372d Rapid Shear Viscosity Calculation by Momentum Impulse Relaxation Molecular Dynamics (Mir-MD)

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Recently, our group introduced a new molecular dynamics method to rapidly compute the viscosity of fluids. The technique, termed *Momentum Impulse Relaxation* (MIR), involves the imposition of a Gaussian velocity profile on an equilibrated system, after which the decay in the profile is monitored as a function of time. By matching the rate of decay of the peak velocity to the corresponding solution to the Navier-Stokes equation, the shear viscosity can be computed. The method was originally applied to simple systems (argon and *n*-butane) and found to give comparable accuracy to conventional equilibrium and non-equilibrium methods, with more than an order of magnitude reduction in computing time.

In this work, we extend and generalize the method to examine larger molecules (like *n*-hexane and a bead-spring model of a polymer) with significantly higher viscosities than have been previously examined. A detailed analysis of the method is given, including the effect the velocity boundary conditions have on the viscosity, the sensitivity of the results to the profile fitting and averaging procedure, and the effect system size and box shape have on the accuracy and speed of the method. We also discuss the use of modified equations of motion to equilibrate or relax the Gaussian profile before the decay of the profile begins.