Canonical Molecular Dynamics

Goal: So far we performed MD simulations at fixed energy, i.e. in the microcanonical ensemble. Now we want to simulate at fixed temperature. There are several approaches trying to achieve this, we will use the Nosé-Hoover thermostat which reproduces the canonical energy distribution.

Coupling our system of particles to a heat bath at fixed temperature T yields the equations of motion

$$m_i \ddot{\mathbf{r}}_i = \mathbf{f}_i - m_i \xi \mathbf{v}_i, \tag{1}$$

$$\dot{\xi} = \frac{1}{Q}\left[\sum_i m_i \mathbf{v}_i^2 - (3N+1)k_B T\right], \tag{2}$$

where $3N+1$ is the number of degrees of freedom and Q is the coupling strength to the heat bath. The friction coefficient ξ is defined as $\xi := \dot{s}/s$, where s is the additional degree of freedom describing the heat bath.

Task 1: Extend your MD code (Exercises 7, 8) to simulate a canonical system with a given temperature.

Task 2: Observe the evolution of the instantaneous temperature

$$T_{\text{inst}} := \frac{1}{k_B \cdot 3(N-1)} \sum_i m_i \mathbf{v}_i^2 \tag{3}$$

for different values of Q as a function of time. Comment on your findings.

Task 3: Once the system reaches thermal equilibrium, sample the energy of the system and visualize its distribution. Comment on what you observe.