Science-2 Project Part A

Lennard Jones Argon Atom-Normal Analysis

- Ayush Sharma
- 2019101004

Table of Content:

Intro

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.

This project accounts for analysing Normal mode of an Argon system of 108 atoms. The project implements the following things:-

- Random initial configuration generation.
- Calculating `LJ Potential` of the generated System.
- Finding minimum energy configuration of generated system (Using Steepest Descent Algorithm)
- Hessian Matrix calculation with Eigen vectors & Eigen values
- Plotting Vibrational Frequencies

For detailed report refer `Report.pdf`

Requirements & code Execution & File structure

Requirements :

```
numpy
matplotlib
tqdm
autograd
multiprocessing
functools
```

Code Execution :

Note: Move to `codes` folder before executing any command.

For each part of the project (total 5), a file has been written (nammed for same) with one other `configuration.py` file.

Part	Execute command	Files Required	Output
1	python3 q1.py	`q1.py`, `configuration.py`	File `init_conf.xyz`

2	python3 q2.py	`q2.py`, `configuration.py`, `init_conf.xyz`	Prints LJ Potential
3	python3 q3.py	`q3.py`, `configuration.py`, `init_conf.xyz`	File `gradient_descent_log.txt`, `final_conf.xyz`
4	python3 q4.py	`q4.py`, `configuration.py`, `final_conf.xyz`	File `hessian.dat`, `eigen_value.dat`, `eigen_vectors.dat`
5	python3 q5.py	`q5.py`, `hessian.dat`	Image for Histogram for vibrational Frequency and File `modes.xyz`

File Structure :

```
├── codes
│   ├── checker_files.py
│   ├── configuration.py
│   ├── outputs
│   │   ├── eigen_values.dat
│   │   ├── eigen_vectors.dat
│   │   ├── final_conf.xyz
│   │   ├── gradient_descent_log.txt
│   │   ├── hessian.dat
│   │   ├── init_conf.xyz
│   │   ├── modes.xyz
│   │   └── vibration_frequency.png
│   ├── q1.py
│   ├── q2.py
│   ├── q3.py
│   ├── q4.py
│   └── q5.py
├── README.md
├── README.pdf
├── Report.pdf
└── Requirements.txt
```

Outputs :

Following is the explanation of what each output contains:-

- `outputs` : This folder contains all files for project submission.
  - `init_conf.xyz` - The initial random configuration in the xyz format.
  - `gradient_descent_log.txt` - Total potenial log while doing potential/energy minization of initial configuration using the steepest descent algorithm.
  - `final_conf.xyz` - The final molecule configuration after minimisation.
  - `eigen_values.dat` - The eigen values for the submission.
  - `eigen_vectors.dat` - The eigen_vectors corresponding to these.
  - `hessian.dat` - The hessian matrix as part of the submission
  - `modes.xyz` - The final normal modes of the system after all calculations in the xyz format. The format is decribed in report.
  - `vibration_frequency.png` - The histogram as part of submission