Am Introduction to the lattice Boltzmann method

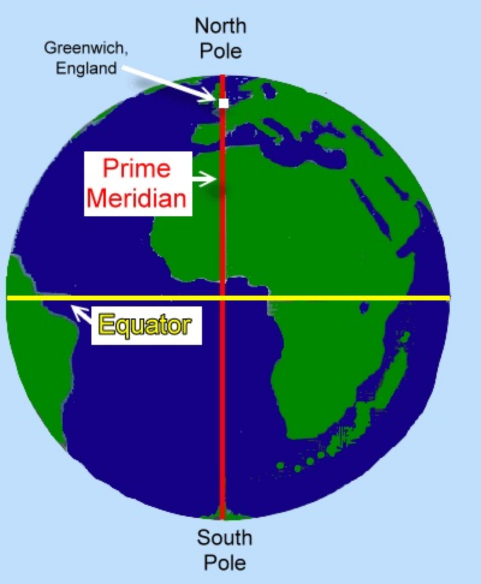
Tim Reis

School of Computing and Mathematical Sciences
University of Greenwich
London, UK

OpenLB Spring School
Mannheim 2019

Acknowledgments : Tim Phillips (Cardiff University), Paul Dellar (University of Oxford)

Where is Greenwich?



Where is Greenwich?

Where is Greenwich?

Greenwich Campus

Greenwich in the Movies

Greenwich in the Movies

Greenwich in the Movies

What is this lecture about?

Fundamental concepts of the LBM

Hopefully addressing some common confusions and misconceptions

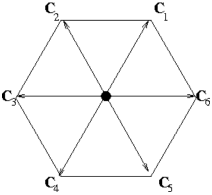
Boltzmann vs lattice Boltzmann vs Navier Stokes

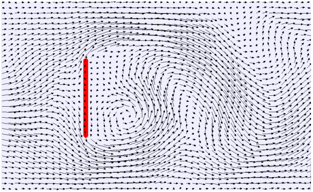
What equations are we solving and why?

A (very) brief historical perspective

LGCA: Hydrodynamics from Boolean operations [Frisch *et al.* 1986]

$$n_i(\mathbf{x} + \mathbf{c}_i, t + 1) = n_i(\mathbf{x}, t) + C(\mathbf{n}), \quad n_i \in \{0, 1\}$$





Eliminate noise and linearise the collision operator

[McNamara and Zanetti 1988,Qian *et al.* 1991], Higuera *et al.* 1989]

$$N_i(\mathbf{x} + \mathbf{c}_i, t + 1) = N_i(\mathbf{x}, t) - \Omega_{ij} \left(N_j - N_j^{(e)} \right)$$

Lattice Boltzmann perspectives

The first LBE review article tells us that [Succi, Benzi, Higuera 1991]

> *The LBE is a nonlinear finite difference equation (even though it does not result from the discretisation of any partial differential equation!)*

The “second generation" of LB is derived from “purely microscopic considerations" and approximates the continuous Boltzmann equation [Chen and Doolen 1998 (which has about 2500 citations!)]

This may suggest that the LBE can go “beyond" Navier-Stokes, *e.g* capture the Knudsen layer in the transition regime - a view also held in the most recent review article [Aidun and Clausen 2010]

Overview

Derivation of the lattice Boltzmann equation

- From kinetic theory to hydrodynamics
- Copying the essentials: from continuous to discrete kinetic theory
- From discrete Boltzmann to lattice Boltzmann (PDEs to numerics)

Multiple relaxation times (MRT)

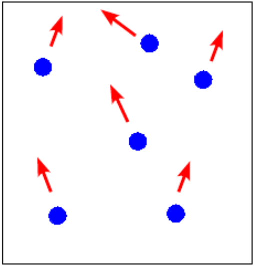
Exact solution of the LBE in Poiseuille flow

The kinetic theory of gases

The Navier-Stokes equations for a Newtonian fluid can be derived from Boltzmann's equation for a monotomic gas

$$\frac{\partial f}{\partial t} + \mathbf{c} \cdot \nabla f = \Omega(f)$$

where $f = f(\mathbf{x}, \mathbf{c}, t)$ is the distribution function of particles at $\mathbf{x}$ and t with velocity $\mathbf{c}$:



$\Omega(f)$ is Boltzmann's binary collision operator.

Hydrodynamics from moments

Hydrodynamic quantities are moments of the distribution function f:

$$\begin{aligned}
\rho(\mathbf{x}, t) &= \int f(\mathbf{x}, \mathbf{c}, t) d\mathbf{c}, \\
\mathbf{u}(\mathbf{x}, t) &= \frac{1}{\rho} \int \mathbf{c} f(\mathbf{x}, \mathbf{c}, t) d\mathbf{c}, \\
\theta(\mathbf{x}, t) &= \frac{1}{3\rho} \int |\mathbf{c} - \mathbf{u}|^2 f(\mathbf{x}, \mathbf{c}, t) d\mathbf{c}.
\end{aligned}$$

The collision operator $\Omega(f)$ drives f back to the Maxwell-Boltzmann distribution

$$f^{(0)} = \frac{\rho}{(2\theta\pi)^{3/2}} \exp\left(-\frac{|\mathbf{c} - \mathbf{u}|^2}{2\theta}\right).$$

From kinetic theory to fluid dynamics

Recall Boltzmann's equation

$$\frac{\partial f}{\partial t} + \mathbf{c} \cdot \nabla f = \Omega(f)$$

Assume f relaxes towards $f^{(0)}$ with a single relaxation time τ:

$$\frac{\partial f}{\partial t} + \mathbf{c} \cdot \nabla f = -\frac{1}{\tau}\left(f - f^{(0)}\right)$$

The zeroth and first moments of the Boltzmann equation give exact conservation laws:

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

Evolution of the momentum flux

The momentum flux $\mathbf{\Pi}$ is given by another moment

$$\mathbf{\Pi} = \int f\mathbf{c}\mathbf{c}d\mathbf{c}, \quad \text{and} \quad \mathbf{\Pi}^{(0)} = \int f^{(0)}\mathbf{c}\mathbf{c}d\mathbf{c}.$$

$\mathbf{\Pi}$ is *not* conserved by collisions. It evolves according to

$$\frac{\partial \mathbf{\Pi}}{\partial t} + \nabla \cdot \boldsymbol{Q} = -\frac{1}{\tau}\left(\mathbf{\Pi} - \mathbf{\Pi}^{(0)}\right),$$

where

$$\mathbf{\Pi}^{(0)} = \rho\mathbf{u}\mathbf{u} + \rho\theta\mathbf{I}, \quad \text{and} \quad \boldsymbol{Q} = \int f\mathbf{c}\mathbf{c}\mathbf{c}d\mathbf{c}.$$

Hydrodynamics follow by exploiting $\tau \ll T$.

Newton's Second Law

Newton's 2nd law following a "blow of fluid" says

$$\rho \frac{d\mathbf{u}}{dt} = \mathbf{F}$$

For a fixed point **x** is space

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

That is, we have an intrinsic non-linearity, even when **F** is linear, as it is for a Newtonian fluid,

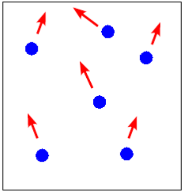
$$\mathbf{F} = \nabla \cdot \left[-c_s^2 \rho \mathbf{I} + \mu \left(\nabla \mathbf{u} + (\nabla \mathbf{u})^T \right) \right]$$

Boltzmann's equation

On the other hand, Boltzmann's equation

$$\frac{\partial f}{\partial t} + \mathbf{c} \cdot \nabla f = \Omega(f)$$

has $f = f(\mathbf{x}, \mathbf{c}, t)$ instead of $\mathbf{u}(\mathbf{x}, t)$.



That is, it has linear advection instead of non-linear convection, but seven independent variables.

Lattice Boltzmann

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

$$\frac{\partial f}{\partial t} + \mathbf{c} \cdot \nabla f = \Omega(f)$$

Lattice Boltzmann

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

LBE squeezes in between: linear advection, few additional degrees of freedom

$$\frac{\partial f}{\partial t} + \mathbf{c} \cdot \nabla f = \Omega(f)$$

What do we need from kinetic theory for hydrodynamics?

Collisions should send $f \to f^{(0)}$ and we need some equilibrium moments (found from the Mazwell-Boltzmann distribution)

$$\begin{aligned}
\rho &= \int f^{(0)} d\mathbf{c}, \\
\rho\mathbf{u} &= \int f^{(0)} \mathbf{c} d\mathbf{c}, \\
\mathbf{\Pi}^{(0)} &= \int f^{(0)} \mathbf{c}\mathbf{c} d\mathbf{c} = \rho\theta\mathbf{I} + \rho\mathbf{u}\mathbf{u}, \\
\mathbf{Q}^{(0)} &= \int f^{(0)} \mathbf{c}\mathbf{c}\mathbf{c} d\mathbf{c},
\end{aligned}$$

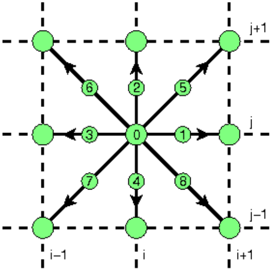
where

$$Q^{(0)}_{\alpha\beta\gamma} = \theta\rho\left(u_\alpha\delta_{\beta\gamma} + u_\beta\delta_{\gamma\alpha} + u_\gamma\delta_{\alpha\beta}\right) + \partial_\alpha\left(\rho u_\alpha u_\beta u_\gamma\right).$$

Discrete kinetic theory

Look to simplify Boltzmann's equation without losing the properties needed to recover the Navier-Stokes equation.

Discetise the velocity space such that $\mathbf{c}$ is confined to a set $\mathbf{c}_0, \mathbf{c}_1, \ldots, \mathbf{c}_N$, e.g



The distribution function is $f(\mathbf{x}, \mathbf{c}, t)$ is replaced by $f(\mathbf{x}, \mathbf{c}_i, t) = f_i(\mathbf{x}, t)$.

The discrete Boltzmann equation

The Boltzmann equation with discrete velocities is

$$\frac{\partial f_i}{\partial t} + \mathbf{c}_i \cdot \nabla f_i = -\frac{1}{\tau}\left(f_i - f_i^{(0)}\right)$$

We now supply the equilibrium function, for example

$$f_i^{(0)} = W_i \rho \left(1 + \frac{1}{\theta}\mathbf{u}\cdot\mathbf{c}_i + \frac{1}{2\theta^2}(\mathbf{u}\cdot\mathbf{c}_i)^2 - \frac{1}{2\theta}|\mathbf{u}|^2\right)$$

The previous integrals are now replaced by summations:

$$\begin{aligned}
\rho &= \sum_i f_i = \sum_i f_i^{(0)}, \\
\rho\mathbf{u} &= \sum_i f_i \mathbf{c}_i = \sum_i f_i^{(0)} \mathbf{c}_i \\
\mathbf{\Pi}^{(0)} &= \sum_i f_i^{(0)} \mathbf{c}_i \mathbf{c}_i = \rho\mathbf{u}\mathbf{u} + \theta\rho\mathbf{I}.
\end{aligned}$$

Moment equations

$$\frac{\partial f_i}{\partial t} + \mathbf{c}_i \cdot \nabla f_i = -\frac{1}{\tau}\left(f_i - f_i^{(0)}\right)$$

Taking the zeroth, first, and second moments of the discrete Boltzmann equation give

$$\begin{aligned}
\frac{\partial \rho}{\partial t} &+ \nabla \cdot (\rho \mathbf{u}) = 0, \\
\frac{\partial \rho \mathbf{u}}{\partial t} &+ \nabla \cdot \mathbf{\Pi} = 0, \\
\frac{\partial \mathbf{\Pi}}{\partial t} &+ \nabla \cdot \boldsymbol{Q} = -\frac{1}{\tau}\left(\mathbf{\Pi} - \mathbf{\Pi}^{(0)}\right)
\end{aligned}$$

Note that we did exactly the same for the continuum Boltzmann equation.

Chapman-Enskog expansion

Hydrodynamics now follows from seeking solutions to

$$\frac{\partial f_i}{\partial t} + \mathbf{c}_i \cdot \nabla f_i = -\frac{1}{\tau}\left(f_i - f_i^{(0)}\right)$$

that vary slowly compared with the timescale τ.

We assume f_i is close to equilibrium and expand:

$$f_i = f_i^{(0)} + \tau f_i^{(1)} + \tau^2 f_i^{(2)} + \dots$$

Or, equivalently,

$$\mathbf{\Pi} = \mathbf{\Pi}^{(0)} + \tau\mathbf{\Pi}^{(1)} + \tau^2\mathbf{\Pi}^{(2)} \dots, \quad \boldsymbol{Q} = \boldsymbol{Q}^{(0)} + \tau\boldsymbol{Q}^{(1)} + \tau^2\boldsymbol{Q}^{(2)} \dots$$

Also expand the temporal derivative:

$$\frac{\partial}{\partial t} = \frac{\partial}{\partial t_0} + \tau\frac{\partial}{\partial t_1} \dots$$

Hydrodynamics from moments

Substituting these expansions into the moment equations and truncating at $\mathcal{O}(1)$ we obtain

$$
\begin{aligned}
\frac{\partial \rho}{\partial t_0} &+ \nabla \cdot (\rho \mathbf{u}) = 0, \\
\frac{\partial \rho \mathbf{u}}{\partial t_0} &+ \nabla \cdot \mathbf{\Pi}^{(0)} = 0, \\
\frac{\partial \mathbf{\Pi}^{(0)}}{\partial t_0} &+ \nabla \cdot \boldsymbol{Q}^{(0)} = -\mathbf{\Pi}^{(1)}
\end{aligned}
$$

The first two equations coincide with the compressible Euler equations if we choose

$$\mathbf{\Pi}^{(0)} = \rho \theta \mathbf{I} + \rho \mathbf{u}\mathbf{u}$$

Calculating the viscous stress tensor

For the Navier-Stokes equation we need to compute the first correction $\mathbf{\Pi}^{(1)}$ to the momentum flux.

$$\frac{\partial \mathbf{\Pi}^{(0)}}{\partial t_0} + \nabla \cdot \boldsymbol{Q}^{(0)} = -\mathbf{\Pi}^{(1)}.$$

Given $\mathbf{\Pi}^{(0)} = \rho\theta\mathbf{I} + \rho\mathbf{uu}$ we can calculate

$$\partial_{t_0} \Pi^{(0)}_{\beta\gamma} = \partial_{t_0} \left(\rho\theta\mathbf{I} + \rho\mathbf{uu}\right)$$

using the leading order equation

$$\begin{aligned} \partial_{t_0} \rho &= -\nabla \cdot (\rho\mathbf{u}) \\ \partial_{t_0}(\rho\mathbf{u}) &= -\nabla\mathbf{\Pi}^{(0)} = -\theta\nabla\rho - \nabla \cdot (\rho\mathbf{uu}) \end{aligned}$$

The yukky bit

After some algebra and frustration we find

$$\begin{aligned}
\partial_{t_0}\Pi^{(0)} &= \theta \mathbf{I}\partial_{t_0}\rho + \mathbf{u}\partial_{t_0}(\rho\mathbf{u}) + \partial_{t_0}(\rho\mathbf{u})\mathbf{u} - \mathbf{u}\mathbf{u}\partial_{t_0}\rho, \\
&= -\theta\mathbf{I}\nabla\cdot(\rho\mathbf{u}) + \mathbf{u}\left(-\theta\nabla\rho - \nabla\cdot(\rho\mathbf{u}\mathbf{u})\right) \\
&\quad + \left(-\theta\nabla\rho - \nabla\cdot(\rho\mathbf{u}\mathbf{u})\right) + \mathbf{u}\mathbf{u}\nabla\cdot(\rho\mathbf{u}), \\
&= -\theta\mathbf{I}\nabla\cdot(\rho\mathbf{u}) - \theta\mathbf{u}\nabla\rho - \theta(\nabla\rho)\mathbf{u} - \nabla\cdot(\rho\mathbf{u}\mathbf{u}\mathbf{u}).
\end{aligned}$$

Note that we replace temporal derivatives with spatial derivatives from lower moment equations.

In suffix notation.

$$\partial_{t_0}\Pi^{(0)}_{\beta\gamma} = -\theta\delta_{\beta\gamma}\partial_\alpha(\rho u_\alpha) - \theta u_\beta\partial_\gamma\rho - \theta u_\gamma\partial_\beta\rho - \partial_\alpha(\rho u_\alpha u_\beta u_\gamma).$$

The yukky bit

The standard lattice Boltzmann equilibria yield

$$
\begin{aligned}
Q^{(0)}_{\alpha\beta\gamma} &= \theta\rho\left(u_\alpha\delta_{\beta\gamma} + u_\beta\delta_{\gamma\alpha} + u_\gamma\delta_{\alpha\beta}\right) \\
\partial_\alpha Q^{(0)}_{\alpha\beta\gamma} &= \theta\delta_{\beta\gamma}\partial_\alpha(\rho u_\alpha) + \theta\partial_\beta(\rho u_\gamma) + \theta\partial_\gamma(\rho u_\beta)
\end{aligned}
$$

Adding the temporal derivative of $\Pi^{(0)}_{\beta\gamma}$ to the divergence of $Q^{(0)}_{\alpha\beta\gamma}$ gives us the viscous stress tensor, since

$$
\frac{\partial \mathbf{\Pi}^{(0)}}{\partial t_0} + \nabla\cdot\mathbf{Q}^{(0)} = -\mathbf{\Pi}^{(1)}.
$$

Assembling the Navier-Stokes equations

The viscous stress is then found to be

$$\mathbf{\Pi}^{(1)} = -\rho\theta\left(\nabla\mathbf{u} + (\nabla\mathbf{u})^T\right) + \mathcal{O}(Ma^3),$$

where $Ma = |\mathbf{u}|/c_s$ is the Mach number ($c_s = \theta^{1/2}$).

We have obtained the (compressible) Navier-Stokes equations

$$\partial_t\rho + \nabla\cdot(\rho\mathbf{u}) = 0, \quad \partial_t(\rho\mathbf{u}) + \nabla\cdot\left(\mathbf{\Pi}^{(0)} + \tau\mathbf{\Pi}^{(1)}\right) = 0.$$

The dynamic viscosity $\mu = \tau\rho\theta$ is proportional to the momentum flux relaxation time τ.

From discrete Boltzmann to lattice Boltzmann

Integrating the discrete Boltzmann equation

$$\frac{\partial f_i}{\partial t} + \mathbf{c}_i \cdot \nabla f_i = \Omega_i(f)$$

along a characteristic for time Δt gives

$$f_i(x + c_i \Delta t, t + \Delta t) - f_i(x, t) = \int_0^{\Delta t} \Omega_i(x + c_i s, t + s)\, ds,$$

Approximating the integral by the trapezium rule yields

$$\begin{aligned} f_i(x+c_i\Delta t, t+\Delta t) - f_i(x,t) &= \frac{\Delta t}{2}\Big(\Omega_i(x+c_i\Delta t, t+\Delta t) \\ &+ \Omega_i(x,t)\Big) + O\left(\Delta t^3\right). \end{aligned}$$

This is an implicit system.

Change of Variables

To obtain a second order explicit LBE at time $t + \Delta t$ define

$$\bar{f}_i(x,t) = f_i(x,t) + \frac{\Delta t}{2\tau}\left(f_i(x,t) - f_i^{(0)}(x,t)\right).$$

The new algorithm is

$$\bar{f}_i(\mathbf{x} + \mathbf{c}_i\Delta t, t + \Delta t) - \bar{f}_i(\mathbf{x}, t) = -\frac{\Delta t}{\tau + \Delta t/2}\left(\bar{f}_i(\mathbf{x}, t) - f_i^{(0)}(\mathbf{x}, t)\right)$$

This could have also been obtained by Strang splitting.

A quick note on forcing

A body force R_i in the discrete Boltzmann equation,

$$\frac{\partial f_i}{\partial t} + \mathbf{c}_i \cdot \nabla f_i = -\frac{1}{\tau}\left(f_j - f_j^{(0)}\right) + R_i,$$

should have the following moments:

$$\sum_i R_i = 0, \quad \sum_i R_i \mathbf{c}_i = \boldsymbol{F}, \quad \sum_i R_i \mathbf{c}_i \mathbf{c}_i = \boldsymbol{F}\mathbf{u} + \mathbf{u}\boldsymbol{F},$$

and implemented as

$$\begin{aligned} \bar{f}_i(x + c_i \Delta t \ , \ t + \Delta t) - \bar{f}_i(x, t) \\ = \quad -\frac{\Delta t}{\tau + \Delta t/2} \left(\bar{f}_i(x,t) - f_i^{(0)}(x,t)\right) + \frac{\tau \Delta t}{\tau + \Delta t/2} R_i(x,t), \end{aligned}$$

Discrete Boltzmann versus continuous Boltzmann

The continuous Boltzmann equation has an infinite hierarchy of moment equations.

The discrete Boltzmann has a truncated system: a q-velocity model has at most q independent moments.

The moments of the DBE differ from those of the BE at $O(Kn^2)$.

The D2Q9 lattice allows us the satisfy the hydrodynamic moments only.

The LBE equilbria are valid in the incompressible limit ($Ma \ll 1$) only, unlike the Maxwell-Boltzmann equilibrium.

The DBE has an order $O(Ma^3)$ error term that breaks Galilean invariance and cannot be eliminated completed on D2Q9.

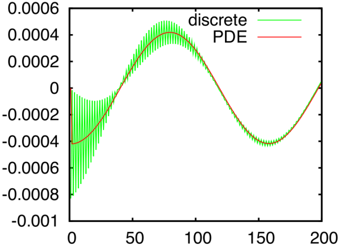
Lattice Boltzmann versus discrete Boltzmann

For spatially uniform solutions

$$\left(\bar{f}_i(t+\Delta t) - f_i^{(e)}(t)\right) = -\left(\frac{1-2\tau/\Delta t}{1+2\tau/\Delta t}\right)\left(\bar{f}_i(t) - f_i^{(e)}(t)\right)$$

For $\tau \ll \Delta t$ the f_i oscillate around equilibrium from timestep to timestep.

In the discrete Boltzmann equation, $f_i \to f_i^{(0)}$ monotonically.



Motivation for non-BGK collisions

We derived the Navier–Stokes equations from evolution equations for the moments ρ, $\rho\mathbf{u}$, and Π.

We used another four independent quantities: Q_{xxx}, Q_{xxy}, Q_{yyx}, Q_{yyy} (but we only needed their equilibrium).

This means we have more degrees of freedom than is needed for the hydrodynamics, but not enough to specify $\mathbf{Q}$.

A multiple-relaxation-time (MRT) collision operator is designed to over-relax the stress, but damp the "ghosts" to equilibrium.

Multi-relaxation time models

MRT models take the form

$$\frac{\partial f_i}{\partial t} + \mathbf{c}_i \cdot \nabla f_i = M^{-1} \Lambda M \left(f_i - f_i^{(0)} \right).$$

Λ is a diagonal matrix of relaxation times.

M is a $q \times q$ matrix which linearly transforms the distribution functions to the velocity moments.

A variety of different collision operators have been proposed

Lallemand and Luo [2000], Succi [2001], Ginzburg *et al.* [2003], Dellar [2003]

Construction of the collision operator

The D2Q9 equilibria can be written as

$$f_i^{(0)} = W_i \left(\rho + 3\rho \mathbf{u} \cdot \mathbf{c}_i + \frac{9}{2}(\rho \mathbf{u}\mathbf{u}) : \left(\mathbf{c}_i \mathbf{c}_i - \frac{1}{3}\mathbf{I} \right) \right)$$

We see now that the equilibria have the interpretation of coefficients multiplying the first 3 Hermite polynomials, $1, \mathbf{c}_i, \mathbf{c}_i\mathbf{c}_i - 1/3\mathbf{I}$. There are 6 vectors here, corresponding to 6 hydrodynamic components.

It seems quite natural to choose the remain 3 vectors to complete the collision matrix using vectors that are orthogonal to these.

Construction of the collision operator

To do this we define Dellar [2003]

$$h_i = (1, -2, -2, -2, -2, 4, 4, 4, 4), \quad X = \sum_i h_i f_i, \quad \mathbf{Y} = \sum_i h_i f_i \mathbf{c}_i.$$

We no have moments containing 9 degrees of freedom. We reconstruct f_i from these moments

$$f_i = W_i \left(\rho + 3\rho \mathbf{u} \cdot \mathbf{c}_i + \frac{9}{2} \left[\mathbf{\Pi} - \frac{\rho \boldsymbol{I}}{3} \right] : \left[\mathbf{c}_i \mathbf{c}_i - \frac{1}{3} \right] + h_i \left[\frac{1}{4} X + \frac{3}{8} \mathbf{c}_i \cdot \mathbf{Y} \right] \right)$$

Implementation

We transform from the basis corresponding to the f_i into a basis of moments. The collision matrix is diagonal in this basis, so it is easy to apply. Finally, we transform back from the moment basis into the original basis.

In other words, we perform collisions directly on the moments, and then reconstruct the post-collision distribution functions.

There is no need to do any matrix inversions!

Implementation

$$
\begin{aligned}
\bar{\mathbf{\Pi}}' &= \bar{\mathbf{\Pi}} - \frac{1}{\tau + \Delta t/2}\left(\bar{\mathbf{\Pi}} - \mathbf{\Pi}^{(0)}\right), \\
\bar{X}' &= \bar{X} - \frac{1}{\tau_X + \Delta t/2}\left(\bar{X} - X^{(0)}\right), \\
\bar{\boldsymbol{Y}}' &= \bar{\boldsymbol{Y}} - \frac{1}{\tau_Y + \Delta t/2}\left(\bar{\boldsymbol{Y}} - \boldsymbol{Y}^{(0)}\right),
\end{aligned}
$$

from which we can reconstruct the post-collision distribution functions

$$
f_i = W_i \left(\rho + 3\rho \mathbf{u} \cdot \mathbf{c}_i + \frac{9}{2}\left[\mathbf{\Pi}' - \frac{\rho \boldsymbol{I}}{3}\right] : \left[\mathbf{c}_i \mathbf{c}_i - \frac{1}{3}\right] + h_i \left[\frac{1}{4} X' + \frac{3}{8} \mathbf{c}_i \cdot \mathbf{Y}'\right] \right)
$$

A very simple and very stable special case

In this basis, $\boldsymbol{Y}^{(0)} = 0$ and $X^{(0)} = 0$. So if we choose $\tau_Y = \tau_X = \Delta t/2$ in

$$
\begin{aligned}
\bar{\mathbf{\Pi}}' &= \bar{\mathbf{\Pi}} - \frac{1}{\tau + \Delta t/2}\left(\bar{\mathbf{\Pi}} - \mathbf{\Pi}^{(0)}\right), \\
\bar{X}' &= \bar{X} - \frac{1}{\tau_X + \Delta t/2}\left(\bar{X} - X^{(0)}\right), \\
\bar{\boldsymbol{Y}}' &= \bar{\boldsymbol{Y}} - \frac{1}{\tau_Y + \Delta t/2}\left(\bar{\boldsymbol{Y}} - \boldsymbol{Y}^{(0)}\right),
\end{aligned}
$$

so that the ghost moments decay instantaneously to their equilibra (of zero) then they do not even have appear in the code!

This MRT was first used by Ladd [1994] and has since been re-discovered/branded as the “regularized” LBE Latt and Chopard [2006]

A snippet from my code

This model is not hard to implement:

```
do k=0,8
rho=rho+f(k,i,j)
ux=ux+f(k,i,j)*cx(k)
uy=uy+f(k,i,j)*cy(k)
Pxx=Pxx+f(k,i,j)*cx(k)*cx(k)
Pxy=Pxy+f(k,i,j)*cx(k)*cy(k)
Pyy=Pyy+f(k,i,j)*cy(k)*cy(k)
enddo
ux=ux/rho
uy=uy/rho
```

```
P0xx = (1d0/3d0)*rho + rho*ux*ux
P0xy = rho*ux*uy
P0yy = (1d0/3d0)*rho + rho*uy*uy

Axx = Pxx - (Pxx-P0xx)/(tau+0.5d0)
Axy = Pxy - (Pxy-P0xy)/(tau+0.5d0)
Ayy = Pyy - (Pyy-P0yy)/(tau+0.5d0)

do k=0,8

f(k,i,j)=w(k)*(2*rho-(3d0/2d0)*rho*(cx(k)**2+cy(k)**2)
        +3*rho*(ux*cx(k)+uy*cy(k))
        +(9d0/2d0)*( Axx*cx(k)**2+2*Axy*cx(k)*cy(k)
        +Ayy*cy(k)**2 ) -(3d0/2d0)*(Axx+Ayy) )

enddo
```

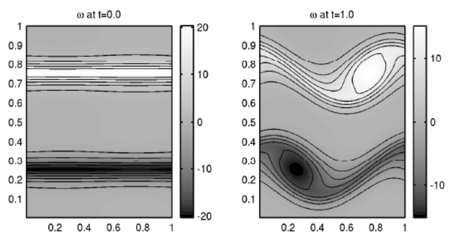
Roll-up of shear waves

Roll-up of shear layers in Minion & Brown [1997] test problem,

$$u_x = \begin{cases} \tanh(\kappa(y - 1/4)), & y \le 1/2, \\ \tanh(\kappa(3/4 - y)), & y > 1/2, \end{cases}$$

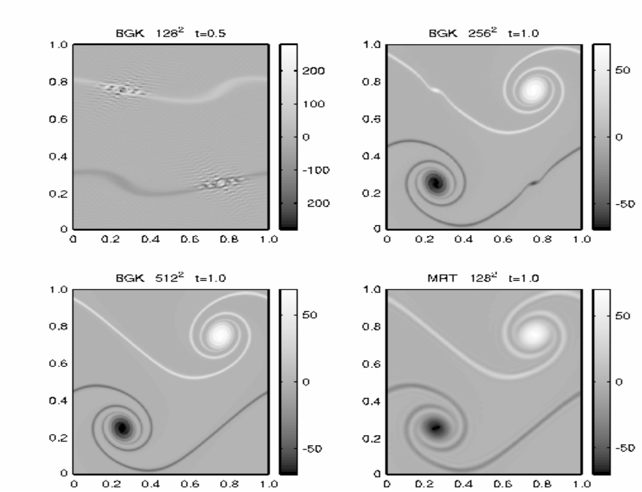
$$u_y = \delta \sin(2\pi(x + 1/4)).$$

E.g: $\kappa = 20$, $\delta = 0.05$ and $Re = 1000$; 256^2 grid



Roll-up of Shear wave with LBE

$Re = 30,000$, $\kappa = 80$ and $\delta = 0.05$



On GPU: 600 MLUPS

TRT models

We never really know how to choose the ghost relaxation times, even though we know they have a huge impact on the stability of LBE

A special case of MRT with two relaxation times, one for odd-order moments and one for even-order moments (TRT model) allows us to simplify the collision operator enough to do some analysis while maintaining good stability properties.

In terms of the MRT construction

$$\begin{aligned}
\bar{\mathbf{\Pi}}' &= \bar{\mathbf{\Pi}} - \frac{1}{\tau + \Delta t/2}\left(\bar{\mathbf{\Pi}} - \mathbf{\Pi}^{(0)}\right), \\
\bar{X}' &= \bar{X} - \frac{1}{\tau_X + \Delta t/2}\left(\bar{X} - X^{(0)}\right), \\
\bar{\boldsymbol{Y}}' &= \bar{\boldsymbol{Y}} - \frac{1}{\tau_Y + \Delta t/2}\left(\bar{\boldsymbol{Y}} - \boldsymbol{Y}^{(0)}\right),
\end{aligned}$$

we'd set $\tau_X = \tau$, which is governed by the Reynolds number, leaving τ_Y as free relaxation time.

More traditionally

TRT is written as

$$\begin{aligned}\bar{f}_i(\mathbf{x}+\mathbf{c}_i, t+1) = \bar{f}_i(\mathbf{x}, t) \quad &- \quad \frac{1}{\tau^+ + 1/2}\left[\frac{1}{2}\left(\bar{f}_i + \bar{f}_{\bar{i}}\right) - f_i^{(0+)}\right] \\ &- \quad \frac{1}{\tau^- + 1/2}\left[\frac{1}{2}\left(\bar{f}_i - \bar{f}_{\bar{i}}\right) - f_i^{(0-)}\right].\end{aligned}$$

An analysis of the TRT LBE shows us that errors and stability are not necessarily governed by each relaxation time but instead their product, $\Lambda = \tau^+\tau^-$.

For example, $\lambda = 1/4$ eliminates the recurrence in higher order moments and leads to very stable simulations Ginzburg [2008], TR[2019]. (This is like setting $\tau = 1/2$ in BGK)

Setting $\lambda = 1/6$ removes a 4th order diffusion error

Setting $\lambda = 1/12$ removes a 3rd order advection error

So, we have good reasons and methods for choosing the relaxation times: τ^+ is set by the Reynolds number and τ^- is adjusted according to the prescribed, numerically favorable, value of Λ

Analytical solution of the LBE

The best way to understand, appreciate, and evaluate an equation/algorithm is to solve it analytically.

General point: Always do the simplest thing first!

The LBE is very hard to solve exactly but we can find analytical solutions in some special cases.

These are usually (but not always) time-independent flows in one dimension!

This is a long way from a real industrial flow but we can learn a lot by looking deeply into a simple problem.

LBE for Poiseuille flow

$$\bar{f}_i(x + c_i\Delta t\ ,\ t + \Delta t) - \bar{f}_i(x,t)$$
$$= \quad -\frac{\Delta t}{\tau + \Delta t/2}\ \left(\bar{f}_i(x,t) - f_i^{(0)}(x,t)\right) + \frac{\tau\Delta t}{\tau + \Delta t/2}\ R_i(x,t)$$

Consider flows satisfying

$$\frac{\partial}{\partial x} = \frac{\partial}{\partial t} = 0, \quad \boldsymbol{F} = (\rho G, 0)$$

Walls located at $j = 1$ and $j = n$

Let $\bar{f}_i^j$ denote the the distribution function $\bar{f}_i$ at node j; similarly for u_j and v_j. Then …

$$
\begin{aligned}
\bar{f}_0^j &= \frac{4\rho}{9}\left(1-\frac{3}{2}\left(u_j^2+v_j^2\right)\right),\\
\bar{f}_1^j &= \frac{\rho}{9}\left(1+3u_j+3u_j^2-\frac{3v_j^2}{2}\right)+\frac{\tau\rho G}{3}\left(2u_j+1\right),\\
\bar{f}_2^j &= \frac{\rho}{9(\tau+1/2)}\left(1+3v_{j-1}+2v_{j-1}^2-\frac{3u_{j-1}^2}{2}\right)+\frac{\tau-1/2}{\tau+1/2}\bar{f}_2^{j-1},\\
\bar{f}_3^j &= \frac{\rho}{9}\left(1-3u_j+3u_j^2-\frac{3v_j^2}{2}\right)+\frac{\tau\rho G}{3}\left(2u_j-1\right),\\
\bar{f}_4^j &= \frac{\rho}{9(\tau+1/2)}\left(1-3v_{j+1}+3v_{j+1}^2-\frac{3u_{j+1}^2}{2}\right)-\frac{\tau-1/2}{\tau+1/2}\bar{f}_4^{j+1},\\
\bar{f}_5^j &= \frac{\rho}{36(\tau+1/2)}\left(1+3u_{j-1}+3v_{j-1}+3u_{j-1}^2+3v_{j-1}^2+9u_{j-1}v_{j-1}\right)\\
&+ \frac{\tau\rho G}{12(\tau+1/2)}\left(1+2u_{j-1}\right)+\frac{\tau-1/2}{\tau+1/2}\bar{f}_5^{j-1},
\end{aligned}
$$

$$
\begin{aligned}
\bar{f}_6^j &= \frac{\rho}{36(\tau+1/2)}\left(1-3u_{j-1}+3v_{j-1}+3u_{j-1}^2+3v_{j-1}^2-9u_{j-1}v_{j-1}\right)\\
&- \frac{\tau\rho G}{12(\tau+1/2)}\left(1-2u_{j-1}\right)+\frac{\tau-1/2}{\tau+1/2}\bar{f}_6^{j-1},\\
\bar{f}_7^j &= \frac{\rho}{36(\tau+1/2)}\left(1-3u_{j+1}-3v_{j+1}+3u_{j+1}^2+3v_{j+1}^2+9u_{j+1}v_{j+1}\right)\\
&- \frac{\tau\rho G}{12(\tau+1/2)}\left(1-2u_{j+1}\right)+\frac{\tau-1/2}{\tau+1/2}\bar{f}_7^{j+1},\\
\bar{f}_8^j &= \frac{\rho}{36(\tau+1/2)}\left(1+3u_{j+1}-3v_{j+1}+3u_{j+1}^2+3v_{j+1}^2-9u_{j+1}v_{j+1}\right)\\
&+ \frac{\tau\rho G}{12(\tau+1/2)}\left(1+2u_{j+1}\right)+\frac{\tau-1/2}{\tau+1/2}\bar{f}_8^{j+1},
\end{aligned}
$$

recurrence relation

This recurrence relation reduces to

$$\frac{u_{j+1}v_{j+1} - u_{j-1}v_{j-1}}{2} = \nu\left(u_{j+1} + u_{j-1} - 2u_j\right) + G,$$

This is the second order finite–difference form of the incompressible Navier–Stokes equations with a constant body force:

$$\frac{\partial(uv)}{\partial y} = \nu\frac{\partial^2 u}{\partial y^2} + G$$

Solution of the difference equation

$$\frac{u_{j+1}v_{j+1} - u_{j-1}v_{j-1}}{2} = \nu \left(u_{j+1} + u_{j-1} - 2u_j\right) + G$$

We can show ρ is constant and $v_j = 0$

The solution to this second order difference equation is

$$u_j = \frac{4U_c}{(n-1)^2}(j-1)(n-j) + U_s, \quad j = 1, 2, \ldots, n$$

where $U_c = H^2 G/8\nu$ is the centre-line velocity and $H = (n-1)$ is the channel height.

So...

$$u_j = \frac{4U_c}{(n-1)^2}(j-1)(n-j) + U_s$$

The first term on the right is the exact solution to Poiseuille flow

The second term on the right is a constant that depend on the boundary conditions

We can NOT capture kinetic (Boltzmann) effects in velocity (because the LBE solution is a perfect parabola, regardless of the boundary conditions used)

A second order algorithm should solve for a quadratic solution exactly

We can find U_s for different boundary conditions (and thus assess them - exact if $U_s = 0$)

Summary

- The D2Q9 LBE retains the properties of the BE needed to derive the Navier–Stokes equations from but *not* beyond
- *“Nonlinearity is local, non-locality is linear"*
- Easy to implement and suitable for parallel processing
- MRT models are far more stable. TRT is stable, accurate, and analytically tractable
- Easy to implement boundary condition??

References

I. Ginzbourg and P. Adler, *Boundary flow condition analysis for the three-dimensional lattice Boltzmann model*, J. Physique II 4 (1994), 191-214

D. d'Humieres and I. Ginzbourg , *Viscosity independent numerical errors for Lattice Boltzmann models: From recurrence equations to "magic" collision numbers*, Comput. Math. Appl 58 (2009), 823-840

X. He, Q. Zou, and L-S Luo, *Analytic solutions and analysis on non-slip boundary conditions for lattice Boltzmann BGK model* J. Comp. Phys 87 (1997), 115-136

M. Junk and Z. Yang, *Analysis of lattice Boltzmann boundary conditions* Proc. Appl. Math. Mech., 3 (2003), 76-79.

References

T. Reis, *On the lattice Boltzmann deviatoric stress: analysis, boundary conditions, and relaxation times*,submitted to IMA J, Numer. Anal.

P.J. Dellar, *Incompressible limits of the lattice Boltzmann equation using multiple relaxation time*, J. Comp. Phys 190 (2003), 351-370

P. Lallemand and L-S Luo, *Theory of the lattice Boltzmann method: Dispersion, dissipation, isotropy, Galilean invariance, and stability*, Phys. Rev. E 61 (2000), 6546