Homework #1 (page 1 of 2)
Simple MD code with Velocity Verlet algorithm

Write the simplest possible one-dimensional "molecular dynamics code" for two particles connected by a spring (Force = $k(x_2-x_1-x_0)$) where $\Delta x=x_2-x_1$ is the distance between particles, x_0 is the equilibrium length of the spring. The equations of motion of the particles should be solved by the Velocity Verlet algorithm.

Your code can have the following structure:

• Define the parameters of the system (k, x_0, m_1, m_2), initial coordinates and velocities of the particles in the system (x_1^0, x_2^0, v_1^0, v_2^0), initial time = 0, time of the simulation, and timestep of integration, Δt.

• Calculate initial force $F^{init} = k(x_2^0 - x_1^0 - x_0)$

• $F^{old} = F^{init}$, $x_1^{old} = x_1^0$, $x_2^{old} = x_2^0$, $v_1^{old} = v_1^0$, $v_2^{old} = v_2^0$

• Time loop:

1. Calculate position at the current time

$$x_1^{new} = x_1^{old} + \Delta t\, v_1^{old} + \Delta t^2 F^{old}/2m_1$$
$$x_2^{new} = x_2^{old} + \Delta t\, v_2^{old} - \Delta t^2 F^{old}/2m_2$$

2. Calculate new forces

$$F^{new} = k(x_2^{new} - x_1^{new} - x_0)$$

3. Calculate new velocities

$$v_1^{new} = v_1^{old} + \Delta t(F^{old} + F^{new})/2m_1$$
$$v_2^{new} = v_2^{old} - \Delta t(F^{old} + F^{new})/2m_2$$

4. Copy new variables to old ones (actually, you do not need to store the values of x and v at two different times, you can use the same variables and write new values over the old ones at steps 1 and 3). Write coordinates and velocities to disc for further analysis.

5. Update time (New time = old time + Δt). If the current time is less than the time of the simulation, go to the time loop and repeat.

• End of the time loop and end of code

1. Attach listing of your code to your homework report.

2. Perform "MD simulation" for two particles using the code you wrote for a few (3-4) different parameters of the system (k, m_1, m_2, x_0). You can choose any set of parameters (a two-atomic molecule, a macroscopic balls with mass of 1 kg each connected by a spring, etc.). If you set $v_1^0 = v_2^0 = 0$, then make sure that $x_2^0 - x_1^0 \neq x_0$.

3. Find timestep of integration, Δt, that allows you to correctly reproduce the dynamics of the system. Provide one plot of the total energy of the system for incorrect choice of timestep and compare it with plots (from task #5 below) for the correct choice of timestep.

4. Make plots of the particle coordinates and velocities versus time for the simulations.

5. Make plots of the kinetic, potential, and total energies versus time for the simulations.

6. How do the vibrational frequency of the pair of particles and the maximum timestep that you can use depend on masses of the particles? Stiffness of the spring?

7. Calculate the vibrational frequency for one of the set of the parameters analytically and compare with the results of your simulations (optional for undergraduates).

8. Modify your code so that the equations of motion are solved by the Euler algorithm instead of the Velocity Verlet one. Repeat one of the simulations you did in #2 with the choice of timestep you made in #3 with the code implementing the Euler algorithm. Compare the particle trajectories and energy conservation obtained with the two methods of integration.