Homework Assignment 1

Due @ 11:59pm Monday 23th February by email serdal@nyu.edu or to ERB 114

🐍 **This sign means python or any kind of scientific computing is needed to get the answer. Please provide your answer with your python code.**

1. A classical liquid of *N* molecules of Oxygen and *N* molecules of Chlorine molecules are in a closed container. Each interacting with the rest with a pairwise Lennard-Jones potential which is given as:

$$V^{LJ}(r_{ij}) = 4\varepsilon_{ij}((\sigma_{ij}/r_{ij})^{12} - (\sigma_{ij}/r_{ij})^6)$$

where *i* and *j* are particle indices and r_{ij} is the distance in between, (ε, σ) are van der Waals parameters that accounts for the polarizability of the particle and effective size respectively. When two different type of particles interact their (ε, σ) is computed by Lorents-Bertholet mixing rule. To compute the (ε, σ) parameter for particle *i* and *j* of different kind we use the following relations:

$$\sigma_{ij} = \frac{1}{2}[\sigma_i + \sigma_j] \quad \text{and} \quad \varepsilon_{ij} = [\varepsilon_i \varepsilon_j]^{1/2}.$$

	ε / k_B	$\sigma (nm)$
Oxygen	61.6	0.295
Chlorine	173.5	0.335

Table1. van der Walls parameters of oxygen and chlorine molecules, epsilon is in units of Boltzmann constant.

a. Plot the potential energy as a function of distance (2.85<r<10 angstrom) between two oxygen molecules, two chlorine 🐍 molecules and one oxygen and one chlorine using the values in table 1. Discuss the difference between the three.

b. Find the point where V^{LJ} is at minimum for oxygen analytically and compute the force at that point for oxygen-oxygen Lennard-Jones interaction.

c. Write down the Newtons' equation of motion explicitly for one oxygen molecule due to the 2*N*-1 molecules of oxygen and chlorine.

d. The positions of atoms for *N*=100 particles is given in the file "O2Cl2.txt". Calculate the total force on particle 7 and 25. Please provide your answer with your python code. 🐍

e. Assuming that each force calculations for one pairwise interaction is six floating point operation. How long does it take to compute the forces for $N=10^{23}$ particles if all BuTinah supercomputer is allocated for your research. How long would it take if you have only 10^4 particles? Please as a unit of time use days.

2. The potential energy of a particle in a single well is given as $U_0(x^2-2)$ where, the strength of the potential is $U_0=2.0$, m=1. Everything is dimensionless so don't worry about the units.

   a. Show that the equations of motion for the particle by using Newton's second Law for a general x_0 and v_0 is $x(t)=x_0\cos\omega t+(v_0/\omega)\sin\omega t$ where $\omega^2=(U_0/m)$ and also derive the equation for $p(t)$. (Hint. Find the general solution of $\dfrac{d^2x}{dt^2}=-\omega^2x$ you will have two initial conditions to satisfy)

   b. Numerical solution of ordinary differential equations is achieved by finite difference methods. The idea is using the information at an earlier step $x(0),p(0)$ to solve the equations at a later time step Δt and obtain $x(\Delta t),p(\Delta t)$. Here Δt must be a very small number to get a correct solution. If you need the positions at time t then you need to repeat the calculation for $n=t/\Delta t$ times to get the answer. Using Taylor series expansion one can write

   $$x(t+\Delta t)=x(t)+\Delta tv(t)+\frac{1}{2}\Delta t^2a(t)+\frac{1}{6}\Delta t^3b(t)+....$$

   if we truncate the function after the second order in Δt then the numerical errors will be in the order of $\approx O(\Delta t^2)$. Write a code and compute the position at $x(\Delta t)$ each of the time steps $\Delta t=\{10^{-4}, 10^{-3}, 10^{-2}, 10^{-1}, 1\}$. Compare your result with the exact result by $Error(\Delta t)=\dfrac{x(\Delta t)^{SIM}-x(\Delta t)^{EXACT}}{\Delta t^2}$. Plot Error versus Δt. Do you see a linear dependence? As initial conditions use p(0)=2, x(0)=0.

   c. Repeat the same calculation for a widely used algorithm in molecular dynamics simulations called velocity Verlet and compare your result for $\Delta t=\{10^{-4}, 10^{-3}, 10^{-2}, 10^{-1}, 1\}$ with the exact solution just like as in b.

$$x(\Delta t) = x(0) + \Delta t \frac{p(0)}{m} + \frac{\Delta t^2}{2m} F(x(0))$$

$$p(\Delta t) = p(0) + \frac{\Delta t}{2}[F(x(0)) + F(x(\Delta t))]$$

d. Repeat velocity Verlet algorithm for n=1000 steps every time using the position and momentum from the one previous step as your initial phase space points and plot Hamiltonian as a function of time. Repeat this for step sizes $\Delta t = \{10^{-4}, 10^{-3}, 10^{-2}, 10^{-1}\}$. Also plot $\frac{\delta H}{\partial t}$ (t) versus time for each time step sizes. What is the optimum step size to use? And explain why? (hint: to compute $\frac{\delta H}{\partial t}$ you can use the finite difference :

$\frac{\delta H}{\partial t} \cong \frac{H(t + \Delta t) - H(t)}{\Delta t}$). Plot them to the same graph with different colors and label x and y axis accordingly.

e. Using the phase space points recorded for initial condition p(0)=2 and x(0)=0 plot the accessible phase space during your numerical simulations of *n*=10000 steps. Repeat the same for another initial conditions, p(0)=4 and x(0)=1. Are they the same? Plot them to the same graph with different colors and label the x and y axis accordingly.