Exploring the accuracy of the Lattice Boltzmann method

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Abstract. Lattice Boltzmann method is a mesoscopic method used for solving hydrodynamics problems of both incompressible and compressible fluids. Although the method is widely used, reliability of the results is unclear. Therefore, we use the method to solve a fundamental problem with a known analytical solution, the Couette flow. We estimate the accuracy of the simulation results obtained by setting different types of spatial grids, boundary conditions, and equilibrium distribution functions. However, the method imposes restrictions on a large number of simulation parameters such as Reynolds and Mach numbers. During simulation we discovered an unexpected behavior of the solution using classical lattice Boltzmann method. In these simulations we find that the conservation law is violated due to an unexpected inflow in the upper corners of the computational domain.

1. Introduction

Fluid dynamics can be described by three main types of approaches: macro-, micro-, and mesoscopic methods. The macroscopic approach relies on the Navier-Stokes equations, where the fluid is treated as a continuous medium characterized by velocity and density fields. Microscopic methods, of which molecular dynamics is a prime example, work on the molecular level, where individual molecules follow the Newtonian dynamics [1].

The lattice Boltzmann method (LBM) is a mesoscopic method, formulated in terms of a distribution of particles in the computational domain. It is derived from Boltzmann transport equation through discretization in velocity space (see e.g., [2, 3] and references therein). The method is extremely effective in solving complex flows, for example, high-speed compressible flows [8] and incompressible multiphase flows [9], and complex geometries, such as corrugated channel [10] and spherical obstacles [11]. However, since LBM involves uncontrollable approximations, precise reliability of LBM results is not always clear-cut.

In this paper, we test the method on a Couette flow problem where the fluid flows in a channel with a moving upper boundary [1]. We choose the Couette flow problem as it is a textbook problem with a known analytical solution. In our simulations, we compare LBM solutions with different boundary conditions to the analytic solution. We find that a naive approach violates the conservation laws, and suggest a way of solving this issue.

2. The Lattice Boltzmann method

Assuming that \( f_i(\mathbf{x}, t) \) is the particle distribution function in \( i \)-th direction, we can write the lattice Boltzmann equation using a standard Bhatnagar-Gross-Krook (BGK) collision operator...
\[ f_i(x + c_i \Delta t, t + \Delta t) = f_i(x, t) - \frac{f_i(x, t) - f_{i,eq}(x, t)}{\tau} \Delta t. \]

Here \( c_i \) is discrete velocity and \( \tau \) is relaxation time.

We obtain the discrete equilibrium distribution function \( f_{i,eq}(x, t) \) from a continuous Maxwell distribution function by decomposing it in terms of Hermite polynomials. We perform numerical simulations using equilibrium distribution functions with one and two expansion terms

\[ f_{i,eq}(x, t) = w_i \rho \left[ 1 + \frac{u \cdot c_i}{c_s^2} \right] + w_i \rho \left[ \frac{(u \cdot c_i)^2}{2c_s^4} - \frac{u \cdot u}{2c_s^2} \right], \]

where \( w_i \) is the weight corresponding to the velocity \( c_i \), \( u \) is the local speed of the fluid, and \( c_s \) is the speed of sound in a fluid during an isothermal process [5].

We use a D2Q9 set of discrete velocities \( c_i \) and weights \( w_i \).

Solving the LBM equation is a repeated application of two steps:

(i) collision

\[ f_i^*(x, t + \Delta t) = f_i(x, t) \left( 1 - \frac{\Delta t}{\tau} \right) + f_{i,eq}(x, t) \frac{\Delta t}{\tau}, \]

(ii) propagation

\[ f_i(x + c_i \Delta t, t + \Delta t) = f_i^*(x, t + \Delta t). \]

**Boundary conditions**

In this study we use three different approaches to specifying the boundary conditions. In the flow direction, we use periodic boundary conditions at the left-hand and right-hand boundaries of the computation domain. Periodic boundary conditions are implemented at the propagation step.

For approximating the boundary conditions on solid walls (top and bottom sides of the computational domain), we use two different approaches: link-wise bounce-back method and wet-node bounce-back method.

In the link-wise bounce-back method, [3] (also known as a mid-grid method in Ref. [2]) the interface between the solid wall and the fluid is between the grid nodes. The crux of this method is that particles that hit the boundary should bounce back to their previous position. In this case

\[ f_i(x_b, t) = f_i^*(x_b, t) - 2w_i \rho_b \frac{c_i \cdot u_b}{c_s^2}, \quad c_i = -c_i, \]

where \( x_b \) are the nodes closest to the physical interface, \( \rho_b \) can be substituted by \( \langle \rho \rangle \) or \( \rho(x_b) \).

An alternative approach is the so-called wet-node bounce-back method [3] (also called the on-grid method in Ref. [2]). Here, we introduce the grid so that the boundary nodes lie as close as possible to the physical interface. First of all, we calculate the density of the fluid on the boundary, and then its distribution on the boundary. We determine the density from the solid wall condition. We find the distribution function on boundary through its nonequilibrium part [4]:

\[ f_{i,neq}(x_b, t) = f_{i,neq}(x_b, t) - \frac{e_b \cdot c_i}{c} N_t, \]

where \( N_t \) is the tangential momentum, \( e_b \) is a unit velocity vector directed along the boundary, and \( f_{i,neq}(x_b, t) = f_i(x_b, t) - f_{i,eq}(x_b, t) \).
3. Numerical experiments

We developed software and implemented the link-wise and wet-node boundary conditions to solve the Couette flow problem [1] where an incompressible fluid is located in a flat vessel with a height of $d$, the lower boundary of the vessel is stationary, and the upper boundary moves at a constant speed $u_0$. This problem has an analytical solution

$$u_x(y) = \frac{u_0}{d} y, \quad u_y = 0.$$  

We note that the link-wise method is known to be stable when the relaxation time $\tau \geq 0.5$ [5].

We compare the standard deviation of $u_x$. Numerical experiments show that adding new expansion terms in the equilibrium distribution function does not improve the accuracy of the method. The wet-node and link-wise methods provide the same solutions to this problem.

![Figure 1. Numerical and analytical solutions of the Couette flow problem for link-wise and wet-node methods and different equilibrium distribution functions.](image)

**Figure 1.** Numerical and analytical solutions of the Couette flow problem for link-wise and wet-node methods and different equilibrium distribution functions.

We find that the wet-node bounce-back method requires slightly less iterations to solve the Couette flow to a given accuracy.

We checked the stability and conservativity of the methods as well.

![Figure 2. Number of iterations for link-wise and wet-node methods.](image)

**Figure 2.** Number of iterations for link-wise and wet-node methods.
4. Palabos

There are several open source and commercial frameworks which implement the LBM methods. In the rest of that paper we use the Palabos open source library [6]. The input parameters are dimensionless values of the velocity \( \tilde{u}_0 \), the relaxation frequency (inverse relaxation time) \( \omega \), the sizes of the area \( l_x \) and \( l_y \), the size of the spatial grid \( N \), and the Reynolds number \( Re \).

We simulate the flow in a wide range of Reynolds and Mach numbers. We analyze the solution obtained for the following values of parameters:

\[
\tilde{u}_0 = 0.01, \quad Re = 1.5, \quad N = 100, \quad \omega = 0.4, \quad l_x = 2, \quad l_y = 1.
\]

The Palabos library allows us to solve this problem with the standard deviation \( err = 1.1 \cdot 10^{-3} \). Despite the high accuracy of the solution, there are some unexpected results, which we concentrate on in the next section.

4.1. Conservativity

In our simulations, we investigate the accuracy of the method as well as its conservativity. To check the fulfillment of conservation laws, we expanded the simulation time up to \( T = 100 \). We checked that simulations conserve energy, with the dimensionless total energy being \( \epsilon = 1.7 \cdot 10^{-5} \).

However, the conservation of the mass is violated: there is a slight increase of the overall density with time, see Fig. 4. In fact, the total density is linearly increasing. Zooming into the computational area, the mechanism of the violation of the conservation law is an unexpected inflow into the upper corners of the simulation domain (i.e. the corners where the moving wall meets the boundaries with periodic boundary conditions).
4.2. Skordos boundary conditions

This problem was solved by using the Skordos boundary conditions as implemented in Palabos [7]. The method is using an extended version of numerical equilibrium distribution function on simulated interface

\[ f_{eq}^*(\mathbf{x}, t) = f_{eq}(\mathbf{x}, t) + w_1 (\mathbf{c}_i \cdot \nabla (\mathbf{c}_i \cdot \rho \mathbf{v})) + w_2 (\nabla \cdot \rho \mathbf{v}). \]

It is commonly used for simulating the flow in the corners of the domain, although it cannot be used for complex geometries [7].

We confirm that using the Skordos boundary conditions restores the conservation of mass. This allows us to solve the problem with even higher accuracy \( err = 2.7 \times 10^{-8} \).

5. Conclusion and Outlook

In this paper, we explore the accuracy of the Lattice Boltzmann method by simulating the Couette flow and comparing the LBM results to the analytical solution. We test several ways of specifying the boundary conditions for solid walls and in the flow direction. For solid walls, we find that link-wise and wet-node bounce-back methods give similar results. We also show that increasing the number of terms in the expansion distribution function does not improve accuracy.

For the boundary conditions in the flow direction, we find that the corners of the domain require special care: unless appropriate boundary conditions are used, simulations fail to fulfill the conservation of mass.

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