**Homework 1**
Due in class Thursday, January 14, 2016.

**Conceptual Questions.**

Q.1. Discuss two important roles for biophysical simulations in relation to theory and experiments.

Q.2. Discuss why and how the numerical approaches to solving the equations of motion for a continuous and a discontinuous (step-wise) potentials are different.

Q.3. Give a numerical argument as to why we do not have to consider gravitational interactions between atoms when writing down the potential function of dense liquids. Express the argument in terms of distance between atoms and give a length beyond which the roles of gravity and interatomic interactions (LJ) will reverse roles. Be concrete and use real numbers.

Q.4. State whether this is an accurate statement: truncation errors arising from the number of significant digits, and round-off errors arising from the accuracy of integration algorithms are inevitable sources of error in simulations. Explain your answer.

Q.5. In class we discussed the predictor-corrector method and expressed the predicted parameters of the simulation using Taylor expansions up to the 3rd order time derivative of position. Express the predictor and corrector step up to 5th order in the position time derivative. (You may leave the $c_i$ coefficients as unknown variables).

Q.6. Show that the Verlet and velocity Verlet algorithms lead to identical trajectories.

Q.7. Another finite difference method is the Leap-Frog algorithm:

$$\begin{aligned} \mathbf{r}(t+\delta t) &= \mathbf{r}(t) + \delta t \mathbf{v}(t+\tfrac{1}{2}\delta t) \\ \mathbf{v}(t+\tfrac{1}{2}\delta t) &= \mathbf{v}(t-\tfrac{1}{2}\delta t) + \delta t \mathbf{a}(t) \end{aligned} \tag{1}$$

Derive the Leap-Frog algorithm by using Taylor expansions for **v**(t+δt/2), **v**(t-δt/2), and **r**(t+δt). In addition, derive an expression for **v**(t) in terms of the velocities at t+δt/2 and at t-δt/2.

**Computer Experiment.**

For this short problem, use the course code version **0.01** posted in learn.

P.1. Calculate the fluctuations in the total energy of simulations using the verlet integrator as a function of time step *dt* by performing the following steps.

1. Make sure you are running a 3D simulation by editing 'defs.h' and uncommenting (and commenting) the appropriate *define* lines.
2. Edit 'main.cc' and uncomment the line that outputs the system properties inside the simulation loop, *sys.output_properties(...).* Make sure that is the only uncommented output.
3. Compile your code by typing 'make'
4. Edit the input file 'input_pos.txt' and change the value of the *total_time* to 2.
5. Do a test run by typing './run_me input_pos.txt' and verifying that the program runs without

problems.

6. Now run 5 simulations, each with *delta_t* = 0.001, 0.002, 0.003, 0.004, 0.005 (change these in 'input_pos.txt') and capture their output properties. For each, graph the total energy (column #6) vs real time (column #2) and obtain the standard deviation of the energy in each case.
7. Plot these standard deviations vs time steps in a log-log plot and determine the slope of a fit.
8. Explain the value of the slope in light of the discussions in class.