

3D case, large resolution

256^3 Simulation (128 grid points/diameter)

Relatively small-amplitude initial azimuthal undulation

Notice reversal of curvature

Show 3D movie
DROPLET IMPACT

DROPLET IMPACT

Relatively larger-amplitude initial azimuthal undulation

Notice

- lift-up of fingers
- no adaptation of wavelength
Thinner layer ($D/h = 8$) and larger horizontal extent ($L_x/D = 4$)
DROPLET IMPACT

The thinner layer creates a thinner corolla which now breaks!
DROPLET IMPACT

There is less uplift by the wind, so the corolla and the fingers are definitely drooping down.
Conclusion: 2005 is not finished!
CAVITATION BUBBLES

Bubbles tend to collapse asymmetrically
- near walls
- in bubble clouds (see recent sonofusion controversy)
Collapsing bubbles form jets.

Lauterborn’s experiment:
Use control points to extrapolate velocity field:
Free axisymmetric oscillations of a bubble:
Comparison experiment/simulation
There is less energy in the real system after rebound:
Breaking bubbles

McIntyre

Simulation
(L. Duchemin)
-- The marker method allows very accurate solutions of the free surface problem with viscosity.

- A critical ratio of distance to compression exists for jet formation near a wall. Surface tension effects remain to be added.

- Simulations of Bubble breaking phenomena show good agreement with experiment. A regime of high-speed, thin jets is found.
LATTICE BOLTZMANN METHOD

Lattice Boltzmann Method (LBM)
Populations are averages, real numbers between 0 and 1.

\[ N_1(x + c_i, t + 1) - N_1(x, t) = N_2(x, t)N_4(x, t) - N_1(x, t)N_3(x, t) \]

With three other equations for \( N_{2,3} \text{ and } 4 \)
In general, the lattice Boltzmann populations obey the equation:

\[ N_i(x + c_i, t + 1) - N_i(x, t) = \Omega_i(N(x, t)) \]

Where \( \Omega_i = \Omega_i(N(x, t)) \) is a complex collision operator.

Equations remain complex. A simpler method is obtained when The right-hand side (the collision operator) is linearized.
LATTICE BOLTZMANN METHOD

Advantages of the LBM

- Simple formulation
- Easy parallelisation
- Automatic phase separation
- Automatic reconnection
- Exact mass and momentum conservation
LATTICE BOLTZMANN METHOD

Applications of the LBM:

• Multiphase flow in porous media (Rothman, Adler).
• Bubbly flow (e.g. work of Sundaresan, collaboration with Tryggvason).
• A commercial code (Powerflow of EXA corporation) exists using an extension of the LBM, mostly marketed to the automotive industry.
LATTICE BOLTZMANN METHOD

How to separate phases in a particle method?

• Introduce repulsive forces between A and B particles, or attractive forces between A and A particles.

Models by

Rothman and Keller 1988
Chen et al. 1989
Equations satisfied by the lattice Boltzmann method found by Chapman-Enskog expansion:

Mass conservation leads to:

\[ \partial_t \rho + \nabla \cdot (\rho \mathbf{u}) = 0 \]

(The LBM is compressible !)
Momentum conservation leads to:

\[
\partial_t (\rho \mathbf{u}) + \nabla \cdot (\rho \mathbf{u} \otimes \mathbf{u}) = -\nabla p + \nabla \cdot \mathbf{S} + \sigma k \delta_s \mathbf{n} + \left( \nabla \sigma \right) \delta_s + \rho \mathbf{g},
\]

Where

\[
S_{ij} = \frac{\mu}{\rho} \left( \frac{\partial \rho u_j}{\partial x_i} + \frac{\partial \rho u_i}{\partial x_j} + \ldots \right)
\]

Compare to the exact (compressible) equation:

\[
S_{ij} = \mu \left( \frac{\partial u_j}{\partial x_i} + \frac{\partial u_i}{\partial x_j} \right) + \mu_2 \left( \nabla \cdot \mathbf{u} \right) \delta_{ij}
\]
LATTICE BOLTZMANN METHOD

The jump conditions are not satisfied: true jump conditions (2D, constant $\sigma$)

a) velocity $[u] = 0$

b) Momentum flux:

\[
\left( p\mathbf{1} + 2\mu \mathbf{D} \right) \cdot \mathbf{n} = \sigma \mathbf{n}
\]

LBM jump conditions

a) Normal velocity $[u \cdot n] = 0$

b) Tangential velocity $[\rho u \cdot t] = 0$

c) Momentum flux:

\[
\left( p\mathbf{1} + S \right) \cdot \mathbf{n} = \sigma \mathbf{n}
\]
Double Poiseuille flow (Irina Ginzburg and Pierre Adler, unpublished) shows that $\rho u$ is continuous, not $u$. 
LATTICE BOLTZMANN METHOD

As a result the LBM is valid/useful only in special cases

- $Re = 0$
- Equal density
- Free surface

Examples: bubbles, flow in porous media.
Simulation, Youngseuk Keehm
QuickTime™ et un décompresseur Vidéo 1 Microsoft sont requis pour visionner cette image.
THE END !
LATTICE BOLTZMANN METHOD

LATTICE GAS CELLULAR AUTOMATA: HISTORY

• Kinetic theory models
• Statistical Physics Models
• Cellular Automata
• Hexagonal FHP gas
• Lattice Boltzmann Method
• Fixed point arithmetic Lattice Boltzmann Methods
LATTICE BOLTZMANN METHOD

Simplest lattice-gas cellular automaton model: the HPP

4 particles per node
One in each directions.

Particles collide and jump from cell to cell.
Momentum and particle number are conserved.
Hexagonal Frisch-Hasslacher-Pomeau (FHP) model:

6 particle velocities, 1 or 0 particle in each state.

Collision rules ensure conservation of mass and momentum and lead to large scale equations resembling Navier-Stokes.
Model later extended to:

- 3 Dimensions
- Two phase flow (two liquids and liquid-gas)
- Models with thermal effects.
- Thermal convection
- Viscoelastic effects.
Difficulties:

• Considerable **noise** affects the results. Vorticity is most noisy, and interface positions fluctuate enormously.
• The lack of **Galilean invariance** is difficult to fix. A fundamental problem of all « Cellular automata » type approaches to modelling is the absence of Noether-like theorems (equivalence between conservation laws and invariance under transforms).
• **Other problems**: compressibility effects, boundary conditions.
FLOW IN POROUS MEDIA

lab experiment by Chatzis and Dullien (1985).
Two-phase LBM: Capillary Pressure - Drainage-type Snap-off (Simulation)

Simulation by Youngseuk Keehm, SRB
Snapshots from two-phase flow sim.

Fontainebleau sandstones

Porosity 22%                            Porosity 16%

Stanford Rock Physics & Borehole Geophysics
Capillary effect on two-phase flow

Low Pressure Gradient

High Pressure Gradient
Capillary effect on two-phase flow

Low Pressure Gradient

High Pressure Gradient