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Tracking of Bubbles using InterSection Marker (ISM) method

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Abstract

In this paper, one of the applications of the InterSection Marker (ISM) method is presented. The ISM method - a hybrid Lagrangian–Eulerian front-tracking algorithm specifically crafted for multi-phase flow simulation, was used to track an air bubble rising in quiescent water under the influence of buoyancy and surface tension forces. Computed bubble terminal velocity and bubble shape of 1 mm size bubble are discussed. The results compared well against the past works, and has laid foundation for the future application of the ISM method in more complex multi-phase flow simulation.

Introduction

Multi-phase flows play an essential role in Nature and Human Engineering applications. Surface wave breaking, raindrops in air, chemical reaction, spray combustion, spray painting, petroleum refining, ship industries, and boiling heat transfer are among many examples. Accurate predictions of such flow behaviours however are a challenge. The complexity arises from the presence of many entities, such as bubbles, drops, or particles within the multi-phase flow, and from their intricate interactions. This phenomenon limits the application of analytical methods. It is also difficult to carry out multi-phase flow experiments with the desired degree of control. Numerical simulation, in this situation, becomes a useful tool for the investigation of multi-phase flow. Using modern computational power and advanced numerical methods, dynamics of multi-phase flows can be studied in great detail. A number of numerical methods have been developed for the study of multi-phase flows, for instance the Volume-of-Fluid and Front-Tracking methods. These methods however have their own merits and shortcomings. To achieve a higher accuracy in multi-phase CFD simulations, an in-house computer code, the InterSection Marker (ISM) method - a hybrid Lagrangian–Eulerian front-tracking algorithm, was used to track an air bubble rising in quiescent water. The ISM method was coupled with a variable-density single-fluid flow solver producing excellent results. This method has the potential for future applications in multi-bubbles dynamics (coalescence/breakage) and in turbulent flow regime (suppression of turbulence by bubbles).

Numerical Methods

During simulation of rising bubbles, a number of challenges and difficulties could be encountered [9]. For instance: (i) the complex interface physics, e.g. the effects of surface tension, thin liquid film dynamics, phase change (heat and mass transfer), and chemical reactions, (ii) the geometric complexity caused by multi-bubbles dynamics (coalescence/breakage), and (iii) the discontinuity of the density and viscosity across the fluid interface tends to cause numerical instability, especially when the jumps in these properties are high. For example, the density ratio of liquid to gas such as in water and air is in the order of 1000:1.

To address these issues, various methods have been developed (comprehensive reviews in [1, 8]), and each method typically has its own characteristics merits and shortcomings. One of the earliest methods to resolve free surface problems is the *Marker-and-Cell* (MAC) method developed by Harlow and Welch [6]. The scheme is based on Eulerian mesh of control volumes. MAC method is computationally very expensive, and at the time was restricted to two dimensional simulations. This method is also unable to evaluate regions involving converging or diverging flows.

Volume-of-Fluid (VOF) methods were developed by Hirt and Nichols [7], Youngs [19], Rudman [13], and Noh and Woodward [10]. The phase is tracked by the volume fraction occupying within each Eulerian control volume mesh. The volume fraction indicates either the presence or absence of the tracked fluid, and tracks total phase occupancy (VOF value of 1), partial occupancy (denoting an interface presence with a VOF value between 0 and 1) or total absence of the tracked phase (VOF value of 0). Two classes of VOF methods can be generally identified with respect to the representation of the interface, namely simple line interface calculation (SLIC) and piecewise linear interface calculation (PLIC). Noh and Woodward [10] and the donor-acceptor algorithm by Hirt and Nichols [7] did pioneering works on earlier SLIC algorithm. Later Youngs [19] proposed more accurate and capable PLIC method. VOF methods are relatively simple and easy to implement, however suffer from artificial coalescence of gas bubbles which occurs when their distance is less than the size of the computational cell.

Level-Set methods, introduced by Osher and Sethian [11] and further developed by Sussman el al. [14] for multiphase flow simulations, have emerged as the main alternative to the volume-of-fluid (VOF) method for the direct advection of a marker function [16]. In this method, different fluid regions are identified by a smooth marker function F(x,t), which is positive in one fluid and negative in the other. The boundary between the fluids is identified by the F(x,t) = 0 level curve. The advection of this level-set (distance) function which moves with the fluid evolves through the solution of the following equation:

$$\frac{DF}{Dt} = \frac{\partial F}{\partial t} + (\bar{u}.\nabla F) = 0 \tag{1}$$

Although conceptually simple and easy to implement, Level set methods have limited accuracy and tend to lose mass for incompressible flow simulations.

In *Front-Tracking* methods (Unverdi and Tryggvason [17], Esmaeeli and Tryggvason [4, 5], Tryggvason et al. [15]), a fixed background grid is used to solve the fluid flow, while a separate interface mesh represented by an unstructured triangulated grid that moves with the fluid is used to track the interface position explicitly. As the interface stretches, points and elements are added and deleted. This method is accurate and robust, however high level of detail comes at the cost of computational requirements.

Combining the strength of the VOF method and the Front-Tracking method, Aulisa's 3D method [2] tracks the interface as a Lagrangian but finds the intersection of the surface mesh with control volume faces and locally remeshes the surface contour whilst preserving the tracked volume. This method however requires permanent markers which cannot be seeded or removed after the simulation is executed, and leads to spherical bubble expansion problem. To improve Aulisa's method, InterSection Marker (ISM) method [8] was devised. ISM method eliminated the need for permanent markers and addressed the local surface issue in volume inflationary type problems. Following section briefly highlights some key aspects of the ISM method. For further reading, Ho et al. [8] should be consulted.

InsterSection Marker (ISM) Method

InterSection Marker (ISM) method, developed by Ho et al. [8], is a hybrid Lagrangian-Eulerian Front-Tracking method which can model an arbitrary 3D shape immersed inside an array of uniform hexahedral control volumes by using a combination of planner polygons. Each planner polygon intersects the edges of the control volume and the combination of cell-edge intersections uniquely identifies the type of polygon a control volume holds.

The ISM interface is made up of its component points (as shown in figure 1): (1) the intersection markers where the interface crosses the control volume cell edges, (2) the cell face conservation points which allow composite curves to be modelled, and (3) the raised centroid whose position is calculated to satisfy volumetric conservation.

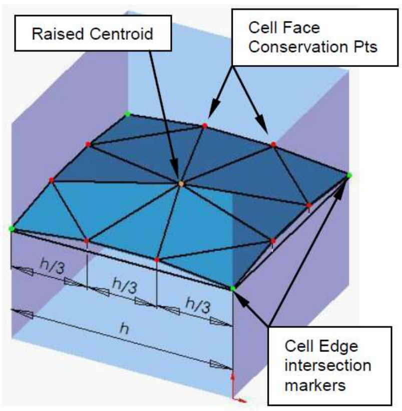

Figure 1. InterSection Marker (ISM) representation of a 2D interface in a rectangular hexahedral control volume.

The ISM method identifies the type of interface residing in a cell by the combination of cell-edge intersections that interface makes. Total of 51 combinations of basic set of planar-type interfaces had been identified: 8 intersection marker combinations for 3 sided interfaces, 15 for 4 sided, 24 for 5 sided, and 4 for 6 sided. These combinations provided a standard look-up table for algorithmic identification. Figure 2 shows four of such arrangements.

To maintain planner surface during translation/deformation, the standard planar surfaces shown in figure 2 needed further subdivision. As such a complex subdivision configuration (figure 3) was selected for the ISM method for its higher interface detail and improved resmoothing capability during the remeshing process. A triangular tessellation pattern is the preferred option because three points randomly translated will always form a plane. Additional intersection-marker combinations of non-planar-type interfaces were also identified (details in [8]), which are necessary to prevent the modelled interface from collapsing and folding onto itself.

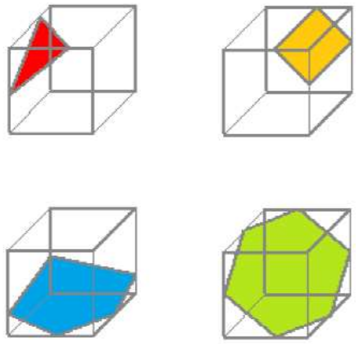

Figure 2. Four examples of different ISM combinations.

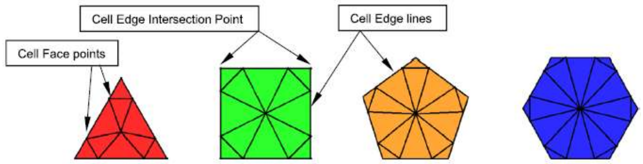

Figure 3. Complex subdivision of planar polygons.

Governing Equations

Both the gas and the liquid phases can be assumed to experience the same 'mixture velocity' at any local point within the computational domain and the two-fluid system can be approximated as one-fluid mixture. In this 'one-fluid' approach, advantage of using a single sets of governing equations (outlined in equations 7.1 – 7.4 of [18]) for both fluids can be taken. Because of space limitation, equations are not presented here.

The immersed boundary method, originally proposed by Peskin [12], was used to model surface tension and buoyancy forces as a smoothed volumetric source term in the momentum equation. Using the Paraboloid Least Square fitting method and taking the input data from the CELL plus the ADJACENT CELL's cell edge intersection points, the local 3D surface curvature was calculated.

Simulation and Results

Coupled with an in-house variable-density single-fluid flow solver, ISM interface tracking method was employed to simulate an air bubble (size 1 mm) rising in quiescent water under the influence of buoyancy and surface tension forces. Simulation was carried out in a computational domain of 31 × 51 × 31 cubic control volumes with an initial spherical bubble of radius 5h (where h is the width of the non-dimensional cubic control volume). The centre of the bubble was located in line with the centre of the cavity, at a distance of 15.5 h from each side wall and at a distance of 15.5 h from the bottom boundary. Non-slip wall conditions were assigned on all boundaries. Simulation air and water properties were taken at standard temperature and pressure (STP) values. Table 1 shows further simulation input parameters. Both the ISM interface tracking algorithm and the flow solver program were compiled using Intel Visual ForTran Composer XE 2011. No ForTran libraries were used to avoid cross-platform and compiler compatibility issues.

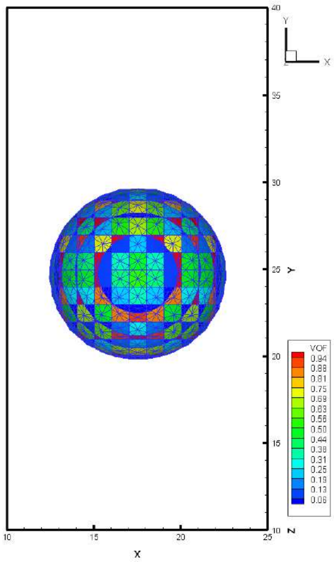

Figure 4. Surface Plot, control volume width = 0.1 mm (Axes denote control volumes [-]). Simulation time = 0.00975 sec.

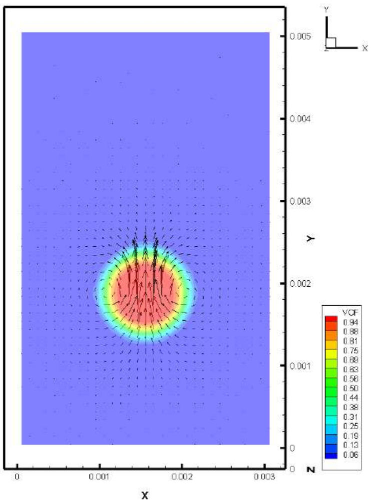

Figure 5. Distributed VOF plot with velocity vectors. (Axes denote physical geometry [m]).

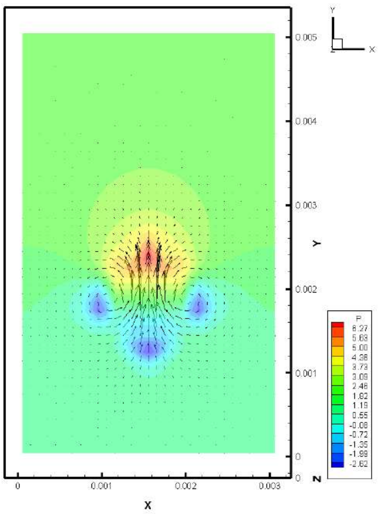

Figure 6. Pressure field plot with velocity vectors (Axes denote physical geometry [m], Pressures are in Pascals).

Water density [kg/m^3]	1000
Air density [kg/m^3]	1
Water viscosity [Pa.s]	1 x 10^{-3}
Air viscosity [Pa.s]	1 x 10^{-5}
Gravity [m/s^2]	-9.81
Surface tension [N/m]	0.072

Table 1. Simulation input parameters.

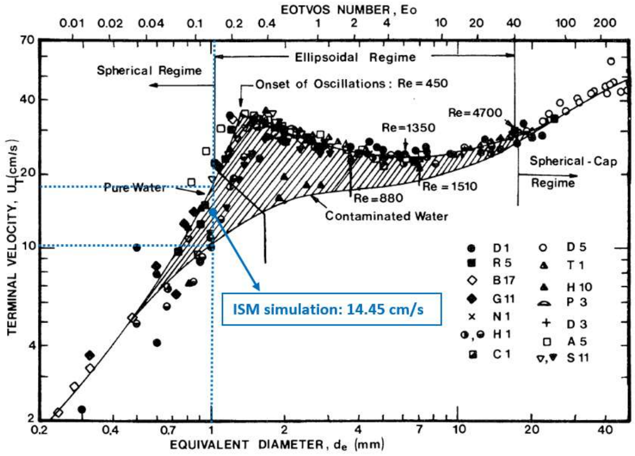

Figure 7. Terminal velocity of air bubbles in water at 20^{0}C [3].

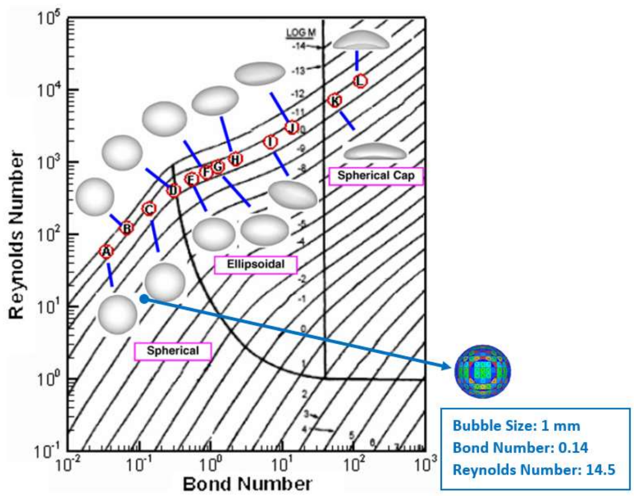

Figure 8. Comparison of 1 mm bubble shape using the ISM method with Hua et al.'s numerically predicted terminal bubble shapes [9].

Figures 4-6 show the shape, distributed VOF field, and pressure field of 1 mm bubble rising under the effects of buoyancy and surface tension. Despite the relatively coarse grid on which the simulation was performed, both the terminal velocity and the bubble shape were in agreement with works previously published. The bubble terminal velocity was compared against the terminal velocities observed in bubble-rise experiments [3], and found to be within the range, as shown in figure 7. The shape of bubble at terminal velocity was of "Spherical" type and was consistent with Hua et al.'s [9] findings – see figure 8.

The Reynolds number and Bond number corresponding to terminal velocity result were calculated according to equations (2) and (3).

$$\mathrm{Re} = \frac{\rho v D_{bubble}}{\mu} \tag{2}$$

$$Bo = \frac{\Delta\rho g (D_{bubble})^2}{\sigma} \tag{3}$$

Advancement and Future work

The ISM method has shown promising results for applications in 3D interface tracking of deformable surfaces (e.g. Sphere, Torus and Red Blood Cell [8]), and in multi-phase flow simulation (i.e. rising single bubble). Current initiatives are underway to fine-tune the application of the ISM method for different sizes single bubble rising in quiescent water under the influence of buoyancy and surface tension forces.

Next logical steps would be to simulate the multi-bubbles dynamics (coalescence/breakage mechanism) by developing interface remeshing subroutines within a control volume. Since bubble Reynolds number was below 1000, no turbulence modelling was considered in the present work. Simulations in laminar and turbulent flow regimes (suppression of turbulence by bubbles) could also be other avenue for the future works.

Conclusions

The ISM method was used to simulate an air bubble (size 1 mm) rising in quiescent water under the influence of buoyancy and surface tension forces. The result was validated successfully against the past works, and has encouraged to pursue further works in advanced multi-phase flow applications, such as multi-bubbles dynamics in quiescent condition, and examining the structure of bubbly flows in laminar and turbulent conditions among other possibilities. These simulations would provide numerical test-bed for developing the closure expressions needed for population balance models which are practical approach for the analysis of bubbly flows in chemical, nuclear and mechanical systems.

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