Introduction to the Lattice Boltzmann Method

A. Kuzmin J. Derksen

Department of Chemical and Materials Engineering
University of Alberta
Canada

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Outline

BGK LATTICE BOLTZMANN EQUATION:

So far we studied the BGK Boltzmann equation:

$$f_i^*(\boldsymbol{x},t) = f_i(\boldsymbol{x},t) - \frac{f_i(\boldsymbol{x},t) - f_i^{eq}}{\tau} + F_i$$
$$f_i(\boldsymbol{x}+\boldsymbol{c_i},t+1) = f_i^*(\boldsymbol{x},t)$$

The BGK equation restores the following macroscopic set of equations:

$$\partial_t \rho + \partial_\alpha \rho u_\alpha^m = 0$$
$$\partial_t \rho u_\alpha^m + \partial_\beta \rho u_\alpha^m u_\beta^m = -\frac{1}{3}\partial_\alpha \rho + F_\alpha + \nu \partial_\beta (\rho \partial_\beta u_\alpha^m + \rho \partial_\alpha u_\beta^m).$$

One can already recognize the disease of the method - there is only one visosity. The classical Navier-Stokes equation is written as:

$$\rho\left(\frac{\partial \boldsymbol{u}}{\partial_t} + \boldsymbol{u}\cdot\boldsymbol{\nabla}\boldsymbol{u}\right) = -\boldsymbol{\nabla}p + \mu\nabla^2\boldsymbol{u} + \eta\boldsymbol{\nabla}(\boldsymbol{\nabla}\cdot\boldsymbol{u})$$

BGK DISADVANTAGES

Overall BGK has certain disadvantages:

- One can recognize through the Chapman-Enskog expansion that the whole procedure depends on the parameter τ. That means that all associated errors depend on the parameter τ. One can refer to works of I. Ginzburg that the associated error for bulk is $\left(\tau - \frac{1}{2}\right)^2$.
- The same is even more related to the boundary conditions (it will be shown later) that for example location of walls is τ dependant.

Why to bother??

Suppose you want to perform simulations which are scaled with the Reynolds number $Re = \frac{U_{LB}N}{\frac{1}{3}(\tau - 1/2)}$. In what follows three "bad" examples are given:

- You choose velocity U_{LB1}, N_1 and τ_1. Suppose you want to perform another set of simulations but with another U_{LB2} or N_2. In this case you to conserve non-dimensional number you pick up another value with τ_2 and obtain absolutely different spatial error.
- If N is limited with the memory requirements - in this case you have to operate with not convenient τ
- The third one is when the physical simulation time step is so small that one wants to increase the lattice Botlzmann velocity to obtain better time step $\Delta t = \frac{U_{LB}}{U}\Delta x$. To keep Reynolds number the same, one needs to increase the relaxation parameter as well.

Naive assumption

What is the solution to this disease? So far one can see that the certain direction probability distribution function is relaxed towards the certain direction equilibrium distribution functions $-\frac{f_i - f_i^{eq}}{\tau}$. The answer is simple - one need to mix probability distribution functions and relax them with different relaxation rates (we omit the force for simplicity reasons):

$$f_i(\boldsymbol{x} + \boldsymbol{c_i}, t+1) = f_i(\boldsymbol{x}, t) - M_{ij} f_j - f_j^{eq}$$

Matrix M should have certain properties. First of all it needs to conserve density and momentum:

$$\sum_i \left(1 c_{ix} c_{iy}\right) M_{ij} f_j - f_j^{eq} = 0$$

Because the moments are defined as $\rho = \sum_i f_i$ and $\rho \boldsymbol{u} = \sum_i f_i \boldsymbol{c_i}$, one can see that the conservation of these quantities means that the matrix M_{ij} has eigenvectors $\{\mathbf{1}\}$, $\{c_{ix}\}$, $\{c_{iy}\}$:

$$\sum_i M_{ij} = s_\rho \{\mathbf{1}\}, \ \sum_i M_{ij} c_{ix} = s_{j_x} c_{ix}, \ \sum_i M_{ij} c_{iy} = s_{j_y} c_{iy}$$

MATRIXES RECONSTRUCTION. EIGENVECTOR DECOMPOSITION

We already see that the eigenvectors somehow are connected with the velocity set. There is a theorem from the linear algebra which states that any matrix can be reconstructed from the set of the eigenvectors:

$$M_{ij} = \sum_k M_i^{(k)} s_k M_j^{(k)}, \tag{1}$$

where s_k are effectively relaxation rates (eigenvalues) and $M^{(k)}$ is the kth eigenvector. Basically, by summing up components of eigenvectors with the eigenvalues one can obtain whole matrix.

Two approaches for the eigenvectors decomposition:

- Hermite polynomials approaches - one can see that the Hermite polynomials are ideal role for the eigenvectors (for example D2Q9 model):

$$\mathcal{H}^{(0)} = \mathbf{1} \qquad \mathcal{H}^{(2)}_{xx} = c_{ix}c_{ix} - \frac{1}{3} \qquad \mathcal{H}^{(3)}_{xxy} = c_{ix}c_{ix}c_{iy} - \frac{c_{iy}}{3}$$

$$\mathcal{H}^{(1)}_{x} = \boldsymbol{c_{ix}} \qquad \mathcal{H}^{(2)}_{xy} = c_{ix}c_{iy} \qquad \mathcal{H}^{(3)}_{xyy} = c_{iy}c_{iy}c_{ix} - \frac{c_{ix}}{3}$$

$$\mathcal{H}^{(1)}_{y} = \boldsymbol{c_{iy}} \qquad \mathcal{H}^{(2)}_{yy} = c_{iy}c_{iy} - \frac{1}{3} \qquad \mathcal{H}^{(3)}_{xxyy} = \left(c^2_{ix} - \frac{1}{3}\right)\left(c^2_{iy} - \frac{1}{3}\right)$$

- The second approach is more commonly used is to use Gramm-Schmidt algorithm to construct basis of vectors.

We start with the Gramm-Schmidt procedure:

THEOREM

Given set of basis vectors $\{e_1, e_2, ..., e_k\}$ *one can obtain the orthonormal basis* $\{n_1, n_2, ..., n_k\}$ *by following the algorithm:*

$$n_1 = \frac{u_1}{\|u_1\|} \qquad u_1 = e_1$$

$$n_2 = \frac{u_2}{\|u_2\|} \qquad u_2 = e_2 - n_1(e_2 \cdot n_1)$$

$$\dots$$

$$n_k = \frac{u_k}{\|u_k\|} \qquad u_k = e_k - \sum_{i=1}^{k-1} n_i(e_k \cdot n_i)$$

COMMON MATRIX

What we want to do is to orthonormalize the following vectors constructed through tensors of different orders from velocity sets, i.e. $\mathbf{1}$,$\boldsymbol{c_i}$,$\boldsymbol{c_i c_i}$, etc. One can follow the procedure of the Gramm-Schmidt orthogonalization and obtain the following eigenvectors:

$$
\begin{aligned}
|\rho\rangle &= |\mathbf{1}\rangle \\
|e\rangle &= -4|\mathbf{1}\rangle + 3(c_{ix}^2 + c_{iy}^2) \\
|\varepsilon\rangle &= 4|\mathbf{1}\rangle - \frac{21}{2}(c_{ix}^2 + c_{iy}^2) + \frac{9}{2}(c_{ix}^2 + c_{iy}^2)^2 \\
|j_x\rangle &= c_{ix} \\
|q_x\rangle &= (-5|\mathbf{1}\rangle + 3(c_{ix}^2 + c_{iy})^2)c_{ix} \\
|j_y\rangle &= c_{iy} \\
|q_y\rangle &= (-5|\mathbf{1}\rangle + 3(c_{ix}^2 + c_{iy})^2)c_{iy} \\
|p_{xx}\rangle &= c_{ix}^2 - c_{iy}^2 \\
|p_{xy}\rangle &= c_{ix}c_{iy}
\end{aligned}
$$

COMMON MATRIX

The matrix consisted from the eigenvectors in terms of numbers is represented as:

$$M = \begin{pmatrix} |\rho\rangle \\ |e\rangle \\ |\varepsilon\rangle \\ |j_x\rangle \\ |q_x\rangle \\ |j_y\rangle \\ |q_y\rangle \\ |p_{xx}\rangle \\ |p_{xy}\rangle \end{pmatrix} = \begin{pmatrix} 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ -4 & -1 & -1 & -1 & -1 & 2 & 2 & 2 & 2 \\ 4 & -2 & -2 & -2 & -2 & 1 & 1 & 1 & 1 \\ 0 & 1 & 0 & -1 & 0 & 1 & -1 & -1 & 1 \\ 0 & -2 & 0 & 2 & 0 & 1 & -1 & -1 & 1 \\ 0 & 0 & 1 & 0 & -1 & 1 & 1 & -1 & -1 \\ 0 & 0 & -2 & 0 & 2 & 1 & 1 & -1 & -1 \\ 0 & 1 & -1 & 1 & -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & -1 & 1 & -1 \end{pmatrix}$$

Note that the collision matrix can be constructed from the eigenvectors matrix M as follows:

$$A_{ij} = \sum_{k=1} 9 M_i^{(k)} \frac{s_k}{\|M^{(k)}\|^2} M_j^{(k)},$$

where s_k as we will see further are the relaxation rates. As far as $M^{-1} = DM^T$, where D is the diagonal matrix which consist of reverse norms of the eigenvectors M, one can write the following matrix equation: $A = M^{-1}SM$.

Let us write the lattice Boltzmann equation in the matrix form:

$$f_i^*(\boldsymbol{x}, t) = f_i(\boldsymbol{x}, t) - A_{ij}(f_j(\boldsymbol{x}, t) - f_j^{eq}(\boldsymbol{x}, t)). \quad f_i(\boldsymbol{x} + \boldsymbol{c_i}, t+1) = f_i^*(\boldsymbol{x}, t)$$

So far this formulation evolves too many operations: at the beginning of calculations one needs to define relaxation rates, then construct matrix Aij and in each iteration one needs to multiply this matrix on the vector $f_j - f_j^{eq}$. The following can be much simplified if we multiply the LBE on M:

$$Mf_i^* = Mf_i(\boldsymbol{x}, t) - MM^{-1}SM(f_j - f_j^{eq})$$

$$Mf_i^* = Mf_i(\boldsymbol{x}, t) - SM(f_j - f_j^{eq})$$

If one introduces so-called moments of the probability distribution function $m_k = M_i^{(k)} f_i$. Then in terms of moments the equation is a simple BGK-like update rule:

$$m_k^* = m_k - s_k(m_k - m_k^{eq}),$$

where s_k is the relaxation rate.

MOMENTS OF THE EQUILIBRIUM FUNCTION

One can take moments of the equilibrium distribution function (we can see that moments are natural expressions already seen before). For example density is the first moment $\rho = M_i^{(1)} f_i = |\rho\rangle f_i$, $\rho u_\alpha = M_i^{(4,6)} f_i = |j_\alpha\rangle f_i$. Overall, the equilibrium moments are as follows:

$$\boldsymbol{m}^{eq} = \begin{pmatrix} \rho \\ -2\rho + 3\rho(u_x^2 + u_y^2) \\ \rho - 3\rho(u_x^2 + u_y^2) \\ \rho u_x \\ -\rho u_x \\ \rho u_y \\ -\rho u_y \\ \rho(u_x^2 - u_y^2) \\ \rho u_x u_y \end{pmatrix} = M f^{eq}$$

Note that conservation laws imply $M_i^{(\rho)} f_i = M_i^{(\rho)} f_i^{eq}$,$M_i^{(j_\alpha)} f_i = M_i^{(j_\alpha)} f_i^{eq}$.

MRT FORMULATION OF THE LBE

Even the collision operator looks simple in the moment space (BGK like collision operator), we cannot propagate moments. Therefore one needs to multiply on matrix M^{-1} to obtain populations to perform streaming. Overall the MRT LBE is performed as follows:

- Calculate ρ and ρu_α from the populations: $\rho = \sum_i f_i$ and $\rho u_\alpha = \sum_i f_i c_{i\alpha}$.
- Calculate equilibrium moments from ρ and ρu_α.
- Calculate moments other than ρ and j_α from distribution functions, for instance $e = M_i^{(e)} f_i$.
- Perform collision in the moment space in BGK like fashion $m_k^* = m_k - s_k(m_k - m_k^{eq})$, with the predefined collision rates s_k. Note that s_ρ and s_{j_α} can be chosen arbitrarily due to the conservation law.
- Obtain populations from the moments by multiplying the vectors of moments on $M^{-1} = DM^T$, where $D = diag(1/9, 1/36, 1/36, 1/6, 1/12, 1/6, 1/12, 1/4, 1/4)$. The equation is $f_i^* = M_{ij}^{-1} m_j^*$
- Perform streaming with the postcollision distribution functions:

$$f_i(\boldsymbol{x} + \boldsymbol{c_i}, t+1) = f_i^*(\boldsymbol{x}, t)$$

- Iterate

NAVIER-STOKES EQUATION

Therefore the MRT LBE has more free parameters to fine tune the viscosity. For example one can restore the full Navier-Stokes equation with the bulk and dynamic viscosity:

$$\rho\Big(\frac{\partial \boldsymbol{u}}{\partial_t} + \boldsymbol{u}\cdot\boldsymbol{\nabla}\boldsymbol{u}\Big) = -\boldsymbol{\nabla}p + \mu\nabla^2\boldsymbol{u} + \eta\boldsymbol{\nabla}(\boldsymbol{\nabla}\cdot\boldsymbol{u}),$$

where for $D2Q9$ model viscosities are given through the following relationships:

$$\mu = \frac{1}{3}\Big(\frac{1}{s_\mu} - \frac{1}{2}\Big)$$
$$\eta = \frac{1}{3}\Big(\frac{1}{s_\eta} - \frac{1}{2}\Big),$$

where $s_\mu = s_{p_{xx}} = s_{p_{xy}}$ and $s_\eta = s_e$. This equation can be obtained through the Chapman-Enskog procedure (same steps plus utilizing the relationship $\sum_i M_i^{(l)} M_{ij} = -s_l M_i^{(l)}$):

$$\epsilon^0 : f_i^{(0)} = f_i^{eq}$$
$$\epsilon^1 : (\partial_{t_0} + c_{i\alpha}\partial_\alpha) f_i^{(0)} = -M_{ij} f_j^{(1)}$$
$$\epsilon^2 : \partial_{t_1} f_i^{(0)} + (\partial_{t_0} + c_{i\alpha}\partial_\alpha) f_i^{(1)} + \frac{(\partial_{t_0} + c_{i\alpha}\partial_\alpha)^2 f_i^{(0)}}{2} = -M_{ij} f_j^{(2)}$$

Advantages of the MRT

There are certain advantages of the MRT:

- More stable
- Better control of the accuracy - can avoid errors which are scheduled as $\left(\tau - \frac{1}{2}\right)^2$.
- 10-20% is slower than BGK
- Precise boundary conditions
- Control of higher-order moments, especially necessary for the non-Newtonian liquids

But still how can I choose other relaxation parameters, given that $s_{p_{xx}}$,$s_{p_{xy}}$, s_e are fixed with viscosities, s_{rho},s_{j_x} and s_{j_y} are not needed to be specified. Three eigenvectors are needed to be specified $9 - 6 = 3$, i.e. s_{q_x},s_{q_y} and s_ε. Usually in simulations they are taken as unity. Moreover, for example P.Lallemand, etc. search best parameters for precision but only through numerical procedures. For example, the best relaxation rate can be as 1.19 or similar. However, more rigorous approach exists and provided for subset of the MRT, so-called two-relaxation time (TRT) model.

TRT CONCEPTS

The choice of relaxation rates is far more than trivial. However, MRT model can be simplified if one uses the symmetric and anti-symmetric components (due to works of Irina Ginzburg). TRT stands for two relaxation time, i.e. the model uses two relaxation rates ω_+ and ω_-. ω_+ is used for even order tensors and ω_- is used for odd order tensors.
For example, for $D2Q9$ formulation given before the moments ρ,e,ε,p_{xx},p_{xy} are even; j_x,q_x,j_y,q_y are odd. That means the algorithm for MRT stands the same except the following choice of the relaxation rates
$s_e = s_\varepsilon = s_{p_{xx}} = s_{p_{xy}} = \omega_+$ and $s_{q_x} = s_{q_y} = \omega_-$.

If one wants to use the TRT concept without using MRT, then one needs to decompose populations on the positive and negative parts:

$$f_i = f_i^+ + f_i^- \qquad f_i^{eq} = f_i^{eq,+} + f_i^{eq,-}$$
$$f_i^+ = \frac{f_i + f_{\bar{i}}}{2} \qquad f_i^{eq,+} = \frac{f_i^{eq} + f_{\bar{i}}^{eq}}{2}$$
$$f_i^- = \frac{f_i - f_{\bar{i}}}{2} \qquad f_i^{eq,-} = \frac{f_i^{eq} - f_{\bar{i}}^{eq}}{2},$$

where the subscript $\bar{i}$ stands for the index of direction opposite to the direction i. After specifying that the LBE is as follows:

$$f_i^*(\boldsymbol{x}, t) = f_i(\boldsymbol{x}, t) - \omega_+(f_i^+(\boldsymbol{x}, \boldsymbol{t}) - f_i^{eq,+}(\boldsymbol{x}, \boldsymbol{t})) - \omega_-(f_i^-(\boldsymbol{x}, \boldsymbol{t}) - f_i^{eq,-}(\boldsymbol{x}, t))$$
$$f_i(\boldsymbol{x} + \boldsymbol{c_i}, t + 1) = f_i^*(\boldsymbol{x}, t)$$

Magic values

We do not show it here, but unless one doesn't have the non-linear problems, all macroscopic errors/quantities of TRT depend on so-called "magic" parameter:

$$\Lambda = \left(\frac{1}{\omega_+} - \frac{1}{2}\right)\left(\frac{1}{\omega_-} - \frac{1}{2}\right).$$

That includes the spatial error, stability, best advection and diffusion. Here is the known list of the best magic parameters:

- $\Lambda = \frac{1}{4}$ is the best stability for the LBE. As well, this number gives the solution for the steady-state case dependant only on the equilibrium function.
- $\Lambda = \frac{1}{12}$ removes the third-order advection error (best advection).
- $\Lambda = \frac{1}{6}$ removes fourth-order diffusion errors (best diffusion).
- $\Lambda = \frac{3}{16}$ gives exact location of bounce-back walls for the Poiseuille flow.

Rule of thumb

The rule of thumb if you want to use MRT use it with TRT because it gives you precise answers. One parameter is usually fixed with viscosity, another one is fixed through the magic number combination.