2. Lattice-Boltzmann method

2.1 Introduction

We now will build a discrete system by using the concepts from kinetic theory as discussed in LN01. The core concept of kinetic theory is the distribution function $f(\mathbf{x},\boldsymbol{\xi},t)$ with $\mathbf{x}$ space (in general in three dimensions), $\boldsymbol{\xi}$ velocity (in general also in three dimensions) and t time. Discretization therefore involves discretization in time, space *and velocity*. The discretization is – to some extent and at some level of abstraction – straightforward. Relating the discrete version of the Boltzmann equation to the Navier-Stokes equation and deriving the discrete version of the equilibrium distribution function are, however, quite elaborate. What we will do in these lecture notes is first present the discrete Boltzmann equation and the discrete version of the equilibrium distribution function and explain the lattice-Boltzmann algorithm. After having explained the algorithm we then relate the lattice-Boltzmann equation to the Navier-Stokes equation (Section 2.4 Chapman-Enskog analysis) and discuss the relation between the continuous and discrete distribution function (Section 2.5 Discrete equilibrium distribution function). These are two section of a more mathematical nature.

2.2 Discretization

We define a discrete and finite set of velocities $\mathbf{c_i}=\left(c_{ix},c_{iy},c_{iz}\right)$ and indicate the distribution function as $f_i(\mathbf{x},t)$ which is now understood as that the density of molecules at $\mathbf{x}$ and t traveling with velocity $\mathbf{c_i}$. Integrations over velocity space (as in Eqs. 1.1 and 1.2 of LN01) now turn into summations over the finite set of velocities

$$\rho(\mathbf{x},t)=\sum_i f_i(\mathbf{x},t) \tag{2.1}$$

$$\rho(\mathbf{x},t)\mathbf{u}(\mathbf{x},t)=\sum_i \mathbf{c_i} f_i(\mathbf{x},t) \tag{2.2}$$

Discretization in space implies that locations where $f_i(\mathbf{x},t)$ is defined are positioned on a simple cubic lattice with the cubes having a side length Δx. Discretization in time implies that $f_i(\mathbf{x},t)$ is defined at moments separated by a time interval Δt.

In these lecture notes I would like to use the practice of using *lattice units*. This means that we choose the units of space and time such that $\Delta x=1$ and $\Delta t=1$.

There are many options when it comes to velocity sets. Velocity sets for solving the Navier-Stokes equation are categorized as D*d*Q*q* with *d* the dimensionality of space (1, 2 or 3), and *q* the number of velocities. The more common velocity sets are D2Q9 and D3Q19; there also are D1Q3, D3Q15, D3Q27 and more. Velocity sets are defined by the velocity vectors $\mathbf{c_i}$ and by a weighing factor per velocity w_i. Finally, as we will see in Section 2.4, each velocity set comes with a constant c_s that relates pressure with density: $p=c_s^2\rho$. This is an (isothermal) ideal gas law with $\dfrac{\partial p}{\partial\rho}=c_s^2$ so that c_s is the speed of sound. In the most common velocity sets, $c_s=\sqrt{1/3}\,\Delta x/\Delta t$ ($c_s=\sqrt{1/3}$ in lattice units).

The discretizations in time, space and velocity lead to the *lattice-Boltzmann equation*:

$$f_i\left(\mathbf{x}+\mathbf{c_i}\Delta t, t+\Delta t\right)= f_i\left(\mathbf{x},t\right)+\Omega_i\left(\mathbf{x},t\right) \tag{2.3}$$

Applying lattice units $\Delta x = 1$ and $\Delta t = 1$ we get

$$f_i\left(\mathbf{x}+\mathbf{c_i}, t+1\right)= f_i\left(\mathbf{x},t\right)+\Omega_i\left(\mathbf{x},t\right) \tag{2.4}$$

In the remainder of these notes we will – for simplicity but without much lack of generality – work in two dimensions and adopt the D2Q9 velocity set with

$$\mathbf{c_0}=\begin{pmatrix}0\\0\end{pmatrix}\mathbf{c_1}=\begin{pmatrix}1\\0\end{pmatrix}\mathbf{c_2}=\begin{pmatrix}-1\\0\end{pmatrix}\mathbf{c_3}=\begin{pmatrix}0\\1\end{pmatrix}\mathbf{c_4}=\begin{pmatrix}0\\-1\end{pmatrix}\mathbf{c_5}=\begin{pmatrix}1\\1\end{pmatrix}\mathbf{c_6}=\begin{pmatrix}-1\\1\end{pmatrix}\mathbf{c_7}=\begin{pmatrix}-1\\-1\end{pmatrix}\mathbf{c_8}=\begin{pmatrix}1\\-1\end{pmatrix} \tag{2.5}$$

and

$$w_0 = 4/9 \quad w_{1-4} = 1/9 \quad w_{5-8} = 1/36 \tag{2.6}$$

and $c_s = \sqrt{1/3}$.

We see (Figure 2.1) that at the end of a time step (which is applying Eq. 2.4 to all nodes on the lattice) a distribution function that started from lattice location **x** ends up in a neighbouring lattice location $\mathbf{x}+\mathbf{c_i}$ (except the distribution with $i=0$ which stays where it was).

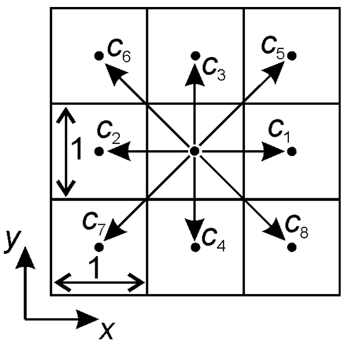

Figure 2.1

The simplest yet effective collision operator is the Bhatnagar, Gross & Krook (BGK) collision operator; see LN01, Eq. 1.12. In discrete form it reads

$$\Omega_i\left(\mathbf{x},t\right)=\Omega_i\left(f\right)=-\frac{1}{\tau}\left(f_i - f_i^{eq}\right) \tag{2.7}$$

The f in $\Omega_i\left(f\right)$ means that the collision operator depends on all distribution functions $f_{0\cdots8}$ at the location-time combination $\left(\mathbf{x},t\right)$. As we will argue later in these notes, the discrete version of the equilibrium distribution function reads

$$f_i^{eq} = w_i \rho \left[1 + \frac{u_\alpha c_{i\alpha}}{c_s^2} + \frac{\left(u_\alpha c_{i\alpha}\right)^2}{2c_s^4} - \frac{u_\alpha u_\alpha}{2c_s^2} \right] \tag{2.8}$$

(note the summation convention: summation over repeated Greek indices). It contains the macroscopic flow variables density and velocity.

It is worthwhile doing a few reality checks. We will perform these for the D2Q9 velocity set as defined in Eqs. 2.5 and 2.6 and $c_s^2 = \frac{1}{3}$.

(1) Mass conservation requires $\sum_i \Omega_i = 0$. Since $\sum_i f_i = \rho$, it then should be that also $\sum_i f_i^{eq} = \rho$. Writing out $\sum_i f_i^{eq}$ for D2Q9 and applying the *summation convention* gets

$\sum_i w_i \rho \left[1 + 3\left(u_x c_{ix} + u_y c_{iy}\right) + \frac{9}{2}\left(u_x c_{ix} + u_y c_{iy}\right)^2 - \frac{3}{2}\left(u_x^2 + u_y^2\right) \right] =$

$\rho\left(1 - \frac{3}{2}u_x^2 - \frac{3}{2}u_y^2\right)\sum_i w_i + 3\rho u_x \sum_i w_i c_{ix} + 3\rho u_y \sum_i w_i c_{iy} + \frac{9}{2}\rho u_x^2 \sum_i w_i c_{ix}^2 + \frac{9}{2}\rho u_y^2 \sum_i w_i c_{iy}^2 + 9\rho u_x u_y \sum_i w_i c_{ix} c_{iy}$

Realize that (see Eqs. 2.5 and 2.6) $\sum_i w_i = 1; \sum_i w_i c_{i\alpha} = 0; \sum_i w_i c_{i\alpha} c_{i\beta} = \frac{1}{3}\delta_{\alpha\beta}$ then indeed $\sum_i f_i^{eq} = \rho$.

(2) Momentum conservation over the collision operation requires $\sum_i \Omega_i c_{i\alpha} = 0$. Since $\sum_i f_i c_{i\alpha} = \rho u_\alpha$, it should be that also $\sum_i f_i^{eq} c_{i\alpha} = \rho u_\alpha$. Again, writing out $\sum_i f_i^{eq} c_{i\alpha}$ and using the symmetry properties of the lattice will get you that indeed $\sum_i f_i^{eq} c_{i\alpha} = \rho u_\alpha$.

It is important to note that the collision operator $\Omega_i\left(f\right)$ only depends on local properties, i.e. the set of distribution functions f_i at the current location at the current moment. This is because the expression for $\Omega_i\left(f\right)$ contains f_i and f_i^{eq} (Eq. 2.7), f_i^{eq} depends on ρ and on u_α, and in turn ρ and u_α can be written in terms of f_i (Eqs. 2.1 and 2.2).

The Chapman-Enskog analysis relates the lattice-Boltzmann equation with the Navier-Stokes equation. We will go through this analysis in Section 2.4. Important results of the analysis are in the first place that the kinematic viscosity of the lattice-Boltzmann fluid relates to the relaxation time according to

$$\nu = c_s^2 \left(\tau - \frac{\Delta t}{2} \right) \tag{2.9}$$

In lattice units and with $c_s^2 = \frac{1}{3}$ this becomes $\nu = \frac{2\tau - 1}{6}$. In the second place the Chapman-Enskog expansion establishes the relation between density and pressure alluded to before: $p = c_s^2 \rho$.

2.3 The lattice-Boltzmann algorithm – time stepping

The lattice-Boltzmann method simply involves applying $f_i\left(\mathbf{x}+\mathbf{c_i},t+1\right)=f_i\left(\mathbf{x},t\right)+\Omega_i\left(\mathbf{x},t\right)$. In practice it means that each time step in a lattice-Boltzmann algorithm is broken up in two parts: *collision* and *streaming*.

In the collision part we execute

$$f_i^*\left(\mathbf{x},t\right)=f_i\left(\mathbf{x},t\right)+\Omega_i\left(\mathbf{x},t\right) \tag{2.10}$$

with $f_i\left(\mathbf{x},t\right)$ the pre-collision distribution function and $f_i^*\left(\mathbf{x},t\right)$ the post-collision distribution function. As already discussed above: executing Eq. 2.10 is a *local operation*. For each lattice node $\mathbf{x}$ it only involves information at $\mathbf{x}$: since $\Omega_i\left(\mathbf{x},t\right)=-\frac{1}{\tau}\left(f_i-f_i^{eq}\right)$ the information required for a collision is $f_i\left(\mathbf{x},t\right)$ and $f_i^{eq}\left(\mathbf{x},t\right)$; the latter depends on $\rho\left(\mathbf{x},t\right)$ and $\mathbf{u}\left(\mathbf{x},t\right)$ which in turn can be determined using $f_i\left(\mathbf{x},t\right)$. Local operations are easily run on parallel compute platforms through domain decomposition: divide the overall simulation domain in subdomains and assign each subdomain to a compute core. The collision operation (Eq. 2.10) does not require any communication between compute cores.

In the streaming part of the LB algorithm we execute

$$f_i\left(\mathbf{x}+\mathbf{c_i},t+1\right)=f_i^*\left(\mathbf{x},t\right) \tag{2.11}$$

i.e. we shift ("stream") the post-collision distribution f_i^* from its current location $\mathbf{x}$ to its neighbouring location $\mathbf{x}+\mathbf{c_i}$ thereby advancing time by one time unit. This is a simple, however non-local operation. In parallel computing the streaming step requires communication over the edges of the subdomains each of which is assigned to a compute core.

2.4 Chapman-Enskog analysis

The aim of the analysis explained in this section is to "derive" the Navier-Stokes equation (Eq. 1.18, LN01) from the lattice-Boltzmann equation. We will be using the LB equation in lattice units and the BGK collision operator. At some point in the derivation we will be needing the specific velocity set for which we will use the D2Q9 set (Eqs. 2.5 and 2.6), as well as the specific expression for the equilibrium distribution for which we take Eq. 2.8.

Here we go: LB equation:

$$f_i\left(\mathbf{x}+\mathbf{c_i},t+1\right)-f_i\left(\mathbf{x},t\right)=-\frac{1}{\tau}\left[f_i\left(\mathbf{x},t\right)-f_i^{eq}\left(\mathbf{x},t\right)\right] \tag{2.12}$$

We expand the distribution function around its equilibrium and introduce the "small" parameter ε:

$$f_i=f_i^{eq}+\varepsilon f_i^{(1)}+\varepsilon^2 f_i^{(2)}+\ldots \tag{2.13}$$

Given that (see above) $\sum_i \left(f_i - f_i^{eq} \right) = 0$ and $\sum_i c_{i\alpha} \left(f_i - f_i^{eq} \right) = 0$, it has to be that $\sum_i f_i^{(n)} = 0$ and $\sum_i c_{i\alpha} f_i^{(n)} = 0$ for $n \geq 1$.

Now comes the – to me – most confusing step in the Chapman-Enskog analysis. It involves expanding the derivatives in the small parameter ε:

$$\frac{\partial f_i}{\partial t} = \varepsilon \frac{\partial^{(1)}}{\partial t} f_i + \varepsilon^2 \frac{\partial^{(2)}}{\partial t} f_i + \ldots; \quad c_{i\alpha} \frac{\partial f_i}{\partial x_\alpha} = \varepsilon c_{i\alpha} \frac{\partial^{(1)}}{\partial x_\alpha} f_i \tag{2.14}$$

The $\partial^{(1)}$ and $\partial^{(2)}$ are not derivatives by themselves, they represent contributions to derivatives with certain orders of magnitude in ε.

Now perform a 2nd order Taylor expansion of the LB equation (Eq. 2.12).

$$\left(\frac{\partial}{\partial t} + c_{i\alpha} \frac{\partial}{\partial x_\alpha} \right) f_i + \tfrac{1}{2} \left(\frac{\partial}{\partial t} + c_{i\alpha} \frac{\partial}{\partial x_\alpha} \right)^2 f_i = -\frac{1}{\tau} \left(f_i - f_i^{eq} \right) \tag{2.15}$$

We want to get rid of the 2nd derivative in Eq. 2.15. We can do so by applying the operator $\frac{1}{2} \left(\frac{\partial}{\partial t} + c_{i\alpha} \frac{\partial}{\partial x_\alpha} \right)$ to Eq. 2.15. This gets us

$$\frac{1}{2} \left(\frac{\partial}{\partial t} + c_{i\alpha} \frac{\partial}{\partial x_\alpha} \right)^2 f_i + hot = -\frac{1}{2\tau} \left(\frac{\partial}{\partial t} + c_{i\alpha} \frac{\partial}{\partial x_\alpha} \right) \left(f_i - f_i^{eq} \right) \tag{2.16}$$

(*hot* stands for *higher-order terms* that we subsequently neglect). Subtracting Eq. 2.16 from 2.15 (and discarding the *hot*) gets us

$$\left(\frac{\partial}{\partial t} + c_{i\alpha} \frac{\partial}{\partial x_\alpha} \right) f_i = -\frac{1}{\tau} \left(f_i - f_i^{eq} \right) + \frac{1}{2\tau} \left(\frac{\partial}{\partial t} + c_{i\alpha} \frac{\partial}{\partial x_\alpha} \right) \left(f_i - f_i^{eq} \right) \tag{2.17}$$

Now we substitute the expansions in Eqs. 2.13 and 2.14 and group the terms by orders of ε. Each group establishes one equation since ε can take any (small) value.

Terms of order ε

$$\left(\frac{\partial^{(1)}}{\partial t} + c_{i\alpha} \frac{\partial^{(1)}}{\partial x_\alpha} \right) f_i^{eq} = -\frac{1}{\tau} f_i^{(1)} \tag{2.18}$$

Terms of order ε^2

$$\left(\frac{\partial^{(1)}}{\partial t} + c_{i\alpha} \frac{\partial^{(1)}}{\partial x_\alpha} \right) f_i^{(1)} + \frac{\partial^{(2)}}{\partial t} f_i^{eq} = -\frac{1}{\tau} f_i^{(2)} + \frac{1}{2\tau} \left(\frac{\partial^{(1)}}{\partial t} + c_{i\alpha} \frac{\partial^{(1)}}{\partial x_\alpha} \right) f_i^{(1)} \tag{2.19}$$

Rewrite Eq. 2.19:

$$\frac{\partial^{(2)}}{\partial t} f_i^{eq} + \left(1 - \frac{1}{2\tau}\right)\left(\frac{\partial^{(1)}}{\partial t} + c_{i\alpha}\frac{\partial^{(1)}}{\partial x_\alpha}\right) f_i^{(1)} = -\frac{1}{\tau} f_i^{(2)} \tag{2.20}$$

Add up Eqs. 2.18×ε and 2.20×ε^2:

$$\varepsilon\frac{\partial^{(1)}}{\partial t} f_i^{eq} + \varepsilon^2\frac{\partial^{(2)}}{\partial t} f_i^{eq} + \varepsilon c_{i\alpha}\frac{\partial^{(1)}}{\partial x_\alpha} f_i^{eq} + \varepsilon^2\left(1 - \frac{1}{2\tau}\right)\left(\frac{\partial^{(1)}}{\partial t} + c_{i\alpha}\frac{\partial^{(1)}}{\partial x_\alpha}\right) f_i^{(1)} = -\varepsilon\frac{1}{\tau} f_i^{(1)} - \varepsilon^2\frac{1}{\tau} f_i^{(2)} \tag{2.21}$$

Revert some expanded derivatives to their ordinary form:

$$\frac{\partial}{\partial t} f_i^{eq} + c_{i\alpha}\frac{\partial}{\partial x_\alpha} f_i^{eq} + \varepsilon^2\left(1 - \frac{1}{2\tau}\right)\left(\frac{\partial^{(1)}}{\partial t} + c_{i\alpha}\frac{\partial^{(1)}}{\partial x_\alpha}\right) f_i^{(1)} = -\varepsilon\frac{1}{\tau} f_i^{(1)} - \varepsilon^2\frac{1}{\tau} f_i^{(2)} \tag{2.22}$$

If we sum Eq. 2.22 over *i*, only the first two terms survive (since $\sum_i f_i^{(n)} = 0$ and $\sum_i c_{i\alpha} f_i^{(n)} = 0$ for $n \geq 1$) and we end up with the continuity equation

$$\frac{\partial}{\partial t}\rho + \frac{\partial}{\partial x_\alpha}\rho u_\alpha = 0 \tag{2.23}$$

Now multiply Eq. 2.22 by $c_{i\beta}$ and sum over *i*:

$$\frac{\partial}{\partial t}\left(\rho u_\beta\right) + \frac{\partial}{\partial x_\alpha}\sum_i c_{i\alpha} c_{i\beta} f_i^{eq} + \left(1 - \frac{1}{2\tau}\right)\frac{\partial}{\partial x_\alpha}\sum_i \varepsilon c_{i\alpha} c_{i\beta} f_i^{(1)} = 0 \tag{2.24}$$

Given the first term, this might be a momentum balance. For interpretation of the other two terms we need to involve the velocity set and the equilibrium distribution (Eqs. 2.5, 2.6 & 2.8). This allows us to derive (with a view to the 2nd term in Eq. 2.24)

$$\sum_i c_{i\alpha} c_{i\beta} f_i^{eq} = \rho u_\alpha u_\beta + \rho c_s^2 \delta_{\alpha\beta} \tag{2.25}$$

We now need to think hard about the term in Eq. 2.24 that contains $\sum_i c_{i\alpha} c_{i\beta} f_i^{(1)}$.

For this we go back to Eq. 2.18, repeated here: $\left(\frac{\partial^{(1)}}{\partial t} + c_{i\alpha}\frac{\partial^{(1)}}{\partial x_\alpha}\right) f_i^{eq} = -\frac{1}{\tau} f_i^{(1)}$, since it contains $f_i^{(1)}$. Multiply Eq. 2.18 by $c_{i\beta} c_{i\gamma}$ and sum over *i*:

$$\frac{\partial^{(1)}}{\partial t}\sum_i c_{i\alpha} c_{i\beta} f_i^{eq} + \frac{\partial^{(1)}}{\partial x_\alpha}\sum_i c_{i\alpha} c_{i\beta} c_{i\gamma} f_i^{eq} = -\frac{1}{\tau}\sum_i c_{i\alpha} c_{i\beta} f_i^{(1)} \tag{2.26}$$

This allows us to express $\sum_i c_{i\alpha} c_{i\beta} f_i^{(1)}$ in terms of the equilibrium distribution and the set of velocities. This is a "hell of a job", the result is

$$\sum_i c_{i\alpha} c_{i\beta} f_i^{(1)} = -\rho c_s^2 \tau \left[\frac{\partial^{(1)} u_\alpha}{\partial x_\beta} + \frac{\partial^{(1)} u_\beta}{\partial x_\alpha} \right] + \tau \frac{\partial^{(1)}}{\partial x_\gamma} \left(\rho u_\alpha u_\beta u_\gamma \right) \tag{2.27}$$

We return to our momentum balance Eq. 2.24 and substitute our findings Eqs. 2.25 and 2.27:

$$\frac{\partial}{\partial t}\left(\rho u_\beta\right) + \frac{\partial}{\partial x_\alpha}\left(\rho u_\alpha u_\beta + \rho c_s^2 \delta_{\alpha\beta}\right) + \left(1 - \frac{1}{2\tau}\right) \frac{\partial}{\partial x_\alpha} \left(-\rho c_s^2 \tau \varepsilon \left[\frac{\partial^{(1)} u_\alpha}{\partial x_\beta} + \frac{\partial^{(1)} u_\beta}{\partial x_\alpha} \right] + \tau \varepsilon \frac{\partial^{(1)}}{\partial x_\gamma} \left(\rho u_\alpha u_\beta u_\gamma \right) \right) = 0$$

This can be simplified: we turn $\varepsilon \frac{\partial^{(1)}}{\partial x_\beta}$ to $\frac{\partial}{\partial x_\beta}$; $\frac{\partial}{\partial x_\alpha}\left(\rho c_s^2 \delta_{\alpha\beta}\right) = c_s^2 \frac{\partial \rho}{\partial x_\beta}$ and we get

$$\frac{\partial}{\partial t}\left(\rho u_\beta\right) + \frac{\partial}{\partial x_\alpha}\left(\rho u_\alpha u_\beta\right) = -c_s^2 \frac{\partial \rho}{\partial x_\beta} + \left(\tau - \tfrac{1}{2}\right) \frac{\partial}{\partial x_\alpha} \left(\rho c_s^2 \left[\frac{\partial u_\alpha}{\partial x_\beta} + \frac{\partial u_\beta}{\partial x_\alpha} \right] - \frac{\partial}{\partial x_\gamma} \left(\rho u_\alpha u_\beta u_\gamma \right) \right) \tag{2.28}$$

We finally argue that the term containing the product of three velocities $\frac{\partial}{\partial x_\gamma}\left(\rho u_\alpha u_\beta u_\gamma\right)$ is negligibly small, at least in the low Mach number limit (the Mach number and a discussion on compressibility will be in LN03).

We now write Eq. 2.28 in a (compressible) Navier-Stokes-like form

$$\frac{\partial}{\partial t}\left(\rho u_\beta\right) + \frac{\partial}{\partial x_\alpha}\left(\rho u_\alpha u_\beta\right) = -\frac{\partial p}{\partial x_\beta} + \nu \frac{\partial}{\partial x_\alpha} \left(\rho \left[\frac{\partial u_\alpha}{\partial x_\beta} + \frac{\partial u_\beta}{\partial x_\alpha} - \tfrac{2}{3} \delta_{\alpha\beta} \frac{\partial u_\gamma}{\partial x_\gamma} \right] + \tfrac{2}{3} \rho \delta_{\alpha\beta} \frac{\partial u_\gamma}{\partial x_\gamma} \right) \tag{2.28}$$

with $p = c_s^2 \rho$ the much anticipated ideal-gas relation between density and pressure, and $\nu = c_s^2 \left(\tau - \tfrac{1}{2}\right)$ the again much anticipated relation between relaxation time and kinematic viscosity. The bulk viscosity is two-thirds of the (shear) viscosity.

2.5 Discrete equilibrium distribution function

A cornerstone of kinetic theory is the Maxwell-Boltzmann equilibrium distribution function, Eq. 1.6 of LN01, repeated here

$$f^{eq}\left(\mathbf{x}, |\mathbf{v}|, t\right) = \rho \left(\frac{1}{2\pi RT} \right)^{3/2} e^{-|\mathbf{v}|^2/(2RT)} \tag{2.29}$$

In the Chapman-Enskog exercise of the previous section we made use of a discrete version of the equilibrium distribution function, Eq. 2.8 (repeated here as Eq. 2.30)

$$f_i^{eq} = w_i \rho \left[1 + \frac{u_\alpha c_{i\alpha}}{c_s^2} + \frac{\left(u_\alpha c_{i\alpha}\right)^2}{2c_s^4} - \frac{u_\alpha u_\alpha}{2c_s^2} \right] \tag{2.30}$$

In this section I would like to show how – globally, not very rigorously – the two expressions (Eqs. 2.29 and 2.30) are related.

As a first step we realize that the velocity **v** in Eq. 2.29 is the random (thermal) velocity of the molecules, i.e. the velocity $\boldsymbol{\xi}$ was decomposed in a bulk velocity **u** and thermal velocity **v**: $\boldsymbol{\xi} = \mathbf{v} + \mathbf{u}$. The second step is to simplify Eq. 2.29. We make it dimensionless and consider isothermal conditions. As a result of these two steps the Maxwell-Boltzmann distribution becomes $f^{eq} = \rho \left(\frac{1}{2\pi} \right)^{3/2} e^{-|(\boldsymbol{\xi}-\mathbf{u})|^2/2}$. If we assume that the bulk speed is much smaller than the thermal speed we can perform a Taylor expansion of f^{eq} around $\mathbf{u} = \mathbf{0}$ and break it off at second order:

$$f^{eq} \approx \rho\, \omega(\boldsymbol{\xi}) \left[1 + \xi_\alpha u_\alpha + \tfrac{1}{2} u_\alpha u_\beta \left(\xi_\alpha \xi_\beta - \delta_{\alpha\beta} \right) \right] \tag{2.31}$$

where we – for brevity – introduced the function $\omega(\boldsymbol{\xi}) \equiv \left(\frac{1}{2\pi} \right)^{3/2} e^{-|\boldsymbol{\xi}|^2/2}$. In Eq. 2.31 we still have a continuous velocity $\boldsymbol{\xi}$, so that the next step is to discretize velocity space. This we can – very naively – do in the following way

$$f_i^{eq} = \rho w_i \left[1 + \xi_{i\alpha} u_\alpha + \tfrac{1}{2} u_\alpha u_\beta \left(\xi_{i\alpha} \xi_{i\beta} - \delta_{\alpha\beta} \right) \right] \tag{2.32}$$

where we have replaced continuous $\omega(\boldsymbol{\xi})$ by discrete w_i and have replaced continuous ξ_α by discrete $\xi_{i\alpha}$. We now can determine w_i and relate $\xi_{i\alpha}$ to $c_{i\alpha}$ (the latter is the discrete set of lattice velocities) by demanding that the BGK collision operator $\Omega_i(f) = -\frac{1}{\tau}\left(f_i - f_i^{eq} \right)$ conserves mass, momentum and energy. The result then is $f_i^{eq} = w_i \rho \left[1 + \frac{u_\alpha c_{i\alpha}}{c_s^2} + \frac{\left(u_\alpha c_{i\alpha}\right)^2}{2c_s^4} - \frac{u_\alpha u_\alpha}{2c_s^2} \right]$ (with $c_s^2 = 1/3$ and w_i as given in Eq. 2.6) which is what we anticipated in Eq. 2.30.

2.6 A few closing remarks

While the LB algorithm is very simple, its mathematical principles are quite complex.

In the next set of lecture notes (LN03) we will be discussing a number of more practical aspects. First and foremost what to do near the boundaries of a flow domain: how to impose no-slip, free slip, periodic etc. boundary conditions. In the second place we need to discuss compressibility. Clearly the method is compressible: information travels with finite speed since a distribution function only travels one lattice distance per time step and also the speed of sound ($c_s = \sqrt{1/3}$) is a finite number. Still, we want to apply the method to incompressible flow. In the third place it needs to be established how to translate a physical flow system (with e.g. SI units) into a LB simulation in lattice units.