Report - Project

The generated configuration is stored in the file `initial.xyz` and the minimized energy configuration is stored in `minConfig.xyz`. The configuration was created by generating random points and checking whether they satisfy the minimum distance requirement of 3.4 angstroms from all other particles.

The initial energy of the configuration was calculated using the following formula:

$\sum_{i=1}^{N} \sum_{j=i+1}^{N} 4\epsilon[(\frac{\sigma}{r_{ij}})^{12} - (\frac{\sigma}{r_{ij}})^{6}]$

```
Potential energy of the initial configuration: -124.65301605762043
```

To minimize the energy, I simply used a brute force method by changing the positions by small amounts, checking if it remains valid and setting the current state to the new state if it has less energy.

```
Minimized energy: -148.533255072374
```

To hessian matrix was calculated by numerical differentiation and all three coordinates of each particle were considered as individual variables. To calculate the eigenvalues and eigenvectors, I used the numpy implementation, and these values were written to the file `hessian_eigen.json`.

To calculate an arbitrary hessian entry,

$\frac{\partial^2 f}{\partial x \partial y} = \frac{U(x+h,y+k) - U(x+h,y-k) + U(x-h,y+k) - U(x-h,y-k)}{4hk}$

if $x = y$,

$\frac{\partial^2 f}{\partial x^2} = \frac{U(x+h) - 2U(x) + U(x)}{hk}$

Frequency histogram:

To plot the frequency histogram, the eigenvalues obtained from the hessian matrix were used.

$C = |eig|^{\frac{1}{2}}$ where C is the constant of vibrational frequencies. These constants were then binned and then ploted as a histogram, which is roughly normal as expected.