NE550 Computer Assignment 1

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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 objectt-oriented features.

3 Results

4 Discussion

5 Summary