

Foundations of Multiscale Modelling: Kinetics.  
Homework 4. Boltzmann equation and hydrodynamics.  
Due 23:59 03 March.

February 22, 2022

**1. Hydrodynamic Equation and transport coefficients (4 points)**

Consider the Boltzmann equation.

(a) Derive the Navier-Stokes equation from the Boltzmann equation for the case of the external force field  $\vec{F}(\vec{r})$  (**2\* points**).

(b) Compute the viscosity coefficient  $\eta$  and thermal conductivity coefficient  $\kappa$  for the BGK model of the Boltzmann equation with the velocity dependent relaxation time:

$$\tau^{-1} = \tau_0^{-1}(V^2/v_T^2),$$

where  $v_T^2 = 2k_B T/m$  (for simplicity use the units where  $k_B = 1$ ) (**2 points**).

*Hint:* Use the Lecture Notes.

**2. Lattice Boltzmann method (10 points)**

**Description of the algorithm**

Let us consider the Lattice Boltzmann algorithm, which is implemented using the D2Q9 model. This model is two dimensional and involves 9 velocity vectors defined by (see Fig. 1)

$$\vec{e}_0 = (0, 0) \tag{1}$$

$$\vec{e}_i = (1, 0), (0, 1), (-1, 0), (0, -1) \quad i = 1, 2, 3, 4 \tag{2}$$

$$\vec{e}_i = (1, 1), (-1, 1), (-1, -1), (1, -1) \quad i = 5, 6, 7, 8 \tag{3}$$

For each particle on the lattice the probability distribution function  $f_i(x, t)$  is associated, which describes the probability of streaming in one particular direction. The macroscopic fluid

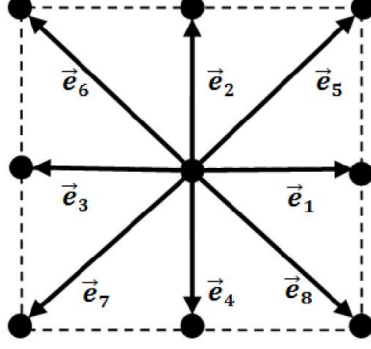


Figure 1: Illustration of a lattice node of the D2Q9 model.

density can be defined as a summation of microscopic particle distribution function

$$\rho(\vec{x}, t) = \sum_{i=0}^8 f_i(\vec{x}, t) \quad (4)$$

The macroscopic velocity is defined in the following way:

$$\vec{u}(\vec{x}, t) = \frac{1}{\rho} \sum_{i=0}^8 f_i(\vec{x}, t) \vec{e}_i \quad (5)$$

The key steps in LBM are the streaming and collision processes which are given by

$$f_i(\vec{x} + \vec{e}_i \Delta t, t + \Delta t) - f_i(\vec{x}, t) = -\frac{[f_i(\vec{x}, t) - f_i^{eq}(\vec{x}, t)]}{\tau} \quad (6)$$

Here  $f_i^{eq}(x, t)$  is the equilibrium distribution and  $\tau$  is considered as relaxation time towards equilibrium. We use the Bhatnagar-Gross-Krook collision model where

$$f_i^{eq}(\vec{x}, t) = \omega_i \rho + \rho s_i(\vec{u}(\vec{x}, t)) \quad (7)$$

$$s_i(\vec{u}) = \omega_i \left( 3(\vec{e}_i \cdot \vec{u}) + \frac{9}{2} (\vec{e}_i \cdot \vec{u})^2 - \frac{3}{2} (\vec{u} \cdot \vec{u}) \right) \quad (8)$$

and the weights  $\omega_i = 4/9$  for  $i = 0$ ,  $\omega_i = 1/9$  for  $i = 1, 2, 3, 4$ ,  $\omega_i = 1/36$  for  $i = 5, 6, 7, 8$ .

### Simulation of the Poiseuille flow by the Lattice Boltzmann approach

We use the following initial and boundary conditions for the velocity components  $u_x$  and  $u_y$  and density  $\rho$ :

$$u_x(x, 0, t) = u_y(x, 0, t) = 0 \quad (9)$$

$$u_x(x, H, t) = u_y(x, H, t) = 0 \quad (10)$$

$$\rho(0, y, t) = \rho_0 \quad (11)$$

$$\rho(L, y, t) = \rho_1 \quad (12)$$

The numerical algorithm can be implemented in the following way:

1. We initialize  $f_i = 1/9$  for all nodes.
2. The streaming step: we move  $f_i$  in the direction of  $\vec{e}_i$  according to:

$$f_1[i][j] = f_1[i-1][j]; \quad (13)$$

$$f_2[i][j] = f_2[i][j-1]; \quad (14)$$

$$f_3[i][j] = f_3[i+1][j]; \quad (15)$$

$$f_4[i][j] = f_4[i][j+1]; \quad (16)$$

$$f_5[i][j] = f_5[i-1][j-1]; \quad (17)$$

$$f_6[i][j] = f_6[i+1][j-1]; \quad (18)$$

$$f_7[i][j] = f_7[i+1][j+1]; \quad (19)$$

$$f_8[i][j] = f_8[i-1][j+1]; \quad (20)$$

Here  $[i]$  corresponds to the position along the x axis,  $[j]$  - along the y axis.

3. The boundary conditions are implemented in the following way. On the left boundary the density is defined according to  $\rho_{in} = 1.5$ . On the right boundary  $\rho_{out} = 0.5$ . On the upper and bottom lines we set the sticking boundary conditions  $u_x = 0$ ,  $u_y = 0$ .

*Lower boundary.*

On the lower boundary we define  $u_x = 0$ ,  $u_y = 0$ . The probability distribution functions  $f_i$  are known for  $i = 1, 3, 4, 7, 8$ . We need to calculate  $f_i$  for  $i = 2, 5, 6$ . Eqs. (4-5) give:

$$f_2 + f_5 + f_6 = \rho - (f_0 + f_1 + f_3 + f_4 + f_7 + f_8) \quad (21)$$

$$f_5 - f_6 = f_3 + f_7 - f_1 - f_8 \quad (22)$$

$$f_2 + f_5 + f_6 = f_7 + f_4 + f_8 \quad (23)$$

In such a way the density  $\rho$  can be determined according to:

$$\rho = f_0 + f_1 + f_3 + 2(f_4 + f_7 + f_8) \quad (24)$$

$f_2$  can be defined according to the bounce-back rule for the non-equilibrium part of the particle distribution:

$$f_2 - f_2^{eq} = f_4 - f_4^{eq} \quad (25)$$

According to Eq. (7)  $f_2^{eq} = f_4^{eq} = \rho/9$  and

$$f_2 = f_4 \quad (26)$$

Solving Eq. (21) and using Eq. (26) one can get:

$$f_2 = f_4 \quad (27)$$

$$f_5 = f_7 - \frac{1}{2}(f_1 - f_3) \quad (28)$$

$$f_6 = f_8 + \frac{1}{2}(f_1 - f_3) \quad (29)$$

*Left boundary.*

On the boundary we define  $\rho_{in} = 1.5$ ,  $u_y = 0$ .  $f_2, f_3, f_4, f_6, f_7$  are known,  $f_1, f_5, f_8$  are unknown. They are defined according to

$$f_1 + f_5 + f_8 = \rho_{in} - (f_0 + f_2 + f_3 + f_4 + f_6 + f_7) \quad (30)$$

$$f_1 + f_5 + f_8 = \rho_{in} u_x + f_3 + f_6 + f_7 \quad (31)$$

$$f_5 - f_8 = -f_2 + f_4 - f_6 + f_7 \quad (32)$$

Using these rules, one can calculate the velocity

$$u_x = 1 - \frac{f_0 + f_2 + f_4 + 2(f_3 + f_6 + f_7)}{\rho_{in}} \quad (33)$$

For the non-equilibrium part the bounceback rule can be used:

$$f_1 - f_1^{eq} = f_3 - f_3^{eq} \quad (34)$$

In such a way, the remaining probability distribution functions can be calculated according to

$$f_1 = f_3 + \frac{2}{3} \rho_{in} u_x \quad (35)$$

$$f_5 = f_7 - \frac{1}{2} (f_2 - f_4) + \frac{1}{6} \rho_{in} u_x \quad (36)$$

$$f_8 = f_6 + \frac{1}{2} (f_2 - f_4) + \frac{1}{6} \rho_{in} u_x \quad (37)$$

*The boundary conditions in the left upper corner.*

Now let us discuss the boundary condition for the corner nodes. Let us consider the left upper corner as an example. Here the probability distributions  $f_2, f_3$  and  $f_6$  are known. The unknown probability distribution functions are determined according to the bounceback condition:

$$f_8 = f_6 \quad (38)$$

$$f_1 = f_3 \quad (39)$$

$$f_4 = f_2 \quad (40)$$

$$f_5 = f_7 = \frac{1}{2} (\rho_{in} - (f_0 + f_1 + f_2 + f_3 + f_4 + f_6 + f_8)) \quad (41)$$

(a) Calculate the boundary conditions for the right boundary with  $\rho_{out} = 0.5$ ,  $u_y = 0$  and for the upper boundary with  $u_x = 0$ ,  $u_y = 0$ . Derive the boundary conditions in the left bottom corner, right upper and right bottom corners (**3 points**).

(b) Implement the Lattice Boltzmann algorithm (D2Q9 model) in two dimensions in order to simulate the Poiseuille flow. Compute and plot the velocity profile ( $u_x$  versus  $y$ ) in the

middle of the channel in the steady state. The number of nodes in the simulation  $N_x = 100$  and  $N_y = 20$ . Check if it agrees with the parabolic Poiseuille flow **(7 points)**.

*Literature*

1. Qisu Zou, Xiaoyi He. *On pressure and velocity boundary conditions for the lattice Boltzmann BGK model*. Phys. Fluids **9**, 1591 (1997).
2. Yuanxun Bill Bao, Justin Meskas. *Lattice Boltzmann method for fluid simulations*. (2011)