

Flow heterogeneity in hard sphere glasses: Connecting MD studies with lattice Boltzmann simulations

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There is growing evidence that the flow of driven amorphous solids is not homogeneous, even if the macroscopic stress is constant across the system [1,2]. Recent event driven molecular dynamics simulations of a hard sphere (HS) glass confirm the heterogeneous nature of the flow but at the same time suggest that, at least for HS glasses, no steady state exists [3]. Due to limitations in the available time and length scales, however, no conclusion could be made on this issue. In this study, we address this and related questions via lattice Boltzmann computer simulations of non-Newtonian fluids. The non-Newtonian character of the fluid enters the LB iteration scheme via a shear rate and density dependent relaxation time, thus encoding the shear rate and density dependence of viscosity. Furthermore, the dependence of the hydrostatic pressure on local density and shear rate is accounted for via a corresponding force term. All the input parameters of the relevant constitutive laws are taken from the preceding molecular dynamics simulations [3]. The present approach thus provides the link between microscopic (MD) simulations and macroscopic hydrodynamic response of the system. The reliability of the lattice Boltzmann simulations is tested by analytic studies of the linear stability phase diagram. As a detailed comparison shows, both the linear stability phase diagram and the dispersion relation for the decay rate of fluctuations in the stable regime are nicely born out by lattice Boltzmann simulations. Studies of the unstable regime, on the other hand, unreveal quite a rich spatio-temporal behavior.

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