Lattice Boltzmann Flows
Seminar Notes

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-modifications:

- corrections by R. Schalkoff, 9/01
- reformulation of pressure and speed of sound terms, 11/03
- addendum on rest density, 11/03

1 Introduction

The goal of this effort is to develop computational alternatives to finite-element techniques for modeling fluid flow through intricate geometries where a million or more nodes may be required to accurately represent behavior. The derivations herein are a synthesis of those found in the reference list, in particular [1, 2, 3, 4, 5, 6], and serve as the basis for the associated code, *flow12.c*.

Lattice-Boltzmann models are derived from cellular automata models, the most famous of which is John Conway's *game of life*. In this game, each node in a rectangular lattice is given a binary state, living or dead. Rules are then applied in a synchronous update, where node states are changed based on the states of the surrounding (8) neighbors:

- A dead node surrounded by 3 living nodes is "born again".
- A living node surrounded by fewer than 2 living nodes dies (isolation).
- A living node surrounded by more than 3 living nodes dies (overcrowding).

The game exhibits complex behavior, and an extensive literature describing its properties has arisen.

Lattice-Boltzmann models are also state-based models with update rules that are to be applied in a synchronous fashion. Although rectangular lattices are computationally convenient, they impose difficulties in achieving isotropic flow behavior. Therefore, we start with a hexagonal lattice of nodes in the plane: We assume a lattice spacing (the distance to the next node), λ, a time step, τ, unit velocity $v = (\lambda/\tau)$, and velocity vectors $\vec{v}_i = v\vec{c}_i$, $i = 0, \ldots, 5$.

The key quantity of interest is the directional density, $f_i(\vec{r}, t)$, which is the particle density at lattice location $\vec{r}$ at time t moving in direction $\vec{c}_i$. Although the general case will have $f_i() \in [0, 1]$, negative densities, $f_i() \in [-1, 0]$, will be convenient.

Quantities of interest related to the $f_i()$s are:

- density, $\rho(\vec{r}, t) = \sum_{i=0}^{5} f_i(\vec{r}, t)$
- velocity field, $\vec{u}(\vec{r}, t) = (\sum_{i=0}^{5} \vec{v}_i f_i(\vec{r}, t))/(\sum_{i=0}^{5} f_i(\vec{r}, t))$
- momentum tensor, $\Pi_{\alpha\beta} = \sum_{i=0}^{5} v_{i\alpha} v_{i\beta} f_i(\vec{r}, t)$, where $\alpha, \beta \in$ {x,y}

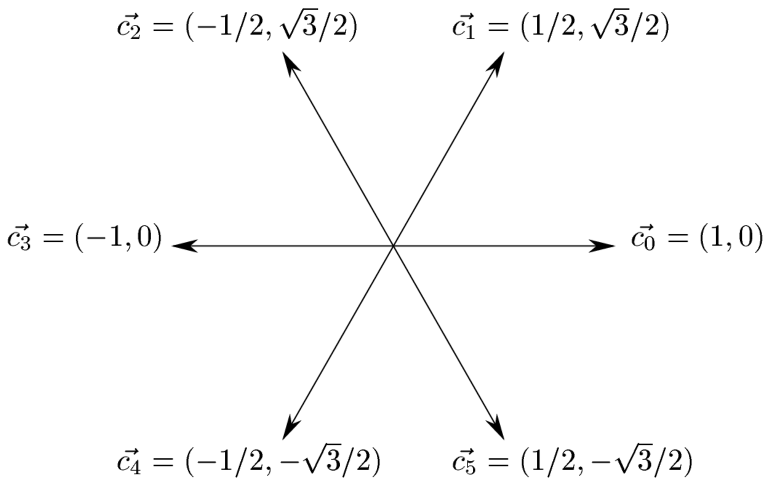

Figure 1: Hex grid

The fundamental system update equation (basis for simulation) is given by:

$$f_i(\vec{r} + \lambda\vec{c}_i, t + \tau) = f_i(\vec{r}, t) + \Theta_i(f(\vec{r}, t)), \qquad \text{i = 0,1, ..., 5} \tag{1}$$

where $\Theta : \Re^6 \to \Re^6$ is a *collision operator*, to be specified. Assuming that Θ is easy to compute, we have an update (1) that is fast and synchronous, so parallelizable. It remains to be seen how this describes fluid flow!

Some important properties of Θ can be specified immediately. From (1) we have

$$f_i(\vec{r} + \lambda\vec{c}_i, t + \tau) - f_i(\vec{r}, t) = \Theta_i(f(\vec{r}, t)), \qquad \text{i = 0,1, ..., 5} \tag{2}$$

and so we can express:

- conservation of mass: $\sum_{i=0}^{5} \Theta_i(f(\vec{r}, t)) = 0$
- conservation of momentum: $\sum_{i=0}^{5} \vec{v}_i \Theta_i(f(\vec{r}, t)) = (0, 0)$

We'll gather other properties along the way before specifying Θ.

2 The First-order Continuity Equation

At this stage we'll need a multi-dimensional (dimension 3, specifically) Taylor expansion. Recall the form [7]:

$$f(x+h, y+k, t+l) = f(x, y, t) + [(h, k, l) \cdot \nabla] f(x, y, t) + \frac{[(h, k, l) \cdot \nabla]^2}{2!} f(x, y, t) + \ldots \tag{3}$$

where the square term is not the Laplacian, in that it includes cross terms. If we apply this to the basic update equation (2) we get:

$$[(\lambda\vec{c}_i, \tau) \cdot \nabla] f_i(\vec{r}, t) + \frac{[(\lambda\vec{c}_i, \tau) \cdot \nabla]^2}{2!} f_i(\vec{r}, t) + \ldots = \Theta_i(f(\vec{r}, t)) \tag{4}$$

We want to consider the limiting behavior here as $\lambda, \tau \to 0$; they can, of course, approach at different rates, and it turns out that two sets of rates are important.

Write

$$t = \frac{t_1}{2\varepsilon} + \frac{t_2}{2\varepsilon^2} \qquad \text{where} \quad t_1 = o(\varepsilon), t_2 = o(\varepsilon^2)$$

$$\vec{r} = \frac{\vec{r}_1}{\varepsilon} \qquad \text{where} \quad \vec{r}_1 = o(\varepsilon)$$

Then

$$\frac{\partial}{\partial t} = \varepsilon \frac{\partial}{\partial t_1} + \varepsilon^2 \frac{\partial}{\partial t_2}$$

$$\frac{\partial}{\partial r_\alpha} = \varepsilon \frac{\partial}{\partial r_{1\alpha}} \qquad \text{for} \quad \alpha \in \{x, y\}$$

So

$$\nabla = (\partial/\partial r_x, \partial/\partial r_y, \partial/\partial t) = (\varepsilon\partial/\partial r_{1x}, \varepsilon\partial/\partial r_{1y}, \varepsilon\partial/\partial t_1 + \varepsilon^2\partial/\partial t_2) \tag{5}$$

We also assume that the solution, $f(\vec{r},t)$, is a small perturbation on this same scale about some local equilibrium, i.e.,

$$f(\vec{r},t) = f^0(\vec{r},t) + \varepsilon f^1(\vec{r},t) \tag{6}$$

and that the macroscopic quantities are carried by the equilibrium value, that is,

- $\rho(\vec{r},t) = \sum_{i=0}^5 f_i^0(\vec{r},t)$
- $\vec{u}(\vec{r},t) = (\sum_{i=0}^5 \vec{v}_i f_i^0(\vec{r},t))/(\sum_{i=0}^5 f_i^0(\vec{r},t))$

Using the gradient expression (5) and the local equilibrium expression (6), we can sum (4) over $i = 0, 1, \ldots, 5$ and equate coefficients of ε^1 to obtain

$$\sum_{i=0}^5 \lambda c_{ix} \frac{\partial f_i^0}{\partial r_{1x}}(\vec{r},t) + \sum_{i=0}^5 \lambda c_{iy} \frac{\partial f_i^0}{\partial r_{1y}}(\vec{r},t) + \sum_{i=0}^5 \tau \frac{\partial f_i^0}{\partial t_1}(\vec{r},t) = 0$$

where the right hand side disappears by conservation of mass. If we now divide by τ, and recall that $\vec{v}_i = \lambda \vec{c}_i/\tau$, we have

$$\left(\frac{\partial}{\partial r_{1x}}, \frac{\partial}{\partial r_{1y}}\right) \cdot \sum_{i=0}^5 \vec{v}_i f_i^0(\vec{r},t) + \frac{\partial}{\partial t_1} \sum_{i=0}^5 f_i^0(\vec{r},t) = 0$$

that is,

$$div_1[\rho(\vec{r},t)\vec{u}(\vec{r},t)] + \partial\rho(\vec{r},t)/\partial t_1 = 0 \qquad \text{(the continuity equation for time scale } t_1) \tag{7}$$

3 The Euler Equation of Hydrodynamics

If we multiply (4) by $\vec{v}_i = (v_{ix}, v_{iy})$, sum over $i = 0, 1, \ldots, 5$, divide by τ, and again equate coefficients of ε^1, we obtain a pair of equations:

$$\frac{\partial}{\partial t_1} \sum_{i=0}^5 v_{i\alpha} f_i^0(\vec{r},t)) + \frac{\partial}{\partial r_{1x}} \sum_{i=0}^5 v_{i\alpha} v_{ix} f_i^0(\vec{r},t)) + \frac{\partial}{\partial r_{1y}} \sum_{i=0}^5 v_{i\alpha} v_{iy} f_i^0(\vec{r},t)) = 0 \qquad \text{for } \alpha \in \{\text{x,y}\} \tag{8}$$

where the right hand side vanishes due to conservation of momentum. This pair can be expressed as

$$\frac{\partial}{\partial t_1}[\rho(\vec{r},t)\vec{u}(\vec{r},t))]_\alpha + \frac{\partial}{\partial r_{1x}}(\Pi^0(\vec{r},t))_{\alpha x} + \frac{\partial}{\partial r_{1y}}(\Pi^0(\vec{r},t))_{\alpha y} = 0 \qquad \text{for } \alpha \in \{\text{x,y}\} \tag{9}$$

where Π^0 denotes the momentum tensor based on the local equilibrium, f^0. This is the Euler Equation of Hydrodynamics, which is just the Navier-Stokes equation without the dissipative effects of viscosity.

4 The Continuity Equation

We can repeat the above procedures for the coefficients of ε^2. If we sum (4) over $i = 0, 1, \ldots, 5$ and equate coefficients of ε^2 we obtain

$$\sum_{i=0}^{5}[\tau\frac{\partial}{\partial t_2}f_i^0(\vec{r},t)+\tau\frac{\partial}{\partial t_1}f_i^1(\vec{r},t)+\lambda c_{ix}\frac{\partial}{\partial r_{1x}}f_i^1(\vec{r},t)+\lambda c_{iy}\frac{\partial}{\partial r_{1y}}f_i^1(\vec{r},t)+\lambda^2(c_{ix}^2/2)\frac{\partial^2}{\partial r_{1x}^2}f_i^0(\vec{r},t)+\lambda^2(c_{ix}c_{iy})$$

$$\frac{\partial^2}{\partial r_{1x}\partial r_{1y}}f_i^0(\vec{r},t)+\lambda^2(c_{iy}^2/2)\frac{\partial^2}{\partial r_{1y}^2}f_i^0(\vec{r},t)+\lambda\tau c_{ix}\frac{\partial^2}{\partial r_{1x}\partial t_1}f_i^0(\vec{r},t)+\lambda\tau c_{iy}\frac{\partial^2}{\partial r_{1y}\partial t_1}f_i^0(\vec{r},t)+(\tau^2/2)\frac{\partial^2}{\partial t_1^2}f_i^0(\vec{r},t)]=0 \quad (10)$$

Because the macroscopic quantities are carried by f^0, we know that $\sum_{i=0}^5 f_i^1(\vec{r},t)=0$ and $\sum_{i=0}^5 \vec{v}_i f_i^1(\vec{r},t)=0$. Thus, after dividing (10) by τ and moving the sum through, we see that the second, third, and fourth terms on the left vanish. We are left with

$$\frac{\partial}{\partial t_2}\rho(\vec{r},t)+(\tau/2)\frac{\partial^2}{\partial t_1^2}\rho(\vec{r},t)+(\tau/2)\sum_{\alpha,\beta\in\{x,y\}}\frac{\partial^2}{\partial r_{1\alpha}\partial r_{1\beta}}\Pi^0_{\alpha\beta}+\tau\sum_{\alpha\in\{x,y\}}\frac{\partial^2}{\partial r_{1\alpha}\partial t_1}\rho(\vec{r},t)\vec{u}(\vec{r},t)_\alpha=0 \quad (11)$$

But, by the order 1 continuity equation,

$$(\tau/2)\frac{\partial^2}{\partial t_1^2}\rho(\vec{r},t)=-(\tau/2)\sum_{\alpha\in\{x,y\}}\frac{\partial^2}{\partial r_{1\alpha}\partial t_1}\rho(\vec{r},t)\vec{u}(\vec{r},t)_\alpha$$

and so the rightmost three summands on the left hand side of (11) sum to

$$(\tau/2)\sum_{\alpha\in\{x,y\}}\frac{\partial}{\partial r_{1\alpha}}[\frac{\partial}{\partial t_1}\rho(\vec{r},t)\vec{u}(\vec{r},t)_\alpha+\sum_{\beta\in\{x,y\}}\frac{\partial}{\partial r_{1\beta}}\Pi^0_{\alpha\beta}] \quad (12)$$

By the Euler equation, the above term in square brackets is 0. Thus we are left with

$$\frac{\partial}{\partial t_2}\rho(\vec{r},t)=0 \quad (13)$$

Density does not change at this time scale. If we now multiply the order 1 continuity equation (7) by ε, multiply (13) by ε^2, and add we obtain

$$div[\rho\vec{u}]+\frac{\partial}{\partial t}\rho=0 \quad (14)$$

which is the standard continuity equation.

5 The Navier-Stokes Equation

The remaining step in this sequence is clear: we need to multiply both sides of (4) by $\vec{v}_i=(v_{ix},v_{iy})$, sum over $i = 0, 1, \ldots, 5$, divide by τ, and equate coefficients of ε^2. Because the notation will become tedious (perhaps it already has), we restrict to the x component.

Of the three terms in (10) that conveniently vanished, only one will be so kind here, specifically,

$$\sum_{i=0}^{5}\tau v_{ix}\frac{\partial}{\partial t_1}f_i^1(\vec{r},t)=0$$

again because the f^0 component carries the velocity field. The other two terms will remain and contribute to f^1 momentum tensor.

Collecting terms, we have

$$\frac{\partial}{\partial t_2}[\rho(\vec{r},t)\vec{u}(\vec{r},t)_x] + \sum_{\alpha\in\{x,y\}}\frac{\partial}{\partial r_{1\alpha}}[\Pi^1(\vec{r},t)]_{\alpha x} + (\tau/2)\frac{\partial^2}{\partial t_1^2}[\rho(\vec{r},t)\vec{u}(\vec{r},t)_x] +$$
$$\tau\frac{\partial}{\partial t_1}\sum_{\alpha\in\{x,y\}}\frac{\partial}{\partial r_{1\alpha}}[\Pi^0(\vec{r},t)]_{\alpha x} + (\tau/2)\sum_{\alpha,\beta\in\{x,y\}}\frac{\partial^2}{\partial r_{1\alpha}\partial r_{1\beta}}[S^0(\vec{r},t)]_{\alpha\beta x} = 0 \quad (15)$$

where S^0 is a third-order tensor,

$$S^0(\vec{r},t)_{\alpha\beta\gamma} = \sum_{i=0}^{5} v_{i\alpha}v_{i\beta}v_{i\gamma}f_i^0(\vec{r},t)$$

The third and fourth summands in (15) can now be collapsed, since, from the Euler equation, we have:

$$(\tau/2)\frac{\partial^2}{\partial t_1^2}[\rho(\vec{r},t)\vec{u}(\vec{r},t)_x] = -(\tau/2)\frac{\partial}{\partial t_1}\sum_{\alpha\in\{x,y\}}\frac{\partial}{\partial r_{1\alpha}}[\Pi^0(\vec{r},t)]_{\alpha x}$$

We are left with:

$$\frac{\partial}{\partial t_2}[\rho(\vec{r},t)\vec{u}(\vec{r},t)_x] + \sum_{\alpha\in\{x,y\}}\frac{\partial}{\partial r_{1\alpha}}\left[\Pi^1(\vec{r},t)_{\alpha x} + (\tau/2)\left(\frac{\partial}{\partial t_1}\Pi^0(\vec{r},t)_{\alpha x} + \sum_{\beta\in\{x,y\}}\frac{\partial}{\partial r_{1\beta}}[S^0(\vec{r},t)]_{\alpha\beta x}\right)\right] = 0 \quad (16)$$

This contains the dissipative contributions to the flow. Multiplying the Euler equation (9) by ε, multiplying the dissipative contributions (16) by ε^2, and adding, we obtain

$$\frac{\partial}{\partial t}[\rho(\vec{r},t)\vec{u}(\vec{r},t)_x] + \sum_{\alpha\in\{x,y\}}\frac{\partial}{\partial r_{\alpha}}\left[\Pi(\vec{r},t)_{\alpha x} + (\tau/2)\left(\varepsilon\frac{\partial}{\partial t_1}\Pi^0(\vec{r},t)_{\alpha x} + \sum_{\beta\in\{x,y\}}\frac{\partial}{\partial r_{\beta}}[S^0(\vec{r},t)]_{\alpha\beta x}\right)\right] = 0 \quad (17)$$

This is the Navier-Stokes equation, although we still need to express Π, Π^0 and S^0 in terms of ρ and $\vec{u}$. This will require specification of the collision operator, Θ. It is worth noting that, to this point, constraints on the specification of the collision operator are minimal.

6 The Collision Operator

The first step in the specification of the collision operator, Θ, is to expand about f^0. Recalling (6), we have:

$$\Theta(f(\vec{r},t)) = \Theta(f^0(\vec{r},t)) + \left[\frac{\partial\Theta_i}{\partial f_j}\right]_{f=f^0}(\varepsilon f^1) + O(\varepsilon^2) \quad (18)$$

Let

$$\Omega_{i,j} = \left[\frac{\partial\Theta_i}{\partial f_j}\right]_{f=f^0}$$

If we now equate powers of ε^0 in (4) we obtain

$$\Theta(f^0(\vec{r},t)) = 0$$

that is, the collision operator vanishes at the local equilibrium.

The fundamental update equation (1) now reads:

$$f_i(\vec{r}+\lambda\vec{c}_i, t+\tau) = f_i(\vec{r},t) + \Omega_i(f(\vec{r},t) - f^0(\vec{r},t)) \quad (19)$$

where Ω_i denotes the i^{th} row of matrix Ω. We can use conservation of mass and conservation of momentum to deduce the structure of Ω.

From conservation of mass (see bullet items following (2)) we have:

$$\begin{aligned}\sum_{i=0}^{5}\Omega_{i,j} &= \sum_{i=0}^{5}\frac{\partial\Theta_i}{\partial f_j}\\ &= \frac{\partial}{\partial f_j}\sum_{i=0}^{5}\Theta_i\\ &= 0\end{aligned}$$

that is, the column sums are 0. Similarly, from conservation of momentum, we have:

$$\begin{aligned}\sum_{i=0}^{5}\vec{v}_i\Omega_{i,j} &= \frac{\partial}{\partial f_j}\sum_{i=0}^{5}\vec{v}_i\Theta_i\\ &= (0,0)\end{aligned}$$

and so weighted column sums are also 0.

More generally, $\Omega_{i,j}$ is the deflection of density f_i in the j^{th} direction. Isotropic flow dictates that its value depends only upon the angle between i and j, which, for our hex-grid, can be only $0^o, 60^o, 120^o$, or 180^o. As a result, we must have:

$$\Omega = \begin{pmatrix} a_0 & a_{60} & a_{120} & a_{180} & a_{120} & a_{60}\\ a_{60} & a_0 & a_{60} & a_{120} & a_{180} & a_{120}\\ a_{120} & a_{60} & a_0 & a_{60} & a_{120} & a_{180}\\ a_{180} & a_{120} & a_{60} & a_0 & a_{60} & a_{120}\\ a_{120} & a_{180} & a_{120} & a_{60} & a_0 & a_{60}\\ a_{60} & a_{120} & a_{180} & a_{120} & a_{60} & a_0 \end{pmatrix} \tag{20}$$

The matrix is symmetric (and circulant), and so the results for column sums apply to row sums. In particular, 0 is a triple eigenvalue with eigenvectors $(1,1,1,1,1,1)$, $(v_{0x}, v_{1x}, v_{2x}, v_{3x}, v_{4x}, v_{5x})$, and $(v_{0y}, v_{1y}, v_{2y}, v_{3y}, v_{4y}, v_{5y})$. Equivalently, we can use $(1,1,1,1,1,1)$, the x components of the $\vec{c}_i$s, $c_x = (1, 1/2, -1/2, -1, -1/2, 1/2)$, and the y components of the $\vec{c}_i$s, $c_y = (0, \sqrt{3}/2, \sqrt{3}/2, 0, -\sqrt{3}/2, -\sqrt{3}/2)$ as the eigenvectors for 0.

It is easy to verify that there are two non-zero eigenvalues, $e_1 = 6a_0 + 6a_{60}$, and $e_2 = -6a_0 - 12a_{60}$. e_1 is a double value with eigenvectors $V_0 = (1,0,-1,1,0,-1)$ and $V_1 = (1,-2,1,1,-2,1)$. The eigenvector for e_2 is $V_2 = (1,-1,1,-1,1,-1)$. This leaves a great deal of flexibility in the choice of Ω, but stability requires that the eigenvalues are $\in (-2,0)$. This is easily seen, since the update step is essentially:

$$f(new) = f(old) + \Omega(f(old) - f^0)$$

which is equivalent to:

$$f(new) - f^0 = [I + \Omega]\,(f(old) - f^0)$$

and so the eigenvalues of $I + \Omega$ must be $\in (-1,1)$.

A further restriction is the target viscosity, μ, which we will see (in section 9) is related to the eigenvalue e_1 according to:

$$\mu = -\frac{\tau v^2}{4}\left(\frac{1}{e_1} + \frac{1}{2}\right) \tag{21}$$

In figure 2 we plot the inequalities $e_1, e_2 \in (-2,0)$ on a_0/a_{60} axes. Since (21) is equivalent to:

$$a_{60} = -a_0 - \frac{\tau v^2}{24\mu + 3\tau v^2} \tag{22}$$

a specification of viscosity, $\mu \in (0, +\infty)$, amounts to selection of a line segment in figure 2 that is parallel to the bounding (lavender) lines $a_{60} = -a_0$ and $a_{60} = -a_0 - 1/3$. Note that a choice of $a_{60} = 1/3$ is convenient in that it is

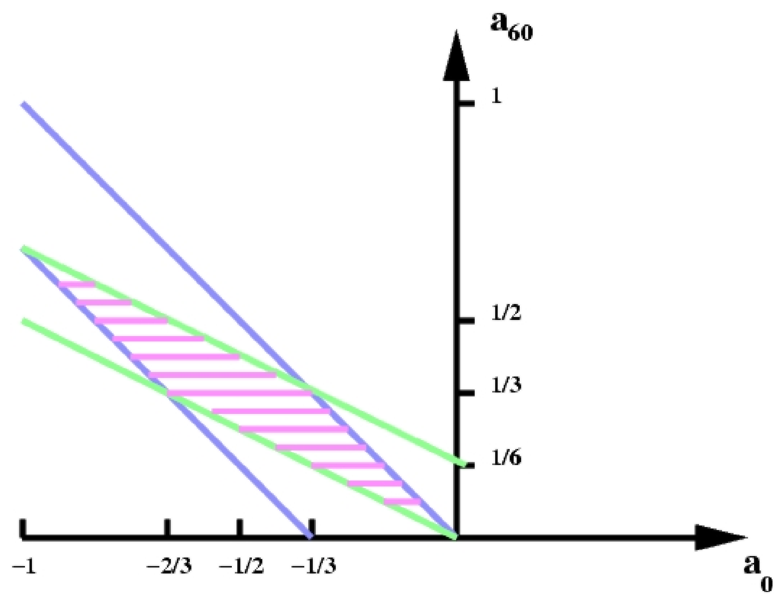

Figure 2: e_1 and e_2 restrictions

available on all such line segments. With this choice, viscosity is then related to a_0 by:

$$a_0 = -\frac{1}{3}\left(\frac{8\mu + 2\tau v^2}{8\mu + \tau v^2}\right) \tag{23}$$

For any $\mu \in (0, +\infty)$, other choices for a_{60} are available, and this flexibility may be valuable later.

7 Power Law Fluids

Although we have yet to specify f^0, it is now easy to see how to simulate non-Newtonian, power-law fluids. The defining characteristic of such fluids is that viscosity depends upon strain rate according to an equation of the form:

$$\mu = K(\dot{e})^n \tag{24}$$

where $\dot{e}$ denotes the so-called second invariant of the rate of deformation tensor, specifically,

$$\dot{e} = \sqrt{\left(\frac{\partial u_x}{\partial x}\right)^2 + \left(\frac{\partial u_x}{\partial y} + \frac{\partial u_y}{\partial x}\right)^2 /2 + \left(\frac{\partial u_y}{\partial y}\right)^2} \tag{25}$$

In this form, the choices, $n = 0$, $n < 0$, and $n > 0$, denote Newtonian, strain-thinning, and strain-thickening fluids.

Given K and n that specify the power-law fluid, we can simulate the flow rather easily. For each node:

1. Use numerical estimates of velocity derivatives to compute $\dot{e}$ by (25).
2. Use (24) to compute target viscosity, μ.
3. Use (23) to compute a_0.
4. Complete specification of Ω by:

$$\begin{aligned} a_{60} &= 1/3 \\ a_{120} &= -(2a_0 + 3a_{60}) \\ a_{180} &= (3a_0 + 4a_{60}) \end{aligned}$$

5. Update $f()$ for this node by (19).

All that remains to completing the description of the code attached in the Appendix is a derivation of f^0.

8 Local Equilibria

An elegant derivation of an f^0 appears in [6], where it is observed that the choice of f^0 is not unique and that the particular value selected can affect the convergence rate of the update scheme. Nevertheless, when that technique is applied to our 6 population, hex-grid model, it yields an overly-constrained system with no (non-trivial) solution. Karlin (personal communication) believes that his 9 population, rectangular grid model is the minimum 2D system for which his technique will yield solutions.

As an alternative, we make the assumption (standard in the literature) that f^0 is quadratic in the velocity components, u_x and u_y, so that

$$f_i^0 = A_i + B_i u_x + C_i u_y + D_i u_x u_y + E_i u_x^2 + G_i u_y^2 \tag{26}$$

The constraints on f^0 are:

$$\sum_i f_i^0 = \rho \tag{27}$$

$$\sum_i v_{ix} f_i^0 = u_x \rho \tag{28}$$

$$\sum_i v_{iy} f_i^0 = u_y \rho \tag{29}$$

$$\sum_i v_{ix} v_{iy} f_i^0 = u_x u_y \rho \tag{30}$$

$$\sum_i v_{ix}^2 f_i^0 = u_x^2 \rho + p \tag{31}$$

$$\sum_i v_{iy}^2 f_i^0 = u_y^2 \rho + p \tag{32}$$

where p denotes pressure. The constraints (27) - (29) were mentioned earlier. The constraints on the momentum tensor (30) - (32) will be required in order to obtain the standard Navier-Stokes equation from our current form (17).

If we are willing to assume that the directional coefficients in (26) are proportional to their velocities, $\vec{v}_i$, we can obtain a unique solution. Specifically, if we write:

$$\begin{aligned} A_i &= A \\ B_i &= v_{ix} B \\ C_i &= v_{iy} C \\ D_i &= v_{ix} v_{iy} D \\ E_i &= (v_{ix}^2 - v^2/2) E \\ G_i &= (v_{iy}^2 - v^2/2) G \end{aligned}$$

then we can apply the following (arithmetic) identities:

$$\sum v_{i\alpha} = 0 \qquad \alpha \in \{x, y\} \tag{33}$$

$$\sum v_{i\alpha}^2 = 3v^2 \qquad \alpha \in \{x, y\} \tag{34}$$

$$\sum v_{ix} v_{iy} = 0 \tag{35}$$

$$\sum v_{i\alpha}^2 v_{i\beta} = 0 \qquad \alpha, \beta \in \{x, y\} \tag{36}$$

$$\sum v_{ix}^2 v_{iy}^2 = (3/4)v^4 \tag{37}$$
$$\sum v_{i\alpha}^3 v_{i\beta} = 0 \qquad \alpha,\beta \in \{x,y\}, \alpha \neq \beta \tag{38}$$
$$\sum v_{i\alpha}^4 = (9/4)v^4 \qquad \alpha \in \{x,y\} \tag{39}$$

to obtain the solution. As an example, if we begin with (27) we have

$$\begin{aligned}
\rho &= \sum_i f_i^0 \\
&= \sum_i A + Bu_x \sum_i v_{ix} + Cu_y \sum_i v_{iy} + Du_x u_y \sum_i v_{ix} v_{iy} + Eu_x^2 \sum_i (v_{ix}^2 - v^2/2) + Gu_y^2 \sum_i (v_{iy}^2 - v^2/2) \\
&= 6A + 0 + 0 + 0 + Eu_x^2(3v^2 - 6v^2/2) + Gu_y^2(3v^2 - 6v^2/2) \\
&= 6A
\end{aligned}$$

and so $A = \rho/6$. Similarly, from (28) we obtain $B = \frac{\rho}{3v^2}$, from (29) we obtain $C = \frac{\rho}{3v^2}$, and from (30) we obtain $D = \frac{4\rho}{3v^4}$

Determining E and G is only slightly more difficult. From (31) and (32) we obtain:

$$\rho u_x^2 + p = \rho v^2/2 + (3/4)v^4 E u_x^2 - (3/4)v^4 G u_y^2 \tag{40}$$

and

$$\rho u_y^2 + p = \rho v^2/2 - (3/4)v^4 E u_x^2 + (3/4)v^4 G u_y^2 \tag{41}$$

The difference is:

$$\rho(u_x^2 - u_y^2) = (3/2)v^4(E u_x^2 - G u_y^2) \tag{42}$$

Because (42) must hold for all values of (u_x, u_y), we must have $E = G = (2\rho)/(3v^4)$. Note that by adding (40) and (41) we can determine that

$$p = \rho(c_s^2 - u^2/2)$$

where $c_s = \sqrt{v^2/2}$ is the speed of sound and $u^2 = u_x^2 + u_y^2$. (Note: for a velocity-independent pressure, see the addendum.)

Thus the final form for f^0 is:

$$f_i^0 = \frac{\rho}{6} + \frac{\rho}{3v^2}[v_{ix}u_x + v_{iy}u_y] + \frac{4\rho}{3v^4}[v_{ix}v_{iy}u_x u_y] + \frac{2\rho}{3v^4}\left[(v_{ix}^2 - v^2/2)u_x^2 + (v_{iy}^2 - v^2/2)u_y^2\right] \tag{43}$$

9 Navier-Stokes Revisited

The remaining task at hand is the development of (17) to express Π, Π^0, and S^0 in terms of ρ and $\vec{u}$. Recall that for any $\alpha,\beta,\gamma \in \{x,y\}$,

$$\Pi_{\alpha\beta}^0 = \sum_{i=0}^{5} v_{i\alpha} v_{i\beta} f_i^0 \tag{44}$$

$$S_{\alpha\beta\gamma}^0 = \sum_{i=0}^{5} v_{i\alpha} v_{i\beta} v_{i\gamma} f_i^0 \tag{45}$$

and f^0 is provided in (43). Thus only the expression for Π will require significant effort. In this regard, we observe that

$$\begin{aligned}
\Pi_{\alpha,\beta} &= \sum_{i=0}^{5} v_{i\alpha} v_{i\beta} f_i \\
&= \sum_{i=0}^{5} v_{i\alpha} v_{i\beta} (f_i^0 + \varepsilon f_i^1)
\end{aligned}$$

and so we really need an expression for f_i^1 in terms of ρ and $\vec{u}$.

We have previously summed (4) over $i = 0, 1, ..., 5$ and equated coefficients of various powers of ε. In section 6 we also equated coefficients of ε^0 in (4) directly, that is, without summing. Following this same path, we now equate coefficients of ε^1 in (4). We obtain

$$\lambda c_{ix}\frac{\partial f_i^0}{\partial r_{1x}} + \lambda c_{iy}\frac{\partial f_i^0}{\partial r_{1y}} + \tau\frac{\partial f_i^0}{\partial t_1} = \Omega_i f^1 \tag{46}$$

or, equivalently,

$$\tau\left(\sum_{\alpha\in\{x,y\}} v_{i\alpha}\frac{\partial f_i^0}{\partial r_{1\alpha}} + \frac{\partial f_i^0}{\partial t_1}\right) = \Omega_i f^1 \tag{47}$$

For the purposes of differentiating f_i^0, we'll regard it as a function of ρ and $\rho\vec{u}$ and use a simplified, order 1 (in $\vec{u}$) approximation,

$$f_i^0 = \frac{\rho}{6} + \frac{v_{ix}}{3v^2}\rho u_x + \frac{v_{iy}}{3v^2}\rho u_y \tag{48}$$

For $\alpha \in \{x,y\}$ a chain-rule differentiation then gives:

$$\begin{aligned}\frac{\partial f_i^0}{\partial r_{1\alpha}} &= \frac{\partial f_i^0}{\partial \rho}\frac{\partial \rho}{\partial r_{1\alpha}} + \frac{\partial f_i^0}{\partial \rho u_x}\frac{\partial \rho u_x}{\partial r_{1\alpha}} + \frac{\partial f_i^0}{\partial \rho u_y}\frac{\partial \rho u_y}{\partial r_{1\alpha}} \\ &= \frac{1}{6}\frac{\partial \rho}{\partial r_{1\alpha}} + \sum_{\beta\in\{x,y\}}\frac{v_{i\beta}}{3v^2}\frac{\partial \rho u_\beta}{\partial r_{1\alpha}}\end{aligned} \tag{49}$$

and, similarly,

$$\begin{aligned}\frac{\partial f_i^0}{\partial t_1} &= \frac{\partial f_i^0}{\partial \rho}\frac{\partial \rho}{\partial t_1} + \frac{\partial f_i^0}{\partial \rho u_x}\frac{\partial \rho u_x}{\partial t_1} + \frac{\partial f_i^0}{\partial \rho u_y}\frac{\partial \rho u_y}{\partial t_1} \\ &= \frac{1}{6}\frac{\partial \rho}{\partial t_1} + \sum_{\beta\in\{x,y\}}\frac{v_{i\beta}}{3v^2}\frac{\partial \rho u_\beta}{\partial t_1}\end{aligned} \tag{50}$$

In this last expression, we can change temporal derivatives to spatial ones by using the continuity equation (7) and the Euler equation (9). We have:

$$\frac{\partial f_i^0}{\partial t_1} = \frac{1}{6}(-div_1(\rho\vec{u})) + \sum_{\beta\in\{x,y\}}\frac{v_{i\beta}}{3v^2}\left[\sum_{\gamma\in\{x,y\}} -\frac{\partial \Pi^0_{\beta\gamma}}{\partial r_{1\gamma}}\right] \tag{51}$$

To differentiate Π^0, we'll again use an order 1 approximation. From (30) - (32) we have $\Pi^0_{\alpha\beta} = \rho u_\alpha u_\beta + p\delta_{\alpha\beta}$, and so, to order 1, $\Pi^0_{\alpha\beta} = \rho\delta_{\alpha\beta}v^2/2$. Thus

$$\frac{\partial f_i^0}{\partial t_1} = \frac{1}{6}(-div_1(\rho\vec{u})) - \sum_{\beta\in\{x,y\}}\frac{v_{i\beta}}{6}\frac{\partial \rho}{\partial r_{1\beta}} \tag{52}$$

We can now substitute (49) and (52) into (47) to obtain a substantially simplified expression:

$$\begin{aligned}\Omega_i f^1 &= \tau\left[-\frac{1}{6}div_1(\rho\vec{u}) + \sum_{\alpha\in\{x,y\}}\sum_{\beta\in\{x,y\}}\frac{v_{i\alpha}v_{i\beta}\partial\rho u_\alpha}{3v^2\partial r_{1\beta}}\right] \\ &= \tau\left[\frac{1}{3}\sum_{\alpha\in\{x,y\}}\sum_{\beta\in\{x,y\}}(c_{i\alpha}c_{i\beta} - \delta_{\alpha\beta}/2)\frac{\partial \rho u_\alpha}{\partial r_{1\beta}}\right]\end{aligned} \tag{53}$$

We cannot, at this stage, obtain an expression for f^1 by inverting Ω (recall, 0 is an eigenvalue of Ω!), but the vectors on the right hand side of (53), $< c_{i\alpha}c_{i\beta} - \delta_{\alpha\beta}/2 >$, are easily seen to be orthogonal to each of the three eigenvectors that span the kernel space of Ω, and thus they are in the image. In particular, we can write each as a linear combination of the two eigenvectors V_0 and V_1 for eigenvalue e_1:

$$\begin{aligned}
< c_{ix}^2 - 1/2 > &= (3/8)V_0 + (1/8)V_1 \\
< c_{iy}^2 - 1/2 > &= -(3/8)V_0 - (1/8)V_1 \\
< c_{ix}c_{iy} > &= (\sqrt{3}/8)V_0 - (\sqrt{3}/8)V_1
\end{aligned}$$

and so we can conclude that

$$f_i^1 = \frac{\tau}{3e_1}\left[(c_{ix}^2 - 1/2)\frac{\partial \rho u_x}{\partial r_{1x}} + (c_{ix}c_{iy})(\frac{\partial \rho u_x}{\partial r_{1y}} + \frac{\partial \rho u_y}{\partial r_{1x}}) + (c_{iy}^2 - 1/2)\frac{\partial \rho u_y}{\partial r_{1y}}\right] \tag{54}$$

We can now return to (17) and assemble all the required terms. The collisional viscosity term, $\Pi_{\alpha x}$, has a first summand

$$\Pi^0_{\alpha x} = \rho u_\alpha u_x + p\delta_{\alpha x} \tag{55}$$

and so

$$\sum_{\alpha\in\{x,y\}} \frac{\partial \Pi^0_{\alpha x}}{\partial r_\alpha} = \frac{\partial}{\partial r_x}\left[\rho u_x^2 + p\right] + \frac{\partial}{\partial r_y}\left[\rho u_x u_y\right] \tag{56}$$

The second summand of the collisional viscosity term is

$$\begin{aligned}
\varepsilon \Pi^1_{\alpha x} &= \sum_{i=0}^{5} \varepsilon f_i^1 v_{i\alpha} v_{ix} \\
&= \frac{\tau v^2}{3e_1}\left[\delta_{\alpha x}(-3/2)div(\rho\vec{u}) + \frac{\partial \rho u_x}{\partial r_x}\frac{1}{v^4}\sum_{i=0}^{5} v_{i\alpha}v_{ix}^3 + (\frac{\partial \rho u_x}{\partial r_y} + \frac{\partial \rho u_y}{\partial r_x})\frac{1}{v^4}\sum_{i=0}^{5} v_{i\alpha}v_{ix}^2 v_{iy} + \frac{\partial \rho u_y}{\partial r_y}\frac{1}{v^4}\sum_{i=0}^{5} v_{i\alpha}v_{ix}v_{iy}^2\right] \\
&= \frac{\tau v^2}{3e_1}\left[\delta_{\alpha x}(-3/4)div(\rho\vec{u}) + (3/4)(\frac{\partial \rho u_x}{\partial r_\alpha} + \frac{\partial \rho u_\alpha}{\partial r_x})\right]
\end{aligned} \tag{57}$$

where we have used $\varepsilon\partial/\partial r_{1\alpha} = \partial/\partial r_\alpha$ and (33)-(39).

If we now differentiate (57) with respect to r_α we obtain

$$\begin{aligned}
&\frac{\tau v^2}{4e_1}\left[\frac{\partial^2 \rho u_x}{\partial r_x^2} - \frac{\partial^2 \rho u_y}{\partial r_x \partial r_y}\right] \qquad \alpha = x \\
&\frac{\tau v^2}{4e_1}\left[\frac{\partial^2 \rho u_x}{\partial r_y^2} + \frac{\partial^2 \rho u_y}{\partial r_x \partial r_y}\right] \qquad \alpha \neq x
\end{aligned}$$

and so their sum gives:

$$\sum_{\alpha\in\{x,y\}} \frac{\partial}{\partial r_\alpha}\varepsilon \Pi^1_{\alpha x} = \frac{\tau v^2}{4e_1}\nabla^2 \rho u_x \tag{58}$$

The two lattice viscosity terms are handled similarly. For the first,

$$\begin{aligned}
\frac{\tau\varepsilon}{2}\frac{\partial}{\partial t_1}\Pi^0_{\alpha x} &= \frac{\tau\varepsilon}{2}\frac{\partial}{\partial t_1}\left[\rho u_\alpha u_x + \delta_{\alpha x} p\right] \\
&\approx \frac{\tau\varepsilon}{2}\frac{\partial}{\partial t_1}\left[\rho\delta_{\alpha x}v^2/2\right] \qquad \text{order } 1 \\
&= \frac{-\tau v^2}{4}div(\rho\vec{u})\delta_{\alpha x}
\end{aligned} \tag{59}$$

where we have again used the continuity equation for time scale t_1. Thus

$$\sum_{\alpha\in\{x,y\}} \frac{\partial}{\partial r_\alpha}\frac{\tau\varepsilon}{2}\frac{\partial}{\partial t_1}\Pi^0_{\alpha x} = \frac{-\tau v^2}{4}\frac{\partial}{\partial r_x}div(\rho\vec{u}) \tag{60}$$

For the second lattice viscosity term, we can use (43) and (33)-(39), to obtain

$$
\begin{aligned}
S^0_{\alpha\beta x} &= \sum_{i=0}^{5} v_{i\alpha} v_{i\beta} v_{ix} f_i^0 \\
&= \frac{\rho}{3v^2} \sum_{i=0}^{5} (v_{i\alpha} v_{i\beta} v_{ix}^2 u_x + v_{i\alpha} v_{i\beta} v_{ix} v_{iy} u_y)
\end{aligned}
\tag{61}
$$

and so

$$
\begin{aligned}
\frac{\tau}{2} \sum_\alpha \sum_\beta \frac{\partial}{\partial r_\alpha} \frac{\partial}{\partial r_\beta} S^0_{\alpha\beta x} &= \frac{\tau v^2}{8} \left[\frac{3\partial^2(\rho u_x)}{\partial r_x^2} + \frac{2\partial^2(\rho u_y)}{\partial r_x \partial r_y} + \frac{\partial^2(\rho u_x)}{\partial r_y^2} \right] \\
&= \frac{\tau v^2}{4} \left[\frac{\partial}{\partial r_x} div(\rho \vec{u}) + (1/2)\nabla^2(\rho u_x) \right]
\end{aligned}
\tag{62}
$$

Finally, by substituting (56),(58),(60), and (62) into the previous version of the Navier-Stokes equation (17) we arrive at:

$$
\frac{\partial}{\partial t}\rho u_x + \frac{\partial}{\partial r_x}\rho u_x^2 + \frac{\partial}{\partial r_y}\rho u_x u_y = -\frac{\partial}{\partial r_x} p - \frac{\tau v^2}{4}\left(\frac{1}{e_1} + \frac{1}{2}\right)\nabla^2(\rho u_x) \tag{63}
$$

If we take derivatives on the left, we obtain

$$
\frac{\partial}{\partial t}\rho u_x + (\vec{u}\cdot\nabla)(\rho u_x) + div(\vec{u})\rho u_x = -\frac{\partial}{\partial r_x} p - \frac{\tau v^2}{4}\left(\frac{1}{e_1} + \frac{1}{2}\right)\nabla^2(\rho u_x) \tag{64}
$$

For incompressible fluids, we have ρ = constant and $div(\rho\vec{u}) = 0$, and so we obtain (for the x component)

$$
\frac{\partial}{\partial t} u_x + (\vec{u}\cdot\nabla) u_x = -(1/\rho)\frac{\partial}{\partial r_x} p - \frac{\tau v^2}{4}\left(\frac{1}{e_1} + \frac{1}{2}\right)\nabla^2(u_x) \tag{65}
$$

and thus for both components:

$$
\frac{\partial \vec{u}}{\partial t} + (\vec{u}\cdot\nabla)\vec{u} = -(1/\rho)\nabla(p) - \frac{\tau v^2}{4}\left(\frac{1}{e_1} + \frac{1}{2}\right)\nabla^2(\vec{u}) \tag{66}
$$

the classical form. Note the appearance of the viscosity term containing e_1 and τv^2. The latter suggests the need for the two time scales.

10 Summary

We have developed a sufficient amount of the Lattice-Boltzmann flow technique to document the attached code, *flow12.c* Remaining tasks include:

- finite element code for validation
- extension to visco-elastic flows [4]
- extension to 3D flows

11 Addendum on Rest Density

One problem with the formulation above is that pressure remains velocity-dependent, $p = \rho(c_s^2 - u^2/2)$. We can eliminate this artifact of the model by adding rest density. This requires a slight change in the expression for the local equilibrium to

$$f_i^0 = A_i + B_i u_x + C_i u_y + D_i u_x u_y + E_i u_x^2 + G_i u_y^2 + H_i u^2 \tag{67}$$

where the coefficients are still proportional to velocity but differ in the proportionality constants for the rest density ($i = 0$) and non-rest density ($i = 1, 2, \ldots, 6$). For $i = 1, 2, \ldots, 6$ we write:

$$\begin{aligned} A_i &= A \\ B_i &= v_{ix} B \\ C_i &= v_{iy} C \\ D_i &= v_{ix} v_{iy} D \\ E_i &= v_{ix}^2 E \\ G_i &= v_{iy}^2 G \\ H_i &= H \end{aligned}$$

For $i = 0$, the only non-zero terms are $A_0 = \hat{A}$, and $H_0 = \hat{H}$. From symmetry we can assume $B = C$ and $E = G$. Constraints (31) and (32) now yield

$$p + \rho u_x^2 = 3Av^2 + u_x^2((9/4)Ev^4 + 3Hv^2) + u_y^2((3/4)Ev^4 + 3Hv^2) \tag{68}$$

and

$$p + \rho u_y^2 = 3Av^2 + u_x^2((3/4)Ev^4 + 3Hv^2) + u_y^2((9/4)Ev^4 + 3Hv^2) \tag{69}$$

Subtracting, we obtain

$$\rho(u_x^2 - u_y^2) = ((3/2)Ev^4)(u_x^2 - u_y^2) \tag{70}$$

and so $E = (2\rho)/(3v^4)$, as before. Adding (68) and (69), we obtain

$$2p + \rho u^2 = 6v^2 A + u^2(2\rho + 6Hv^2) \tag{71}$$

and so, if we select $H = -\rho/(6v^2)$, we have $p = 3Av^2$.

From constraint (27), we have

$$\rho = 6A + \hat{A} + u^2(3Ev^2 + 6H + \hat{H}) \tag{72}$$

and so if $\hat{H} = -\rho/v^2$, we have $\rho = 6A + \hat{A}$.

We let R denote the ratio of rest density to non-rest density, specifically, $R = \hat{A}/A$. Then

$$p = \rho \frac{3v^2}{6 + R}, \tag{73}$$

now independent of u^2, where the speed of sound is determined by

$$c_s^2 = \frac{3v^2}{6 + R} \tag{74}$$

Changes to the collision matrix, and hence the eigenvalues, are also required. One of the (3) non-zero eigenvalues is still constrained by viscosity. The other two can be forced to -1, so that the associated eigenvalues of $I + \Omega$ are zero. See the code, flow12.c, for details.

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