CE 530
Molecular Simulation

Assignment #6 Due: 4 April 2017

1. Show that the Verlet and velocity Verlet algorithms lead to identical trajectories.

2. Derive the leap-frog algorithm by using Taylor expansions for $v(t+\frac{\Delta t}{2})$, $v(t-\frac{\Delta t}{2})$, $x(t+\Delta t)$, and $x(t)$.

3. One should be very careful with calculation of diffusion constant via the mean squared displacement when periodic boundaries are used. Why?

4. The accompanying file contains data for the trajectory of a single Lennard-Jones atom in an NVE simulation. The first three columns list the *x, y, z* coordinates of the atom at each MD step, and the last three columns are the corresponding velocity components. The time step is 0.01 (in LJ units where σ and ε/*k* are unity).

   Averages for temperature and pressure are 0.925 and 0.659, respectively (in Lennard-Jones units). The simulated system contains 2700 atoms at a density of 0.8.

   Compute the velocity autocorrelation function from these data, and estimate the diffusivity from this. Compare your result to the following correlation in terms of pressure and temperature.

$$\log_{10} D = 0.05 + 0.07\,p - \frac{1.04 + 0.1p}{T}$$

   Optional bonus question: evaluate and plot the mean-squared displacement as a function of time, and examine the limiting (long-time) slope to estimate the diffusivity from this result. Beware of the issue in problem 3.

   Note: even though there appears to be a lot of data in the file, it really is not sufficient to obtain results with good precision, so do not worry too much if your results seem less than perfect.