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# A Lattice Boltzmann model for the simulation of fluid flow

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**Abstract.** We set out the theory for a Lattice Boltzmann algorithm capable of mimicking the Navier-Stokes equation for fluid flow in two dimensions (2D). The solution satisfies criteria of Galilean invariance and isotropy, and viscosity is obtained by direct reference to the viscous term in the Navier-Stokes equation. It is possible to specify directly the viscosity and other hydrodynamic parameters without reference to specific collision modes. The model was tested by simulating 2D flow through a plane channel (Poiseuille flow). A parabolic flow profile was obtained, in excellent agreement with the analytical Navier-Stokes solution. We conclude that the algorithm can be used to model 2D fluid flow.

## 1. Introduction

The Lattice Boltzmann (LB) approach has been proposed as a method for solving problems of fluid flow by the direct computation of local Boltzmann equilibrium upon a regular lattice in 2D or 3D [1, 2]. The LB approach originated as a by-product of the derivation of wholly discrete Lattice Gas Cellular Automata (LGCA) models [3, 4]; however, recent demonstrations of the capability of the LB approach, for example the simulation of flow past a symmetric sudden expansion [5], indicate that in many applications it is superior to LGCA [6], despite the latter's apparent advantage of only employing integer arithmetic.

In section 2 we present the analysis for an LB model for mimicking the Navier-Stokes equation for fluid flow in 2D. The equilibrium (non-viscous) term is well known and not original, although our version of its derivation (section 2.3) is perhaps easier to understand than most. The non-equilibrium term and its derivation (section 2.4) is, we believe, original, in that it is obtained by direct reference to the viscous term in the Navier-Stokes equation, rather than by expanding about the LB equilibrium term (as in other models). Viscosity is obtained without referring to specific collision modes; therefore it is possible to specify directly the viscosity and other hydrodynamic parameters. The solution satisfies criteria of Galilean invariance and isotropy. Generalization of the model to include 3D flows has not been considered here but should be straightforward.

Section 3 describes the application of the model to the simulation of 2D flow through a plane channel (Poiseuille flow). As expected, a parabolic velocity profile was obtained, while the computed maximum velocity at the centre of the channel differed from the Navier-Stokes solution by less than 2%.

## 2. Analysis

### 2.1. Orientation

In the following we shall use the notation  $f_i(\mathbf{r}, t)$  to denote the density  $f$  of particles moving in direction  $i$  ( $i = 0, 1, 2, \dots, 6$ ,  $i = 0$  denotes stationary particles) at node  $\mathbf{r}$  on the 2D hexagonal grid, measured at time  $t$ . In the LB model  $f$  is a continuous variable while  $i$ ,  $\mathbf{r}$  and  $t$  are discrete.

The aim of this analysis is to construct an LB model leading to the Navier–Stokes equation. In doing so we will find explicit forms for  $f_i(\mathbf{r}, t)$ .

### 2.2. From LB to Navier–Stokes

We write the LB equation as [4]

$$f_i(\mathbf{r}, t+1) = f_i(\mathbf{r} - \mathbf{c}_i, t) + \Delta_i \quad (1)$$

where  $\Delta_i$  is the collision function and  $\mathbf{c}_i$  are the directional vectors at a node:

$$\begin{aligned} \mathbf{c}_0 &= \mathbf{0} \\ \mathbf{c}_1 &= \frac{1}{2}\hat{x} + \frac{\sqrt{3}}{2}\hat{y} & \mathbf{c}_4 &= -\frac{1}{2}\hat{x} - \frac{\sqrt{3}}{2}\hat{y} \\ \mathbf{c}_2 &= -\frac{1}{2}\hat{x} + \frac{\sqrt{3}}{2}\hat{y} & \mathbf{c}_5 &= \frac{1}{2}\hat{x} - \frac{\sqrt{3}}{2}\hat{y} \\ \mathbf{c}_3 &= -\hat{x} & \mathbf{c}_6 &= \hat{x} \end{aligned} \quad (2)$$

The density  $\rho(\mathbf{r}, t)$  and velocity  $\mathbf{u}(\mathbf{r}, t)$  at a node are defined by

$$\begin{aligned} \rho(\mathbf{r}, t) &= \sum_i f_i(\mathbf{r}, t) = \sum_i f_i(\mathbf{r} - \mathbf{c}_i, t-1) \\ \rho(\mathbf{r}, t)\mathbf{u}(\mathbf{r}, t) &= \sum_i \mathbf{c}_i f_i(\mathbf{r}, t) = \sum_i \mathbf{c}_i f_i(\mathbf{r} - \mathbf{c}_i, t-1) \end{aligned} \quad (3)$$

for collisions conserving density and momentum. Taking the Taylor expansion to first order, (1) may be written

$$\frac{\partial f_i}{\partial t}(\mathbf{r}, t) = f_i(\mathbf{r} - \mathbf{c}_i, t) - f_i(\mathbf{r}, t) + \Delta_i = -\mathbf{c}_i \cdot \nabla f_i(\mathbf{r}, t) + \Delta_i. \quad (4)$$

In this equation the time derivative is with respect to fixed coordinates. The time rate of change following the fluid (the substantive derivative) is given by

$$\frac{Df_i}{Dt} = \frac{\partial f_i}{\partial t} + \mathbf{u} \cdot \nabla f_i = (\mathbf{u} - \mathbf{c}_i) \cdot \nabla f_i + \Delta_i. \quad (5)$$

Henceforth we abbreviate  $f_i(\mathbf{r}, t)$  as  $f_i$ , and likewise with other variables. Noting that the time and space derivatives of  $\mathbf{c}_i$  are zero, and that [4]

$$\sum_i \Delta_i = 0 \quad \sum_i \mathbf{c}_i \Delta_i = 0 \quad (6)$$

we obtain the continuity equation by summing (5) over  $i$ :

$$\frac{\partial \rho}{\partial t} + \nabla(\mathbf{u}\rho) = 0. \quad (7)$$

Multiplying (5) by  $c_i$  and summing over  $i$  yields

$$\rho \frac{\partial}{\partial t} (\mathbf{u}\rho) + \mathbf{u} \cdot \nabla (\mathbf{u}\rho) = \sum_i (\mathbf{u} - \mathbf{c}_i) \nabla (f_i c_i). \tag{8}$$

Subtracting  $\mathbf{u}$  times (7) from (8), and using tensor notation, we find that

$$\rho \frac{\partial}{\partial t} u^\alpha + \rho u^\beta \nabla^\beta u^\alpha = \nabla^\beta \left( -\sum_i (u^\alpha - c_i^\alpha)(u^\beta - c_i^\beta) f_i \right). \tag{9}$$

We now make contact with the Navier-Stokes equation,

$$\rho \frac{\partial}{\partial t} u^\alpha + \rho u^\beta \nabla^\beta u^\alpha = \nabla^\beta \sigma^{\alpha\beta} \tag{10}$$

by equating the right-hand side of (9) with the stress tensor  $\sigma^{\alpha\beta}$

$$\sigma^{\alpha\beta} = -p\delta^{\alpha\beta} + \sigma'^{\alpha\beta} = -\sum_i (u^\alpha - c_i^\alpha)(u^\beta - c_i^\beta) f_i \tag{11}$$

where  $\sigma'^{\alpha\beta}$  represents the viscous effects. To obtain the Navier-Stokes equation we need to find  $f_i$  such that (in 2D) [7]

$$\begin{aligned} -\sum_i (u^\alpha - c_i^\alpha)(u^\beta - c_i^\beta) f_i \\ = -p\delta^{\alpha\beta} + \eta(\nabla^\alpha u^\beta + \nabla^\beta u^\alpha - \delta^{\alpha\beta} \nabla^\gamma u^\gamma) + \zeta \delta^{\alpha\beta} \nabla^\gamma u^\gamma \end{aligned} \tag{12}$$

where  $\eta$  and  $\zeta$  are the coefficients of viscosity. By writing  $f_i$  as

$$f_i = \bar{f}_i + \delta f_i \tag{13}$$

we follow the analysis by separately considering an equilibrium term  $\bar{f}_i$  and a viscous term  $\delta f_i$ ;

$$-\sum_i (u^\alpha - c_i^\alpha)(u^\beta - c_i^\beta) \bar{f}_i = -p\delta^{\alpha\beta} \tag{14}$$

$$-\sum_i (u^\alpha - c_i^\alpha)(u^\beta - c_i^\beta) \delta f_i = \eta(\nabla^\alpha u^\beta + \nabla^\beta u^\alpha - \delta^{\alpha\beta} \nabla^\gamma u^\gamma) + \zeta \delta^{\alpha\beta} \nabla^\gamma u^\gamma. \tag{15}$$

### 2.3. Equilibrium distribution

In the following analysis it is convenient to work in terms of normalized particle number  $n_i$ ,

$$n_i = \bar{f}_i / \rho \tag{16}$$

such that (equation (3))

$$n_0 + \sum_i n_i = 1 \quad \sum_i \mathbf{c}_i n_i = \mathbf{u} \tag{17}$$

where the summation is now taken to be over just the six non-stationary components. We obtain the equilibrium solution by imposing a Boltzmann distribution locally:

$$n_i(\mathbf{u}) = n_i(0) Z e^{\mu \cdot \mathbf{c}_i}, \quad n_0(\mathbf{u}) = n_0(0) Z \tag{18}$$

where the partition function  $Z$  is given by

$$Z = \frac{1}{n_0(0) + \sum_i n_i(0) e^{\mu \cdot \mathbf{c}_i}}. \tag{19}$$

For  $\mathbf{u} = \mathbf{0}$  all  $n_i$  will be equal (in a single-velocity model), but may be different from  $n_0$ :

$$n_i(0) = n(0) = \frac{1 - n_0(0)}{6}. \tag{20}$$

We proceed by expanding the exponential in (18) to order  $\mu^2$ :

$$n_i(\mathbf{u}) = n(0) \left( 1 + \mu \cdot \mathbf{c}_i + \frac{1}{2} (\mu \cdot \mathbf{c}_i)^2 \right) / \left( n_0(0) + 6n(0) + \frac{1}{2} n(0) \sum_i (\mu \cdot \mathbf{c}_i)^2 \right) \tag{21}$$

$$n_0(\mathbf{u}) = n_0(0) / \left( n_0(0) + 6n(0) + \frac{1}{2} n(0) \sum_i (\mu \cdot \mathbf{c}_i)^2 \right).$$

Noting that (equation (2))

$$\sum_i c_i^\alpha c_i^\beta = 3\delta^{\alpha\beta} \tag{22}$$

we find (to second order)

$$n_i(\mathbf{u}) = n(0) \left( 1 + \mu \cdot \mathbf{c}_i + \frac{1}{2} (\mu \cdot \mathbf{c}_i)^2 - \frac{3}{2} n(0) \mu^2 \right) \quad n_0(\mathbf{u}) = n_0(0) \left( 1 - \frac{3}{2} n(0) \mu^2 \right). \tag{23}$$

Multiplying  $n_i(\mathbf{u})$  by  $c_i$  and summing, we obtain

$$\mathbf{u}^\alpha = \sum_i c_i^\alpha n_i(\mathbf{u}) = n(0) \mu^\alpha \sum_i c_i^\alpha c_i^\beta \tag{24}$$

and therefore (equation (22))

$$\mu = \frac{\mathbf{u}}{3n(0)}. \tag{25}$$

Back-substituting  $\mu$  in (23) gives

$$n_i(\mathbf{u}) = n(0) \left[ 1 + \frac{\mathbf{u} \cdot \mathbf{c}_i}{3n(0)} + \frac{(\mathbf{u} \cdot \mathbf{c}_i)^2}{18n(0)^2} - \frac{\mathbf{u}^2}{6n(0)} \right] \tag{26}$$

$$n_0(\mathbf{u}) = n_0(0) \left( 1 - \frac{\mathbf{u}^2}{6n(0)} \right) = n_0(0) - \frac{n_0(0) \mathbf{u}^2}{1 - n_0(0)}. \tag{27}$$

To determine the free parameter  $n_0(0)$  we need to impose another condition upon the system. In particular, Galilean invariance has not yet been taken into account. This condition may be expressed as follows:

$$\sum_i c_i^\alpha c_i^\beta n_i(0) = \sum_i (c_i^\alpha - u^\alpha)(c_i^\beta - u^\beta) n_i(\mathbf{u}) \tag{28}$$

where the summation includes stationary particles. Expanding the right-hand side, we obtain

$$\begin{aligned} & \sum_i c_i^\alpha c_i^\beta (n_i(0) - n_i(\mathbf{u})) \\ &= -u^\alpha \sum_i c_i^\beta n_i(\mathbf{u}) - u^\beta \sum_i c_i^\alpha n_i(\mathbf{u}) + u^\alpha u^\beta \sum_i n_i(\mathbf{u}) = -u^\alpha u^\beta. \end{aligned} \tag{29}$$

Therefore we find

$$\sum_i (n_i(0) - n_i(\mathbf{u})) = -(\mathbf{u}_x^2 + \mathbf{u}_y^2) = -\mathbf{u}^2 \tag{30}$$

where the summation no longer includes stationary particles since  $c_0 = 0$ . Using (17) we obtain

$$n_0(\mathbf{u}) = n_0(0) - \mathbf{u}^2 \tag{31}$$

and hence (equations (27) and (31))

$$n_0(0) - \mathbf{u}^2 = n_0(0) - \frac{n_0(0)\mathbf{u}^2}{1 - n_0(0)}$$

or

$$n_0(0) = \frac{1}{2}. \tag{32}$$

Therefore (equation (20))

$$n(0) = \frac{1}{12} \tag{33}$$

and the equilibrium distribution is given by (equations (16), (26) and (27))

$$\bar{f}_i = \frac{\rho}{12} (1 + 4\mathbf{u} \cdot \mathbf{c}_i + 8(\mathbf{u} \cdot \mathbf{c}_i)^2 - 2\mathbf{u}^2) \quad \bar{f}_0 = \rho(\frac{1}{2} - \mathbf{u}^2). \tag{34}$$

#### 2.4. Viscous effects

To determine the viscous term  $\delta f_i$ , we adopt the general forms

$$\delta f_i = A \nabla^\gamma u^\gamma + B c_i^\alpha c_i^\beta \nabla^\beta u^\alpha \quad \delta f_0 = C \nabla^\gamma u^\gamma \tag{35}$$

where  $A$ ,  $B$  and  $C$  need to be found. Using these expressions in equation (15), it can be shown that

$$\begin{aligned} & \eta(\nabla^\alpha u^\beta + \nabla^\beta u^\alpha - \delta^{\alpha\beta} \nabla^\gamma u^\gamma) + \zeta \delta^{\alpha\beta} \nabla^\gamma u^\gamma \\ &= -3\delta^{\alpha\beta} A \nabla^\gamma u^\gamma - \frac{3}{4} B (\nabla^\alpha u^\beta + \nabla^\beta u^\alpha + \delta^{\alpha\beta} \nabla^\gamma u^\gamma) \\ & \quad - u^\alpha u^\beta (6A + 3B + C) \nabla^\gamma u^\gamma. \end{aligned} \tag{36}$$

In obtaining the right-hand side terms of this equation, use has been made of the following:

- (i) equation (22);
- (ii) the conditions

$$\sum_i c_i^\alpha = 0 \quad \sum_i c_i^\alpha c_i^\beta c_i^\gamma = 0 \tag{37}$$

- (iii) the isotropy of the fourth-order term [4, 8]:

$$\sum_i c_i^\alpha c_i^\beta c_i^\gamma c_i^\delta = X(\delta^{\alpha\beta} \delta^{\gamma\delta} + \delta^{\alpha\gamma} \delta^{\beta\delta} + \delta^{\alpha\delta} \delta^{\beta\gamma}). \tag{38}$$

Taking a double trace (for which  $\delta^{\alpha\alpha} = \delta^{\gamma\gamma} = 2$ ,  $\delta^{\alpha\gamma} \delta^{\alpha\gamma} = \delta^{\alpha\alpha} = 2$ ), we obtain

$$\sum_i c_i^\alpha c_i^\alpha c_i^\gamma c_i^\gamma = 6 = 8X \tag{39}$$

i.e. the coefficient for the 'B' term in equation (36) is  $X = 3/4$ . Equating terms in (36):

$$-\frac{3}{4} B = \eta \quad -3A - \frac{3}{4} B = \zeta - \eta \quad 6A + 3B + C = 0. \tag{40}$$

Therefore

$$B = -\frac{4}{3}\eta \quad A = \frac{1}{3}(2\eta - \zeta) \quad C = 2\zeta \tag{41}$$

the viscous terms then reading as follows (equation (35)):

$$\delta f_i = \frac{1}{3}(2\eta - \zeta) \nabla^\gamma u^\gamma - \frac{4}{3}\eta c_i^\alpha c_i^\beta \nabla^\beta u^\alpha \quad \delta f_0 = 2\zeta \nabla^\gamma u^\gamma. \tag{42}$$

2.5. Summary of model

We have constructed an LB model which leads to the Navier–Stokes equation. Galilean invariance and isotropy are built into the model. The calculation steps are as follows:

(i) Calculate density and velocity using data from the previous time step (equation (3)).

(ii) Calculate the gradients as follows:

$$\begin{aligned} \frac{\partial u_x}{\partial x}(\mathbf{r}, t) &= \frac{1}{3} \sum_i c_{i,x} u_x(\mathbf{r} + \mathbf{c}_i, t) \\ \frac{\partial u_x}{\partial y}(\mathbf{r}, t) &= \frac{1}{3} \sum_i c_{i,y} u_x(\mathbf{r} + \mathbf{c}_i, t) \\ \frac{\partial u_y}{\partial x}(\mathbf{r}, t) &= \frac{1}{3} \sum_i c_{i,x} u_y(\mathbf{r} + \mathbf{c}_i, t) \\ \frac{\partial u_y}{\partial y}(\mathbf{r}, t) &= \frac{1}{3} \sum_i c_{i,y} u_y(\mathbf{r} + \mathbf{c}_i, t) \end{aligned} \tag{43}$$

noting that

$$\nabla^\alpha u^\beta = \frac{1}{3} \sum_i c_i^\alpha c_i^\gamma \nabla^\gamma u^\beta \quad c_i^\gamma \nabla^\gamma u^\beta = u^\beta(\mathbf{r} + \mathbf{c}_i, t) - u^\beta(\mathbf{r}, t).$$

(iii) Calculate  $f_i(\mathbf{r}, t)$  and  $f_0(\mathbf{r}, t)$  as follows (equations (13), (34) and (42)):

$$\begin{aligned} f_i &= \frac{\rho}{12} (1 + 4(c_{i,x} u_x + c_{i,y} u_y) + 8(c_{i,x} u_x + c_{i,y} u_y)^2 - 2(u_x^2 + u_y^2)) \\ &\quad + \frac{1}{3} (2\eta - \zeta) \left( \frac{\partial u_x}{\partial x} + \frac{\partial u_y}{\partial y} \right) - \frac{4}{3} \eta \left( c_{i,x}^2 \frac{\partial u_x}{\partial x} + c_{i,y}^2 \frac{\partial u_y}{\partial y} + c_{i,x} c_{i,y} \left( \frac{\partial u_x}{\partial y} + \frac{\partial u_y}{\partial x} \right) \right) \end{aligned} \tag{44}$$

$$f_0 = \rho \left( \frac{1}{2} - (u_x^2 + u_y^2) \right) + 2\zeta \left( \frac{\partial u_x}{\partial x} + \frac{\partial u_y}{\partial y} \right) \tag{45}$$

(with  $c_{i,x}$  and  $c_{i,y}$  given by equation (2)).

2.6. Physical parameters

In the LB model it is possible to specify directly the initial density and velocity (typically as an equilibrium distribution). It is also possible to specify the coefficients of viscosity; usually one can set  $\zeta = 0$ , with the kinematic viscosity being given by  $\nu = \eta / \rho$ .

The pressure of the system is given by ((14), (34))

$$p \delta^{\alpha\beta} = \frac{\rho}{12} \sum_i (u^\alpha - c_i^\alpha)(u^\beta - c_i^\beta) (1 + 4u^\gamma c_i^\gamma + 8(u^\gamma c_i^\gamma)^2 - 2u^{\gamma 2}) + \rho u^\alpha u^\beta \left( \frac{1}{2} - u^{\gamma 2} \right). \tag{46}$$

Taking  $\alpha = \beta$ , we find

$$p = \frac{\rho}{4} (1 - u^4). \tag{47}$$

Sound velocity is given by

$$c_s = \sqrt{\partial p / \partial \rho} = \frac{1}{2} - O(u^4). \tag{48}$$

### 3. Application to flow in a plane channel

As a verification exercise the proposed LB algorithm was used to compute the flow profile for steady flow through a 2D plane channel in response to a uniform pressure gradient. For incompressible viscous flow with no-slip boundary conditions at the walls, the Navier-Stokes equation gives, for the velocity of fluid along the channel ( $u_x$ ) [6, 7],

$$u_x = \frac{1}{2\nu\rho} \frac{\partial p}{\partial x} \left( \left( \frac{W}{2} \right)^2 - y^2 \right)$$

where  $x$  and  $y$  are measured parallel and perpendicular to the channel respectively ( $y=0$  at the centre of the channel), and  $W$  is the width of the channel. If  $F$  is the force on the fluid in length  $L$  of channel, the pressure gradient may be written

$$\frac{\partial p}{\partial x} = \frac{F}{LWZ}$$

where  $Z$  is a notional distance in the third direction. Writing the volumetric density  $\rho$  in terms of the density per lattice site  $\rho_s$ ,

$$\rho = \frac{\rho_s}{lwZ}$$

where  $l$  and  $w$  are the length and width of a single lattice site ( $l=1$ ,  $w=\sqrt{3}/2$ ), we obtain for the fluid velocity

$$u_x = \frac{\sqrt{3} F}{16\nu\rho_s} \frac{W}{L} \left( 1 - \left( \frac{2y}{W} \right)^2 \right).$$

If  $L$  has the same number of lattice spacings as  $W$ , this expression gives

$$u_x = \frac{3}{32} \frac{F}{\nu\rho_s} \left( 1 - \left( \frac{2y}{W} \right)^2 \right).$$

This equation is in a form which allows a direct comparison with simulation. In the LB model the channel was specified to be 32 lattice points square, with bounce-back boundaries top and bottom and periodic boundaries left and right. A force was applied to the (initially static) fluid by replacing 0.001 stationary particles with 0.001  $x$ -moving particles at each non-boundary lattice site on each time step. The kinematic viscosity and density per lattice site were specified as 1.0 and 0.2 respectively. Noting that at each bounce-back boundary the true wall position is half a lattice spacing outside the grid [5], the width of the channel is exactly  $W = 32\sqrt{3}/2$  lattice spacings.

Using these values the LB program was run for 1000 time steps. The resulting flow profile, which was steady after 400 time steps, is plotted in figure 1. Also plotted is the parabolic profile obtained using the above equation. The fit is excellent; at the centre of the channel the simulation and Navier-Stokes values differ by less than 2%.

### 4. Conclusion

We have derived and verified an LB algorithm which can be used to simulate 2D Navier-Stokes flow.



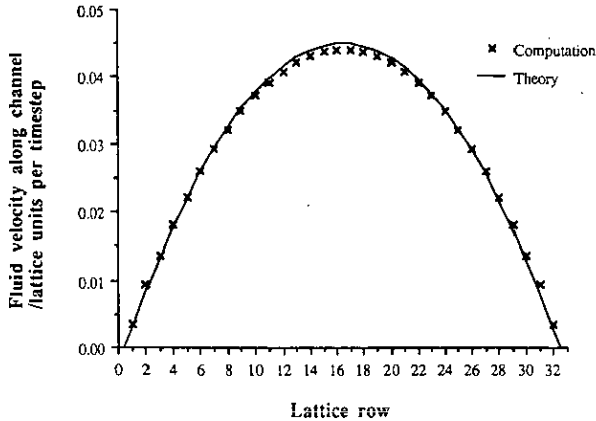


Figure 1. Cross section of 2D plane channel, showing the fluid velocity along the channel.

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