Notes on Lattice Boltzmann Method for Thermal Flows

Jakub Šťavina
stavina.jakub@gmail.com

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Disclaimer: These notes were largely adapted from [1] and are not meant for publication or distribution.

1 Abstract

These notes aim to review and collect the concepts and formulas necessary for writing a simulation of a thermal flow such as the Rayleigh-Benard convection using the lattice Boltzmann method. At first, we will provide a high-level overview and setup of the problem in terms of the Navier-Stokes equations coupled with the convection-diffusion equation via so-called Boussinesq approximation. We briefly discuss the Boltzmann transport equation as a means to motivate the lattice Boltzmann equation (LBE). We will highlight its utility in fluid dynamics and convection-diffusion simulation by applying it to the thermal flow problem at hand. Finally, we address some specific aspects of implementation of the LBE such as the computational algorithm, initialization and boundary conditions. We provide an example simulation with a simple 2D setup and the Dirichlet boundary condition.

2 Problem setup

The problem we aim to solve, with its relevance in nature and industry, is the coupled dynamics of momentum and convection-diffusion in a thermal flow. The momentum transport will be modelled by the (incompressible) Navier-Stokes equations (NSE), which in their conservation form read

$$\nabla \cdot \mathbf{u} = 0, \tag{1}$$

$$\frac{\partial \mathbf{u}}{\partial t} + \nabla \cdot (\mathbf{u} \otimes \mathbf{u}) = -\frac{1}{\rho_0}\nabla p + \nu \nabla^2 \mathbf{u} + \frac{\mathbf{F}_b}{\rho_0}. \tag{2}$$

Meanwhile, the convection and diffusion of the temperature field T will be modelled by the equation

$$\frac{\partial T}{\partial t} + \nabla \cdot (T\mathbf{u}) = \varkappa \nabla^2 T \tag{3}$$

where the local convection velocity is the fluid velocity $\mathbf{u}$. The coupling of temperature back to the fluid is realized through the fluid's temperature-dependent density. We shall assume, that the temperature variation is small, such that the fluid density may be modelled by the linear relationship $\rho(T) = \rho_0(1 - \alpha(T - T_0))$. The small temperature changes lead to density fluctuations, which in turn give rise to a buoyancy force density

$$\mathbf{F}_b = -\alpha\rho_0(T - T_0)\mathbf{g}. \tag{4}$$

This is the Boussinesq approximation, physical motivation for which is that the effect of the density difference on inertia is much smaller than the buoyancy. This justifies keeping the density constant elsewhere in the NSE.

3 Lattice Boltzmann method

3.1 Boltzmann transport equation

The statistical behavior of a thermodynamic system out of equilibrium is described by means of a probability density function $f = f(t, \mathbf{x}, \mathbf{v})$. Boltzmann transport equation (BTE) equates that the total derivative of f equals the collision term Ω which is in turn given by Boltzmann's *molecular chaos assumption*. BTE then reads

$$\frac{\partial f}{\partial t} + \mathbf{v} \cdot \nabla_{\mathbf{x}} f + \frac{\mathbf{F}}{m} \cdot \nabla_{\mathbf{v}} f = \Omega. \tag{5}$$

In the total derivative on the left-hand side of EQN 5, the time derivatives of the phase-space coordinates $(\mathbf{x}, \mathbf{v})$ are replaced by velocities and forces as per Newton's second law. The probability density function f relates to physical quantities such as density ρ, local flow velocity $\mathbf{u}$, pressure p and temperature T via its moments. These are given by the formulas

$$\rho = \int f \, d^3\mathbf{v}, \qquad \rho\mathbf{u} = \int \mathbf{v} f \, d^3\mathbf{v}, \qquad p = \rho RT = \frac{1}{3}\int |\mathbf{v} - \mathbf{u}|^2 f \, d^3\mathbf{v}. \tag{6}$$

Much of the complexity of the BTE lies in the collision term Ω which is not given here in its full generality. For our purposes, we only consider a simplification to the collision term due to Bhatnagar, Gross and Krook (BGK) which states that the effect of particle collisions at time t is to force the velocity distribution $f(\mathbf{v}) = f(t, \mathbf{x}_0, \mathbf{v})$ at the point $\mathbf{x}_0$ into a local Maxwellian equilibrium distribution

$$f^{eq.} = \frac{\rho}{(2\pi RT)^{d/2}} \exp\left(-\frac{(\mathbf{v} - \mathbf{u})^2}{2RT}\right), \tag{7}$$

over a relaxation time τ. The collision term is thus given by $\Omega = -(f - f^{eq.})/\tau$. We will see these ideas mirrored in the lattice Boltzmann equation - a discrete version of BTE.

3.2 Lattice Boltzmann equation

The lattice Boltzmann equation is given by first splitting time to intervals of length Δt and discretizing space on a uniform lattice (typically taken to be rectangular with spacing Δx between adjacent sites). Velocities are then discretized by associating the lattice sites with velocity set such that a particle travelling from a lattice site $\mathbf{x}$ with a discrete velocity $\mathbf{v}_i$ from the velocity set will in time Δt arrive at a lattice site $\mathbf{x}'$. The discrete particle populations f_i will then at each lattice site $\mathbf{x}$ specify the number of particles travelling with the velocity $\mathbf{v}_i$. A typical example would be the the rectangular lattice with $\Delta x = \Delta t = 1$ and the D2Q9 velocity set

$$\mathbf{v}_i = \binom{0}{0}, \binom{1}{0}, \binom{0}{1}, \binom{-1}{0}, \binom{0}{-1}, \binom{1}{1}, \binom{-1}{1}, \binom{-1}{-1}, \binom{1}{-1}; \qquad i = 0, 1, \ldots, 8. \tag{8}$$

In the absence of external forces, we can then directly write down discrete Boltzmann equation in each of the particle populations f_i - the lattice Boltzmann equation as

$$\frac{1}{\Delta t}(f_i(\mathbf{x} + \mathbf{v}_i\Delta t, t + \Delta t) - f_i(\mathbf{x}, t)) = \Omega_i = -\frac{1}{\tau}(f_i(\mathbf{x}, t) - f_i^{eq.}(\mathbf{x}, t)). \tag{9}$$

The fluid density and fluid velocity are then obtained as the discrete moments

$$\rho(\mathbf{x}, t) = \sum_i f_i(\mathbf{x}, t), \qquad \rho(\mathbf{x}, t)\mathbf{u}(\mathbf{x}, t) = \sum_i f_i(\mathbf{x}, t)\mathbf{v}_i. \tag{10}$$

Perhaps the single most important equation in these notes is the expression for the equilibrium distribution $f_i^{eq.}(\mathbf{x}, t)$, the discrete version of EQN 7, which is often taken as

$$f_i^{eq} = w_i\rho\left(1 + \frac{\mathbf{u}\cdot\mathbf{v}_i}{c_s^2} + \frac{(\mathbf{u}\cdot\mathbf{v}_i)^2}{2c_s^4} - \frac{\mathbf{u}\cdot\mathbf{u}}{2c_s^2}\right). \tag{11}$$

Here, c_s is the "speed of sound" on our lattice and w_i are lattice-dependent weights. For the D2Q9 lattice,

$$c_s^2 = \frac{\Delta x^2}{3\Delta t^2} \qquad \text{and} \qquad w_i = \frac{4}{9}, \frac{1}{9}, \frac{1}{9}, \frac{1}{9}, \frac{1}{9}, \frac{1}{36}, \frac{1}{36}, \frac{1}{36}, \frac{1}{36}; \qquad i = 0, 1, \ldots, 8. \tag{12}$$

It can be shown by Chapman-Enskog analysis that the fluid velocity $\mathbf{u}$ obtained from the LBE approximates the weakly-compressible Navier-Stokes equations

$$\frac{\partial}{\partial t}\rho + \nabla\cdot(\rho\mathbf{u}) = 0, \tag{13}$$

$$\frac{\partial}{\partial t}(\rho\mathbf{u}) + \nabla\cdot(\rho\mathbf{u}\otimes\mathbf{u}) = -\nabla p + \nu\nabla\cdot\left[\rho\left(\nabla\mathbf{u} + (\nabla\mathbf{u})^{\mathsf{T}}\right)\right]. \tag{14}$$

This analysis also show that the relaxation time τ is related to the kinematic viscosity ν by $\nu = c_s^2(\tau - \Delta t/2)$.

3.3 Forces

A a first step in order to include forces in the LBE requires a modification to the fluid velocity

$$\rho \mathbf{u} = \sum_i f_i \mathbf{v}_i + \frac{\mathbf{F}\Delta t}{2}. \tag{15}$$

The LBE is then modified by adding a sourcing term S_i and thus reads

$$\frac{1}{\Delta t}(f_i(\mathbf{x} + \mathbf{v}_i \Delta t, t + \Delta t) - f_i(\mathbf{x}, t)) = \Omega_i + S_i, \tag{16}$$

where the sourcing term is given by

$$S_i = \left(1 - \frac{\Delta t}{2\tau}\right) w_i \left(\frac{\mathbf{F} \cdot \mathbf{v}_i}{c_s^2} + \frac{(\mathbf{F} \cdot \mathbf{v}_i)(\mathbf{u} \cdot \mathbf{v}_i)}{c_s^4} - \frac{\mathbf{F} \cdot \mathbf{u}}{c_s^2} \right). \tag{17}$$

3.4 LBM for the convection-diffusion equation

The BTE describes the full physical situation of the thermal flow with the temperature and velocity fields arising from the moments of f readily coupled. Hence, there is in principle no need to resort to using the system of EQN 1, 2 and 3 coupled via approximations such as EQN 4. However, capturing the dynamics of higher moments such as the ones required to define T in practice requires use of more complicated velocity sets than D2Q9 which in turn results in less stable numerical methods. Instead, a second set of populations g_i is introduced, such that the temperature field is calculated as $T = \sum_i g_i$ and which obey the LBE

$$\frac{1}{\Delta t}(g_i(\mathbf{x} + \mathbf{v}_i \Delta t, t + \Delta t) - g_i(\mathbf{x}, t)) = -\frac{1}{\tau_g}(g_i(\mathbf{x}, t) - g_i^{eq}(\mathbf{x}, t)). \tag{18}$$

This approach can be motivated by the formal similarity of EQN. 13, 14 and the EQN. 3 which may lead to the expectation that a suitable choice of the equilibrium distribution $g_i^{eq.}$ will approximate EQN. 3. It turns out, that the equilibrium distribution required for this has a simpler form compared to $f_i^{eq.}$

$$g_i^{eq.} = w_i T \left(1 + \frac{\mathbf{v}_i \cdot \mathbf{u}}{c_s^2}\right), \tag{19}$$

with the relaxation time τ_g being related to the diffusion coefficient by $\varkappa = c_s^2(\tau_g - \Delta t/2)$. Note that here the velocity $\mathbf{u}$ is provided externally.

4 The implementation

4.1 Lattice Boltzmann method

A single step of the LBM can be summarized as follows:

1. Determine the force density $\mathbf{F}$ for the time step,
2. Compute the fluid density ρ and velocity $\mathbf{u}$,
3. Using ρ and $\mathbf{u}$ compute the equilibrium populations f_i^{eq},
4. Compute the source term S_i using $\mathbf{F}$ and ρ,
5. Find the post-collision populations: $f_i^*(\mathbf{x}, t) = f_i(\mathbf{x}, t) + \Delta t(\Omega_i + S_i)$,
6. Propagate the populations: $f_i(\mathbf{x} + \mathbf{v}_i \Delta t, t + \Delta t) = f_i^*(\mathbf{x}, t)$,
7. Increment the time by Δt.

4.2 Thermal Lattice Boltzmann method

The implementation of LBM for the thermal flow model follows the steps:

1. Initialise the two sets of populations, f_i and g_i. Specify gravity $\mathbf{g}$, viscosity ν, thermal conductivity $\varkappa$ and thermal expansion coefficient α. Define a reference temperature T_0 as the average temperature of the system. Implement boundary conditions for the NSE and the EQN. 3 as specified below.
2. Using the fluid velocity $\mathbf{u}$ as external velocity, perform one time step of the LBM for g_i as detailed in 4.1 omitting the steps 1. and 4. Evaluate the temperature $T(\mathbf{x})$.
3. Compute the buoyancy force density $\mathbf{F}_b(\mathbf{x})$ from EQN 4.
4. Perform one time step of the as for the populations f_i, following 4.1, use the buoyancy force $\mathbf{F}_b(\mathbf{x})$ to drive the flow. Evaluate the new fluid velocity $\mathbf{u}$.
5. Go back to step 2 for the next time step.

4.3 Initialization and boundary conditions

Supposing that the initial velocity $\mathbf{u}$ and temperature T fields are known, we initialize the populations f_i and g_i to their respective equilibria given by $f_i^{eq.}$ and $g_i^{eq.}$. More accurate initializations are available, but this will suffice for our purposes.

For $\mathbf{u}$, we shall use the no-slip boundary condition, which is in LBM implemented via the bounce-back scheme

$$f_i(\mathbf{x}_b, t + \Delta t) = f_{\bar{i}}^*(\mathbf{x}_b, t) \tag{20}$$

where $\mathbf{x}_b$ is a boundary node and the unknown population f_i is determined by a post-collision population $f_{\bar{i}}^*$ from the opposite direction: for example in D2Q9 for $i = 0, 1, 2, 3, 4, 5, 6, 7, 8$ we have $\bar{i} = 0, 3, 4, 1, 2, 7, 8, 5, 6$. For the Dirichlet boundary condition on the temperature filed T, the anti-bounce-back scheme is used

$$g_i(\mathbf{x}_b, t + \Delta t) = -g_{\bar{i}}^*(\mathbf{x}_b, t) + 2w_{\bar{i}} T_{wall}, \tag{21}$$

where T_{wall} is the wall temperature. Note the negative sign in front of $g_{\bar{i}}^*$ and weights $w_{\bar{i}}$ in front of T_{wall}.

5 Results

To demonstrate the use of LBM for thermal flows, we performed a simulation of the Rayleigh-Bénard convection. The geometrical setup for the Rayleigh-Bénard convection consists of two parallel plates distance H apart. The bottom plate is kept at $T = T_{bot}$, while the top plate is at T_{top}, such that $T_{bot} > T_{top}$. The plates are subject to thermal Dirichlet boundary condition. Both plates are subject to no-slip boundary condition for fluid momentum. On the vertical sides, periodic boundary condition is imposed. We have chosen the initial condition with vanishing fluid velocity and a uniform temperature T_0 perturbed by a function of the form $0.005 \sin(12\pi x/(W-1)) \sin(\pi y/H)$.

Quantity	Symbol	Value
Time step	Δt	1
Space step	Δx	1
Total width	W	400
Total height	H	100
Top temperature	T_{top}	0.5
Bottom temperature	T_{bot}	1.5
Initial temperature	T_0	1
Initial density	ρ_0	1
Thermal conductivity	κ	0.002
Kinematic viscosity	ν	1/6
Buoyancy strength	$g\alpha$	0.015

Table 1: Summary of the simulation parameters used to generate the figures in this section.

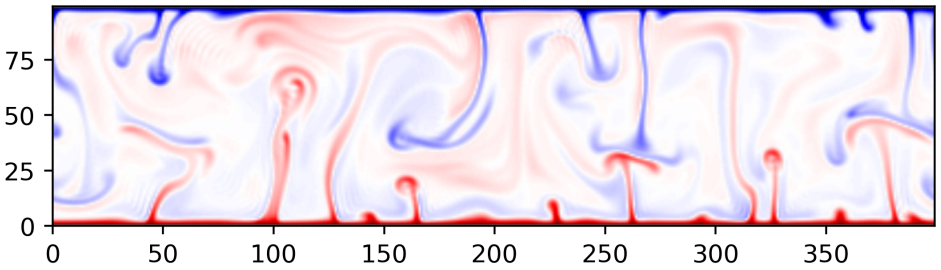

Figure 1: Temperature filed T after $N_t = 20000$ time steps.

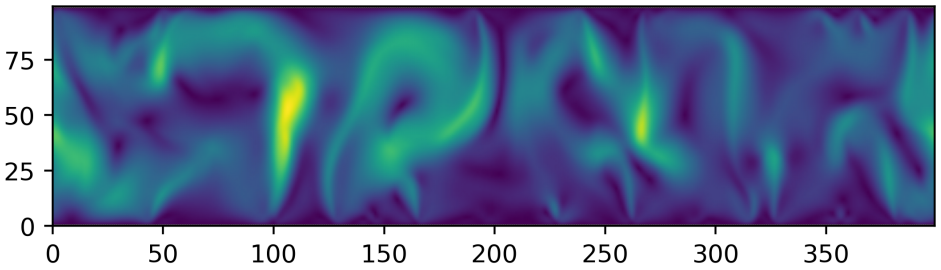

Figure 2: Caption

Figure 3: Absolute value of fluid velocity $|\mathbf{u}|$ after $N_t = 20000$ time steps.

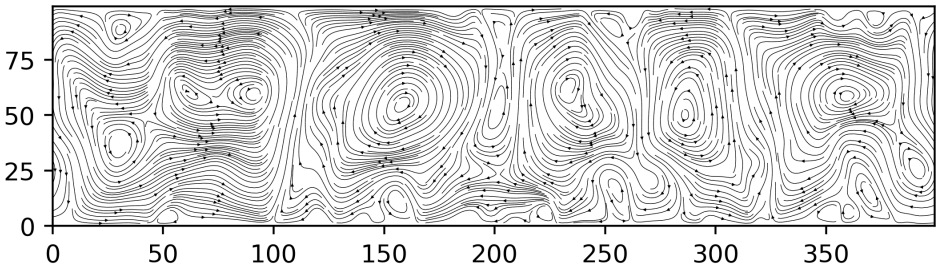

Figure 4: Streamlines after $N_t = 20000$ time steps.

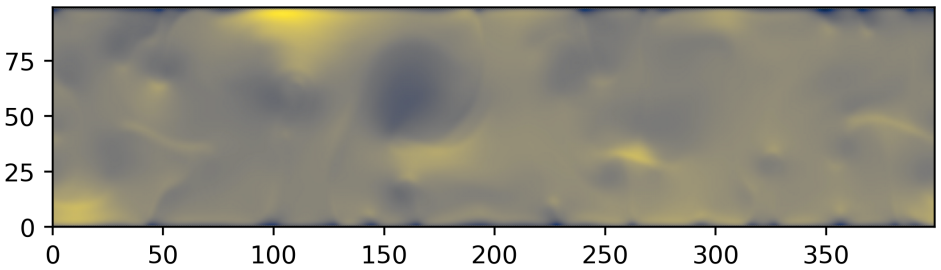

Figure 5: Fluid density ρ after $N_t = 20000$ time steps.

References

[1] T. Kruger, H. Kusumaatmaja, A. Kuzmin, O. Shardt, G. Silva, and E. M. Viggen, *The lattice Boltzmann method*. Graduate Texts in Physics, Cham, Switzerland: Springer International Publishing, Apr. 2018.