Sharp Surface Tension Force for Level-Set Method in Multiphase Flow Modeling

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Abstract

A new algorithm suitable for level-set method in multiphase flow modeling is introduced to calculate the magnitude of the sharp surface tension force by evaluating the interfacial area contained within a cell located on the interface. This algorithm is successfully tested by measuring the area of a three dimensional closed geometries. To demonstrate the effects the proposed algorithm has on a typical interface capturing method, a static droplet was simulated using level-set method. The results are presented before and after applying the algorithm. The enhanced accuracy of the calculated pressure jump across the interface, the more uniform pressure distribution in the vicinity of the interface, and the smoothness of the interface indicate the effectiveness of the algorithm.

Introduction

For more than four decades researchers have been trying to develop and improve different methods of capturing an interface between two fluids. Early papers on this subject focused on Volume of Fluid method (VOF) that uses mass conservation law to advect a sharp color function [1][2][3][4][5][6]. To reduce the singularity issues inherent to the VOF method, Level Set method was proposed, in which a continuous distance-function is defined within the physical domain as the shortest distance to the interface, with a positive sign in one of the fluids and a negative sign in the other [7][8][9].

One drawback that mostly relates to Volume of Fluid (VOF) and level set (LS) methods is the difficulty in determination of the forces applied on the cells located on the interface. For example, the surface tension force is difficult to implement mainly due to the large discretization errors in evaluating the surface curvature and the direction along which the force is applied. The magnitude of the force is also difficult to estimate because it depends on the area of the interface contained within an interface cell. Watanabe *et.al.* [13] approximated the surface area contained within a unit cube and measured the surface area and volume of simple geometries by considering that the interface is aligned with one of 15 lattice directions in a cubic cell structure. Youngs [11] mathematically derived formulas for the volume fraction of the cut cell for each of the formed shapes. However, he did not calculate the interfacial area that is required in calculating the surface tension force. Bussman *et.al.* used Youngs' formulations in their VOF-based code to simulate the surface tension force for uniform cubic cells [12]. In sharp implementation of surface tension, the area term in the surface tension force expression ($\sigma\kappa A_c$) is usually approximated by the area of one of the faces in the cell [13], so called "stair-stepped" method, which usually overestimates the surface tension force and produces the need for distributing the force on neighboring cells. The goal of this work is to present a methodology to accurately evaluate the surface tension force by calculating the correct interfacial area contained within an interface cell. This paper presents an algorithm to evaluate this area through analytical formulas for the area contained in a cuboid cell. This algorithm is designed so that it can be conveniently used in codes that use Level Set methodology.

Algorithm to Evaluate Interfacial Area for Cuboid Interfacial Cells

The area of the interface contained within a cell depends on the shape of the cell, the direction of the normal vector to the interface, and the intercept of the interface. The intercept in the Volume of Fluid (VOF) method is determined by a parameter f which is the volume fraction of one of the phases and the normal vector is in the direction of the gradient of f. In the level set methodology, the intercept is determined by φ, a distance function. In the level set method the normal vector to the interface is defined as $\hat{n} = \vec{\nabla}\varphi\big|_{interface}$. Moving interfaces in Level-Set method are modeled though the following relation [8]:

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$$\frac{D\varphi}{Dt} = \frac{\partial\varphi}{\partial t} + \vec{U}.\vec{\nabla}\varphi = 0$$

To preserve the geometrical interpretation of the distance function, it should be reinitialized after each time step [7][8].

This section presents analytical formulas for evaluating the truncated area of a plane (normal vector: $\hat{n} = n_x\hat{x} + n_y\hat{y} + n_z\hat{z}$, distance function: φ) within a cuboid cell of sides Δx, Δy, and Δz. The truncated interface can be triangular, quadrilateral, pentagonal, or hexagonal. These cases are schematically illustrated in Figure 1. Consider the transformation $X = x/\Delta x$, $\mathrm{Y} = y/\Delta y$, and $Z = z/\Delta z$ that transforms the cuboid cell to a unit cube in an scaled system of coordinates. The components of the normal vector of the crossing plane in the scaled coordinate system will be $n_x\Delta x/\alpha$, $n_y\Delta y/\alpha$, and $n_z\Delta z/\alpha$, where $\alpha = \sqrt{(n_x\Delta x)^2 + (n_y\Delta y)^2 + (n_z\Delta z)^2}$ is the normalization factor. The coordinate system can be rotated such that the components of the normal vector in the scaled coordinate (N_1^s, N_2^s, and N_3^s) are, respectively, the minimum, middle and maximum values of $\left|n_x\Delta x/\alpha\right|$, $\left|n_y\Delta y/\alpha\right|$, and $\left|n_z\Delta z/\alpha\right|$. Such transformations transform the original geometry to a unit cube crossed by a plane whose normal vector is $\left[N_1^s, N_2^s, N_3^s\right]$. Let H_1^s, H_2^s, and H_3^s denote the x, y and z intercepts in the transformed coordinate system, and let T^s be the distance between the origin and the plane interface. The intercepts satisfy the relation $H_i^s = T^s/N_i^s$ in all directions (i=1,2,3) and therefore $0 \le N_1^s \le N_2^s \le N_3^s$ ensures that $H_1^s \ge H_2^s \ge H_3^s \ge 0$. Assuming that the volume fraction of the cut cell on the side of the origin (f^s) is less than half, the shape of the truncated plane within the unit cube can be categorized into 5 cases, illustrated in Figure 2 [11]: triangle (when $H_1^s \le 1$), quadrilateral (when $H_1^s > 1$ and $H_2^s \le 1$), pentagon (when $H_2^s > 1$, $H_3^s \le 1$, and $T^s \le N_1^s + N_2^s$), quadrilateral (when $H_2^s > 1$, $H_3^s \le 1$, and $T^s > N_1^s + N_2^s$), and hexagon (when $H_3^s > 1$). If f^s is more than half, a simple $f^{s\prime}$= 1- f^s transformation, which preserves the area, can be applied. Analytical formulas for the volume in the scaled coordinate system (f^s) in each of these cases are presented in [11]. Multiplying f^s by $\Delta x\Delta y\Delta z$ scales it to the original coordinate system, i.e. the volume in a cuboid cell (f) is equal to $f^s\Delta x\Delta y\Delta z$.

The interfacial area contained in the unit cube can be derived by differentiating f^s with respect to T^s in the scaled coordinate system (*i.e.* $A^s = df^s/dT^s$). Similarly, this relation in the original coordinate system is written as $A = df/dT$, which reduces to

$$A = \frac{df}{dT} = \frac{df}{dT^s}\frac{dT^s}{dT} = \frac{df^s}{dT^s}\frac{\Delta x\Delta y\Delta z}{\alpha} \tag{1}$$

in which the scaling factor $dT/dT^s = \alpha$ is applied. Applying equation (1) on the above mentioned categorized cases provides the expressions for the interfacial area and the volume fraction in terms of the components of the normal vector and the distance function in the original coordinate system. They are summarized as follow:

1. Triangular section is formed when $T^s \le N_1^s$. (Figure 2.a)

$$f = \frac{T^3}{6N_1^sN_2^sN_3^s}\Delta x\Delta y\Delta z$$

$$A_c = \frac{T^2}{2N_1^sN_2^sN_3^s}\frac{\Delta x\Delta y\Delta z}{\alpha}$$

2. Quadrilateral section is formed when $T^s > N_1^s$ and $T^s \le N_2^s$. (Figure 2.b)

$$f = \frac{T^3 - (T - N_1^s)^3}{6N_1^s N_2^s N_3^s} \Delta x \Delta y \Delta z$$

$$A_c = \frac{T^2 - (T - N_1^s)^2}{2N_1^s N_2^s N_3^s} \frac{\Delta x \Delta y \Delta z}{\alpha}$$

3. Pentagonal section is formed when $T^s > N_2^s$, $T^s \leq N_3^s$, and $T^s \leq N_1^s + N_2^s$. (Figure 2.c)

$$f = \frac{T^3 - (T - N_1^s)^3 - (T - N_2^s)^3}{6N_1^s N_2^s N_3^s} \Delta x \Delta y \Delta z$$

$$A_c = \frac{T^2 - (T - N_1^s)^2 - (T - N_2^s)^2}{2N_1^s N_2^s N_3^s} \frac{\Delta x \Delta y \Delta z}{\alpha}$$

4. Quadrilateral section is formed when $T^s > N_2^s$, $T^s \leq N_3^s$ and $T^s > N_1^s + N_2^s$. (Figure 2.e)

$$f = \frac{T - (N_1^s + N_2^s)/2}{N_3^s} \Delta x \Delta y \Delta z$$

$$A_c = \frac{1}{N_3^s} \frac{\Delta x \Delta y \Delta z}{\alpha}$$

5. Hexagonal section is formed when $T^s > N_3^s$. (Figure 2.d)

$$f = \frac{T^3 - (T - N_1^s)^3 - (T - N_2^s)^3 - (T - N_3^s)^3}{6N_1^s N_2^s N_3^s} \Delta x \Delta y \Delta z$$

$$A_c = \frac{T^2 - (T - N_1^s)^2 - (T - N_2^s)^2 - (T - N_3^s)^2}{2N_1^s N_2^s N_3^s} \frac{\Delta x \Delta y \Delta z}{\alpha}$$

Implementation of Surface Tension in Level Set Method

The accurate computation of surface tension is essential for any multiphase flow modeling technique. The challenge peculiar to surface tension in modeling fluid interfaces is the presence of spurious currents [10] that are interpreted as small velocity fields produced due to a slight unbalance between stresses in the interfacial region. Although different techniques are used for implementation of body forces [7], it is crucial for all of them to accurately estimate the magnitude and direction of the forces. The surface tension force, expressed as $\vec{F}_{\text{S.T.}} = \sigma \kappa A_c \vec{n}$, is proportional to the exposed surface area (A_c) and its local curvature (κ). To correctly evaluate the body force representing the surface tension in Navier-Stokes equation in a discretized space, one needs to calculate both κ and A_c. Overlooking the area enclosed in a numerical cell produces an unrealistic pressure jump and may result in uneven interface motion.

In this section the proposed method of calculating the surface tension force is compared to a conventional approximate method by presenting the numerical results of modeling a static two dimensional drop in a non-gravitational space. The drop of radius 2 and it is placed in an 8 × 8 square domain. To embolden the effects of surface tension and to limit the effects other phenomena have on the simulation results, the density ratio is assumed to be 1 and exact curvature is assigned for simulations. Surface tension property of water is used ($\sigma = 72$).The effect of surface tension should result in satisfaction of the pressure jump equation across the interface:

$$\Delta p\big|_{\text{interface}} = \sigma \kappa = 36\ Pa \tag{2}$$

In order to explain the implementation of the surface tension force, Navier-Stokes equation is presented in the X-direction as:

$$\rho \frac{Du}{Dt} = -\frac{\partial p}{\partial x} + \nu \nabla^2 u + [\, f_V \,]_{\mathrm{x}} \qquad ; \qquad \frac{D}{Dt} = \frac{\partial}{\partial t} + u_i \frac{\partial}{\partial x_i} \tag{3}$$

This force can be either applied as a Sharp Surface Force (SSF) [13], or it can be applied as a Continuous Surface Force (CSF) [14]. In the current simulation, the tension force is implemented as a sharp surface force. The volumetric force in Equation (3) can be accurately calculated by converting the enclosed surface force to a volumetric force. The enclosed surface force is then estimated as:

$$F_x\big|_{\mathrm{s}} = \sigma\kappa A_c \hat{n}\cdot\hat{x} = \sigma\kappa A_c \cos(\alpha) \tag{4}$$

converting it to a volumetric force applying only to the control volume in which interface passes through, reads as:

$$[\, f_{\mathrm{v}} \,]_x = \frac{\sigma\kappa A_c \hat{n}\cdot\hat{x}}{\Delta x \Delta y \Delta z} \tag{5}$$

The surface force, $F_x\big|_{\mathrm{s}}$, is schematically depicted for two cells in

Figure 3. As a result, in this method, surface force is first converted to a volumetric force and then it is implemented in flow equations. We denote this method as “areal method”, since estimating the enclosed area distinguishes it from the conventional SSF method presented in [13]. For this method, we therefore estimate the interfacial force if $|\varphi(i,j,k)| \le \frac{1}{2}\sqrt{\Delta x^2 + \Delta y^2 + \Delta z^2}$.

Conventional SSF method avoids calculating the enclosed area and therefore the numerical discretization basically assumes A_c equal to one of the faces in the cell. For sake of comparison, the presented discretization in [13] can be derived for X-direction using:

$$F_x\big|_{\mathrm{s}} = \sigma\kappa A_{\text{enclosed interface}} \approx \sigma\kappa \Delta y \Delta z \tag{6}$$

in which the enclosed area is approximated with one of the faces in the cell.

Figure 3 illustrates why this may not be a good approximation for A_c: In cell 1, A_c is smaller than $\Delta y \Delta z$, while in cell 2, A_c is larger than $\Delta y \Delta z$ .Consequently, converting it to a volumetric force, it reads:

$$[\, f_{\mathrm{v}} \,]_x = \frac{\sigma\kappa \Delta y \Delta z}{\Delta x \Delta y \Delta z} = \frac{\sigma\kappa}{\Delta x} \tag{7}$$

and this is the formulation which is used in conventional SSF method. This implementation can be referred as ‘stair-stepped’ method in a sense explained in [13].

Navier-Stokes equation was solved on a collocated variable arrangement [15] to numerically simulate a drop. The resulting pressure contours in the numerical domain are presented in Figure 4. It is clearly demonstrated that the areal method produces a more uniform pressure distribution inside and outside the drop and a more acceptable pressure jump value: while the least error for $(\Delta p)_{partial}$ for the conventional method, stair-stepped method, is more than .08%, the proposed algorithm produces an error around .004%.

Furthermore, the effect of mesh refinement on the predicted pressure jump value was tested on both methods, and the results are summarized in Figure 5. The error associated with the areal method reasonably decreases with increasing the number of meshes, as expected.

Conclusion

A new algorithm was introduced to estimate the surface tension force by calculating the interfacial area contained in an interface cell. Analytical formulas were derived for the case of a cuboid cell crossed by a planar interface. The proposed formulation and algorithm were applied and tested on a Level-Set computational fluid dynamic code by simulating a static drop. The results were compared against the results of a conventional method of estimating surface tension force and demonstrated significant improvements: 1) The pressure jump value predicted by the proposed method was found to be in a better agreement with the theoretical prediction; 2) It resulted in a more uniform pressure distribution in the vicinity of the interface; 3) It also resulted to less spurious currents around interface.

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Figures:

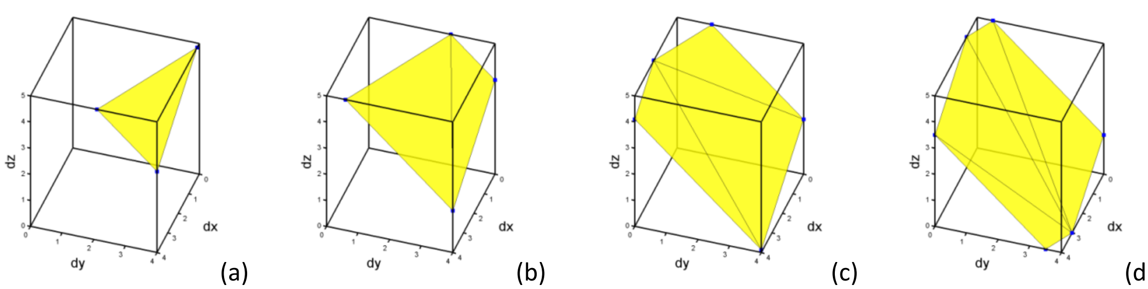

Figure 1. Interfacial area representation for $\hat{n} = [1/3, 2/3, 2/3]$, dx=4, dy=4, dz=5 (arb. unit length) . The formed polygon is (a) hexagonal (φ =0), (b) pentagonal (φ =0.4), (c) quadrilateral (φ =1.4), or (d) triangular (φ=2.4)

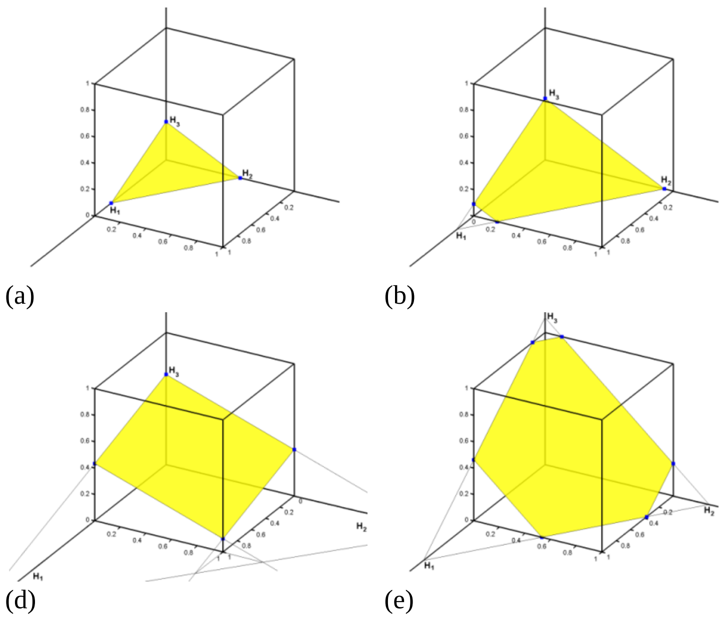

Figure 2. Any cell crossed by the phase interface can be transformed into a unit cube crossed by a plane. Figures (a) to (e) illustrate cases 1 to 5 respectively.

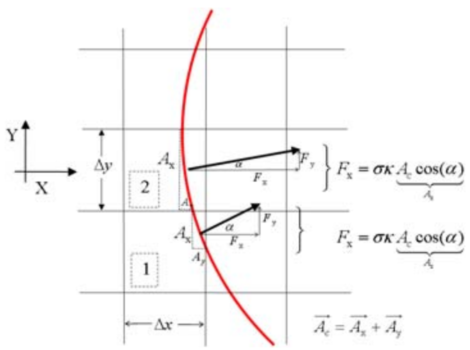

Figure 3. Expressions for the exact surface tension force are presented.

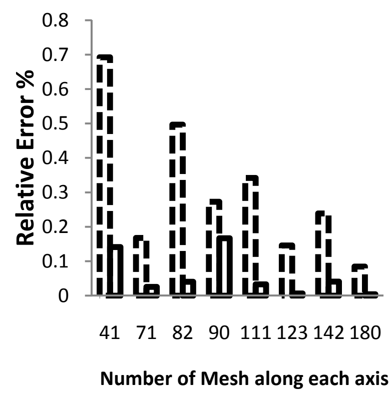

Figure 5. Relative error for $(\Delta p)_{partial}$ is demonstrated in simulating of a 2D drop using different numerical resolutions. The dashed line represents error for stair-step method of estimating surface tension force and the solid line areal method. It is shown that for each resolution the areal method results in less error than the stair-step method.

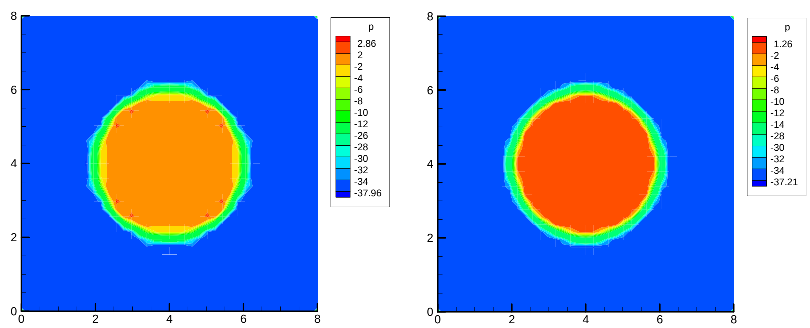

Figure 4. Pressure jump in a 2D stationary water droplet using 41x41 cells. Theoretical pressure jump value is 18.20 Pa. Left: the stair-stepped (conventional) approximate method. Right: the improved interfacial area algorithm, areal method.