Introduction to the Lattice Boltzmann Method

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Outline

1. Introduction
2. Non-dimensionalization
3. Velocity discretization
4. Time and space discretization
5. Navier-Stokes
6. Numerical implementation

Boltzmann equation in BBGKY hierarchy

Quantum mechanics:

$$i\hbar\partial_t\Psi = \hat{H}\Psi$$

Molecules motion:

$$m_i\partial_\alpha V_{i\alpha} = F_{i\alpha} = -\sum_{ij}\partial_\alpha V_{ij\alpha}$$

Boltzmann equation:

$$\partial_t f + v_\alpha\partial_\alpha f + \frac{F_\alpha}{m}\partial_{v_\alpha} f = J$$

Macroscopic hydrodynamic equations:

$$\partial_\alpha u_\alpha + u_\beta\partial_\beta u_\alpha = -\frac{\partial_\alpha p}{\rho} + \nu\partial^2_{\beta\beta}u_\alpha$$

BOLTZMANN EQUATION

After integration of the molecules motion one can obtain the Boltzmann equation:

$$\partial_t f + v_\alpha \partial_\alpha f + \frac{F_\alpha}{m} \partial_{v_\alpha} f = J,$$

where J is the collision operator, and f is the probability function. Collision operator is a complicated function usually written as:

$$J = \int_{\boldsymbol{v}'} \mathrm{d}\sigma(\Omega) \int \mathrm{d}\boldsymbol{v}' |\boldsymbol{v} - \boldsymbol{v}'| (f' \bar{f}' - f \bar{f}),$$

where $f = f(\boldsymbol{v})$ $\bar{f} = f(\bar{\boldsymbol{v}})$, $f' = f(\boldsymbol{v}')$,$\bar{f}' = f(\bar{v})$, $\sigma(\Omega)$ is the differentinal scattering cross section responsible for changing two molecules directions $(\boldsymbol{v}, \hat{\boldsymbol{v}}) \rightarrow (\boldsymbol{v}', \hat{\boldsymbol{v}})'$. TODO: insert image with the directions.

Boltzmann equation key assumptions

Boltzmann equation has certain assumptions:

- It is used only for binary collisions, i.e. the media is dillute gas.
- The collisions are performed under "molecular chaos" assumptions: velocity and position of the molecule are uncorrelated.

Most importantly (it's what we use later on) is that the collision integral is conserving:

$$\int J \begin{pmatrix} 1 \\ v_\alpha \\ \varepsilon \end{pmatrix} \mathrm{d}v_\alpha = 0$$

BGK collision operator

BGK collision operator is one of the most useful generalizations:

$$\partial_t f + v_\alpha \partial_\alpha f + \frac{F_\alpha}{m} \partial_{v_\alpha} f = J(f) = -\frac{\boldsymbol{f - f^{eq}}}{\boldsymbol{\tau}},$$

where τ is the relaxation rate towards the equilibrium presented by the Maxwell-Boltzmann distribution:

$$f^{eq}(\boldsymbol{r}, \boldsymbol{v}, t) = \rho(\boldsymbol{r}) \left[\frac{m}{2\pi k T(\boldsymbol{r})}\right]^{3/2} \exp\left[-\frac{m(\boldsymbol{v} - \boldsymbol{v_0}(\boldsymbol{r}))^2}{2kT(\boldsymbol{r})}\right].$$

The BGK collsion operator is more general than the usual Boltzmann collision integral. Moreover, it is conserving as the Boltzmann collision integral:

$$\int \frac{f - f^{eq}}{\tau} \begin{pmatrix} 1 \\ v_\alpha \\ \varepsilon \end{pmatrix} \mathrm{d}v_\alpha = 0$$

INTEGRALS OF THE EQUILIBRIUM FUNCTION

As soon as the equilibrium function is specified one can find the moments of the equilibrium function in the velocity space:

$$\begin{cases} \displaystyle\int f^{eq} \mathrm{d}\boldsymbol{v} = \rho(\boldsymbol{r}) \\ \displaystyle\int f^{eq} \boldsymbol{v} \mathrm{d}\boldsymbol{v} = \rho(\boldsymbol{r}) \boldsymbol{v_0}(\boldsymbol{r}) \\ \displaystyle\int f^{eq} \frac{(\boldsymbol{v} - \boldsymbol{v_0})^2}{2} = \frac{kT(\boldsymbol{r})}{m} \end{cases}$$

Non-dimensional form

It is hard to work with the probability distributon function which has dimensions of $\left[\frac{\text{kg s}^3}{\text{m}^6}\right]$. In what follows for simplicity we stick with the isothermal case $T(\boldsymbol{r}) = const$. For the nondimensalization the following quantities need to be non-dimensionalized: time, coordinate and velocity. For velocity if we look to the equilibrium distribution function it suggests us the natural scaling for the velocity as $c_0 = \sqrt{\frac{kT}{m}}$ which is the speed of sound for the ideal gas law. For coordinate we choose a natural scale L_0. The non-dimensionalization becomes as follows:

$$\frac{\partial \frac{f}{\rho(\frac{kT}{m})^{3/2}}}{\partial t \frac{c_0}{L_0}} + \frac{v_\alpha}{c_0} \frac{\partial \frac{f}{\rho(\frac{kT}{m})^{3/2}}}{\partial \frac{x_\alpha}{L_0}} + \frac{F_\alpha L_0}{m c_0^2} \frac{\frac{f}{\rho(\frac{kT}{m})^{3/2}}}{\partial \frac{v_\alpha}{c_0}} = -\frac{f - f^{eq}}{\rho(\frac{kT}{m})^{3/2}} \frac{1}{\tau \frac{c_0}{L_0}}.$$

NON-DIMENSIONAL FORM

After algebra one obtains the following:

$$\partial_{\hat{t}}\hat{f} + \hat{v}_\alpha \partial_{\hat{\alpha}}\hat{f} + \hat{F}_\alpha \partial_{\hat{v}_\alpha}\hat{f} = -\frac{\hat{f} - \hat{f}^{eq}}{\hat{\tau}}.$$

For the sake of simplicity from hereon hat symbols will be omitted. One can already see the next step as the expansion of the probability distribution functions in the Knudsen number series expansion.

HERMITE POLYNOMIAL EXPANSION

As we already mentioned, the collision operator is conserving. We search the solution for the probability distribution function as a series of the Hermite polynomials in space:

$$f(\boldsymbol{x}, \boldsymbol{v}, t) = \omega(\boldsymbol{v}) \sum_{n=0}^{\infty} \frac{1}{n!} \boldsymbol{a}^{(n)}(\boldsymbol{x}, t) \mathcal{H}^{(n)}(\boldsymbol{v}),$$

where the coefficient $\boldsymbol{a}^{(n)}(x, t) = \int f(\boldsymbol{x}, \boldsymbol{v}, t) \mathcal{H}^{(n)}(\boldsymbol{\xi})$. Hermite polynomial in the velocity space is defined through the generation weight function $\omega(\boldsymbol{v})$:

$$\mathcal{H}^{n}(\boldsymbol{v}) = \frac{(-1)^n}{\omega(\boldsymbol{v})} \boldsymbol{\nabla}^n \omega(\boldsymbol{v}),$$

where the weight function has the Maxwell-Boltzmann equilibrium distribution form:

$$\omega(\boldsymbol{v}) = \frac{1}{(2\pi)^{D/2}} \exp\left(-v^2/2\right)$$

EXPANSION OF COEFFICIENTS

Some Hermite polynomials expansions:

$$\mathcal{H}^{(0)}(\boldsymbol{v}) = \rho \qquad \mathcal{H}^{(1)}_{\alpha}(\boldsymbol{v}) = v_\alpha$$

$$\mathcal{H}^{(2)}_{\alpha\beta}(\boldsymbol{v}) = v_\alpha v_\beta - \delta_{\alpha\beta} \qquad \mathcal{H}^{(3)}_{\alpha\beta\gamma}(\boldsymbol{v}) = v_\alpha v_\beta v_\gamma - v_\alpha \delta_{\beta\gamma} - v_\beta \delta_{\alpha\gamma} - v_\gamma \delta_{\alpha\beta}$$

According to Shan and et. al. (JFM, 2006) and Cerciagnini (Mathematical Methods in Kinetic Theory, 1965) one can rewrite coefficients for the a few first coefficients for the Hermite polynomial expansion:

$$\boldsymbol{a}^{(0)} = \rho \qquad \boldsymbol{a}^{(1)} = \rho \boldsymbol{v_0}$$

$$\boldsymbol{a}^{\boldsymbol{(2)}} = \boldsymbol{P} + \rho(\boldsymbol{u}^2 - \boldsymbol{\delta}) \qquad \boldsymbol{a}^{(3)} = \boldsymbol{Q} + u\boldsymbol{a}^2 - (D-1)\rho\boldsymbol{u}^3$$

HERMITE EXPANSION OF EQUILIBRIUM

Non-dimensional equilibrium distribution function is represented as $f^(0) = \rho\omega(v - v_0)$. This right away gives the following expansion coefficients for the equilibrium distribution function:

$$\boldsymbol{a}_{eq}^{(0)} = \rho$$
$$\boldsymbol{a}_{eq}^{(1)} = \rho\boldsymbol{v_0}$$
$$\boldsymbol{a}_{eq}^{(2)} = \rho\boldsymbol{v_0}^2$$
$$\boldsymbol{a}_{eq}^{(3)} = \rho\boldsymbol{v_0}^3$$

A few notes:

- As we told before the collision operator is conserving (in isothermal case it is conserving density and momentum). One can see it as $\boldsymbol{a}^{(0)} = \boldsymbol{a}_{eq}^{(0)} = \rho$, $\boldsymbol{a}^{(1)} = \boldsymbol{a}_{eq}^{(1)} = \rho\boldsymbol{v_0}$.
- The expansion of the equilibrium function upto the second order gives the following function in the velocity space:

$$f^{eq}(\boldsymbol{v}) = \omega(\boldsymbol{v})\rho(1 + \boldsymbol{v}\cdot\boldsymbol{v_0} + \frac{1}{2}[(\boldsymbol{v}\cdot\boldsymbol{v_0}) - v_0^2])$$

Velocity discretization

The nicest feature of the Gauss-Hermite integrals is exact integration in the discrete space. Let us look it at the expansion coefficients:

$$\boldsymbol{a}^n(\boldsymbol{x},t) = \int \omega(\boldsymbol{v}) \sum_{m=0}^{\infty} \frac{1}{m!} \boldsymbol{a}^{(m)} \mathcal{H}^{(n)}(\boldsymbol{v}) \mathcal{H}^{(m)}(\boldsymbol{v}) \mathrm{d}\boldsymbol{v} = \int \omega(v) p(\boldsymbol{x},\boldsymbol{v},t) \mathrm{d}\boldsymbol{v},$$

where $p(\boldsymbol{x},\boldsymbol{v},t)$ is the polynomial. The Gauss quadrature rule states the following:

$$\int \omega(v) p(\boldsymbol{x},\boldsymbol{v},t) \mathrm{d}\boldsymbol{v} = \sum_{i=1}^{d} \frac{w_i}{\omega(\boldsymbol{v_i})} f(\boldsymbol{x},\boldsymbol{v_i},t) \mathcal{H}^{(n)}(\boldsymbol{v_i}),$$

where $\boldsymbol{v_i}$ is the discrete velocity set, w_i is weights set.
Using the Gauss quadrature rule for the equilibrium distribution function coefficients $\boldsymbol{a}_{eq}^{(0)} = \rho$ and $\boldsymbol{a}_{eq}^{(1)} = \rho \boldsymbol{v}$ one can obtain the following:

$$\rho = \boldsymbol{a}_{eq}^{(0)} = \sum_{i=1}^{d} \frac{w_i}{\omega(\boldsymbol{v_i})} \omega(\boldsymbol{v_i}) (1 + \boldsymbol{v_i} \cdot \boldsymbol{v_0} + \frac{1}{2}[(\boldsymbol{v_i} \cdot \boldsymbol{v_0})^2 - v_0^2]) \times 1$$

$$\rho \boldsymbol{v} = \boldsymbol{a}_{eq}^{(1)} = \sum_{i=1}^{d} \frac{w_i}{\omega(\boldsymbol{v_i})} \omega(\boldsymbol{v_i}) (1 + \boldsymbol{v_i} \cdot \boldsymbol{v_0} + \frac{1}{2}[(\boldsymbol{v_i} \cdot \boldsymbol{v_0})^2 - v_0^2]) \times \boldsymbol{v_i}$$

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Velocity discretization

Therefore one can define the equilibrium function as to be:

$$f_i^{eq}(\boldsymbol{x}, \boldsymbol{v_i}, t) = w_i \rho (1 + \boldsymbol{v_i} \cdot \boldsymbol{v_0} + \frac{1}{2}[(\boldsymbol{v_0} \cdot \boldsymbol{v})^2 - v_0^2]),$$

with the following macroscopic quantities:

$$\rho = \sum_i f_i^{eq} = \sum_i f_i$$

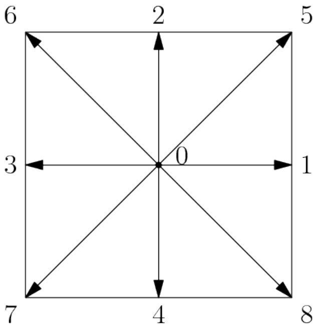
$$\rho \boldsymbol{v_0} = \sum_i f_i^{eq} \boldsymbol{v_i} = \sum_i f_i \boldsymbol{v_i},$$

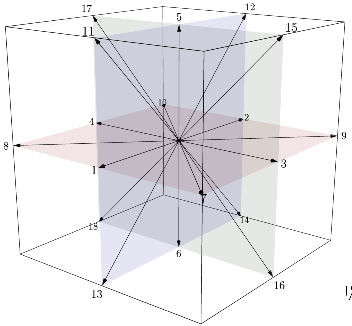
where the initial distribution function is redefined $\frac{w_i f_i}{\omega(v_i)} \to f_i$ for simplicity calculation reasons.

Velocity sets

It's time to tell what are the weights and velocity sets to calculate Hermite integrals. We present only a few popular LBM models as an example ($P(\boldsymbol{v})$ stands for the permutations):

D2Q9 $\boldsymbol{v_i}$	D2Q9 w_i	D3Q19 $\boldsymbol{v_i}$	D3Q19 w_i
$(0,0)$	$\frac{4}{9}$	$(0,0,0)$	$\frac{1}{3}$
$P(\sqrt{3},0)$	$\frac{1}{9}$	$P(\sqrt{3},0,0)$	$\frac{1}{18}$
$(\pm\sqrt{3},\pm\sqrt{3})$	$\frac{1}{36}$	$P(\pm 3,\pm 3,0)$	$\frac{1}{72}$





How do I avoid $\sqrt{3}$ in velocities? The answer is non-dimensiolization. Right now velocities are irrational numbers. Thus, we introduce the scaling factors:

$$\boldsymbol{c_i} = \frac{\boldsymbol{v_i}}{\sqrt{3}} \qquad \boldsymbol{u} = \frac{\boldsymbol{v_0}}{3}$$

After substituting it to the equilibrium function one can come up with the equilibrium function as:

$$f_i^{eq} = w_i \rho \Big(1 + 3\boldsymbol{u} \cdot \boldsymbol{c_i} + \frac{9}{2} \big(c_{i\alpha} c_{i\beta} - \delta_{\alpha\beta} 3 \big) u_\alpha u_\beta \Big).$$

OVERALL

We came up with the discretized continuous Boltzmann equation which conserves density and momentum (no forcing):

$$\partial_t f_i + c_{i\alpha} \partial_\alpha f_i = -\frac{f_i - f_i^{eq}}{\tau}.$$

At this particular time we introduce the discretized forcing term through the same Hermite polynomial expansion in the continous space and tell that it is incorporated smoothly:

$$F_\alpha \partial_{v_\alpha} f = \omega(\boldsymbol{v}) \sum_{n=1}^{\infty} \frac{n}{n!} \boldsymbol{F}\boldsymbol{a}^{(n-1)} \mathcal{H}^{(n)}$$

Taken upto to two orders of the expansion one can obtain the following:

$$F(\boldsymbol{v}) = \omega(\boldsymbol{v})\rho(1 + \boldsymbol{v} \cdot \boldsymbol{F} + (v_\alpha v_\beta - \delta_{\alpha\beta})F_\alpha v_\beta),$$

or in the discrete velocity space it will become as follows:

$$F_i = w_i \rho(1 + 3\boldsymbol{c_i} \cdot \boldsymbol{F} + \frac{9}{2}[c_{i\alpha} c_{i\beta} - \frac{\delta_{\alpha\beta}}{3}]F_\alpha u_\beta)$$

DISCRETIZATION

We start from the continuos discretized velocities BGK Boltzmann equation:

$$\partial_t f_i + c_{i\alpha}\partial_\alpha f_i = -\frac{f_i - f_i^{eq}}{\tau} + F_i.$$

One can see that the left hand side can be readily integrated along the characteristic. The right hand side can be integrated using the trapezoidal rule

$$f_i(\boldsymbol{x} + \boldsymbol{c_i}\Delta t, t + \Delta t) - f_i(\boldsymbol{x}, t) = \frac{\Delta t}{2}\left[-\frac{f_i(\boldsymbol{x} + \boldsymbol{c_i}, t + \Delta t) - f_i^{eq}(\boldsymbol{x} + \boldsymbol{c_i}, t + \Delta t)}{\tau} + F_i(\boldsymbol{x} + \boldsymbol{c_i}, t + \Delta t) - \frac{f_i(\boldsymbol{x}, t) - f_i^{eq}(\boldsymbol{x}, t)}{\tau} + F_i(\boldsymbol{x}, t)\right]$$

The equation above is implicit and cannot be readily integrated. Therefore we introduce the change of the variable as:

$$\bar{f}_i(\boldsymbol{x}, t) = f_i(\boldsymbol{x}, t) + \frac{\Delta t}{2}\left[\frac{f_i(\boldsymbol{x}, t) - f_i^{eq}(\boldsymbol{x}, t)}{\tau} - F_i(\boldsymbol{x}, t)\right].$$

NEW VARIABLE

The inverse of the new variable is $f_i = \frac{\bar{f}_i + \frac{\Delta t}{2\tau} f_i^{eq} + \frac{\Delta t}{2} F_i(\boldsymbol{x}, t)}{1 + \frac{\Delta t}{2\tau}}$. One can see that the integrated equation is rewritten as:

$$\bar{f}_i(\boldsymbol{x} + \boldsymbol{c_i}\Delta t, t + \Delta t) = \bar{f}_i(\boldsymbol{x}, t) - \Delta t \left[\frac{f_i(\boldsymbol{x}, t) - f_i^{eq}}{\tau} + F_i(\boldsymbol{x}, t) \right]$$

$$\bar{f}_i(\boldsymbol{x} + \boldsymbol{c_i}\Delta t, t + \Delta t) = \bar{f}_i(\boldsymbol{x}, t) - \Delta t \left[\frac{\frac{\bar{f}_i(\boldsymbol{x}, t) + \frac{\Delta t}{2\tau} f_i^{eq} + \frac{\Delta t}{2} F_i(\boldsymbol{x}, t)}{1 + \frac{\Delta t}{2\tau}} - f_i^{eq}}{\tau} + F_i(\boldsymbol{x}, t) \right]$$

After simple algebra one can obtain the following explicit update rule:

$$\bar{f}_i(\boldsymbol{x} + \boldsymbol{c_i}\Delta t, t + \Delta t) = \bar{f}_i(\boldsymbol{x}, t)\left(1 - \frac{\Delta t}{\tau + \frac{\Delta t}{2}}\right) + f_i^{eq}(\boldsymbol{x}, t)\frac{\Delta t}{\tau + \frac{\Delta t}{2}} + \frac{F_i \Delta t}{1 + \frac{\Delta t}{2\tau}}.$$

One only needs to check the macroscopic variables:

$$\sum_i f_i = \rho$$

$$\sum_i \bar{f}_i = \sum_i f_i + \frac{\Delta t}{2}\Big[\frac{\sum_i f_i - f_i^{eq}}{\tau} - \sum_i F_i\Big] = \rho$$

$$\sum_i f_i \boldsymbol{c_i} = \rho u_\alpha$$

$$\sum_i \bar{f}_i \boldsymbol{c_i} = \sum_i f_i \boldsymbol{c_i} + \frac{\Delta t}{2}\Big[\frac{\sum_i (f_i - f_i^{eq})\boldsymbol{c_i}}{\tau} - \sum_i F_i c_i\Big] = \rho u_\alpha - \frac{\boldsymbol{F}\Delta t}{2}$$

Therefore, the macroscopic variables can be found as:

$$\rho = \sum_i \bar{f}_i, \quad \rho u_\alpha = \sum_i \bar{f}_i c_{i\alpha} + \frac{F_i \Delta t}{2}$$

Note that all the moments for force populations F_i are apriori known from the continuous theory which we presented before.

Implicit and Explicit LB schemes

The scheme presented before is believed to be second order accurate in time and space. However it is much more common used another formulation of the Lattice Boltzmann equation which can be obtained by simply changing $\tau + \frac{1}{2} \to \tau$. Therefore the lattice boltzmann equation in the usual form can be formulated as:

Lattice Boltzmann equation

$$f_i(\boldsymbol{x} + \boldsymbol{c_i}\Delta t, t + \Delta t) = \frac{\Delta t}{\tau} f_i^{eq}(\boldsymbol{x}, t) + f_i(\boldsymbol{x}, t)\left(1 - \frac{\Delta t}{\tau}\right) + F_i \Delta t \left(1 - \frac{1}{2\tau}\right),$$

where the force term (Guo formulation, PRE 2002) and the equilibrium functions are calculated with the shifted, so-called macroscopic velocity calculated as:

$$\rho \boldsymbol{u} = \sum_i f_i \boldsymbol{c_i} + \frac{\boldsymbol{F}\Delta t}{2}$$

KNUDSEN NUMBER EXPANSION

Still even we know how to discretize in space, velocity space and time and be able to conserve quantities, we don't know what macroscopic equations can be obtained. This is the topic of the Chapman-Enskog expansion. If we look more closely to the Knudsen number definition as:

$$\epsilon = Kn = \frac{\lambda}{L_0},$$

where λ is the mean free path. One can state that the relaxation rate towards the equilibrium distribution function is close to the time between molecule collisions (the average molecule speed is close to the speed of sound). That can suggest right away the scaling of the non-dimensional time is the Knudsen number:

$$\frac{\tau}{\frac{L_0}{c_0}} \approx \frac{\frac{\lambda}{c_0}}{\frac{L_0}{c_0}} = \frac{\lambda}{L}$$

Therefore one can suggest the natural scaling of the problem through the Knudsen number expansion:

$$f = \sum_{n=0}^{\infty} \epsilon^n f^{(n)}.$$

Chapman-Enskog expansion

If one substitutes the expansion to the continuous Boltzmann equation one can obtain the following (we drop the force for the simplicity reason):

$$\partial_t \sum_{n=0}^{\infty} \epsilon^n f^{(n)} + c_{i\alpha}\partial_\alpha \sum_{n=0}^{\infty} \epsilon^n f^{(n)} = -\frac{\sum_{n=0}^{\infty} f^{(n)} - f^{eq}}{\tau}.$$

The equilibrium function gives the same density and momentum. It means the following:

$$\sum_i f_i = \sum_{n=0}^{\infty} \epsilon^n \sum_i f_i^{(n)} = \sum_i f_i^{(0)} + \epsilon \sum_i f_i^{(1)} + ... = \rho$$

By taking that $f_i^{(0)} = f_i^{eq}$ one can obtain the following summations for higher order terms:

$$\sum_i f_i^{(n)} = \sum_i f_i^{(n)} c_{i\alpha} = 0, \text{ for } n > 0$$

By summing up the equation in velocity space one can obtain the following:

$$\partial_t \rho + \partial_\alpha \rho u_\alpha = 0$$

$$\partial_t \rho u_\alpha + \partial_\beta (\rho u_\alpha u_\beta + \sum_{n=1} \epsilon^n \sum_i f_i^{(n)} c_{i\alpha} c_{i\beta}) = 0$$

TIME SCALES

At this particular stage one can see the separation of the time scales as follows:

$$\partial_{t_0}\rho = 0 \quad \partial_{t_0}\rho u_\alpha = -\partial_\beta \rho u_\alpha u_\beta$$

$$\partial_{t_1}\rho = 0 \quad \partial_{t_1}\rho u_\alpha = -\partial_\beta \sum_i f_i^{(1)} c_{i\alpha} c_{i\beta}$$

Therefore one can introduce the separation of time scales as:

$$\partial_t = \partial_{t_0} + \epsilon\partial_{t_1} + \epsilon^2\partial_{t_2}$$

Chapman-Enskog expansion in Δt

To be able to capture the expansion at the level of Knudsen number we need to specify the Knudsen number. As far as the Knudsen number is not specified since the BGK collision operator is different in comparison with the Boltzmann collision integral. Let us specify departure from the equilibrium, i.e. Knudsen number, controlled by the non-dimensional time step, i.e. $\epsilon = Kn = \Delta t$. Therefore, the lattice Boltzmann equation becomes:

$$f_i(\boldsymbol{x} + \epsilon \boldsymbol{c_i}, t + \epsilon) - f_i(\boldsymbol{x}, t) = -\epsilon \frac{f_i - f_i^{eq}}{\tau} + \epsilon F_i (1 - \frac{\epsilon}{2\tau}). \quad (1)$$

As we discussed before parameter τ is of Knudsen number order of magnitude. Thus, let us rescale $\frac{\tau}{\epsilon} \to \tau$, where a new τ is of unity order of magnitude. Thus, the LBE becomes:

$$f_i(\boldsymbol{x} + \epsilon \boldsymbol{c_i}, t + \epsilon) - f_i(\boldsymbol{x}, t) = -\frac{f_i - f_i^{eq}}{\tau} + \epsilon F_i (1 - \frac{1}{2\tau}). \quad (2)$$

CHAPMAN-ENSKOG EXPANSION

Let us do a multivariable Taylor expansion for the left hand side of the LBE:

$$\sum_{n=0}^{\infty} \epsilon^n \frac{(\partial_t + c_{i\alpha}\partial_\alpha)^n}{n!} f_i = \sum_{n=0}^{\infty} \epsilon^n \frac{(\partial_t + c_{i\alpha}\partial_\alpha)^n}{n!} \sum_{m=0}^{\infty} \epsilon^m f_i^{(m)}$$

$$= -\frac{\sum_{n=1}^{\infty} \epsilon^n f_i^{(n)}}{\tau} + \epsilon F_i (1 - \frac{1}{2\tau}).$$

Let us take consequtive approximation by ϵ:

$$\epsilon^0 : f_i^{(0)} = f_i^{eq}$$

$$\epsilon^1 : (\partial_{t_0} + c_{i\alpha}\partial_\alpha) f_i^{(0)} = -\frac{f_i^{(1)}}{\tau} + F_i\left(1 - \frac{1}{2\tau}\right)$$

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

CONTINUITY EQUATION

One can simplify the term with ϵ^2 by substiting the expression for $(\partial_{t_0} + c_{i\alpha}\partial_\alpha) f_i^{(0)}$:

$$\epsilon^2 : \partial_{t_1} f_i^{(0)} + (\partial_{t_0} + c_{i\alpha}\partial_\alpha)\left(1 - \frac{1}{2\tau}\right)\left[f_i^{(1)} + \frac{F_i}{2}\right] = -\frac{f_i^{(2)}}{\tau}$$

Another condition what we need to establish are the moments of the functions:

$$\sum_i f_i^{(0)} = \rho, \qquad \sum_i f_i^{(n)} = 0 \text{ for } n > 0$$

$$\sum_i f_i c_{i\alpha} = \sum_{i,n} \epsilon^n f_i^{(n)} c_{i\alpha} = \rho u_\alpha \qquad \sum_i f_i^{(0)} c_{i\alpha} = \rho u_\alpha + \epsilon \frac{F_\alpha}{2}$$

$$\sum_i f_i^{(1)} c_{i\alpha} = -\frac{F_\alpha}{2} \qquad \sum_i f_i^{(n)} c_{i\alpha} = 0 \text{ for } n > 0$$

The continuity equation can be obtained by summing three equations by i:

$$\epsilon : \quad \partial_{t_0}\rho + \partial_\alpha \sum_i f_i^{(0)} c_{i\alpha} = 0$$

$$\epsilon^2 : \quad \partial_{t_1}\rho + \left(1 - \frac{1}{2\tau}\right)\partial_\alpha\left(\sum_i c_{i\alpha} f_i^{(1)} + \frac{\sum_i c_{i\alpha} F_i}{2}\right) = 0$$

CONTINUITY EQUATION

Overall one can obtain the continuity equation:

$$\epsilon: \quad \partial_{t_0}\rho + \partial_\alpha \sum_i f_i^{(0)} c_{i\alpha} = 0$$

$$\epsilon^2: \quad \partial_{t_1}\rho + \left(1 - \frac{1}{2\tau}\right)\partial_\alpha\left(-\frac{F_\alpha}{2} + \frac{F_\alpha}{2}\right) = 0$$

$$(\partial_{t_0} + \epsilon\partial_{t_1}) + \partial_\alpha(\rho u_\alpha + \epsilon F_\alpha/2)) = 0$$
$$\partial_t\rho + \partial_\alpha \rho u_\alpha^m = 0,$$

where $\rho u_\alpha^m = \sum_i f_i c_{i\alpha} + \epsilon F_\alpha/2$ is the so-called macroscopic velocity, already discussed in the continous space formulation.

NAVIER-STOKES EQUATION

The same summation with the vector $c_{i\alpha}$ can be applied to obtain the Navier-Stokes equation:

$$\epsilon: \quad \partial_{t_0}(\rho u_\alpha + \epsilon F_\alpha/2) + \partial_\beta \sum_i f_i^{(0)} c_{i\alpha} c_{i\beta} = F_\alpha$$

$$\epsilon^2: \quad \partial_{t_1}(\rho u_\alpha + \epsilon F_\alpha/2) + \left(1 - \frac{1}{2\tau}\right)\partial_{t_0}\left(\sum_i f_i^{(1)} c_{i\alpha} + \frac{\sum_i F_i c_{i\alpha}}{2}\right)$$

$$+ \left(1 - \frac{1}{2\tau}\right)\partial_\beta\left(\sum_i f_i^{(1)} c_{i\alpha} c_{i\beta} + \frac{\sum_i F_i c_{i\alpha} c_{i\beta}}{2}\right) = 0$$

NAVIER-STOKES EQUATION

Note that $\sum_i f_i^{(1)} c_{i\alpha} + \frac{\sum_i F_i c_{i\alpha}}{2} = 0$. For the rest one can obtain the following expression from the original Chapman-Enskog expression on order of ϵ:

$$f_i^{(1)} + \frac{F_i}{2} = \tau[F_i - (\partial_{t_0} + c_{i\alpha}\partial_\alpha) f_i^{(0)}]$$

Therefore the expression for $\sum_i \left(f_i^{(1)} + \frac{F_i}{2}\right) c_{i\alpha} c_{i\beta}$ can be obtained through the moments of $f_i^{(0)}$:

$$\begin{aligned}\sum_i \left(f_i^{(1)} + \frac{F_i}{2}\right) c_{i\alpha} c_{i\beta} =& \tau \sum_i F_i c_{i\alpha} c_{i\beta} - \tau \partial_{t_0} \sum_i f_i^{(0)} c_{i\alpha} c_{i\beta} \\ & - \tau \partial_\gamma \sum_i c_{i\alpha} c_{i\beta} c_{i\gamma} f_i^{(0)}.\end{aligned}$$

Few terms are known from the continuous theory, i.e.

$$\sum_i F_i c_{i\alpha} c_{i\beta} = F_\alpha u_\beta^m + F_\beta u_\alpha^m$$

$$\sum_i f_i^{(0)} c_{i\alpha} c_{i\beta} c_{i\gamma} = \rho u_\alpha^m u_\beta^m u_\gamma^m + \frac{\rho u_\alpha^m}{3} \delta_{\beta\gamma} + \frac{\rho u_\beta^m}{3} \delta_{\alpha\gamma} + \frac{\rho u_\gamma^m}{3} \delta_{\alpha\beta}.$$

Calculations

Let us calculate the time derivative $\partial_{t_0} \sum_i f_i^{(0)} c_{i\alpha} c_{i\beta}$:

$$\partial_{t_0} \sum_i f_i^{(0)} c_{i\alpha} c_{i\beta} = \partial_{t_0} \left(\frac{\rho}{3} \delta_{\alpha\beta} + \rho u_\alpha^m u_\beta^m \right)$$

$$\partial_{t_0} \frac{\rho}{3} = \frac{1}{3} \left(-\partial_\gamma \rho u_\gamma^m \right)$$

$$\partial_{t_0} \rho u_\alpha^m u_\beta^m = \partial_{t_0} \frac{\rho u_\alpha^m \rho u_\beta^m}{\rho} = u_\alpha^m \partial_{t_0} \rho u_\beta^m + u_\beta^m \partial_{t_0} \rho u_\alpha - u_\alpha^m u_\beta^m \partial_{t_0} \rho$$

$$\partial_{t_0} \rho u_\alpha^m = F_\alpha - \frac{1}{3} \partial_\alpha \rho - \partial_\beta \rho u_\alpha^m u_\beta^m$$

$$\partial_{t_0} \rho u_\alpha^m \rho_\beta^m = u_\alpha^m \left(F_\beta - \frac{1}{3} \partial_\beta \rho - \partial_\gamma \rho u_\beta^m u_\gamma^m \right) + u_\beta^m \left(F_\alpha - \frac{1}{3} \partial_\alpha \rho - \partial_\gamma \rho u_\alpha^m u_\gamma^m \right)$$

At this particular moment we assume the low Mach limit that means $\boldsymbol{u^m}$ is small and we neglect all the terms with the order $O((\boldsymbol{u^m})^3)$:

$$\partial_{t_0} \sum_i f_i^{(0)} c_{i\alpha} c_{i\beta} \approx -\frac{\delta_{\alpha\beta}}{3} \partial_\gamma \rho u_\gamma^m + u_\alpha^m F_\beta + u_\beta^m F_\alpha - \frac{u_\alpha}{3} \partial_\beta \rho - \frac{u_\beta}{3} \partial_\alpha \rho$$

$$\partial_\gamma \sum_i f_i^{(0)} c_{i\alpha} c_{i\beta} c_{i\gamma} \approx \frac{1}{3} \left[\partial_\beta \rho u_\alpha^m + \partial_\alpha \rho u_\beta^m + \delta_{\alpha\beta} \partial_\gamma \rho u_\gamma^m \right].$$

Calculations

After substitution of found terms one can obtain the following:

$$\begin{aligned}
\sum_i \left(f_i^{(1)} + \frac{F_i}{2}\right) c_{i\alpha} c_{i\beta} = {} & \tau(F_\alpha u_\beta^m + F_\beta u_\alpha^m) - \frac{\tau}{3}\left[\partial_\beta \rho u_\alpha^m + \partial_\alpha \rho u_\beta^m + \delta_{\alpha\beta}\partial_\gamma \rho u_\gamma^m\right] \\
& - \tau\left[-\frac{\delta_{\alpha\beta}}{3}\partial_\gamma \rho u_\gamma^m + u_\alpha^m F_\beta + u_\beta^m F_\alpha - \frac{u_\alpha}{3}\partial_\beta \rho - \frac{u_\beta}{3}\partial_\alpha \rho\right] \\
\sum_i \left(f_i^{(1)} + \frac{F_i}{2}\right) c_{i\alpha} c_{i\beta} = {} & -\frac{\tau}{3}\left[\rho \partial_\beta u_\alpha^m + \rho \partial_\alpha u_\beta^m\right]
\end{aligned}$$

One can substitute all found terms to the Chapman-Enskog system to restore the Navier-Stokes equation:

$$\begin{aligned}
\epsilon : \quad & \partial_{t_0} \rho u_\alpha^m + \partial_\beta \rho u_\alpha^m u_\beta^m = -\frac{1}{3}\partial_\alpha \rho + F_\alpha \\
\epsilon^2 : \quad & \partial_{t_1} \rho u_\alpha^m - \left(1 - \frac{1}{2\tau}\right)\frac{\tau}{3}\partial_\beta\left[\rho \partial_\beta u_\alpha^m + \rho \partial_\alpha u_\beta^m\right] = 0
\end{aligned}$$

NAVIER-STOKES EQUATION

This is exactly the Navier-Stokes equation:

OUR GOAL:

$$(\partial_{t_0} + \epsilon\partial_{t_1})\rho u_\alpha^m + \partial_\beta \rho u_\alpha^m u_\beta^m = -\frac{1}{3}\partial_\alpha \rho + F_\alpha + \nu\partial_\beta(\rho\partial_\beta u_\alpha + \rho\partial_\alpha u_\beta),$$

where $\nu = \frac{1}{3}(\tau - \frac{1}{2})$ is the kinematic viscosity.
Alltogether, the lattice Boltzmann method restores the slightly compressible Navier-Stokes equation with the certain limits - small Knudsen number (closiness to the equilibrium) and small Mach number (truncation of $\boldsymbol{u}^3$ terms).

Why to bother: Advantages vs Disadvantages

Hydrodynamics: The complications come from the term $(\boldsymbol{u} \cdot \boldsymbol{\nabla})\boldsymbol{u}$:

- Highly non-linear
- Non-local integration through complex fluid trajectories

Lattice: Advantages:

- Transport is linear and exact $(\boldsymbol{c} \cdot \boldsymbol{\nabla})f$
- Interaction is local $J(f)$
- Complex geometries
- Multiscal physics
- Massive parallelization

Disadvantages:

- Stability issues
- Boundary conditions

Lattice Boltzmann equation

Usually lattice Boltzmann is represented through two step procedure (collision and streaming):

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

While collision is local, streaming takes a value of the function and stream it in the certain direction $\boldsymbol{c_i}$.

Lattice Boltzmann algorithm

So far we were dealing only with equations. The question remains how to do calculations? The procedure is the following:

- Define your non-dimensional numbers and match them with the lattice Boltzmann numbers. For example it's easy to obtain a matching lattice spacing $\Delta x = \frac{L}{N}$ and $\Delta t = \frac{U_{LB}}{U}\Delta x$. Remember that U_{LB} should be small. As well Knudsen number $Kn \propto Ma \cdot Re$ - usually $Kn \propto \frac{1}{N}$. Remember about that to be stable parameter $\tau > 1/2$. However, for large τ the accuracy of the method deteriorate.
- Choose your grid size N, relaxation parameter τ, lattice Boltzmann velocity U_{LB}. Map your domain to the grid.
- Initialize your distribution function values with the equilibrium function values.
- Iterate:
  - Calculation of the macroscopic variables $\rho = \sum_i f_i$, $\rho \boldsymbol{u} = \sum_i f_i \boldsymbol{c_i} + \frac{F}{2}$. If force is not constant calculate it before.
  - Do collision procedure
  - Boundary conditions can be here or before the calculation of the macroscopic variables
  - Perform streaming
  - Loop

Next lecture

Next lecture is about TRT and MRT.