Computational Physics II

Homework 7

Submission: January 07 (Tuesday), 2020

Simulating interacting particles in a box (10 points)

Consider a system of N particles (in a box of length L with periodic boundary conditions) interacting with each other via Lennard-Jones potential of the form

$$V(r) = 4\epsilon\Big[(\sigma/r)^{12} - (\sigma/r)^{6}\Big]. \tag{1}$$

In Eq. (1) you can take $\epsilon = 1$ and $\sigma = 1$.
The Hamiltonian of the system is given by

$$H = \frac{1}{2}\sum_i m_i v_i^2 + \frac{1}{2}\sum_{i\neq j} V(|r_i - r_j|). \tag{2}$$

You can use $m_i = 1$ for all the particles.

- Write a program to simulate the system using Verlet integration scheme (Use sufficiently small δt for the updates. You can choose, say, $\delta t = 0.001$. Use the cut-off $r_c = 2.5$ for the LJ potential.)
- Measure the total energy as well as the potential energy of the system and plot them as a function of time (two seperate plots). Is the total energy conserved?
- Choose 2-3 different δt of your choice (not very large!) to look at its influence on the total energy.