Chapter 2
The Boltzmann Equation

Ludwig Eduard Boltzmann (1844–1906), the Austrian physicist whose greatest achievement was in the development of statistical mechanics, which explains and predicts how the properties of atoms and molecules (microscopic properties) determine the phenomenological (macroscopic) properties of matter such as the viscosity, thermal conductivity, and diffusion coefficient. The distribution function (probability of finding particles within a certain range of velocities at a certain range of locations at a given time) replaces tagging each particle, as in molecular dynamic simulations. The method saves the computer resources drastically.

In this chapter, the main concept of the Boltzmann equation is introduced.

2.1 Boltzmann Transport Equation

A statistical description of a system can be explained by distribution function $f(r, c, t)$, where $f(r, c, t)$ is the number of molecules at time $t$ positioned between $r$ and $r + dr$ which have velocities between $c$ and $c + dc$, as mentioned in the previous chapter. An external force $F$ acting on a gas molecule of unit mass will change the velocity of the molecule from $c$ to $c + Fdt$ and its position from $r$ to $r + cdt$ (Fig. 2.1).

The number of molecules, $f(r, c, t)$, before applying the external force is equal to the number of molecules after the disturbance, $f(r + cdt, c + Fdt, t + dt)$, if no collisions take place between the molecules. Hence,

$$f(r + cdt, c + Fdt, t + dt) dr dc - f(r, c, t) dr dc = 0 \quad (2.1)$$

However, if collisions take place between the molecules there will be a net difference between the numbers of molecules in the interval $dr dc$. The rate of change between final and initial status of the distribution function is called collision operator, $\Omega$. Hence, the equation for evolution of the number of the molecules can be written as,
Dividing the above equation by $dt$, yields

$$\frac{df}{dt} = \Omega(f)$$  \hfill (2.3)

The above equation states that the total rate of change of the distribution function is equal to the rate of the collision. Since $f$ is a function of $r$, $c$ and $t$, then the total rate of change can be expanded as,

$$df = \frac{\partial f}{\partial r} dr + \frac{\partial f}{\partial c} dc + \frac{\partial f}{\partial t} dt$$  \hfill (2.4)

Dividing by $dt$, yields

$$\frac{df}{dt} = \frac{\partial f}{\partial r} \frac{dr}{dt} + \frac{\partial f}{\partial c} \frac{dc}{dt} + \frac{\partial f}{\partial t}$$  \hfill (2.5)

The vector $r$ can be expressed in 3-D Cartesian coordinate system as $r = xi + yj + zk$, where $i$, $j$, and $k$ are unit vectors along $x$, $y$, and $z$-direction, respectively.

Equation 2.5 can be written as,

$$\frac{df}{dt} = \frac{\partial f}{\partial r} c + \frac{\partial f}{\partial c} a + \frac{\partial f}{\partial t}$$  \hfill (2.6)

where $a$ is equal to $dc/dt$, the acceleration and can be related to force $F$ by Newton’s second law, $a = F/m$.

Therefore, the Boltzmann transport equation (2.3) can be written as,
\[
\frac{\partial f}{\partial t} + \frac{\partial f}{\partial r} \cdot c + \frac{F}{m} \cdot \frac{\partial f}{\partial c} = \Omega \tag{2.7}
\]

The \( \Omega \) is a function of \( f \) and need to be determined to solve the Boltzmann equation.

For system without an external force, the Boltzmann equation can be written as,

\[
\frac{\partial f}{\partial t} + c \cdot \nabla f = \Omega \tag{2.8}
\]

Note that \( c \) and \( \nabla f \) are vectors.

Equation 2.8 is an advection equation with a source term (\( \Omega \)), or advection with a reaction term, which can be solved exactly along the characteristic lines that is tangent to the vector \( c \), if \( \Omega \) is explicitly known. The problem is that \( \Omega \) is a function of \( f \) and Eq. 2.8 is an integro-differential equation, which is difficult to solve.

The relation between the above equation and macroscopic quantities such as fluid density, \( \rho \), fluid velocity vector \( u \), and internal energy \( e \), is as follows

\[
\rho(r,t) = \int mf(r,c,t) \, dc \tag{2.9}
\]

\[
\rho(r,t)u(r,t) = \int mcf(r,c,t) \, dc \tag{2.10}
\]

\[
\rho(r,t)e(r,t) = \frac{1}{2} \int mu_a^2 f(r,c,t) \, dc \tag{2.11}
\]

where \( m \) is the molecular mass and \( u_a \) the particle velocity relative to the fluid velocity, the peculiar velocity, \( u_a = c - u \).

Equations 2.9, 2.10, and 2.11 are conservation of mass, momentum, and energy, respectively.

From the kinetic theory, as discussed before, the internal energy can be expressed as,

\[
e = \frac{3}{2m} k_B T \tag{2.12}
\]

2.1.1 Example 2.1

In a road intersection, if there is no car collisions, the cars from section A move (stream) to \( A' \) and cars from section B move to \( B' \) without any problem. This case represents Eq. 2.8 with \( \Omega = 0 \), see Fig. 2.2. However, if there is a collision at the intersection, then cars at section A cannot smoothly move to \( A' \) or from B to \( B' \). The time needed to reach smooth traffic (equilibrium conditions) depend on the type of the collision and the response of the policeman (relaxation time). In this case \( \Omega \) is not zero.
2.2 The BGKW Approximation

It is difficult to solve Boltzmann equation because the collision term is very complicated. The outcome of two body collisions is not likely to influence significantly, the values of many measured quantities (Cercignani, 1990). Hence, it is possible to approximate the collision operator with simple operator without introducing significant error to the outcome of the solution. Bhatnagar, Gross and Krook (BGK) in 1954 introduced a simplified model for collision operator. At the same time Welander (1954), independently, introduced similar operator. The collision operator is replaced as,

\[ \frac{1}{s} \left( \frac{f^{eq}}{C_0} f \right) \]  

where \( x = \frac{1}{s} \)  

The coefficient \( x \) is called the collision frequency and \( s \) is called relaxation factor. The local equilibrium distribution function is denoted by \( f^{eq} \), which is Maxwell–Boltzmann distribution function.

After introducing BGKW approximation, the Boltzmann equation (Eq. 2.8, without external forces) can be approximated as,

\[ \frac{\partial f}{\partial t} + c \cdot \nabla f = \frac{1}{\tau} (f^{eq} - f) \]  

where \( \omega = 1/\tau \)

The coefficient \( \omega \) is called the collision frequency and \( \tau \) is called relaxation factor. The local equilibrium distribution function is denoted by \( f^{eq} \), which is Maxwell–Boltzmann distribution function.

After introducing BGKW approximation, the Boltzmann equation (Eq. 2.8, without external forces) can be approximated as,

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In Lattice Boltzmann method, the above equation is discretized and assumed it is valid along specific directions, linkages. Hence, the discrete Boltzmann equation can be written along a specified direction as,

\[ \frac{\partial f_i}{\partial t} + c_i \nabla f_i = \frac{1}{\tau} (f^{eq}_i - f_i) \]  

The above equation is the working horse of the lattice Boltzmann method and replaces Navier–Stokes equation in CFD simulations. It is possible to derive Navier–Stokes equation from Boltzmann equation. We can make comments as the followings about Eq. 2.15:
1. The equation is a linear partial differential equation.
2. The equation looks like an advection equation with a source term.
3. The right-hand side of the equation represents the advection (streaming).
4. The left-hand side term represents the collision process, source term.

Equation 2.15 can be discretized as

$$f_i(r + c_i \Delta t, t + \Delta t) = f_i(r, t) + \frac{\Delta t}{\tau} [f_i^e(r, t) - f_i(r, t)]$$  \hspace{1cm} (2.16)

The local equilibrium distribution function with a relaxation time determine the type of problem needed to be solved. The beauty of this equation lies in its simplicity and can be applied for many physics by simply specifying a different equilibrium distribution function and source term (external force). Adding a source term (force term) to the above equation is straightforward. However, there are a few concerns, which will be discussed in the following chapters. Also, the details of implementing the above equation for different problems, such as momentum, heat and mass diffusion, advection–diffusion without and with external forces, will be presented in the following chapters.

It is possible to use finite difference or finite volume to solve partial differential equation (2.15). Some authors used this approach to solve fluid dynamic problems on non-uniform grids. The main focus of the book is to solve Eq. 2.15 in two steps, collision and streaming.

In LBM, the solution domain need to be divided into lattices. At each lattice node, the factitious particles (distribution function) reside. Some of these particles streams (move) along specified directions to the neighboring nodes. The number of direction, linkage, depends on the lattice arrangement. Different lattice arrangements will be discussed in the following section.

2.3 Lattice Arrangements

The common terminology used in LBM is to refer to the dimension of the problem and the number of speed is using $DnQm$, where $n$ represent the dimension of the problem (1 for 1-D, 2 for 2-D and 3 for 3-D) and $m$ refers to the speed model, number of linkages. In the following paragraphs different lattice arrangements used for 1-D, 2-D, and 3-D will be discussed.

2.3.1 One-Dimensional

In general, two models can be used for lattice arrangements, called D1Q3Q and D1Q5Q, as shown in Fig. 2.3. D1Q3 is the most popular one. The black nodes are the central node, while the gray nodes are neighboring nodes. The factitious
particles stream from the central node to neighboring nodes through linkages with a specified speed, called lattice speed.

### 2.3.1.1 D1Q3 and D1Q2

For D1Q3, there are three velocity vectors \((c_0, c_1, c_2)\) for \(f_0, f_1, \text{and } f_2\), which equal to 0, 1, and \(-1\), respectively. Note that we assumed that \(dx = dt\), otherwise, \(c_1 = \frac{\Delta x}{\Delta t}\) and \(c_2 = -\frac{\Delta x}{\Delta t}\), where \(\Delta x\) and \(\Delta t\) are the linkage length and time step, respectively. For this arrangement, the total number of factitious particles at any instant of time cannot exceed three particles. One stagnant particle (zero velocity) resides on the central site. The other two particles move either to the left or to the right node in the streaming process. The weighting factors, \(\omega_i\), has values of \(4/6, 1/6\) and \(1/6\) for \(f_0, f_1\), and \(f_2\), respectively. The speed of sound, \(c_s\), in lattice units for D1Q3 is \(1/\sqrt{3}\). It is also possible to use other arrangement called D1Q2. The weighting factors, \(\omega_i\), has values of \(1/2\) and \(1/2\) for \(f_1\) and \(f_2\), respectively. The speed of sound for this arrangement is \(1/\sqrt{2}\). These schemes, D1Q2 and D1Q3, are mostly used. However, it is possible to involve more sites and use higher order schemes, such as, D1Q5.

### 2.3.1.2 D1Q5

For this arrangement, the total number of factitious particles at any instant of time cannot exceeded five particles. The weighting factors, \(\omega_i\), are \(6/12, 2/12, 2/12, 1/12\), and \(1/12\) for \(f_0, f_1, f_2, f_3, \text{and } f_4\), respectively. The speed of the sound in lattice units is \(1/\sqrt{3}\).

### 2.3.2 Two-Dimensional

#### 2.3.2.1 D2Q5 and D2Q4

D2Q5 model has four velocity vectors issued from the central nodes, Fig. 2.4. One of the particle resides at the central node, hence its speed is zero, noted as \(c(0,0)\). The distribution function \(f_1\) and \(f_2\) move with \(c(1,0)\) and \(c(-1,0)\) (to the east and west), respectively, while \(f_3\) and \(f_4\) move with speed \(c(0,1)\) and \(c(0,-1)\) (to the north and south), respectively. Note that it is assumed that \(\Delta x = \Delta y = \Delta t\).
The weighting factors for $f_0, f_1, f_2, f_3,$ and $f_4$ are $2/6, 1/6, 1/6, 1/6,$ and $1/6$, respectively. It is worthy to mention that this arrangement cannot be used to simulate fluid flows. This issue will be discussed latter on. D2Q4 has four velocity vectors and there is no particle residing on the centre node. The weighting factor for each direction is $1/4$. We will discuss implementations and applications of each scheme in the following chapters. The numbering of lattice links is arbitrary. However, for computer programming algorithm, proper numbering may reduce simplifying the computer code.

2.3.2.2 D2Q9

This model is very common, especially for solving fluid flow problems. It has high velocity vectors, with the central particle speed being zero, 2.5. The speeds are $c(0,0), c(1,0), c(0,1), c(-1,0), c(0,-1), c(1,1), c(-1,1), c(-1,-1)$ and $c(1,-1)$ for $f_0, f_1, f_2, f_3, f_4, f_5, f_6, f_7$ and $f_8$, respectively. The weighting factors for corresponding distribution functions are $4/9, 1/9, 1/9, 1/9, 1/9, 1/36, 1/36, 1/36,$ and $1/36$ (Fig. 2.5).

2.3.3 Three-Dimensional

In general two models are used in simulation of three dimensional problems, D3Q15 and D3Q19.

Fig. 2.4 Lattice arrangements for 2-D problems, D2Q4 and D2Q5.
2.3.3.1 D3Q15

In this model 15 velocity vectors are used, Fig. 2.6, the central distribution function, \( f_0 \) has zero speed. D3Q15 is most commonly used for 3-D simulations. Notice that nodes 1, 2, 3, and 4 are on the center of the east, north, west, and south faces, respectively. Nodes 5 and 6 are on the center of the front and back faces, respectively. The nodes 7, 8, 9, 10, 11, 12, 13, and 14 are on the corners of the lattice. The 15 velocity vectors for the distribution functions of \( f_0 \), \( f_1 \) to \( f_6 \), \( f_7 \) to \( f_9 \), \( f_{10} \), \( f_{11} \), \( f_{12} \), \( f_{13} \) and \( f_{14} \) are

\[
\begin{align*}
 c(0,0,0), & \quad c(1,0,0), \quad c(0,1,0), \quad c(-1,0,0), \quad c(0,-1,0), \quad c(0,0,1), \quad c(0,0,-1), \\
 c(1,1,1), & \quad c(1,1,-1), \quad c(1,-1,-1), \quad c(1,-1,1), \quad c(-1,1,1), \\
 c(-1,-1,1) & \quad \text{and} \quad c(-1,-1,-1),
\end{align*}
\]

respectively. The weighting factors are 16/72 for \( f_0 \)
8/72 for \( f_1 \) to \( f_6 \) and
1/72 for \( f_7 \) to \( f_{14} \).

2.3.3.2 D3Q19

This model has 19 velocity vectors, with central vector of speed zero, Fig. 2.7. The weighting factors are:

- for \( f_0 \) is 12/36
- for \( f_1 \) to \( f_6 \), is 2/36
- for \( f_7 \) to \( f_{18} \), is 1/36.

It is possible to use D3Q7 or D2Q6 similar to D2Q5 and D2Q4 for advection–diffusion problems.

Fig. 2.6  Lattice arrangements for 3-D problems, D3Q15.
2.4 Equilibrium Distribution Function

The key element in applying LBM for different problems is the equilibrium distribution function, \( f_{eq} \). As we will see in the following chapters that the procedure of solving diffusion, advection–diffusion, momentum, and energy equations is the same. The difference mainly depends on the equilibrium distribution function. In fact, different physical problems (such as a wave propagation problem, etc.) can be solved by LBM provided that a proper equilibrium distribution function is used.

For particles moving in a medium with macroscopic velocity \( u \): The normalized Maxwell’s distribution function (Eq. 1.38) can be written as,

\[
\frac{q^2}{3} e^{-\frac{q}{C_0^2} \left( \frac{c}{C_0} u \right)^2} \]

which can be written as,

\[
\frac{\rho}{2\pi/3} e^{-\frac{1}{2} (c-u)^2} \]

(2.17)

where \( c^2 = c \cdot c \) and \( u^2 = u \cdot u \). Recall that Taylor series expansion for \( e^{-x} \) is,

\[
e^{-x} = 1 - x + x^2/2 - x^3/(3!) \cdots
\]

(2.19)

Hence Eq. 2.18 can be expanded around the stationary state as,

\[
f = \frac{\rho}{2\pi/3} e^{-\frac{1}{2} (c-u)^2} \left[ 1 + 3(c \cdot u) - \frac{3}{2} u^2 + \cdots \right]
\]

(2.20)

The general form of the equilibrium distribution function can be written as,
\[ f_i^{eq} = \Phi \omega_i \left[ A + B c_i \cdot u + C (c_i \cdot u)^2 + D u^2 \right] \quad (2.21) \]

where \( u \) is the macroscopic flow velocity vector; \( A, B, C, \) and \( D \) are constants and need to be determined based on the conservation principle (mass, momentum, and energy). \( \Phi \) stands for scalar parameter, such as density (\( \rho \)), temperature (thermal energy density), or species concentration, which is equal to summation of all the distribution functions, i.e.,

\[ \Phi = \sum_{i=0}^{i=n} f_i^{eq} \quad (2.22) \]

where \( n \) is the number of the lattice links. For example, in a diffusion process, the flow is stagnant, velocity is zero, then Eq. 2.17 can be reduced to:

\[ f_i^{eq} = \Phi A \omega_i \quad (2.23) \]

It turns out that \( A \) is equal to unity, where \( \sum_{i=0}^{i=n} \omega_i = 1 \). In the following chapters more details will be given about the equilibrium distribution function.