

PSCM - Final Project

[Documentation](#)

Install requirements.txt

Use following command:

```
pip3 install requirements.txt
```

Automated Script Instruction for 300 ITERATIONS

Run the following command:

```
python3 main.py
```

then you will be prompted by a command line interface, type "run" i.e.

```
>> run
```

This will execute the complete code for ITERATIONS = 300, while for the van hove plot as it takes time to generate van_hove correlation values, the code uses backup file (generated before).

Technologies Used

Language: Python

Modules: numpy, matplotlib, pickle, copy, tqdm

Description

Following steps are implemented:

1. Initially 108 Argon atoms are generated randomly such that length of the box is 18 Angstrom
 2. Potential Energy is minimized using gradient descent.
 3. Initial velocities are sampled using Maxwell-Boltzman distribution with T = 300 Kelvin
 4. Trajectory is generated for ITERATIONS = 300
 5. Following plots are plotted:
 - Mean Square Displacement Plot
 - Van Hove Correlation
 - Velocity Correlation
 - Dynamic Structure Factor
 - Distance Frequency Graph
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Features

1. Command Line Interface
 2. The frames once generated for X number of iterations is saved as a file "frames_{ITERATIONS}.pkl"
 3. Van hove correlation matrix can also be saved as a file "vanhove_{ITERATIONS}.pkl"
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Instructions

Instructions to execute the program:

```
> python3 main.py
```

After this a command line interface will be available, showing this

```
>> help
```

Execute "help" function for the functions which can be called in the program.

HELP

The following functions are available for command line interface.

```
ls ---->          |Print the pkl file names in the current directory
gen ITERATIONS ----> |Generate ITERATIONS and save in file
load INPUT_FILE ----> |Provide Input File
load vanhove INPUT_FILE |Provide Input File
plot msd ---->       |Plot Mean Square Displacement
plot vanhove ---->    |Plot Van Hove Correlation
plot vel ---->        |Plot Velocity Correlation
plot df ---->         |Plot Dynamic Factor
exit ---->           |EXIT
```

Constants

```
N = 108 # Number of atoms
LEN = 18e-10 # Angstrom
EPSILON = 1.66e-21 # 0.238 kcal/mol
SIGMA = 3.4e-10 # Angstrom
MIN_DIST = 3.4e-10 # Angstrom

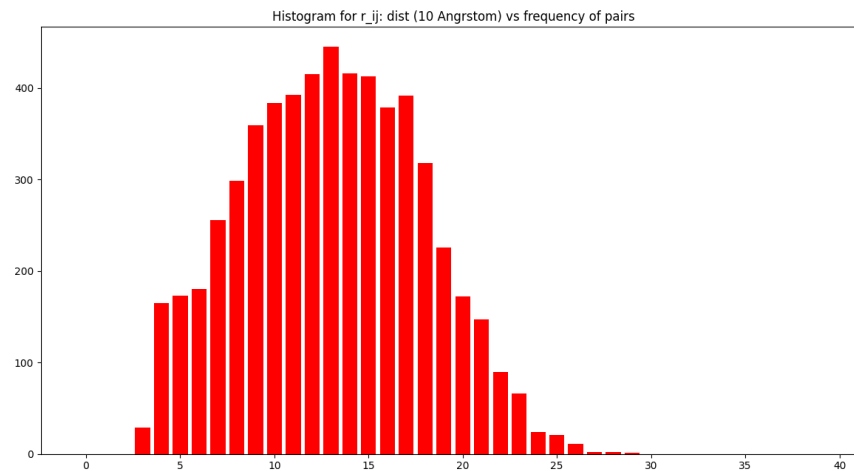
# For gradient descent
DELTA = 0.01 # energy difference to break gradient descent
ETA = 0.1 # learning rate

# For trajectory generation
ITERATIONS = 300 # can be taken as an input too
TIME_STEP = 4e-15 # 4 femto seconds
MASS = 6.63359936e-26 # mass of Argon (in Kg)

#For Sampling velocities
K = 1.38e-10 # Boltzman Constant
TEMP = 300 # Temperature = 300 Kelvin
```

Sample Plots for 300 ITERATIONS & Inferences

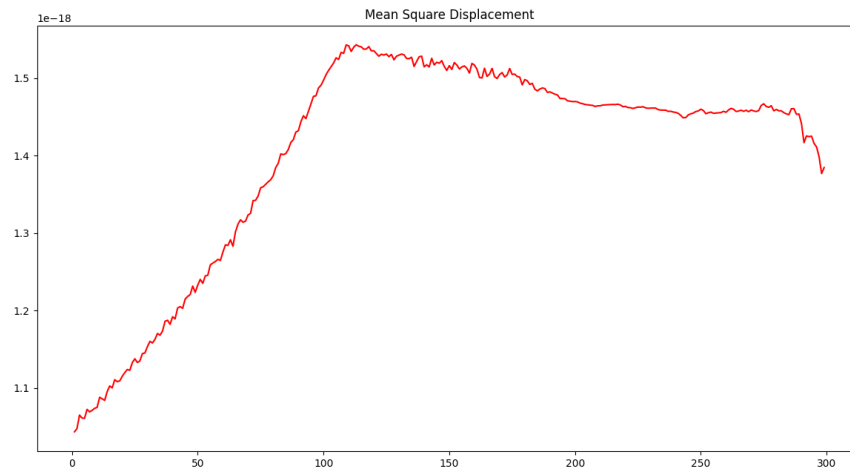
Pair Distance Bar Graph



As the minimum distance was given to be 3.4 Angstrom, hence it can be seen in the graph that there is no pair of atoms with distance less than 3.4 Angstrom.

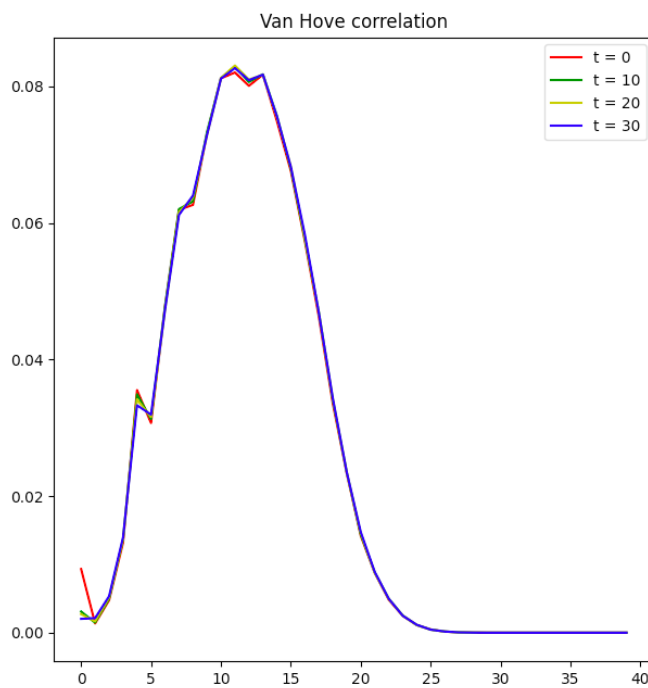
For this graph, the distances were rounded off to the nearest integer. Also, it can be seen that the curve is somewhat follows ~gaussian distribution. This can be due to the random sampling for 108 atoms, and central limit theorem.

Mean Square Displacement



It can be seen that, MSD value increases as time-difference gap increases initially as a quadratic relation. And then it seems to drop a bit which can be due to application of periodic-boundary conditions. As 1st kind of periodic boundary conditions is used, i.e. if the atom moves left to the box, another atom comes from the right.

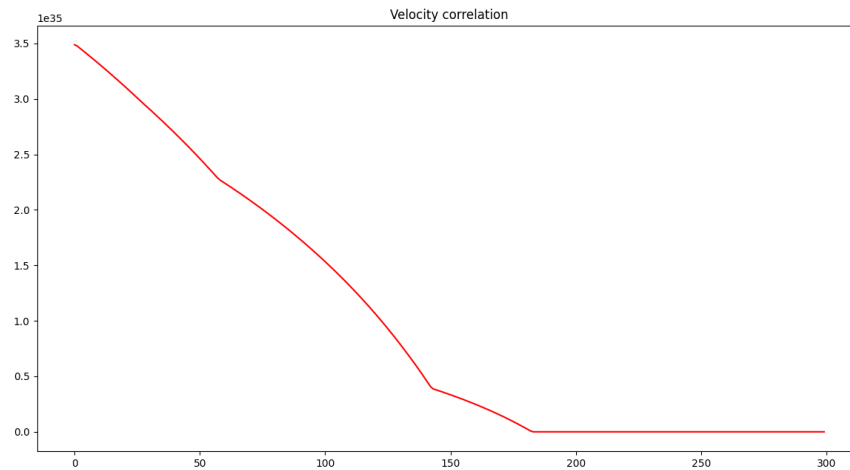
Van Hove Correlation



This can be seen to be in line with the Van Hove Correlation function graphs available online, and it follows some kind of ~maxwell distribution i.e. increases first and then after reaching a peak decreases.

For all time-gaps, the graphs seems to be following similar pattern.

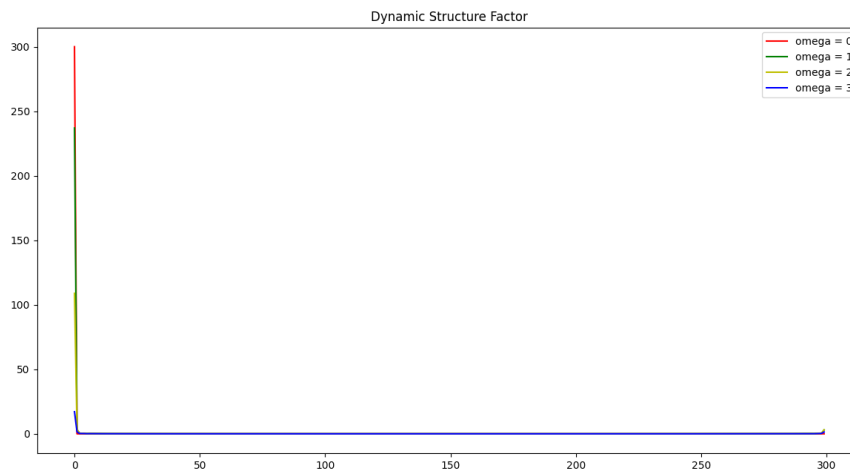
Velocity Correlation



It can be seen that initially the value is the highest and then it drops and becomes flat as time-gap increases. This is because initially when the time difference is less, the vectors for all atoms are somewhat aligned (due to less random nature ~ coming from small time difference) and hence the dot product which is proportional to $\cos(\theta)$ takes the maximum value.

While as time-gap increases, the velocity vectors become highly disaligned compared to the initial position leading to flattening of the curve (due to random nature), and hence showing near to 0 correlation.

Dynamic Structure Factor



The **intermediate scattering** function is the spatial Fourier transform of the van Hove function (which was calculated above), while the **dynamic structure factor** is basically temporal Fourier transform of intermediate scattering function.

And in the graph it can be seen that there is a spike initially around k near to 0.

Deadline

Phase-1: 20th April 2021

Final : 25th April 2021

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