Simulating interacting diatomic molecules in a box

Goal: Learn simulating interacting molecules using constraint forces.

Consider a system of N diatomic molecules in a 3-dimensional square box of side-length L with periodic boundary conditions. We will assume the pairwise intermolecular interactions are described by the Lennard-Jones potential

$$V(r) = 4\left(r^{-12} - r^{-6}\right), \tag{1}$$

where r is the separation between two particles.

The intramolecular interactions that hold the molecules together are modelled by a constraint that pairs of atoms in a molecule have a fixed distance r. This can be ensured by adding the constraint forces

$$\begin{aligned} \vec{g}_1 &= \lambda r, \\ \vec{g}_2 &= -\lambda r, \end{aligned} \tag{2}$$

to the equations 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.

Keep in mind the following points:

- The distance between the two atoms in a molecule should be small enough such that other molecules do not travel across their bond.
- It might be easier to test your implementation in the 2-dimensional case before going to the 3-d case.

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