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Density fluctuations in lattice-Boltzmann simulations of multiphase fluids in a closed system

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Abstract

A two-dimensional single component two-phase lattice Boltzmann model was used to simulate the Rayleigh–Taylor instability in a closed system. Spatiotemporally variable densities were generated by gravity acting on the fluid density. The density fluctuations were triggered by rapid changes in the fluid velocity induced by changes in the interface geometry and impact of the dense fluid on the rigid lower boundary of the computational domain. The ratio of the maximum density fluctuations to the maximum fluid velocity increased more rapidly at low velocities than at high velocities. The ratio of the maximum density fluctuations in the dense phase to its maximum velocity was on the order of the inverse of the sound speed. The solution became unstable when the density-based maximum local Knudsen number exceeded 0.13.

Keywords: Multiphase flow; Lattice-Boltzmann; Density fluctuations

1. Introduction

The lattice-Boltzmann (LB) method is a mesoscale simulation technique that lies between microdynamics at a molecular scale and the macroscopic continuum mechanics of fluids [1–3]. In LB models, the fluid is represented as an ensemble of particles that synchronously stream along the bonds of a regular lattice and undergo mass and momentum conserving collisions at the nodes. The microdynamic conservation principles that govern the collisions ensure the local conservation of mass and momentum, which is essential for the macroscopic behavior to be consistent with the Navier–Stokes equation. Because the LB method is based on a microscopic description of fluid dynamics, large-scale hydrodynamics emerges naturally [4], and the interfacial dynamics in multiphase systems can be simulated more easily by using LB models [5,6] than by using conventional grid-based Navier–Stokes solvers. In multiphase LB simulations, problems such as interface

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broadening and grid entanglement are avoided; however, the interface is spread over a few lattice nodes. In this article we focus on the simulation of two-dimensional multiphase flow in a closed system using an LB model that includes the fluid–fluid interactions proposed by Shan and Chen [6] and the solid–fluid interactions proposed by Martys and Chen [5]. Macroscopic equations governing the motion of each component in the Shan–Chen model have been derived [4] using the Chapman–Enskog method [7]. A one-component two-phase formulation of the Shan–Chen model has been used to simulate bubble growth on, and detachment from, horizontal and vertical surfaces [8], to study two-phase flow in a two-dimensional homogeneous and regularly packed synthetic porous system [9], and to simulate interfacial configurations in partially-saturated porous media [10].

The LB method can be used to simulate single-phase flow governed by the incompressible Navier–Stokes equation in the limit in which temporal variations in the fluid density are small. The fluid density is related to the pressure through the square of the sound velocity, c_s, and a finite c_s^2 (which is a characteristic of all LB models) introduces density fluctuations. However, the density fluctuations associated with multiphase flows are much larger than the density fluctuations associated with the single-phase flows with similar characteristic velocities, because of the large rates of change in velocity and momentum density when fluid impact on solid surfaces and/or capillary barriers are overcome leading to Haines jumps [11]. The purpose of this article is to investigate the relationships between the average density fluctuations in the dense fluid and its spatially-averaged velocity when the fluids were acted on by gravity with different strengths in a closed system, and to relate the findings to the velocity of the sound (density) waves before and after the dense fluid contacts the rigid boundaries of the flow domain.

2. Lattice–Boltzmann method (LBM)

LB models are based on a discrete microscopic population distribution function and the microdynamics of the LB model with a single relaxation time (BGK) model [12] is described by

$$f_k(\mathbf{x}+\mathbf{e}_k\Delta t, t+\Delta t) - f_k(\mathbf{x}, t) = \frac{f_k^{eq}(\mathbf{x}, t) - f_k(\mathbf{x}, t)}{\tau}, \tag{1}$$

where $f_k(\mathbf{x}, t)$ is the population density at the lattice node at position $\mathbf{x}$ at time t along the velocity vector $\mathbf{e}_k$, f_k^{eq} is the equilibrium Maxwell–Boltzmann distribution function, τ is the relaxation parameter, and Δt is the time increment. A 2D 9-velocity (D2Q9) model was used in this study. The discrete velocity vector basis for the D2Q9 model consists of the null vector, four vectors of length unity directed towards the nearest neighbor nodes, and four vectors of length $\sqrt{2}$ directed towards the next-nearest neighbor nodes. The discrete equilibrium Maxwell–Boltzmann distribution is approximated by the low-Mach number mass and momentum conserving expansion [13]:

$$f_k^{eq} = w_k\rho\left(1 + \frac{\mathbf{e}_k\cdot\mathbf{u}}{c_s^2} + \frac{(\mathbf{e}_k\cdot\mathbf{u})^2}{2c_s^4} - \frac{\mathbf{u}\cdot\mathbf{u}}{2c_s^2}\right), \tag{2}$$

where w_k is the weight coefficient for the kth vector (4/9 for the null vector, $\frac{1}{9}$ for the nearest neighbor vectors and $\frac{1}{36}$ for the next-nearest neighbor vectors). The local macroscopic density and velocity at a lattice site can be computed from the distribution functions at that site as $\rho = \sum_{k=0}^{8} f_k$ and $\rho\mathbf{u} = \sum_{k=0}^{8} f_k\mathbf{e}_k$. With the equilibrium distribution in Eq. (2), the Navier–Stokes equations can be recovered through a Chapman–Enskog expansion, which shows that the kinematic viscosity of the fluid is $v = c_s^2(\tau - \frac{1}{2})$, and the sound velocity is $c_s = 1/\sqrt{3}$ in lattice units, when $\Delta x = \Delta t = 1$.

First-order phase separation processes can be incorporated into the LBM by modifying the net momentum at the lattice sites to represent the effects of density dependent fluid–fluid interaction forces. Such interactions can be simulated by introducing fluid–fluid interactions that involve only neighboring nodes separated by a distance of $|\mathbf{e}_k|$ (when $\Delta t = 1$). The resulting rate of momentum change at each lattice site for a two-phase