Molecular dynamics simulation with Lennard-Jones potential and Verlet algorithom

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Programming Language: Python
Version: 3.10

1 Theory

Molecular dynamic simulation is a classical many-body problem where the position and momentum of a particle can be calculated simultaneously. As all particles behave deterministically, we can simulate them in a computer using the necessary algorithms.

Lennard-Jones potential: The Lennard-Jones potential is an intermolecular pair potential. Out of all the intermolecular potentials, the Lennard-Jones potential is the one that has been the most extensively studied. It is considered an archetype model for simple yet realistic intermolecular interactions. The Lennard-Jones potential models soft repulsive and attractive interactions. Hence, the Lennard-Jones potential describes electronically neutral atoms or molecules. It is named after John Lennard-Jones. The commonly used expression for the Lennard-Jones potential is,

$$U(r) = 4\epsilon \left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6} \right]$$

Where, ϵ and σ are constants, depends on molecule. Now if we put $4\epsilon\sigma^{12} = A$ and $4\epsilon\sigma^{6} = B$ then equation become,

$$U(r) = \frac{A}{r^{12}} - \frac{B}{r^{6}}$$

$$\therefore f_x = -\frac{\partial U}{\partial x} = x\left(\frac{12A}{r^{14}} - \frac{6B}{r^{8}}\right)$$

$$\therefore f_y = -\frac{\partial U}{\partial y} = y\left(\frac{12A}{r^{14}} - \frac{6B}{r^{8}}\right)$$

$$\therefore f_z = -\frac{\partial U}{\partial z} = z\left(\frac{12A}{r^{14}} - \frac{6B}{r^{8}}\right)$$

Where, f_x, f_y, f_z are components of force.

Algorithm:-

1. Generate random uniform distribution of array of 500×3 within range which is position matrix of particles. Where each row representing different particles and column 0,1,2 are representing x, y, z coordinates of particles.

2. Do the same for velocity coordinates of particles.

3. Determine the distance matrix(r_{ij}) of the position matrix.

   Note: In mathematics, computer science and especially graph theory, a distance matrix is a square matrix (two-dimensional array) containing the distances, taken pairwise, between the elements of a set.

4. Calculate $1/r_{ij}$ of each element of the distance matrix and remove divide by zero using necessary code.

5. Calculate f_x, f_y, f_z using formula given above and sum row wise to get total force by all particles.

   Note: After this operation we will get a force array of shape 500×3. Which can be used easily to update position and velocity arrays(or matrix).

6. Update position and velocity arrays by Verlet approximation method which telles,

$$r_{i+1} = r_i + v_i dt + \frac{1}{2}\frac{f_i}{m}dt^2$$

$$v_{i+1} = v_i + \frac{1}{2}\left(\frac{f_i + f_{i+1}}{m}\right)dt$$

7. Repeat 3 to 6 several times to achieve equilibrium.