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Evaluation of the finite element lattice Boltzmann method for binary fluid flows

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ABSTRACT

In contrast to the commonly used lattice Boltzmann method, off-lattice Boltzmann methods decouple the velocity discretization from the underlying spatial grid thereby potentially increasing the geometric flexibility of the method. The current work combines characteristic-based integration of the streaming step with the free-energy based multiphase model by Lee and Lin (2005). This allows for simulation time steps more than an order of magnitude larger than the relaxation time. Unlike previous work by Wardle and Lee (2013) that integrated intermolecular forcing terms in the advection term, the current scheme applies collision and forcing terms locally for a simpler finite element formulation. A series of thorough benchmark studies reveal that this does not compromise stability and that the scheme is able to accurately simulate flows at large density and viscosity contrasts.

1. Introduction

The lattice Boltzmann method has become popular as a numerical solver for multiphase flows. Several models have been proposed in the literature during the last two decades that can generally be classified into four categories: The chromodynamic model by Gunstensen et al. [1,2] which was used for the earliest simulations, the phenomenological interparticle-potential model by Shan and Chen [3,4], the free-energy model by Swift et al. [5] and the mean-field model by He et al. [6,7] were based on the kinetic theory for dense fluids. With the exception of the latter, these models are restricted to Boussinesq flows in their original formulations, a limit which has been pushed by the many recent developments described in several reviews, see *e.g.* [8–10].

In addition to these four categories, more recent development by Mazloomi et al. has applied the entropic lattice Boltzmann stabilization mechanism to multiphase flows including fluid–solid interactions [11,12]. This enables simulations of real-world phenomena such as binary droplet collisions [13,14].

1.1. Overview

Simulating binary flows beyond the Boussinesq approximation is generally a challenging issue due to the sharp changes in density across the interface. In an attempt to remedy this, He et al. [6] introduced an incompressible transformation in their kinetic model, changing the particle distribution function for mass and momentum into that for hydrodynamic pressure and

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momentum. Adding to this transformation, Lee and Lin [15] enhanced stability of their free-energy based model by adopting the stress form of the surface tension force for the pressure–momentum lattice Boltzmann equation (LBE) and the potential form of the surface tension force for the LBE of the order parameter. They furthermore introduced discretization schemes that comply with the second-order accuracy of the lattice Boltzmann method, and their model has recently been augmented to allow arbitrary wetting properties of the two phases [16]. All of the above models have been shown to produce stable and accurate results for density ratios of up to 1000 and viscosity ratios up to 60. Here, we shall consider further the model of Lee and Lin [15].

1.2. Off-lattice Boltzmann methods

The traditional, regular-grid based setting limits the application of the lattice Boltzmann method to uniform Cartesian grids. However, extensions have been made to irregular grids by introducing a class of off-lattice Boltzmann schemes consisting of finite volume [17,18] and finite element schemes [19,20]. Inherent to all of these is the standard Courant–Friedrichs–Lewy (CFL) condition on the time step δt, a necessary condition for the stability of any kind of advection equation. Certain schemes employ an explicit treatment of the collision term, thereby imposing the more restrictive condition $\delta t < 2\tau$ for forward Euler time integration and $\delta t < \tau$ for Strang splitting, where τ is the relaxation time [21–23].

Characteristic-based schemes generally tend to provide better numerical stability compared to other time-integration schemes such as Runge–Kutta [24] and furthermore allow for implicit integration of the collision term. This property is utilized in [19] to allow for CFL numbers up to 100 at the expense of increased computation time per time step by employing an iterative solver for the implicit term. In more recent work a variable transformation is often employed that masks the implicitness while preserving mass and momentum conservation [20,25,26]. Combining this with explicit, second-order accurate time integration, Bardow et al. [20] successfully overcome the restrictive time step condition.

The current work applies the BGK-collision and forcing locally in the collision step. This simplifies the scheme, yet still allows for time steps more than an order of magnitude larger than the relaxation time when combined with explicit, second-order accurate advection along characteristics.

2. Numerical method

2.1. Lattice Boltzmann method

The current study uses the model initially presented in [15] in three dimensions, which introduces two particle distribution functions f_α and g_α. The distribution function f_α recovers the order parameter (density) that tracks the interface between the two different phases and g_α recovers the hydrodynamic flow fields (pressure and momentum) of the two fluids. As the two distribution functions have different purposes, the stress and potential forms of the surface tension force are selectively adopted to match their roles.

Integrating the governing discrete Boltzmann equation for f_α and g_α over a time step δt and applying the trapezoidal rule leads to [15]

$$f_\alpha(x_i + e_{\alpha i}\delta t, t + \delta t) - f_\alpha(x_i, t) = +(-\Omega_{f_\alpha} + F_\alpha)|_{(x_i,t)} + (-\Omega_{f_\alpha} + F_\alpha)|_{(x_i+e_{\alpha i}\delta t, t+\delta t)} \tag{1}$$

and

$$g_\alpha(x_i + e_{\alpha i}\delta t, t + \delta t) - g_\alpha(x_i, t) = +(-\Omega_{g_\alpha} + G_\alpha + \mathcal{G}_\alpha)|_{(x_i,t)} + (-\Omega_{g_\alpha} + G_\alpha + \mathcal{G}_\alpha)|_{(x_i+e_{\alpha i}\delta t, t+\delta t)} \tag{2}$$

where the intermolecular forcing terms F_α and G_α and the BGK-operator Ω_{ψ_α} for a given distribution function $\psi \in \{f, g\}$ are given by

$$\Omega_{\psi_\alpha} = +\frac{1}{2\tau}(\psi_\alpha - \psi_\alpha^{\mathrm{eq}}) \tag{3}$$

$$F_\alpha = +\frac{\delta t}{2}\frac{(e_{\alpha i} - u_i)[\partial_i \rho c_s^2 - \rho\partial_i(\mu_\varphi - \kappa\partial_k\partial_k\rho)]}{c_s^2}\Gamma_\alpha(u_i) \tag{4}$$

$$G_\alpha = +\frac{\delta t}{2}\frac{(e_{\alpha i} - u_i)\partial_i\rho c_s^2}{c_s^2}[\Gamma_\alpha(u_i) - \Gamma_\alpha(0)] + \frac{\delta t}{2}\frac{(e_{\alpha i} - u_i)[\kappa\partial_i(\partial_k\rho\partial_k\rho) - \kappa\partial_j(\partial_i\rho\partial_j\rho)]}{c_s^2}\Gamma_\alpha(u_i) \tag{5}$$

and $\mathcal{G}_\alpha$ is a volumetric body force. Here $e_{\alpha i}$ denote the 19 discrete particle velocities in directions α of the D3Q19 model, $c_s = 1/\sqrt{3}$ the constant speed of sound, u_i the macroscopic velocity, ρ the mixture density and μ_φ the chemical potential. The dimensionless relaxation parameter τ is proportional to the kinematic viscosity ν through $\nu = c_s^2\tau\delta t$. The equilibrium distribution functions f_α^{eq} and g_α^{eq} are given by

$$f_\alpha^{\mathrm{eq}} = w_\alpha\rho\left[1 + \frac{e_{\alpha i}u_i}{c_s^2} + \frac{(e_{\alpha i}e_{\alpha j} - c_s^2\delta_{ij})u_iu_j}{2c_s^4}\right] \tag{6}$$

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