24-623 2010 HW#2

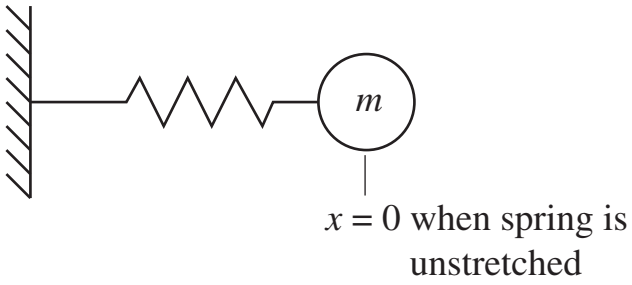
Assigned: January 18, 2010.
Due: February 3, 2010 at the beginning of class. Please use the Blackboard discussion board to ask questions of the instructor or the other students.

1. (10 points) Prove:

$$\text{(a)} \quad \frac{1}{2m_i}\frac{\partial|\mathbf{p}_i|^2}{\partial \mathbf{p}_i} = \frac{\mathbf{p}_i}{m_i}$$

$$\text{(b)} \quad \frac{\partial r_{ij}}{\partial \mathbf{r}_i} = \frac{\mathbf{r}_{ij}}{r_{ij}}$$

2. (15 points) In this problem, you will write a program to analyze the behavior of a mass-spring system and compare the results to analytical solutions. The system of interest is shown below. The variable x denotes the displacement of the mass from its equilibrium position, where the spring is unstretched. Assume that all quantities are dimensionless. Take the mass to be 1. We will consider two cases: (i) $U_s = x^2/2$ and (ii) $U_s = x^4 - 2x^2 + 1$.



(a) Using the Hamiltonian mechanics discussed in class, derive the equations of motion for the mass in terms of the spring potential energy, U_s. Present you answer as both two first-order equations and one second-order equation. Don't just write the equations down. You must show the derivation. (2 points)

(b) For case (i) (a linear spring) write down the equations of motion, and solve them analytically in terms of general initial conditions (you can solve the second-order equation if you like). Plot the position and momentum of the mass for $x(0) = 0$ and $p(0) = \sqrt{2}$ for $0 < t < 20$. Prove that energy is conserved. Why is momentum not conserved? (3 points)

(c) Write a computer program that numerically integrates the equation of motion for case (i) using the velocity Verlet scheme described in class. Explain how you chose the time step. Show that energy is conserved. Plot the results for $x(0) = 0$ and $p(0) = \sqrt{2}$ and compare them to the solution of part (b). Also plot the solution points "on top" of the potential energy function. (5 points)

(d) Using the computer program from part (d), investigate case (ii). Consider a number of different initial conditions so that you fully explore the energy surfaces for total energies of 0.25, 1, and 2. Is the time step from part (e) still valid? For each energy, include plots of the position as a function of time. Plot the solution points "on top" of the potential energy function. (5 points)

3. (25 points) In this problem, you will begin developing your MD code. Your first task is to model LJ nanoparticles. An input file for a 10-atom nanoparticle is on Blackboard. Start by developing a code that

- works in dimensionless LJ variables
- reads in the initial positions from an input file
- initializes the particle momenta
- integrates the equations of motion in three dimensions using the velocity Verlet scheme (use a dimensionless time step of 0.002)
- calculates force and potential energy using the LJ potential
- calculates kinetic energy
- generates data that can be visualized using Chime

In addition to submitting your code electronically, provide plots, written explanations, etc., showing the following for the 10-atom nanoparticle:

- time variation of kinetic, potential, and total energy (which should be conserved)
- conservation of momentum in the x, y, and z directions

Note: You do not need to give the system any initial momenta for the atoms to start moving. The center of mass of the nanoparticle should not move if the equations of motion have been properly implemented. Make your code as general as possible (e.g., it should work for an arbitrary number of atoms). *Do not do anything with cutoffs or periodic boundary conditions.*

BONUS (15 points)

(i) Generate input files for nanoparticles with $2 \leq N \leq 9$.

(ii) By writing the equations of motion as

$$\begin{aligned} \dot{\mathbf{r}}_i &= \frac{\mathbf{p}_i}{m_i} \\ \dot{\mathbf{p}}_i &= \mathbf{F}_i - \eta \mathbf{p}_i, \end{aligned}$$

and taking η to be a constant, positive number we can slowly remove kinetic energy from the system (i.e, a quench). In the Verlet scheme, the integration for the x-direction will proceed as:

$$\begin{aligned} &1.\, p_{i,x}(t + \Delta t/2) = p_{i,x}(t) + [F_{i,x}(t) - \eta p_{i,x}(t)]\Delta t/2 \\ &2.\, r_{i,x}(t + \Delta t) = r_{i,x}(t) + p_{i,x}(t + \Delta t/2)\Delta t/m_i \\ &3.\, p_{i,x}(t + \Delta t) = [p_{i,x}(t + \Delta t/2) + F_{i,x}(t + \Delta t)\Delta t/2]/(1 + \eta \Delta t/2) \end{aligned}$$

Implement this scheme in your MD code. Quench the structures you developed in part (i) to find their minimum energies. Plot the energy per atom in the relaxed structures as a function of N. Try different initial structures for a few values of N. Are their multiple minima? How does your choice of η affect the results? The dimensionless energy of the atoms at zero temperature in the bulk fcc crystal is -7.46. How do your values compare to this value?