Homework 5
Due in class Tuesday, February 16, 2016.

Problem:

Q.1. Given a bidisperse system with particle sizes σ_0 and σ_1, and depths of Lennard-Jones interactions ϵ_0 and ϵ_1 respectively, (i) derive dimensionless expressions for the inter particle <u>potentials</u> V_{00}, V_{01}, and V_{11} – involving 0-0, 0-1, and 1-1 particle interactions – as done in class. (ii) Derive also the three dimensionless <u>forces</u> between these interaction pairs to find $\ddot{r}_{00}$, $\ddot{r}_{01}$, and $\ddot{r}_{11}$. (iii) Lastly, derive dimensionless expressions for the total <u>energy</u> and <u>temperature</u> in this bidisperse system. Note that the pairwise interactions are given by $\epsilon_{00}=\epsilon_0$, $\epsilon_{11}=\epsilon_1$, $\epsilon_{01}=\sqrt{\epsilon_0\epsilon_1}$, and distances by $\sigma_{00}=\sigma_0$, $\sigma_{11}=\sigma_1$, $\sigma_{01}=(\sigma_0/2+\sigma_1/2)$. For all of the transformations, use $r\rightarrow\sigma_0 r$, $E\rightarrow E\sqrt{\epsilon_0\epsilon_1}$, and $t\rightarrow t\sqrt{m\sigma_0^2/\sqrt{\epsilon_0\epsilon_1}}$.

Computer Experiment:

<u>Event-Driven Dynamics.</u> For the following computer experiment, use the LJ code (NOTE: use version **0.09** available from the course website). For this problem:

- make sure you compile in **two** dimensions (file 'defs.h' uncomment line “#define NDIM 2”)
- build the program by typing: 'make 1'
- run it with: './run_me input_v09_pset5.txt' (this file is available from the Learn website)

P.1. Find an estimate for the density below which DMD dynamics will be faster than an equivalent MD system with t=0.005. Do this by:

1. <u>running</u> several realizations of the DMD system with different densities (at least **5 densities** lower than 0.845 by changing the first line in 'input_v09_pset5.txt'),
2. <u>capture</u> the on-screen numeric output of the run to a file (the output is a two-column list consisting of 'simulation time' and 'collision time'),
3. <u>discard</u> data before equilibration and do a histogram of collision times,
4. <u>fit</u> the histograms to a decaying exponential function to obtain the characteristic collision time for each density, similarly to the way shown in class.
5. <u>Plot</u> the characteristic collision time vs density and thus determine the density for the crossover.

NOTE: You need to present enough evidence of your work to get appropriate credit. Just a graph of collision time vs density is not enough for full credit.