Course - CVL867
Assignment 3 Solutions
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Units: **Note: Absolute units are ignored for quantities such as energy, velocity, position, etc. They are perceived in a relative sense to understand what is happening in step wise dynamics of system.**

Code:

0.1 Description of code:

a) utils/lj_pot.py — functions to compute pairwise lj potential, total lj potential and gradient of lj potential.

b) utils/gradient_descent.py — function executing gradient descent to solve minimization ploblem.

c) utils/utils_.py — contains utility functions for - plotting, velocity-verlet, gaussian to sample initial velocity, total kinetic energy and saving trajectory for ovito

d) main.py — executes the entire assignment.

0.2 How to run the code:

Just run python main.py

1 Write a function to calculate the potential energy between two particles interacting via Lennard jones potential given by following equation.

- see file utils/lj_pot.py - function: lj_potential(r, eps, sigma)

2 Using the above function write a function to calculate potential energy of the complete system taking into consideration the periodic boundaries and atom type information. Test the function on the following system, the configuration for which is provided.

- see file utils/lj_pot.py - function: total_lj_potential(positions, species, box_length, eps_AA, eps_AB, eps_BB, sigma_AA, sigma_AB, sigma_BB, rc)

- Energy: -798

3 Write a program to perform energy minimization. Use any energy minimization algorithm discussed in class. You can also use functions from any standard optimization libraries.

- see file utils/gradient_descent.py

Please see plots is figure 1 which emphasises the point of step size.

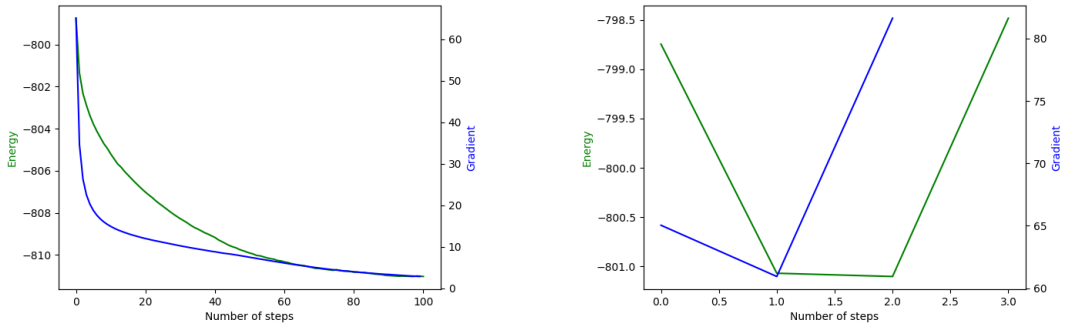

Figure 1: Gradient above means norm of the gradient. For step size 0.001 and 0.002, higher step-size(0.002) diverges quickly in just 3 steps here

4 Write a function to assign velocities to the particles corresponding to a given temperature using gaussian distribution. Use this function to assign velocities corresponding to a temperature of T=2.0 to the given LJ configuration.

- see file utils/utils_.py - function assign_velocities

Please see figure 2: distribution of sampled velocities.

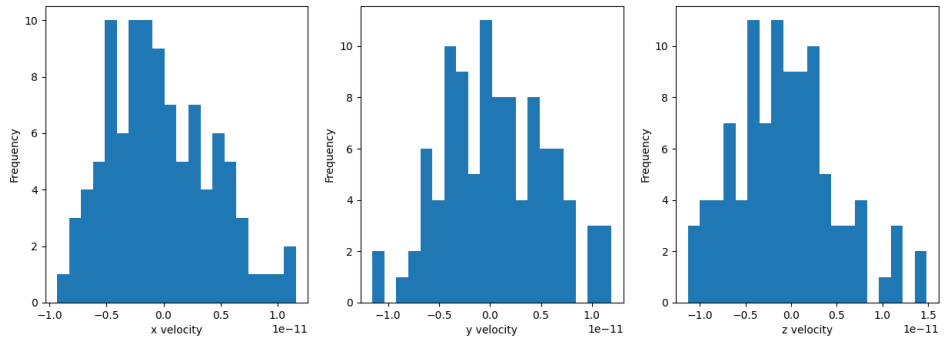

Figure 2: Velocity histogram

5 Write a function to calculate force and acceleration on each particle for the given LJ interaction and perform one step of NVE simulation, using velocity-verlet algorithm.

- see file utils/util_.py - function: velocity_verlet(pos, vel, species, box_length, eps_AA, eps_AB, eps_BB, sigma_AA, sigma_AB, sigma_BB, dt, rc):

6 Using above function generate a trajectory of 1000 steps, with timestep=0.003. Save it as a numpy array.

- see file main.py - attached file in submission trajectory.npy

trajectory.npy - shape is 1000*100*7, 1000: nsteps, 100: natoms, 7: pos in xyz, vel in xyz and atom type [**0 or 1**].

Please see figure 3: total energy is held constant while gradient descent(Q3) was not energy conserving.

7 Bonus: Write a function to save the trajectory in Ovito

- see file utils/utils_.py - function save_xyz_trajectory(trajectory, filename)

Contained a gif file in submission

Please see figure 4: a snapshot of system.

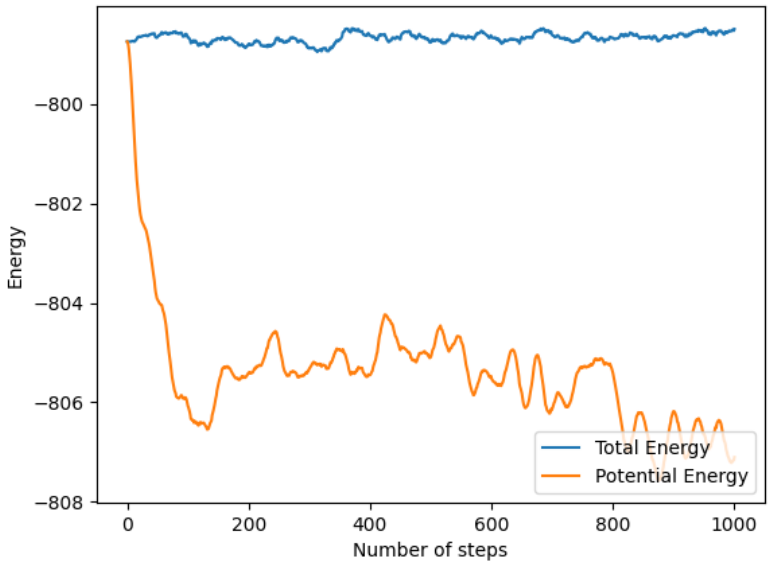

Figure 3: Energy vs steps in NVE ensemble

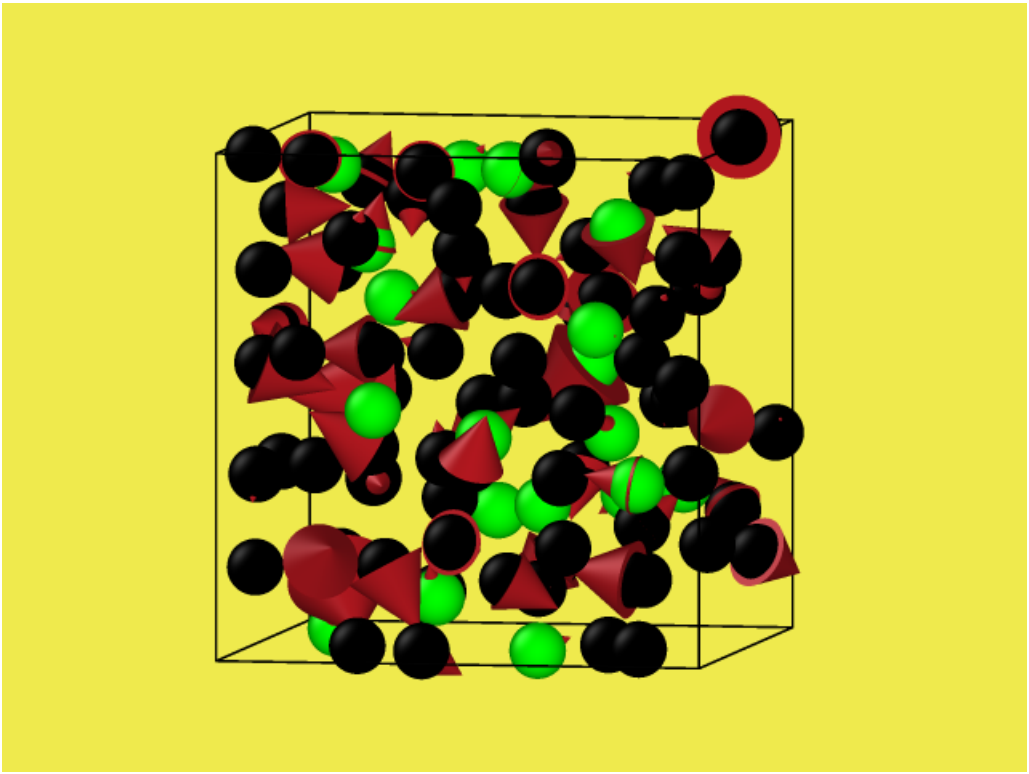

Figure 4: Screenshot of the video, black: A atoms, green: B atoms, red arrow: velocity (size of arrow) and direction representing velocity direction Note: the particle radius has been rescaled in ovito for better visualization.