

Analytical Solution for a Simple Shear Flow Using Lattice Boltzmann Methods

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Motivation

There are few analytical solutions to the Lattice Boltzmann Equation (LBE). Those that do exist are very powerful since they allow close analysis of the method itself.

Zou et al.¹ calculated analytical solutions for the Poiseuille and the Couette flow. However, as will be shown, discrepancies were found for the validity of their solution for the Couette flow.

¹J. Stat. Phys., Vol. 81, (1995), pp. 3

Motivation

For a simple shear flow (couette), the macroscopic velocities at different positions only differ by constant amounts. Perhaps the $\{f_i\}_{i=0}^8$ are related to each other similarly, so a Galilean transformation assumption is proposed as the major assumption. The LBE is just a huge system of equations, so the system decouples, and now focus is required only on the $\{f_i\}$ at one point.

This assumption may not necessarily produce an analytical solution, but it is shown that the (unique) derived solution fulfills the LBE. The solution derived agrees with experiment to machine accuracy. It's also interesting to pursue a solution solely in terms of the equilibrium distribution. Finally, looking at this simpler case may provide insights to more complicated flows.

The Lattice Boltzmann Method

Define $\{f_i(x, t)\}$ as local probability densities associated with a lattice velocity \vec{v}_i . Macroscopic quantities can be calculated via moments of these functions. Density is

$$\sum f_i(x, t) = \rho(x, t) \quad (1)$$

and the local momentum is

$$\sum f_i(x, t) v_{i\alpha} = \rho(x, t) u_\alpha(x, y) \quad (2)$$

The $\{f_i\}$ evolve due to the Lattice Boltzmann Equation

$$f_i(\vec{x} + \vec{v}_i, t + \Delta t) = f_i(\vec{x}, t) + \Omega_i \quad (3)$$

We shall use the BGK approximation for the collision operator Ω_i :

$$\Omega_i = \Delta t \omega (f_i^0(\rho, \vec{u}) - f_i(x, t)) \quad (4)$$

where ω is a relaxation time parameter.

The Lattice Boltzmann Method

The local density equilibrium f_i^0 is given by the Maxwell-Boltzmann distribution:

$$f_i^0(\rho, \vec{u}) = w_i \left(1 + 3v_{i\alpha}u_\alpha + \frac{9}{2}v_{i\alpha}u_\alpha v_{i\beta}u_\beta - \frac{3}{2}u_\alpha^2 \right) \quad (5)$$

where w_i are the lattice weights ($w_0 = \frac{4}{9}$, $w_i = \frac{1}{9}$ for $i \in \{1, 2, 3, 4\}$, $w_i = \frac{1}{36}$ for $i \in \{5, 6, 7, 8\}$). Einstein summation convention is used. $\Delta t = 1$ and lattice spacing $\Delta x = 1$ is henceforth assumed. Assuming that the f_i are stationary (time-independent), (3) now becomes

$$f_i(\vec{x} + \vec{v}_i) = f_i(\vec{x})(1 - \omega) + \omega f_i^0(\rho, \vec{u}) \quad (6)$$

A computer program can recursively implement (6), (1), and (2) to simulate fluid flow.

Problem Characteristics

For the simple steady-state shear flow that we are interested in, the velocity has the following form in Cartesian coordinates (x -direction is parallel with movement)

$$u_x(y) = \dot{\gamma}y \quad (7)$$

$$u_y = 0 \quad (8)$$

Thus (6) becomes (assume $\rho = 1$ uniformly)

$$f_i(y + v_{iy}) = f_i(y)(1 - \omega) + \omega f_i^0(\dot{\gamma}y) \quad (9)$$

Boundary Conditions for Actual Simulation

How to put experiment and theory on common ground to compare?

- Boundary conditions are quite important, for discrepancies easily transmit into the bulk.
 - ▶ First: boundary = local equilibrium distribution, failed
- Second: boundary = analytical sol.
 - ▶ first guess
 - ▶ Zou
 - ▶ final solution

Major Assumption

As an ansatz, it is assumed that the f_i at different positions can be related to each other through a Galilean transformation. Wagner and Paganobarraga² provide the following form from a Taylor Series expansion (taylor expand the LBE to first order, reinsert into itself, 2nd order terms are 0):

$$\begin{aligned}\Delta f_i &= f_i(y + v_{iy}) - f_i(y) \\ &= f_i^0(\dot{\gamma}(y + v_{iy})) - f_i^0(\dot{\gamma}y) \\ &\quad - \tau \left(v_{i\alpha} \partial_\alpha [f_i^0(\dot{\gamma}(y + v_{iy})) - f_i^0(\dot{\gamma}y)] + \partial_t [f_i^0(\dot{\gamma}(y + v_{iy})) - f_i^0(\dot{\gamma}y)] \right) \\ &\quad + O(\partial^2) \\ &= f_i^0(\dot{\gamma}(y + v_{iy})) - f_i^0(\dot{\gamma}y) - \tau \left(v_{i\alpha} \partial_\alpha (f_i^0(\dot{\gamma}(y + v_{iy})) - f_i^0(\dot{\gamma}y)) \right)\end{aligned}\tag{10}$$

where $\tau = \frac{1}{\omega}$. The higher order $O(\partial^2)$ terms are 0 by the nature of the simple shear flow, and the time derivative is 0 since the flow is steady state.

First Guess

The first iteration of the Galilean Invariance Assumption was

$$\Delta f_i = f_i^0(\dot{\gamma}(y + v_{iy})) - f_i^0(\dot{\gamma}y)$$

Plugging this into (9), there results (using a change of variables)

$$\begin{aligned} f_i(y) &= f_i(\dot{\gamma}(y - v_{iy}))(1 - \omega) + \omega f_i^0(\dot{\gamma}(y - v_{iy})) \\ &= (f_i(y) + f_i^0(\dot{\gamma}(y - v_{iy})) - f_i^0(\dot{\gamma}y))(1 - \omega) + \omega f_i^0(\dot{\gamma}(y - v_{iy})) \\ \iff f_i(y) &= \frac{f_i^0(\dot{\gamma}(y - v_{iy})) - f_i^0(\dot{\gamma}y) + \omega f_i^0(\dot{\gamma}y)}{\omega} \end{aligned} \quad (11)$$

of course if $\omega \neq 0$

Problems

(11) doesn't even solve the LBE, though!

$$\begin{aligned} & \frac{f_i^0(\dot{\gamma}y) - f_i^0(\dot{\gamma}(y + v_{iy})) + \omega f_i^0(\dot{\gamma}(y + v_{iy}))}{\omega} \\ &= \frac{f_i^0(\dot{\gamma}(y - v_{iy})) - f_i^0(\dot{\gamma}y) + \omega f_i^0(\dot{\gamma}y)}{\omega} (1 - \omega) + \omega f_i^0(\dot{\gamma}y) \\ &\iff (-2f_i^0(\dot{\gamma}y) + f_i^0(\dot{\gamma}(y + v_{iy})) + f_i^0(\dot{\gamma}(y - v_{iy}))) (\omega - 1) = 0 \end{aligned}$$

Using (5) and that $u(y + v_{iy}) = u_x(y) + \dot{\gamma}v_{iy}$, it is clear that

$$f_i^0(\dot{\gamma}(y \pm v_{iy})) = w_i \left(1 + 3v_{ix}(u_x \pm \dot{\gamma}v_{iy}) + \left(\frac{9}{2}v_{ix}^2 - \frac{3}{2}\right)(u_x \pm \dot{\gamma}v_{iy})^2 \right) \quad (12)$$

Plugging in and canceling and grouping, the result is

$$\begin{aligned} & (-2f_i^0(\dot{\gamma}y) + f_i^0(\dot{\gamma}(y + v_{iy})) + f_i^0(\dot{\gamma}(y - v_{iy}))) (\omega - 1) = 0 \\ &\iff (3w_i(3v_{ix}^2 - 1)v_{iy}^2\dot{\gamma}^2) (\omega - 1) = C_i(\omega - 1) = 0 \quad (13) \end{aligned}$$

But the quantity C_i is in general not equal to 0. Hence, (11) is a solution only when $\omega = 1$ (since i spans the set $\{0, 1, 2, \dots, 8\}$). This is peculiar.

Problems

Moreover, the "solution" doesn't even solve the first iteration of the Galilean Invariance Assumption:

$$\begin{aligned} & \frac{f_i^0(\dot{\gamma}y) - f_i^0(\dot{\gamma}(y + v_{iy})) + \omega f_i^0(\dot{\gamma}(y + v_{iy})) - f_i^0(\dot{\gamma}(y - v_{iy})) + f_i^0(\dot{\gamma}y) - \omega f_i^0(\dot{\gamma}y)}{\omega} \\ &= f_i^0(\dot{\gamma}(y + v_{iy})) - f_i^0(\dot{\gamma}y) \\ &\iff -2f_i^0(\dot{\gamma}y) + f_i^0(\dot{\gamma}(y + v_{iy})) + f_i^0(\dot{\gamma}(y - v_{iy})) = 0 \\ &\iff C_i = 0 \iff \mathbf{F} \end{aligned}$$

The solution was obtained by assuming these two equations, so how doesn't it satisfy them anymore?

Solution

The derived analytical solution is

$$f_i(y) = \frac{f_i^0(\dot{\gamma}(y - v_{iy})) - f_i^0(\dot{\gamma}y) + \omega f_i^0(\dot{\gamma}y)}{\omega} + \frac{(1 - \omega)C_i}{\omega^2} \quad (14)$$

where $C_i = \frac{1}{2}v_{iy}^2(v_{ix}^2 - \frac{2}{3})\dot{\gamma}^2$. Algebra shows that

$$C_i = \frac{1}{2}v_{iy}^2(v_{ix}^2 - \frac{2}{3})\dot{\gamma}^2 = 3w_i(3v_{ix}^2 - 1)v_{iy}^2\dot{\gamma}^2.$$

Sufficiency

Equation (14) solves (6) and (10).

$$\begin{aligned} & \frac{f_i^0(y) - f_i^0(y + v_{iy}) + \omega f_i^0(y + v_{iy})}{\omega} + \frac{(1 - \omega)C_i}{\omega^2} \\ &= \omega f_i^0(y) + (1 - \omega) \left(\frac{f_i^0(y - v_{iy}) - f_i^0(y) + \omega f_i^0(y)}{\omega} + \frac{C_i(1 - \omega)}{\omega^2} \right) \\ &\iff (-2f_i^0(y) + f_i^0(y + v_{iy}) + f_i^0(y - v_{iy}))(\omega - 1) = C_i(\omega - 1) \\ &\iff C_i = C_i \end{aligned}$$

($\omega = 1$ works). Moreover, looking at equation (10),

$$\begin{aligned} & v_{ix} \partial_x [f_i^0(\dot{\gamma}(y + v_{iy})) - f_i^0(\dot{\gamma}y)] + v_{iy} \partial_y [f_i^0(\dot{\gamma}(y + v_{iy})) - f_i^0(\dot{\gamma}y)] \\ &= 3w_i(3v_{ix}^2 - 1)v_{iy}^2 \dot{\gamma}^2 = C_i \end{aligned}$$

after using (12) and since $\partial_x u = 0$ and $\partial_y u = \dot{\gamma}$. Hence, the needed corrective factor is present, so it solves it.

Necessity

Combing equations (10) and (9), equation (14) is obtained. This makes sense because the extra factor of $\frac{C_i}{\omega}$ is present.

Comparison to Zou et al.

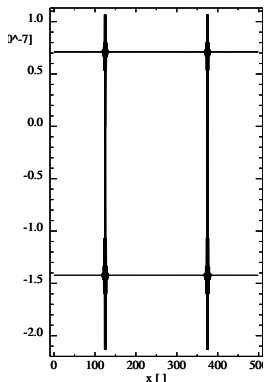


Figure: $\omega = 1.5$ Zou diff

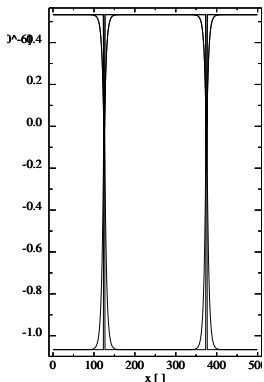


Figure: $\omega = 0.2$

The Zou solution is basically eq. 11 (first guess) plus $\frac{C_i}{\omega^2} a$. While analyzing these to the left differences, Prof. Wagner brilliantly suggested to multiply a factor of $(1 - \omega)$ to $\frac{C_i}{\omega^2}$, hence the proposed analytical solution (14).

^aJ Stat Phys 81, 319–334 (1995)

Numerical Verifications

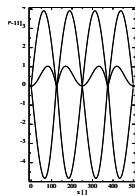
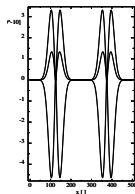


Figure:

$\omega =$

Figure: $\omega = 1.5$

1.9 error between analytical solution and implementation

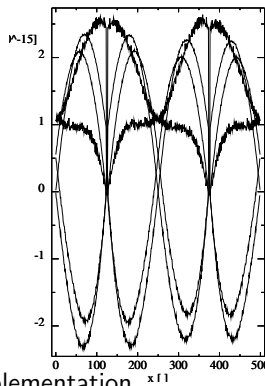


Figure: $\omega = 0.2$

Importance of Second Order Correction

The second iteration of the Galilean transformation adds a non-zero constant to

$$\Delta f_i^0$$

meaning that $\Delta f_i \neq \Delta f_i^0$ for this flow. The correction term increases as $\omega \rightarrow 0$ (which is where we were seeing larger deviations).

The quantity $-2f_i^0(\dot{\gamma}y) + f_i^0(\dot{\gamma}(y + v_{iy})) + f_i^0(\dot{\gamma}(y - v_{iy}))$ shows up a lot (averaging, Laplace's eq.). For simple shear flow, it is simply C_i . In fact, you can work backwards from this to also get the analytical solution, which is what we saw at first, but we thought it wouldn't make sense to just add a constant to the Gal. transformation.

For other flows, the correction term is not constant.

Outlook

- Galilean transformation assumption turns out to be a valid way to get a solution.
- Flows for which $\Delta f_i = \Delta f_i^0$?
- (stationary) simple shear flow, 2nd order terms are 0
- Apply Galilean Transformation with correction to other flows
- Need to keep higher orders
- Lees-Edwards Boundary Conditions
- Different equilibrium distributions, collision operators