Exercise 1. Simulating interacting molecules in a box

Goal: This week we are going to learn how interacting molecules can be simulated using constraint forces.

Consider a system of N diatomic molecules (in a box of length L with periodic boundary conditions) that interact with each other. For simplicity we assume that all atoms are identical. Atoms of different molecules interact via the Lennard-Jones potential

$$V(r) = 4\left[\left(\frac{1}{r}\right)^{12} - \left(\frac{1}{r}\right)^{6}\right]$$

with each other. To ensure that the two particles in a molecule keep their distance r we have to add the constraint forces

$$\boldsymbol{g}_1 = \lambda \boldsymbol{r}$$
$$\boldsymbol{g}_2 = -\lambda \boldsymbol{r}$$

to the equation(s) of motion.

Task 1: Derive an analytical expression for the Lagrange multiplier λ.

Task 2: Simulate the system using the Verlet scheme as described in the lecture notes.

Hint: The distance between the two atoms in a molecule should be small enough such that other molecules do not cross their bond.

Hint: It might be easier to consider the 2D case and check if the behaviour of the molecules is correct before you go to the 3D case.

Task 3 (OPTIONAL): Extend your program to simulate three-component molecules.