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An efficient lattice Boltzmann multiphase model for 3D flows with large density ratios at high Reynolds numbers

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ABSTRACT

We report on the development, implementation and validation of a new Lattice Boltzmann method (LBM) for the numerical simulation of three-dimensional multiphase flows (here with only two components) with both high density ratio and high Reynolds number. This method is based in part on, but aims at achieving a higher computational efficiency than Inamuro et al.'s model (Inamuro et al., 2004). Here, we use a LBM to solve both a pressureless Navier–Stokes equation, in which the implementation of viscous terms is improved, and a pressure Poisson equation (using different distribution functions and a D3Q19 lattice scheme); additionally, we propose a new diffusive interface capturing method, based on the Cahn–Hilliard equation, which is also solved with a LBM. To achieve maximum efficiency, the entire model is implemented and solved on a heavily parallel GPGPU co-processor. The proposed algorithm is applied to several test cases, such as a splashing droplet, a rising bubble, and a braking ocean wave. In all cases, numerical results are found to agree very well with reference data, and/or to converge with the discretization.

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1. Introduction

In recent years, the lattice Boltzmann method (LBM) has become an increasingly attractive, fast, and accurate, alternative modeling method to standard continuum mechanics numerical models, for solving a variety of complex single and multiple-fluid flow problems [1]. Besides its versatility, this is in part due to the LBM's ability to be efficiently parallelized for implementation on General Purpose Graphical Processor Units (GPGPUs). Specifically, it has been shown in various publications [2–4] that LBM methods are especially well-suited for a GPGPU implementation, due to the locality of collision and propagation operators and the explicit nature of the method.

The LBM is based on the Boltzmann equation, which governs the dynamics of molecular probability distribution functions from a microscopic point of view. In the standard LBM implementation, the Boltzmann equation is discretized on an Eulerian mesh, a.k.a. the *lattice*, yielding a numerical method for computing macroscopic distribution functions on the lattice, in which the macroscopic hydrodynamic quantities, such as pressure and velocity, are obtained as low-order moments of these distribution functions [5,1]. To the limit of small time step and grid spacing, the LBM solution can be shown to converge towards the solution of the governing macroscopic equations of continuum mechanics [6]. Hence, with the proper

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selection of the LBM collision operator and distribution functions, the LBM solution can be made to converge to that of the Navier–Stokes equations (NS), including in the presence of a free surface (e.g., Janssen et al. [7]). The explicit nature of the method and the linear formulation of advection terms in the LBM collision–propagation equation provide the numerical scheme with several advantages, such as: (i) a relatively easy implementation (as far as uniform grids are concerned); and (ii) the locality of numerical operators, which allows for a more efficient parallel implementation, particularly on GPGPUs, than for more traditional finite volume of finite element algorithms. These characteristics have made the LBM a widely used tool for solving various complex fluid mechanics problems, such as multiphase flows, micro- and nanoscale flows, flows in porous media, and other fluid flow types [8,9,1].

Although many studies of multiphase flows using the LBM have been reported [10,11], most of these had two significant limitations: (i) the maximum density ratio between fluids is typically limited to 5–10, due to the triggering of local instabilities near the fluid-phase interface for larger ratios; (ii) most of the schemes cannot simulate high Reynolds number flows, due to instabilities resulting from the low relaxation times required for high Reynolds numbers (Re). The effects of either one of these problems are sufficient to make simulations unstable, even in the absence of the other problem.

The practical applications that motivated this research deal with air–sea interactions at the ocean surface in high wind conditions, hence with turbulent (i.e., very large Re values around 10^8) two-fluid flows with a high density ratio (order 1000). Hence, our main goal has been to develop an efficient LBM model that overcame these two limitations.

Several LBM studies of multiphase flows with a high density ratio have been proposed; Zheng et al. [12] proposed an LBM scheme for high density ratio, but in their work they used an artificial density ratio defined as the mean of densities of two fluid system. The deficiencies and limitations of their work have been explained in [13,14]. Two promising concepts were proposed by Lee et al. [8] and Inamuro et al. [9]. Lee et al. [8] used an approach similar to that of He et al. [15], in which they transformed the classical single phase discrete Boltzmann equation, from a mass–momentum to a pressure–momentum formulation. This decreased potential instabilities that could occur due to large fluid density gradients near the phase interface. Also, they split up the intermolecular forces for a non-ideal gas into hydrodynamic pressure, thermodynamic pressure, and surface tension force contributions. They reported that "parasitic currents" at the phase interface affected the numerical results due to the imbalance between thermodynamic pressure and surface tension forces, resulting from truncation errors related to curvature computations. They nearly eliminated this problem by using a thermodynamic identity to recast the intermolecular forcing term from a stress to a potential formulation. Furthermore, to stabilize their numerical scheme for large density ratios, they used different discretization patterns (i.e., central, biased and mixed differences) at different stages of the simulations. With this scheme, they were able to simulate two-phase flows with density ratio up to 1000. However, they could not achieve high Reynolds numbers, because stability issues related to low relaxation times were not addressed, and in their scheme relaxation time was still a function of the Reynolds number. To eliminate the numerical instabilities resulting from high density ratios, Inamuro et al. [9] removed the density from the advection part of the LBM equilibrium distribution functions. This in effect eliminated the pressure gradient from the corresponding macroscopic momentum equation, which thus became a "pressureless" NS equations. To retrieve the complete momentum equations and satisfy mass conservation, they subsequently corrected the velocity field by solving a Poisson equation for the pressure field. In their method, unlike in classical LBMs, the fluid viscosity is no longer related to the relaxation time and hence results stay more stable at high Reynolds numbers. Finally, in Inamuro et al.'s method, viscous effects are modeled by specifying the viscous stress tensor as a body force in the LBM collision operator. Proceeding this way, however, yields additional non-physical terms in the corresponding momentum equation, which decreases the model accuracy. In earlier work [5], we modified Inamuro et al.'s method to solve two-dimensional (2D) two-phase flows with high density ratio, by removing the non-physical terms from the momentum equation and formulating the phase interface tracking equations in a more rigorous way, based on the Cahn–Hilliard equations [16]. Additionally, we efficiently implemented our model for a massively parallel solution on a GPGPU. In doing so, we solved all the governing equations for each fluid, the interface, and the Poisson equation (required for correcting the velocity field) with a LBM scheme, thus achieving an even higher computational efficiency on the GPGPU. Our method, however, only worked for low Reynolds number flows.

In this paper, in light of this earlier work, we develop a new three-dimensional (3D) LBM model, also based on Inamuro et al.'s [9] approach. As before, we introduce new equilibrium distribution functions to both retrieve NS equations and improve the formulation of surface tension and viscous forces. For the interface capturing part, as in [5], we solve the Cahn–Hilliard equation using a LBM scheme with improved equilibrium distribution functions. In this new 3D model, however, we formulate the latter functions to be able to achieve high Reynolds numbers in the applications without suffering from instability problems. The resulting numerical scheme is computationally demanding, as the Poisson equation must be (iteratively) solved for each time step of the solution, in order to obtain the velocity field correction terms. As before, to achieve high computational efficiency, our LBM code is parallelized and implemented on a GPGPU using the nVIDIA CUDA framework. This approach provides access to the latest generation of GPGPU boards, such as the nVIDIA Tesla C2070 that was used in the present work (448 computing cores; 6 GB of memory; and a double precision computing capability).

The paper is organized as follows. We first develop the LBM equations used to solve for multiphase flows with high density ratios and detail their numerical implementation. The method is then validated for a series of applications, by comparing the present numerical results to reference solutions, for the splashing of droplets on a thin fluid layer, for a rising bubble, and for breaking ocean waves. Finally, we draws some conclusions and provide perspectives for future work.

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