Assignment One

CL 469 - Lattice Boltzmann method for fluid flow

Date: 10-03-25 **Submission due date: 19-03-25**

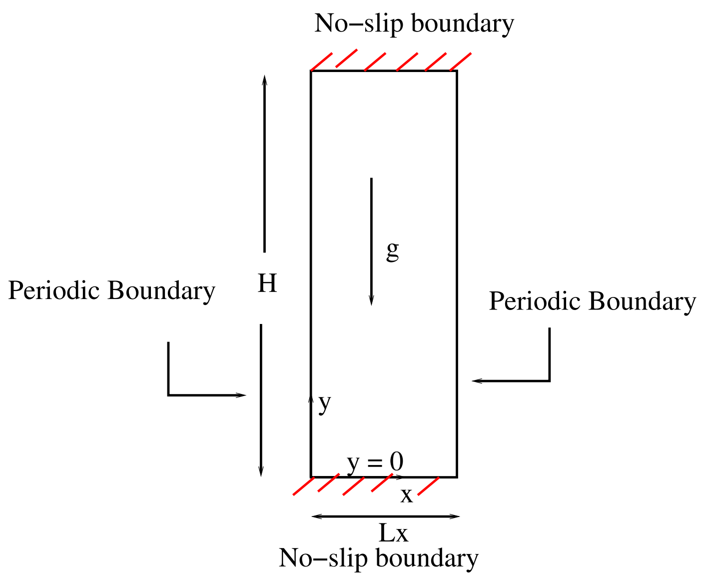
Maximum Marks: 10 **Weightage: 10%**

- The assignment needs to be submitted individually. You are encouraged to write your own lattice Boltzmann code. It is perfectly fine to use external sources (including snippets given in the course tutorial, ChatGPT, Deepseek, Gemini Code Assist and other online resources) to develop your version of the code. In all cases, **it is necessary** to mention which resources you have consulted in the assignment report. Failure to report the use of external resources will be treated as academic malpractice.

- A report (pdf format) and the code used for the assignment need to be submitted as a single compressed/zip file. Name the zip file as *assignment_one_your_roll_number.zip*. To keep the size of the zip file manageable, please ensure that data generated during simulations is **not** included in the zip file. The code file(s) is expected to be $\sim 10 - 100$ KB, while the report is less than ~ 5 MB. Ensure that the code compiles and produces results that are consistent with the answers/data in the pdf report.

- It is okay to discuss the questions asked in the report preparation with class fellows, the teaching assistant and the course instructor. Copying the code and answers from class fellows will be considered academic malpractice.

Problem statement: Consider an air column of height H above the ground. Assume ideal gas behaviour for the air with the equation of state being $p = \rho c_s^2$. For simplicity, consider a two-dimensional situation where gravity is acting downwards (in $-y$ direction) and switched on at $t = 0$. Walls close the air column at the top and bottom. Boundary conditions on lateral sides are periodic. The initial density is ρ_0 and fluid velocity $\mathbf{u} = 0$ everywhere. Gravity $g_y = 9.8\ \frac{m}{s^2}$, air column height $H = 4730\ m$, air density $\rho_0 = 1\ \frac{kg}{m^3}$, speed of sound in air $c_{\text{s,air}} = 340\ m/s$ and kinematic viscosity $\nu = 2 \times 10^{-5}\ \frac{m^2}{s}$. Find the steady-state density and pressure profile in the column.



The mass and momentum balance equations are

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0$$

$$\rho \left(\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} \right) = -\nabla p + \mu \nabla^2 \mathbf{u} + \rho \mathbf{g}$$

with the equation of state

$$p = \rho c_s^2 = \rho R T, \tag{1}$$

where R is specific gas constant and T is temperature.

Assuming that the system reaches a steady state with zero fluid velocity everywhere (referring to a case where pressure and fluid velocity do not change with time in some reference frame),

Force balance in y direction using the equation of state gives,

$$0 = -\frac{\partial p}{\partial y} - \rho g_y$$

Using equation of state $p = \rho c_s^2 = \rho R T$

$$0 = -c_s^2 \frac{\partial \rho}{\partial y} - \rho g_y$$

or

$$\rho = \rho_b \exp\left[-\frac{y g_y}{c_s^2}\right], \qquad p = p_b c_s^2 \exp\left[-\frac{y g_y}{c_s^2}\right], \tag{2}$$

where ρ_b, p_b are density and pressure at the $y = 0$, respectively. To find fluid density at the bottom ρ_b, we use the mass conservation principle

$$m = \int_0^{\Delta z} \int_0^{L_x} \int_0^{H} \rho \; \mathrm{d}y \; \mathrm{d}x \; \mathrm{d}z \tag{3}$$

$$= \rho_b L_x \Delta z \left(-\frac{c_s^2}{g_y}\right) \exp\left[-\frac{y g_y}{c_s^2}\right]\Bigg|_{y=0}^{y=H} \tag{4}$$

$$\rho_0 H L_x \Delta z = \rho_b L_x \Delta z \frac{c_s^2}{g_y}\left[1 - \exp\left[-\frac{H g_y}{c_s^2}\right]\right], \tag{5}$$

which is equal to the initial mass of the air column $m = \rho_0 H L_x \Delta z$.

$$\rho_b = \rho_0 \frac{H g_y}{c_s^2} \frac{1}{\left[1 - \exp\left[-\frac{H g_y}{c_s^2}\right]\right]} \tag{6}$$

$$= \frac{\rho_0 \alpha}{[1 - \exp[-\alpha]]}, \qquad \alpha = \frac{H g_y}{c_s^2} \tag{7}$$

Combining Eqs.(7 and 2)

$$\rho = \frac{\rho_0 \alpha}{[1 - \exp[-\alpha]]} \exp\left[-\frac{\alpha y}{H}\right], \qquad \alpha = \frac{H g_y}{c_s^2} \tag{8}$$

lattice Boltzmann algorithm:

1. Initial fluid velocity $\mathbf{u}(\mathbf{x}, t = 0)$ and density $\rho(\mathbf{x}, t = 0)$ distribution are given everywhere. Equilibrium fluid populations at time t=0 can then be found. Initialize the fluid populations with equilibrium fluid populations. In this problem, the initial velocity is zero everywhere and density is uniform ρ_0

$$f_i(\mathbf{x}, t = 0) = f_i^{\mathrm{eq}}(\mathbf{x}, t = 0) = w_i \rho_{lb} \tag{9}$$

2. Time iteration loop

(a) Update density and velocity

$$\rho = \sum_i f_i \tag{10}$$

$$\rho \mathbf{u} = \sum_i f_i \mathbf{c}_i + \frac{\Delta t}{2}\mathbf{F} \tag{11}$$

Note the presence of a force term (force per unit volume) on the right-hand side of Eq. (11). We will discuss the inclusion of force terms in the Chapman-Enskog analysis in the coming sessions. How to code force inclusion is discussed in the class. In the current problem $\mathbf{F} = \rho \mathbf{g}$ and $\mathbf{F} \neq \mathbf{g}$.

(b) Collide fluid populations

$$f_i^* = \left(1 - \frac{\Delta t}{\tau}\right) f_i + \frac{\Delta t}{\tau} f_i^{\mathrm{eq}} + F_i \tag{12}$$

Here, we have used the BGK collision operator, and f_i^* are post-collision fluid populations. We use the Guo scheme to include the force term

$$F_i = \left(1 - \frac{\Delta t}{2\tau}\right) w_i \left(\frac{\mathbf{c}_i - \mathbf{u}}{c_\mathrm{s}^2} + \frac{(\mathbf{c}_i \cdot \mathbf{u})}{c_\mathrm{s}^4}\mathbf{c}_i\right) \cdot \mathbf{F}\Delta t, \tag{13}$$

$\mathbf{F}$ in the equations 13 and 11 are the same. The lattice force terms F_i are 13 and 12 are the same.

(c) Propagate fluid populations

$$f_i(\mathbf{x} + \mathbf{c}_i \Delta t, t + \Delta t) = f_i^*(\mathbf{x}, t) \tag{14}$$

(d) Apply boundary conditions
we have discussed the no-slip (bounce-back) and periodic boundary conditions. Sufficient for this problem. Periodic boundaries at $x = 0$ and $x = L_x$ and bounce-back at top ($y = L_y$) and bottom ($y = 0$).

3. Exit the code

Choice of simulation parameters and corresponding conversion factors (sections 7.1 and 7.2 textbook):

General considerations

1. The time step $\Delta t = 1$ and grid spacing $\Delta x = 1$ are fixed. Simulation parameters are always reported in lattice units, which are dimensionless. For example, relaxation parameter $\tau = 1$, kinematic viscosity $\nu = 1$, density $\rho = 1$, gravity component $g = 10^{-6}$ and so on.

2. For the moment, we know only the simple BGK collision operator. For simple flows, BGK operator works for relaxation parameters in the range $0.55 < \tau < 1.5$. The lower limit on τ is related to the stability, while the upper limit results from slip on solid walls. It may, of course, work outside the said range, too, if the flow is unidirectional.

3. The problems we are interested in this course are incompressible/weakly compressible flow situations. Thus, we do not match the Mach number in the real world and in our simulations. The current problem involves only steady state with $\mathbf{u} = 0$ resulting in zero Reynolds Number $\mathrm{Re} = 0$ and Mach number $\mathrm{Ma} = 0$. The Mach number in simulations is lattice Mach number $\mathrm{Ma} = \frac{|\mathbf{u}|}{c_\mathrm{s}}$ has to be kept much smaller than 1 at all times. This means that although the Mach number is zero at steady-state, we have to ensure that at no point (in space and time) the fluid velocity becomes comparable to the lattice speed of sound. A general rule of thumb is to keep Ma less than 10^{-2} or fluid velocity magnitude $|\mathbf{u}|$ less than 10^{-3} at all times.

4. The Highest possible velocity in simulation at any time can be estimated by dimensional analysis. There are multiple ways of generating velocity dimensions from the given quantities.
   (a) From Eq. (11), we note that $\rho\mathbf{u} \sim \mathbf{F}\Delta t$. $\sim$ stands for scales as. In the current problem, $F_y = \rho g_y$. Given that $\frac{|\mathbf{u}|}{c_s} \ll 1$, it is necessary that $\rho g_y \Delta t \ll \rho c_\mathrm{s}$.
   (b) Combining kinematic viscosity and gravity $u \sim \frac{g_y}{\nu} L^2 \ll c_\mathrm{s}$. L here is typical lattice (grid) points that resolve the space between two solid surfaces or typical characteristic length scale.
   (c) Combining gravity and height of the column $u \sim \sqrt{g_y H} \ll c_\mathrm{s}$. You might remember from high-school physics lessons about Torricelli's law $u = \sqrt{g_y H}$ for a frictionless fluid flowing out of a container with height H. This scaling tells the speed gathered by an object falling freely under gravity g_y through a height H. This scaling in the current problem corresponds to the case of no wall at the bottom. That is, the scaling over-predicts the maximum possible velocity in the simulations.

   As we shall see scaling given by points 4b, 4c is too restrictive for the current one-dimensional problem.

for the current problem

Let C_l, C_t and C_ρ be the conversion factors. Real units are given with subscript phys while the lattice Boltzmann units are without subscript.

1. BGK operator allows a small window of possible kinematic viscosity values. Given that we are working with the BGK operator, the kinematic viscosity then sets the constraint for the choice of simulation parameters. Choose the kinematic viscosity $\nu = 0.1$ that corresponds to relaxation parameter $\tau = \frac{1}{c_\mathrm{s}^2}\nu + 0.5\Delta t = 0.8$.

$$\nu \frac{C_l^2}{C_t} = \nu_\mathrm{phys} = 2 \times 10^{-5} \frac{m^2}{s} \tag{15}$$

2. We set the vertical dimension (in y direction) in the simulation to $L_y = 200$. Meaning that we have chosen 100 grid points to represent an exponential function.

$$L_y C_l = H_\mathrm{phys} = 4730m, \tag{16}$$

3. The dimensionless number we have to match is

$$\frac{g_y L_y}{c_\mathrm{s}^2} = \alpha = 0.4 = \frac{g_\mathrm{phys} H_\mathrm{phys}}{c_\mathrm{s,\ phys}^2}$$
$$g_y = \alpha \frac{c_\mathrm{s}^2}{L_y} = 6.67 \times 10^{-4} \tag{17}$$

   The lattice speed of sound is fixed with the D2Q9 lattice. Thus, selecting the number of grid points in y direction L_y already decides the gravity strength in the simulations.

$$g \frac{C_l}{C_t^2} = \alpha \frac{c_\mathrm{s}^2}{L_y} \frac{C_l}{C_t^2} = g_\mathrm{phys} \tag{18}$$

4. Speed of sound

$$c_\mathrm{s} \frac{C_l}{C_t} = c_\mathrm{phys} \tag{19}$$

5. Density (mass) conversion

$$\rho C_\rho = \rho_\mathrm{phys} \tag{20}$$

Report preparation:

1. The final (steady-state) density profile does not depend upon the fluid viscosity. Explain the role of fluid viscosity in the problem.

2. For incompressible fluids, we know that pressure varies linearly with depth. Show that when density changes are small $\frac{\Delta\rho}{\rho_0} \ll 1$, the pressure variation given by Eq. (8) is indeed linear. $\Delta\rho$ refers to highest possible density variation in the system and ρ_0 is the initial uniform density. Small density variations correspond to weakly compressible flow.

3. What are the initial kinetic and potential energies of the system? What are the final kinetic and potential energies of the system? If there is any difference in the sum of kinetic and potential energies of the system at the initial and final time, what is the reason for the change?

4. Does the density profile depend upon the length in x direction L_x?

5. The length conversion factor C_l is decided by one Eq. (16). It seems the time conversion factor C_t can be decided by one of the Eqs. (18,19,15). How should C_t be decided then?

6. Take the reference parameters as $\nu = 0.1, g_y = 6.667 \times 10^{-4}$ and $L_y = 200$. Find (by trial and error) and report the minimum kinematic viscosity that will still produce stable simulations.

7. Compare analytical and simulation density profile as a function of y at steady-state. Pay attention to the effective location of the boundary at the fluid-solid interface.

8. Report maximum velocity magnitude $|\mathbf{u}|$ in the simulation. At what time t and position y the maximum velocity occurs? Scale the time t with viscous time scale $t_{\text{visc}} = H^2/\nu$ and position y with column height H. That is report the dimensionless time and position t/t_{visc}, y/H at which maximum fluid velocity is observed.

9. Do the fluid populations (at any time t and position $\mathbf{x}$) ever become negative in the simulations? Report maximum and minimum values of the fluid populations throughout the simulation for the reference case in point 6.

10. Repeat the simulations with no-slip boundary conditions on the lateral sides (instead of the periodic boundary). Explain if the steady-state density profile would change with the change of boundary conditions on lateral sides. Compare maximum velocity magnitude $|\mathbf{u}|$ when lateral boundaries are periodic and no-slip (bounce-back) for the reference case in point 6.