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Artoli, A.M.M.

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Chapter 3

Numerical Method

"It is the People's method."

Li-Shi Luo, Shanghai, Discrete Fluids Conference, 2002.

"Reaching full maturity is just a matter of time and labour, no conceptual hurdles in sight."

Sauro Succi, 2001.

In this chapter, the theory of lattice Boltzmann methods is reviewed. The advantages and drawbacks in comparison with the classical computational fluid dynamics (CFD) techniques are highlighted. The accuracy and performance of the method are briefly discussed.

3.1 Introduction

For many years to come, a necessity for efficient and robust numerical CFD solvers will be demanded by computational scientists who work at the edge of available computer power. It has been realised by many authors that transport phenomena can be studied from a kinetic theory point of view (e.g. Caflisch, 1983; Ramaswamy, 2001), where an alternative description is given through the Boltzmann equation for the density function $f(t, \vec{x}, \vec{\xi})$ for particles of velocity $\vec{\xi}$ at point $\vec{x}$ and time t. The Boltzmann equation is derived from Newton's laws of motion in the limit of a large number of particles. Although the Boltzmann equation was mainly developed for ideal gases, nevertheless, in the limit of small mean free path between molecular collisions, a gas may be considered as a continuum fluid[1]. The main advantage over solving the Boltzmann equation instead of the Navier-Stokes equations is that Navier-Stokes equations are not adequate to model flows in which the local Knudsen number lies in the continuum regime, since they are based on small deviation from local thermodynamic equilibrium, while the capability of the Boltzmann solution to

[1]The number of gas molecules in a cubic centimetre is given by Loschmidt number $N = p/kT$.

capture complex fluid behaviour even near shocks is a fact (see Cerignani (1975) for details and Pareschi and Russo (2001) for recent developments). After the link between the Boltzmann equation and hydrodynamics was well established (Cercignani 1971; Caflisch, 1983), a need for efficient solvers was raised, since the Boltzmann equation is hard to solve. Perturbation techniques such as the Chapmann-Enskog and Hilbert techniques were the common numerical solvers (Cercignani, 1971), with the solutions obtained as asymptotes to the Boltzmann equation, after simplifying the collision operator.

Soon after Frisch, Hasslacher and Pomeau (1986) introduced the lattice gas cellular automata (LGCA), an automata that is capable of capturing complex fluid nature by just obeying conservation laws, a few shortcomings of LGCA were recognised and intensively investigated. Those are, among others, the lack of Galilean invariance, statistical noise[1], low Reynolds number (high viscosity) and exponential complexity of the collision operator (Succi, 2001; Rothman and Zaleski, 1997; Chopard and Droz, 1998). The earliest lattice Boltzmann method was introduced by McNamara and Zanetti (1988) and Higuera and Jimenez (1989) to circumvent these shortcomings. Although the idea was simply to replace the Boolean LGCA occupation numbers n_i with ensemble-averaged populations $f_i =< n_i >$, the system became capable to capture many features in the evolving nature, but complex enough, due to the complexity of non-equilibrium statistical mechanics, needed to understand it. In the next section a brief review on the hydrodynamics of the lattice Boltzmann method will be presented for completeness. More details on the theory behind the lattice Boltzmann method and the developments in that direction are available in literature (e.g. Qian *et al.*, 1992; Succi *et al.*, 1993; Qian, 1993; Flekkϕy and Herrmann, 1993; Chopard and Droz, 2001; Succi, 2001) and interested readers may consult the last two books or the proceedings of the 9th (2000), the 10th (2001) International Conferences on Discrete Simulation of Fluid Dynamics, the DFG and Konwihr Workshop on Lattice Boltzmann methods (LSTM Erlangen, 2001) and the 11th International Conference on Discrete Simulation of Fluid Dynamics and Condensed Matter Physics (Fudan University, 2002). There exist a number of lattice Boltzmann models, based on more complex collision operators (known as Generalised LBE models) than the BGK approximation. As a first step, however, we believe that the lattice Boltzmann BGK (simply the lattice BGK) model is quite adequate for the recent study that deals with Newtonian fluids under laminar regimes. Use of Generalised models is recommended in future work.

[1] An insight can be gained from these 'physically sound' fluctuations. For details see Rivet and Boon (2001).

3.2 The Lattice Boltzmann Model

Although the lattice Boltzmann model historically evolved from the lattice gas automata, it was soon realised as a special discretisation of the Boltzmann equation

$$\frac{\partial f}{\partial t} + \vec{\xi} \cdot \vec{\nabla} f = -J_i(f_i) \tag{3.1}$$

with the collision term $-J_i(f_i)$ later simplified by Bhatnagar Groos and Krook (BGK) in 1954
to describes the evolution of the single particle distribution function $f \equiv f(x, \vec{\xi}, t)$ for particles that move with a microscopic velocity $\vec{\xi}$, collide with collision relaxation time λ till they relax to the Maxwell-Boltzmann equilibrium distribution function g. Equation 3.1 then becomes

$$\frac{\partial f}{\partial t} + \vec{\xi} \cdot \vec{\nabla} f = -\frac{1}{\lambda}(f - g), \tag{3.2}$$

A numeric solution for f is obtained by discretising Eq. (3.2) in the velocity space $\vec{\xi}$ using a finite set of velocities $\vec{e}_i$, $i = 0, 1, ..., N$, without violating the conservation laws of the hydrodynamic moments. This gives

$$\frac{\partial f_i}{\partial t} + \vec{e}_i \cdot \vec{\nabla} f_i = -\frac{1}{\lambda}\left(f_i - f_i^{(eq)}\right). \tag{3.3}$$

where $f_i(\vec{x},\ t) \equiv f_i(\vec{x},\ \vec{e}_i,\ t)$ and $f_i^{(eq)} = f_i^{(0)}(\vec{x},\ \vec{e}_i,\ t)$ are the distribution function and the equilibrium distribution function of $\vec{e}_i$, respectively. The equilibrium distribution function, obtained by Taylor expansion of the Maxwellian distribution, usually takes the following form in the limit of low Mach number

$$f_i^{(eq)} = \rho w_i \left(1 + \frac{3}{v^2}\vec{e}_i \cdot \vec{u} + \frac{9}{2v^4}(\vec{e}_i \cdot \vec{u})^2 - \frac{3}{2v^2}\vec{u} \cdot \vec{u}\right), \tag{3.4}$$

where w_i is a weighting factor, $v = \delta_x/\delta_t$ is the lattice speed, and δ_x and δ_t are the lattice spacing and the time step, respectively. The values of the weighting factor and the discrete velocities depend on the used lattice Boltzmann model (LBM) and can be found in the literature (see e.g. Mei *et al.*, 2000). In this chapter, without loss of generalisation, we use the D2Q9 model (Chen and Doolen, 1998) and and its incompressible candidate D2Q9i, which has three types of particles on each node; a rest particle, four particles moving along x and y principal directions with speeds $|\vec{e}_i| = 1$, and four particles moving along diagonal directions with speeds $|\vec{e}_i| = \sqrt{2}$. The hydrodynamic density, ρ, and the macroscopic velocity, $\vec{u}$, are determined in terms of the particle distribution functions from

$$\rho = \sum_i f_i = \sum_i f_i^{(eq)} \tag{3.5}$$

and

$$\rho\, \vec{u} = \sum_i \vec{e}_i\, f_i = \sum_i \vec{e}_i\, f_i^{(eq)}\ . \tag{3.6}$$

Equation (3.2) is then discretised in space and time into the well-known lattice BGK equation

$$f_i(\vec{x}+\vec{e}_i\,\delta_t,\, t+\delta_t) \;-\; f_i(\vec{x},\, t) = \;-\;\frac{1}{\tau}[f_i(\vec{x},\, t) \;-\; f_i^{(0)}(\vec{x},\, t)] \tag{3.7}$$

where $\tau = \frac{\lambda}{\delta_t}$ is the dimensionless relaxation time. Taylor expansion of Eq. (3.7) up to $O(\delta_t^2)$ and application of the multi-scale Chapmann-Enskog technique (e.g. Chopard and Droz, 1998) by expanding f_i about $f_i^{(0)}$ and introducing two time scales[1] $t_0 = t$ and $t_1 = t\delta_t$ (assuming that $\lambda \sim \delta_t$), we can write the evolution equation as

$$(\partial t_0 \;+\; \vec{e}_i \cdot \vec{\nabla}) f_i^{(0)} \;=\; -\frac{1}{\tau} f_i^{(1)} \tag{3.8}$$

to the first order, and

$$\partial t_1 f_i^{(0)} + (\partial t_0 + \vec{e}_i \cdot \vec{\nabla})(1 - \frac{1}{2\tau}) f_i^{(1)} = -\frac{1}{\tau} f_i^{(2)} \tag{3.9}$$

to the second order. From the last two equations, the macroscopic density, ρ, and velocity, $\vec{u}$, can be obtained to the first and the second order in δ_t by taking the sum of Eq.(3.8) over all directions and velocities to yield the continuity equation

$$\partial t_0 \rho + \vec{\nabla} \cdot (\rho \vec{u}) = 0 \tag{3.10}$$

to the first order. Also, by multiplying Eq.(3.10) by $\vec{e}_i$ and taking the summation over all directions and velocities, we reach

$$\partial t_0 (\rho \vec{u}) + \vec{\nabla} \cdot \Pi^{(0)} = 0 \tag{3.11}$$

where

$$\Pi_{\alpha\beta}^{(0)} \;=\; \rho\; c_s^2 \delta_{\alpha\beta} + \rho u_\alpha u_\beta \tag{3.12}$$

is the momentum flux tensor, to the first approximation. Here, c_s is the speed of sound which is given by

$$c_s = \sqrt{C}\; v \tag{3.13}$$

where C is a geometric parameter which depends on the used lattice Boltzmann model. For the D2Q9 and D3Q19 models, $C = 1/3$. Similarly, from Eq.(3.9) we get

$$\partial t_1 \rho = 0, \tag{3.14}$$

and

$$\partial t_1 \;(\rho\; \vec{u}) + \vec{\nabla} \cdot \left(1 - \frac{1}{2\tau}\right) \Pi^{(1)} = 0, \tag{3.15}$$

[1]Using the full Taylor expansion of the Boltzmann equation does not need two time scales. A single time scale approach is adopted by Holdych *et al.* (2002).

where

$$\Pi^{(1)}_{\alpha\beta} = \sum_i f_i^{(1)} \vec{e}_{i\alpha} \vec{e}_{i\beta}$$
$$= \delta_t v^2 \tau \left[\left(\frac{c_s^2}{v^2} - C\right) \delta_{\alpha\beta} \vec{\nabla} \cdot (\rho \vec{u}) - C(\partial_\beta \rho u_\alpha + \partial_\alpha \rho u_\beta) \right] \tag{3.16}$$

is the momentum flux tensor, to the second order approximation (e.g. Chopard and Droz, 1998). For incompressible fluids, $\vec{\nabla} \cdot (\rho \vec{u}) = 0$, and therefore Eq. (3.16) becomes

$$\Pi^{(1)}_{\alpha\beta} = \rho \delta_t v^2 \tau \left[- C \left(\partial_\beta u_\alpha + \partial_\alpha u_\beta \right) \right] \tag{3.17}$$

or, equivalently,

$$\Pi^{(1)}_{\alpha\beta} = - 2\rho \, \delta_t \, v^2 \, \tau \, C \, S_{\alpha\beta}. \tag{3.18}$$

The strain rate tensor is therefore

$$S_{\alpha\beta} = - \frac{1}{2 \, C \, \delta_t \, v^2 \, \tau \, \rho} \, \Pi^{(1)}_{\alpha\beta}. \tag{3.19}$$

The Navier-Stokes equation can be derived from Eq. (3.7):

$$\partial_t \, \vec{u} + (\vec{u} \cdot \vec{\nabla}) \vec{u} = - \frac{1}{\rho} \vec{\nabla} \, p + \nu \, \vec{\nabla}^2 \, \vec{u} \tag{3.20}$$

where $p = \rho c_s^2$ is the scalar pressure and ν is the kinematic viscosity of the lattice Boltzmann model, given by

$$\nu = C \, v^2 \, \delta_t \, (\tau - \frac{1}{2}) \tag{3.21}$$

Substituting these formulas for the pressure and viscosity into Eq. (2.15) yields

$$\sigma_{\alpha\beta} = - \rho c_s^2 \, \delta_{\alpha\beta} - \left(1 - \frac{1}{2\tau} \right) \sum_{i=0} f_i^{(1)} e_{i\alpha} \, e_{i\beta}. \tag{3.22}$$

This equation gives the stress tensor components in lattice units and is valid for all of the known lattice BGK models. We emphasise that the quantity $f_i^{(1)} e_{i\alpha} \, e_{i\beta}$ is usually computed during the collision process. Therefore, the stress tensor components can be obtained without almost any additional computational cost. This significantly enhances the lattice Boltzmann BGK method, as other CFD methods are more elaborate and estimate the stress tensor components from the simulated velocity field. As this approximation is of second order in the Knudsen number, the stress tensor components are also accurate up to the second order in the Knudsen number.

3.3 A Priori Error Analysis

There have been many theoretical investigations on the analysis of the lattice Boltzmann method under study. Realisation of the error behaviour depends on the way it is analysed. However, the method is in general of second order in space and first order in time. The following paragraphs briefly attempt to analyse the lattice Boltzmann equation.

3.3.1 Analytical Solutions

Analytical solutions for the lattice Boltzmann equation have been obtained for some flows in the context of simple and exact boundary conditions. Luo *et al.* (1991) solved the generalised hydrodynamics of two-dimensional lattice-gas automata in the linearised Boltzmann approximation and derived the dependence of the transport coefficients upon wave number. Cornubert *et al.* (1991) analytically solved the Kramers problem[1] and classified the boundary conditions into two categories, producing isotropic and anisotropic Knudsen layers. Ginzbourg and Adler (1995) computed first and second order deviations of f_i from their equilibrium. Machine accuracy was obtained by Noble *et al.*(1995) for the plain Poiseuille flow with lattice BGK. This was later analysed by Zou *et al.* (1995), He *et al.* (1997) and Luo (1997) who analytically solved the lattice BGK for the Poiseulle and the Couette flow (see next chapter). Recently, kinetic theory approach to the lattice Boltzmann methods has flourished (He and Luo, 1997b and 1997c; Abe, 1997; Shan and He, 1998). These studies have remarked that the lattice Boltzmann schemes are directly connected to the mescoscopic Boltzmann equation. A need to link lattice Boltzmann models to LGA is no more needed, except for historical reasons. Although studies on formal error analysis of the lattice Boltzmann methods for unsteady flows are quite rate (He and Luo, 1997a; Artoli *et al.*, 2001; Holdych *et al.*, 2002), additional conclusions may be drawn from studies on steady flows, especially those by Holdych *et al.*, (2002). In the last-named reference it was shown that the error varies with the product of Δx^2 and polynomials in the relaxation time τ that multiply high order derivatives and suggested the roots of these polynomials as optimum values for τ. The analysis is performed by inserting a Taylor series expansion of the equilibrium distribution f_i^{eq} into the lattice Boltzmann equation. The compressibility error C.E. and the momentum error M.E. were then computed for 2D models. Although a lot has been done in order to understand the error behaviour in three dimensions, the most popular way is via performing benchmark simulations, as it is very difficult to isolate compressibility errors, momentum errors and discretisation errors in three dimensional Cartesian grids. We will study both approaches (see Chapter 4 and Chapter 5).

[1] A standard problem in kinetic theory caused by the modification of the bulk equilibrium by an obstacle.

3.4 Accuracy of the Lattice Boltzmann Equation

In numerical solvers, differential operators are usually replaced with corresponding finite difference discretisations. The accuracy of a numerical method is said to be of degree n (or n^{th} order accurate), where n is the degree of the polynomial after which the error vanishes (Succi, 2001).
It can be shown that the lattice Boltzmann equation is equivalent to a second order discretisation of the Navier-Stokes equation if the viscosity is defined by Eq. 3.21 and the pressure is defined as $p = \rho c_s^2$. Therefore, the hydrodynamic quantities can be computed with the lattice Boltzmann equation up to second order accuracy in both space and time[1] (Succi, 2001). This accuracy may be enhanced by considering influence of more neighbours through adding further discrete speeds (Succi, 2001). On the other hand, the accuracy of LBE is commonly degraded by four major sources. These are the boundary conditions, the compressibility error, the discretisation error and the momentum error. These errors will not be discussed here in details unless necessary, depending on each benchmark case. Nevertheless, a short briefing would complete the idea of the behaviour of this numerical scheme.

3.4.1 Discretisation Errors

Although Cartesian grids are quite comfortable to work with in parallel computing, they produce large errors when representing fluid boundaries of non-uniform geometry such as vessel structures. Three ways to deal with discretisation errors are to consider realistic models by the aid of scanning techniques (such as magnetic resonance and Computed Tomography), to use curved boundary conditions or finite volume-like LBMs, and to use fine grids at regions of interest. The first treatment is limited by scanner resolution and the other two techniques exploit computational power. Nevertheless, even with a very coarse grid, the lattice Boltzmann solvers return acceptable accuracy, far better than the required engineering accuracy, as will be seen in the next few chapters.

3.4.2 Boundary Conditions

As mentioned above, Kramer's problem arises when the fluid meets an obstacle. Therefore, accurate boundary conditions are needed. The role of a boundary condition in lattice Boltzmann schemes is to give the evolving fluid information from the obstacle which is normally of different physical characteristics (solid, another fluid, gas, etc.). This information is transported by particle distributions streaming from the obstacle into the fluid bulk. As they are unknown (due to the fact that the number of specifying equations is less than the number of the unknowns), heuristic assumptions

[1]First order accuracy in time may be theoretically argued. The lattice Boltzmann equation is a first order in time discretisation of the original Boltzmann equation. I am grateful to Li-Shi Luo who explained to me the potential for confusion in a short remark "It depends on the way you look at it."

are needed to close the system at the boundary. These heuristics depend on the nature of the boundary, whether it is an inlet, outlet or a containing surface. Since this issue is sophisticated, and since the boundary conditions are numerous, only the used boundary conditions will be discussed in association with the models implementing them. For an introduction on Boundary conditions the reader is referred to a chapter written by Succi (2001) and to cited literature in this study.

3.4.3 Compressibility Errors

The lattice Boltzmann method is a compressible discretisation of the Boltzmann equation. Under the fluid dynamic limit, the incompressible NS equations can be derived. This makes the compressibility effect an undesired error source when dealing with incompressible fluids. To correct this, a few incompressible models have been proposed (Zou *et al.*, 1995; He and Luo, 1997; Guo *et al.*, 2000; Guo and Zhao, 2002), most of them are for steady flows. Although some can be used for unsteady flow, they may either complicate the model or hardly enhance the overall error unless more restrictions are fed into the system. Moreover, three dimensional incompressible lattice BGK models are not well tested in the literature. In this study, the standard lattice BGK is used for the sake of simplicity. The compressibility effects are reduced by inventing a new technique based on reducing the Mach number on the fly (see Chapter 7).

3.4.4 Momentum Error

This is the error that appears in the momentum equation and is usually a function of the dimensionless hydrodynamic numbers. It was shown by Holdych *et al.*(2002) that if the viscosity is considered as the independent parameter, this error is a multiple function of Δx^2 and polynomials in the relaxation parameter τ, which include the Reynolds number and the viscosity. The major terms suggest that the error increases linear with the Reynolds number. The τ- dependent polynomials suggests some values for τ at which the error is minimum (solutions for the polynomials). It was shown in the same study that the momentum error is inversely proportional to the Reynolds number if Δt is seen as the independent variable in the error analysis[1].

3.5 Summary

Many solution methods have been developed to solve various flow problems on High Performance Computers, and several new techniques were used to enhance their performance. It may be very difficult to compare between these methods in accuracy and performance, and we can hardly draw constructive conclusions from such comparisons. However, it would be possible to justify why some numerical solvers such as the lattice Boltzmann schemes are superior to other ones in certain cases.

[1]We need to remember that $\Delta x = c\Delta t$.

An elegant flow solver, nevertheless, is required to satisfy many desired features, the most important of which are accuracy and performance. In terms of accuracy, lattice Boltzmann is known to be of second order in space and time. The stress tensor is obtained from the non-equilibrium parts of the distribution functions without any need to approximate the shear-rate. This last featureis of help to researchers in haemodynamics since the shear stress is believed to play a major role in the development of arterial diseases.

For its orthogonal (Cartesian) grid, grid generation in lattice Boltzmann methods is negligible when compared to that in body fitted grid methods. Although Cartesian grid generation is coarse, many near-obstacle features are captured with comparable accuracy to body fitted grids.

The Cartesian grid is an advantage when solving large scale applications in parallel computing environment, as, for instance, load balancing can be satisfactorily achieved. The lattice Boltzmann is also an adaptive method (see next chapter). The explicit nature of time discretisation is another feature that is useful for simulating time-dependent flows.

On the other hand, the lattice BGK is quasi-compressible, thermodynamically inconsistent, very difficult to stabilise at high Reynolds numbers and may harldly involve fluid-structure interaction. So far, many achievements have been made to enhance the method. Many of these drawbacks can be eliminated with the use of the generalised lattice Boltzmann equation (GLBE) (d'Humieres *et al.*, 1992; D'Humeres *et al.*, 2002), but at a cost of 15% in performance (D'Humeres *et al.*, 2002). The method has also been developed to model fluid turbulence (see e. g. Chen et al., 2003 for higlights of benefits over the NS solvers).

Although only recently developed, this study proves that the method is useful in computational haemodynamics. Bearing in mind the hydrodynamic constraints in this study, the lattice-BGK is adequate enough in dealing with simplified blood flow models such as Newtonian flow in the aorta.

In the next chapter, simple 2D steady flow benchmarks are used to test the accuracy of the method while Chapter 5 deals with pulsatile flows. Computational issues are discussed afterwards.