Readme

This program is an implementation of the Molecular dynamics project as part of COMP6464 course.

- To compile the C code and load dependent modules: type "make"

- To run code with simulation run :

    python3 md1-simulation.py x x x x or python3 md2-simulation.py x x x x

- For a normal run:

    python3 md1.py x x x x or python3 md2.py x x x x

Notes:

Python3 should be used to run the application.

The various errors that could be generated in computation and the issues faced in connecting C and python using ctypes is mentioned in the report.