Exercise 1. Canonical Molecular Dynamics

Goal: So far, we considered microcanonical MD simulations where the total energy of the system is conserved. In this week's exercise we will simulate a system in contact with a thermal reservoir at fixed temperature T. There are several techniques to do this (see lecture notes). We will use the Nosé-Hoover thermostat which is the best in the sense that it reproduces the correct energy distribution corresponding to a canonical system.

The final equations of motion for our system are given by

$$\begin{aligned} m_i \ddot{\boldsymbol{r}}_i &= \boldsymbol{f}_i - m_i \xi \boldsymbol{v}_i \\ \dot{\xi} &= \frac{1}{Q}\left(\sum_i m_i \boldsymbol{v}_i^2 - (3N+1)k_B T\right) \end{aligned}$$

where $3N+1$ is the number of degrees of freedom, T the desired temperature of the system and Q the coupling strength to the heat bath. The friction coefficient ξ is defined as

$$\xi = \frac{\dot{s}}{s}$$

where s is the additional degree of freedom introduced by the heat bath. Note that s itself does not appear in the simulation.

Task 1: Extend your already existing MD code (exercise sheet 07) to simulate a canonical system with a given temperature.

Task 2: Observe the behavior of the instantaneous temperature $\mathcal{T}$ over time.

Hint: Start with an initial configuration with instantaneous temperature $\mathcal{T}_0$, set the desired temperature T to a different value and observe the behavior of $\mathcal{T}$ over time.

Task 3: When the system reaches thermal equilibrium, calculate the total energy of the system and plot the distribution. Can you observe the correct distribution?

Task 4: Repeat task 2 for different values of Q. What do you notice?