Homework 2

Due in class Thursday, January 21, 2016.

Questions:

Q.1. Discuss the relative importance of speed, closeness to classical trajectories, conservation laws, and time reversibility to the choice of particular finite difference integration methods.

Q.2. Explain the basic differences between starting from a lattice vs random positions in the initial particle configurations. Elaborate on the benefits and caveats of each in a simulation.

Q.3. Explain the qualitative difference between the pair correlation function of crystals and fluids.

Q.4. Explain why it might be better to use the mean squared displacement as opposed to the velocity autocorrelation when calculating the diffusion coefficient for simple liquids.

Problems:

For the following, use the LJ code version **0.02** (only) to find solutions to the following (note that this version is slightly different from version 0.01).

P.1. Identify the line of code in file 'ensemble.cc' that implements zero total linear momentum when assigning initial velocities to particles. Indicate your find by stating the line number and by copying and pasting this line in your answer.

P.2. Identify the lines of code in file 'forces.cc' and 'base/macros.h' where the cubic periodic boundary conditions are implemented. Indicate your find by stating the line numbers and by copying and pasting these lines in your answer.

P.3. Edit 'main.cc' to print intial and final *speeds* by uncommenting the appropriate lines of code before and after the MAIN LOOP. Make sure you are running a two-dimensional system (check 'defs.h'). Compile and run the code (see the README) using 'input_P3.txt'. Plot and do a histogram of both sets of speeds (at t=0 and $t=t_{max}$). Discuss their differences. Compare your histograms with the Maxwell distribution of speeds $f(v)=4\pi\rho\left(\frac{1}{2\pi T}\right)^{d/2} v^{d-1} e^{-v^2/2T}$ by overlaying this distribution over your histogram (determine the value of *T* from the output of your simulation). *d* is the dimensionality of the system. Now, repeat in three dimensions and using 'input_P3_3D.txt'.

P.4. In class we showed how to use a random uniform distribution from [0,1] to obtain a normal distribution. (i) Reproduce these results by using Method # 1 (i.e. plot histograms of both, the uniform and normal distributions). (ii) Now, use the formula given in class (chapter 3 of notes, section 3.1) to adjust this normal distribution to a new normal distribution with average <x> = 3 and variance σ = 0.5. You may use the code in the “tests/gaussian_dist” directory for this question by:

1. editing 'main.cc' and choosing your number distribution,
2. compiling by typing 'make',
3. running and plotting the data as done in class,
4. adjusting the distribution to the new distribution and plotting.

P.5. **Graduate Students only.** Use a random uniform distribution $\{\xi_i\}$ in the range from [0,1] to obtain distributions using Method # 2 discussed in class, but now using the formula:

$$x = \sum_{i=1}^{n} \xi_i - \frac{n}{2} \quad .$$

Do normalized distributions of {x} using n = 6, 8, 10, 12, and 14. Plot all of these distributions in the same graph and overlay over them the corresponding analytical gaussian distribution function. Decide and report based on your data, which value of n approximates best the true gaussian distribution.