Practical Aspects of the Simulation of Two-Dimensional Flow Around Obstacle with Lattice Boltzmann Method (LBM)

Phadungsak Ratanadecho
Department of Mechanical Engineering, Faculty of Engineering, Thammasat University (Rangsit Campus), Klong Luang, Pathumthani 12121
Tel (02) 564-3001 Fax (02) 564-3010
E-mail: ratphadu@engr.tu.ac.th

Abstract

The lattice Boltzmann method (LBM) based on the D2Q9 model and a single relaxation time method called the lattice-BGK method are described. Numerical results for a discrete microscopic description of a low Reynolds number flow in a two-dimensional channel flow are reported and its practical relevance was investigated by comparing it with the analytical results. It is found that this approach improves the understanding of the flow pattern in highly complex geometries and to obtain a reliable model for its operating behaviour and design.

Keywords: lattice Boltzmann method, simulation, porous media, obstacle, D2Q9.

1. Introduction

Recently, lattice gas automata (LGA) and lattice Boltzmann automata approaches (Frich et al. [1] and Frich et al. [2]) have been shown to be attractive alternatives to classical methods in CFD, e.g., finite volume methods and Finite element methods for the solution of the partial differential equations (PDE), i.e., Navier-Stokes equations (Noble et al. [3] and Noble et al. [4]). Partial differential equations (PDE) have been the only and most tractable way to describe dynamical and spatially extended system, for a long time.

However, as more difficult problems are considered, PDE may be less adequate and cannot always be formulated when complicated local dynamics involving thresholds or discontinuity are studied. Finally, the sophisticated numerical schemes used to solve PDE often screen out the nature of the process being analyzed and prevent their generalization to new phenomena. In these situations, a description based on a simple model of reality, instead of an exact equation, is quite powerful. The solution procedure is replaced by a direct computer simulation of the model, from which predictions can be made, as in a laboratory experiment. The crucial justification of this methodology is the observation that in many fields of sciences, there are several levels of reality.

The LBM is a derivative of the lattice gas automata method which was first proposed about a dozen years ago by a number of physicists. Nowadays, the method has quickly found its way in dealing with a number of engineering flow problems. Unlike classical methods which solve the discretized macroscopic Navier-Stokes equations, the LBM is based on microscopic particle models and mesoscopic kinetic equations. The fundamental concept of the LBM is to "construct simplified kinetic models that incorporate the essential physics of microscopic or mesoscopic processes so that the macroscopic averaged properties obey the desired macroscopic equations".

The LBM is especially useful for modeling interfacial dynamics, flows over porous media, flow problems in highly complex geometries and various thermodynamic properties of a fluid system, such as the multiphase flows problem (Ratanadecho et al., [5]-[7] and Ratanadecho [8]-[9] and Bernsdorf et al. [10]), in a relatively straightforward way. In addition, the LBM
The objective of the study is to develop an algorithm based on lattice Boltzmann (BGK) automata (Qian et al. [11]) to investigate a two-dimension flow around an arbitrary obstacle mounted in a channel for a range of Reynolds numbers between 80 and 300 as well as flow around a highly complex obstacle. In order to check the accuracy, the calculations from the present LBM model are compared with the theoretical result for the single phase channel flow problem.

2. Description of Numerical Method

The concept of LBM treats the fluid on a statistical level, simulating the movement and interaction of single particles or ensemble-averaged particle density distributions by solving a velocity discrete Boltzmann-type equation. The lattice-Boltzmann method has been shown to be a very efficient tool for flow simulation in highly complex geometries discretized by up to several million grid points.

2.1 Numerical schemes

All numerical simulations presented in this paper will be briefly described here. For simplicity, an equidistant orthogonal lattice is chosen for common LBM computation. This could be done without a significant loss of memory and performance, since the LBM requires much less memory and CPU time than classical methods. On every lattice node \( \vec{r}_i \), a set of \( i \) real numbers, the particle density distributions \( f_i \), is stored. The updating of the lattice basically consists of two steps: a streaming process, where the particle densities are shifted in discrete time steps \( t \), through the lattice along the connection lines in direction \( \vec{c}_i \), to their next neighboring nodes \( \vec{r}_i + \vec{c}_i \), and a relaxation step, where locally a new particle distribution is computed by evaluating an equivalent to the Boltzmann collision integrals (\( \Delta_i^{\text{Boltz}} \)). For every time step, all quantities appearing in the Navier-Stokes equations (density, velocity, pressure gradient and viscosity) can locally be computed in terms of simple functions of this density distribution and (for the viscosity) of the relaxation parameter \( \omega \).

For the present computation, a 2D nine-speed (D2Q9) lattice-Boltzmann automata with single time Bhatnagar-Gross-Krook (Bhatnagar et al. [12]) relaxation collision operator \( \Delta_i^{\text{Boltz}} \) proposed by Qian et al. [11] is used:

\[
f_i(\vec{r}_{i+1}, \vec{r}_i + \vec{c}_i) = f_i(\vec{r}_i, \vec{c}_i) + \Delta_i^{\text{Boltz}}(\vec{r}_i, \vec{c}_i)
\]

with a local equilibrium distribution function \( N_i^{\text{eq}} \):

\[
f_i^{\text{eq}} = \rho \left[ 1 + \frac{c_{\alpha} U_\alpha}{c_i^2} \right] \frac{c_{\alpha} U_\alpha}{c_i^2} \frac{c_{\beta} U_\beta}{c_i^2} - \delta_{\alpha \beta} \left( \frac{c_{\alpha} c_{\beta}}{c_i^2} \right)
\]

This local equilibrium distribution function \( f_i^{\text{eq}} \) has to be computed every time step for every node from the components of the local flow velocities \( U_\alpha \) and \( U_\beta \), the fluid density \( \rho \), a lattice geometry weighting factor \( t_p \), and the speed of sound \( c_i \), which we chose to recover the incompressible time-dependent Navier-Stokes equations (Qian et al. [11]):

\[
\partial_t \rho + \partial_\alpha \left( \rho U_\alpha \right) = 0
\]

\[
\partial_t \left( \rho U_\alpha \right) + \partial_\beta \left( \rho U_\alpha U_\beta \right) = -\partial_\alpha \rho + \partial_\beta \left( \partial_\beta U_\alpha + \partial_\alpha U_\beta \right)
\]

In addition, the left side of Eq. (1) is analogous to the "translation" stage in LBM, and the right to the "collision" stage. For example, in the two-dimensional "D2Q9" model, there are 9 velocities (\( \vec{c}_i \)) on a square lattice: one has speed=0 and corresponds to a "rest" particle; four have speed=1 and are at 0, 90, 180 and 270 degrees; and four have speed=\( \sqrt{2} \) at 45, 135, 225 and 315 degrees, as shown in Fig. 1.
Fig. 1 Schematic 2D lattice Boltzmann calculation on a square lattice, after the translation step. Shown are 6 fluid sites and 3 wall sites (the wall is shown with a brick pattern).

Through careful choice of the equilibrium distribution, the macroscopic quantities (density, velocity, pressure gradient and viscosity) fulfilling the Navier-Stokes equation can be obtained in terms of the moments of the particle distribution function \( f_i(t,r) \) at each site, e.g. for the D2Q9 model:

- **Density:**
  \[
  \bar{\rho} = \sum_i f_i(r,t)
  \]
  (6)

- **Flow velocity:**
  \[
  \bar{v} = \sum_i f_i(r,t) c_i / \bar{p}
  \]
  (7)

- **Pressure:**
  \[
  p = \rho c^2
  \]
  (8)

- **Viscosity:**
  \[
  \nu = \frac{1}{6} \left( \frac{2}{\omega} - 1 \right)
  \]
  (9)

2.2 Boundary conditions

**Wall boundary conditions**

There is a long and still ongoing discussion on the proper use of boundary conditions within the framework of LBM. Although it is known that simple bounce-back wall boundary conditions are of first-order accuracy whereas the lattice-Boltzmann equation is of second order, these bounce-back conditions are the most efficient ones for arbitrary complex geometries. Furthermore, previous investigations showed that the error produced by the bounce-back boundary conditions is sufficiently small if the relaxation parameter \( \omega \) is close enough to 2. Therefore, we believe that the bounce-back conditions can still be used without any influence on the order of the LBM scheme, if \( \omega \) is chosen within a suitable range. Furthermore, the bounce-back boundary conditions are the most efficient ones for arbitrary complex geometries, which are most typical for the application of LBM.

**Inlet and outlet boundary conditions**

In order to simulate a fully developed laminar channel flow, a parabolic velocity profile with a maximum velocity \( u_{\text{max}} \) is prescribed at the channel inlet whereas fixed pressure outlet boundary conditions are chosen.

**Initial boundary conditions**

For the validation test cases, the equilibrium distribution function \( f_i^{\text{eq}} \) was computed from given velocity fields for uniform pressure distribution and taken as the initial solution for the density distribution function \( f_i \). The flow field for the arbitrary obstacle is initialized with the equilibrium distribution function \( f_i^{\text{eq}} \) for zero velocity and uniform pressure, and the inlet velocity had slowly been increased during the first few thousand iterations, to avoid the generation of pressure waves.

3. Result and Discussion

In order to check the accuracy, the calculations from present LBM model are compared with the theoretical result for the single phase channel flow problem. Comparison of the velocity profile in Fig. 2 shows the same trend although the spatial variation of the velocity profile near the center of channel predicted by our model is slightly higher than the theoretical result. This might be due to the initialization of the densities with equilibrium distribution \( f_i^{\text{eq}} \) because of lower iteration numbers.
The good results for the above test case clearly show the possibility of performing accurate numerical simulation for various single phase channel flow problem with the present implementation of the lattice Boltzmann method. Especially, as is already known from the lattice Boltzmann theory, where this quantity could be taken into account for a proper definition of viscosity, no problems with the numerical dissipation have been observed.

3.1 Flow around a square obstacle

The flow around a square obstacle positioned inside a channel was simulated for a range of Reynolds number Re between 80 and 300, defined by the length of the obstacle d, the maximum flow velocity \( u_\text{max} \) of the parabolic inflow profile and the dynamic viscosity \( \nu \) as:

\[
Re = \frac{u_\text{max} d}{\nu} \quad (10)
\]

In this region, it is known from experiments and other numerical studies that vortex shedding is observed and a two-dimensional time dependent flow evolves. At a Reynolds number Re above approximately 300, the flow might become three-dimensional, and two-dimensional computations will therefore not produce physical results.

According to the computational domain as shown in Fig. 3, obstacles of sizes ranging from \( d \times d = 10 \times 10 \) up to \( d \times d = 40 \times 40 \) lattice units are positioned vertically centered in the first third section of the computational domain with sizes between \( l \times h = 500 \times 80 \) and \( l \times h = 2000 \times 320 \) lattice units.

For the wall, a no-slip boundary condition is realized by particle density bounce-back. A parabolic velocity inflow profile is applied, and the outlet pressure is fixed.

The only quantity taken into account in the present analysis is the Strouhal number \( St \), computed from the obstacle diameter \( d \), the measured frequency of the wakes \( f \) and the maximum velocity \( u_\text{max} \), as defined in Eq. (11):

\[
St = \frac{fd}{u_\text{max}} \quad (11)
\]

All computations are done on one processor of the Pentium III. Starting with zero flow velocity and uniform pressure, after a sufficient number of iterations, time-dependent flow evolves with a fixed frequency \( f \). This frequency \( f \) was determined by spectral analysis of the temporal evolution of the \( v \)-component of the flow velocity at several points in the wake behind the obstacle.

For this quantity, the numerical convergence of the scheme with respect to grid resolution was investigated first. What is known from fluid mechanics, and can be reproduced very well by our simulations (see Fig.4), is the fact that the topology of the vortex shedding behind a square obstacle changes significantly with the Reynolds number. For a Reynolds number of 80 the separation point of the vortices is observed to be the rear edge of the obstacle, whereas it moves from the rear to the front edge of the obstacle for higher Reynolds numbers. At Re = 266, small secondary vortices can be found at the top and
bottom of the obstacle. A sufficient resolution of this secondary vortex appears to be crucial for the development of a correct shedding frequency f, which results in the necessity for finer grids for higher Reynolds numbers.

The dependence of the Strouhal number St on grid resolution can be seen for Reynolds numbers between 80 and 266 in Fig.5. The values indicate second-order convergence of the scheme, and lattice sizes of \( l \times h = 2000 \times 320 \) for obstacles of dimension \( d = 40 \) product results with good accuracy for Reynolds numbers up to 300. For Reynolds numbers < 100, near dependence of Strouhal number on grid resolution can be observed, which is in accordance with our observations concerning secondary vortices.

For one full period, the streamlines of a shedding vortex are shown in Fig.6 at \( Re = 80 \). One can see a small vortex developing at the rear top edge of the square obstacle, which is moving downwards while growing, and moves upwards while growing, to separate finally from the top rear edge of the obstacle.

![Fig.5 Strouhal number St as a function of linear lattice dimension l for different Reynolds Number Re](image)

**3.2 Flow around a highly complex obstacle**

For practical applications, this simple procedure as explained in the previous section allows for an easy implementation of arbitrary complex structures (e.g. the flow simulation through a porous structure as presented in Fig. 7) or to change the obstacle structure during the computation, which is necessary for problems with time varying flow geometry. To illustrate the capabilities of LBM, the flow contours and velocity vector fields during fluid flow through a highly complex porous structure are presented in Fig. 8. It is evident from the figure that regardless of the complexity of the pores, the flow features expected are well captured by using LBM simulation.

**4. Conclusion**

With two classical flow studies, this paper is able to show that our implementation of the lattice BGK automata yields reliable results for time-dependent flows. Strouhal numbers St for two-dimensional channel flows around a square obstacle with a blockage ratio of \( b = 0.125 \) and Reynolds numbers between 80 and 300 are measured numerically. It is shown that for a correct evaluation of the Strouhal number higher
grid resolutions are necessary for higher Reynolds numbers owing to the generation of small secondary vortices below and above the obstacle, which have to be resolved numerically.

In addition, concerning complex geometries, the CPU time for the LBM first decreased with increasing complexity of the obstacle structure (e.g. the flow simulation through a porous structure as presented in Fig. 8) and become almost independent from it for highly complex structures. In summary, the LBM method strengthens the often stressed opinion that this method is competitive with respect to the application of CFD especially for problems involving complex geometries such as porous media.

The next step in research in this area is to measure the performance of LBM model against experiment.
Fig. 6 One period of vortex shedding behind a square obstacle at $Re=80$
Fig. 7 Obstacle structure with increasing complexity

Fig. 8 Flow through 2D porous media
5. Acknowledgment
This work was supported by the Department of Chemical Engineering & Materials Science University of Minnesota, Twin Cities under Post Doctoral Grant.

6. References