

# Contents

<b>1</b>	<b>Introduction</b>	<b>3</b>
<b>2</b>	<b>Methods</b>	<b>4</b>
2.1	Integration . . . . .	4
2.2	Potentials . . . . .	4
2.2.1	Lenard-Jones-Potential . . . . .	4
2.2.2	Neighborhood-Search Algorithm . . . . .	5
2.2.3	Embedded-Atom Method Potentials . . . . .	5
2.2.4	Berendsen-Thermostat . . . . .	5
<b>3</b>	<b>Implementation</b>	<b>6</b>
<b>4</b>	<b>Results</b>	<b>7</b>
4.1	Results from the Lenard-Jones Potential with direct Summation . . . . .	8
4.2	Result from the Simulation with the Berendsen Thermostat . . . . .	10
4.3	Results from the Simulation with the Neighborhood-List . . . . .	10
4.4	Results from the Simulation with the Gupta-Potential . . . . .	12
<b>5</b>	<b>Conclusion</b>	<b>14</b>

# List of Figures

4.1	Simulation with different timesteps . . . . .	8
4.2	Simulation Snapshot . . . . .	9
4.3	Simulation Snapshot . . . . .	9
4.4	Simulation Snapshot . . . . .	9
4.5	Simulationtime with the Berendsen Thermostat from 8 to 192 Atoms . . . . .	10
4.6	Simulationtime with the Neighborhood-list . . . . .	11
4.7	Gold Cluster Simulation . . . . .	12
4.8	Melting Point, Heat Capacity and Latent Heat vs Clustersize . . . . .	13

# Chapter 1

## Introduction

1

# Chapter 2

## Methods

The goal of a molecular dynamics simulation is to determine the motion of each individual atom. For this we have to solve the equations of motion and compute the forces that affect each atom.

$$\vec{f}_k = -\frac{\partial}{\partial \vec{r}_k} E_{pot}(\{\vec{r}_k\}) \quad (2.1)$$

The forces can be derived from the potential Energy as shown in 2.1 [cf. 4]. The simulation was run in a discretized space, so all updates to the motion of atoms was only done after a time step.

### 2.1 Integration

From the equation 2.1 we can obtain the force at each individual atom with it's acceleration, velocity and position as shown in 2.1.

$$\vec{f}_i = \frac{\partial E_{pot}}{\partial \vec{r}_i} = m_i \vec{a}_i = m_i \vec{v}_i = m_i \vec{r}_i \quad (2.2)$$

### 2.2 Potentials

$$\vec{f}_k = -\frac{\partial E_{pot}}{\partial \vec{r}_k} = \sum_i \frac{\partial V}{\partial r_{ik}} \hat{r}_{ik} \quad (2.3)$$

#### 2.2.1 Lenard-Jones-Potential

$$V(r) = 4\epsilon \left[ \left( \frac{\sigma}{r} \right)^{12} - \left( \frac{\sigma}{r} \right)^6 \right] \quad (2.4)$$

```
[4]: import sympy as sp
import warnings
warnings.filterwarnings('ignore')
sp.init_printing()
eps = sp.Symbol("ε")
sig = sp.Symbol("σ")
rad = sp.Symbol("r")
```

```
energyRad = 4 * eps * ((sig/rad)**12 - (sig/rad)**6)
energyRad.diff(rad)
```

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

### 2.2.2 Neighborhood-Search Algorithm

### 2.2.3 Embedded-Atom Method Potentials

### 2.2.4 Berendsen-Thermostat

$$\lambda = \sqrt{1 + \left( \frac{T_0}{T} - 1 \right) \frac{\Delta t}{\tau}} \quad (2.5)$$

$$T(t) = T_0 + (T_1 - T_0)e^{-t/\tau} \quad (2.6)$$

## Chapter 3

# 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, alternatively this could also have been done directly in CLion with a plugin. Additional libraries used were: googletest [3] for the unit-tests and eigen [1] for the arrays used for data storage in the container-class. Further software from the course was used for reading xyz-data and for the implementation of the Neighborhood-Search and Gupta-Potential algorithms [4]. To visualize the simulation the positions of the atoms at a given time were recorded and then put into OVITO Basic [2] to be able to look at them.

The code is parted into a headerfile (.h) and a codefile (.cpp). The functions were generally structured into a related header- and codefile. For example all functions regarding the Lennard-Jones-Potential can be found in an appropriately named filecombo. Furthermore a test file exists where the unit-tests can be found.

The implementation itself just followed the milestones given in the course and went up till milestone seven. In case any mistakes happened the main of each milestone was saved into an extra file and just commented into the code again in the true main.cpp file.

For further information it would be best to just look at the code itself as it should be well commented [5].

## **Chapter 4**

# **Results**

## 4.1 Results from the Lenard-Jones Potential with direct Summation

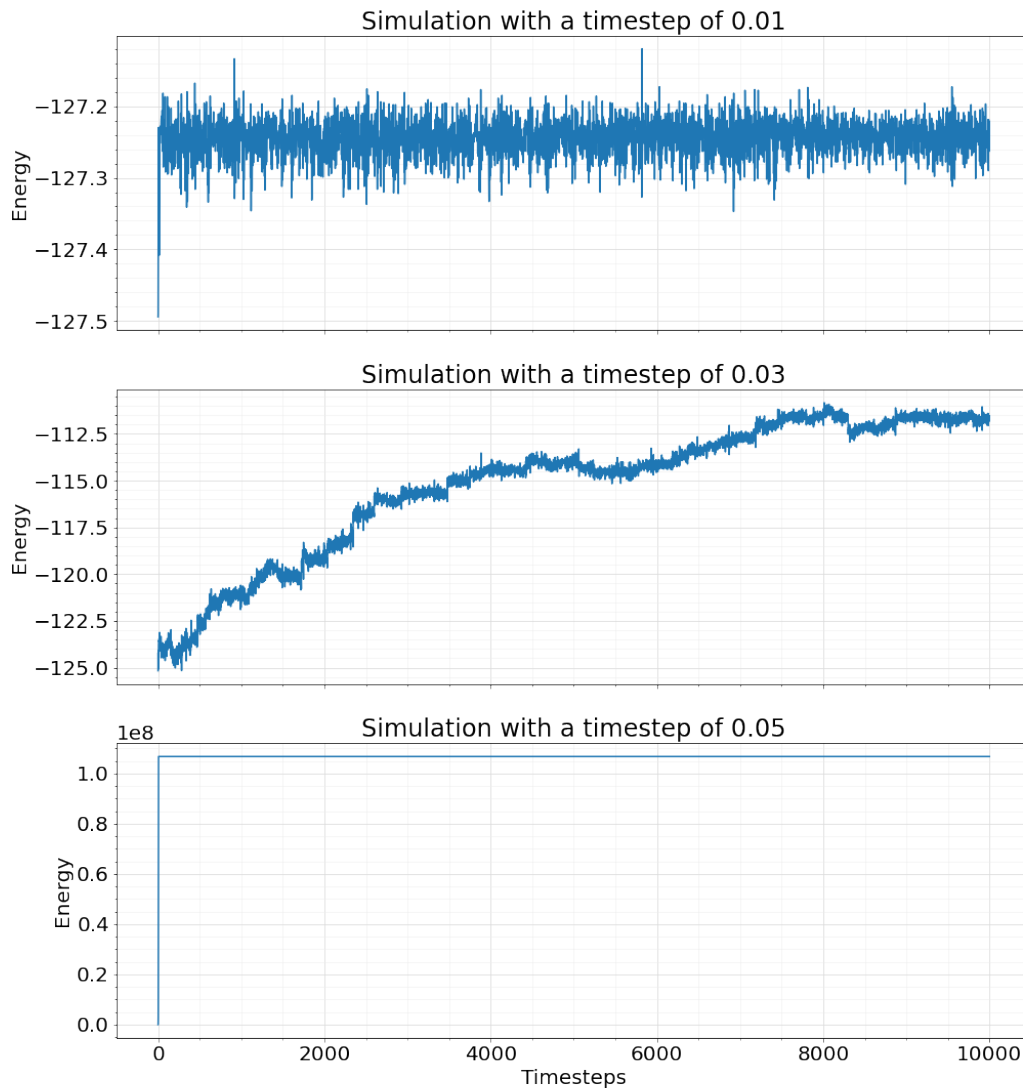


Figure 4.1: Simulation with different timesteps

The first task of the course asks to plot the total energy of the simulation for different time steps. The units were in a Lenard-Jones equivalent and not given here. As can be seen in the sequence 4.1, with a bigger and bigger timestep the energy in the simulation goes from stable (timestep 0.01) over a drifting behavior (timestep 0.03) to being unstable (timestep 0.05). A good timestep for this simulation would be 0.01.



To visualize the simulation OVITO [2] was used and this series of images was created.



Figure 4.2: Simulation Snapshot

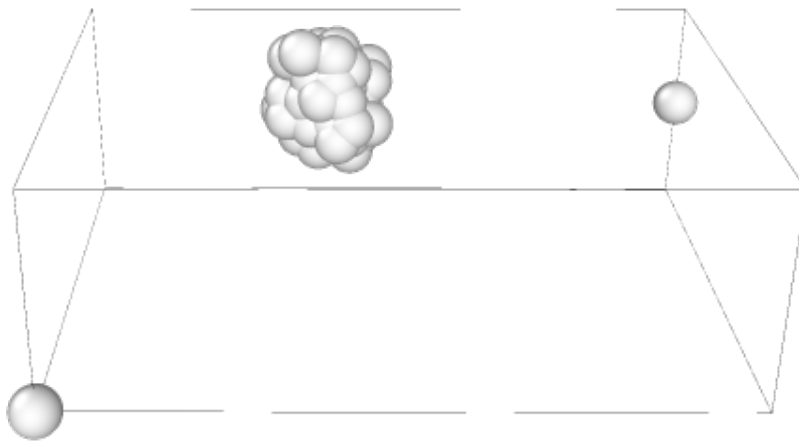


Figure 4.3: Simulation Snapshot



Figure 4.4: Simulation Snapshot

As it can be seen in the images 4.2, 4.3 and 4.4 the Atoms are initially ordered into a blob, which was given in the course. Later in the simulation some of the atoms escape the initial blob and fly outward separately.

## 4.2 Result from the Simulation with the Berendsen Thermostat

After incorporating the Berendsen Thermostat into the code it is interesting to look at the computational complexity of the simulation. With growing numbers of atoms the computation of should follow an order of something like  $O(N^2)$ . The main culprit for this is the force-computation, as each interaction with all the other atoms in the simulation has to be computed. This is also shown in the next figure as the computation time follows a quadratic function.

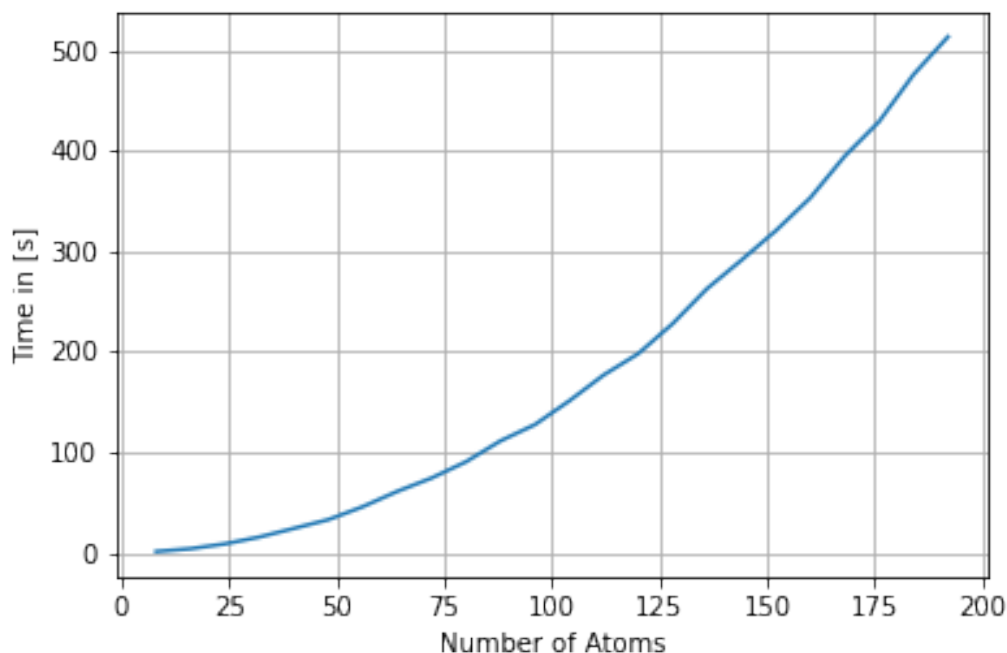


Figure 4.5: Simulationtime with the Berendsen Thermostat from 8 to 192 Atoms

Although all the interaction between all the atoms are computed they do not carry the same weight to the force that affects the atom. It should be rather clear that, the further apart atoms are, the smaller the force gets. After a certain distance it gets so small that it can be ignored. This leads to the idea to use neighborhood-lists that ignore the atoms outside of a certain radius, which was done in the next section.

## 4.3 Results from the Simulation with the Neighborhood-List

After running the simulation in the previous section, it was clear that they follow a computational complexity of the order  $O(N^2)$ . This can be reduced to a linear order  $O(N)$  with the usage of

neighborhood-lists. Only the atoms in a certain radius around the atom will be computed and a force will be added to the total force affecting the atom.

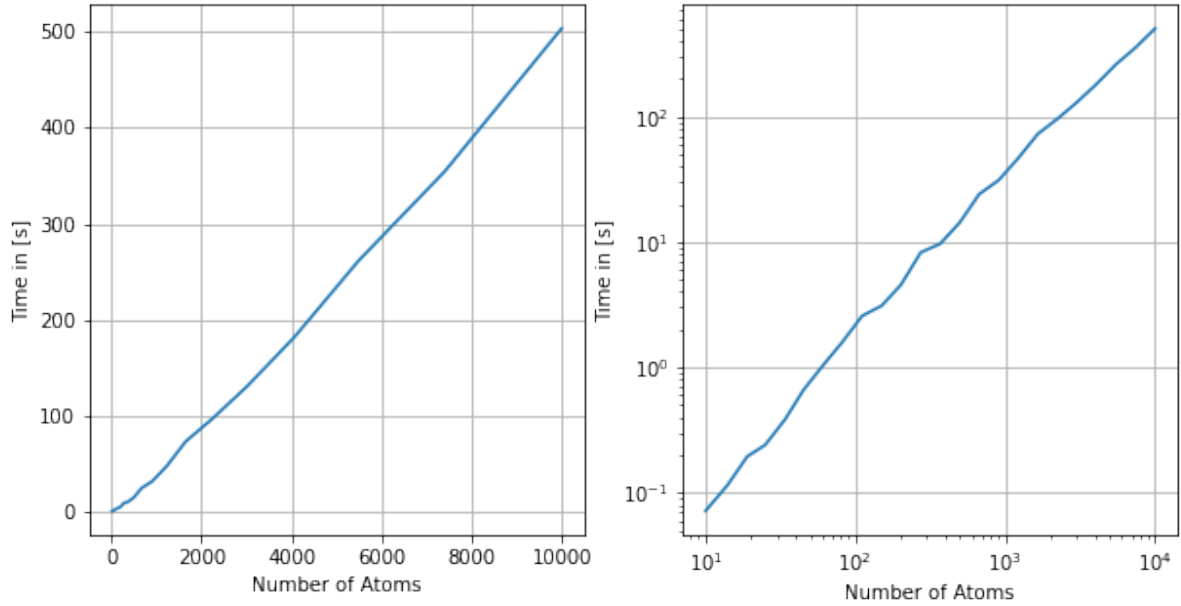


Figure 4.6: Simulationtime with the Neighborhood-list

This can be seen in figure 4.6 on a linear and a logarithmic scale.

## 4.4 Results from the Simulation with the Gupta-Potential

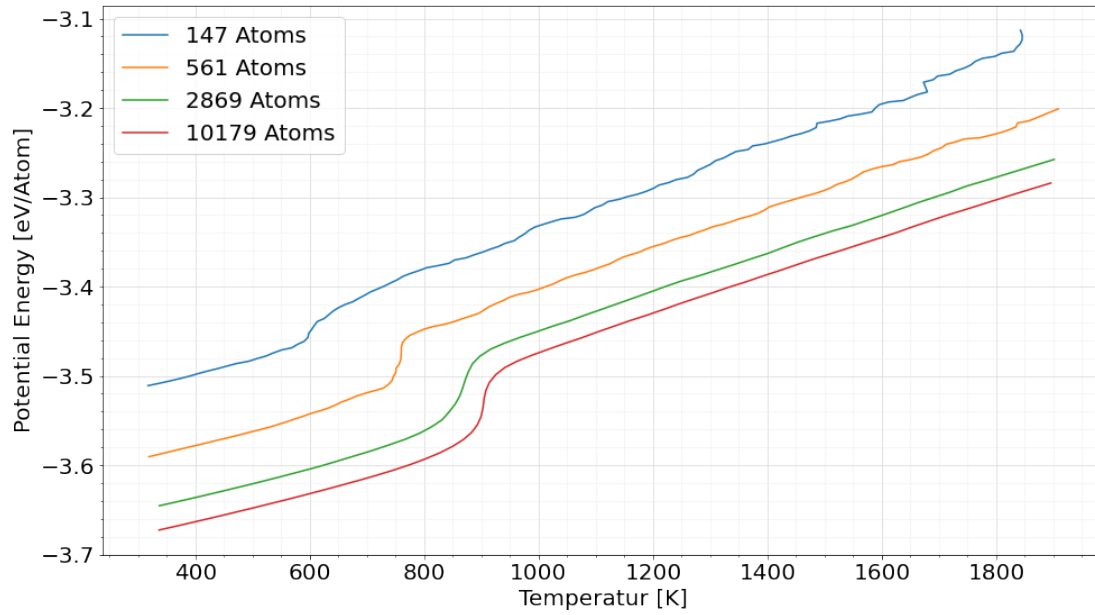


Figure 4.7: Gold Cluster Simulation

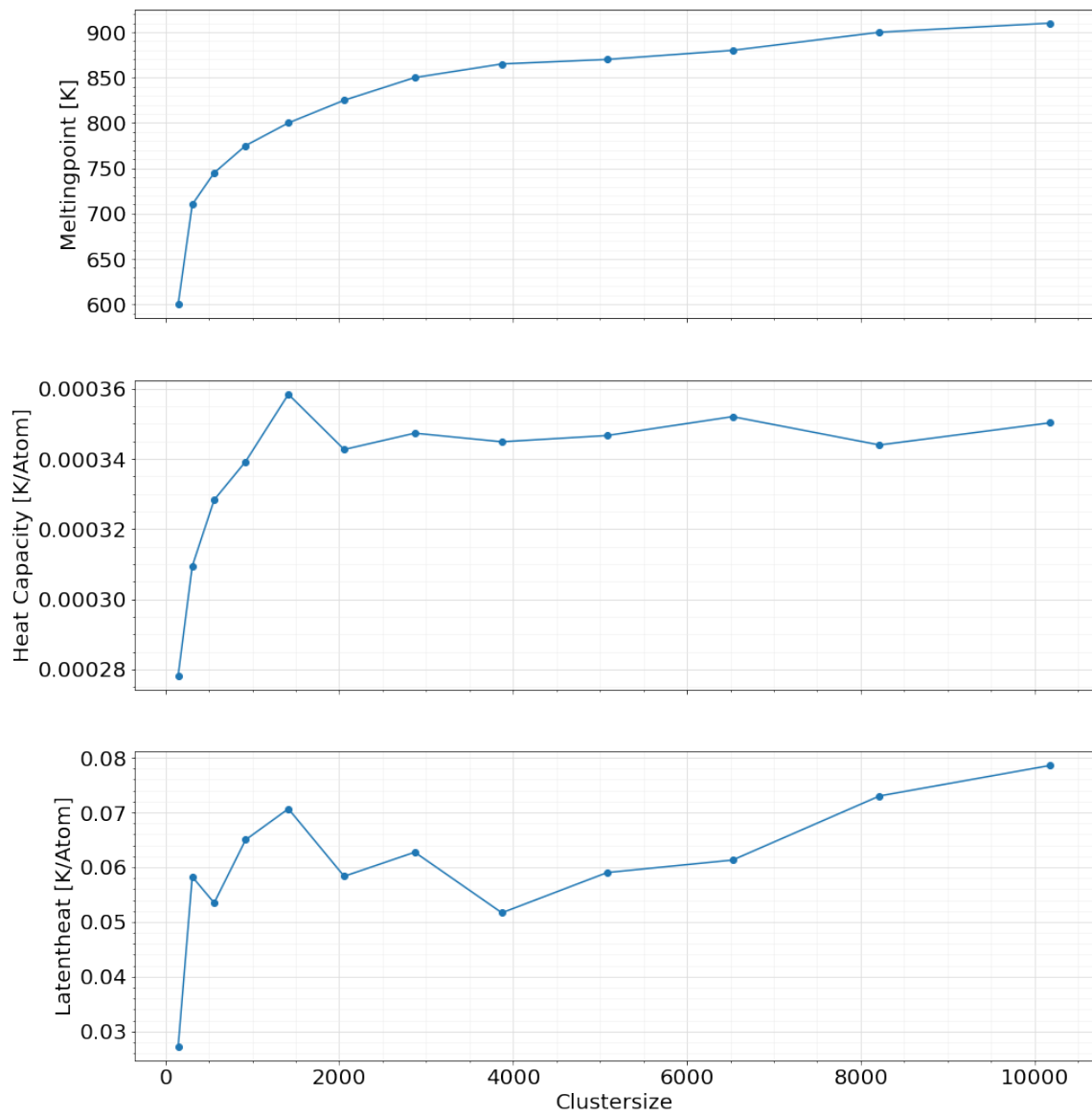


Figure 4.8: Melting Point, Heat Capacity and Latent Heat vs Clustersize

## **Chapter 5**

## **Conclusion**

# Bibliography

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