Assignment 5: Molecular Dynamics

December 2020

1 Introduction

Molecular dynamics (MD) is a method for simulating the movements of atoms and molecules and is wildly used to study properties of molecular systems in chemical physics, materials science, and biophysics. Hereby, the time-evolution of the molecular system is studied by propagating it according to its equations of motion. In the most common cases, the system follow simply the numerical solutions of Newton's equation of motion, where usually the Leapfrog or Velocity-Verlet scheme are used to propagate the system.

In the following you are asked to write a small MD code, that uses the Velocity-Verlet alogrithm to propagate the H_2 molecule.

$$x(t) = x_0 + v(t)dt + 0.5a(t)dt^2 \tag{1}$$
$$a(t) = F(x(t))/m \tag{2}$$
$$v(t) = v_0 + 0.5(a(t) + a_0)dt \tag{3}$$

where $F(x(t))$ is the force $(\frac{\partial V}{\partial x})$ of the system and m its mass. The code should read in the initial structure from an 'XYZ'-format file (see assignemnt 3), then propagate the system. For the computation of the forces on the atoms you should use a common morse-potential:

$$V = D_e \left(1 - e^{-a(R-R_0)}\right)^2 \tag{4}$$

and its associate gradient.

The parameters for H_2 are:

$$D_e = 0.176 \tag{5}$$
$$a = 1.02 \tag{6}$$
$$R_0 = 1.40 \tag{7}$$
$$\tag{8}$$

in atomic units.

The code should print the three energies: total energy (for check on energy conservation), kinetic energy, potential energy of the system as well as optionally the trajectory of structures in XYZ-format.