NE550 Computer Assignment 1

Dr. Eapen
Arvin Kushwaha

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Contents

1 Objective

In this Computer Assigment, we aim to produce a molecular dynamics code using the C languageto use the Lennard-Jones potential with a cutoff at $2^{\frac{1}{6}}\sigma$ to represent a soft-sphere interaction. Using this code we investigate the temperature, potential and kinetic energy, as well as total momentum, total energy, and pressure. Of these quantities, temperature and pressure are thermodynamic properties that arise out of the statistical nature of energy and are only well-defined for suffiiciently large systems.

2 Approach

To write this code, I use the C++ language, an extension onto the C language that allows additional object-oriented features. The code consists of a struct representing 2D vectors along with the respective operato overloads, and a struct to store the macrostates of our system. The class also contains a class representing the system, which handles the initialization and updating of the system, along with computation of the macrostates.

3 Results

4 Discussion

5 Summary