# Science-2 Project Part A

# **Lennard Jones Argon Atom-Normal Analysis**

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### 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:**

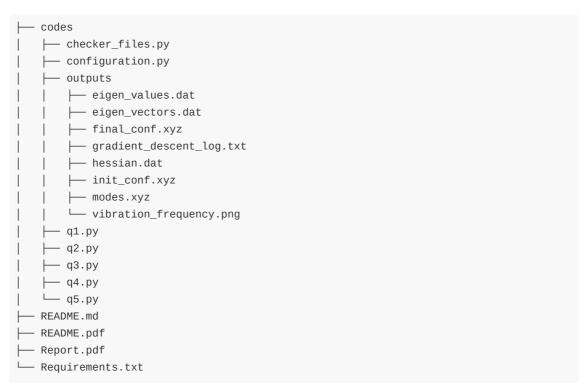
Note: Move to codes folder before executing any command.

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	<pre>q2.py, configuration.py, init_conf.xyz</pre>	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:



### 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