CL469 - Lattice Boltzmann method for fluid flows

Scaling and Parameter Selection

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1 Unit System in Lattice Boltzmann

It is important to work with a consistent unit system to quantitatively assess a physical phenomena. In case of fluid flows, we need units to quantify flow properties such as velocity, force, stress, etc. and fluid properties such as density, viscosity, etc. Most commonly the unit system that we come across are the SI unit system, CGS system or the Imperial unit system, which we shall refer to as physical unit systems. In lattice Boltzmann simulations, we introduce a new unit system called the **lattice unit (lu)** system. To study some physical phenomena, say, by validating with experimental data or analytical data, it is imperative we come up with a mapping between the physical unit systems and lattice unit systems. Thankfully, we already have a simple way to do that. This method is simply known as **Scaling**.

Every quantity in lattice units is related to its physical counter-part through a scale factor. For example, if we consider length l, then

$$l^* \text{ (length in lattice units)} = \frac{l_p \text{ (length in physical units)}}{C_l}, \tag{1}$$

where C_l denotes the conversion factor for length, which is decided by us. It can be anything as long as we remember the fact that l^* and l_p denote the same quantity, just in different unit systems. If the physical unit system is SI unit system, then C_l has units m/lu. Also, note that even though there can be no wrong choice for C_l, there can be more relevant choices which make calculations/computations easier. Similar to the conversion factor for length, we can have convserion factors for time and density as

$$t^* = \frac{t_p}{C_t},\ \rho^* = \frac{\rho_p}{C_\rho}, \tag{2}$$

where C_t and C_ρ denotes the conversion factor for time and density respectively.

Now, the question is, do we require similar scaling factors for force, pressure and velocity? To understand this we must revisit Non-dimensionalization.

2 Non-dimensionalization and Derived Conversion Factors

We know that any physical quantity in fluid flow (p_1) which is a function of some fluid properties (α_i), flow parameters (β_i) and geometric parameters (γ_i), can be written as

$$p_1 = \psi(\alpha_1, \alpha_2, .., \beta_1, \beta_2, ..., \gamma_1, \gamma_2, ...). \tag{3}$$

From Buckingham-Π theorem, we know that Eq (3) can be written in terms of non-dimensional groups denoted as Π_i

$$\Pi_1 = \varphi(\Pi_2, \Pi_3, ...), \tag{4}$$

which significantly reduce the size of the parameter space, and make the operating parameters and output parameters independent of any unit system. Recall, that to derive these dimensionless groups for fluid flow, we only used three fundamental dimensions $[M\ L\ T]$, denoting mass, length and time. Similarly, we only need the three fundamental

scale factors C_ρ (density is mass per unit volume), C_l and C_t to derive scale factors for force, velocity and pressure.

One can show that, by making use of Buckingham-Π theorem, and representing the quantities in the form in Eq. (4), the derived scale factors for velocity, pressure, force density and kinematic viscosity (ν) can be obtained as

$$C_u = \frac{C_l}{C_t},\ C_p = \frac{C_\rho C_l^2}{C_t^2},\ C_F = \frac{C_\rho C_l}{C_t^2},\ \text{and}\ C_\nu = \frac{C_l^2}{C_t} \tag{5}$$

respectively.

(For more details, refer to Section 7.1.1 and 7.1.2 in Timm Krüger's book).

From the law of similarity, we also know that it is very advantageous to characterize fluid flow through non-dimensional numbers. The most important non-dimensional number for single-phase fluid flow is the Reynolds number (Re), which gives a comparison of the inertial forces with the viscous forces. It is written as

$$\mathrm{Re} = \frac{U_p L_p}{\nu_p}, \tag{6}$$

where U_p is the characteristic velocity scale, L_p is the characteristic length scale and ν_p is the kinematic viscosity.

Since, Reynolds number is non-dimensional, it must be independent for the unit system used. To check this, replace $U_p = C_u U^* = \frac{C_l}{C_t} U^*$, $L_p = C_l L^*$ and $\nu_p = C_\nu \nu^* = \frac{C_l^2}{C_t}\nu^*$. This gives

$$\mathrm{Re} = \frac{U^* L^*}{\nu^*}. \tag{7}$$

Thus, no matter what the unit system is that we are using, it is necessary to match Re between both the unit systems to ensure we are simulating the same physical system.

Now, the next question is what should the scale factors be?

In simulations, the physical length scale, time-scale and mass is chosen as the grid size (Δx_p), time-step (Δt_p) and some reference density ρ_p. For the ease of implementation and convenience, we choose their lattice counterparts as $\Delta x^* = 1\ lu$, $\Delta t^* = 1\ lu$ and $\rho^* = 1\ lu$.

Thus, we get

$$\Delta x^* = \frac{\Delta x_p}{C_l},\ \Delta t^* = \frac{\Delta t_p}{C_t},\ \rho^* = \frac{\rho_p}{C_\rho}. \tag{8}$$

Substituting for $\Delta x^*, \Delta t^*$ and ρ^*, we get the scale factors as the physical quantities themselves, i.e., $C_l = \Delta x_p$, $C_t = \Delta t_p$ and $C_\rho = \rho_p$.

Now that we have the scale factors, how to decide the parameters to choose for the simulations?

3 Parameter Selection

To decide what parameters to use for simulations, let us first list out the constraints the parameters must satisfy to give accurate and meaningful results.

- the relaxation time (τ^*) in lattice units must be more than 0.5 to ensure stability of the BGK collision operator. It is also required maintain a grid Reynolds number $\mathrm{Re}_g = \dfrac{U^*_{\max}\Delta x^*}{\nu^*}$ small ($< \mathcal{O}(10)$). Physically this means that all local hydrodynamic length scales must be resolved.

- Maximum velocity must be much smaller than the lattice speed of sound (c^*_s) ($U^*_{\max} \ll c^{*2}_s$). In other words it means Mach number (Ma) is small. For D2Q9 lattice, the lattice speed of sound is $c^*_s = \dfrac{1}{\sqrt{3}} \approx 0.577$. Practically this means that $U^*_{\max}$ must be much smaller than 0.1. A smaller value of $U^*_{\max}$ ensures that the higher order truncation errors in the equilibrium distribution function are small.

- To reach steady state (if any), one must simulate the system up until multiple factors of the viscous time-scale $\dfrac{L^2_p}{\nu_p}$.

To illustrate the process of parameter selection abiding by the constraints listed above, let us consider a case of 2D Couette flow.

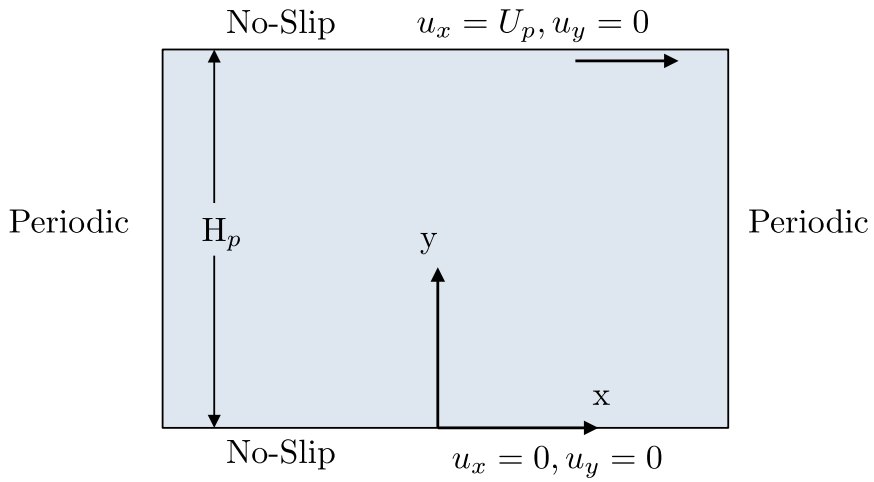

Figure 1: Schematic of a 2D Couette flow.

Problem Statement: A plane Couette flow is being driven between two parallel plates by moving the top plate with a constant velocity of 10^{-1} m/s. The width of the channel is 10^{-3} m. The density and the kinematic viscosity of the fluid is 10^3 Kg/m^3 and 10^{-6} m^2/s. Choose the simulation parameters for a lattice Boltzmann simulation to simulate this system upto the steady state.

We denote plate velocity as $U_p = 10^{-1}$ m/s, channel width as $H_p = 10^{-3}$ m and kinematic viscosity as $\nu_p = 10^{-6}$ m^2/s. Let us first calculate the Reynolds number,

$$\mathrm{Re}_p = \frac{U_p H_p}{\nu_p} = \frac{10^{-1}(m/s)10^{-3}(m)}{10^{-1}(m^2/s)} = 100. \tag{9}$$

Note that we have used the plate velocity and the channel width as the characteristic velocity scale and length scale respectively. This Reynolds number must also be same for

the quantities in lattice units in order to get the same physical system. The analytical velocity profile for this case is given as

$$u_x = \frac{U_p}{H_p} y, \tag{10}$$

where u_x is the x-component of velocity and y is the vertical coordinate across channel width.

Like characteristic velocity and length scale, there is also a characteristic time scale. This time scale is chosen as the viscous time scale given as $t_\nu = \frac{H_p^2}{\nu_p}$, since it governs the momentum diffusion across the channel. At steady state, we expect that the changes in flow parameters are negligible. Question is in simulations, how does one check that? There can be two approaches to this problem. Typically we want the errors in velocity field compared to the analytical solution to be very small at steady state. However, we may not have analytical solutions for many complex flow situations. In such cases, we use a rule of thumb which requires we simulate the system up until multiple factors of the viscous time scale. From some experience that it should be at least $10\,t_\nu$. Thus, for the current problem we get $t_\nu = 1\ s$ and we choose to simulate the system up to a physical time of $10\ s$.

Usually, in any simulation we intend to choose the number of grid points used to resolve the channel width. Let us choose 5 grid points, which correspond to $H^* = 5\ lu$, i.e., width in lattice units. Since, the width of the channel in physical units is $H_p = 10^{-3}\ m$, we get $\Delta x_p = 2 \times 10^{-4}\ m$.

Thus, the mapping between channel width in physical and lattice units can be written as

$$H^* = \frac{H_p}{C_l} = \frac{10^{-3}}{2 \times 10^{-4}} = 5\ lu. \tag{11}$$

Now, we can use the relation between relaxation time and kinematic viscosity in lattice units $(\tau^* - 1/2)c_s^{*2} = \nu^*$. Further, we can use this relation to obtain the time-step in physical units as

$$\Delta t_p = (\tau^* - 1/2)c_s^{*2}\frac{\Delta x_p^2}{\nu_p}. \tag{12}$$

To stay well above the stability limit, let us choose $\tau^* = 0.8$. Thus, using $\nu_p = 10^{-6}\ m^2/s$, $\Delta x_p = 2 \times 10^{-4} m$ and $\tau^* = 0.8$ in Eq. (12), we get $\Delta t_p = 4 \times 10^{-3}\ s$.

This means, to simulate $1\ s$ of physical time, which is also the viscous time scale, we must run the simulation for $\frac{1}{4 \times 10^{-3}} = 250$ iterations. Similar to C_l, one can show that $C_t = \Delta t_p = 4 \times 10^{-3}\ s/lu$.

Next, we must find the plate velocity in lattice units. To do this we can use two approaches.

- Using C_l and C_t, we can construct $C_u = \frac{C_l}{C_t} = \frac{\Delta x_p}{\Delta t_p}$. Now using, $U^* = \frac{U}{C_u} = 1$ which is larger than c_s^*. Thus, this choice of parameters violates the constraints we laid out before. As a check however, one can plug in this value of U^* in the Reynolds number using properties in lattice units and $\mathrm{Re} = \frac{U^* H^*}{\nu *} = 100$. Thus, the law of similarity is abided by construction.

- The same value of U^* can similarly be found by explicitly using the fact that $\text{Re} = \dfrac{U^* H^*}{\nu *} = 100$. Either way, the choice of parameters doesn't satisfy the constraints.

There can be many ways to tune parameters such that the constraints are satisfied. For example, tuning grid size and relaxation time. In this example, we choose the latter. Consider $\tau^* = 0.56$ instead of 0.8. This gives $\Delta t_p = 8 \times 10^{-4}\ s$. Thus, we have increased the temporal resolution such that to simulate 1 s of physical time, we must run the simulation for 1250 iterations. Following the same method as before we can find the plate velocity in lattice units as $u^* = 0.2\ lu$. Note that even though this velocity is less than c_s^*, it is still high enough to cause the truncation errors be significant. However, for the simple case of Couette flow, this still works.

The last parameter to choose is the total time up until which we should simulate to ensure the system has reached steady state. As discussed, we should simulate upto multiple factors of the viscous time-scale $t_\nu = \dfrac{H_p^2}{\nu_p} = 1\ s$ which translates to 1250 iterations. The rule of thumb that we consider is that the total time to simulate should be atleast $10 t_\nu = 10\ s$ or 12500 iterations.

Thus we have all the simulation parameters to simulate the system. Note, however, this set of parameters is not unique and one can have infinite such combinations.

In the book of Timm Krüger, Section 7.2.3 and 7.3 has extensive discussion on the constraints and an example on gravity driven Poisueille flow.

Sometimes, it is possible that we only know the Reynolds number for the flow. In such a case we can choose the width of the channel in lattice units $H^* = 5\ lu$, which is essentially the number of grid points used to discretize the channel width.

Then choose $\tau^* = 0.56$ and use $\nu^* = (\tau^* - 0.5) c_s^{*2}$ to find the kinematic viscosity in lattice units as $\nu^* = 0.02$.

From here, use the fact that $\text{Re} = \dfrac{U^* H^*}{\nu^*} = 100$ to find the plate velocity as $U^* = 0.2\ lu$.

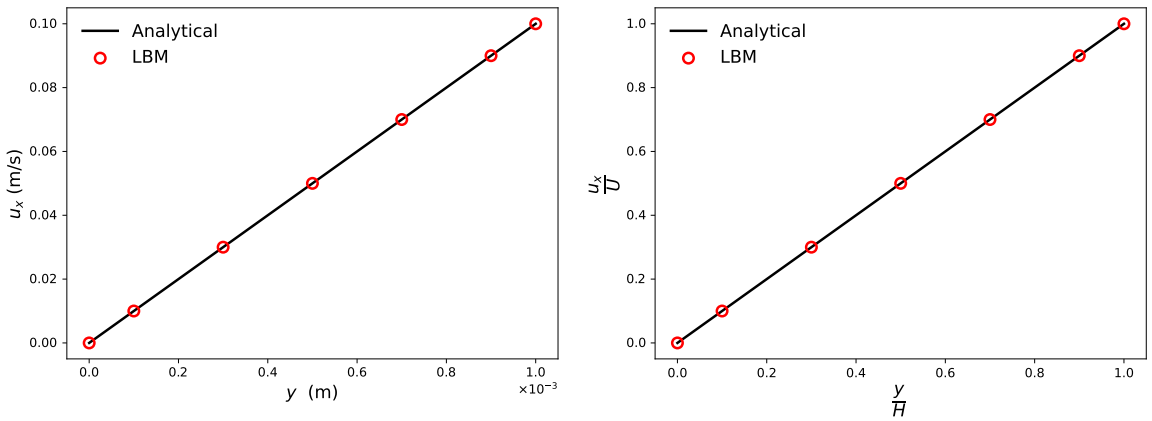

Figure 2: Velocity profiles in (a) dimensional form and (b) non-dimensional form compared with the analytical solution.

Once the results from simulations are available, one can use the scale factors to convert

the quantities in lattice units to physical units. However, it is good idea to always report results in non-dimensional variables so that it remains independent of the choice of the unit system. The results for Couette flow for the derived parameters in physical units and non-dimensional variables are shown in Fig. (2).