ChemE I5800 **Molecular Simulation** **Spring 2019**

Problem Set 8 – due April 17

This problem concerns the MD simulation of Couette and Poiseuille flow, and involves modifications of the equilibrium LJ program to incorporate atomic walls and a forced flow.

Start from the standard program lj.f and reset the number of particles to 1372 (i.e., change *nc* from 5 to 7). The upper and lower planes of fcc cells will be assigned to the walls, and the remaining five planes (or 10 layers of atoms) will be the flowing liquid. From the code, these walls will be parallel to the x-y plane. Note that in the position/velocity/force/... arrays, the lower wall will correspond to the first group of atoms, the liquid to the middle group and the top wall to the last group, so it is easy to isolate the three atom types..

To make the upper and lower atoms into a "wall", add an interaction which tethers them to their original lattice positions with harmonic springs: $\mathbf{F}_i \to \mathbf{F}_i - k(\mathbf{r}_i - \mathbf{r}_{0i})$, where $\mathbf{r}_{0i}$ is the original lattice position of atom i, with $k = 10$. In principle, the mass of the wall atoms to be equal to k (so that the spring oscillation period is comparable to that of the LJ interaction, or else the timestep should be reduced, but you need not bother here.

Run the modified code at density 0.8 and temperature 1.0 with no other changes and with temperature fixed by kinetic energy rescaling until the potential energy stabilizes. Measure the density profile in the fluid – divide the gap region into sampling bins in z in the form of slabs parallel to the walls and find the number of atoms within each slab. You should see an density oscillation close to the walls, which decays going into the interior of the fluid, and a small fluctuating velocity.

For Poiseuille flow, apply an acceleration $g = 0.05$ to each fluid atom along the x direction parallel to the walls. Measure the density profile as above, along with the profiles of x-velocity, pressure, shear stress (σ_{xz}) and temperature. To see a clean result in this small system use very long runs (100000 steps or more) and average over long intervals. You should see the density oscillation persist, perhaps with reduced strength, along with a parabolic velocity profile, and a linear stress profile. For Couette flow, translate one of the wall tether sites $\mathbf{r}_{0i}$ at velocity 0.1 - shift each atom's reference position by v*delta at each step. Obtain the same profiles as in the previous case, which should have a linear velocity and constant shear stress.

If you do not use a thermostat in the accelerated part of the calculation the liquid should heat up. *Do not* blindly use the built-in constant-KE thermostat; it treats the entire system at once, whereas temperature is really defined with respect to the local average velocity, and the latter will vary across the channel. The simplest correct thermostat method is to use a Langevin thermostat in the neutral (y) direction only. The complicated method is to apply a thermostat to each layer of liquid, acting on the difference between the atom velocities and the local average.