Hands on session 10: Common Non-Equilibrium Calculations

1. Common Non-Equilibrium Calculation: Shear Viscosity
   In this hands-on session we will calculate the viscosity of a Lennard-Jones (LJ) fluid. The temperature and density will be the same as assumed in the previous hands-on session. There we used a viscosity of 1.01 for the fluid, let's see if we were justified in doing so. The viscosity of a system of fluid particles (atoms or colloids) can be found in a number of ways: (i) perturbed equations of motion; (ii) reverse perturbation method (Muller-Plathe) technique; (iii) dragging a wall; and (iv) from the long-time integral of the pressure autocorrelation function. Our specific goal in this session is to use LAMMPS to calculate the viscosity for an LJ fluid using two of these methods: (i) and (ii). Input script templates have been provided ("in.nemd" and "in.mp", respectively), but, as previously, they are missing several key command lines for performing the desired simulations. Your task is to complete the input scripts, run them, analyze the results, and report back to the group your findings. Below are the steps to guide you through the process.
   a. Extra credit: verify the zero/low shear-rate viscosity using method (iv)
   b. Extra, extra credit (follow-up on after short course): combine this LJ system with the colloids of the previous one double check the diffusion coefficient of the colloids now that you've measured the viscosity of the pure LJ solvent
2. The input script template
   As mentioned, we will calculate the viscosity of an atomistic Lennard-Jones solvent at a particular temperature and pressure. The outline of the scripts is: create atoms and initialize velocities, equilibrate, shear until steady-state is reached, shear again while collecting data.
3. Fill in pair style
   a. Fill in the pair lj/cut command
      1. Set "sigma" equal to 1.0
      2. Set "epsilon" equal to 1.0
      3. Set the cutoff distance to 2.5σ.
      4. Note the use of non-dimensional or "LJ" units!
   ii. Don't forget the pair coeff command! (see doc pages)
4. Fill in thermostat/integrators
   a. Equilibrate system
      i. Let's equilibrate via fix langevin + fix nve integrator
         1. Fill in the fix langevin command
            a. Set the fix "id" to 2. This is because the template is set up to switch off ("unfix") this command after equilibration run (cf. couple lines down).

b. As before you need to specify the "damp" and the "temperature" parameters among others (see doc page)
c. "damp" has units of time and again represents a momentum relaxation time. In this case, however, there is no connection to a background solvent and its viscous drag on the LJ atom. Instead, damp simply represents a rate of relaxation of the temperature. Set its value to 0.1.
d. Set "temperature" to 1.0

2. Fill in fix nve command

b. Shear system twice; once to reach steady-state, and then again while collecting data
   i. For Method (i)
      1. Fill in the fix nvt/sllod command in the location indicated in the nemd template (see doc page)
         a. Use the "temp" keyword and set "Tstart" and "Tstop" to 1.0
         b. Set "Tdamp" to 0.1
      2. The fix deform command is given for you. Take a minute to review this command (see doc pages). Also note carefully that the simulation region "simbox" above was defined to be a prism for use with this command.
   ii. For Method (ii)
      1. Fill in the fix viscosity command in both locations indicated in the mp template (see doc page)
         a. Set up the shear in the xy-plane
         b. Set a swap rate of 50

5. Define a viscosity variable named "visc" (see doc page)
   a. For method (i)
      i. At low shear rate, the viscosity is found from the linear relation between stress and shear rate ($\mu = -\sigma_{xy}/\dot{\gamma}_{xy}$).
         1. Note we are shearing in the xy-plane so for LAMMPS the predefined variable "pxy" is the stress we need. Also, shear rate (units of 1/time) is found using the predefined variables "srate" (the shear flow velocity) divided by "ly" (the box length).
   b. For method (ii)
      i. We use the total momentum swap accumulated in the fix viscosity to calculate the physical momentum flux in the system instead of the shear stress ($j_y(p_x) = P_{tot}/(2tL_xL_z)$).
         1. Define a momentum flux variable using the predefined variables "step", "lx", "lz" and the scalar total momentum swap (P_{tot})

accumulated in the fix viscosity command. You can access this for your variable using "f_<id>", where "id" is the name you gave the fix viscosity command. Note, t is time. This can be found by $t = 0.005*($step-<number of equilibration steps>$)$. Where <number of equilibration steps> is the number of steps you ran for equilibration and shearing to reach steady state (sum of the two previous run commands). Where does the numerical value of 0.005 come from?

   a. Note when starting data collection the denominator (time) will be zero initially. So, add a small constant ("$1.0e\text{-}10$") to avoid divide by zero error, i.e., $j_y(p_x) = P_{tot}/(2tL_xL_z + 1.0e - 10)$.

2. Now the viscosity can be found similar to SLLOD by $\mu = -j_y(p_x)/\dot{\gamma}_{xy}$. To determine the shear rate, a variable "dVx" has been defined for you from quantities obtained by the fix ave spatial command to calculate the average flow field. Take a minute to review this command (see doc pages). To access this variable in a lammps variable command line use "v_dVx". The difference between the flow velocity in the middle bin and top bin ("dVx") divided by half the box length ("lx/2") gives an approximation to the velocity gradient.

6. Fill in run commands
   a. Careful! How long should you run for to get reasonable results? In this case we may not know a priori what the relevant time scale is to "ballpark" the run time, but we can always run for a "long time" and watch for the time beyond which the observables are no longer time dependent. This is the steady-state. Once this is reached we can obtain data for viscosity.
   b. For the two methods fill in the first run command. You can use trial and error for the length of this first run (not too long for practical reasons) to reach the steady state. Once this is determined, fill in the second run command and collect data for the viscosity calculation.
7. Now it's time to get a number for μ.
   a. For both methods
      i. In a terminal window, issue the "gnuplot" command to start the plotting program.
      ii. Plot the viscosity variable, "visc", vs. time by issuing the command "plot 'log.lammps' using <timestep_column>:<compute_ave_viscosity_variable_column>"; where <timestep_column>, and <compute_ave_viscosity_variable_column> should be replaced with the integer values of the columns in the lammps log output file that contain

the time step (column 1) and average viscosity variable values (column 7), respectively.

iii. Now you should be able to see the viscosity variable fluctuating about some value. Is it close to 1.01?

1. Note you should only be looking at the data during time steps related to the final, data gathering run. You can focus on this range by setting the xrange in gnuplot. Issue the command "set xrange[<low_end_of_data_run_steps>:<high_end_of_data_run_steps>]", where "<low_end_of_data_run_steps>" is the first time step of the data gathering run and "<high_end_of_data_run_steps>" the last time step.
2. You can use gnuplot to get a quick-and-dirty average once you've set the xrange to bracket that data run timesteps. Issue the successive commands in gnuplot: (1) "a1=1.01"; (2) "f1(x)=a1"; (3) "fit f1(x) 'log.lammps' using 1:7 via a1". What is the value the fit command reports for a1?
3. You can view the velocity profile by plotting the output of the ave spatial command in the profile.nemd file. Issue the command "gnuplot". The issue the command "plot 'profile.<method>' using 2:4", where <method> = "nemd" or "mp". You can use the "replot <m>*x" command to get a value of shear rate <m>.