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Computation of the curvature field in numerical simulation of multiphase flow

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Abstract

An essential ingredient in the simulation of multiphase fluid flow with surface tension is the accurate computation of the interface curvature. Curvature effects become more significant as we decrease the length scale of the problem at hand and thus accurate computation of curvature is especially important when considering microscale multiphase flows. We compared the curvature field calculated by three methods: the front capturing approach exemplified by the Level Set Method, the front tracking approach exemplified by Tryggvason's original Front Tracking method and a new Hybrid approach used in the context of the Level Contour Reconstruction Method, LCRM [S. Shin, S.I Abdel-Khalik, V. Daru and D. Juric, Accurate representation of surface tension using the level contour reconstruction method, JCP 203 (2005) 493–516]. We find that both the Level Set and Hybrid LCRM show great improvement if curvature is first calculated directly on the phase boundary and then redistributed back to the underlying grid. © 2006 Elsevier Inc. All rights reserved.

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1. Introduction

Popular numerical techniques used for multiphase based on using a fixed Eulerian grid with additional interface advection schemes all use the concept of a curvature field on the Eulerian grid to account for the interfacial effects of surface tension. Therefore, the accurate computation of curvature is an essential ingredient in simulation of multiphase fluid flow although it is a notoriously difficult quantity to compute with high fidelity. Despite its importance, the nature of the curvature field relative to various numerical treatments has not been clearly addressed and compared. In this article we compare the curvature field calculated by several popular methods: the front capturing approach exemplified by the Level Set Method [1], the Front Tracking approach exemplified by Tryggvason's original Front Tracking method [2] and a new Hybrid approach used in the context of the level contour reconstruction method, LCRM [3,4].

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2. Numerical formulation of surface tension force

The surface tension force term, \mathbf{F} in the single field formulation of the governing Navier–Stokes equations can be treated in different ways but here we briefly describe three approaches. Firstly, front capturing type methods such as the Level Set method use the form

$$\mathbf{F}_{\mathrm{LS}} = \sigma \boldsymbol{\kappa}_{\mathrm{LS}} \nabla H \tag{1}$$

where all quantities are calculated solely on an Eulerian grid. Here, σ is the surface tension coefficient (assumed constant) and κ is the interface curvature field. *H* is a Heaviside function which has the value of 1 in one phase and 0 in the other. The subscript "LS" stands for the Level Set formulation. The Volume of Fluid method uses an analogous concept by replacing *H* with a color function, *C*.

On the other hand, Front Tracking methods suggested by Tryggvason et al. [2] use direct information from the interface (interface elements or points) to calculate geometric quantities such as curvature:

$$\mathbf{F}_{\mathrm{FT}} = \int_{\Gamma(t)} \sigma \kappa_{\Gamma} \mathbf{n}_{\Gamma} \delta(\mathbf{x} - \mathbf{x}_{\Gamma}) \,\mathrm{d}s \tag{2}$$

Here, \mathbf{n}_{Γ} is the unit normal to the interface, $\mathbf{x}_{\Gamma} = \mathbf{x}(s, t)$ is a parameterization of the interface $\Gamma(t)$, κ_{Γ} in this case is the local mean curvature calculated on the interface, and $\delta(\mathbf{x} - \mathbf{x}_{\Gamma})$ is a three-dimensional Dirac distribution that is non-zero only when $\mathbf{x} = \mathbf{x}_{\Gamma}$. The subscript "FT" stands for the Front Tracking formulation.

Finally, in [4] we describe a Hybrid formulation for the surface tension force that uses aspects of both front capturing and Front Tracking methods:

$$\mathbf{F}_{\mathrm{H}} = \sigma \boldsymbol{\kappa}_{\mathrm{H}} \nabla I \tag{3}$$

The subscript "H" stands for the Hybrid approach. The Indicator function, I, has essentially the same characteristics as the Heaviside function, H.

3. Calculation of the curvature field

Front capturing type methods such as the Level Set Method calculate the curvature field as

$$\boldsymbol{\kappa}_{\rm LS} = \nabla \cdot \mathbf{n} = \nabla \cdot \left(\frac{\nabla \phi}{|\nabla \phi|}\right) \tag{4}$$

Here, ϕ is the level-set distance function. In VOF methods ϕ would be replaced by the volume fraction or in some versions a (mollified) color function, C.

In the original Front Tracking method the local curvature on the interface, κ_{Γ} , is calculated by parameterization of the interface, in 2D:

$$\kappa_{\Gamma} = \frac{\frac{d^2x}{ds^2}\frac{dy}{ds} - \frac{d'y}{ds^2}\frac{dx}{ds}}{\left[\left(\frac{dx}{ds}\right)^2 + \left(\frac{dy}{ds}\right)^2\right]^{3/2}}$$
(5)

Numerically, this is usually done with the aid of a curve fit between neighboring interface elements. Here, *s* represents arc length along the interface. This local curvature value at the interface element is distributed onto the Eulerian grid to obtain the curvature field, κ_{FT} ,

$$\boldsymbol{\kappa}_{\rm FT} = \frac{\sum_e \kappa_{\Gamma_e} w_e}{\sum_e w_e} \tag{6}$$

Here, w_e represents a weighting function and summation is performed over four (or sometimes 16) grid cells near each interface point in each x, y, and z direction.

The curvature field in the Hybrid approach [4] is found by

$$\boldsymbol{\kappa}_{\mathrm{H}} = \frac{\mathbf{F}_{\mathrm{L}} \cdot \mathbf{G}}{\sigma \mathbf{G} \cdot \mathbf{G}} \tag{7}$$

where in this equation the force, \mathbf{F}_{L} , is an alternative Front Tracking formulation for the surface tension force based on the tension, \mathbf{f}_{e} , on each surface element (a line element in 2D or plane triangle in 3D) (see [3] for details):

$$\mathbf{F}_{\mathrm{L}} = \int_{\Gamma(t)} \mathbf{f}_{\mathrm{e}} \delta(\mathbf{x} - \mathbf{x}_{\Gamma}) \,\mathrm{d}s \tag{8}$$

And G is geometric information computed directly on the interface and then distributed onto an Eulerian grid.

$$\mathbf{G} = \int_{\Gamma(t)} \mathbf{n}_{\Gamma} \delta(\mathbf{x} - \mathbf{x}_{\Gamma}) \,\mathrm{d}s \tag{9}$$

4. Results and discussion

Fig. 1 shows the local curvature values for a circle placed in 10×10 box with radius 2.5. Seventy-eight interfacial points are uniformly distributed around the circle (Fig. 1a). Local curvature values for the Level Set and Hybrid methods have been found by interpolating their field values to the interfacial points. As we can see in Fig. 1b, the Front Tracking formulation is the most accurate and the Hybrid formulation gives a comparable result but the value is slightly overestimated. The reason for the discrepancy in Hybrid formulation is due to the Eulerian grid resolution and vanishes with increased grid resolution. Maximum error of the curvature value was 0.081% with a 50×50 grid, 0.020% with a 100×100 grid, and 0.005% with a 200×200 grid. The Hybrid formulation exhibits good accuracy since the curvature field has been computed from Eulerian quan-



Fig. 1. Local curvature distribution of a circle with uniformly distributed points with radius 2.5 placed in 10×10 box: (a) interfacial point distribution and (b) local curvature values computed using each method.

tities which have already been distributed from the Lagrangian grid. The level set formulation shows an oscillating behavior for the local curvature value around the circle.

The Front Tracking (Fig. 2a) and Hybrid formulation (Fig. 2b) generate very uniform nearly constant curvature fields around the interface whereas, due to the nature of its calculation from the distance function, curvature in the Level Set formulation (Fig. 2c) shows not a constant but a monotonically decreasing curvature from the inside to the outside of the interface zone.

To check the importance of the relative spacing of interfacial points (or element sizes) in Front Tracking method, we generated the same circle as in Fig. 1 except that the interfacial point spacing is unevenly distributed (Fig. 3a). The interface points here are randomly perturbed with a 50% deviation from the average point spacing used to generate the circle in Fig. 1. The curve is fit by a Lagrange polynomial parameterized by arclength. Arclength parameterization yields more complex formulas for the curve and its derivatives but the results are vastly superior to simple point index formula. However, this also points to the computationally intensive nature of an accurate calculation of the curvature especially when dealing with 3D flows and the need to fit a surface. As expected the Front Tracking formulation gives the most accurate curvature results (Fig. 3b). The Hybrid formulation gives comparable results but suffers slightly from the uneven distribution of element sizes. The level set curvature is unaffected since it is a purely Eulerian method.

If we examine the curvature field from the Hybrid formulation (Fig. 4), we notice the interesting characteristic that the higher errors in curvature exist away from the interface towards the edge of the interfacial zone. In calculating the curvature using Eq. (7), due to the compact support of the numerical Dirac delta distribution, the denominator \mathbf{G} (Eq. (8)) is only non-zero in this zone around the interface. It will have values near zero at the edges of this zone, thus any errors become more sensitive to the data away from the interface.



Fig. 2. Curvature field of a circle with uniformly distributed points with radius 2.5 placed in 10×10 box: (a) Front Tracking formulation; (b) Hybrid formulation; and (c) Level Set formulation.



Fig. 3. Local curvature distribution of a circle with unevenly distributed points with radius 2.5 placed in 10×10 box: (a) interface point distribution and (b) local curvature value computed using each method.



Fig. 4. Curvature field of a circle with unevenly distributed points with radius 2.5 placed in 10×10 box with Hybrid formulation.

Considering that the error tends to increase away from the phase boundary in the Hybrid formulation, we propose the following remedy: calculate the curvature values still using the form of Eq. (7) but now applied locally at the interfacial points and then redistribute the result back to the Eulerian grid. Chen et al. [5] used a similar idea in the case of velocity extrapolation in the Stefan problem using the Level Set method. The exten-

sion to 3D being straightforward we will focus on describing the idea in two-dimensions. Expressing the vector components of Eqs. (8) and (9) as

$$\mathbf{F}_{\mathbf{L}} = (F_x^{\mathbf{L}}, F_y^{\mathbf{L}}) \quad \mathbf{G} = (G_x, G_y) \tag{10}$$

We then interpolate the components to the interface points using a procedure proposed by Torres and Brackbill [6]. Continuous and smooth field values can be interpolated using B-spline interpolation functions. For example, the value of F_x^L at an arbitrary location can be found by interpolation of the grid values:

$$F_x^{\mathbf{L}}(\mathbf{x}) = \sum_g F_x^{\mathbf{L}}(i, j, k) S(\mathbf{x} - \mathbf{x}_g)$$
(11)

Here, $S(x - x_g)$ is a tensor product of one-dimensional B-splines, M, given by:

$$S(\mathbf{x} - \mathbf{x}_g) = M(x - x_g; \Delta x)M(y - y_g; \Delta y)$$
(12)

We use the cubic B-spline kernel $M_3(x; h)$ for which a detailed description can be found in Torres and Brackbill [6]. With B-spline interpolation to the interface points (x_e, y_e) , the equation to calculate curvature at the interface points analogous to Eq. (7) is



Fig. 5. Curvature field of a circle with unevenly distributed points with radius 2.5 placed in 10×10 box: (a) New Hybrid formulation and (b) New Level Set formulation.

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$$\kappa_{\rm N_H}(x_{\rm e}, y_{\rm e}) = \frac{F_x^{\rm L}(x_{\rm e}, y_{\rm e})G_x(x_{\rm e}, y_{\rm e}) + F_y^{\rm L}(x_{\rm e}, y_{\rm e})G_y(x_{\rm e}, y_{\rm e})}{\sigma[G_x(x_{\rm e}, y_{\rm e})^2 + G_y(x_{\rm e}, y_{\rm e})^2]}$$
(13)

Here, x_e and y_e represent the x and y locations of each individual element midpoint. The local curvature values obtained with Eq. (13) can now be redistributed back to the underlying Eulerian grid as in Eq. (6) to obtain the curvature field

$$\boldsymbol{\kappa}_{\mathrm{N_H}} = \frac{\sum_{e} \kappa_{\mathrm{N_H}}(x_{e}, y_{e}) w_{e}}{\sum_{e} w_{e}}$$
(14)

We will refer to the procedure in Eqs. (13), (14) as the "New Hybrid formulation".

The level set curvature field (Eq. (4)) can also be modified in the same way. The local curvature values can be calculated at given interface points (x_e , y_e):

$$\kappa_{\text{N}_\text{LS}}(x_{\text{e}}, y_{\text{e}}) = \nabla \cdot \left(\frac{\nabla \phi(x_{\text{e}}, y_{\text{e}})}{|\nabla \phi(x_{\text{e}}, y_{\text{e}})|} \right)$$
(15)

These local curvature values can now be redistributed back to the fixed grid again as in Eq. (14) to obtain the curvature field

$$\boldsymbol{\kappa}_{\text{N}_\text{LS}} = \frac{\sum_{e} \kappa_{\text{N}_\text{LS}}(x_e, y_e) w_e}{\sum_{e} w_e} \tag{16}$$

However, this procedure will only be applicable to the Level Set method in general if there is some way of identifying individual interface points. The recent Particle Level Set Method of Enright et al. [7] may take advantage of this New Level Set formulation because the interface location is known owing to the existence of tracked particles in their method but is limited to certain velocity fields. Since we happen to have these points for our test cases we will generate such a modified level set curvature field for comparison purposes and refer to the procedure here as the "New Level Set" formulation. Fig. 5a and b shows the superior results obtained for the curvature field calculated using Eq. (14) for the New Hybrid and New Level Set formulations using Eq. (16), respectively.

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