

Chapter 1

Milestone 4

1.1 Force-Derivation from the Lenard Jones Potential

$$\vec{f}_k = \sum_i \frac{\partial V}{\partial r_{ik}} \hat{r}_{ik} \quad (1.1)$$

$$V(r) = 4\epsilon \left[\left(\frac{\sigma}{r} \right)^{12} - \left(\frac{\sigma}{r} \right)^6 \right] \quad (1.2)$$

$$\frac{\partial V}{\partial r_{ik}} = 4\epsilon \left(\frac{6\sigma^6}{r_{ik}^6} - \frac{12\sigma^{12}}{r_{ik}^{13}} \right) \quad (1.3)$$

```
[4]: import sympy as sp
import warnings
warnings.filterwarnings('ignore')
sp.init_printing()
eps = sp.Symbol("e")
sig = sp.Symbol("s")
rad = sp.Symbol("r")
energyRad = 4 * eps * ((sig/rad)**12 - (sig/rad)**6)
energyRad.diff(rad)
```

```
[4]:
```

$$4e \left(\frac{6s^6}{r^7} - \frac{12s^{12}}{r^{13}} \right)$$

1.2 Different Time Steps

1.3 Simulation Snapshots

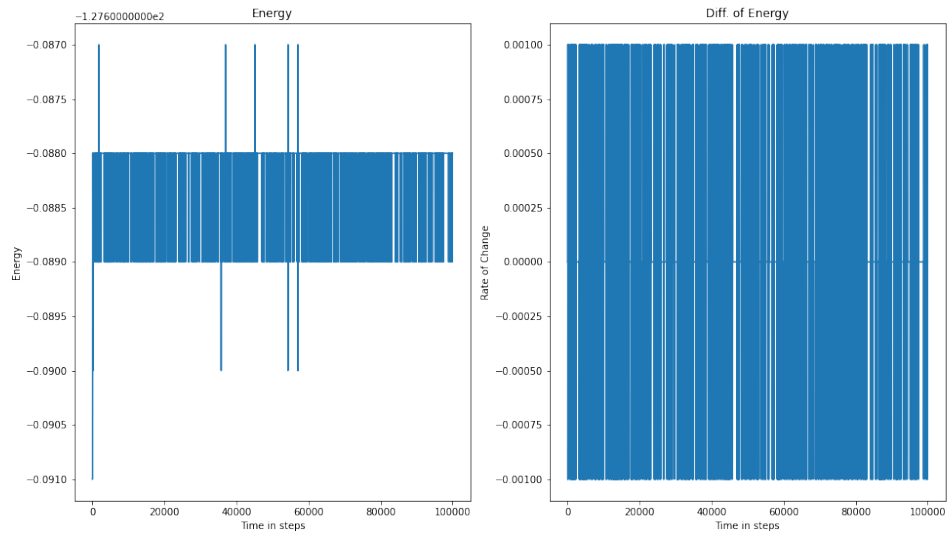


Figure 1.1: Simulation with a time step of 0.001

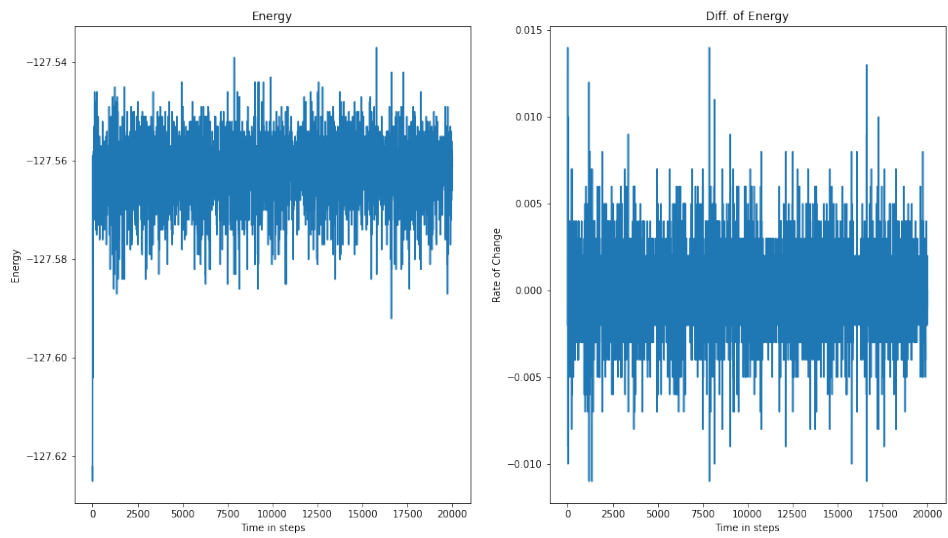


Figure 1.2: Simulation with a time step of 0.005

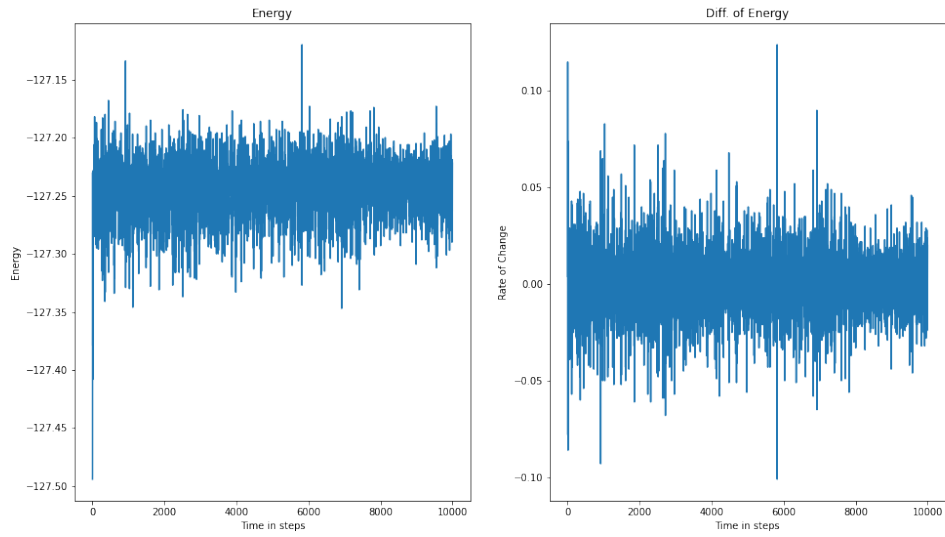


Figure 1.3: Simulation with a time step of 0.01

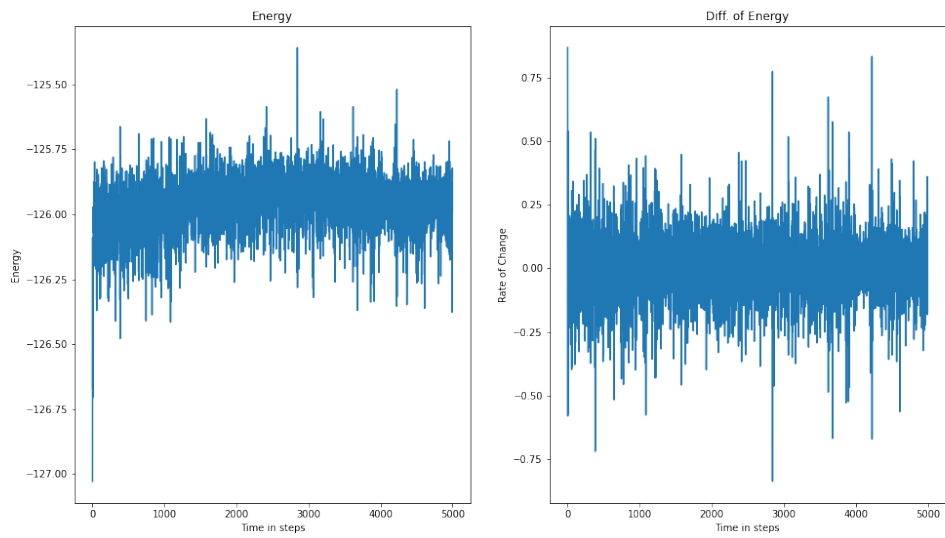


Figure 1.4: Simulation with a time step of 0.02

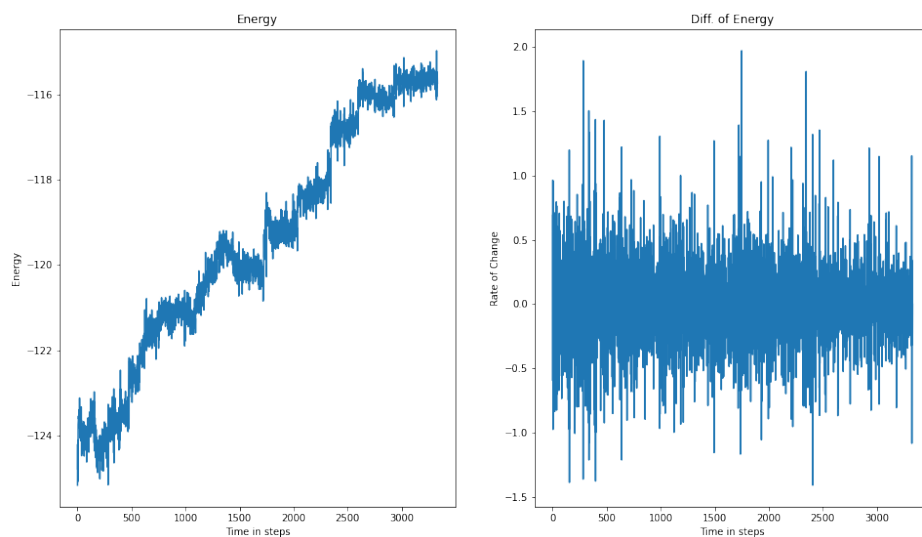


Figure 1.5: Simulation with a time step of 0.03

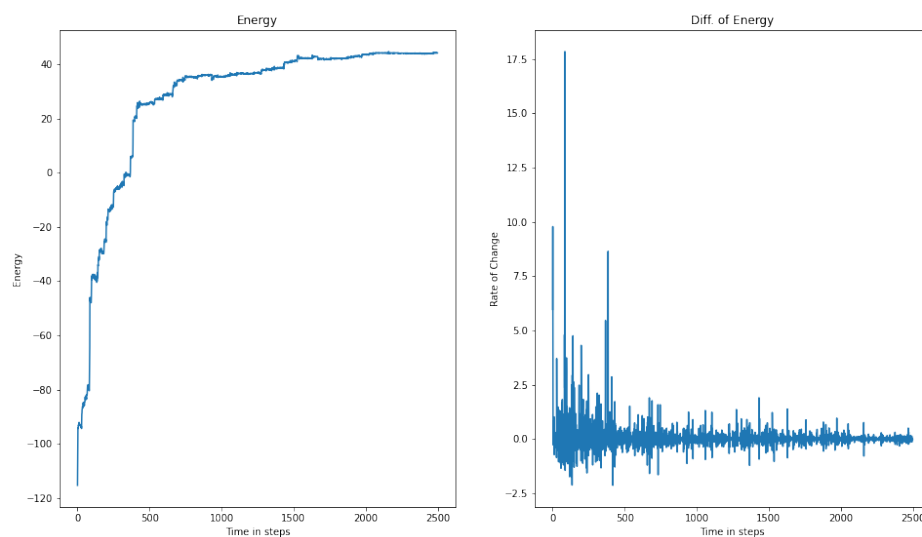


Figure 1.6: Simulation with a time step of 0.04



Figure 1.7: Simulation

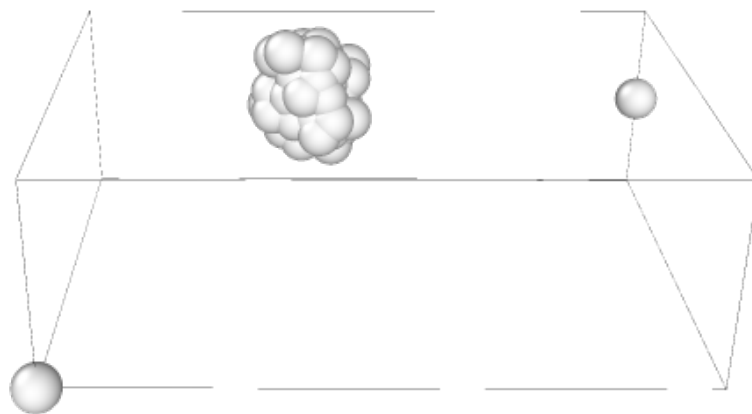


Figure 1.8: Simulation



Figure 1.9: Simulation



Figure 1.10: Simulation

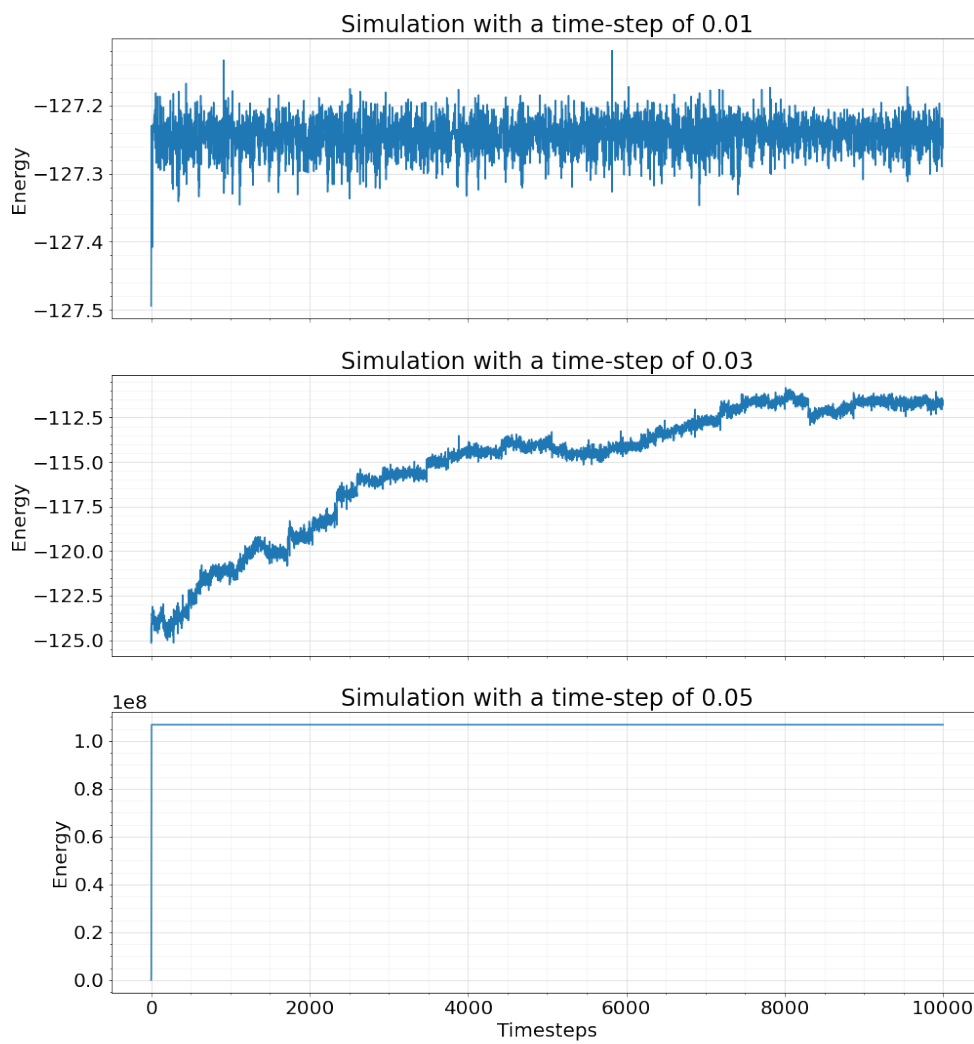


Figure 1.11: Simulation

Chapter 2

Milestone 5

2.1 Berendsen Thermostat Teststrategy

$$\lambda = \sqrt{1 + \left(\frac{T_0}{T} - 1\right) \frac{\Delta t}{\tau}} \quad (2.1)$$

$$T(t) = T_0 + (T_1 - T_0)e^{-t/\tau} \quad (2.2)$$

2.2 Simulation Time

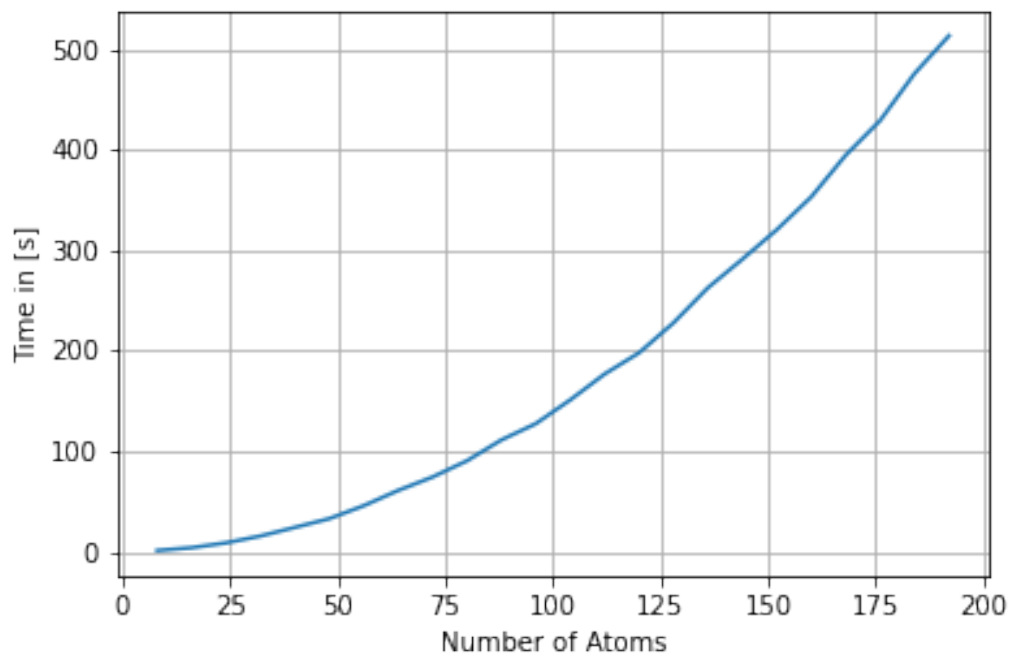


Figure 2.1: Simulationtime from 8 to 192 Atoms

Chapter 3

Milestone 6

The Images are outdated!!!!

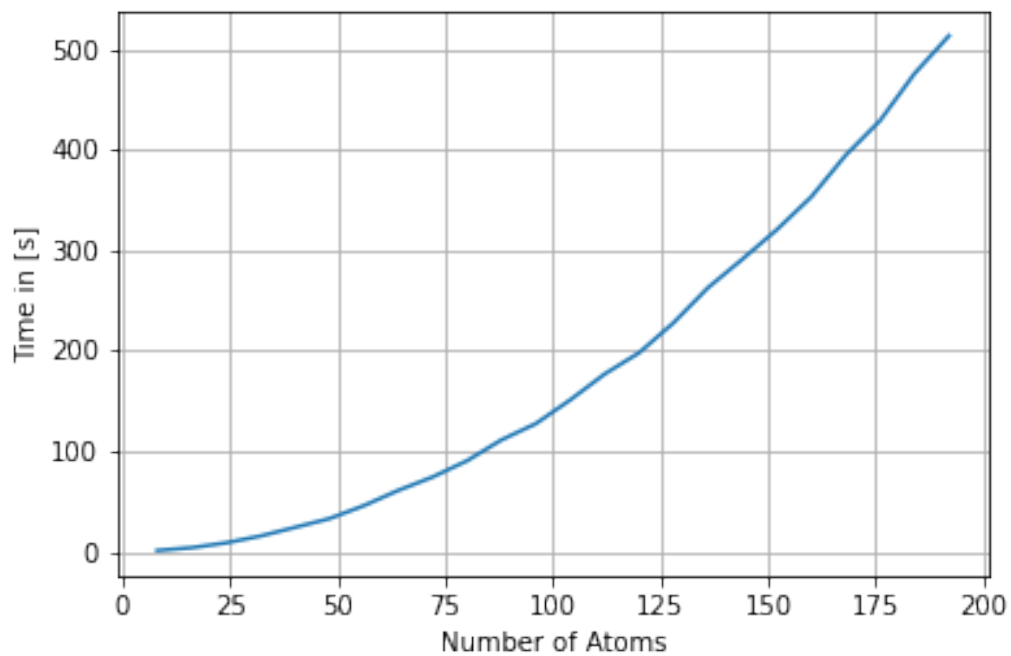


Figure 3.1: Simulationtime without Neighborlist

New images that are correct.

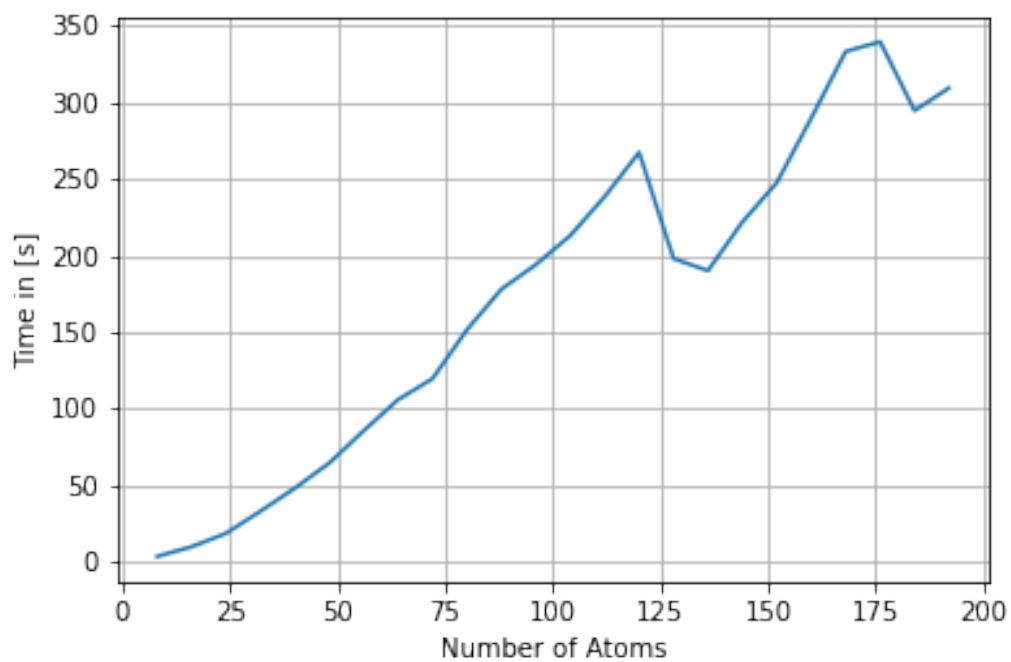


Figure 3.2: Simulationtime with the old Neighborlist

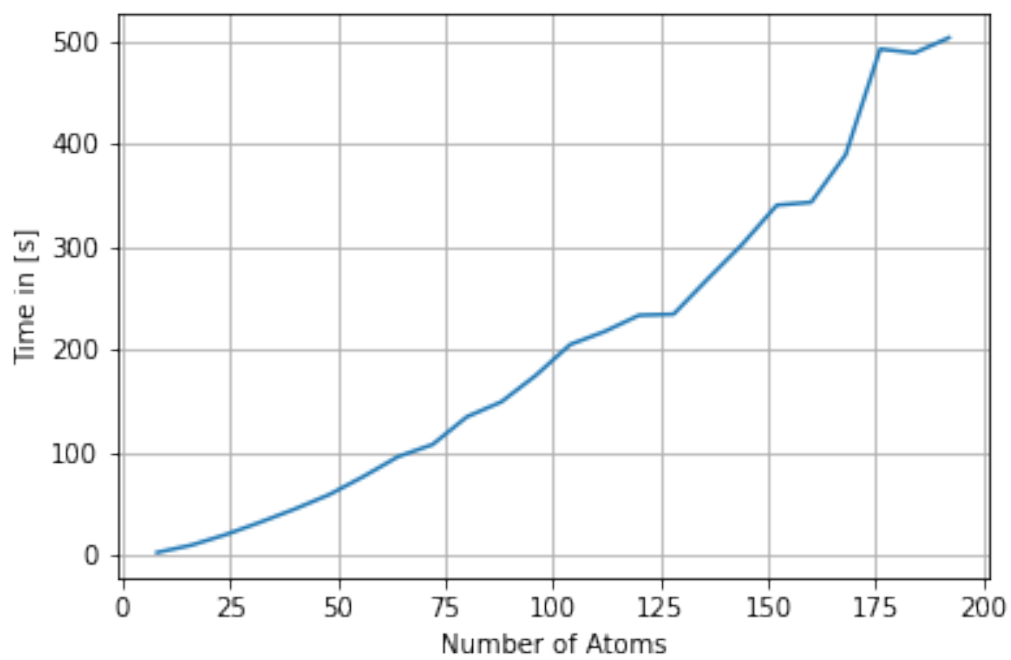


Figure 3.3: Simulationtime with the new Neighborlist

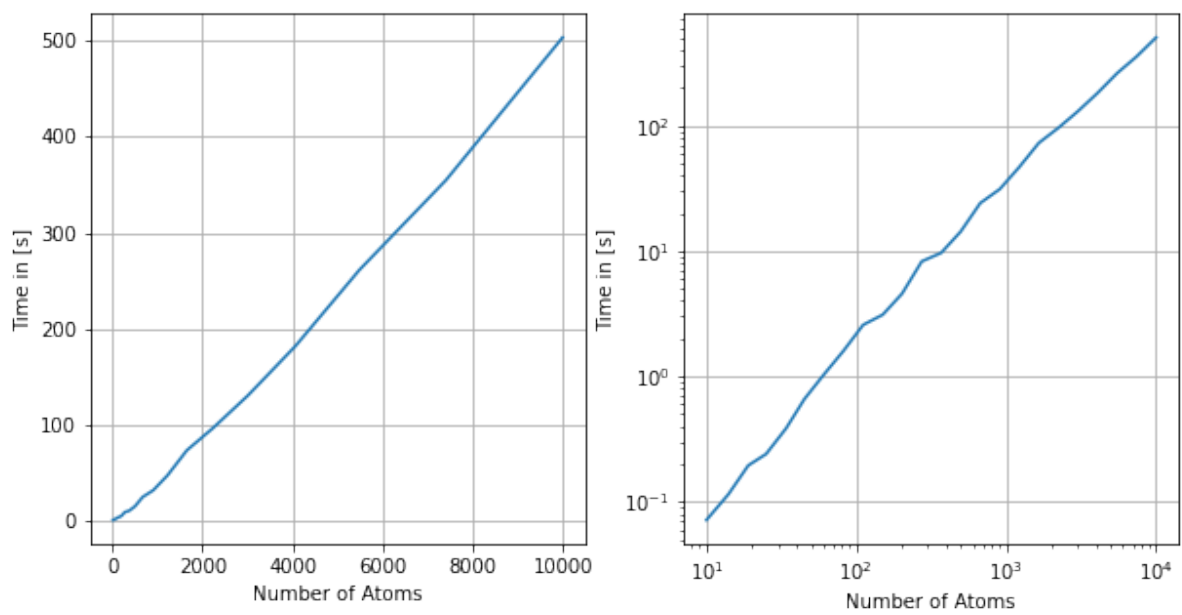


Figure 3.4: Simulationtime with the new Neighborlist

Contents

1	Milestone 4	1
1.1	Force-Derivation from the Lenard Jones Potential	1
1.2	Different Time Steps	1
1.3	Simulation Snapshots	1
2	Milestone 5	10
2.1	Berendsen Thermostat Teststrategy	10
2.2	Simulation Time	10
3	Milestone 6	12
4	Methods	17
4.1	Integration	17
4.2	Potentials	17
4.2.1	Lenard-Jones-Potential	17
4.2.2	Neighborhood-Search Algorithm	17
4.2.3	Embedded-Atom Method Potentials	17
5	Implementation	18
6	Results	19
6.1	Results from the Lenard-Jones Potential with direct Summation	19
6.2	Result from the Simulation with the Berendsen Thermostat	19
6.3	Results from the Simulation with the Neighborhood-List	19
6.4	Results from the Simulation with the Gupta-Potential	20

List of Figures

1.1	Simulation	2
1.2	Simulation	2
1.3	Simulation	3
1.4	Simulation	3
1.5	Simulation	4
1.6	Simulation	4
1.7	Simulation	5
1.8	Simulation	6
1.9	Simulation	7
1.10	Simulation	8
1.11	Simulation	9
2.1	Simulationtime	11
3.1	Simulationtime without Neighborlist	12
3.2	Simulationtime with the old Neighborlist	13
3.3	Simulationtime with the new Neighborlist	13
3.4	Simulationtime with the new Neighborlist	14
6.1	Simulation	19
6.2	Simulation	20
6.3	Simulation	21
6.4	Simulation-time with the Berendsen Thermostat from 8 to 192 Atoms	22
6.5	Simulation-time with the Neighbor-list	22
6.6	Gold Cluster Simulation	23
6.7	Melting Point, Heat Capacity and Latent Heat vs Clustersize	24

Chapter 4

Methods

4.1 Integration

4.2 Potentials

4.2.1 Lenard-Jones-Potential

4.2.2 Neighborhood-Search Algorithm

4.2.3 Embedded-Atom Method Potentials

Chapter 5

Implementation

The simulation code was written in C++, most of it just as functions, although the positions, velocities, etc. of the individual atoms were saved in a container-class. While writing the functions, these were also tested with unit-tests. Plots generation and automation for running the project were written in python.

The C++-code was developed in CLion, an IDE which bundles many useful features together (CMake, GDB and Git). The python-code was written in jupyter-notebook. Additional libraries used were: googletest for the unit-tests and eigen for the arrays used for data storage in the container-class.

Chapter 6

Results

6.1 Results from the Lenard-Jones Potential with direct Summation



Figure 6.1: Simulation

6.2 Result from the Simulation with the Berendsen Thermostat

6.3 Results from the Simulation with the Neighborhood-List

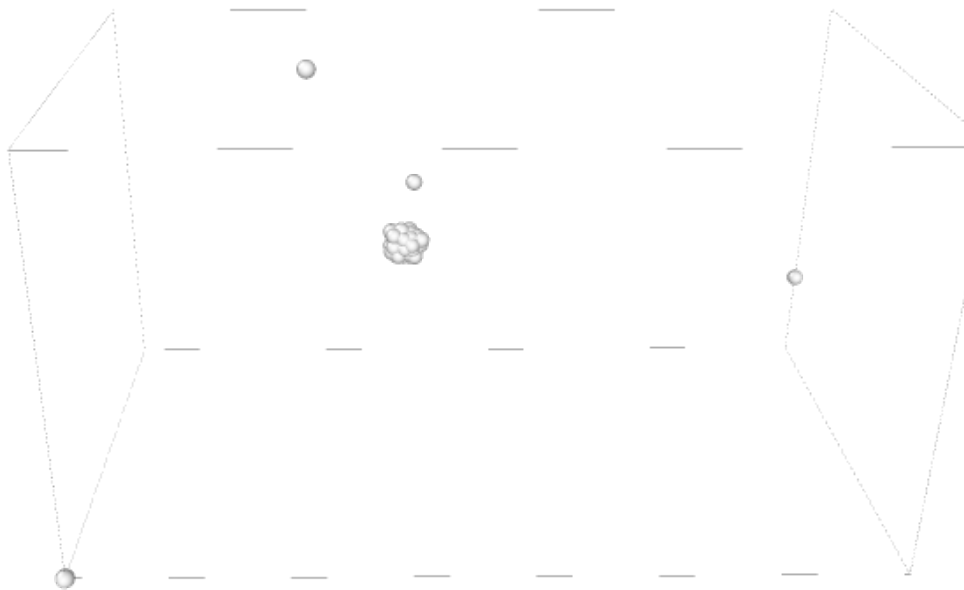


Figure 6.2: Simulation

6.4 Results from the Simulation with the Gupta-Potential

Random citation [1]

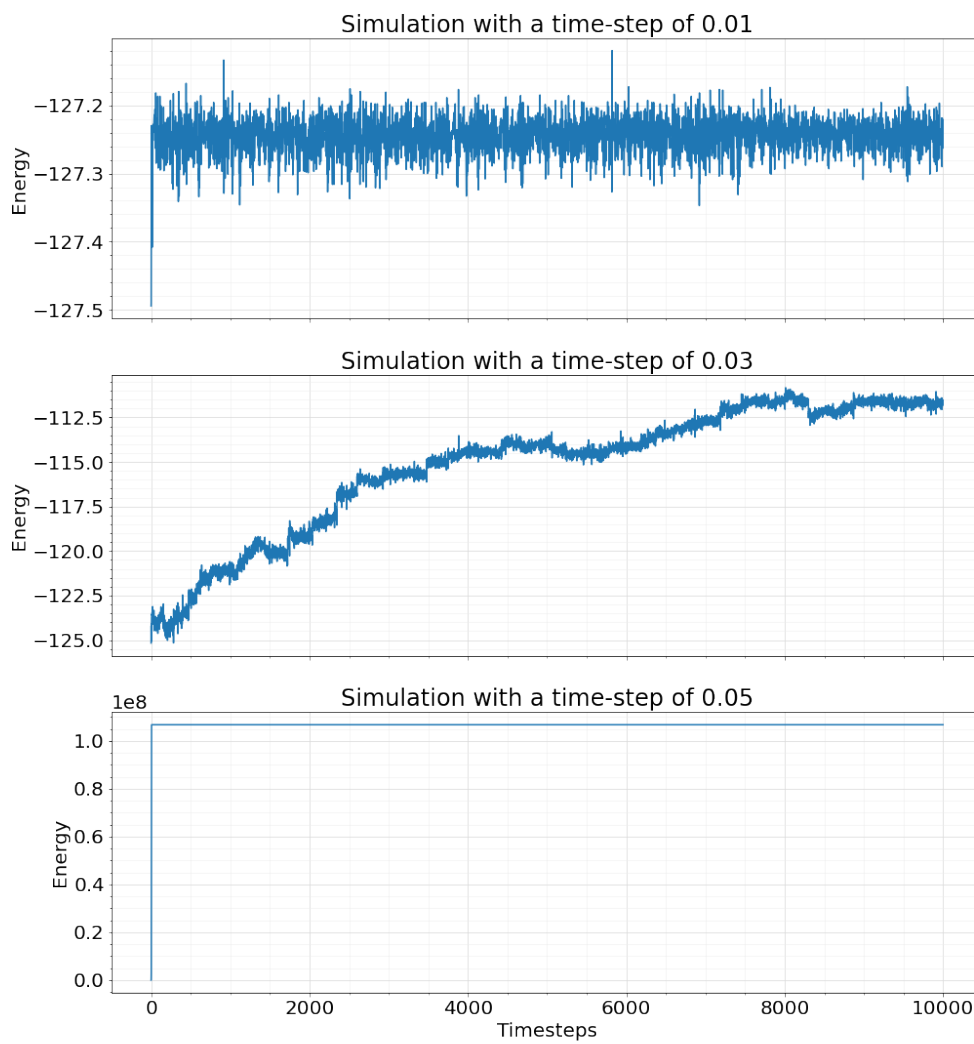


Figure 6.3: Simulation

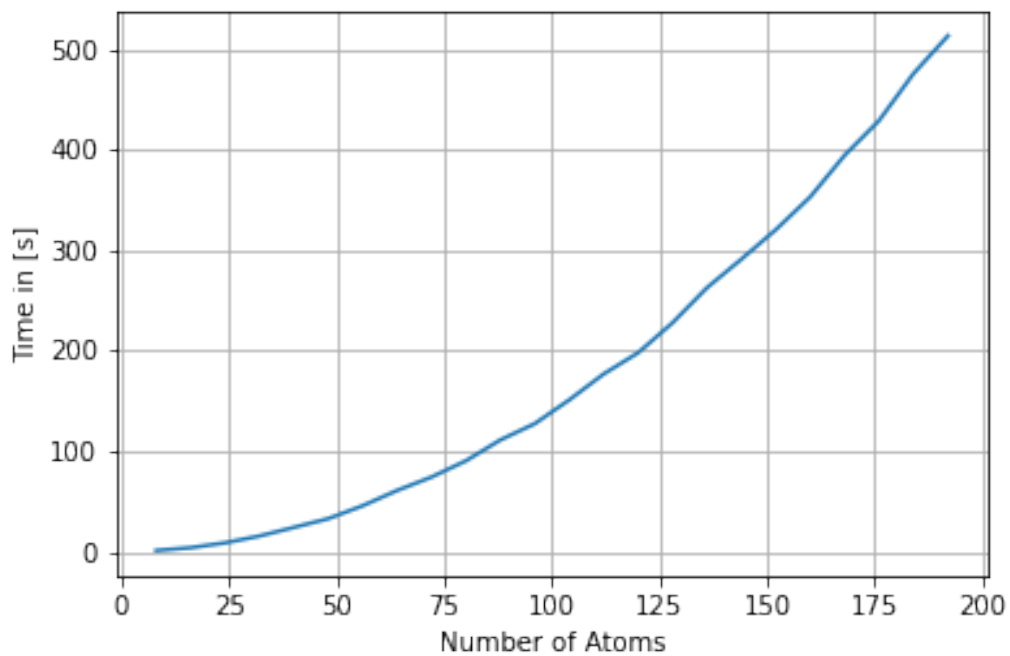


Figure 6.4: Simulation-time with the Berendsen Thermostat from 8 to 192 Atoms

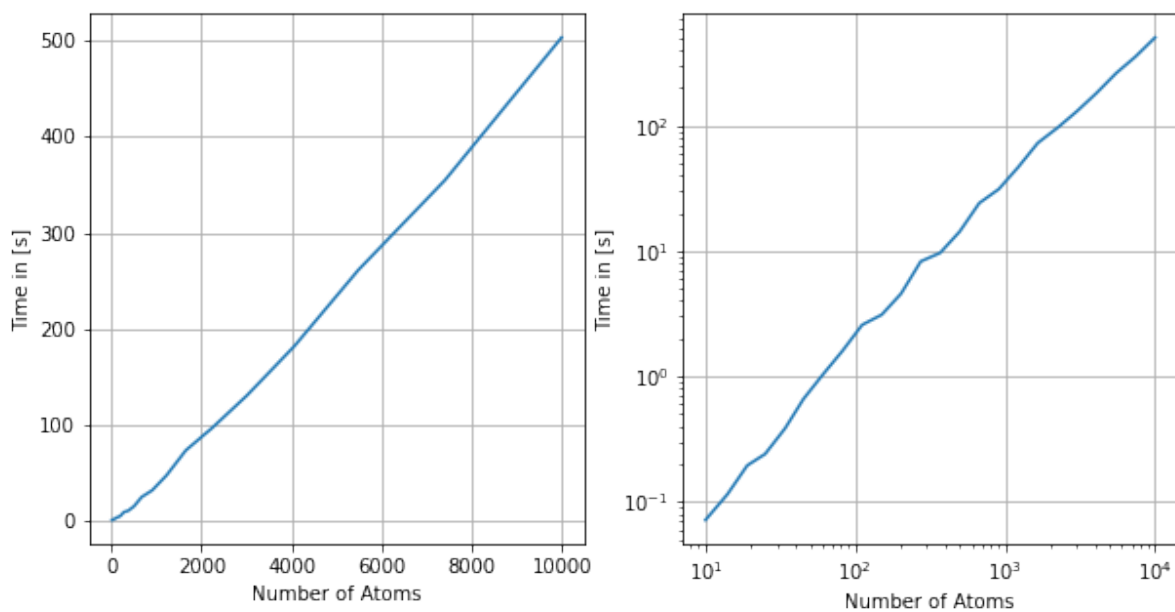


Figure 6.5: Simulation-time with the Neighbor list

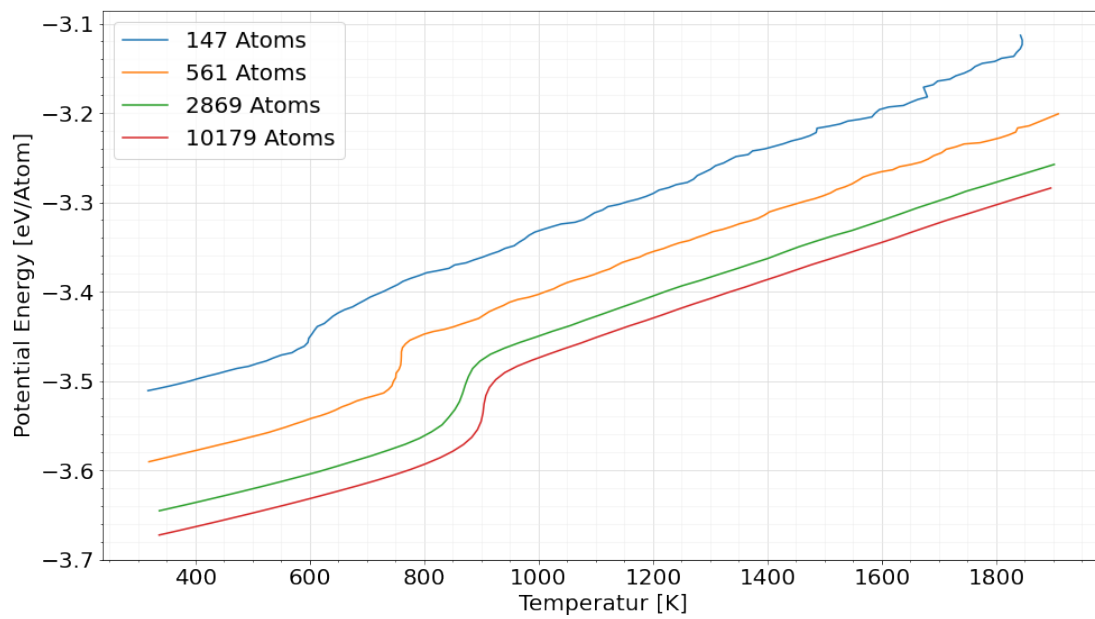


Figure 6.6: Gold Cluster Simulation

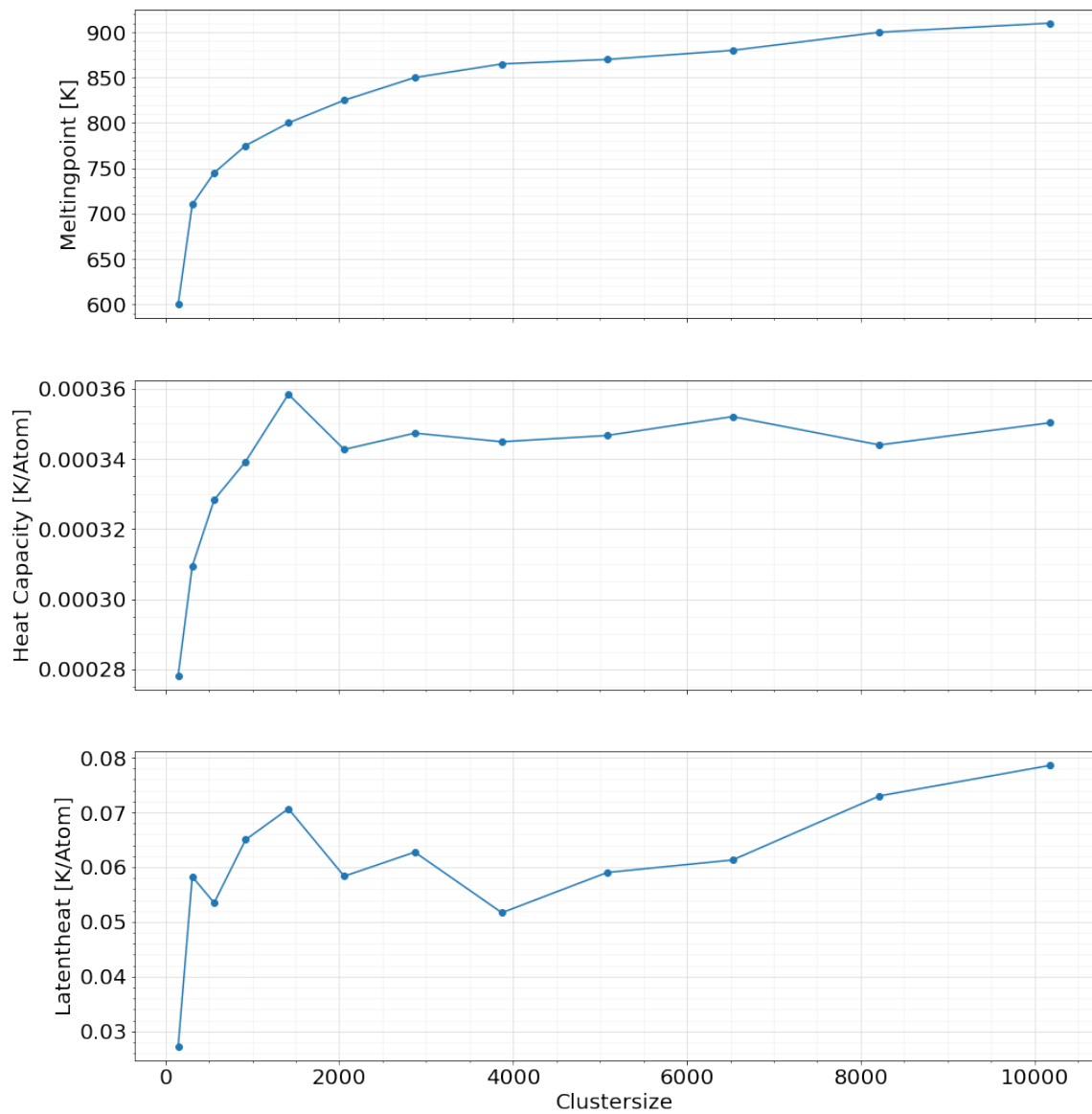


Figure 6.7: Melting Point, Heat Capacity and Latent Heat vs Clustersize

Bibliography

- [1] MultiMedia LLC. *MS Windows NT Kernel Description*. 1999. URL: <http://web.archive.org/web/20080207010024/http://www.808multimedia.com/winnt/kernel.htm> (visited on 09/30/2010).