360.243 Numerical Simulation and Scientific Computing II (VU 3,0) 2022S

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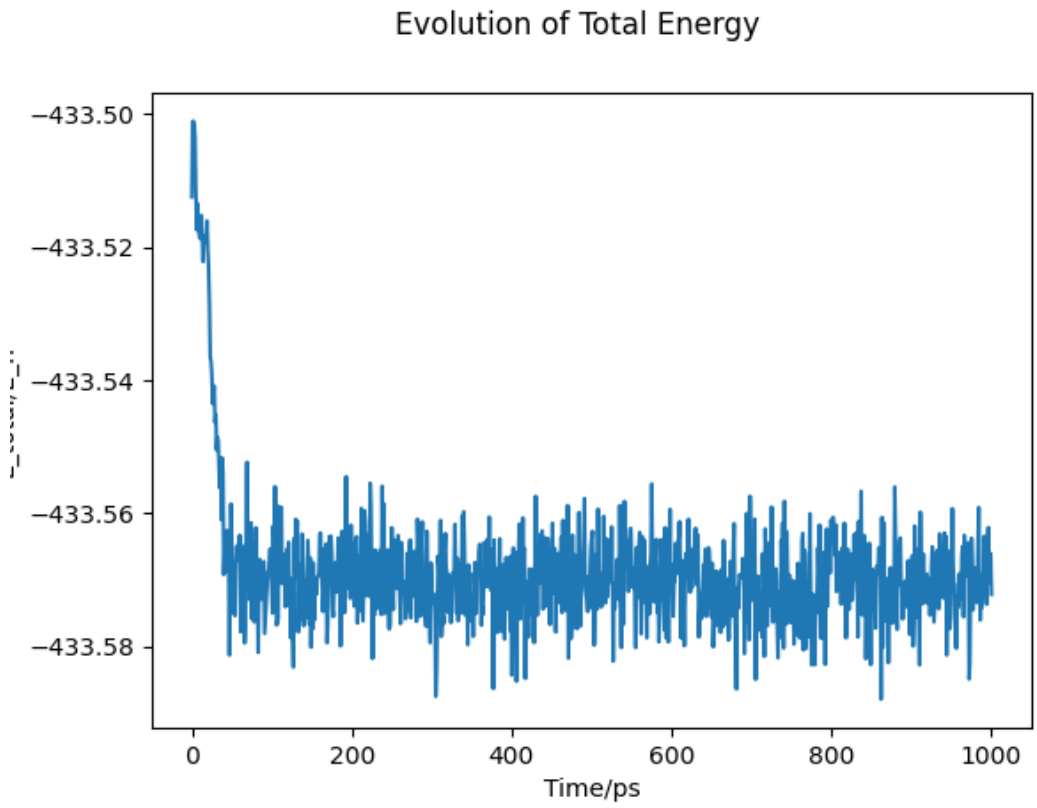
Exercise 2 - Task 4

1. Plot Energy conservation

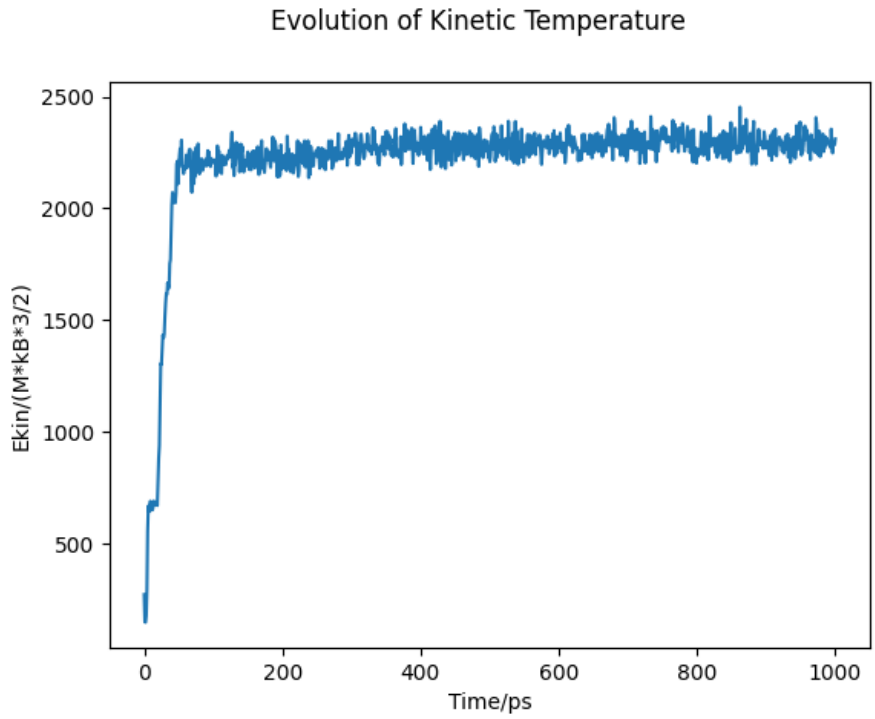


Plot 1: Total system energy

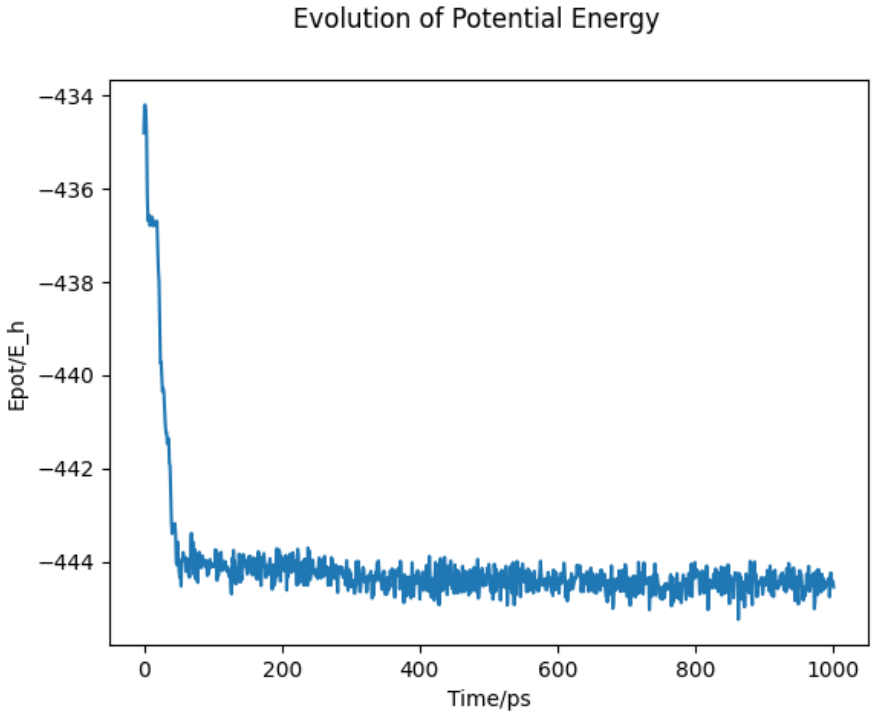
Discussion:

As expected the system conserves the total energy. The value oscillates (although only very slightly) due to model imprecisions (Newton`s equations of motion) and also due to the fact that only every 1000st step of the trajectory calculation was saved and subsequently used for plotting. The drop in the beginning could be explained by the initial setting. The Unit of energy used is Eh (see Task1).

2. Plot Evolution of the kinetic temperature and potential energy



Plot 2: Kinetic temperature



Plot 3: Potential energy

Discussion:

Corresponding to the conservation of the whole system energy, the kinetic and potential energy is also conserved.

3. Specific heat of the system

Formula for the computation:

$$c_v = k_\mathrm{B}\frac{\langle E_\mathrm{kin}\rangle^2}{\sigma^2_{E_\mathrm{kin}}}, \text{ where } \sigma^2_{E_\mathrm{kin}} = \left\langle (E_\mathrm{kin} - \langle E_\mathrm{kin}\rangle)^2 \right\rangle.$$

Calculated Value:

$$6.071680671051434e-17\ \mathrm{E_{Hartree}/Kelvin}$$

4. Plot of fraction of interatomic pairs against radius – Pair Correlation Function