24-623/12-623 2017 HW#2

Total points: 50
Assigned: September 13, 2017.
Due: September 28, 2017, midnight to Canvas. Please use the Canvas discussion board to ask questions of the instructor, the CA, or the other students.

1. (a) (7 points) Prove:

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

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

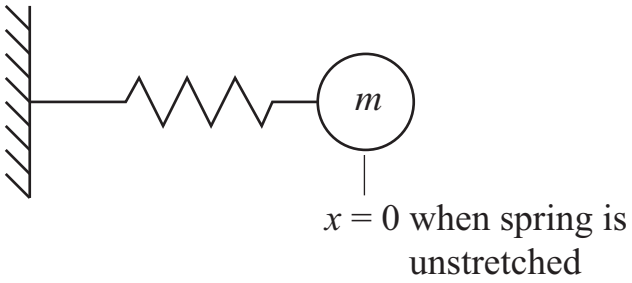
(iii) The Hamiltonian equations of motion conserve the total system momentum.

(b) (3 points) The velocity Verlet algorithm for particle i in the x direction is

1. $v_{i,x}(t + \Delta t/2) = v_{i,x}(t) + F_{i,x}(t)\Delta t/(2m_i)$
2. $r_{i,x}(t + \Delta t) = r_{i,x}(t) + v_{i,x}(t + \Delta t/2)\Delta t$
3. $v_{i,x}(t + \Delta t) = v_{i,x}(t + \Delta t/2) + F_{i,x}(t + \Delta t)\Delta t/(2m_i)$

In class, we derived the first two steps. Now, derive the third step.

2. (20 points total) 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. You will consider two cases: (i) $U_s = x^2/2$ and (ii) $U_s = x^4 - 2x^2 + 1$.



(a) (2 points) 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 as one second-order equation. Don't just write the equations down. You must show the derivation.

(b) (4 points) For case (i) (a linear spring) write down the equations of motion and solve them analytically in terms of the general initial conditions $x(0) = x_0$ and $v(0) = v_0$ (you can solve the second-order equation if you like). Plot the position and velocity of the mass for $x_0 = 0$ and $v_0 = \sqrt{2}$ for $0 \leq t \leq 20$. Prove that energy is conserved. Why is momentum not conserved?

(c) (7 points) 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 $v_0 = \sqrt{2}$ and compare them to the solution of part (b). Plot the solution position and velocity points as a constant energy manifold.

(d) (7 points) Using the computer program from part (c), investigate case (ii) for $0 \leq t \leq 20$. 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 (c) still valid? For each energy, include plots of the position as a function of time. Plot the potential energy function versus position. On the same graph, plot your solution points for each total energy so that they lie on the potential energy function. Plot the solution position and velocity points for each total energy as constant energy manifolds on the same graph.

3. (20 points) In this problem, you will begin developing your MD code. Your first task is to model a Lennard-Jones (LJ) nanoparticle. An input file for a 10-atom nanoparticle (10.txt) is in the HW#2 folder on Blackboard. The coordinates in this file are dimensionless. Start by writing a code that

- Works in dimensionless LJ units
- Reads in the initial positions from an input file
- Initializes the particle velocities to zero
- Integrates the equations of motion in three dimensions using the velocity Verlet scheme and 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 VMD

In addition to submitting your code electronically, provide plots, written explanations, etc., showing the following for the 10-atom nanoparticle for $0 \leq t \leq 2$:

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

Also include a snapshot of the nanoparticle from VMD. Note: The center of mass of the nanoparticle will 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 (10 points)

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

(ii) By writing the equations of motion as

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

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:

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

Implement this scheme in your MD code. Quench the structures you developed in part (i) to find their minimum energies. Plot the potential 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 potential energy of each atom at zero temperature in the bulk fcc crystal is -7.46. How do your values compare to this value?