Homework 3
Due in class Thursday, January 28, 2016.

Questions:

Q.1. Explain the role that temperature plays when utilizing a minimizing algorithm to find minima and thus lower the energy of a starting configuration.

Q.2. (i) Explain the meaning of the first and second peaks in the pair correlation function, g(r), of a liquid. (ii) Explain the origin of the asymptotic value of g(r) as $r \rightarrow \infty$.

Q.3. Rework the line search example from section 4.1.a of the Notes "*3.Starting Up"* by first starting at point (5,4), finding all of the direction vectors, search line equations, minima along each direction, and final absolute minimum of *f(x,y).*

Problems:

For the following problems, use the LJ code (NOTE: use only version **0.09** available from BBLearn) presented in class to find solutions to the following.

Outputs of the program are contained in a subdirectory called 'results'. Output for the pair correlation function are in the file 'results/gr.dat'. For timing the execution time, you may use the Unix command 'time' as shown in class.

P.1. (i) Compute the number of nearest neighbors, or coordination number, in two dimensions for several densities by integrating g(r) as done in class. Do this by using ρ = {0.845, 0.8, 0.7, 0.6, 0.5}.

1. Make sure NDIM is 2 in 'defs.h'. Compile by typing 'make 1'.
2. Invoke the program by running: './run_me input_v09.txt.gr2D'.
3. Change densities by adjusting the *requested_particle_density* parameter in the input file.

Note in the input file that since *time_measurement* is 20 and *total_time* is 100, you will end up with 5 graphs for g(r), corresponding to different periods of time. Be careful to discard results belonging to times previous to equilibration of the system and only use equilibrated g(r) graphs.

(ii) Graph the number of nearest neighbors vs density and give an **interpretation** for your results.

P.2. (i) Repeat the above in **three dimensions** (NDIM is 3 in 'defs.h') but only for ρ = 0.845. Use 'input_v09.txt.gr3D' and note that *time_measurement* is now 10. (ii) Compare your result with the coordination number for the FCC crystal.

P.3. **Graduate Students only.** Using the numerical g(r) from the previous problem, calculate:

$$4\pi\rho \int_0^{L/2} g(r) r^2 dr \qquad (1)$$

and compare with the theoretical number of particles inside a sphere of radius L/2 and density ρ. For both cases, use the actual density used in the simulation given in the 'results/params.dat' file, the third number in that file. Also, note that L is given in the input file. Discuss the results of your comparison.