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A LATTICE BOLTZMANN FOR DISORDERED FLUIDS

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A variant of the lattice Boltzmann scheme is presented as a mesoscopic model of glassy behavior. A hierarchical density-dependent interaction potential is introduced, which allows the coexistence and competition of multiple density minima. We find that this competition allows to model geometrical frustration which produces disordered patterns with sharp density contrasts and no phase-separation. A way of modeling mechanical arrest of real glasses is also proposed and discussed.

1. Introduction

The behavior of glassy materials and related disordered systems is one of the most debated and still open problems in modern condensed matter physics. Glasses exhibit anomalous relaxation, namely long-lived departures from local equilibria, which result from the trapping of atoms around fixed positions in space according to a disordered pattern. The numerical simulation of glassy behavior relies mainly on Molecular Dynamics and Monte Carlo techniques.[1,2] Both methods incorporate details of microscopic behavior and, as a result, they fall short of reaching spatio-temporal scales of macroscopic interest. Coarse-grained lattice gas models represent a step ahead in reaching larger scales: On the one hand there are spin-glasses[3,4] and on the other their modern lattice glass variants.[5,6] Clearly, these lattice models cannot reach the same degree of physical fidelity as truly atomistic methods.

It is in the spirit of mesoscopic models that the lattice Boltzmann equation (LBE) was originally introduced for simulating hydrodynamic behavior in ordinary fluids.[7] Over the years, LBE has proved quite flexible in describing situations beyond the mere fluid dynamics framework.[8] It appears therefore reasonable to explore whether LBE can be extended in such a way to cover glassy behavior as well. We present in the following some preliminary results of a lattice Boltzmann model which allows to catch some features of glassy systems.

2. The Model

We use a modified lattice Boltzmann equation with a single relaxation parameter,[9] which reads as follows:

$$f_i(\mathbf{r}+\mathbf{c}_i,t+1)-(1-q)f_i(\mathbf{r}+\mathbf{c}_i,t)-qf_i(\mathbf{r},t)=-\omega\left(f_i(\mathbf{r},t)-f_i^{eq}(\mathbf{r},t)\right) \qquad (1)$$

where $f_i(\mathbf{r},t)\equiv f(\mathbf{r},\mathbf{v}=\mathbf{c}_i,t)$ is a discrete distribution function of particles moving along the direction i with discrete speed $\mathbf{c}_i$. We use a nine-velocity model on a square lattice with $c_i=(\pm1,0)$, $(0,\pm1)$, $(\pm1,\pm1)$. The constant q is a parameter which allows to control the propagation rate between neighboring sites. It varies in the range $]0,1]$ with the case $q=1$ corresponding to the usual LBE. The right-hand side represents the relaxation to a local equilibrium f_i^{eq} in a time lapse of the order of ω^{-1}. The distribution functions are related to the fluid density ρ and to the fluid momentum $\rho\mathbf{u}$ by

$$\rho=\sum_i f_i\ , \qquad \rho\mathbf{u}=\sum_i f_i\mathbf{c}_i\ . \qquad (2)$$

Using the multiscale technique, after some algebra, we get the following equations at second order:

$$\partial_t\rho+q\partial_\alpha(\rho u_\alpha)+\frac{q}{2}(q-1)\left[\partial_\alpha\partial_\alpha(c_s^2\rho)+\partial_\alpha\partial_\beta(\rho u_\alpha u_\beta)\right]=0 \qquad (3)$$

$$\begin{aligned}\partial_t(\rho u_\beta)+q\partial_\alpha(\rho u_\alpha u_\beta)&=-q\partial_\beta p+q\partial_\alpha\left[\rho\Big(qc_s^2(\frac{1}{\omega}-\frac{1}{2})\partial_\beta u_\alpha+c_s^2(\frac{q}{\omega}-\frac{1}{2})\partial_\alpha u_\beta\Big)\right]\\&-q(q-1)c_s^2\left(u_\alpha\partial_\beta\rho+\frac{1}{2}u_\beta\partial_\alpha\rho\right)-q\left(\frac{q}{\omega}+\frac{q}{2}-1\right)\partial_\alpha\partial_\gamma(\rho u_\alpha u_\beta u_\gamma)\end{aligned} \qquad (4)$$

where $p=c_s^2\rho$ is the equation of state. Note that the major physical quantities scale as follows: $u_\alpha\to qu_\alpha$, $p\to q^2p$, $\nu\to q^2\nu$, plus corrections scaling with $q-1$, so that the standard equations for a quasi-incompressible fluid[10] are recovered in the limit $q\to1$.

In order to describe light and heavy phases with a single species fluid we follow the approach of Shan and Chen[11] and introduce a non ideal-gas behavior within the LBE formalism by means of a phenomenological pseudo-potential which describes the effects of potential energy interactions.

We introduce a repulsive Lennard-Jones potential interaction, which takes the following expression on the lattice:

$$V(r)=\begin{cases}G\Psi(\rho)r^{-12} & \text{if } 1\le r\le\sqrt{2}\\ 0 & \text{otherwise}\end{cases} \qquad (5)$$

where G is a positive parameter controlling the strength of the interaction. The structure of $\Psi(\rho)$ is in the form of nested polynomials, whose density zeroes are distributed according to a binary tree whose depth depends on the number of generations N_g:

$$\Psi(\rho) = (\rho - \rho_0) \prod_{g=2}^{N_g} \frac{-1}{(1 + (\frac{\rho-\rho_0}{\overline{\rho}_0/2})^{2^{g-1}})^2} \prod_{k=1}^{2^{g-1}} \frac{(\rho - \rho_{gk})}{(\rho_{gk} - \rho_0)} \tag{6}$$

where $\overline{\rho}_0$ controls the density gap. This hierarchical potential implements the presence of $N_\rho = 2^{N_g} - 1$ competing density extrema.

The denominator in Eq. (5) is such to let $\Psi \to 0$ outside the hierarchical range of zeroes ρ_{gk}. The result is an effective potential alternating stable repulsive regions ($\Psi' = \frac{\partial \Psi}{\partial \rho} > 0$) with unstable attractive ones ($\Psi' < 0$), distributed approximately in the density range $\rho_\mp = \rho_0(1 \mp \overline{\rho}_0(1-2^{-N_g}))$. The presence of unstable regions causes the appearance of phase transitions which determine the separation of light and heavy phases inside the fluid. In this case we should not observe the typical patterns of phase separation in binary fluids where coherent regions of the two phases grow in time until they span completely the system. The LBE with hierarchical interactions takes the final form

$$\begin{aligned} f_i(\mathbf{r} + \mathbf{c}_i, t+1) - (1-q) f_i(\mathbf{r} + \mathbf{c}_i, t) - q f_i(\mathbf{r}, t) \\ = -\omega \left(f_i(\mathbf{r}, t) - f_i^{eq}(\mathbf{r}, t) \right) + F_i(\mathbf{r}, t) \end{aligned} \tag{7}$$

where $F_i = -G \frac{\rho}{\rho_0} \nabla \Psi(\rho) \cdot \mathbf{c}_i$.

3. Numerical results

We have simulated the fluid on a 2D lattice of size 256×256 with the following parameters: $\omega = 1.0$, $\rho_0 = 1.0$, $N_g = 3$, $\overline{\rho}_0 = 0.5$, G and q are varied in the ranges $[0, 1]$ and $[0.8, 1]$, respectively. The initial condition is $\rho(\mathbf{r}) = \rho_0 \; (1 + \xi)$ where ξ is a random perturbation uniformly distributed in the range $[-0.01, 0.01]$. The effects due to propagation (left hand side of Eq. (7)) between neighboring sites and to the non-linear potential $\Psi(\rho)$ make the density distribution to spread out in time, so that an instability is triggered as soon as G exceeds the critical threshold G_c.

We find analytically $G_c \sim 0.089 \; q^2$. Numerically we can verify this prediction by monitoring the value of G, keeping q fixed, for which the quantity $\Delta\rho \equiv \rho_{max} - \rho_{min}$ becomes non zero. The density gap $\Delta\rho$ starts up at $G = G_c \sim 0.09 \; q^2$ in good agreement with the analytical result and rapidly fills the available range of states between ρ_- and ρ_+, as the interaction strength is increased. In Fig. 1 we show for the case $G = 0.45$, $q = 1$ the probability distribution function of ρ as a function of time. The density ρ distributes in time within the available range of values according to a gaussian distribution, characterized by decreasing fluctuations around the mean value as time goes on. The analysis of the spatial distribution of the density field shows no phase-separation, but rather a disordered coexistence of light and dense phases. This shows that the potential allows to model sharp density contrasts over a disordered spatial distribution.

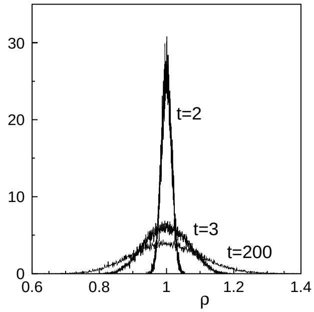

Fig. 1. The probability distribution function of ρ at different times for the case $G = 0.45$, $q = 1$.

4. Conclusion

The proposed LBE produces a number of encouraging results. Geometrical frustration is qualitatively captured by a hierarchical density-dependent potential, alternating repulsive and attractive interactions. This potential gives rise to disordered patterns with short-range, sharp density contrasts. However, anomalous time relaxation is not captured even by introducing a conditional propagation, i.e. $q \neq 1$. Nevertheless we believe this is a route to be explored in future work: possible strategies include a density-dependent relaxation frequency ω and/or density-dependent site-to-site hopping rates.[12]

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