

Computational Physics II

Homework 8

Submission: January 14, 2020

Verlet list or neighbor-list

As the force calculation part is a time consuming one during each step of the MD simulation, it may be useful to construct a neighbor-list and use it (good approximation when force is short-ranged).

1. Write a program to implement the neighbor-list in your MD code.
2. Plot the total energy both from your old (without neighbor-list) and this modified code and compare them.

Simulation at constant temperature (4 points)

Write a program to implement the Andersen thermostat for MD simulation in canonical ensemble.

1. Plot the total energy and the kinetic energy (or temperature) versus time.
2. compare the total energy for different values (2-3) of the collision frequency ν .