Normal-Mode-Analysis

Science-2 Project Part A for Analysing the Normal Modes of an Argon System of 108 atoms following the Lennard Jones Potential. The code generates a initial random configuration of 108 atoms based on the given conditions, implements Periodic Boundary Conditions, Reduces the system of the random configuration using the Steepest Descent Algorithm for minimisation, then it generates a Hessian Matrix , and the eigen values and eigen vectors for it. It also plots a histogram of the frequencies. All Questions (5 of them) given as the project has been solved. A detailed report is included with theory and implementation details as Report.pdf.

Running the Code

python3 main.py

The code takes some time to run. This is because of many computations required for the project and python is very slow in such cases. The **get energy** method takes in a geom and gives the TotalEnergy of the system following the Lennard Jones Potential. FrequenciesClass is responsible for normal modecalculation from Hassien Matrix, and given molecular structure. Further calculation is done by using a type of generalised Gradient Descend Algorithm to calculate minimum energy configuration. Hessian class which is responsible for Hassian Matrix calculation, eigen values and eigen vectors.The code uses the Finite Differences Method for Partial derivatives which

have been explained in the Report.

Directory Structure

Following is the directory and code structure

eigen_values.dat- The eigen values for the submission

eigen_vectors.dat- eigen_vectors corresposing to these

hessian.dat- The hessian matrix as part of the submission

hist.png- The histogram as part of submission

init.png- The VMD Visualisation of the initial random configuration

modes.xyz- The final normal modes of the system after all calculations in the xyz format. Theformat is decribed in report.

molecule.xyz- The initial random configuration in the xyz format

new_molecule.xyz- The new molecule configuration after minimising the energy using thesteepest descent algorithm in the xyz format.

new.png- The VMD Output for the minimised configuration