Computers and Fluids 161 (2018) 74–88

Contents lists available at ScienceDirect

Computers and Fluids

journal homepage: www.elsevier.com/locate/compfluid

Computing interface curvature from volume fractions: A hybrid approach

H.V. Patel, J.A.M. Kuipers, E.A.J.F. Peters*

Multiphase Reactors Group, Department of Chemical Engineering and Chemistry, Eindhoven University of Technology, 5600 MB Eindhoven, P.O. Box 513, The Netherlands

ARTICLE INFO

Article history:
Received 29 June 2017
Revised 13 November 2017
Accepted 19 November 2017
Available online 21 November 2017

Keywords:
Volume of Fluid
Hybrid interface curvature
Balanced-force
Convolution
Generalized height function

ABSTRACT

The Volume of Fluid method is extensively used for the multiphase flows simulations in which the interface between two fluids is represented by a discrete and abruptly-varying volume fractions field. The Heaviside nature of the volume fractions field presents an immense challenge for the accurate computation of the interface curvature and induces the spurious velocities in the flows with surface-tension effects. A 3D hybrid approach is presented combining the Convolution and Generalized Height Function method for the curvature computation. The volumetric surface tension forces are computed using the balanced-force continuum surface force model. It provides a high degree of robustness at lower grid resolutions with first-order convergence and high accuracy at higher grid resolutions with second-order convergence. The present method is validated for several test cases including a stationary droplet, an oscillating droplet and the buoyant rise of gas bubbles over a wide range of Eötvös (*Eo*) and Morton (*Mo*) numbers. Our computational results show an excellent agreement with analytical/experimental results with desired convergence behavior.

1. Introduction

Multiphase flows involving fluid-fluid interfaces are ubiquitous in nature and technology. Rain drops, atomizing water jet, spray driers, emulsions, bubble swarms and trickle bed reactors are just a few examples. Typically these flows have high density and/or viscosity ratios with high surface tension effects which tend to produce topologically complex and dynamically evolving interfaces. So, the accurate numerical simulation of such flows has attracted a lot of attention among researchers.

Numerical simulations of multiphase flows need to address two primary challenges: (i) mass-conserving advection of the fluid phases and (ii) accurate computation of the surface tension forces at the fluid-fluid interface. A wide range of multi-fluid interface tracking/capturing methods have been developed to simulate multiphase flows and they mainly differ with respect to the way they tackle aforementioned challenges. A holistic overview of these methods is presented by Scardovelli and Zaleski [1]. Examples include the Volume of Fluid [2], Level Set [3], Front-Tracking [4], multiphase Lattice-Boltzmann [5] and moving-grids [6] methods.

The Volume of Fluid (VOF) method uses a discrete and abruptly-varying volume fractions (F) field to represent the fractional amount of a reference fluid present in each computational cell. Advection of F is treated by a pseudo-Lagrangian geometrical advection schemes to minimize numerical diffusion. Interface reconstruction is required for geometrical advection of F which is done by piecewise linear interface calculation (PLIC) following Youngs [7]. Weymouth and Yue [8] shows that the VOF method can be 'exactly' mass conservative however negligible mass errors may arise due to finite machine precision during numerical computations.

The volumetric surface tension force is computed using the continuum surface force (CSF) model proposed by Brackbill et al. [9]. CSF model suggests that the accuracy of the surface tension force is mostly determined by the computed local interface curvature. Accurate computation of the curvature is particularly difficult due to the discontinuous nature of F field. Inaccurate curvature, however, along with the improper discretization of the surface tension force creates an imbalance of pressure and surface tension forces at the interface which induces spurious velocities in the flow field. A detailed analysis of generation and scaling of spurious velocities in VOF simulations can be found in [10]. So, to reduce/eliminate these spurious velocities two problems need to be tackled distinctly: (i) surface tension and pressure forces need to be discretized at the same location (balanced-force concept by

* Corresponding author.
E-mail address: E.A.J.F.Peters@tue.nl (E.A.J.F. Peters).

https://doi.org/10.1016/j.compfluid.2017.11.011

Francois et al. [11]) and (ii) accurate computation of the interface curvature.

Interface curvature can be computed as a second order spatial derivative of the abruptly-varying F field. Different methods are available for the numerical computation of interface curvature and an excellent comparison is presented by Cummins et al. [12] and Francois et al. [11]. The Convolution (CV) method uses a smoothing kernel to convolute the F field before differentiating it. This removes the high frequency aliasing error which otherwise would occur due to the numerical differentiation of F (Heaviside function). Accuracy and convergence of the CV method depends upon the length of the smoothing kernel. The Height Function (HF) method computes the heights by summing the F field across the interface which produces differentiable heights from an abruptly-varying F field. A Standard Height Function (SHF) method uses a fixed 7×3 stencil in 2D ($7 \times 3 \times 3$ in 3D) for this summation process. A Generalized Height Function (GHF) method [13] uses an adaptive stencil to compute heights which produces a better curvature estimate especially in the case of complex topologies and interface merging/breakup. Reconstructed distance function (RDF) method computes a distance function from the interface in the VOF framework. This distance function is smoothly varying and hence curvature is directly computed from the numerical differentiation of the same. RDF method is similar to the one used for the coupled VOF-Level Set simulations by Sussman and Puckett [14]. A Least Squared (LS) method is another option which computes the curvature by fitting a parabola in 2D (paraboloid in 3D) either on the volume fractions directly [15] or on a set of interfacial points [13].

Only a few attempts have been made to develop hybrid methods for curvature computation. Popinet [13] presents a hybrid method on adaptive grids which uses the GHF method at higher grid resolutions and the LS method at lower grid resolutions. The LS method is computationally expensive and requires a complex implementation compared to other methods. Owkes and Desjardins [16] presents a mesh decoupled HF method where HF stencils are constructed in the direction of the interface normal which may not be aligned with the underlaying Eulerian grid. Embedded height-function technique by Ivey and Moin [17] constructs HF stencils on unstructured non-convex polyhedral meshes. This method embeds traditional HF stencils in the unstructured mesh and geometrically interpolates the volume fraction information from the mesh to the HF stencil. Both of these methods uses fixed length HF stencils which drastically reduces the curvature accuracy during interface merging or breakup.

Cummins et al. [12] concluded that the CV or RDF method exhibits a greater robustness over the HF method and doesn't breakdown catastrophically when the interfacial length scale (radius of curvature) is not adequately resolved by the grid. On the other hand, the HF method computes very accurate curvatures which converges with second-order when the interface is adequately resolved. So, the choice of appropriate curvature finding method depends on the number of grid cells across the radius of curvature. They called for a hybrid/unified curvature finding method which uses a robust CV or RDF method at lower and an accurate HF method at higher grid resolutions. Such a hybrid method should have a branching algorithm to decide which curvature finding method is to be used based on the local interface topology.

In this paper, a 3D hybrid approach (CV-GHF) is presented which combines the CV and GHF methods for the curvature computation. The volumetric surface tension force is computed using the balanced-force CSF model. The present method computes highly accurate curvatures with second-order convergence at higher grid resolutions. A branching algorithm is an in-built part of the present method which automatically switches the curvature computation method from GHF to CV at lower grid resolutions. The method is quite robust and shows first-order convergence at lower grid resolutions. The paper is organized as follows: First, we describe the governing Navier-Stokes equations for multiphase flows along with the balanced-force CSF model in VOF framework. Subsequently, we discuss the CV, HF and hybrid CV-GHF method with the branching algorithm in detail. Next, we lay down different scenarios where the GHF method exhibits better performance than the SHF method. Curvature errors are then quantified for the present CV-GHF method to check the convergence behavior. Finally, an extensive validation of the method is reported with different test cases including a stationary droplet, an oscillating droplet and the buoyant rise of gas bubbles over a wide range of physical properties of the gas-liquid system.

2. Numerical method

In this section the governing equations for the multiphase flow are described along with the discretization and solution methodology in brief. The main focus will be based on the balanced-force concept which is used to discretize the surface tension force in present work.

2.1. Governing equations

For the incompressible, unsteady, Newtonian multiphase flows the mass and momentum conservation (Navier-Stokes) equations can be represented in terms of the single velocity field ($\mathbf{u}$) formalism:

$$\nabla \cdot \mathbf{u} = 0 \tag{1}$$

$$\rho \frac{\partial \mathbf{u}}{\partial t} + \rho \nabla \cdot (\mathbf{u}\mathbf{u}) = -\nabla p + \nabla \cdot \boldsymbol{\tau} + \rho \mathbf{g} + \mathbf{F}_\sigma \tag{2}$$

where $\boldsymbol{\tau} = \mu[\nabla \mathbf{u} + (\nabla \mathbf{u})^T]$ is the fluid stress tensor, $\mathbf{g}$ is the acceleration due to gravity and $\mathbf{F}_\sigma$ is the local surface tension force accounting for the presence of curved deformable fluid-fluid interfaces. The local averaged density (ρ) is evaluated by the linear averaging of the densities of the individual fluid phases:

$$\rho = F\rho_1 + (1 - F)\rho_2 \tag{3}$$

Note that we use volume fraction $F = 1$ and 0 for the computational cells fully occupied by fluid 1 and fluid 2, respectively. $0 < F < 1$ indicates that the cell contains a fluid-fluid interface. The local averaged dynamic viscosity (μ) is calculated by harmonic averaging [18]:

$$\frac{\rho}{\mu} = F\frac{\rho_1}{\mu_1} + (1 - F)\frac{\rho_2}{\mu_2} \tag{4}$$

Advection of F depends on the local fluid velocity and is governed by the following conservation equation:

$$\frac{DF}{Dt} = \frac{\partial F}{\partial t} + \mathbf{u} \cdot \nabla F = 0 \tag{5}$$

The volumetric surface tension force ($\mathbf{F}_\sigma$) is computed using the continuum surface force (CSF) model [9]:

$$\mathbf{F}_\sigma = \sigma \kappa \mathbf{n} \tag{6}$$

where σ is the coefficient of surface tension, κ is local interface curvature and $\mathbf{n}$ is the interface normal. $\mathbf{F}_\sigma$ is non-zero only at the interface. $\mathbf{n}$ and κ are first and second order derivative of F respectively as follow:

$$\mathbf{n} = \nabla F \tag{7}$$

$$\kappa = -\nabla \cdot \frac{\nabla F}{|\nabla F|} = -\nabla \cdot \frac{\mathbf{n}}{|\mathbf{n}|} = \frac{1}{|\mathbf{n}|}\left[\frac{\mathbf{n}}{|\mathbf{n}|} \cdot \nabla|\mathbf{n}| - (\nabla \cdot \mathbf{n})\right] \tag{8}$$