1 From Boltzmann to Lattice Boltzmann

We start from the Boltzmann equation:

$$\partial_t f + v \cdot \nabla_x f = -\frac{1}{\tau}(f - f^{eq}) \tag{1}$$

Step 1: Discretisation of velocity space → Restrict to discrete velocity set c_i, $i = 1, ..., Q$

$$\Rightarrow \partial_t f_i + c_i \cdot \nabla_x f_i = -\frac{1}{\tau}(f_i - f_i^{eq}), \quad i = 1, ..., Q \tag{2}$$

- Derivation of f_i^{eq}: See next section

Step 2: Discretisation of left hand side of Eq. (2):

- $\partial_t f_i \approx \frac{f_i(x,t+dt) - f_i(x,t)}{dt}$ → Euler timestepping
- $c_i \cdot \nabla_x f_i \approx \|c_i\| \cdot \frac{f_i(x+c_i dt, t+dt) - f_i(x,t+dt)}{\|c_i\| dt}$ → time-implicit integration along (discrete characteristic) c_i

Step 3: Discretisation of right hand side of Eq. (2): Crank-Nicolson (for reasons of accuracy)

$$-\frac{1}{\tau}(f_i - f_i^{eq}) \approx \frac{1}{2}\left(-\frac{1}{\tau}(f_i(x,t) - f_i^{eq}(x,t)) - \frac{1}{\tau}(f_i(x + c_i dt, t + dt) - f_i^{eq}(x + c_i dt, t + dt))\right) \tag{3}$$

Setting Step 2 and 3 into Eq. (2) results in:

$$f_i(x + c_i dt, t + dt) + \frac{dt}{2\tau}\left(f_i(x + c_i dt, t + dt) - f_i^{eq}(x + c_i dt, t + dt)\right) \quad = \quad f_i(x,t)\left(1 - \frac{dt}{2\tau}\right) + \frac{dt}{2\tau} f_i^{eq}(x,t) \tag{4}$$

Step 4: Re-definition of distribution functions

- Define

  $$\overline{f}_i(x,t) := f_i(x,t) + \frac{dt}{2\tau}(f_i(x,t) - f_i^{eq}(x,t)), \tag{5}$$

  which is equivalent to

  $$f_i(x,t) = \frac{2\tau}{2\tau + dt}\overline{f}_i(x,t) + \frac{dt}{2\tau + dt} f_i^{eq}(x,t). \tag{6}$$

- Setting Eq. (5),(6) into Eq. (4), yields:

  $$\overline{f}_i(x + c_i dt, t + dt) = \frac{2\tau}{2\tau + dt}\left(1 - \frac{dt}{2\tau}\right)\overline{f}_i(x,t) + \frac{dt}{2\tau + dt}\left(1 - \frac{dt}{2\tau}\right) f_i^{eq}(x,t) + \frac{dt}{2\tau} f_i^{eq}(x,t) \tag{7}$$

- Evaluating the coefficients in Eq. (7) yields:

  $$\frac{2\tau}{2\tau + dt}\left(1 - \frac{dt}{2\tau}\right) \quad = \quad 1 - \frac{dt}{\tau + dt/2} \tag{8}$$

  $$\tag{9}$$

  $$\frac{dt}{2\tau + dt}\left(1 - \frac{dt}{2\tau}\right) + \frac{dt}{2\tau} \quad = \quad \frac{dt}{\tau + dt/2} \tag{10}$$

  Hence, we obtain the LBM:

  $$\overline{f}_i(x + c_i dt, t + dt) = \overline{f}_i(x,t) - \frac{dt}{\tau + dt/2}\left(\overline{f}_i(x,t) - f_i^{eq}(x,t)\right) \tag{11}$$

Remarks:

- In order to make our populations fly to the direct neighbour cells, it must hold that $\|x_i\| = \|c_i\| \cdot dt$ where $\|x_i\|$ is the distance between the cell midpoints.
- A dimensionless form can be obtained by scaling the time units by dt and the length units by dx. Within the Lab Course, we refer to this scaling.
- Compared to the worksheet, the derived LBM equation looks a bit different $(-\frac{1}{\tau} \Leftrightarrow -\frac{dt}{\tau+dt/2})$. With the scaling $dt = 1$ and a re-definition $\tau' := \tau + \frac{1}{2}dt = \tau + \frac{1}{2}$, you exactly obtain the update formula from the worksheet. From this re-definition, one can also understand the lower bound for the relaxation time to be $\frac{1}{2}$ and NOT 0 in LBM!

2 Derivation of the discrete equilibrium distribution

The continuous Boltzmann-Maxwellian distribution is given as:

$$f^{eq}(x,v,t) = \left(\frac{m_p}{2\pi k_B T}\right)^{D/2} e^{-\frac{m_p(v-u(x,t))^2}{2k_B T}} \tag{12}$$

where $u(x,t)$ denotes the average velocity at (x,t), that is $u(x,t) = \frac{1}{\rho}\int f^{eq}(x,v,t)v dv$. For the sake of compact writing, I introduce $C_0 := \left(\frac{m_p}{2\pi k_B T}\right)^{D/2}$ and $C_1 := \frac{m_p}{2k_B T}$. Using this, we obtain

$$f^{eq}(x,v,t) = C_0 e^{-C_1 v^2} \cdot e^{C_1(2uv-u^2)} \tag{13}$$

The LBM is based on the *small Mach number* assumption. At this, we assume that the average velocities u in the system are very small compared to the single molecular velocities v. Using this assumption, we can expand the exponential of f^{eq} into a polynomial in u. Therefore, we define a function $g^{eq}_{x,v,t}(u) := f^{eq}(x,v,t)$ (actually, we just keep all parameters in f^{eq} constant and only consider the average velocity u) and expand using the Taylor technique:

$$g^{eq}_{x,v,t}(u) = g^{eq}_{x,v,t}(0) + \nabla g^{eq}_{x,v,t}(0) \cdot u + ... \tag{14}$$

Evaluating the single terms in the Eq. (14) yields:

$$\begin{aligned} g^{eq}_{x,v,t}(u=0) &= C_0 e^{C_1 v^2} \\ \partial_{u_d} g^{eq}_{x,v,t}(u=0) &= C_0 e^{-C_1 v^2} \cdot e^{C_1(2uv-u^2)} \cdot C_1(2v_d - 2u_d) \overset{u=0}{=} C_0 e^{-C_1 v^2} 2C_1 v_d \end{aligned} \tag{15}$$

Setting these expressions into the taylor expansion form gives:

$$g^{eq}_{x,v,t}(u) \approx C_0 e^{-C_1 v^2}(1 + 2C_1(v \cdot u) + ...) \tag{16}$$

Comparing this form with the equilibrium distribution in the LBM scheme, we can clearly see how they actually relate to each other. However, the single weights $w_i = C_0 e^{-C_1 v^2}$ have not been determined yet. They arise from the requirement, that discrete integrations over all equilibrium states need to conserve the overall mass, momentum,... in the system. For example, considering the mass, we require that $\sum_i g^{eq}_{x,v,t}(c_i) = \rho$. Putting all respective requirements together, we obtain a linear equation system for the lattice weights w_i which then can be solved, using the isotropy relations that are required on the lattice. The arising weights differ for each velocity space discretisation (D3Q15,D3Q19,D3Q27 etc.). For the D3Q19 case, they are defined on worksheet 2.

3 Chapman-Enskog Expansion

Until now, we only said that we can model the flow either on the continuum scale (using the Navier-Stokes equations) or on the mesoscopic scale by LBM. However, it would also be nice to see how those scales relate to each other. The *Chapman-Enskog expansion* has been developed which shows that in the low Mach-number limit (as discussed together with the equilibrium expansion in the previous section), the Boltzmann equation – or the LBM – yields the Navier-Stokes equations. Carrying out the whole expansion is out of scope for the Lab Course. We will only consider a small outtake, deriving the continuity equation (conservation of mass) from the LBM.
In the general Navier-Stokes case, the continuity equation reads:

$$\partial_t \rho + \nabla_x \cdot (\rho u) = 0^* \tag{17}$$

Starting from the LB update rule

$$f_i(x + c_i dt, t + dt) = f_i(x,t) - \frac{dt}{\tau'}(f_i - f_i^{eq}) \tag{18}$$

where develop the left hand side into a Taylor series:

$$f_i(x + c_i dt, t + dt) = f_i(x,t) + \nabla_x f_i(x,t) c_i dt + \partial_t f_i(x,t) dt + ... \tag{19}$$

Using this expansion in Eq. (18) and splitting the distribution into equilibrium and non-equilibrium part according to $f_i = f_i^{eq} + f_i^{neq}$ results in:

$$\nabla_x f_i^{eq} c_i dt + \partial_t f_i^{eq} dt + \nabla_x f_i^{neq} c_i dt + \partial_t f_i^{neq} dt = -\frac{dt}{\tau'} f_i^{neq} \tag{20}$$

To obtain a valid expression for the fluid density (or the mass, respectively) of our system, we need to integrate over all particle populations in velocity space. In the discrete LBM form, this corresponds to a summation over i:

$$\begin{aligned} & \textstyle\sum_i \left(\nabla_x f_i^{eq} c_i dt + \partial_t f_i^{eq} dt + \nabla_x f_i^{neq} c_i dt + \partial_t f_i^{neq} dt\right) && = \textstyle\sum_i \left(-\frac{dt}{\tau'} f_i^{neq}\right) \\ \Leftrightarrow\ & dt \nabla_x \textstyle\sum_i (f_i^{eq} c_i) + dt \partial_t \sum_i (f_i^{eq}) + dt \nabla_x \sum_i (f_i^{neq} c_i) + dt \partial_t \sum_i (f_i^{neq}) && = -\frac{dt}{\tau'} \textstyle\sum_i (f_i^{neq}) \end{aligned} \tag{21}$$

We already know that it holds $\rho = \sum_i f_i = \sum f_i^{eq}$, $\rho u = \sum_i f_i c_i = \sum f_i^{eq} c_i$. From this, we can easily follow that

$$\begin{aligned} \textstyle\sum_i f_i^{neq} &= 0 \\ \textstyle\sum_i f_i^{neq} c_i &= 0. \end{aligned} \tag{22}$$

Setting these results into Eq. (21) and dividing by dt yields the general continuity equation.

4 References:

Chapman, S. and Cowling, T.G., The mathematical theory of nonuniform gases, Cambridge University Press, London, 1970

*For the incompressible case where $\rho = const.$, this equation becomes $\nabla \cdot u = 0$.

Dellar, P., An interpretation and derivation of the lattice Boltzmann method using Strang splitting, to appear in the ICMMES 2010 proceedings.

He, X. and Luo, L.-S., Theory of the lattice Boltzmann method: From the Boltzmann equation to the lattice Boltzmann equation, Phys. Rev. E 56(6), 1997