Project Report

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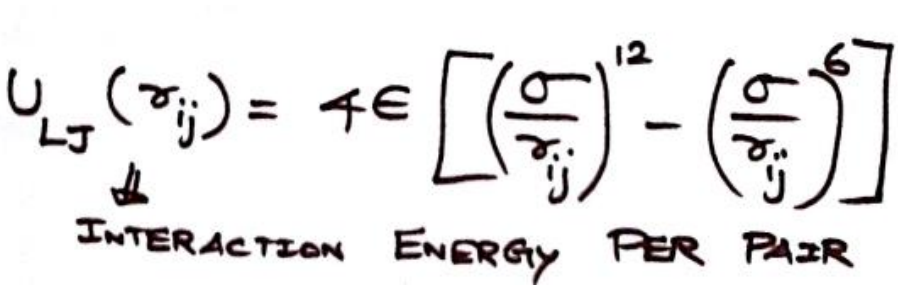
Answer 1

For this question I have generated the random configuration using the random restart approach. In this the code generates random coordinate within the bounds of the box and if the new coordinate is at a minimum distance of sigma, then the coordinate is accepted and added to the configuration. If at any time we are unable to add a new coordinate in the configuration for 10000 trials (attempts), we delete the entire previous configuration and start from new. This is because it is possible that during the initial creation of the configuration, we might generate sparse coordinates with distance > sigma but less than 2 * sigma (closer to this bound), which makes adding new coordinates in between these two points not possible and thus we discard the whole configuration and start fresh.

Answer 2

To calculate the potential energy of the system, we must calculate the potential energy between all the possible pairs of molecules and add these energies together. To calculate the potential energy between the two molecules, we must calculate the distance between those two molecules using Periodic Boundary Conditions I.e., the start, and end of the box are joined together. This distance is plugged into the potential energy function to find the energy between two molecules.



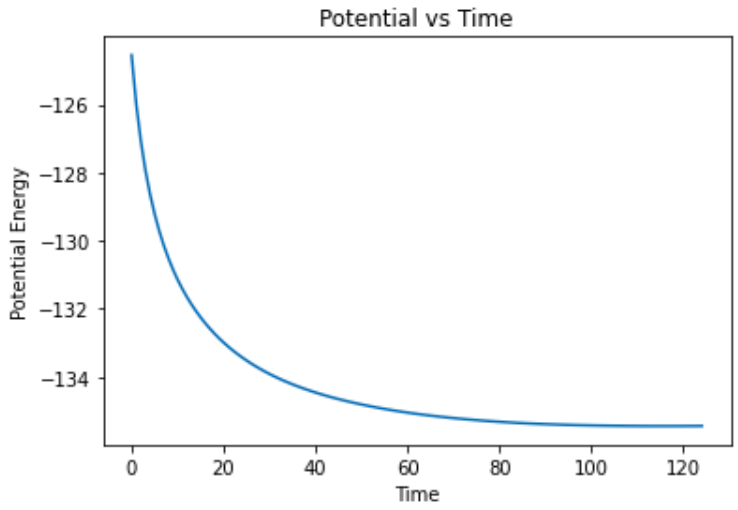
Finally, we must sum all these energies up over all possible pairs of molecules.

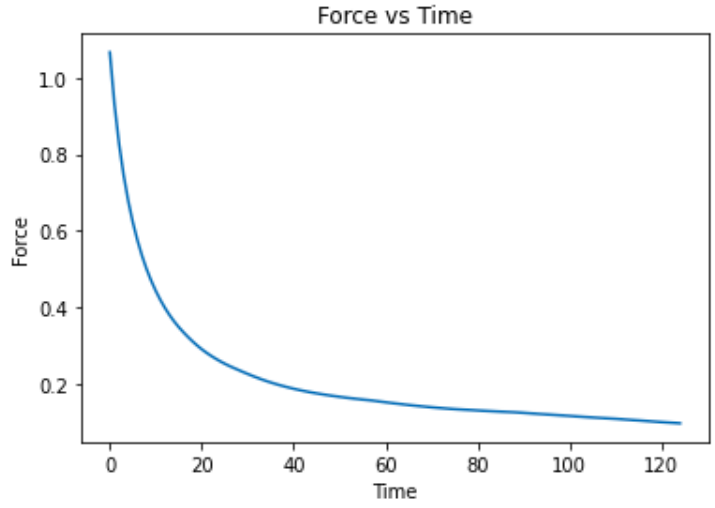
```
config = read_config('config.xyz')
potential_energy(config)
```

```
-124.54543403057832
```

Answer 3

To find the minimum energy U, we try to change the configuration at each timestep by slightly moving the molecules in the configuration according to the resultant force applied on the molecule by all the other molecules in the configuration. For example, for molecule 1 we consider the force exerted on this molecule by all the other 107 molecules and find the resultant direction of the net force. After finding this, we displace particle 1 slightly in this direction according to the magnitude of this force. This process is done simultaneously for all the molecules. This process is repeated for 125 iterations to reach the minimum potential energy or until the net magnitude of movement / force becomes less than a certain threshold (0.01). This approach is since as we move the particles away from each other, we reduce the force acting between the particles and thus the configuration approaches to a more stable configuration and the net potential energy of the system also decreases with time.





Answer 4

In this to first find the hessian matrix we must find the double derivatives of the potential energy function of the net system with the 3 * N (N = 108, x y & z coordinate of each molecule) independent variables of the system. Thus, the hessian matrix would be of size 3 * N × 3 * N. To fine the double derivative of such a function we go to the roots of derivative. We displace the configuration by a small factor h in the positive and negative direction for each independent variable and then calculate the potential energy of the new system. This is also done for each pair of the independent variables in which we slightly displace two

independent variables in the +h and -h direction and then again calculate the potential energy of the new system. Finding all these energies is highly time intensive and computationally very expensive so we parallelize this process by using multiprocessing which considerably speeds up the process. After finding all these energies we calculate the elements of the hessian matrix. The diagonal elements of the hessian matrix are given by d^2U/dx_i^2, x_i is the i^{th} independent variable and thus the value of diagonal element is given by:

$$\frac{\mathrm{d}^2 f}{\mathrm{d}x^2} \approx \frac{f(x+h) - 2f(x) + f(x-h)}{h^2}$$

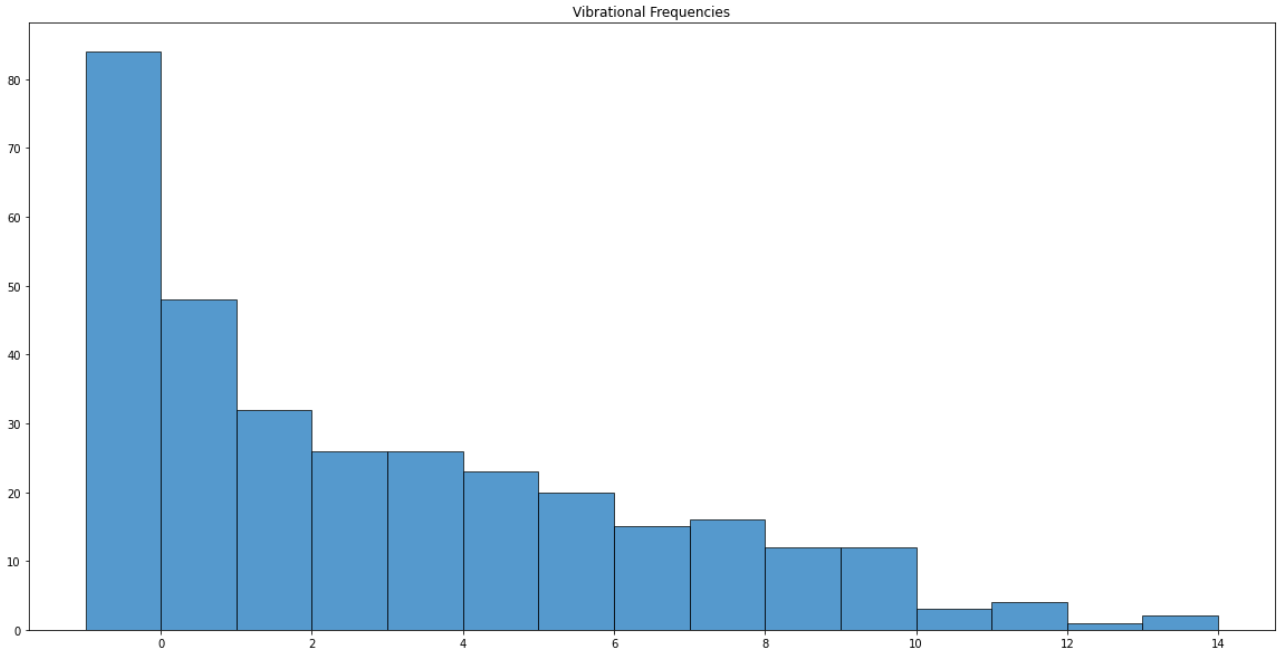
Similarly, the non-diagonal elements of the hessian are symmetric and finding only one triangular half is sufficient. To find d^2U/dx_ix_j, x_i and x_j are the i^{th} and j^{th} independent variables respectively, we use the formula:

$$f_{xy}(x,y) \approx \frac{f(x+h,y+k) - f(x+h,y) - f(x,y+k) + 2f(x,y) - f(x-h,y) - f(x,y-k) + f(x-h,y-k)}{2hk},$$

This gives us the final hessian matrix.

Answer 5

After calculating the final hessian matrix, we must find its Eigen values which are the vibrational frequencies of the system. These Eigen values are then plotted on a histogram with appropriate bin size and the resultant graph is obtained.


Vibrational Frequencies
0
10
20
30
40
50
60
70
80
0
2
4
6
8
10
12
14