LATTICE BOLTZMANN MODELS FOR COMPLEX FLUIDS

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Abstract

We present various Lattice Boltzmann Models which reproduce the effects of rough walls, shear thinning and granular flow. We examine the boundary layers generated by the roughness of the walls. Shear thinning produces plug flow with a sharp density contrast at the boundaries. Density waves are spontaneously generated when the viscosity has a nonlinear dependence on density which characterizes granular flow.

PACS numbers: 03.40.Gc 47.50.+d 81.35.+k

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1. Introduction

Many fluids in our daily life have rather complex rheological behavior. Pastes, suspensions, liquid crystals, dense polymers and granular media are usually non-Newtonian and can exhibit many flow anomalies, prominent ones being shear thinning or thickening and the spontaneous formation of density fluctuations in granular flow. Within the framework of classical fluid dynamics it is in general not simple to take into account these nonlinearities. Therefore it is of interest to look for alternative techniques to model the behavior of complex fluids.

As one alternative to the direct solution of the equations of motion the so-called Lattice Boltzmann Models (LBM) have been proposed\cite{1,2}. These models are defined on a lattice with velocity vectors that can only point into few discrete directions and all have the same length. This simplification is somewhat compensated by the fact that on each site one has more real degrees of freedom (six on a triangular lattice) than in the classical numerical techniques allowing for the definition of a local shear or a local rotation.

Two important questions concerning the LBM models can be asked: 1. How well do they reproduce solutions of the phenomenological equations of motion, like Navier Stokes? and 2. How well do they reproduce nature? The first question has been extensively addressed in the literature\cite{1−6}. If certain assumptions are made on the length and time scales over which the variables can change the incompressible Navier Stokes equation can be derived using the Chapman Enskog scheme. It is, however, known that straightforward simulations of the LBM can give inhomogeneous densities violating this incompressibility restriction. In this paper we will investigate these spatial and temporal density fluctuations in more detail. In fact, we want to address mainly the second question: Can LB models describe real phenomena like shear thinning, density waves or the perturbations arising from the roughness of walls?

For that purpose we will investigate the flow through a pipe along which the particles are accelerated through gravity. We want to see what happens if the walls of the pipe are rough and study constitutive laws that produce plug flow and
clogging. The typical experimental materials to which our investigations should apply, are suspensions with shear thinning in the case of plug flow, and granular media in the case of clogging.

In the following section we describe the model and the various variants used in this paper. The next section is devoted to the effects of wall roughness. Section 4 discusses models that give shear thinning and section 5 presents data for a model that spontaneously generates density waves.

2. Description of the model

We consider a triangular lattice, and on each site $\vec{x}$ we have six real variables $N_i(\vec{x}, t)$, $i = 1, \ldots, 6$, representing (counted counter clockwise) the densities of the particles going in the direction $i$ of the lattice. (For convenience we will in the following omit the site index $\vec{x}$ and denote by $N'_i$ the value of the particle density after collision.) One updating of the system ($t \to t + 1$) is given by two steps: (1.) The collision step at which the six $N_i$ are updated at each site through

$$
N'_i = N_i + \lambda (N_i - N_{eq}^i)
$$

and (2.) the propagation step at which each $N_i$ is shifted to the site of the nearest neighbor in direction $i$. Eq. (1) produces a relaxation towards the equilibrium densities $N_{eq}^i$ which is numerical stable provided the relaxation constant $-2 < \lambda < 0$. The value of $\lambda$ sets the kinematic viscosity of the fluid. The equilibrium densities are given by

$$
N_{eq}^i = \frac{\rho}{6} (1 + 2\vec{u} \cdot \vec{c}_i + 4(\vec{u} \cdot \vec{c}_i)^2 - 2\vec{u}^2)
$$

where $\rho$ is the mass density at site $\vec{x}$

$$
\rho = \sum_i N_i
$$

$\vec{c}_i$ the unity vector along direction $i$ and $\vec{u}$ the velocity vector at site $\vec{x}$ defined through the momentum density per site

$$
\rho \vec{u} = \sum_i \vec{c}_i N_i
$$
The equilibrium distribution $N_i^{eq}$ given in Eq. (2), is chosen to give mass and momentum conservation in the collision step. The flow will be forced into the direction of the gravity $\vec{g}$, which is pointing parallel to the walls of the pipe. For that purpose an additional step is added after the collision step which is defined by $N_i'' = N_i' + \frac{1}{3} \vec{c}_i \cdot (\rho \vec{g})$. Periodic boundary conditions are imposed in the direction of gravity in which the system has a length of $L_1$. In the perpendicular direction one has walls separated by $L_2$ lattice spacings. The lattice orientation is such that one of the lattice directions is parallel to the walls. At the beginning of the simulation the average density $\bar{\rho}$ is fixed. It is an important parameter of the model which because of mass conservation stays constant in time. We initialize the system by having the same values of the $N_i$ on each site and then let the system evolve to its steady state. In the case of the stable flows steady state is reached after 2000 or 3000 time steps. In the case of the unstable flows that develop density waves, the simulations might take up to 20000 time steps to reach steady state.

The sites lying on the walls of the system only have two directions a and b. Usually two different collision steps can be applied on these sites\textsuperscript{[4]}, either the specular condition, i.e. $N'_a = N_b$ and $N'_b = N_a$, or the bounce-back condition, i.e. $N'_{a,b} = N_{a,b}$. In the propagation step for these sites the direction in which the $N_i$ are shifted is inverted. We want to be able to implement walls that are not smooth but rugged, i.e. that have (quenched) disorder. For this purposes we introduce a mixed boundary condition defined through

$$N'_a = xN_a + (1 - x)N_b \quad \text{and} \quad N'_b = (1 - x)N_a + xN_b$$

(5)

where $x = y^\alpha$ and $y$ is a random variable chosen from a homogeneous distribution between 0 and 1. Setting $\alpha = 0$ will give the pure bounce-back condition whereas $\alpha = \infty$ corresponds to the pure specular reflection condition.

The relaxation parameter $\lambda$ depends on the material properties including the kinematic and the bulk viscosities. Usually complex fluids are phenomenologically described by “constitutive laws” given e.g. by the functional dependence of the viscosities upon the shear velocity, the density or the pressure. We want to investigate the effect of rather typical nonlinear constitutive laws on the flow properties.
Since an exact relation between $\lambda$ and the material constants is not known we will lean on some approximative arguments\textsuperscript{[1,13]} that predict a vanishing bulk viscosity. In that case one can relate $\lambda$ directly to the kinematic viscosity $\nu$ through $\lambda = -\frac{1}{2}(0.25 + 2\nu)^{-1}$. We will consider two cases: (1.) $\nu$ is a function of the local shear rate $\dot{\tau}$ and (2.) $\nu$ is a function of the local density $\rho$. The detailed functional forms used here will be described in sections 4 and 5.

Our calculations were performed on a Connection Machine CM-2 at GMD (Bonn) using 32-bit precision. The program needs less than one minute to make 50 updates of a system of size $1024^2$. The program was also benchmarked on a CM-5 at I.P.G. in Paris\textsuperscript{[7]}.

3. The effects of rugged walls

As already mentioned, it is well known that LB models produce inhomogeneities in the density when used to simulate for instance flow through a pipe. In the middle of the pipe the density is higher than at the walls\textsuperscript{[13]} by a factor $1/(1-u^2)$. This is seen in fig. 1 which shows the density in a cross section through the pipe. For $\alpha = 0$, i.e. the case of smooth walls the density profile has precisely the predicted shape of $\rho_{wall}/(1-u^2)$ as can be seen from the line showing the pressure \textsuperscript{[13]} $p = (\rho/2)(1-u^2)$. In the case of rough walls, for which we have chosen in $\alpha = 1$ in fig. 1, the density has a minimum close to the walls. Also, the pressure has a minimum at the wall and a lower, but still constant value in the center. As expected there are some random fluctuations close to the walls.

In fig. 2 we see the density variation along the center of the pipe. Since the values taken at different times coincide very well one is in the steady state. Clearly the randomness of the reflection properties of the wall still have some effect but the relative variation is of the order of 0.0001, i.e. extremely weak.

The roughness at the walls therefore seems to be screened very efficiently. This is seen more clearly in fig. 3 which shows the entire density profile in the pipe. The boundary layer has a thickness of a few mean free paths (the mean free path in this context is the characteristic length over which a perturbation in the $N_i$’s will be damped and has typical length of $1/\lambda$) where the distribution of the
Ni’s is clearly different from that in the bulk of the material. In this sense it may be characterized as a Knudsen layer.

4. Shear thinning and plug flow

Shear thinning can be phenomenologically explained by a non-Newtonian constitutive law given by a decrease of the viscosity as a function of the shear rate. Within the context of the LBM the shear rate \( \dot{\tau} \) can be defined through

\[
\dot{\tau}(\vec{x}) = \frac{1}{3} \left| \sum_i \vec{c}_i u_\parallel(\vec{x} + \vec{c}_i) \right|
\]

where \( u_\parallel \) is the projection of \( \vec{u} \) into the direction of the pipe. We consider a constitutive law of the form \( \nu = \nu_1 \) for \( \tau \leq \tau_0 \) and \( \nu = \nu_2 \) for \( \tau > \tau_0 \) and \( \nu_1 > \nu_2 \).

In fig. 4 we show the velocity profile in a cross section through the pipe. In the simulations the flow was initialized with a relatively strong forcing, \( g = 5 \times 10^{-5} \). During this initial phase the shearthinned regions at the walls appear, and the flow velocity increases to approximately its steady state value. Then the forcing was reduced by a factor 10 to \( g = 5 \times 10^{-6} \) and the system allowed to reach steady state.

We see that the profile is rather flat in a broad central region which ends at a sharp kink after which one finds a rather steep velocity gradient towards the walls where the fluid is in the thinned phase. This kind of behavior is usually called plug flow. It was checked that the flow is really in a steady state by performing longer runs. In a recent preprint\(^9\) a simulation of a similar LBM has been presented which also finds plug flow by taking a constitutive law in which the viscosity decreases with the shear rate like a power law. This seems to indicate that the appearance of plug flow is rather independent on the detailed form of the constitutive law as long as \( \nu \) is a decreasing function of \( \dot{\tau} \).

5. Density waves

A salient feature of granular media is the spontaneous formation of density waves, similar in fact to traffic jams on highways. One possibility to explain the effect that generates these waves is to assume that the viscosity depends on density.
Within the kinetic gas theory of granular media\textsuperscript{[10,11]} the relation $\nu \propto (\rho - \rho_c)^{1/3}$ has been derived. Since the above relation imposes a maximum density $\rho_c$ it is rather difficult to implement it directly within the context of the LBM where the particles do not have an exclusive volume. We therefore chose a piecewise linear relation of the form $\nu = \nu_{\text{min}}$ if $\rho \leq \rho_t$ and $\nu = \nu_0 + \gamma(\rho - \bar{\rho})$ for $\rho > \rho_t$ (see fig. 5). $\bar{\rho}$ is the average density and the threshold density $\rho_t$ is chosen to make $\nu$ a positive continuous function of the density. Fig. 6 shows results from simulations where $\rho_t = 2.962$ and the slope $\gamma = 6.25$ corresponding to a minimum cut-off viscosity $\nu_{\text{min}} = 0.01$.

In order to generate density waves we found it necessary to introduce a small perturbation producing a 0.3\% relative density difference. This perturbation was performed by introducing a small amount of momentum on one line across the pipe, keeping the mass unchanged. In fig. 6 we see that this initially very weak perturbation dramatically builds up and develops into a density wave of over 10\% density contrast. For a pipe of same width but half the length, i.e. a different aspect ratio the wave has a less pronounced profile. This dependence on the aspect ratio is not to be confounded with finite size effects. Our mean free path is typically one lattice spacing so that the strong finite size effects encountered in some lattice gas models\textsuperscript{[14]} should not be relevant here. The maximum flow velocity $u_{\text{max}}$ at the later times is $u_{\text{max}} = 0.039$ and $u_{\text{max}} = 0.048$ for the channel lengths 256 and 512 respectively and same width 64. The forcing $g = 3.33 \times 10^{-5}$ is the same for both system lengths. For the present parameter values the initial perturbation relaxes, leaving a time independent density field, if the value of $\gamma$ is less than 3.75. This effect can be understood qualitatively by observing that there are two competing mechanisms in the system: On one hand, the viscous relaxation of density perturbations will tend to smoothen density contrasts. On the other hand, the rather steep increase of viscosity with density combined with the presence of the walls will tend to increase the contrasts. A small increase in the density at the wall will give a local increase in viscosity and slow down the flow. Due to the inertia of the surrounding flow this in turn will lead to a
further increase in the density and so on. If this instability dominates the relaxing mechanism the density wave will form.

By triggering the density wave by two spatially separated perturbations, rather than just a single one, we checked that the complex shape of the waves does not reflect the detailed way in which they were initiated. We also observe that there seems to be no characteristic wavelength: Fig. 6 shows that the waves have roughly the same shape on the scale of the channel length although the amplitude depends on the system size.

Fig. 7 shows this amplitude as a function of time during 60,000 time steps. The insert shows the initial unstable phase leading to the rather drastic increase of the amplitude at the time 10,000. The first small increase in the density is due to the acceleration of the flow and can be understood from the velocity dependence in the pressure. The small jump at the time 2500 results from the perturbation. Before the instability is triggered at the time 10,000, small oscillations in the amplitude are observed. It was checked that the amplitude indeed has its’ steady state value at the time 60,000 by running the simulations ten times longer. The complicated relaxation towards the fully developed density wave indicates that strong non-linear effects come into play rendering a linear stability analysis meaningless. It would be interesting to understand this behaviour further.

In fig. 8 one can see the density wave propagating. The fronts are actually sharpest at the boundary and the left gradient which is less sharp than the right one has some weak spatial oscillations. The fact that the waves are of the order of the length of the pipe again shows that there is no characteristic length scale. The periodic boundary conditions seem crucial to reinforce the steady state. One therefore has the typical behaviour of a kinetic wave as also found in traffic jam models\cite{15}.

6. Conclusion

We have presented various versions of Lattice Boltzmann Models which can reproduce rather complex flow behavior. On one hand we investigated how the laminar flow screens the asperities arising from rugged walls by forming Knudsen
layers close to the wall. When a shear thinning constitutive law is introduced we find plug flow. Finally, when the viscosity is an increasing function of density we observe a range of parameters for which the material spontaneously produces density waves traveling upstream. These density waves are triggered by some perturbation that apparently is unstable, but the final shape of the wave is independent of the initial disturbance.

Plug flow and density waves are common phenomena in non-Newtonian fluid dynamics and have been investigated recently in detail for granular media[12]. It seems therefore that LB models can be a powerful tool to handle complex fluids numerically. This approach is, however, yet quite preliminary. One has to determine the physical parameters for which the proposed models do match a real experiment and then compare measured and simulated results. Work in this direction is in progress.

Acknowledgements

We thank Dan Rothman and Einat Aharonov for illuminating comments and discussions.

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Figure Captions

Fig. 1 Density as a function of the position $Y$ across the channel for $\alpha = 0$ (squares) and $\alpha = 1$ ($\times$). Also $2p = \rho(1 - u^2)$ is shown for $\alpha = 0$ ($\bigcirc$) and $\alpha = 1$ ($+$). $L_1 = 256, L_2 = 64, \bar{\rho} = 3, g = 3.33 \times 10^{-5}$ and $\nu = 0.25$. The figure shows the steady state profile after 7500 iteration steps. The maximum flow velocity $u_{\text{max}} = 0.52$.

Fig. 2 Density in the center of the pipe as a function of the position $X$ along the channel for $\alpha = 1$ and otherwise the same parameters as in fig. 1. The two lines correspond to two measurements 25 iteration steps apart.

Fig. 3 Density contrast in the pipe for the same parameters as in fig. 1 and fig. 2. White denotes the lowest density and black the largest one.

Fig. 4 Velocity as a function of the position, $Y$ across the channel measured at steady state after 5000 iteration steps. The insert shows the viscosity’s dependence on the local shearrate. In this simulation $\nu_1 = 1.0, \nu_2 = 0.1, \tau_0 = 10^{-3}$, $\bar{\rho} = 3.0, L_1 = 256$ and $L_2 = 64$. The forcing is $g = 5 \times 10^{-6}$.

Fig. 5 The density dependence of the viscosity chosen in the simulations.

Fig. 6 The density in the center of the channel as a function of the position $X$ along the channel for $\rho_t = 2.962, \bar{\rho} = 3.0, g = 3.33 \times 10^{-5}$ and $L_2 = 64$. The curve of crosses is for $L_1 = 256$ and 60,000 iteration steps after the initial perturbation. The other curves correspond to $L_1 = 512$ and 5000 (thick line), 60,000 (full line) and 60,025 (dashed line) iterations after the perturbation was applied. The slope $\gamma = 6.25$ and the minimum viscosity $\nu_{\text{min}} = 0.01$.

Fig. 7 The amplitude, i.e. difference between largest and smallest density, along the center of the pipe as a function of time measured in units of 100 iteration
steps for $L_1 = 256$ and otherwise the same parameters as in fig. 5. The insert is a blow-up of the behavior at early times.

**Fig. 8** Density contrast in the pipe for the same parameters as in fig. 5 and fig. 6 after 60,000 (upper) and 60,025 (lower) iteration steps. White denotes the lowest and black the largest density.