Lattice Boltzmann Simulations for Glass-Forming Liquids

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In order to bridge the scales in the simulation of the flow of glass-forming liquids, mesoscopic simulations based on continuum-mechanics principles are performed. The Lattice Boltzmann technique is an efficient method to solve the Navier-Stokes equations of ordinary, linear-response Newtonian liquids, in the low-Mach-number limit. However, in glass-forming systems, the interplay of slow structural relaxation and flow fields causes nonlinear response effects such as shear-thinning, and the appearance of a finite yield stress separating flowing from non-flowing states under the application of external forces. On the level of the Navier-Stokes equation, these effects arising from the micro-scale need to be captured by nonlinear closure relations, called constitutive laws, that link the stress tensor that appears in the equations back to the velocity fields. On a microscopic level, the mode-coupling theory of the glass transition gives a qualitative description rooted in first-principles statistical physics. We present an extension of the lattice Boltzmann scheme to include the nonlinear integral-equation-constitutive laws arising from this microscopic description, to simulate larger-scale flow behavior of glass-forming fluids.