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A mass-conserving lattice Boltzmann method with dynamic grid refinement for immiscible two-phase flows

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ABSTRACT

A mass-conserving lattice Boltzmann method (LBM) for multiphase flows is presented in this paper. The proposed LBM improves a previous model (Lee and Liu, 2010 [21]) in terms of mass conservation, speed-up, and efficiency, and also extends its capabilities for implementation on non-uniform grids. The presented model consists of a phase-field lattice Boltzmann equation (LBE) for tracking the interface between different fluids and a pressure-evolution LBM for recovering the hydrodynamic properties. In addition to the mass conservation property and the simplicity of the algorithm, the advantages of the current phase-field LBE are that it is an order of magnitude faster than the previous interface tracking LBE proposed by Lee and Liu (2010) [21] and it requires less memory resources for data storage. Meanwhile, the pressure-evolution LBM is equipped with a multi-relaxation-time (MRT) collision operator to facilitate attainability of small relaxation rates thereby allowing simulation of multiphase flows at higher Reynolds numbers.
Additionally, we reformulate the presented MRT-LBM on nonuniform grids within an adaptive mesh refinement (AMR) framework. Various benchmark studies such as a rising bubble and a falling drop under buoyancy, droplet splashing on a wet surface, and droplet coalescence onto a fluid interface are conducted to examine the accuracy and versatility of the proposed AMR-LBM. The proposed model is further validated by comparing the results with other LB models on uniform grids. A factor of about 20 in savings of computational resources is achieved by using the proposed AMR-LBM. As a more demanding application, the Kelvin–Helmholtz instability (KHI) of a shear-layer flow is investigated for both density-matched and density-stratified binary fluids. The KHI results of the density-matched fluids are shown to be in good agreement with the benchmark AMR results based on the sharp-interface approach. When a density contrast between the two fluids exists, a typical chaotic structure in the flow field is observed at a Reynolds number of 10000, which indicates that the proposed model is a promising tool for direct numerical simulation of two-phase flows.

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1. Introduction

Sharp-interface and diffuse-interface models [1,2] are commonly used for numerical simulation of multiphase flows. The basic idea behind diffuse-interface models is to spread the interfacial region onto a finite number of grid points, which is typically around $3 \sim 6$ cells, and to employ a continuum (volumetric) force, instead of a singular Dirac δ function, to represent the surface tension. Numerically speaking, diffuse-interface models are preferred over sharp-interface models, particularly in phase-change problems [3], mainly because the computations for complex flows are performed much easier and irregular topological changes are readily captured by solving a phase-field equation. Diffuse-interface models are especially suitable for problems that involve interface disintegration and coalescence and in simulation of contact line dynamics.

Rooted in the kinetic theory, the lattice Boltzmann method (LBM) is a mesoscopic approach for simulation of fluid flows [4–6], and it is favorable because phase interface boundaries are essentially mesoscopic in nature. As a diffuse-interface model, the multiphase LBM has become a well established computational tool for numerical study of nonideal gases and complex fluids [7–11]. Several lattice Boltzmann (LB) models have been implemented and developed by other researchers. Among the existing two-phase LB models [12–21], the pressure-evolution LBM equipped with stencil discretization schemes has proved to be a promising method for studying the fluid dynamics of a variety of phenomena [21,22]. This model is an improved version of the model proposed by He and colleagues [8,16] in that instead of using the Carnahan–Starling equation of state the chemical potential is used. In addition, thanks to stable discretization stencils [18], the pressure-evolution LBM can handle large density differences and suppress spurious velocity currents to the machine precision [22].

The original pressure-evolution LBM, however, has two major drawbacks. First, as pointed out by Guo et al. [23], it suffers from the lack of mass conservation. Second, it is restricted to moderate Reynolds numbers. The lack of mass conservation stems from the force imbalance in the interface tracking equation, which is due to the use of biased finite-difference (FD) scheme in the calculation of the gradient of the composition in the lattice Boltzmann equation (LBE) from which the Cahn–Hilliard equation [23] is derived. On the other hand, using a single-relaxation-time (SRT) collision operator [24] in the pressure-evolution equation for recovering the hydrodynamic properties limits the applicability of the model to relatively small Reynolds numbers.

From the computational point of view, simulation of multiphase flows on small scales is a challenging task. Given that the characteristic interfacial thickness is small and must be resolved by a sufficient number of computational points, higher resolution is required in the vicinity of the interface between different fluids. Solving the governing equations, which are usually in the form of partial differential equations, requires a high-fidelity numerical method. This is complicated by the fact that often we are dealing with high-Reynolds-number flows where higher grid resolution is desired, for example, in the vicinity of the interface between different fluids. Using a structured uniform grid throughout the computation domain could be costly and inefficient. Therefore, adaptive mesh refinement (AMR) techniques are employed.

There are many AMR algorithms proposed in the literature. Berger and co-workers [25,26] utilized rectangular, overlapping grid patches to solve the two-dimensional (2D) hyperbolic equations in the conservative form. De Zeeuw and Powel [27] proposed a 2D AMR scheme with a quad-tree data structure. To overcome the computational overhead of the tree-based approach, a fully threaded tree AMR was developed by Khokhlov [28]. Ji et al. [29] replaced the tree data structure with a hash table and proposed a cell-based AMR. Recently, another AMR algorithm without the need to maintain or modify a tree-type data structure was proposed by Fakhari and Lee [30].

There are also numerous AMR packages available [31–36]. Among them, the Paramesh toolkit [31] is designed to extend an existing serial code for uniform grids to a parallel routine with dynamic grid adaptation. In the author's opinion, however, the Paramesh is not written efficiently. Constructing a parallel AMR algorithm is yet another demanding topic. There is ongoing research in developing AMR algorithms in parallel and optimizing the load balancing techniques associated with them. Interested readers are referred to the comprehensive discourse by Rantakokko and Thuné [37, chap. 5].

The LBM has also been incorporated into the AMR strategy. Tölke et al. [38] proposed an AMR-LBM for simulation of multiphase flows. They invoked a data structure consisted of the hierarchy of tree-type grids. Yu and Fan [39] used the Paramesh toolkit [31] to implement an AMR-LBM for simulation of bubble rising due to buoyancy force. Inspired by the idea proposed in Paramesh, Fakhari and Lee [40] developed a block-structured AMR algorithm for both standard LBM and FD-LBM using the cell-centered data structure.

Most of the existing LB models for interface tracking [41–43] are based on the Cahn–Hilliard (CH) theory [44,45]. As it has been shown recently [46], using the CH equation causes small droplets to disappear once their radius is below a critical value. From the numerical point of view, another undesired feature of the CH models is the calculation of the Laplacian of the chemical potential. This implies the computation of a 4th-order derivative because the Laplacian of the composition or index function is required to compute the chemical potential. Consequently, another class of interface tracking equation, herein called the phase-field equation, is proposed by Sun and Beckermann [47]. The phase-field equation was recently reformulated in the conservative form by Chiu and Lin [48]. It requires only 2nd-order derivatives, which can be reduced to the calculation of 1st-order derivatives, or even no derivatives if central moments are invoked, in the LBM framework [49].

Recently, we developed a conservative phase-field LBE [49] which was more efficient than the original interface-tracking equation proposed in Ref. [21]. In the present study, we will combine the phase-field LBE for interface tracking equation [49] and the pressure-evolution LBM with a multiple-relaxation-time (MRT) collision operator [50,51] to propose a mass-conserving LB model for simulation of two-phase flows at higher Reynolds numbers. In addition, we will extend the recently