Homework 6
Due in class Tuesday, February 23, 2016.

Problem:

Q.1. Derive the limiting forms of equations 66 and 67 from Chapter 2 of the Notes for the case of $\gamma\Delta t \to 0$. Do so by expanding equations 68-70. You may express your answer in terms of $\boldsymbol{v}(t)=(d\boldsymbol{r}/dt)_t$ and $\boldsymbol{a}(t)=(d^2\boldsymbol{r}/dt^2)_t$. Relate your answers to the corresponding simulation demo shown in class.

Q.2. Derive the limiting forms of $\Delta\mathbf{r}^G$ and $\Delta\mathbf{v}^G$ and equations 66 and 67 from Chapter 2 of the Notes in the limit of $\gamma\Delta t >> 1$. Describe the motion.

Q.3. Show that for $\gamma \to 0$ equations 71 and 72 from Chapter 2 of the Notes for chapter 2 for $\mathbf{r}(t+\delta t)$ and $\mathbf{v}(t+\delta t)$ reduce to the equivalent velocity Verlet finite difference equations.

Computer Experiment:

Langevin Dynamics. For the following computer experiment, use the LJ code version 0.09 and 'input_v09_pset6.txt' (both available from the Learn website).

- make sure you compile in **three** dimensions (file 'defs.h' uncomment line “#define NDIM 3”)
- recompile with: % make 1
- run it by typing: % ./run_me input_v09_pset6.txt

P.1. Run the program for γ = {5,6,7,8,9,10,12,15,20} by changing the value of the 'damping_constant' parameter in the input file. For each of these values:

1. measure average temperatures (from the 'thermo.dat' file, 3rd column),

2. calculate the diffusion coefficients (proportional to slopes of 'r2t.dat').

Present your results in a table with all of your values of γ, slopes, D, T, and T/ γ.

Plot D vs T / γ and calculate the slope.

Discuss the meaning of the slope in light of the expression given in class.

NOTE: you will get cleaner results if you average all 10 curves given in 'r2t.dat' to obtain an average curve from which to obtain each slope, as done in class.