Development and applications of a Level Set Method for interface tracking

Sébastien Tanguy, Alain Berlemont

UMR6614-CORIA
Technopôle du Madrillet
BP 12 Avenue de l'Université
76801 Saint-Etienne-du-Rouvray Cedex

Abstract

Level set technique for interface tracking is presented, both for the continuum surface force approach and the ghost fluid method approach. A projection method is used to solve incompressible Navier Stokes equations which are coupled to a transport equation for the level set. Results are presented for droplet collisions in 2D and 3D, in the reflexive coalescence regime with satellites formation.

1 Introduction

Numerical simulation for multiphase flows requires a specific approach to describe interface behaviors, such droplet coalescence or break-up. Front tracking methods[1] are based on the Lagrangian tracking of marker particles; they are more efficient when the interface curvature does not exhibit stiff behaviors. However it appears that topological changes, which are involved in droplet coalescence, depend on an interaction time parameter of great influence. Volume of Fluid method is describing the volumetric fraction of each phase in grid cells. The main disadvantage of the method is the interface reconstruction that appears quite difficult on 2D domain, and numerically prohibitive on 3D domain. A consequence is the uncertainty on interface curvature and thus on surface tension forces. Our work deals with a Level Set method of Osher and Sethian[2] which describes the interface with the zero level curve of a continuous function. This function is defined as the signed distance to the interface. Its advancement is updated with a convection equation, coupled with a constraint that ensures that the function is always a signed distance. Different numerical methods can be implemented to take into account for surface tension forces, which depend on the curvature of zero level curve, in Navier Stokes equations. We provide the advantages and the drawbacks of this method and we discuss about its potential improvements. The main target of this study is to reach a better understanding of primary and secondary atomization processes, studying jet stability and droplets collisions.

2 Description of the method

Level Set methods are based on the use of a continuous function ϕ to describe the interface between two mediums [3,4]. That function is defined as the algebraic distance between any point of the domain and the interface, and the interface is thus described by the 0 level of that function. Solving a convection equation determines the evolution of the interface in a given velocity field[3] **V**:

$$\frac{\partial \phi}{\partial t} + \mathbf{V}.\nabla\phi = 0 \qquad (1)$$

That propagating interface equation is of hyperbolic type. Specific care has to be devoted on the discretization method, as discontinuities are often observed in the results. To avoid singularities in the distance function field, we thus use 5th order WENO scheme for convective terms.

One advantage of the level set method is its ability to represent topological changes both in 2D or 3D geometry quite naturally. Moreover, geometrical information on the interface, such as normal vector **n** or curvature κ, are easily obtained through:

$$\mathbf{n} = \frac{\nabla\phi}{|\nabla\phi|} \qquad (2) \qquad \kappa(\phi) = \nabla \cdot \mathbf{n} \qquad (3)$$

However some problems arise when the level set method is developed: numerical dissipation when solving interface transport equation lead to mass deficit, which can be important when the flow is under-resolved. Moreover high velocity gradient can produce large spreading and stretching of level set, such as ϕ will no more remain a distance function. A redistancing algorithm [4] is then applied to keep ϕ as the algebraic distance to interface. The algorithm is base on the iterative resolution of the following equation:

$$\frac{\partial d}{\partial \tau} = \text{sign}(\phi)(1 - |\nabla\phi|) \qquad \text{where} \quad d(x,t,\tau)_{\tau=0} = \phi(x,t) \qquad (4)$$

That hyperbolic type equation is solved with 5th order WENO scheme for spatial derivatives

The main advantage of the above algorithm is to provide us with the required property for ϕ without changing the position and velocity of the interface.

However numerical computation of equation (4) can produce mass loss in the results. That scheme is thus coupled with a constraint[4] which helps in minimizing the mass error.

3 Projection method

The Level Set method is coupled with projection method for the direct numerical simulation of the incompressible Navier-Stokes equations expressed as follows:

$$\frac{\partial \mathbf{V}}{\partial t} + (\mathbf{V}\cdot\nabla)\mathbf{V} + \frac{\nabla p}{\rho} = \frac{\nabla(2\mu\mathbf{D})}{\rho} + \mathbf{g} \qquad \mathbf{D} = \tfrac{1}{2}(\nabla\mathbf{V} + \nabla\mathbf{V}^T) \qquad (5)$$

$$\nabla \cdot \mathbf{V} = 0 \qquad (6)$$

p is the pressure, ρ and μ are the fluid density and viscosity respectively.

Three main steps are carried out:

- estimate velocity **V*** from velocity at time t_n:

$$\mathbf{V}^* = \mathbf{V}^n - dt * ((\mathbf{V}^n \cdot \nabla)\mathbf{V}^n - \frac{\nabla(2\mu\mathbf{D})}{\rho} - \mathbf{g}) \qquad (7)$$

  where **g** is the gravity vector.

- solve Poisson equation for divergence free velocity:

$$\nabla \cdot (\frac{\nabla p^{n+1}}{\rho}) = \frac{\nabla \cdot \mathbf{V}^*}{dt} \tag{8}$$

- update velocities

$$\mathbf{V}^{n+1} = \mathbf{V}^n - dt * \frac{\nabla p^{n+1}}{\rho} \tag{9}$$

The above method is well known but requires special attention. Spatial derivatives are estimated with 2nd order central scheme, but convective terms are approximated by 5th order WENO scheme discretization in order to ensure a robust behavior of the solution. Temporal derivatives are approximated with at least 2nd order Runge-Kutta scheme.
Equation (8) is numerically solved with a conjugate gradient method which is pre-conditioned by an incomplete Choleski factorization.

4 Discontinuities

The interface is defined by two different medium and discontinuities have to be handled on density, viscosity and pressure. Specific treatment is thus needed to numerically describe the jump conditions. Formally, these conditions are defined by:

$$\lambda(\phi) = \lambda_g + (\lambda_l - \lambda_g) H(\phi) \tag{10}$$

where λ stands for ρ or μ and $H(\phi)$ is the Heaviside function centered on the interface.
The pressure jump related to surface tension σ and the interface curvature reads:

$$[p] = \sigma \kappa(\phi) \tag{11}$$

Two different approaches can be used to represent the above conditions, namely the continuum surface force (delta formulation) or the ghost fluid method [5].

4.1 Continuum surface force

In the continuum surface force (CSF) approach, the Heaviside function is smoothed on two or three nodes on each side of the interface as follows:

$$H_\varepsilon(\Phi) = \begin{cases} 0 & \text{if } \phi < \varepsilon \\ 1/2\left[1 + \phi/\varepsilon + 1/\pi \sin\left(\pi\phi/\varepsilon\right)\right] & \text{if } |\phi| \le \varepsilon \\ 1 & \text{if } \phi > \varepsilon \end{cases} \tag{12}$$

In order to take into account for surface tension force, an additional term is involved in Navier Stokes equations, which is written:

$$-\sigma\kappa(\phi)\delta_\varepsilon(\phi)\nabla\phi \tag{13}$$

where δ_ε is the derivative of $H_\varepsilon(\phi)$.
That approach has been proved to be robust and leads to interesting results, but two main problems can be noticed. The first one is linked to the smoothing of the Heaviside function which introduces an interface thickness which depends on the mesh size, and thus an uncertainty on the interface exact position. The second problem is parasitic currents, which can appear for very high curvature of the interface that can generate slight spurious velocities due to high surface tension forces.

4.2 Ghost fluid method

In the Ghost Fluid method (GFM) ghost cells are defined[5,6] on each side of the interface and appropriated schemes are applied for jump conditions. The interface is as above defined through the distance function, and jump conditions are extrapolated on some nodes around the interface. Following these jump conditions, the discontinued functions are continuously prolongated and then derivatives are estimated. Let us consider variable f which is discontinuous across the interface such as the jump of f is $[f]_\Gamma=a(x)$. The f derivative is then expressed in cells i which are crossed by the interface by:

$$\left.\frac{\partial f}{\partial x}\right|_{i+\frac{1}{2}} = \frac{f_{i+1}-f_i}{dx} - \frac{a_\Gamma}{dx} \qquad a_\Gamma = \frac{a_i|\phi_{i+1}| + a_{i+1}|\phi_i|}{|\phi_i| + |\phi_{i+1}|} \tag{14}$$

The above scheme can be applied for any kind of discontinuities, with assumption that the interface can be localized inside a grid mesh and that the jump of the discontinuous variables (pressure, density and viscosity in our simulations) is known.

5 Results

The main problem arising in droplet collisions concerns the description of thin liquid layers in the process. That problem is illustrated on figure 1 which shows droplet collision process on time where initial kinetic energy of the droplets has been almost transformed in surface energy. The resulting droplet structure looks like a tore with classic external ring, but with a very thin layer inside the ring. The inside membrane surface energy is negligible due to its curvature with tends towards 0. However, when its thickness is of the order of the grid mesh, a rupture of the membrane can occur which may produce some discrepancies in the results. To avoid such problem, grid refinement is used in the present work.

Figure 1: Thin layer during droplet coalescence

We have carried put numerous simulations to validate our codes (among them: Zalezak's disk, single vortex flow, periodic double shear layer, Rayleigh-Taylor instability). Moreover both approaches, namely CSF and GFM, have been compared and it appears that GFM method should be mainly preferred when the liquid membrane thickness is small.

5.1 2D axi-symmetric simulations

Recent results droplet collisions[7] providing collision regime diagram as function of Weber number and impact parameter have used to validate our simulation. The Weber number is defined with the droplet relative velocity, namely:

$$We = \frac{\rho d U_{rel}^2}{\sigma} \tag{15}$$

In the following results, we consider ethanol droplet collision in air. Physical properties are:

σ=0.02275 kg.s^{-2} ρ_{liq}=791 kg.m^{-3} μ_{liq}=1.20.10^{-3} ρ_{gas}=1.226kg.m^{-3} μ_{gaz}=1.78.10^{-5}

The first set of results concerns head on collision (impact parameter =0) of two identical droplets of initial diameter 400 μm and the Weber number is equal to 61. Ghost fluid method is used on a 120x360 grid and the time step satisfies 0.5 CFL condition.

Following experimental results[7], the coalescence regime is reflexive separation with one satellite. Qualitative agreement is satisfactory, as we can observe that behavior on figure 2, where the collision is shown on different times. Quantitative comparisons are not straightforward, but following Estrade[7] observations the satellite diameter d_s should be:

$$\frac{d_s}{d_g(1+\Delta)} = 0.008(We - We_2) - 0.1734 \tag{16}$$

where d_g is the larger particle diameter, Δ is the ratio of particle initial diameters (Δ=1 here) and We_2 is a critical Weber number for transition between coalescence and reflexive separation given par Qian et al[8]. In the presented results, one obtain: d_s=190 μm. The simulation produces a slightly larger diameter, namely 230 μm. The satellite diameter is larger when the Weber number increases and this tendency has been verified in our simulations. However when the Weber number increases the internal membrane is thinner which requires more and more grid nodes and thus computer time.

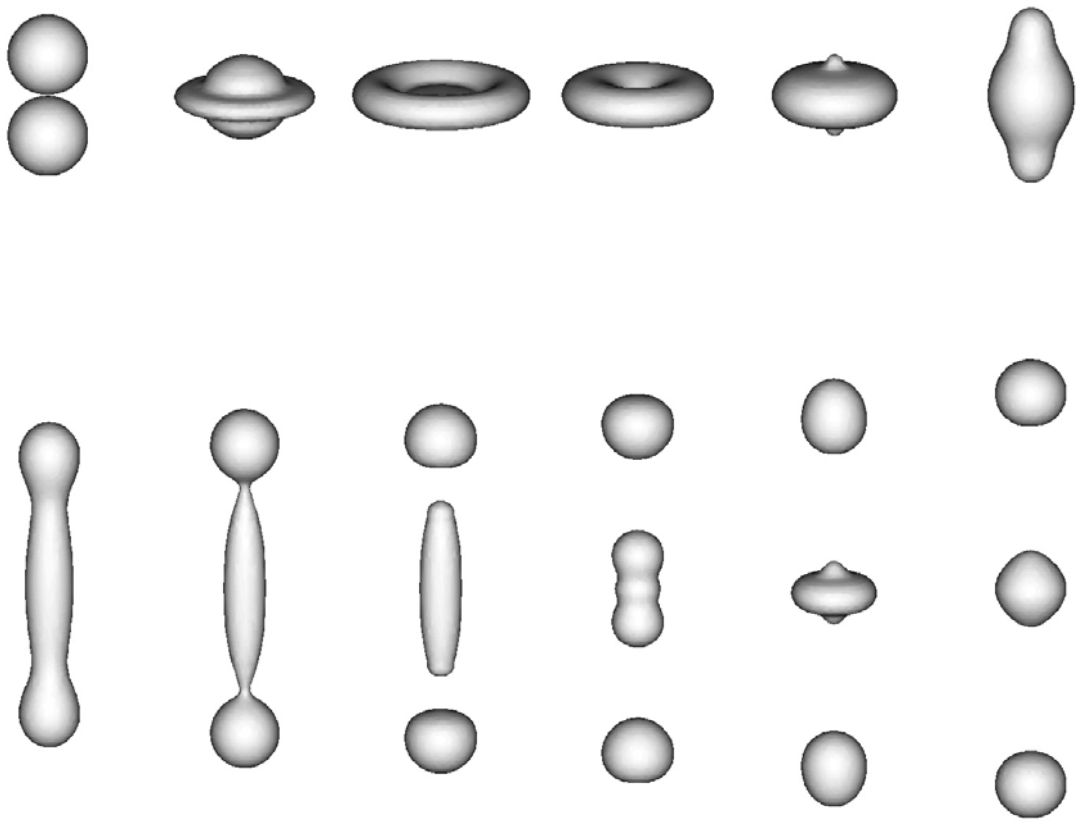

Figure 2: Head on droplet collision for We=61

5.2 3D simulations

The code has been extended to 3D configurations and we present below some preliminary results on droplet coalescence with the continuum surface force method.
Ethanol droplet collision is considered, the Weber number is 80, the impact parameter is equal to 0.5, and particle diameter is 400 μm. The grid is 160x160x34 equally spaced nodes. The obtained results are presented on figure 3 (12 images) and we observe the droplet reflexive separation with formation of three satellites. That behavior is in qualitative agreement with experiments[7] but as it can be seen on the figure (image 5), the internal membrane is broken denoting a too small number of grid nodes. It is clear that optimization of the code is required to compare more precisely the simulations with experimental results. Note that the "cross" deformation on image 9 has been experimentally observed.

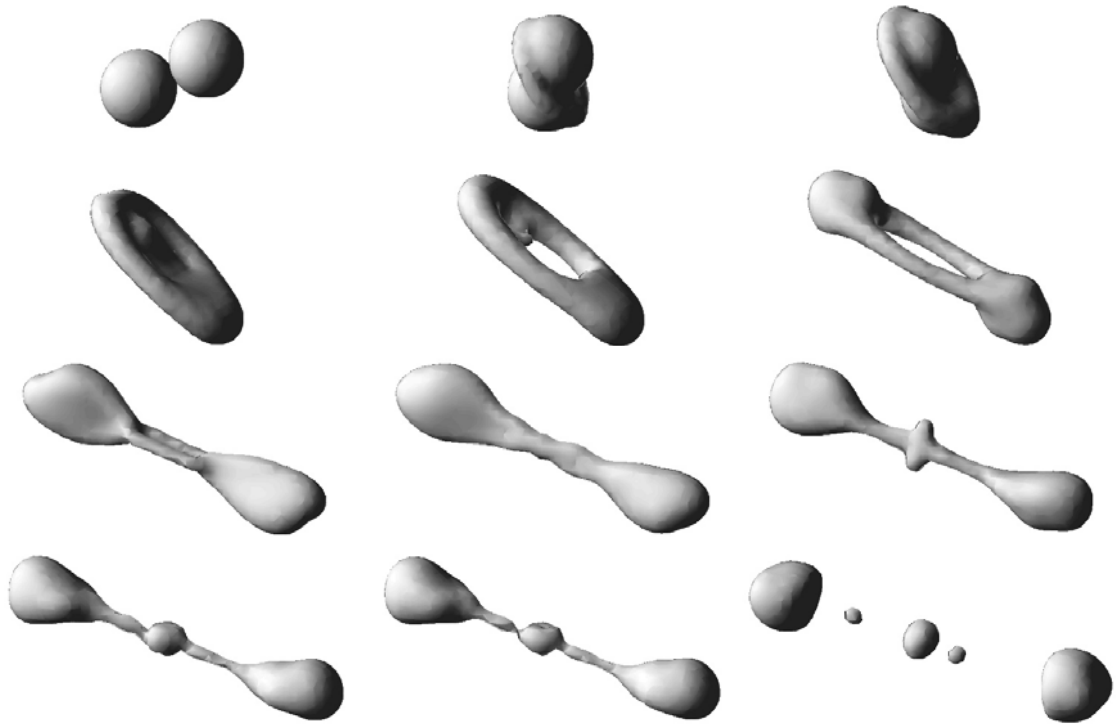

Figure 3: Reflexive separation of droplet collisions We=80 I=0.5

6 Conclusion

Two different methods have been set up for interface tracking with the level set method in 2D and 3D configurations. Results are encouraging and new developments are currently carried out. The ghost fluid method appears to be slightly more precise than the continuum surface force and seems to be a bit faster. That behavior is linked to the Poison equation solver which requires less iterations with GFM than with CSF.
However improvements are necessary in both formulations since the level set method accuracy is quite poor in under resolved regions where mass loss can arise. That behavior is quite important in cases of thin membranes and has to be evaluated more precisely. The constraint, which is used in the present paper in the re-distancing algorithm, should be better replaced by the particle level set method[9], which insures mass conservation and allows a fine description of the interface.

References

[1] Nobari J Trygvason G 1994 *Head on collision of drops: a numerical investigation*, *Physics of Fluids*, 8

[2] Osher S., Sethian J. 1988 *Front propagating with curvature dependent speed, J. Comp.Phys.*, 79, 1.

[3] Sethian J A 1999 *Level Set Method and fast marching methods*. Cambridge Univ.Press.

[4] Sussman M Fatemi E Smereka P Osher S 1997 *An improved Level Set method for incompressible two-phase, Computers and Fluids*, 27.

[5] Kang M Fedkiw R Liu X D 2000 *A Boundary Condition Capturing Method for Multiphase Incompressible Flow, J. Sci. Comput*. 15, 323-360.

[6] Liu X D Fedkiw R Kang M 2000 *A Boundary Condition Capturing Method for Poisson equation on irregular domains, J. Sci. Phys*., 151-178.

[7] Estrade J.P. 2000, *Etude expérimentale et numérique de la collision de gouttelettes*, *PhD Thesis*, Université de Toulouse, France.

[8] Quian J Law C K 1994 *Effects of liquid ambient gas properties on droplets collision, AIAA Journal,* 1-13.

[9] Enright D Fedkiw R Ferziger J Mitchell I. 2002 *A Hybrid Particle Level Set Method for Improved Interface Capturing ‚J. Comput. Phys.* 183, 83-116.