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A multiphase lattice Boltzmann method for simulating immiscible liquid-liquid interface dynamics

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ABSTRACT

The simulation of immiscible liquid–liquid interface dynamics using the lattice Boltzmann method is studied in this work. The capabilities of the proposed model are investigated and validated with the inclusion of an external forcing term, e.g. the force of gravity. Fundamental tests are performed to further validate the performance of the method for computing multiphase flows. Four theoretical test cases are studied: (1) two-phase Poiseuille flow with variable density and viscosity ratios; (2) two-phase flow subject to hydrostatic pressure; (3) two-dimensional bubble dynamics; and (4) capillary-gravity wave. The four test cases provide clear quantitative results. In particular, the results of the proposed formulation for the test case with two-dimensional bubble dynamics are compared with the results of three different finite element methods. We found that the proposed lattice Boltzmann method is consistent with these standard approaches, and that the relative standard deviation between all codes is less than 1% for several flow quantities. Most of the test cases in this study use real liquid properties for the dimensionless density and viscosity ratios. In this context, the real immiscible liquids are mercury, water, and hexane. In addition, a final application test case is studied, where a hexane bubble under gravity is initially trapped inside a structured pore that is completely water-wet. A methodology using the bisection method to find the critical Bond number for which the transition from a trapped to a non-trapped bubble occurs is proposed.

1. Introduction

In recent years, the lattice Boltzmann method (LBM) for fluid flow simulation has undergone considerable development. This may be attributed to several factors, but an important one is its ability to model multiphase flow systems relatively easily, compared to standard approaches like the finite element or finite volume methods. The simulation of multiphase flows with LBM can be subdivided into the following class:

- Color-gradient method from Rothman and Keller [1] and Gunstensen et al. [2];
- Pseudo-potential from Shan and Chen [3];
- Free-Energy from Swift et al. [4];
- Mean-Field from He et al. [5]; and
- Field-Mediator from Santos et al. [6].

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This list is not exhaustive, but the above methods encompass most of the topic and so can serve as the starting point for newcomers interested in researching the LBM simulation of multiphase flows. For the interested reader, books on the general lattice Boltzmann method can be found in Refs. [7–9]. A book on multiphase lattice Boltzmann modeling has recently been published by Huang et al. [10]. Because the main aim of this work is to study the color-gradient method, we review some aspects (not all) of its development. Gunstensen et al. [2] first proposed an LB model based on the lattice-gas model of Rothman and Keller [1] for simulating immiscible fluids.

Single-phase operator. Most color-gradient models are based on a basic single-relaxation-time for the single-phase collision operator. Recently, a multiple-relaxation-time (MRT) single-phase operator has been introduced into the color-gradient model [11–13]. Introducing the lattice Boltzmann relaxation process into the moment space has resulted in a significant increase in the stability of the model, and this has greatly broadened the range of stable parameters, especially for the simulation of flow at low viscosity. For flow with unit density ratios, Leclaire et al. [14] introduced a cascaded single-phase collision operator into the color-gradient model. For a given surface tension force, the model has been shown to be unconditionally stable within the limit of zero viscosity.

Perturbation operator. It has been shown that the original perturbation operator of Gunstensen et al. [2] does not recover the correct form of the macroscopic capillary stress tensor [15]. The color-gradient model has been extended to the common D2Q9 lattice by Reis and Phillips [15] and the perturbation operator was modified, so that the model now complies with the correct form of the capillary stress tensor. The perturbation operator has been further extended by Liu et al. [16] for the D3Q19 lattice.

Recoloring operator. One characteristic of the color-gradient model for addressing multiphase flows is a recoloring operator intended to render the various fluids immiscible. The original recoloring operator of Gunstensen et al. [2] results in the creation of large numerical artifacts, which may introduce numerical instability into the model and lead to simulation divergence. In particular, the interface is so thin with the original model that large numerical errors occur when the color-gradient is evaluated. These errors may also translate into parasitic currents. All multiphase flow models that we know suffer to some extent from these parasitic currents. The problem has led to some changes to the recoloring operator. Back in 2002, Tölke et al. [17] redesigned it to create a thicker interface between the fluids. However, the thickness of that interface was not adjustable. Latva-Kokko and Rothman [18] modified the original Gunstensen et al. recoloring operator [2] in order to introduce a new parameter that enable manual adjustment of the interface thickness between the fluids. In Leclaire et al. [19], the authors show the superiority of the Latva-Kokko and Rothman algorithm versus the original Gunstensen et al. [2] recoloring operator. In fact, their new recoloring operator extends the range of stable parameters of the method and improves the steady state convergence rate, as well as significantly reducing the lattice pinning problem of the original method. The recoloring operator was further improved in Ref. [13], where a new expression for the recoloring parameter was introduced. This allows to control the numerical dimensionless Cahn number, i.e. the ratio between the numerical interface thickness and a typical macroscopic scale, by means of lattice refinement. Note that with a diffuse based interface simulation method, the numerical Cahn number is usually much greater than the real physical Cahn number given by the ratio between the true physical interface thickness and the typical macroscopic scale. To a lesser extent, the same comment could also apply to sharp interface simulation methods, such as the original Gunstensen et al. model [2], as even one discrete spatial step Δx is considered thick for modeling the physical interface thickness. One advantage of this new expression is that it has been shown to control the spurious currents at steady state with lattice refinement, while ensuring that the numerical Cahn number still converges to zero. We also believe, although cannot yet prove, that the proposed modified recoloring operator can also control the spurious currents with lattice refinement in the unsteady regime. The numerical approach proposed in this latter work can also be used to improve the initial condition of a multiphase color-gradient method simulation. An interesting diffusion process was proposed by Li et al. [11] in order to correct the antidiffusive property of the recoloring algorithm of Gunstensen et al. [2].

Variable density and viscosity ratios. Variable viscosity ratios were first achieved by Grunau et al. [20], who used an interpolation of the relaxation factor. Since then, different types of viscosity interpolation have been proposed in the scientific literature [21]. While the choice of the viscosity interpolation is rather ad hoc and problem-dependent, the use of viscosity interpolation at the interface is a very commonly used methodology with the multiphase flow model to calculate the viscosity ratios between the fluids. The simulation of variable density ratios between fluids has been shown to be a much more difficult task, however. Grunau et al. [20] modified the Gunstensen et al. [2] model to achieve this. By using the free degree of liberty available in the lattice speed of sound, a stable fluid interface can be obtained because the lattice sound speed is chosen such that the pressure field is continuous across the interface. However, only much later was it found that this numerical approach was insufficient to simulate multiphase flow with variable density ratios. In fact, correct momentum discontinuity (or velocity continuity) across the interface is not guaranteed by the Grunau et al. [20] approach. This problem is referred to as the *discontinuity problem* of the multiphase LBM [19,21–23]. Many multiphase LBMs (not only the color-gradient model) can be affected by this problem. To partially solve it in the color-gradient model, two approaches have been proposed: one using a corrective source term [24], and the other using enhanced equilibrium distribution functions [25]. With the color-gradient model, the simulation of multiphase flow with variable density ratios has also been improved with the introduction of an isotropic gradient operator for the color-gradient [26].