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### Large Scale Lattice-Boltzmann Simulations: Computational Methods and Applications

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## Theoretical background

### 2.1 Lattice-Boltzmann models

In the previous chapter we introduced the basic concepts of lattice gases. The main philosophy is to model fluid dynamics by a particle propagation - and collision process on a regular lattice. Although lattice gases have proven to be very useful for modeling hydrodynamics, one major drawback of the method is the statistical noise in the computed hydrodynamic fields. This shortcoming is a direct consequence of the single particle boolean dynamics. To obtain accurate results for the hydrodynamical fields, averaging over a large number of time steps and/or lattice points are often required and therefore the simulations may be rather inefficient.

It has been shown that a simple modification of the LG idea can reduce the noisy dynamics. In fact, by tracing a density of particles along each bond of the lattice, *cf.* following the motion of an average number of particles, the noise in the results can be eliminated. This is the key idea of the so-called lattice-Boltzmann methods (LBM). However, it must be emphasized that this modification has one major consequence for the simulated physical behavior. In this refinement of the method it is assumed that there are no particle correlations in the system, *cf.* the boolean variables  $n_i$  can be considered as independent random variables. This is the so-called Boltzmann molecular chaos assumption from kinetic theory [17]. To further understand this assumption we consider the ensemble average of a part of the two-body collision operator,  $\langle D_i \rangle$ . The term  $D_i$  is a boolean valued expression that is true when only two particles are entering a lattice point along the bonds  $i$  and  $i+3$  and otherwise it is false. It is a part of the two body collision rule discussed in the previous chapter (for more details see Ref. [16]). Its ensemble average is defined as,

$$\langle D_i \rangle = \langle n_i n_{i+3} (1 - n_{i+1}) (1 - n_{i+2}) (1 - n_{i+4}) (1 - n_{i+5}) \rangle .$$

If it is assumed that the particle-particle correlations decay very fast due to the collisions between particles, the molecular chaos assumption is valid. This enables us to evaluate the ensemble averages  $\langle n_k n_l n_m \dots \rangle$  in a simple way, and

the following equality will hold,

$$\langle D_i \rangle = \langle n_i \rangle \langle n_{i+3} \rangle \langle 1 - n_{i+1} \rangle \langle 1 - n_{i+2} \rangle \langle 1 - n_{i+4} \rangle \langle 1 - n_{i+5} \rangle .$$

In general, it is very difficult to show whether the molecular chaos assumption is valid. In kinetic theory it is argued that this assumption is reasonable for fluid flow at a macroscopic scale [17]. However, in many applications fluctuations and correlations play an important role, e.g. fluctuating hydrodynamics [18], reaction-diffusion systems [16] and diffusion of colloidal particles in a fluid [19]. In these cases the LGA are definitely more realistic than LBM.

In this chapter, we focus on the macroscopic behavior of the Lattice-Boltzmann models. The objective is to underline the basic physical assumptions and related limitations for modeling fluid flow by means of LBM. The complete derivation is based on Ref. [16]. First, a general equation for the macroscopic behavior of LBM is derived. Next, the different terms in the general equation are connected with the known hydrodynamic properties, e.g. velocity, pressure, speed of sound and viscosity. And finally, we present a brief overview of the development of the LGA and LBM in order to illustrate the latest improvements.

## 2.2 The general Lattice Boltzmann equation

The lattice-Boltzmann models can be described by the following equation,

$$f_i(\mathbf{r} + \Delta t \mathbf{v}_i, t + \Delta t) = f_i(\mathbf{r}, t) + \Omega_i(\mathbf{r}, t) \quad (2.1)$$

where  $f_i(\mathbf{r}, t)$  is the probability of finding a particle with velocity  $\mathbf{v}_i$  at position  $\mathbf{r}$  and time  $t$ ,  $\Delta t$  is the time step and  $\mathbf{v}_i$  is the velocity along link  $i$ . The first term in Eq. 2.1 represents the streaming part and the second term,  $\Omega_i$ , is the collision operator. The main difference between Eq. 2.1 and the regularly used continuous Boltzmann equation from kinetic theory [20], is the strict discretization of the phase space. In Eq. 2.1 the time and space variables are discrete and in the velocity space only a small number of values are allowed. For the time being we do not specify the exact form of the collision operator, but we state only the main requirements imposed on it, namely:

- conservation of mass, that is  $\sum_{i=1}^n \Omega_i(\mathbf{r}, t) = 0$  ( $n$  is the number of links per lattice point) and
- conservation of momentum,  $\sum_{i=1}^n \Omega_i(\mathbf{r}, t) \mathbf{v}_i = \mathbf{0}$ .

The macroscopic variables, density  $\rho(\mathbf{r}, t)$  and velocity  $\mathbf{u}(\mathbf{r}, t)$  are defined as moments of the discrete velocity distribution  $f_i(\mathbf{r}, t)$  as

$$\rho(\mathbf{r}, t) = \sum_{i=1}^n f_i(\mathbf{r}, t)$$

$$\mathbf{u}(\mathbf{r}, t) = \frac{\sum_{i=1}^n f_i(\mathbf{r}, t) \mathbf{v}_i}{\rho(\mathbf{r}, t)}$$

As stated in the introduction, our main objective is to derive the macroscopic behavior of Eq. 2.1 in terms of the hydrodynamic fields,  $\rho$  and  $\mathbf{u}$ . To obtain a continuum description we first apply a Taylor expansion to the left hand side of Eq. 2.1 up to second-order in time and space around  $(\mathbf{r}, t)$ ,

$$\Delta r \partial_t f_i + \Delta r (\mathbf{c}_i \cdot \nabla) f_i + \frac{\Delta r^2}{2} \partial_t^2 f_i + \frac{\Delta r^2}{2} (\mathbf{c}_i \cdot \nabla)^2 f_i + \Delta r \Delta t (\mathbf{c}_i \cdot \nabla) \partial_t f_i = \Omega_i, \quad (2.2)$$

where  $\partial_x = \frac{\partial}{\partial x}$ ,  $\Delta r$  is the lattice spacing and the vector  $\mathbf{c}_i$  denotes the coordinates of the neighbor along link  $i$ . In fact we have assumed here that the distribution  $f_i$  is a smooth and sufficiently differentiable function in time and space. This can be justified when the lattice spacing is much bigger than the mean free path\* [16]. Notice that the traditional derivation of the Navier-Stokes equations from the basic conservation laws is based on similar arguments (the so-called continuum limit approximation)[3].

To proceed further with the derivation, we apply the Chapman-Enskog expansion [16, 17]. The Chapman-Enskog expansion is commonly used in statistical mechanics to solve the Boltzmann equation. It consists of three basic approximations,

- First the particle distribution function  $f_i$  is expanded into terms of different order of magnitude (with  $\varepsilon$  a small perturbation parameter),

$$f_i = f_i^0 + \varepsilon f_i^1 + \varepsilon^2 f_i^2 + \dots$$

This expansion is analogous to the regularly used perturbation methods for solving differential equations.

- Furthermore, two different time-scales are introduced, the multi-scale expansion, for describing the time evolution of the macroscopic variables. It is known that in hydrodynamic phenomena the main physical processes are the convection of fluid parcels (determined by the local velocity of the fluid) and viscous effects as a results of diffusion of momenta. These two processes take place at different time-scales. Therefore, we expand the time and space variable as follows,

$$t = \frac{t_1}{\varepsilon} + \frac{t_2}{\varepsilon^2} \quad \partial t = \varepsilon \partial_{t_1} + \varepsilon^2 \partial_{t_2}$$

$$\mathbf{r} = \frac{\mathbf{r}_1}{\varepsilon} \quad \frac{\partial}{\partial r_\alpha} = \varepsilon \partial_{1\alpha},$$

where  $\alpha$  denotes the spatial coordinate (in two-dimensions the  $x$  or  $y$  coordinate) and  $t_1$  and  $t_2$  are the convective and diffusive time-scale respectively.

- Finally the  $f_i^j$  should satisfy the following constraints,

$$\rho = \sum_{i=1}^n f_i^0 \quad \text{and} \quad \rho \mathbf{u} = \sum_{i=1}^n f_i^0 \mathbf{v}_i$$

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\*The mean free path is the average distance that molecules travel between collisions

and

$$\sum_{i=1}^n f_i^l = 0 \quad \text{and} \quad \sum_{i=1}^n f_i^l \mathbf{v}_i = \mathbf{0}$$

for  $l \geq 1$ . These constraints are necessary in order to find a consistent and unique solution for the distribution function  $f_i$ . As we will see in the next section,  $f_i^0$  is considered as the equilibrium distribution.

For a more detailed description of the Chapman-Enskog expansion we refer the interested reader to standard text books on kinetic theory [17, 20]. Also, a nice introduction of this technique in the case of the diffusion automaton (a HPP type of model) is discussed in Ref. [16]. This description discusses the necessity for the different approximations in the Chapman-Enskog expansion in more detail. Having introduced the Chapman-Enskog expansion, we can now derive balance equations for different order of the perturbation parameter  $\varepsilon$ . Notice that to obtain relations for the hydrodynamic fields we need to sum over all the lattice bonds. By applying the Chapman-Enskog expansion to Eq. 2.2, and taking the sum over all links, we can derive the following balance equations for  $O(\varepsilon)$ ,

$$\partial_{t_1} \rho + \partial_{1\alpha} \rho u_\alpha = 0 \quad (2.3)$$

and

$$\partial_{t_1} \rho u_\alpha + \partial_{1\beta} \Pi_{\alpha\beta}^{(0)} = 0 \quad (2.4)$$

where

$$\Pi_{\alpha\beta}^{(0)} = \sum_{i=1}^n v_{i\alpha} v_{i\beta} f_i^0(\mathbf{r}, t)$$

and the Einstein summation convention is used implicitly, meaning that repeated indices imply summation over space coordinates, e.g. in 2D,

$$c_{i\beta} \partial_{1\beta} = c_{ix} \partial_{1x} + c_{iy} \partial_{1y}.$$

Eq. 2.3 states that the density fluctuations at time-scale  $t_1$  are balanced by the net inflow of mass into a fluid element. And Eq. 2.4 states a similar balance for the momentum. These equations are similar to the Euler equations for inviscid fluid flows [3]. In an analogous way a balance equation can be derived for  $O(\varepsilon^2)$ ,

$$\partial_{t_2} \rho + \frac{\Delta t}{2} \partial_{t_1}^2 \rho + \frac{\Delta t}{2} \partial_{1\alpha} \partial_{1\beta} \Pi_{\alpha\beta}^{(0)} + \Delta t \partial_{t_1} \partial_{1\alpha} \rho u_\alpha = 0 \quad (2.5)$$

and

$$\partial_{t_2} \rho u_\alpha + \partial_{1\beta} \Pi_{\alpha\beta}^{(1)} + \frac{\Delta t}{2} \partial_{t_1}^2 \rho u_\alpha + \frac{\Delta t}{2} \partial_{1\beta} \partial_{1\gamma} S_{\alpha\beta\gamma}^{(0)} + \Delta t \partial_{t_1} \partial_{1\beta} \Pi_{\alpha\beta}^{(0)} = 0 \quad (2.6)$$

where

$$S_{\alpha\beta\gamma}^{(0)} = \sum_{i=1}^n v_{i\alpha} v_{i\beta} v_{i\gamma} f_i^0 \quad \text{and} \quad \Pi_{\alpha\beta}^{(1)} = \sum_{i=1}^n v_{i\alpha} v_{i\beta} f_i^1.$$

Notice that in these equations we have some terms associated with time scale  $t_1$  that can be further simplified using the balance equations 2.3 and 2.4. By taking the time derivative  $\partial_{t_1}$  of Eq. 2.3 the following relation can be derived,

$$\frac{\Delta t}{2} \partial_{t_1}^2 \rho = -\frac{\Delta t}{2} \partial_{t_1} \partial_{1\alpha} \rho u_\alpha.$$

Using this expression and Eq. 2.4 it is easy to show that the following relation holds,

$$\frac{\Delta t}{2} \partial_{t_1}^2 \rho + \frac{\Delta t}{2} \partial_{1\alpha} \partial_{1\beta} \Pi_{\alpha\beta}^{(0)} + \Delta t \partial_{t_1} \partial_{1\alpha} \rho u_\alpha = \frac{\Delta t}{2} \partial_{1\alpha} [\partial_{t_1} \rho u_\alpha + \partial_{1\beta} \Pi_{\alpha\beta}^{(0)}] = 0.$$

We can now use this property to simplify Eq. 2.5 and obtain the following simple form,

$$\partial_{t_2} \rho = 0.$$

This expression states that at time scale  $t_2$  the density can be assumed to be constant. Thus in fact the density fluctuations are completely determined by the physical process that take place at time scale  $t_1$ , namely convection. Similarly the following relation can be derived by taking the time-derivative  $\partial_{t_1}$  of Eq. 2.4,

$$\frac{\Delta t}{2} \partial_{t_1}^2 \rho u_\alpha = -\frac{\Delta t}{2} \partial_{t_1} \partial_{1\beta} \Pi_{\alpha\beta}^{(0)}.$$

Using this expression in Eq. 2.6 gives,

$$\partial_{t_2} \rho u_\alpha + \partial_{1\beta} [\Pi_{\alpha\beta}^{(1)} + \frac{\Delta t}{2} (\partial_{t_1} \Pi_{\alpha\beta}^{(0)} + \partial_{1\gamma} S_{\alpha\beta\gamma}^{(0)})] = 0. \quad (2.7)$$

Eq. 2.7 contains the dissipative contribution to the Euler equation. The term,  $\Pi_{\alpha\beta}^{(1)}$  is the dissipative part of the momentum tensor. It will be shown later that the second term,  $\frac{\Delta t}{2} (\partial_{t_1} \Pi_{\alpha\beta}^{(0)} + \partial_{1\gamma} S_{\alpha\beta\gamma}^{(0)})$ , accounts for the discreteness of the lattice. Due to the special form of LBM this term can be included as a correction factor in the kinematic viscosity. This is exactly the reason why the scheme is second-order convergent in space and time while it is based on first-order space and time difference methods (see addendum A). Combining the  $O(\epsilon)$  and  $O(\epsilon^2)$  terms we get the following general equation for the macroscopic description of the Lattice-Boltzmann equation:

$$\partial_t \rho + \nabla \cdot (\rho \mathbf{u}) = 0 \quad (2.8)$$

$$\partial_t \rho u_\alpha + \frac{\partial}{\partial r_\beta} [\Pi_{\alpha\beta} + \frac{\Delta t}{2} (\epsilon \partial_{t_1} \Pi_{\alpha\beta}^{(0)} + \frac{\partial}{\partial r_\gamma} S_{\alpha\beta\gamma}^{(0)})] = 0 \quad (2.9)$$

In summary, we derived the continuity equation, Eq. 2.8, and the momentum equation, Eq. 2.9, from general constraints for mass and momentum conservation. In fact these macroscopic equations are now expressed in terms of first-order, second-order and third-order tensor relation of the particle distribution function and the lattice velocities. In order to derive the final equations in terms of the velocity and the density (the macroscopic variables) we need to express  $f_i^0$  and  $f_i^1$  as functions of the local velocity and density and evaluate these tensorial functions.

## 2.3 The Lattice-BGK model

To proceed further with the derivation we need to consider the details of the collision term. In the simulations that will be reported in this thesis we use a special class of LBM, namely the lattice-Boltzmann BGK (Bhatnager, Gross and Krook) methods (LBGK). For simplicity we consider here the derivation of the macroscopic behavior of the so-called  $D_2Q_8$  lattice-BGK model which is based on a two-dimensional square lattice (see Figure 2.1). In this model,  $\mathbf{c}_i = (\cos(\frac{2\pi}{8}(i-1)), \sin(\frac{2\pi}{8}(i-1)))$  and the velocity  $\mathbf{v}_i = \frac{\Delta x}{\Delta t} \mathbf{c}_i$  for the horizontal and vertical directions, and  $\mathbf{v}_i = \sqrt{2} \frac{\Delta x}{\Delta t} \mathbf{c}_i$  for the diagonal directions.

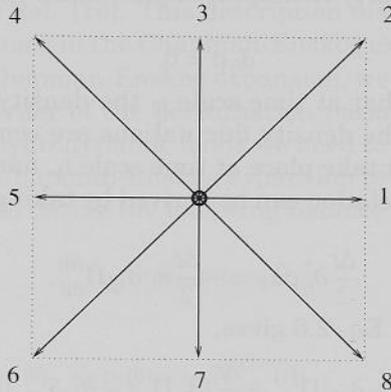


Figure 2.1: The grid stencil of the D2Q8 model.

### 2.3.1 Single time relaxation approximation

In LGA collisions are modeled by scattering of incoming particles. This can be expressed in a mathematical form by for example the Boolean operator  $D_i$ . However, in the context of LBM a direct connection can be made with the continuous Boltzmann equation from kinetic theory and thus existing knowledge may be used for modeling the collision term. In this way Qian et al. [21] and Chen et al. [22] independently proposed the single time relaxation approximation in which the collision process is modeled by a relaxation to the local equilibrium distribution function, the so-called Lattice-BGK model. This approximation has already been proposed by Bhatnager, Gross and Krook (BGK) in 1954, as an alternative collision model in the case of the continuous Boltzmann equation [17, 20]. In this model the collision term  $\Omega_i$  is defined as,

$$\Omega_i = \frac{1}{\tau} (f_i^0(\mathbf{r}, t) - f_i(\mathbf{r}, t)),$$

where  $\tau$  is the so-called relaxation parameter. The main assumption in the BGK model is that the fluid is locally close to thermal equilibrium and thus the dimensions of unit fluid volumes are much bigger than the microscopic scale (the

mean-free path). The idea is that collisions tend to drive the system towards an equilibrium state,  $f_i^0$ , which is defined as [16],

$$f_i^0 = m_i \rho \left( a + \frac{b}{v^2} \mathbf{v}_i \cdot \mathbf{u} + \frac{e}{v^2} u^2 + \frac{h}{v^4} (\mathbf{v}_i \cdot \mathbf{u})^2 \right), \quad (2.10)$$

where  $m_i$ ,  $a$ ,  $b$ ,  $e$  and  $h$  are coefficients which should be determined according to mass and momentum conservation and the desired macroscopic behavior, as will be shown in the next section. Notice that Eq. 2.10 is a second-order expansion in velocity of the well known Maxwellian distribution [23] in the limit of small velocities (low Mach number).

### 2.3.2 The first-order distribution function

For the complete evaluation of Eq. 2.9, we still need to determine  $f_i^{(1)}$  in terms of the density and the velocity. Here we do not go into the details of the derivation, but we state only the final results. The derivation is based on a Taylor expansion of the collision operator around the equilibrium state. After some algebraic manipulations and using the previously derived balance equations, the following expression can be derived [16]

$$f_i^{(1)} = -\Delta t \tau \frac{b}{v^2} m_i (v_{i\alpha} v_{i\beta} - \frac{av^2}{b} \delta_{\alpha\beta}) \partial_{1\alpha} \rho u_\beta. \quad (2.11)$$

### 2.3.3 Lattice symmetries

In standard hydrodynamics the tensors in the momentum equation should be isotropic. This is due to the fact that in a real fluid stress effects relax equally in each direction. This implies that the tensors in Eq. 2.9 should be isotropic. This is the reason why in lattice Gas and lattice Boltzmann models only special lattices are used. For a square lattice isotropy is guaranteed by taken  $m_i = 1$  for the diagonal links and  $m_i = 4$  otherwise [16]. The following relations can then be derived,

$$\sum_{i=1}^8 m_i v_{i\alpha} = 0 \quad \sum_{i=1}^8 m_i v_{i\alpha} v_{i\beta} = 12v^2 \delta_{\alpha\beta} \quad \sum_{i=1}^8 m_i v_{i\alpha} v_{i\beta} v_{i\gamma} = 0$$

and

$$\sum_{i=1}^8 m_i v_{i\alpha} v_{i\beta} v_{i\gamma} v_{i\delta} = 4v^4 (\delta_{\alpha\beta} \delta_{\gamma\delta} + \delta_{\alpha\gamma} \delta_{\beta\delta} + \delta_{\alpha\delta} \delta_{\beta\gamma}),$$

with  $\delta_{\alpha\beta}$  the Kronecker delta function.

## 2.4 The Navier-Stokes equations

By using the expression for  $f_i^0$ ,  $f_i^1$  and the isotropy identities we can compute  $\Pi_{\alpha\beta}^{(0)}$ ,  $S_{\alpha\beta\gamma}^{(0)}$  and  $\Pi_{\alpha\beta}^{(1)}$ . First, it is easy to see that the constraints

$$\rho = \sum_{i=1}^8 f_i^0 \quad \text{and} \quad \rho \mathbf{u} = \sum_{i=1}^8 f_i^0 \mathbf{v}_i,$$

and the isotropy identities, yield the following results for the coefficients of the equilibrium distribution function,

$$a = \frac{1}{20}, \quad b = \frac{1}{12},$$

and

$$12h + 20e = 0. \quad (2.12)$$

Using the tensor identities and the definition of the equilibrium distribution function,  $\Pi_{\alpha\beta}^{(0)}$  can be simplified as follows,

$$\Pi_{\alpha\beta}^{(0)} = \sum_{i=1}^8 v_{i\alpha} v_{i\beta} f_i^0(\mathbf{r}, t) = 12v^2 \left( a + \left( e + \frac{h}{3} \right) \frac{u^2}{v^2} \right) \rho \delta_{\alpha\beta} + 8h\rho u_{\alpha} u_{\beta}.$$

Due to Galilean invariance the coefficient in front of the convective term should be equal to 1 and therefore  $h = \frac{1}{8}$ . Furthermore, using Eq. 2.12 it is easy to see that  $e = \frac{-3}{40}$  and thus  $\Pi_{\alpha\beta}^{(0)}$  can be rewritten as,

$$\Pi_{\alpha\beta}^{(0)} = p \delta_{\alpha\beta} + \rho u_{\alpha} u_{\beta}, \quad (2.13)$$

where the pressure  $p$  is defined as,

$$p = \frac{3}{5} v^2 \left( 1 - \frac{2}{3} \frac{u^2}{v^2} \right) \rho = c_s^2 \rho + O(u^2),$$

and  $c_s$  is the speed of sound. Notice that the pressure is velocity dependent. This unphysical effect can be eliminated by introduction of rest particles in the model [24]. By using the tensor identities and the relations for  $f_i^0$  and  $f_i^1$  we can analogously derive expressions for  $\Pi_{\alpha\beta}^{(1)}$  and  $S_{\alpha\beta\gamma}^{(0)}$  [16],

$$\varepsilon \Pi_{\alpha\beta}^{(1)} = \Delta t v^2 \tau [12a - 4b] \delta_{\alpha\beta} \nabla \cdot \rho \mathbf{u} - 4b (\partial_{\beta} \rho u_{\alpha} + \partial_{\alpha} \rho u_{\beta}) \quad (2.14)$$

(here we have used  $\varepsilon \partial_{1\gamma} = \partial_{\gamma}$ ) and

$$S_{\alpha\beta\gamma}^{(0)} = \frac{v^2}{3} \rho (u_{\gamma} \delta_{\alpha\beta} + u_{\beta} \delta_{\alpha\gamma} + u_{\alpha} \delta_{\beta\gamma}) \quad (2.15)$$

respectively. Substituting these computed expressions in Eq. 2.9 the following macroscopic equation can be derived after some algebraic manipulations [16],

$$\begin{aligned} \partial_t \rho u_\alpha + \rho u_\beta \partial_\beta u_\alpha + u_\alpha \nabla \cdot \rho \mathbf{u} = & -\partial_\alpha p + \Delta t v^2 \left( \frac{\tau}{3} - \frac{1}{6} \right) \nabla^2 \rho u_\alpha + \\ & \Delta t v^2 \left[ \tau \left( \frac{2}{3} - 12a \right) - \left( \frac{1}{3} - 6a \right) \right] \partial_\alpha \nabla \cdot \rho \mathbf{u} \end{aligned} \quad (2.16)$$

In the case of an incompressible fluid one has  $\nabla \cdot \rho \mathbf{u} = 0$  and we recover the usual Navier-Stokes equation

$$\partial_t \mathbf{u} + (\mathbf{u} \cdot \nabla) \mathbf{u} = -\frac{1}{\rho} \nabla p + \nu_{lb} \nabla^2 \mathbf{u} \quad (2.17)$$

where  $\nu_{lb}$  is the kinematic viscosity of the fluid in lattice units,

$$\nu_{lb} = \frac{\Delta t v^2}{3} \left( \tau - \frac{1}{2} \right). \quad (2.18)$$

Summarizing, the Lattice BGK model is based on the following physical constraints:

- The Boltzmann molecular chaos assumption;
- The Chapman Enskog expansion and the single time relaxation to the equilibrium distribution are only valid in the limit of low Knudsen number (the Knudsen number is the ratio of mean free path to the characteristic flow length);
- The expansion of the equilibrium distribution function is only valid in the limit of low Mach numbers;
- The lattice and the coefficients in the equilibrium distribution function must be chosen such that the macroscopic equations are isotropic.

## 2.5 Regularly used LBGK models

Many different formulations of the lattice-BGK model can be found in the literature. The differences mainly lie in the connectivity of the lattice used. In two dimensions 7 or 9 links per lattice point (the  $D_2Q_7$  and  $D_2Q_9$  models, respectively) are frequently used, while in three dimensions 15 or 19 links per lattice point (the  $D_3Q_{15}$  and  $D_3Q_{19}$  models, respectively) are regularly used, in addition to models without rest particles (the  $D_3Q_{14}$  and  $D_3Q_{18}$  models). In this thesis the  $D_2Q_9$  model is used in the two-dimensional simulations, whereas in three dimensions the  $D_3Q_{15}$  and the  $D_3Q_{19}$  models are considered. In the  $D_2Q_9$  model each lattice point is connected to its eight nearest and diagonal neighbors. In the  $D_3Q_{19}$  model each lattice point is connected to its six nearest and twelve diagonal neighbors at a distance of  $\sqrt{2}$ , while in the  $D_3Q_{15}$  model each lattice point

is connected to its six nearest and eight diagonal neighbors at a distance of  $\sqrt{3}$  (see Fig. 3.7). Rest particles are included in all three models.

The time evolution of the lattice-BGK model is described in the previous section. However, we will use a commonly used formulation for the equilibrium distribution function [21]

$$f_i^0 = t_i \rho \left( 1 + \frac{1}{c_s^2} (\mathbf{c}_i \cdot \mathbf{u}) + \frac{1}{2c_s^4} (\mathbf{c}_i \cdot \mathbf{u})^2 - \frac{1}{2c_s^2} u^2 \right), \quad (2.19)$$

where  $t_i$  is a weight factor depending on the length of the vector  $\mathbf{c}_i$ , and  $c_s$  is the speed of sound.

Model	<b>0</b>	<b>I</b>	<b>II</b>	<b>III</b>
$D_2Q_9$	$\frac{4}{9}$	$\frac{1}{9}$	$\frac{1}{36}$	0
$D_3Q_{15}$	$\frac{2}{9}$	$\frac{1}{9}$	0	$\frac{1}{72}$
$D_3Q_{19}$	$\frac{1}{3}$	$\frac{1}{18}$	$\frac{1}{36}$	0

Table 2.1: The coefficients  $t_i$  in the equilibrium distribution function  $f_i^{(0)}$  for the different lattice-BGK models [21, 24]. 0 indicates a rest particle, I is for links pointing to the nearest neighbors, II is for the links pointing to the next-nearest neighbors, and III is for the next-next-nearest neighbors.

For the weight factors used in the different models see table 2.1.

The lattice-Boltzmann models presented here yield the correct hydrodynamic behavior for an incompressible fluid in the limit of low Mach and Knudsen numbers [21]. The kinematic viscosity of the simulated fluid  $\nu$  and the speed of sound  $c_s$  expressed in lattice units, are  $\nu_{lb} = \frac{\tau - \frac{1}{2}}{3}$  and  $c_s = \sqrt{\frac{1}{3}}$  [21]. The fluid pressure  $p(\mathbf{r}, t)$  is given by

$$p(\mathbf{r}, t) = c_s^2 (\rho(\mathbf{r}, t) - \bar{\rho}), \quad (2.20)$$

where  $\bar{\rho}$  is the mean density of the fluid.

## 2.6 Taxonomy of LGA and LBM

In the previous sections we have shown that under specific assumptions the lattice BGK model simulate the behavior of incompressible fluid flow at a macroscopic scale. During the last years many different models have been developed (see Fig. 2.2). In this section we present an overview of these models.

As stated previously, the first particle based model that was proposed for simulating fluid flow was a lattice gas automaton on a square lattice, the so-called

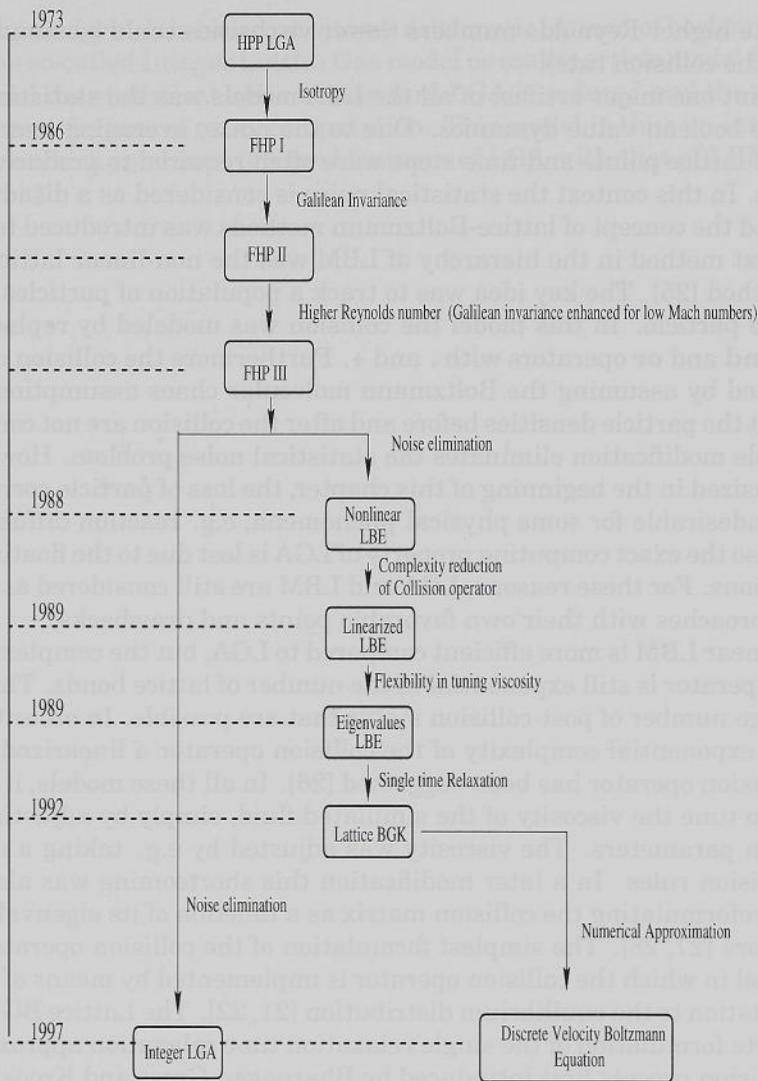


Figure 2.2: The development of the Lattice Gas and Boltzmann models.

HPP model [14, 15]. Although the basic ingredients for modeling the macroscopic behavior of fluid flow correctly, namely conservation of mass and momentum, were present in the HPP model, the viscous stress relaxation was not isotropic. Later, it was realized that isotropic behavior could be obtained by using a hexagonal lattice (FHP I model). However, as stated in the previous chapter these models were not Galilean invariant. This was due to a  $g(\rho)$  factor in front of the convection term. By introducing rest particles in the model (FHP II) this  $g(\rho)$  term could be set close to 1. In a next development the set of collisions that were allowed was extended (the FHP III model) in order to be able

to simulate higher Reynolds numbers (lower viscosities could be simulated by affecting the collision rate).

At this point one major artifact of all the LGA models was the statistical noise due to the boolean value dynamics. Due to the noise, averaging over a large number of lattice points and time steps were often required to produce smooth flow fields. In this context the statistical noise is considered as a disadvantage of LGA and the concept of lattice-Boltzmann methods was introduced to reduce it. The first method in the hierarchy of LBM was the non-linear lattice Boltzmann method [25]. The key idea was to track a population of particles instead of a single particle. In this model the collision was modeled by replacing the boolean **and** and **or** operators with  $\cdot$  and  $+$ . Furthermore the collision operator is factorized by assuming the Boltzmann molecular chaos assumption, which states that the particle densities before and after the collision are not correlated. This simple modification eliminates the statistical noise problem. However, as we emphasized in the beginning of this chapter, the loss of particle correlations may be undesirable for some physical phenomena, e.g. reaction diffusion processes. Also the exact computing property of LGA is lost due to the floating point computations. For these reasons, LGA and LBM are still considered as two different approaches with their own favorable points and drawbacks.

The nonlinear LBM is more efficient compared to LGA, but the complexity of its collision operator is still exponential in the number of lattice bonds. This is due to the large number of post-collision states that are possible. In order to break down the exponential complexity of the collision operator a linearized version of the collision operator has been suggested [26]. In all these models, it was not possible to tune the viscosity of the simulated fluid, simply by adjusting some simulation parameters. The viscosity was adjusted by e.g. taking a different set of collision rules. In a later modification this shortcoming was also eliminated by reformulating the collision matrix as a function of its eigenvalues and eigenvectors [27, 28]. The simplest formulation of the collision operator is the BGK model in which the collision operator is implemented by means of a single time relaxation to the equilibrium distribution [21, 22]. The Lattice BGK model is a discrete formulation of the single relaxation time relaxation approximation of the collision process first introduced by Bhatnager, Gross and Krook in 1954 [17]. Note that the development of the different lattice models is much in the same line as the development of the Boltzmann equations in standard kinetic theory.

A few years ago it has been argued that the lattice-BGK scheme is a numerical discretization of the continuous Boltzmann-BGK transport equation for a discrete set of velocities (see addendum A) [29]. More specifically stated, the Lattice-BGK method can be derived from the discrete velocity Boltzmann equation by applying a first-order upwind space discretization and a first-order Euler time integration scheme. This similarity between LBGK and the discrete velocity Boltzmann equations seems to be promising in extending the standard Lattice-BGK scheme to simulations on for example non uniform lattices, thermal models, multi-phase flows etc.

Closely related to the spirit of LGA on the other hand, a new type of model has

been proposed which is based on integer arithmetic instead of boolean computations, the so-called Integer Lattice Gas model or multiparticle model [30, 16]. In this model the statistical noise of standard LGA is reduced and the model still has the nice feature of exact computation. This model is thus an intermediate approach which combines the good features of LGA with that of LBM.

