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On an Improved Sharpening Method for Interfacial Flow

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Abstract

Numerical simulations of multiphase flow for tracking free surface is studied, using finite volume method, finite difference method with volume of fluid. These methods are based on a set of equations that control the two liquid phases as one phase with variable properties. This set of Navier-Stokes equations and volume fraction function equation are solved on a structured staggered grid. Surface tension is computed at the interface by a continuum surface force CSF. Due to smearing of the discontinuity in the numerical solution from upwind schemes in the advection equation, a proposed solution to reduce the interface thickness is written in a homemade C++ code, which consists of coupling a modified artificial compression method with the present smoothing method to reduce oscillations and nonlinear instabilities.

Keywords: Multiphase Flow, volume of fluid, free surface, surface tension, finite volume, interfacial smoothing, artificial compression method.

INTRODUCTION

The two-phase flows are present in many industrial applications and even in everyday life include the flow of the water in the pipes, the liquid sloshing in a tank, transportation of oil, condensations operations, chemical separations, droplets splashing etc., and in each process mentioned above we have an interface between immiscible fluid as in our case.

An interface between a liquid and a gas is often stated as a free surface. The aim why we talk about the word "free" is the difference concerning the densities of gas and liquid (e.g., the quotient of the density between the water and the air is 1000). In the numerical processing of the free surface flows, the accurate representation of the sharp interfaces requires robust methods.

The following methods are extensively used to simulate free surface flows, we quote: (a) The surface fitting method, where the interface is followed by attaching it to a mesh surface, which is forced to move with the interface, this can be considered a Lagrangian mesh method. (b) The surface capturing method, where an indicator function is used to mark the fluids on either side of the free surface. In addition, the mesh is fixed. Consequently, there shall be an Eulerian and (c) the surface tracking method, where the interface is represented explicitly and followed by special markers points. The grid also remains fixed. It can therefore, be considered as an hybrid method of Eulerian-Lagrangian grid [1].

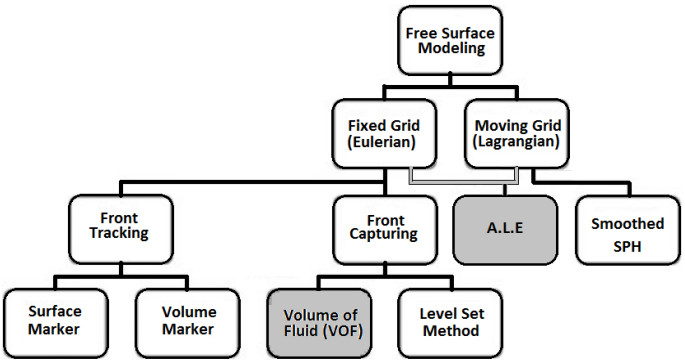

Figure 1: Interface modeling techniques.

Among the methods mentioned above, a simple but powerful one is introduced by Hirt and Nichols at Los Alamos Laboratory in 1979 [2]. This method is based, on the concept of fractional volume of fluid (VOF). Like any method that has pros and cons, and due to the discontinuity of one or more variables in the interface, different problems arise, among them, the one discussed here, the numerical diffusion that smear the interface considerably.

Several researchers have participated with their contributions to improve the boundary between the liquid and gas phase, by developing and modifying, new schemes and methods, and the recently proposed high-order central difference schemes for conservation laws have a propensity of smearing linear discontinuities

The early work of Neumann and Richtmyer [3], gave rise to the concept of shock capturing, in computing solutions of the discontinuity of hyperbolic problems. The capture shock approach is not without shortcomings: everyday finite

difference schemes approaching a discontinuity problem by a continuous transition that occupies 3-5 cells.

Finite difference schemes with higher-order produce overshoots or undershoots when crossing the discontinuity. These oscillations cause nonlinear instabilities [4].

Special schemes were designed to overcome this instability such the anti-diffusion method of Boris and Book [5], they developed the Flux-Corrected Transport method, which uses an anti-diffusive term, in the convective equation to reduce numerical diffusion. The use of non-centered differencing by Van Leer [6], and Warming and Beam [7], and the method of artificial compression (ACM) developed by Harten [8][9]. The performance of the ACM depends on the choice of an indicator of discontinuities. Luckily, the mass fraction in the advection equation, of one of the two fluids may be used directly to perform this task.

EQUATIONS OF MULTIPHASE FLOWS

The behavior of liquids and gases, which are both considered fluids, can be observed in almost all areas of life ranging from complex technical applications (e.g. gas-petroleum separation) to the most trivial of everyday life situations (e.g. liquid flow pipe).

The Volume of Fluid method (VOF) is a universal technique in monitoring the two-phase interfaces and free surface flows. It is based on a characteristic function *C*, the value of "1" in one phase and "0" in the other phase. Thus, fluids are assumed incompressible and immiscible.

The model selection is undertaken depending on the nature of the flows that are of interest. For a case of flows with a fixed topology or dispersed phases, it is better to treat the two phases separately. This is referred to as a two-fluid model approach. On the other hand, if the flow is characterized by a topology that changes over time, it is not possible to model interfacial transfers appropriately. The set of physical information is now contained in the mixture formed by the two phases. This approach leads to a model of one fluid. The phases are no longer considered individually and the flow appears as a two-phase mixture with variables physical properties (density, viscosity). This approach can handle a wide range of two-phase flows.

Two-phase medium equations: The momentum equation of varying density and viscosity:

$$\rho\frac{\partial u}{\partial t}+\rho\,\nabla\cdot uu=-\nabla p+\rho g+\nabla\mu\left(\nabla\mathbf{u}+\nabla^{T}\mathbf{u}\right)+f \qquad (1)$$

Momentum equations in 2D:

$$\rho\left(\frac{\partial u}{\partial t}+\frac{\partial uu}{\partial x}+\frac{\partial uv}{\partial y}\right)=-\frac{\partial p}{\partial x}+\rho g_x+\frac{\partial}{\partial x}2\mu\frac{\partial u}{\partial x}+\frac{\partial}{\partial y}\mu\left(\frac{\partial u}{\partial y}+\frac{\partial v}{\partial x}\right)+f_x \qquad (2)$$
$$\rho\left(\frac{\partial v}{\partial t}+\frac{\partial uv}{\partial x}+\frac{\partial vv}{\partial y}\right)=-\frac{\partial p}{\partial y}+\rho g_y+\frac{\partial}{\partial x}\mu\left(\frac{\partial u}{\partial y}+\frac{\partial v}{\partial x}\right)+\frac{\partial}{\partial y}2\mu\frac{\partial v}{\partial y}+f_y$$

With f, f_x, f_y, the forces acting other than the force of gravity (e.g.: surface tension). Even if the density varies from one place to another, it is assumed, constant in each fluid as the fluid element travels with the flow of fluids. The density hence changes according to:

$$\frac{\partial\rho}{\partial t}+\mathbf{u}\cdot\nabla\rho=0 \qquad (3)$$

Equation (3) represents the advection of density, we can discretize this equation by a direct method (DNS), but if you want to use a VOF method we must use a similar equation called a volume fraction equation $C\left(\vec{x},t\right)$:

$$\frac{\partial C}{\partial t}+\mathbf{u}\cdot\nabla C=0 \qquad (4)$$

$$\text{with}\quad C(\vec{x},t)=\begin{cases}1 & \text{in the liquid (water)}\\ 0 & \text{in the air}\\ 0<C<1 & \text{at the interface}\end{cases}$$

This description assumes especially the absence of phase change and local slip between phases. To close the model, it is necessary to clarify the law of variation of the physical properties and the surface tension force. The following relation defines density unambiguously:

$$\rho=C\rho_l+(1-C)\rho_g \qquad (5)$$

Where ρ_l, ρ_g are density of liquid and density of gas respectively, concerning the viscous effects, several levels of modeling is possible. In the simplest, one viscosity model, it is constructed similarly to equation (5) without a theoretical justification of this analogy:

$$\mu=C\mu_l+(1-C)\mu_g \qquad (6)$$

In this case, the equation of mass conservation for an incompressible flow is reduced to:

$$\nabla\cdot\mathbf{u}=0 \qquad (7)$$

In two dimensions:

$$\frac{\partial u}{\partial x}+\frac{\partial v}{\partial y}=0 \qquad (8)$$

Discretization and Computer Approach:

In the first case, we start by writing a simple **C++** solver for a flow with variable density and viscosity. We will discretized

surface tension by a method of continuum surface forces (CSF) [10]. Integration of the first order is used for time. To solve the advection of the volume fraction function (4), upwind scheme is used. Since the viscosity is variable, the complete deformation tensor is used to calculate the viscous stress. Thus, the discretization is based on the simplified equations:

$$\rho\frac{\partial \mathbf{u}}{\partial t}+\rho\nabla\cdot\mathbf{uu}=-\nabla p+\rho g+\nabla\bullet\mu\left(\nabla\mathbf{u}+\nabla^{T}\mathbf{u}\right)+\mathbf{f} \quad (9)$$

$$\nabla\cdot\mathbf{u}=0 \quad (10)$$

In time we can integrate this equation as follows, we divided the equation of motion (10), using the Chorin decomposition [11]:

$$\frac{\mathbf{u}^{*}-\mathbf{u}^{n}}{\Delta t}=-\mathbf{A}^{n}+\mathbf{g}+\frac{1}{\rho^{n}}\mathbf{D} \quad (11)$$

$$\frac{\mathbf{u}^{n+1}-\mathbf{u}^{*}}{\Delta t}=-\frac{\nabla p}{\rho^{n}} \quad (12)$$

Where **A** is a discrete estimation of the advection term, and **D** is an approximation diffusion term. Taking the divergence of (12), and using the continuity equation to remove ∇n^{n+1} a Poisson equation is obtained for the pressure:

$$\nabla\cdot\left(\frac{1}{\rho^{n}}\nabla p\right)=\frac{1}{\Delta t}\nabla\cdot\mathbf{u}^{*} \quad (13)$$

As soon as the pressure found, equation (13) can be used to find the estimated velocity at instant *(n +1).*

Advection of the Volume Fraction Function:

The volume fraction function is advected using a first order upwind scheme, isolating the temporal derivative, and rewriting equation (4) in the conservative form, since the flow field is incompressible, we get:

$$\frac{\partial C}{\partial t}=-\nabla\cdot\left(C\,\mathbf{u}\right) \quad (14)$$

Thus the discrete form of (14):

$$\begin{aligned}C_{i,j}^{n+1}=C_{i,j}^{n}-\frac{\Delta t}{2dx}\Big[&u_{i+1/2,j}\left(C_{i+1,j}+C_{i,j}+\left\langle u_{i+1/2,j}\right\rangle\left(C_{i,j}-C_{i+1,j}\right)\right)\\&-u_{i-1/2,j}\left(C_{i,j}+C_{i-1,j}+\left\langle u_{i-1/2,j}\right\rangle\left(C_{i-1,j}-C_{i,j}\right)\right)\Big]\\-\frac{\Delta t}{2dy}\Big[&v_{i,j+1/2}\left(C_{i,j+1}+C_{i,j}+\left\langle v_{i,j+1/2}\right\rangle\left(C_{i,j}-C_{i,j+1}\right)\right)\\&-v_{i,j-1/2}\left(C_{i,j}+C_{i,j-1}+\left\langle v_{i,j-1/2}\right\rangle\left(C_{i,j-1}-C_{i,j}\right)\right)\Big]\end{aligned} \quad (15)$$

with $$\left\langle u_{i+1/2,j}\right\rangle=\begin{cases}+1 & \text{if } u_{i+1/2,j}>0\\ -1 & \text{if } u_{i+1/2,j}<0\\ 0 & \text{otherwise}\end{cases}$$

Surface Tension Modeling:

The surface tension is a set of forces acting on each point of the surface, parallel to the surface. These cohesive forces between the molecules of the substance acting without chemical bonding.

In simulations of immiscible multiphasic flow, we are often involved in length scales, where the surface tension is significant. The force per unit area is specified by:

$$\mathbf{f}=\sigma\kappa\left|\nabla C\right|\mathbf{n} \quad (16)$$

With σ tension coefficient of air / liquid surface, we must assume constant, κ a local estimate of the curving of the liquid and **n** an approximation of the normal to the free surface. The surface tension at the interface is modeled with a localized force by volume prescribed by a continuum surface force model [12], for a volume fraction, the normal is estimated by:

$$\mathbf{n}=-\frac{\nabla C}{\left|\nabla C\right|} \quad (17)$$

We substitute (17) in (16) we obtain:

$$\mathbf{f}=-\sigma\kappa\nabla C \quad (18)$$

With:

$$\kappa=-\nabla\mathbf{n} \quad (19)$$

Using the finite difference we obtain, the discretized form of the surface tension that can be added as a source term:

$$\begin{aligned}f^{x}_{i+1/2,j}&=-\frac{\sigma}{2\Delta x}\left(C_{i+1,j}-C_{i,j}\right)\left(\kappa_{i+1,j}+\kappa_{i,j}\right)\\ f^{y}_{i,j+1/2}&=-\frac{\sigma}{2\Delta y}\left(C_{i,j+1}-C_{i,j}\right)\left(\kappa_{i,j+1}+\kappa_{i,j}\right)\end{aligned} \quad (20)$$

Harten's artificial compression:

A. Harten [8], introduced an artificial compression term to equation (14), to reduce smearing near the interface, this method has a great benefit to make interface sharp, but when exaggerated it shows free surface oscillations. Olsson and al [13], rewrite the artificial compression method to preserve the profile and thickness of the interface constant.

$$\frac{\partial C}{\partial\tau}+\nabla\cdot C\left(1-C\right)\mathbf{n}=\nabla\cdot\varepsilon\nabla C \quad (21)$$

Equation (21) is advanced in pseudo-time τ, consists of a compression streams $\nabla\cdot C\left(1-C\right)\mathbf{n}$ that acts at sharpening the shape, and of a diffusion term $\nabla\cdot\varepsilon\nabla C$ that guarantee the profile remains of typical thickness ε, which is the smallest distance between two nodes in the structured domain grid.

The modified Harten's artificial compression (MHAC):

The MHAC consists of the following equation:

$$\frac{\partial C}{\partial \tau}=\nabla\cdot C\left(1-C^{2}\right)\mathbf{n}\beta+\nabla\cdot\varepsilon\nabla C \tag{22}$$

Where β is a constant, it can be discretized as follow:

$$\frac{\partial C}{\partial \tau}=\frac{\partial F}{\partial x}+\frac{\partial G}{\partial y} \tag{23}$$

Applying finite difference method to (23):

$$C_{i,j}^{n+1}=C_{i,j}^{n}+\Delta\tau\left[\frac{1}{\Delta x}\left(F^{+}-F^{-}\right)+\frac{1}{\Delta y}\left(G^{+}-G^{-}\right)\right] \tag{24}$$

Where F^{+}, F^{-} are discretized as follow:

$$\begin{aligned}F^{+}&=1/2nx_{1}\left(C_{i+1,j}^{n}+C_{i,j}^{n}\right)\left(1-1/2\left(C_{i+1,j}^{n}+C_{i,j}^{n}\right)^{2}\right)\beta+\varepsilon/\Delta x\left(C_{i+1,j}^{n}-C_{i,j}^{n}\right)\\ F^{-}&=1/2nx_{2}\left(C_{i,j}^{n}+C_{i-1,j}^{n}\right)\left(1-1/2\left(C_{i,j}^{n}+C_{i-1,j}^{n}\right)^{2}\right)\beta+\varepsilon/\Delta x\left(C_{i,j}^{n}-C_{i-1,j}^{n}\right)\end{aligned} \tag{25}$$

β is a constant approximated between 10.0 to 25.0.

The normal approximation in 2D, was discretized as follow, forward and backward:

$$\begin{aligned}nx&=-\frac{\nabla Cx}{\sqrt{\left(\nabla Cx\right)^{2}+\left(\nabla Cy\right)^{2}}}\\ ny&=-\frac{\nabla Cy}{\sqrt{\left(\nabla Cx\right)^{2}+\left(\nabla Cy\right)^{2}}}\end{aligned} \tag{26}$$

The pseudo-time $\Delta\tau$ and ε where approximated as follow:

$$\begin{aligned}\varepsilon&=\left[\min\left(\Delta x,\Delta y\right)\right]^{1-d}\\ \Delta\tau&=Cof\left[\min\left(\Delta x,\Delta y\right)\right]^{2}/\varepsilon\end{aligned} \tag{27}$$

Where Cof and ε are constants with approximate values respectively, $d\approx 0.1,\ Cof\approx 0.2\times 10^{-5}$

The Proposed model of smoothed sharpening method (SSM):

The proposed SSM, is based on calculating a mean volume fraction value at each time step, from the neighboring cells around the $C_{i,j}$ cell, and compressing the interface to its smallest value "$\min\left(\Delta x,\Delta y\right)$".

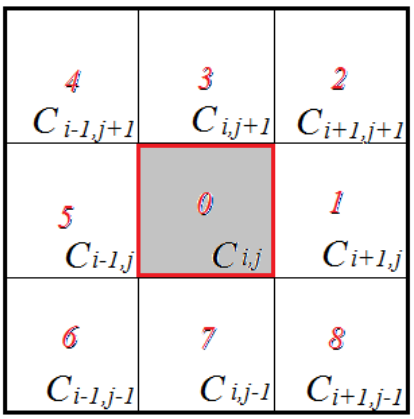

Figure: 2 The eight neighbors of $C_{i,j}$ cell, used for smoothing

Let us define *Cs*, the smoothed value of the volume fraction function.

$$Cs_{i,j}=\frac{3}{4}Cs_{i,j}+\frac{1}{4}\left(\frac{C_{i+1,j}+C_{i-1,j}+C_{i,j+1}+C_{i,j-1}+C_{i+1,j+1}+C_{i-1,j+1}+C_{i+1,j-1}+C_{i-1,j-1}}{8}\right) \tag{28}$$

After smoothing, we compress the interface as follow:

$$\begin{aligned}&if\ \ 0<Cs\le 0.5\ then\ Cs=0.5\\ &if\ \ 0.5\le Cs<1\ then\ Cs=0.5\end{aligned} \tag{29}$$

We add a smallest amount of the smoothed value to the initial value of the volume fraction function to smear a little bit the interface, such as:

$$C_{i,j}=\alpha C_{i,j}+\left(1-\alpha\right)Cs_{i,j} \tag{30}$$

Where α is a constant value that should not be below 0.9995, such as $0.9995\le\alpha<1$. (Moreover, It works). With a smaller value of α the simulation no longer progress, and it can take very long time.

RESULTS AND DISCUSSION

Rising bubble:

A central difference scheme with diffusion and anti-diffusion in 30x90 grid, without any sharpening method fig. 3, and an upwind scheme with the proposed SSM and the MHAC implementation fig. 4. We can see from the fig. 3 that a considerable mass loss occurs that ends up with no more or a little quantity of air, which is due to a large smearing. In the other hand and with the same first order upwind scheme and using the proposed model of SSM technique, we get no more mass loss and this without surface reconstruction.

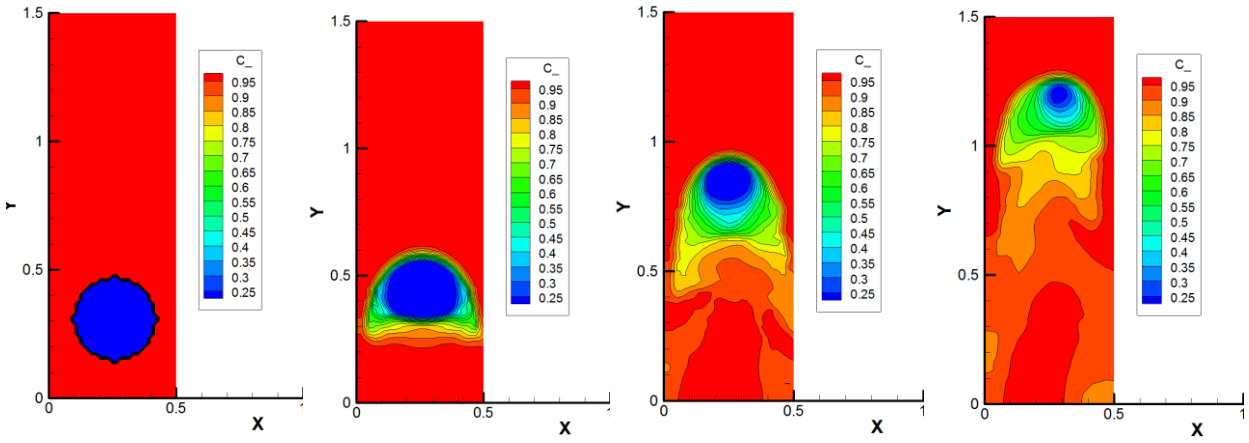

Figure 3: Bubble rising without any sharpening, mass loss and interfacial smearing

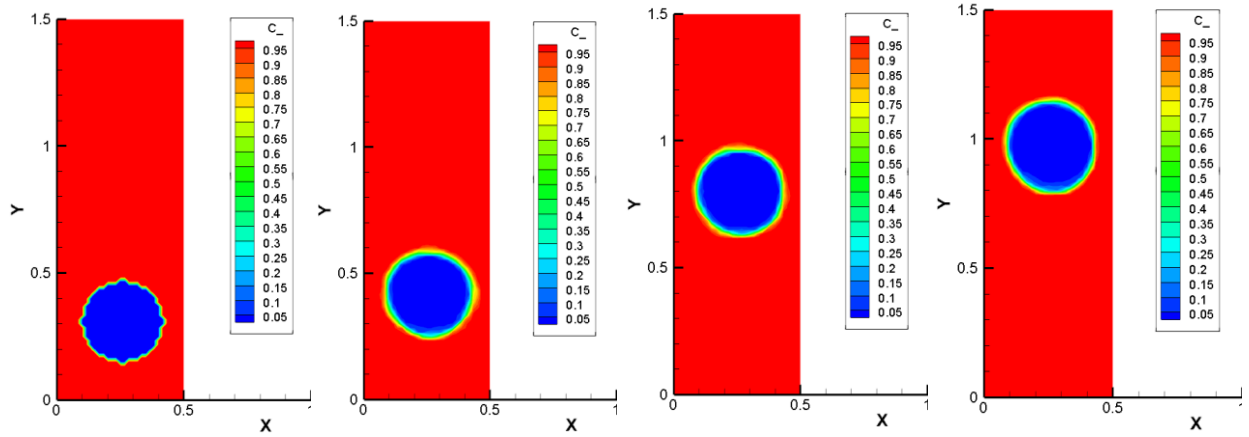

Figure 4: Bubble rising with interfacial sharpening, without mass loss and no interfacial smearing

Break dam:

We have a nearly good result concerning break dam simulation since the effect of the surface tension is negligible, even the mass loss was very limited. The thickness of the interface is limited to no more than three (3) cells.

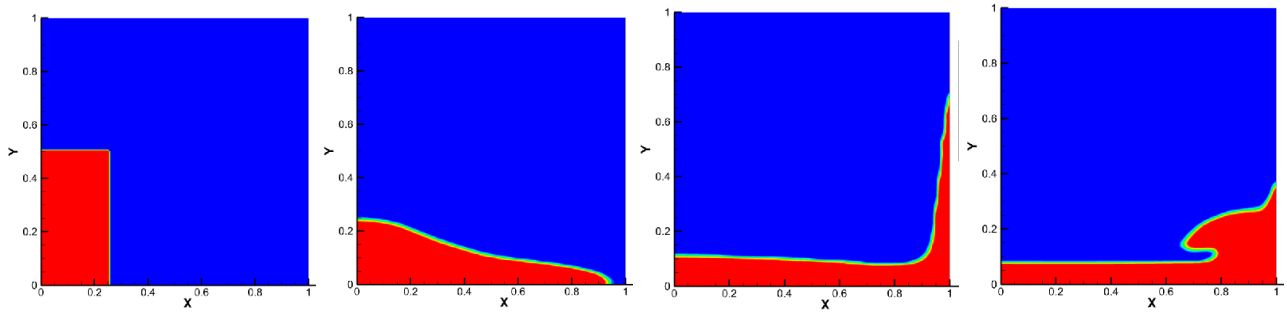

Figure 5: Break dam with interfacial sharpening, without mass loss and no interfacial at different time

Bubbles coalescence:

This method is very suitable with bubbles coalescence. It gives good results that are close to reality. In addition, we can see the interface is very thin, even if displaying the 19 lines interface from 0.05 to 0.95, as seen in fig. 6.

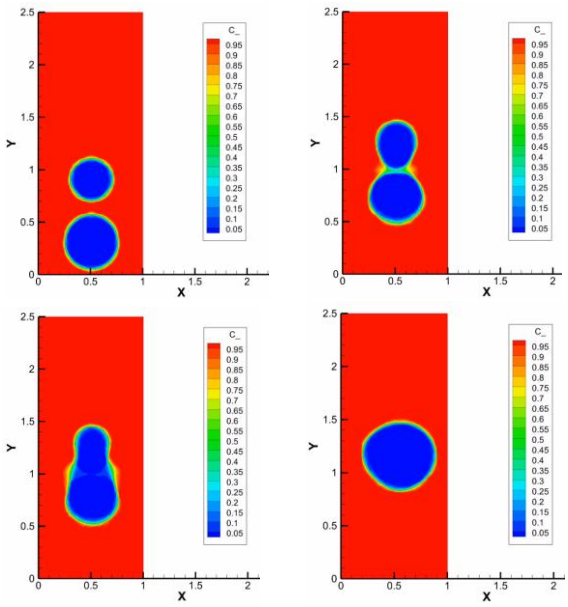

Figure 6: Bubbles coalescence with interfacial sharpening.

CONCLUSIONS

In this work, we focused on developing a C++ solver for direct numerical simulation of two-phase flows. Many industrial applications require this type of tool. However, depending on the purpose of the application and the physical processes involved, different simulation methods are used. Our work has started with the analysis of existing studies in the field of modeling multiphase flows. The main subject in our study is sharpening the interface as thin as possible without having oscillations; we had to tune much constant values to achieve our goal.

In this work, I start by improving the method of interface monitoring to limit the influence of numerical diffusion and mass loss due to the interface reconstruction problem. Discretization techniques of advection and methods of correction where used, The results obtained in the framework of this paper, are a very significant first step in the design of a numerical solver that can simulate two-phase immiscible flow with sharp interface, where the density ratio can reach 1/1000th. Many of them can be viewed as animations at this url: http://www.youtube.com/watch?v=o1m3ZJa2AoI&list = UUBxM-TRE9IBbqrGEBO2MuZw

In the numerical tool development for the simulation of two-phase flow, we have considered only the hydrodynamic aspects of the movement of the interface. In fact, parts of the dispersed liquid also experience thermodynamic interactions that are partly due to electrostatic forces, something that is not considered in our study.

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