Droplet collisions using a Level Set method: comparisons between simulation and experiments

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Abstract

Level Set methods are based on defining a continuous function where the zero level curve is the interface. That function is initialized as the signed distance to the interface in the computation field. Solving a convection equation allows one to follow the interface displacements in a given velocity field. One advantage is its ability to represent topological changes and geometrical information on the interface, such as the normal vector or curvature, which are obtained through a level set function gradient. To avoid the spreading and stretching of a level set, a re-distancing algorithm is applied to ensure that the function remains the signed distance to the interface.

The Level Set method is coupled with the projection method for the direct numerical simulation of the incompressible Navier-Stokes equations. Spatial derivatives are estimated with the 2nd order central scheme, but convective terms are approximated by the 5th order WENO scheme discretization in order to get a robust behavior of the solution. Temporal derivatives are approximated with the Adams Bashforth scheme. The linear system deduced from the Poisson equation is solved with a multigrid algorithm for preconditioning the conjugate gradient method. To handle interface discontinuities the ghost fluid method is used. Numerical codes have been developed for 2D, 2Daxi and 3D geometries, with MPI parallelization. The results are presented for head-on droplets collisions in a coalescence regime and a reflexive regime with 2D axi-symmetric code, and for off-center droplets collision code in a separation regime for a large impact parameter with 3D code. Simulations provide realistic and various droplet collision behaviors and they correspond to experimental observations.

Keywords: Level Set, ghost fluid, interface tracking, droplet collision simulation.
1 Introduction

Numerical simulations for interface tracking can be carried out using either “front tracking” methods or “front capturing” methods. Front tracking methods (Nobari et al. [1]) are based on the Lagrangian tracking of marker particles that are attached to the interface motion. They appear suitable when irregularities on the interface curvature are not too large, but they are not well adapted to describing topological changes of the interface. Moreover on 3D geometries they rapidly require too large computer resources and they do not appear of interest for industrial purpose. We have thus developed a front capturing method.

Two main approaches can be used in front capturing methods, namely the Volume of Fluid method (VOF) and the Level Set method. The VOF method describes the volumetric fraction of each phase in grid cells. The main difficulty of the method is that 2D interface reconstruction appears quite difficult, and 3D reconstruction is numerically prohibitive on 3D domain. A consequence can be some uncertainties on the interface curvature and thus on the surface tension forces. Nevertheless, let us mention that realistic and predictive simulations can be carried out (Rieber and Frohn [2], Gueyffier et al. [3]). Interface reconstruction can be avoided by assuming a continuous volumetric fraction throughout the whole computational domain, which means that an interface thickness is introduced (Benkenida and Magnaudet [4]). The method is then quite similar to the Level Set method in its continuous force formulation. Osher and Sethian [5] proposed a Level Set method which describes the interface with the zero level curve of a continuous function defined by the signed distance to the interface. To describe the interface discontinuities, two approaches can be used, namely the Continuous Surface Force (“delta” formulation), which assumes that the interface thickness is 2 or 3 grid meshes wide, and the ghost fluid method (GFM), which has been derived by Fedkiw et al. [6] to capture jump condition on the interface.

We first present the Level set method and its coupling with incompressible Navier Stokes equations. The Ghost Fluid Method is described and results are then presented and compared with experiments for different droplet collision configurations, leading to different collision regimes, namely coalescence, separation after minor deformation and separation with the formation of satellites in the break up process. Simulations are carried out with the 2D-axi code for head-on collisions and the 3D code for off-center collisions.

2 Numerical approach

2.1 Level set method

Level Set methods are based on the use of a continuous function $\phi$ to describe the interface between two mediums [7,8]. 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 $\mathbf{V}$:
Specific care is put 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 \( \mathbf{n} \) or curvature \( \kappa \), are easily obtained through:

\[
\mathbf{n} = \frac{\nabla \phi}{|\nabla \phi|} \quad \kappa(\phi) = \nabla \cdot \mathbf{n}
\]

Some problems arise when the level set method is developed, namely high velocity gradient can produce wide spreading and stretching of level set, and \( \phi \) will no longer remain a distance function. A redistancing algorithm [8] is then applied to keep \( \phi \) as the signed distance to interface. The algorithm is based on the iterative resolution of the following equation:

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

where \( \tau \) is a fictitious time. We solve equation (3) until steady state is reached, thus close to the exact steady state solution namely either \( \text{sign}(\phi) = 0 \), meaning that we are on the droplet interface, or \( |\nabla d| = 1 \) which mathematically defines a distance function. We then replace \( \phi(x,t) \) by \( d(x,t,\tau_{\text{steady}}) \).

It is well known that numerical computation of eqns. (1) and (3) can generate mass loss in under-resolved regions. This is the main drawback of level set methods, but to improve mass conservation two main extensions of the method can be developed, namely the particle level set (Enright et al. [9]) and a coupling between VOF and Level Set (Sussman and Puckett [10]). These extensions have not been carried out here, but we have quantified mass loss in the simulations and ensured that it was negligible (<1%).

### 2.2 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:

\[
\frac{\partial \mathbf{V}}{\partial t} + (\mathbf{V} \cdot \nabla) \mathbf{V} + \frac{\nabla p}{\rho} = \frac{\nabla (2\mu \mathbf{D})}{\rho} + \mathbf{g} \quad \mathbf{D} = \frac{1}{2}(\nabla \mathbf{V} + \nabla \mathbf{V}^T) \quad \nabla \cdot \mathbf{V} = 0
\]

\( \mathbf{p} \) is the pressure, \( \rho \) and \( \mu \) are the fluid density and viscosity respectively. Spatial derivatives are estimated with 2nd order central scheme, but convective terms are approximated by 5th order WENO scheme discretization in order to get a robust behavior of the solution. Temporal derivatives are approximated Adams Bashforth formulation. Linear system deduced from Poisson equation is solved with a multigrid algorithm for preconditioning conjugate gradient method (Tanguy [11]).
2.3 Discontinuities: ghost fluid method

The interface is defined by two different phases and discontinuities must be taken into account for density, viscosity and pressure. For example, the pressure jump related to surface tension $\sigma$ and to the interface curvature reads (Brackbill et al. [12])

$$
[p] = \sigma \kappa(\phi) + 2[\mu] (\nabla u \cdot n, \nabla v \cdot n, \nabla w \cdot n) \cdot n
$$

where $[.]$ represents a jump in the variable considered.

Specific treatment is thus needed to describe the jump conditions numerically. Two different approaches can be used to represent the above conditions, namely the continuum surface force (CSF formulation) or the Ghost Fluid Method (GFM). The CSF approach has been proved to be robust and leads to interesting results, but two main problems can be noticed. Smoothing the Heaviside function introduces an interface thickness which depends on the mesh size, and thus an uncertainty on the exact location of the interface. To overcome that smoothing, the Ghost Fluid Method, has been developed by Fedkiw et al. [6]. The formalism respects jump discontinuities across the interface, and avoids an interface thickness. Discretization of discontinuous variables is more accurate, and spurious currents in the velocity field are thus much lower than with CSF methods. We have used this procedure to discretize all discontinuous variables, namely density, viscosity, pressure and viscous tensors ([11], Kang et al. [13]).

In the GFM, ghost cells are defined on each side of the interface and appropriated schemes are applied for jump conditions. As above defined the distance function defines the interface, and jump conditions are extrapolated on some nodes on each side of the interface. Following the jump conditions, the discontinued functions are extended continuously and then derivatives are estimated. Let us consider variable $f$ which is discontinuous across the interface such as the jump of $f$ is $[f]_I = a(x)$.

The $f$ derivative is then expressed in cells $i$ which are crossed by the interface by:
\[
\frac{\partial f_i}{\partial x} \bigg|_{x_{i+\frac{1}{2}}} = \frac{f_{i+1} - f_i}{dx} - a_{\Gamma} \quad \quad a_{\Gamma} = \frac{a_{\Gamma}^i \phi_{i+1} + a_{\Gamma}^{i+1} \phi_i}{\phi_i + \phi_{i+1}}
\]

(7)

where Ghost values \(f_{i+1}^{-g}\) and \(f_i^{g+}\) are defined by:

\[
f_{i+1}^{-g} = f_{i+1} - a_{\Gamma} \quad \quad f_i^{g+} = f_i + a_{\Gamma}
\]

(8)

The method is 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 is known. More details can be found in Liu et al. [14] on implementing the Ghost Fluid Method to solve the Poisson equation with discontinuous coefficients and obtain solution with jump condition. All the simulations presented here are thus carried out with the Ghost Fluid Method. Numerical codes have been developed for 2D, 2Daxi and 3D geometries, and MPI parallelization is used.

3 Results

Experimental droplet collision studies (Ashgriz and Poo [15], Qian and Law [16]) are providing us with different correlations to decide what happens when droplet collision occurs. The main parameters are the surface tension coefficient \(\sigma\), liquid viscosity \(\mu\), liquid density \(\rho\), droplet relative velocity \(U_c\), the impact parameter \(I\), and the ratio of droplet diameters \(\Delta\). The following non-dimensional numbers are thus defined by most authors to characterize droplet collisions, namely:

\[
We = \frac{\rho U_c^2 D_s}{\sigma} \quad \quad Oh = \frac{\mu}{\sqrt{\rho \sigma D_s}} \quad \quad \Delta = \frac{D_s}{D_b} \quad \quad I = \frac{2b}{D_s + D_b}
\]

(9)

where \(We\) is the Weber number and \(Oh\) the Ohnesorge number, and it is assumed that \(D_b\) is the bigger droplet diameter and \(D_s\) is smaller droplet diameter. The impact parameter \(I\) characterizes the eccentricity of the collision, and \(b\) is defined as the distance from the center of one droplet to the relative velocity vector placed on the center of the other droplet.

Several simulations have been carried out for head on droplet collision (2D-axi), off center droplet collisions (3D), for different Weber number and Ohnesorge number. Different collision regimes have thus been observed, namely coalescence, coalescence followed by separation with or without formation of satellites, and all the comparisons with experimental studies are in very good agreement and some of them are very impressive (Tanguy and Berlemont [17]).

Some results are now described in order to illustrate the ability of the method to comply with experimental observations. As previously mentioned, mass conservation might not be satisfied in Level set methods and we thus evaluated mass loss during all simulations to check that it was negligible (<1%). Moreover we carried out convergence tests to check that coalescence and break-up of interface was independent of the mesh size [17].
3.1 **Coalescence followed by separation for head-on collisions**

Collision has been observed by Ashgriz and Poo [15] for two identical water droplets, with a Weber number equal to 23, and impact parameter nearly equal to zero (0.05). Simulation results are presented for water droplets, with the same Weber number, and with an impact parameter equal to 0, a droplet radius of 400 µm, and a droplet relative velocity of 1.44 ms\(^{-1}\). The grid size is 60x120 in the 2D axi configuration.

Comparisons between our results and experimental visualization are shown on figures 1.a and 1.b.

![Figure 1: (a) Head on collision, We=23, from Ashgriz and Poo [15]; (b) Head on collision, We=23, Oh=0.0047, our simulation.](image)

The qualitative agreement between simulation and experiments in the different pictures is quite good. The final state is well predicted (two droplets without satellites) and moreover, the liquid phase behavior during the collision process is very similar in both image sequences.

3.2 **Head on collision for two droplets with different sizes**

Experimental conditions given by Ashgriz and Poo [15] are the Weber number (We=56), the droplet radius ratio (0.5) and the impact parameter (0.). We thus chose one radius equal to 400 µm, the smallest radius is 200 µm, and the relative velocity for We=56 is equal to 3.175 ms\(^{-1}\). The grid size is 60x240.
As can be observed on figures 2.a and 2.b the agreement between the experimental pictures and the simulation results is very impressive. The shape evolution of the liquid phase is quite identical on both image sequences, and the last images of the two resulting droplets prove the quality of the whole collision process simulation.

![Image of figure 2](image)

**Figure 2:** (a) Head on collision, $\text{We}=56$, radius ratio 0.5 from Ashgriz and Poo [15]; (b) Head on collision, $\text{We}=56$, $\text{Oh}=0.0047$, radius ratio 0.5, simulation.

### 3.3 Off-center collision

In order to check the method in 3D configurations, collision between two droplets with non-zero impact parameter has been studied. We chose ethanol droplet, droplet radius is $100\,\mu\text{m}$, impact parameter is 0.5 and relative velocity is $2.94\,\text{ms}^{-1}$ which gives a Weber number equal to 60. The grid size is $64\times128\times256$ and symmetry condition is imposed on the parallel direction of the droplet velocity vectors. MPI parallelization is used and calculations are carried out on 8 processors on IBM 1600 cluster.

The chosen initial configuration is in the transition regime between separation with one satellite and separation with three satellite. Simulation results are presented on Figure 3.a. Collision process leads to coalescence followed by separation with formation of two satellites.

Ashgriz and Poo [15] showed a collision with very similar behavior as shown on figure 3.b, but with a slightly different configuration, namely water droplets, $\text{We}=83$ and impact parameter is 0.43. A difference appears on image 2 in figures 3.a and 3.b where the thin membrane is broken in the simulation but seems to experimentally remain during the collision.
The numerical description of very thin liquid layers in the collision process is a difficult problem to handle. As shown on figure 4 the thin membrane which is observed in the 3D simulation first breaks near the liquid ring, and then the bridge on the center of the liquid shape is elongated until it also breaks and a small droplet appears in the center. The ring is then stretched until its two sides collapse on the vertical axis and the small droplet is captured and merges with the whole liquid. Ashgriz and Poo [15] never seem to observe this behavior. We can assume that the break-up in the interface topology is induced by under-resolved numerical simulation of the very thin interface. However, while it remains quite impossible to check the spatial convergence of the results in 3D configurations, such behavior has also been observed in 2D simulations, namely for $We=23$ in the above results. Refining the grid can, in some cases, allow the interface motion to be described without any rupture, but we found some cases
where the membrane break-up occurs at the same time on the same location whatever the grid size we used (the finest grid mesh was less than 2 µm). We observed that these thin membranes rupture during head-on droplet collisions for quite small Weber numbers.

Figure 4: Thin membrane break in 3D simulation.

![Figure 4: Thin membrane break in 3D simulation.](image)

Figure 5: Comparison between simulation and experiments for transition between coalescence and separation in (Oh,We) space for droplet head on collision.

3.4 Quantitative comparison

Quantitative comparisons can be biased by a lack of experimental operating conditions or detailed measurement data. However experimental studies (Qian and Law [16]) provide the critical Weber versus Ohnesorge number for the transition between coalescence regime and separation regime for droplet head on collision. Figure 5 compares our results with Qian and Law [16] experimental correlation, and Rieber and Frohn [18] simulations. The agreement between our simulations and experimental data is very satisfactory and confirms that Level Set method with Ghost Fluid approach are accurate tools numerical simulations of droplet collisions.
References


