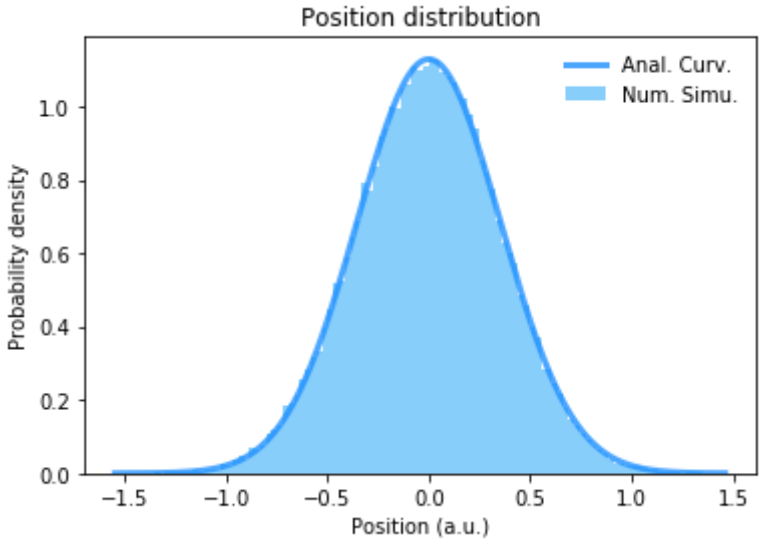
Tests of Andersen Thermostat (general)

1 Side scheme

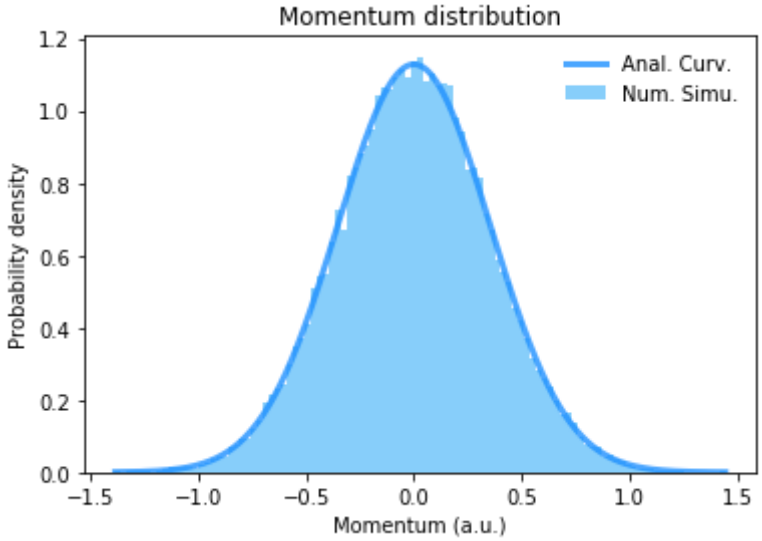
1.1 Case 1: 3-dimensional harmonic oscillator

- potential: $V(r) = m\omega^2 r^2/2$
- simulation parameters:
  - run time: 10^5 fs
  - step size: $2.418884326509 \times 10^{-3}$ fs (0.1 a.u.)
  - data collection period: 1000
- system information: $m = 1$ a.u., $\omega = 1$ a.u., $\beta = 8$ a.u.

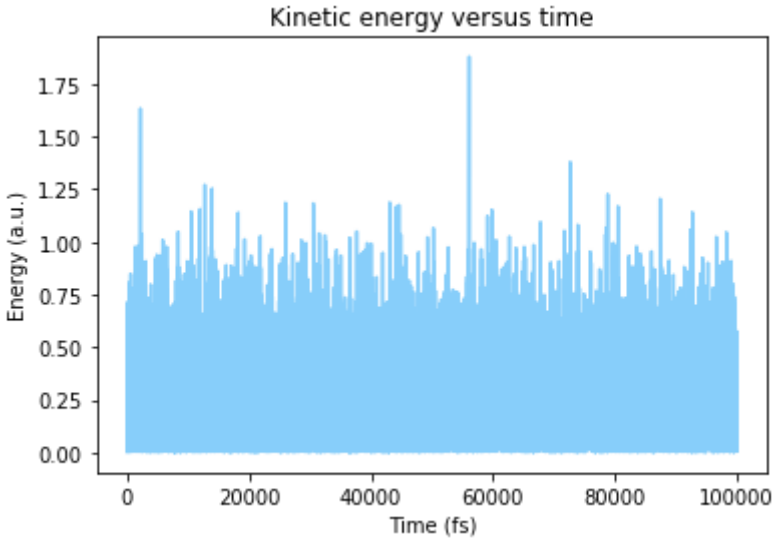
The position distribution of the first degree of freedom:



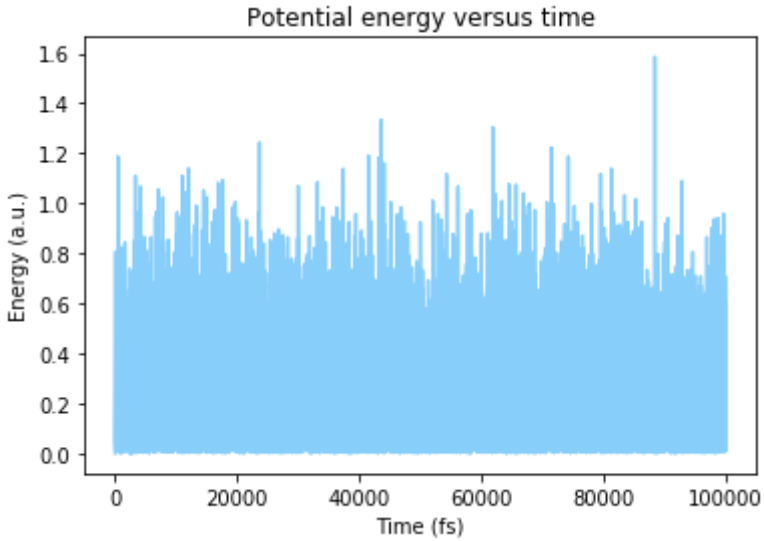
The momentum distribution of the first degree of freedom:



The evolution of kinetic energy:



The evolution of potential energy:



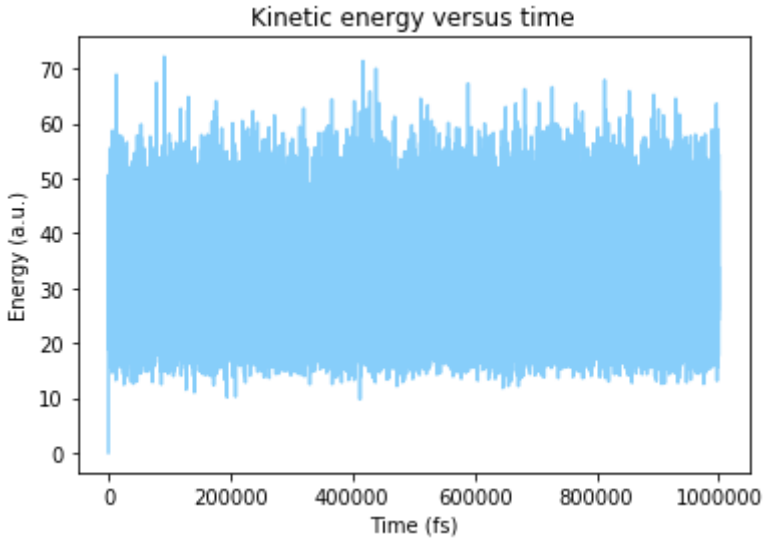
1.2 Case2: $(\mathrm{Ne})_{13}$ molecular system

- potential:

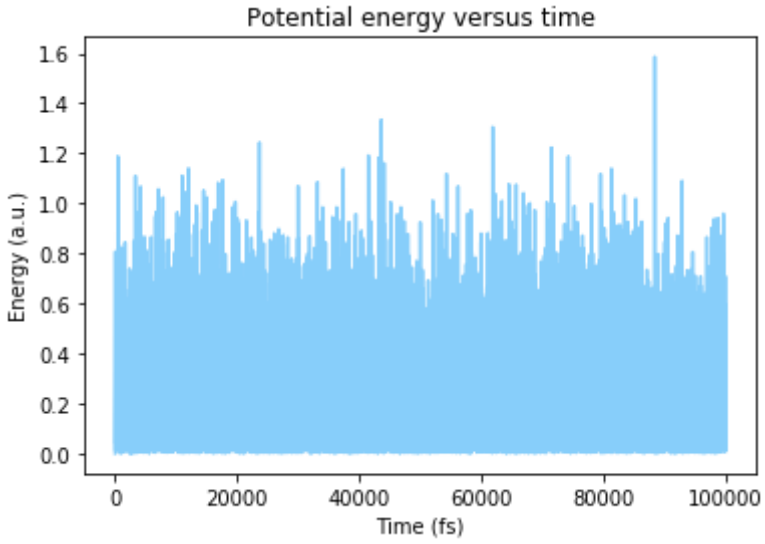
$$V(r_{ij}) = 4\epsilon \left[\left(\frac{\sigma}{r_{ij}} \right)^{12} - \left(\frac{\sigma}{r_{ij}} \right)^{6} \right].$$

- simulation parameters:
  - run time: 10^6 fs
  - step size: 0.1 fs
  - data collection period: 100
- system information: $m(\mathrm{Ne}) = 3.35 \times 10^{-26}$ kg, $T = 14$ K, $\epsilon = 35.6$ K, $\sigma = 2.749$ Å

The evolution of kinetic energy:



The evolution of potential energy:

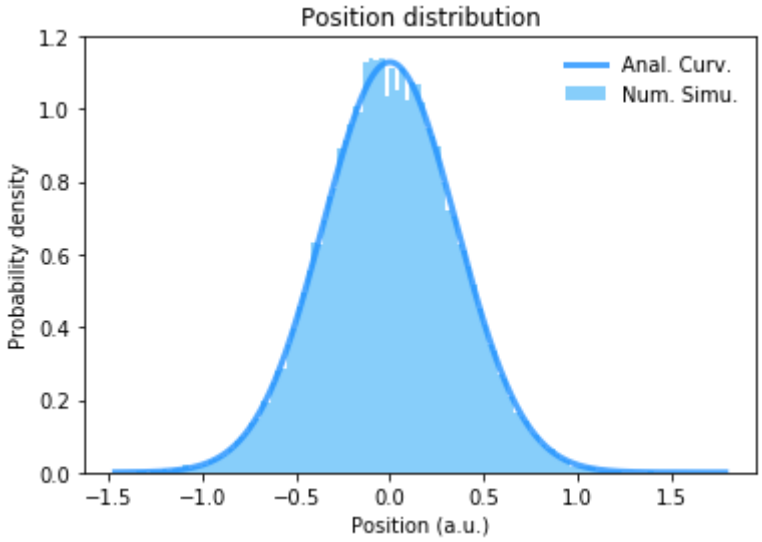


2 Middle scheme

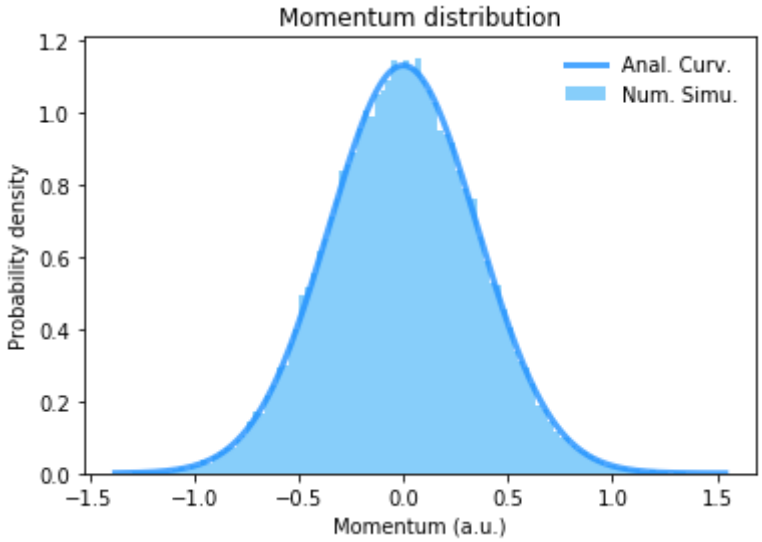
2.1 Case 1: 3-dimensional harmonic oscillator

- potential: $V(r) = m\omega^2 r^2/2$
- simulation parameters:
  - run time: 10^5 fs
  - step size: $2.418884326509 \times 10^{-3}$ fs (0.1 a.u.)
  - data collection period: 1000
- system information: $m = 1$ a.u., $\omega = 1$ a.u., $\beta = 8$ a.u.

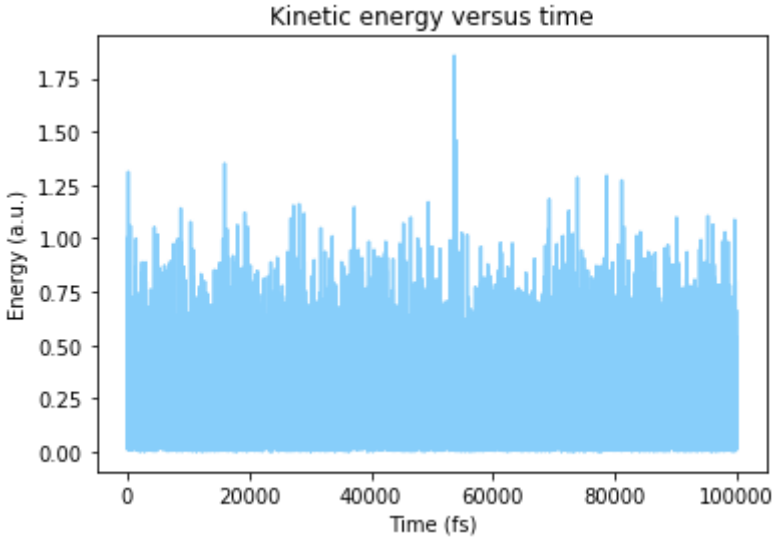
The position distribution of the first degree of freedom:



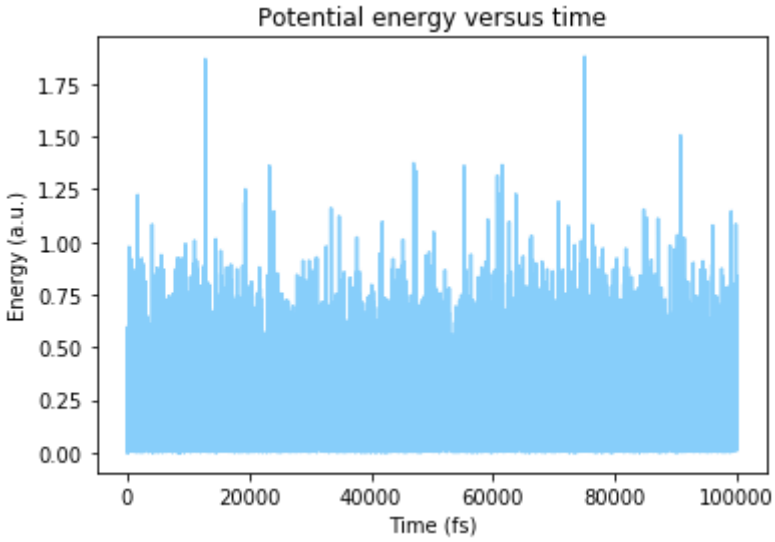
The momentum distribution of the first degree of freedom:



The evolution of kinetic energy:



The evolution of potential energy:



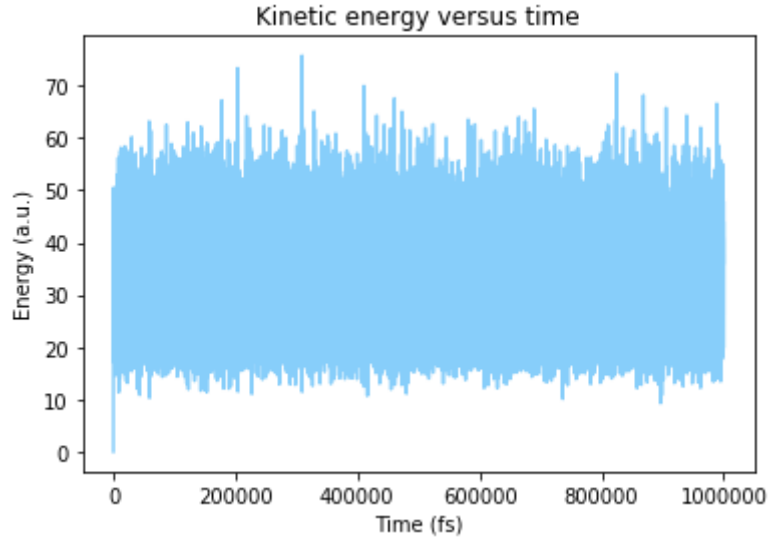
2.2 Case2: $(\mathrm{Ne})_{13}$ molecular system

- potential:

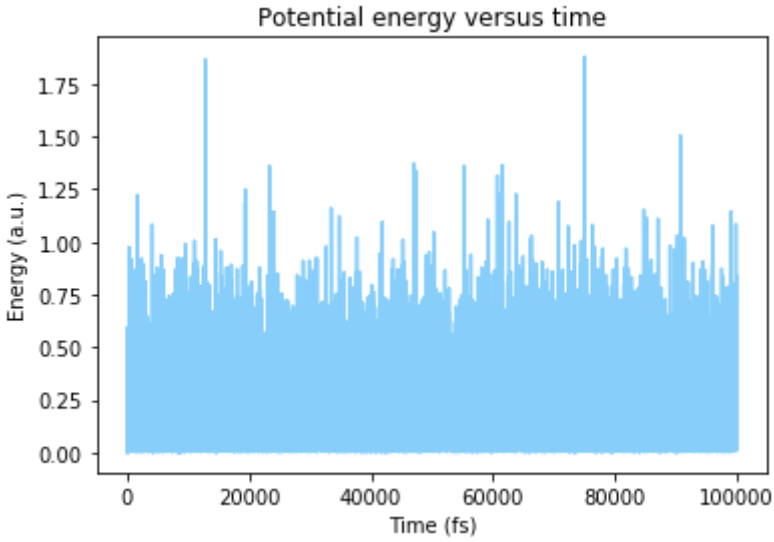
$$V(r_{ij}) = 4\epsilon \left[\left(\frac{\sigma}{r_{ij}} \right)^{12} - \left(\frac{\sigma}{r_{ij}} \right)^{6} \right].$$

- simulation parameters:
  - run time: 10^6 fs
  - step size: 0.1 fs
  - data collection period: 100
- system information: $m(\mathrm{Ne}) = 3.35 \times 10^{-26}$ kg, $T = 14$ K, $\epsilon = 35.6$ K, $\sigma = 2.749$ Å

The evolution of kinetic energy:



The evolution of potential energy:


Potential energy versus time
Energy (a.u.)
1.75
1.50
1.25
1.00
0.75
0.50
0.25
0.00
0
20000
40000
60000
80000
100000
Time (fs)