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Axisymmetric multiphase lattice Boltzmann method for generic equations of state

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A B S T R A C T

We present an axisymmetric lattice Boltzmann model based on the Kupershtokh et al. multiphase model that is capable of solving liquid–gas density ratios up to 10^3. Appropriate source terms are added to the lattice Boltzmann evolution equation to fully recover the axisymmetric multiphase conservation equations. We validate the model by showing that a stationary droplet obeys the Young–Laplace law, comparing the second oscillation mode of a droplet with respect to an analytical solution and showing correct mass conservation of a propagating density wave.

1. Introduction

The lattice Boltzmann method (LBM) [1,2] is an efficient numerical tool to solve the Navier–Stokes equations. This numerical method can be systematically derived from the Boltzmann equations by means of a Hermite expansion approach [3]. In many physically realistic flow problems one has to deal with multiphase flows such as the contact angle hysteresis of a moving droplet on a surface, a capillary rise in a cylindrical tube and droplet impact on solid surfaces. To this end, several extensions have been proposed to support multiphase flows in the LBM. In an early attempt, Gunstensen et al. [4] studied a two-component fluid lattice-gas method. Shan et al. [5,6] were the first to incorporate intermolecular interactions to achieve phase separation in LBM. A different approach to model a multiphase fluid was developed by Swift et al. [7], who associated a free energy functional to the fluid. In their original form, these models lack the ability to achieve high density ratios across fluid interfaces and suffer from spurious currents near the liquid–vapor interface. In many engineering applications density ratios range from $10^1 to 10^3$, posing a serious limitation to the applicability of these lattice Boltzmann models in their original form. Recently, Lee et al. [8] showed that the spurious currents are caused by discretization errors in the computation of the multiphase force. These spurious currents can be reduced to machine precision by employing a potential form of the non-ideal pressure and a isotropic central difference approximation scheme for the multiphase force. Kupershtokh et al. [9] showed that it is possible to achieve density ratios of 10^6 when the multiphase force is discretized by just a single-neighbour discretization scheme. The ability to achieve high density ratios makes this model applicable to many engineering applications. However, in this scheme the surface tension cannot be varied independently and spurious currents still exist.

Recently the LBM was extended to support axisymmetric multiphase flows. These axisymmetric simulations are effectively 2D simulations in a cylindrical coordinate system. Therefore, the computational cost for axisymmetric 3D flow problems is significantly lower in comparison to the same problem in a full 3D simulation. Halliday et al. [10] was the first to implement an axisymmetric LBM for single-phase flows. They introduced additional source and sink terms to the evolution equation and showed that they recover the 2D axisymmetric Navier–Stokes equations. This model was improved by Lee et al. [11] who corrected a missing source term related to the radial velocity. In addition, the method of Halliday et al. was extended to support non-ideal flows. Premnath et al. [12] were the first to implement an axisymmetric multiphase LBM. Their model is able to achieve density ratios up to 10 and was further improved by Mukherjee et al. [13] to support density ratios up to 10^3 and perform stable computations at lower viscosities. In this improved model, they use a pressure-evolution based LBM combined with a multiple-relaxation-time (MRT) collision model. Another axisymmetric multiphase LBM model by Srivastava et al.

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[14] is based upon the widely used Shan–Chen model. In this model, they add an extra contribution to the Shan–Chen multiphase force to fully recover three-dimensionality in the system. However, large density ratios (>30) could not be achieved due to the limits of the original Shan–Chen model.

In this paper, we introduce a novel and easy-to-implement axisymmetric isothermal multiphase model for high density ratio fluids. The proposed model is based on the axisymmetric LBM of Srivastava et al. [14] combined with the multiphase model of Kupershtokh et al. [9]. The combined model inherits all advantages and disadvantages of the existing multiphase model by Kupershtokh et al., which we will not discuss in detail here. An extensive study to the accuracy and stability of the Kupershtokh et al. multiphase method can be found in [15]. Our implementation is discussed in Section 2. In Section 3 we present three validation tests. First, we verify that a stationary droplet obeys the Young–Laplace law. Then, we compare the second oscillation mode of an oscillating droplet with an incompressible analytical solution. Finally, we show that the method correctly describes the propagation of a density wave towards and away from the longitudinal z-axis. Our main conclusions and limitations of the method are discussed in Section 4.

2. Model derivation

We first introduce the standard LBM. In the following subsections, we will gradually show the changes necessary to obtain a fully functional axisymmetric isothermal multiphase LBM.

2.1. The lattice Boltzmann method

We use the common D2Q9 LBM, based on a two-dimensional Eulerian lattice with nine velocities. For the time evolution of the distribution function f_i, we use the BGK approximation with a single relaxation parameter τ [2]. The time evolution is given by

$$f_i(\boldsymbol{x}+\boldsymbol{e}_i\delta t, t+\delta t) = f_i(\boldsymbol{x}, t) + \frac{\delta t}{\tau}(f_i^{\mathrm{eq}}(\boldsymbol{x}, t) - f_i(\boldsymbol{x}, t)) + \delta t S_i(\boldsymbol{x}, t), \quad (1)$$

where $\boldsymbol{x}$ is the position, t is the time, δt is the time step, τ is the relaxation time, $S_i(\boldsymbol{x}, t)$ is a source term, f_i^{eq} is the local equilibrium distribution and $\boldsymbol{e}_i$ is a discrete velocity set given by

$$\boldsymbol{e}_i = \begin{cases} (0,0) & i=0, \\ (1,0)_{\mathrm{FS}} & i=(1,2,3,4), \\ (\pm 1, \pm 1) & i=(5,6,7,8), \end{cases}$$

where the subscript $_{\mathrm{FS}}$ denotes a fully symmetric set of points. The local equilibrium distribution function f_i^{eq} is a second-order Taylor expansion of the Maxwell–Boltzmann distribution [2] and is given by

$$f_i^{\mathrm{eq}}(\boldsymbol{x}, t) = w_i\rho(\boldsymbol{x}, t)\left[1 + \frac{1}{c_s^2}(\boldsymbol{e}_i\cdot\boldsymbol{u}(\boldsymbol{x}, t)) + \frac{1}{2c_s^2} \times \left(\frac{1}{c_s^2}(\boldsymbol{e}_i\cdot\boldsymbol{u}(\boldsymbol{x}, t))^2 - ||\boldsymbol{u}(\boldsymbol{x}, t)||^2\right)\right], \quad (2)$$

where $c_s^2 = 1/3$ is the lattice speed of sound in this single-phase model and w_i are the quadrature weights given by

$$w_i = \begin{cases} 4/9 & i=0, \\ 1/9 & i=(1,2,3,4), \\ 1/36 & i=(5,6,7,8). \end{cases}$$

The hydrodynamic quantities of the fluid, such as density ρ and velocity $\boldsymbol{u}$ are calculated as weighted sums of the distribution function f_i

$$\rho(\boldsymbol{x}, t) = \sum_i f_i(\boldsymbol{x}, t), \quad (3)$$

$$\boldsymbol{u}(\boldsymbol{x}, t) = \frac{\delta t\boldsymbol{F}(\boldsymbol{x}, t)}{2\rho(\boldsymbol{x}, t)} + \sum_i \frac{\boldsymbol{e}_i f_i(\boldsymbol{x}, t)}{\rho(\boldsymbol{x}, t)}, \quad (4)$$

where $\boldsymbol{u}(\boldsymbol{x}, t)$ is shifted by means of an internal/external force $\boldsymbol{F}$. In the past, different implementations of a body force, $\boldsymbol{F}$, were proposed [16]. Here we use the forcing scheme by Guo et al. [17]

$$S_i(\boldsymbol{x}, t) = w_i\left(1 - \frac{\delta t}{2\tau}\right)\left(\frac{(\boldsymbol{e}_i - \boldsymbol{u})\cdot\boldsymbol{F}}{c_s^2} + \frac{(\boldsymbol{e}_i\cdot\boldsymbol{u})(\boldsymbol{e}_i\cdot\boldsymbol{F})}{c_s^4}\right). \quad (5)$$

2.2. The extension to an axisymmetric method

In an axisymmetric flow (Fig. 1), there is no flow in the azimuthal direction ($u_\theta = 0$) and mass conservation reads

$$\frac{\partial\rho}{\partial t} + \nabla_{\mathrm{c}}\cdot(\rho\boldsymbol{u}) = -\frac{\rho u_r}{r} \quad (6)$$

where $\nabla_{\mathrm{c}} \equiv (\partial/\partial z, \partial/\partial r)$ is the gradient operator in a two-dimensional Cartesian coordinate system ($x \to z$, $y \to r$) and $\boldsymbol{u} = (u_z, u_r)$ is the fluid velocity. The momentum equation reads

$$\rho\left(\frac{\partial\boldsymbol{u}}{\partial t} + \boldsymbol{u}\cdot\nabla_{\mathrm{c}}\boldsymbol{u}\right) = -\nabla_{\mathrm{c}}P + \mu\nabla_{\mathrm{c}}\cdot[\nabla_{\mathrm{c}}\boldsymbol{u} + \nabla_{\mathrm{c}}\boldsymbol{u}^{\mathrm{T}}] + \boldsymbol{C} \quad (7)$$

where P is the fluid pressure which in a single-phase LBM is given by $P = c_s^2\rho$ and $\boldsymbol{C}$ is given by

$$C_z = \frac{\mu}{r}\left(\frac{\partial u_z}{\partial r} + \frac{\partial u_r}{\partial z}\right), \quad C_r = 2\mu\frac{\partial}{\partial r}\left(\frac{u_r}{r}\right), \quad (8)$$

with μ the fluid viscosity. It is clear that Eqs. (6) and (7) have additional contributions to the mass and momentum conservation equations in comparison to 2D flow in the (z, r)-plane. These contributions ensure local conservation of mass and momentum when fluid is moving towards or away from the longitudinal z-axis. The single-phase LBM can be supplemented with appropriate source-terms to recover the axisymmetric conservation Eqs. (6) and (7) [14]. To this end, the evolution Eq. (1) is rewritten with an additional source term h_i

$$f_i(\boldsymbol{x}+\boldsymbol{e}_i\delta t, t+\delta t) = \frac{\delta t}{\tau}(f_i^{\mathrm{eq}}(\boldsymbol{x}, t) - f_i(\boldsymbol{x}, t)) + f_i(\boldsymbol{x}, t) + \delta t S_i(\boldsymbol{x}, t) + \delta t h_i\left(\boldsymbol{x} + \boldsymbol{e}_i\frac{\delta t}{2}, t + \frac{\delta t}{2}\right). \quad (9)$$

where h_i is evaluated at fractional time steps. Srivastava et al. [14] showed by means of a Chapman–Enskog (CE) expansion that when h_i has the following form

$$h_i = w_i\left(-\frac{\rho u_r}{r} + \frac{1}{c_s^2}(e_{iz}H_z + e_{ir}H_r)\right), \quad (10)$$

with $\boldsymbol{e}_i = (e_{iz}, e_{ir})$ and

$$H_z = \frac{e_{iz}}{r}\left(\mu\left(\frac{\partial u_z}{\partial r} + \frac{\partial u_r}{\partial z}\right) - \rho u_r u_z\right), \quad (11a)$$

$$H_r = \frac{e_{ir}}{r}\left(2\mu\left(\frac{\partial u_r}{\partial r} + \frac{u_r}{r}\right) - \rho u_r^2\right), \quad (11b)$$

the resulting LBM solves the axisymmetric conservation equations given by (6) and (7) in the limit of small Mach number. The velocity derivatives inside (11) are approximated by a isotropic fifth-order