CE 530
Molecular Simulation

Assignment #2 Due: 21 February 2017

1. Download the data file given with this problem (URL is given below - I suggest though using the one on the CE 530 site, right clicking and choosing to save it to disk). The file contains 25,000 data points from a very simple simulation (exclude the first entry in the file, which is just the number of data points). Analyze the data to estimate the average, and determine a 68% confidence limit for your result. Note that the data points are not independent. Explain your calculations. Do you need to discard any initial values (does the system need much time to "relax")? How does the choice of the block size affect your confidence limit?

   http://www.eng.buffalo.edu/~kofke/ce530/Assignments/random.dat

2. Program several implementations of the central-image algorithm for cubic periodic boundary conditions, and perform timing tests to see which implementation is fastest. You should submit at least 4 results (more are ok), varying any of the following.

   - The basic algorithm, selecting among the implementations discussed in class, and/or others you can think of that might be more efficient.
   - Use of a unit cell size, or another size of arbitrary length.
   - Origin at the cell corner (coordinates ranging from 0 to 1) or at the center of the cell (coordinates from -1/2 to +1/2).
   - Choice of programming language.
   - Choice of computing platform.

   Each test should select multiple x-values at random, ranging over at least one full periodic image on either side of (and including) the central image, and perform the central-image algorithm on each. Select enough values so that the program spends at least a few seconds of cpu on each algorithm, allowing you to get accurate timing value. Use functions that allow you to measure the cpu time programmatically (rather than by hand, with a timer).

   Prepare a table describing your results, summarizing the method for each timing value reported.

3. Construct a molecular simulations using one of the classes in the package *etomica.simulation.prototypes*. Modify the class in at least three ways (even if just to change the number of atoms being simulated), with each member of your group choosing at least one of the ways. You can set up *etomica* in *eclipse* following the instructions here: http://rheneas.eng.buffalo.edu/wiki/Source.

   Make a self-contained executable jar file following the instructions here:

   http://rheneas.eng.buffalo.edu/wiki/Runnable_JARs

   Email the jar file to me to complete the assignment.