

Shear Banding from lattice kinetic models with competing interactions

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We present numerical simulations based on a Boltzmann kinetic model aimed at the characterization of rheological properties of soft-glassy materials. The kinetic approach is directly inspired by lattice models with competing (frustrating) self interactions and is shown to give rise to shear banding effects when frustration is enhanced. The present methodological framework may result as a valuable tool for the theoretical/computational investigation of the emergence of such non linear and non trivial rheological properties which are at the heart of the understanding of many soft glassy materials.

Keywords: Soft Glassy Materials, Non Linear Rheology, Lattice Kinetic models, frustrated phase separation

1. Introduction

Many applications in modern science, engineering and biology have prompted the recent blossoming of research in the rheology of soft-flowing and nonergodic materials, such as emulsions, foams, gels (Larson 1999, Coussot 2005, Chaikin & Lubensky 1995, Lyklema 1991, Evans & Wennerström 1999, Degennes 1979, Doi & Edwards 1986, Grosberg & Khokhlov 1994, Weaire & Hutzler 1999). The theoretical understanding of such materials sets interesting questions on its own. Indeed, since soft-materials share simultaneously many distinctive features of the three basic states of matter (solid, liquid and gas), their quantitative description does not fall in the traditional methods of equilibrium and/or non-equilibrium statistical mechanics. New concepts and theoretical paradigms are indeed required to adjust many non-standard features, such as rheology, long-time relaxation, dynamic disorder, ageing and related phenomena. In particular, under simple shear conditions, some of these complex fluids may separate into bands of widely different viscosities. This phenomenon is known as “shear banding” (Berret 2005) and involves inhomogeneous flows where macroscopic bands with different shear rates or shear stresses coexist in the sample. Although shear banding is attributed to a shear-induced transition from a microscopic organization of the fluid structure to another, it still raises lots of theoretical and experimental challenges (Manneville *et al.* 2007, Sollich *et al.* 2009, Fardin *et al.* 2010).

Simultaneously, the need for new tools of analysis also emerges for computational studies, which typically involve many interacting space and time scales, the latter

case being particularly acute in view of the aforementioned long-time relaxation. In the recent past, we presented a new conceptual/computational scheme for the numerical simulation of soft-flowing materials (Benzi *et al.* 2009, Bernaschi *et al.* 2009, Benzi *et al.* 2010). The scheme is based on a (Lattice) Boltzmann (LB) formulation (Bathnagar, Gross & Krook 1954, Benzi *et al.* 1992, Chen & Doolen 1998, Gladrow 2000) for interacting binary fluids (Shan & Chen 1993,1994), in which, by a proper combination of short-range attraction and mid-range repulsion (competing self interactions), an effective form of frustration was encoded within the physics of the binary mixture (Benzi *et al.* 2009). More specifically, by tuning the above interactions in such a way as to bring the surface tension down to nearly vanishing values, many typical signatures of soft-glassy behaviour, such as long-time relaxation, dynamical arrest, ageing, and non-linear Herschel-Bulkley rheology, have been clearly detected in numerical studies (Benzi *et al.* 2009, Bernaschi *et al.* 2009, Benzi *et al.* 2010). In this paper we further elaborate along these lines by performing confined numerical simulations and looking at the rheological properties of the model, i.e. the relation between the applied shear and the developed stress by the fluid. Performing numerical simulations on a wide range of shear rates we detect the emergence of shear banding effects, i.e. a stress plateau is shown to correspond to a wide range of stationary shear rates. These results lend further credit to the Boltzmann kinetic formulation as a systematic tool to study the emergence of non linear rheological properties from the mesoscopic scale.

2. The Model: Lattice Boltzmann equation with competing self interactions

In this section we review the main properties of the lattice Boltzmann model used in the numerical simulations. Further details can be found in our recent work (Benzi *et al.* 2009). The starting point is the lattice transcription of the generalized Boltzmann equation (Bathnagar, Gross & Krook 1954, Benzi *et al.* 1992, Chen & Doolen 1998, Gladrow 2000) for a multicomponent fluid with S species as inspired by the work of Shan & Chen (Shan & Chen 1993, Shan & Doolen 1995):

$$f_{is}(\vec{r} + \vec{c}_i \Delta t, t + \Delta t) - f_{is}(\vec{r}, t) = -\frac{\Delta t}{\tau_s} [f_{is}(\vec{r}, t) - f_{is}^{(eq)}(\rho_s, \vec{u} + \tau_s \vec{F}_s / \rho_s)]. \quad (2.1)$$

In the above, $f_{is}(\vec{r}, t)$ is the probability density function of finding a particle of species $s = 1 \dots S$ at site \vec{r} and time t , moving along the i -th lattice direction, defined by the discrete speeds \vec{c}_i with $i = 0 \dots b$. For simplicity, the characteristic propagation time lapse Δt is taken equal to unity ($\Delta t = 1$) in the following. The left hand-side of (2.1) stands for molecular free-streaming, whereas the right-hand side represents the collisions as a simple time relaxation towards the local Maxwellian equilibrium $f_{is}^{(eq)}(\rho_s, \vec{u})$ on a time scale τ_s . The local Maxwellian is truncated at second order, an approximation that is enough to recover the correct isothermal hydrodynamic balance

$$f_{is}^{(eq)}(\rho_s, \vec{u}) = w_i^{(eq)} \rho_s \left(1 + \frac{(u_a c_{ia})}{c_S^2} + \frac{(c_{ia} c_{ib} - c_S^2 \delta_{ab})}{2c_S^4} u_a u_b \right)$$

with c_S^2 the square of the sound speed in the model and δ_{ab} the Kronecker delta with a, b indicating the Cartesian components (repeated indices are summed upon).

The $w_i^{(eq)}$'s are equilibrium weights used to enforce isotropy of the hydrodynamic equations (Benzi *et al.* 1992, Gladrow 2000, Chen & Doolen 1998). The equilibrium for the s species is a function of the local species density

$$\rho_s(\vec{r}, t) = \sum_i f_{is}(\vec{r}, t)$$

and the common velocity, defined as

$$\vec{u}(\vec{r}, t) = \frac{\sum_s \frac{1}{\tau_s} \sum_i f_{is}(\vec{r}, t) \vec{c}_i}{\sum_s \frac{1}{\tau_s} \rho_s(\vec{r}, t)}.$$

The common velocity receives a shift from the force \vec{F}_s acting on the s species (Shan & Chen 1993, Shan & Doolen 1995). This force may be an external one or due to intermolecular interactions. The pseudo-potential forces embed the essential features to achieve phase separation and a mechanism of frustration achieved through competing self interactions. More specifically, within each species, the forces consist of an attractive (denoted with (*attr*)) component, acting only on the first Brillouin region (belt, for simplicity), and a repulsive (denoted with (*rep*)) one acting on both belts, whereas the force between species (X) is short-ranged and repulsive. In equations:

$$\vec{F}_s(\vec{r}, t) = \vec{F}_s^{(attr)}(\vec{r}, t) + \vec{F}_s^{(rep)}(\vec{r}, t) + \vec{F}_s^X(\vec{r}, t)$$

where

$$\vec{F}_s^{(attr)}(\vec{r}, t) = -G_s^{(attr)} \psi_s(\vec{r}, t) \sum_{i \in \text{belt1}} w_i \psi_s(\vec{r}_i, t) \vec{c}_i \quad (2.2)$$

$$\vec{F}_s^{(rep)}(\vec{r}, t) = -G_s^{(rep)} \psi_s(\vec{r}, t) \sum_{i \in \text{belt1}} p_i \psi_s(\vec{r}_i, t) \vec{c}_i - G_s^{(rep)} \psi_s(\vec{r}, t) \sum_{i \in \text{belt2}} p_i \psi_s(\vec{r}_i, t) \vec{c}_i \quad (2.3)$$

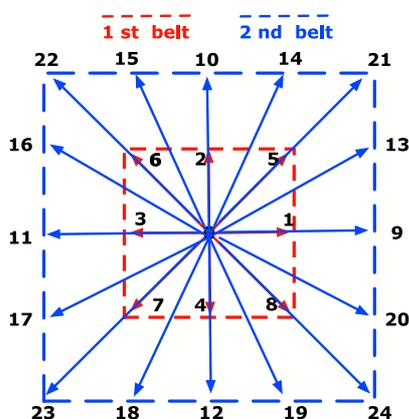
$$\vec{F}_s^X(\vec{r}, t) = -\frac{1}{(\rho_0^{(s)})^2} \rho_s(\vec{r}, t) \sum_{s' \neq s} \sum_{i \in \text{belt1}} G_{ss'} w_i \rho_{s'}(\vec{r}_i, t) \vec{c}_i. \quad (2.4)$$

In the above, the groups “belt 1” and “belt 2” refer to the first and second Brillouin zones in the lattice and \vec{c}_i , p_i , w_i are the corresponding discrete speeds and associated weights (see figure 1 and table 1). The interaction parameter $G_{ss'} = G_{s's}$, $s' \neq s$, is the cross-coupling between species, ρ_0 is a reference density to be defined shortly and, finally, $\vec{r}_i = \vec{r} + \vec{c}_i$ are the displacements along the \vec{c}_i velocity vector. These interactions are sketched in Figure 1 for the case of a two component fluid (say species A and B). This model bears similarities to the NNN (next-to-nearest-neighbor) frustrated lattice spin models (Shore & Sethna 1991, Shore, Holzer & Sethna 1992). However, in our case, a high lattice connectivity (Sbragaglia 2007) is required to ensure compliance with macroscopic non-ideal hydrodynamics, which is at the core of the complex rheology to be discussed in this work. To this purpose, the first belt is discretized with 8 speeds, whereas the second with 16, for a total of $b = 25$ connections (including rest particles). All the weights take the values illustrated in Table 1.

Forcing Weights (for $\vec{F}_s^{(rep)}$)	
$p_i = 247/420$	$i = 0$
$p_i = 4/63$	$i = 1, 4$
$p_i = 4/135$	$i = 5, 8$
$p_i = 1/180$	$i = 9, 12$
$p_i = 2/945$	$i = 13, 20$
$p_i = 1/15120$	$i = 21, 24$

Forcing Weights (for $\vec{F}_s^{(attr)}$ and \vec{F}_s^X)	
$w_i = 4/9$	$i = 0$
$w_i = 1/9$	$i = 1, 4$
$w_i = 1/36$	$i = 5, 8$

Table 1. Links and weights of the two belts, 25-speeds lattice.

Figure 1. The discrete 25-speed lattice. Both belts are illustrated with the corresponding velocities. Further details can be found in the paper by Benzi and coworkers (Benzi *et al.* 2009).

3. Results

4. conclusions

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