International Journal of Heat and Fluid Flow 70 (2018) 59–78

Contents lists available at ScienceDirect

International Journal of Heat and Fluid Flow

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

Simulating liquid droplets: A quantitative assessment of lattice Boltzmann and Volume of Fluid methods

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ARTICLE INFO

Keywords:
Multiphase flows
Pseudopotential Lattice Boltzmann
Volume of fluid
Emulsions
Liquid droplets

ABSTRACT

While various multiphase flow simulation techniques have found acceptance as predictive tools for processes involving immiscible fluids, none of them can be considered universally applicable. Focusing on accurate simulation of liquid-liquid emulsions at the scale of droplets, we present a comparative assessment of the single-component multiphase pseudopotential lattice Boltzmann method (PP-LB, classical and modified) and the Volume of Fluid method (VOF, classical and modified), highlighting particular strengths and weaknesses of these techniques. We show that a modified LB model produces spurious velocities 1–3 orders of magnitude lower than all VOF models tested, and find that LB is roughly 10 times faster in computation time, while VOF is more versatile. Simulating falling liquid droplets, a realistic problem, we find that despite identical setups, results can vary with the technique in certain flow regimes. At lower Reynolds numbers, all methods agree reasonably well with experimental values. At higher Reynolds numbers, all methods underpredict the droplet Reynolds number, while being in good agreement with each other. Particular issues regarding LB simulations at low density ratio are emphasized. Finally, we conclude with the applicability of VOF vis-à-vis PP-LB for a general range of multiphase flow problems relevant to myriad applications.

1. Introduction

Multiphase flow simulations are becoming commonplace in describing and designing engineering applications, which has led to the development of numerous numerical techniques (Prosperetti and Tryggvason, 2009; Tryggvason et al., 2011). In addition, this has provided unprecedented insight into flow physics at the scale of individual droplets and bubbles which in many cases is relevant at the larger scale of reactors or processes. This has in turn greatly benefited emulsion research dealing with liquid-liquid flows (Loewenberg and Hinch, 1996; Cristini and Tan, 2004; Roudsari et al., 2012), where performing experiments to obtain high resolution spatio-temporal data is often not feasible. Many food and personal care products consist of liquid-liquid emulsions with a low density ratio. In the oil industry, separating water from oil (in particular downhole water/oil separation, leaving the water underground) is a tremendously relevant issue (Kokal et al., 2002), as many oil sources not just produce oil and gas but also water in increasing amounts. Also the concept of Enhanced Oil Recovery (EOR) (Lake, 1989) in which steam is injected into oil containing reservoirs to increase oil production results in large amounts of fine liquid-liquid emulsions which need treatment. In the polymer industry, quite a few polymers are produced by means of emulsion polymerization processes Arshady (1992). Reliable simulations of these widely different processes require an accurate description of the flow physics at the droplet scale. The existence of myriad simulation techniques presents another caveat - which method is most applicable to a specific problem? This calls for studies that reveal particular strengths and shortcomings of these simulation techniques when directly compared, however in the case of interface resolving multiphase flows, such studies are difficult to come by.

To the best of the authors' knowledge, among the very few other studies comparing a mesoscopic technique to a continuum technique for multiphase flow are the comparison between a two fluid free energy LB approach and a volume of fluid method by Takada et al. (2000), between a pseudopotential LB and a front-tracking finite-difference method for rising bubbles by Sankaranarayanan et al. (2003) and between a free energy LB formulation and a phase field method by

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https://doi.org/10.1016/j.ijheatfluidflow.2017.12.001
Received 16 August 2017; Received in revised form 8 November 2017; Accepted 5 December 2017

Scarbolo et al. (2013). We compare two widely used techniques based on very different principles, namely the finite volume based Volume of Fluid (VOF) method and the mesoscopic, single-component multiphase pseudopotential lattice Boltzmann method (PP-LB) and focus on specific challenges faced when simulating fluids at low density ratio. Generally, multiphase flows can contain single or multiple fluid components in different phases, for instance a fluid existing simultaneously in its liquid and vapour phase, or two immiscible liquids like oil and water. The most elusive problem here is the accurate representation of the phase separating interface, that essentially emerges from the microscopic interactions at the molecular level, detached from the continuum regime of hydrodynamics, and which can undergo complex deformations during the evolution of the flow. VOF and PP-LB differ greatly in how they simulate interface dynamics. Both techniques have particular points of strength, but they also bring a set of shortcomings that are easily overlooked - we address them both in the course of our study.

VOF is one of the first techniques developed for multiphase flow simulations based on the finite volume method (FVM) (Hirt and Nichols, 1981). Using VOF, one solves an additional advection equation for a boolean valued phase indicator function, marking the two *immiscible* fluids. In principle, at the interface, this indicator value changes rapidly from 0 to 1 (or vice-versa) marking the two phase regions. Further, all physical properties are modeled as phase averages, hence working with an effective *single-fluid* formulation of the Navier-Stokes equation. This method has been demonstrated to perform well for a wide range of multiphase flow problems and can reproduce an appreciably sharp interface undergoing arbitrarily large deformations (Gopala and van Wachem, 2008).

Also over the past two decades, PP-LB has emerged as a versatile alternative to conventional finite volume techniques for simulating multiphase flows (Chen et al., 2014). It was first proposed by Shan and Chen (1993, 1994) and is based on a mesoscopic kinetic equation for particle distribution functions, and has been used for various fluid mechanics and engineering problems (Chen et al., 1995; Chen and Doolen, 1998). In this method, particle interactions are modeled by an interparticle force which causes a single-component fluid to spontaneously segregate into two phases of different densities that change smoothly from one bulk value to another. The interface emerges automatically and is characterized by monitoring the variation in density, and is therefore no longer a mathematical boundary and no explicit interface tracking/capturing technique is required. Moreover, surface tension effects emerge automatically from the underlying Boltzmann dynamics. The single-component PP-LB is the most widely used LB based model due to its simplicity and versatility, remarkable computational efficiency and clear representation of the underlying microscopic physics.

Evidently, VOF and PP-LB simulate multiphase flows very differently, the first being a continuum approach and the latter mesoscopic. The main point of departure is that in VOF, the two (or more) fluids are completely immiscible and interfacial dynamics is modeled with a specified surface tension force. While in single-component PP-LB, the two fluids are modeled as the liquid and vapor phases of the same non-ideal component (Swift et al., 1995), which coexist due to phase separation (Yuan and Schaefer, 2006). Immiscibility of the two phases in PP-LB is ensured by a repulsive interaction parameter, consequently leading to surface tension effects. Owing to these differences, a direct comparison between the strengths and weaknesses of the two methods can benefit a user by providing motivation for selecting either technique, for one might be better suited to a specific problem than the other. Previously (Mukherjee et al., 2016), the authors attempted such an intercomparison and it was observed that even after a careful formulation of identical test cases, predicted results can vary between the two methods. In this study, we investigate this discrepancy further to more conclusively remark on the predictive aspects of VOF vis-à-vis PP-LB.

We begin with a description of PP-LB (our own in-house code implementation using FORTRAN 90 as well as an implementation in the open source Parallel Lattice Boltzmann solver Palabos-v1.5r1), and the VOF method (using the standard OpenFOAM and FLUENT VOF solvers, along with modifications to the OpenFOAM solver). We first address the so-called spurious velocities that emerge in both methods as numerical artifacts and can be a limiting constraint on the accuracy of results. We also compare the thickness of the interface as produced by these methods, and show that sharper interfaces are achieved at the cost of higher spurious velocities. Next we simulate falling droplets with a low density ratio (2D and 3D in VOF, and 2D in LB) to compare how well the methods predict the velocity evolution, terminal Reynolds number and droplet shape. This comparison is performed in a small region of the phase-space governing falling droplets, corresponding to the spherical and ellipsoidal regions of the shape regime map of Clift et al. (2005) (henceforth called the Clift map). We then discuss the specific challenges faced for the two methods and conclude with our main findings.

2. Numerical methods

2.1. Single-component PP-LB

The standard lattice Boltzmann equation with a single relaxation time (Succi, 2001) is written as

$$\frac{f_i(\mathbf{x}+\mathbf{e}_i\Delta t,\, t+\Delta t)-f_i(\mathbf{x},\, t)}{\Delta t}=\frac{1}{\tau}(f_i(\mathbf{x},\, t)-f_i^{\mathrm{eq}}(\mathbf{x},\, t))+\mathbf{S}_i \tag{1}$$

where $f_i(\mathbf{x},\, t)$ is the density distribution function associated with discrete velocity direction i, and $\mathbf{S}_i$ represents a general source term added into the lattice Boltzmann equation (which is related to all thermodynamic and hydrodynamic forces). The discrete velocities $\mathbf{e}_i$ in the ith - direction, for the D2Q9 lattice are given by $\mathbf{e}_0=0$ and $\mathbf{e}_i=\lambda_i(\cos\theta_i,\,\sin\theta_i)$ with $\lambda_i=1$, $\theta_i=(i-1)\pi/2$ for $i=1-4$ and $\lambda_i=\sqrt{2}$, $\theta_i=(i-5)\pi/2+\pi/4$ for $i=5-8$. The order numbers $i=1-4$ and $i=5-8$ represent the rectangular and the diagonal directions of the lattice respectively. In Eq. (1), f_i^{eq} is the equilibrium distribution function and is calculated as

$$f_i^{\mathrm{eq}}=w_i\rho\left[1+\frac{(\mathbf{e}_i\cdot\mathbf{u}^{\mathrm{eq}})}{c_s^2}+\frac{(\mathbf{e}_i\cdot\mathbf{u}^{\mathrm{eq}})^2}{2c_s^4}-\frac{(\mathbf{u}^{\mathrm{eq}}\cdot\mathbf{u}^{\mathrm{eq}})}{2c_s^2}\right] \tag{2}$$

where $c_s^2=1/3$ is the lattice speed of sound, w_i are the weighting factors equal to 4/9 for $i=0$, 1/9 for $i=1-4$ and 1/36 for $i=5-8$, and $\mathbf{u}^{\mathrm{eq}}$ is the equilibrium velocity. Also, the local mass density, local velocity and the viscosity in the lattice units for each component are calculated as $\rho=\sum_i f_i$, $\mathbf{u}=(\sum_i \mathbf{e}_i f_i)/\rho$ and $\nu=(\tau-0.5)/3$ respectively.

The force $\mathbf{F}$ acting on a multiphase system includes external body forces, $\mathbf{F}_{\mathrm{body}}$ (e.g. gravity) and the mean field inter-particle interaction force, $\mathbf{F}_{\mathrm{int}}$, and is written as $\mathbf{F}=\mathbf{F}_{\mathrm{body}}+\mathbf{F}_{\mathrm{int}}$. Based on the original pseudopotential model (Shan and Chen, 1994), the so called $\beta-$scheme (Gong and Cheng, 2012) has been introduced for the interaction force for a single-component multiphase system as follows:

$$\begin{aligned}\mathbf{F}_{\mathrm{int}}=&-\beta\left[\psi(\mathbf{x},\, t)G\sum_i\psi(\mathbf{x}+\mathbf{e}_i\Delta t,\, t)\mathbf{e}_i\Delta t\right]\\&+\frac{1-\beta}{2}\left[G\sum_i w_i[\psi(\mathbf{x}+\mathbf{e}_i\Delta t,\, t)]^2\mathbf{e}_i\Delta t\right]\end{aligned} \tag{3}$$

where $\Delta t=1$ is the time interval and G denotes the interaction parameter, with $G<0$ representing an attractive force between the particles. Compared to the original pseudopotential interaction force, the $\beta-$scheme has more isotropy and by choosing a proper value for β, the thermodynamic inconsistency and magnitude of spurious velocities can be greatly reduced (Gong and Cheng, 2012; Zarghami et al., 2015; Zarghami and Van den Akker, 2017). It has been shown that by setting $\beta=1.25$ the density ratio in LB matches well with the analytical equation of state (EOS) (Zarghami et al., 2015). Note that by choosing