Homework 4
Due in class Thursday, February 4, 2016.

Problem:

Q.1. (i) Starting from Poisson's equation, derive the potential due to a spherically symmetric Gaussian distribution of charge,

$$\rho_i(r) = q_i \frac{\alpha^3}{\pi^{3/2}} e^{-\alpha^2 r^2} \qquad (1)$$

where α is a constant and q_i is the charge.

(ii) Discuss the limits of your expression for the potential at both, r = 0 and r → ∞.

Computer Experiment:

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

Remember that 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. Timing of Verlet lists: recompile the program for **two dimensions** (NDIM 2 in 'defs.h').

1. Run the system with 'input_v09.txt.N2' and write down the time that it took to complete. This is an L=45, ρ = 0.845 system using an N^2 force calculation (N=1711).

2. Run the same system but now using a cutoff at distance r_c=2.5 (use 'input_v09.txt.Cutoff'). Write down the execution time. Discuss the reason for the discrepancy in execution times between the N^2 and the cutoff calculation.

3. You will now run using Verlet lists fixing r_c and varying the value of r_l. The input file for this part is 'input_v09.txt.VerletLists'. Run the program for r_l from 2.6 to 4.5 in steps of 0.1, and from 4.5 to 6.5 in steps of 0.5, and obtain the execution time for each value of r_l. You do this by editing the input file, the line for *rl_cutoff*. Graph execution time vs r_l. Discuss and explain the shape and behavior of your graph.