

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

1.2 Different Time Steps

1.3 Simulation Snapshots

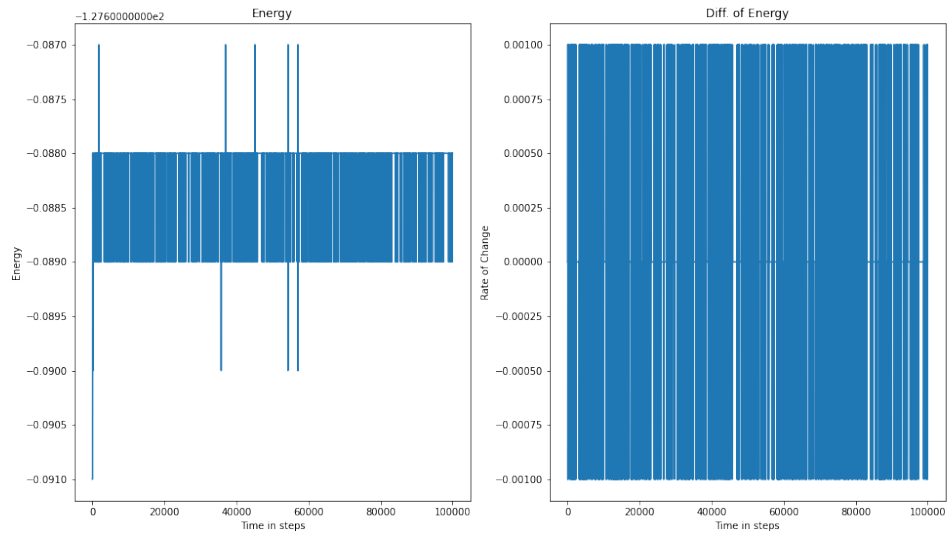


Figure 1.1: Simulation with a time step of 0.001

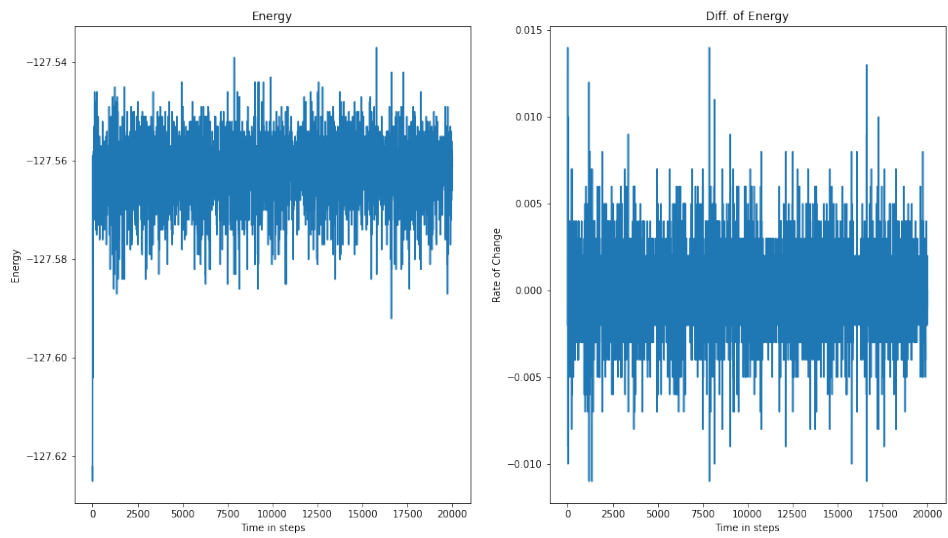


Figure 1.2: Simulation with a time step of 0.005

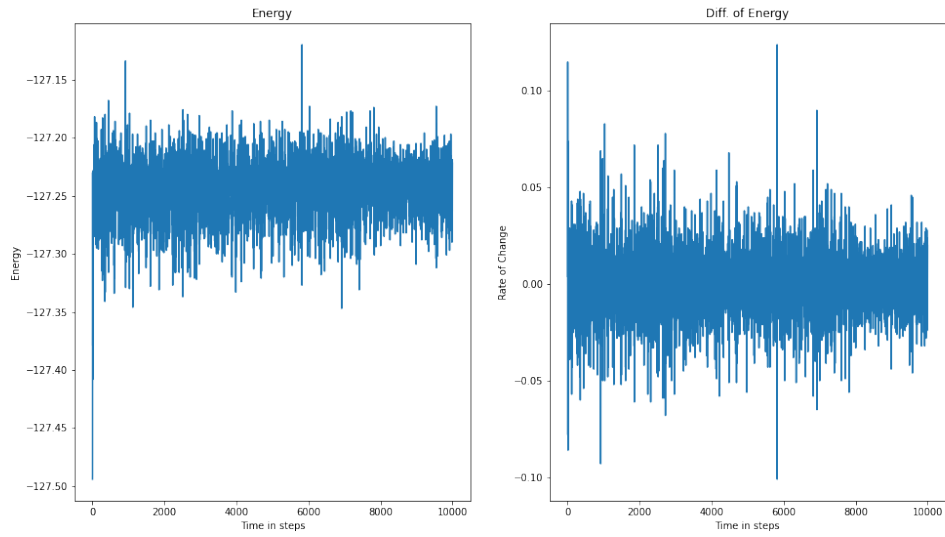


Figure 1.3: Simulation with a time step of 0.01

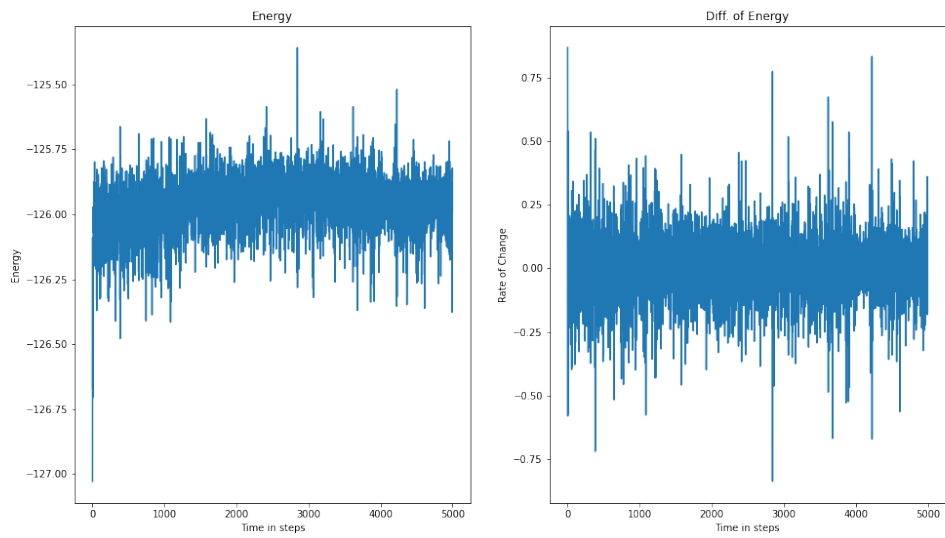


Figure 1.4: Simulation with a time step of 0.02

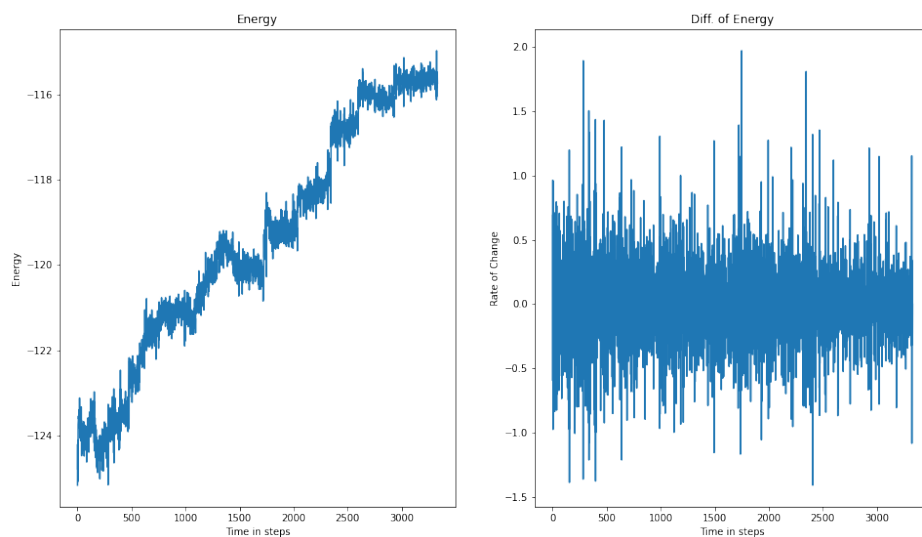


Figure 1.5: Simulation with a time step of 0.03

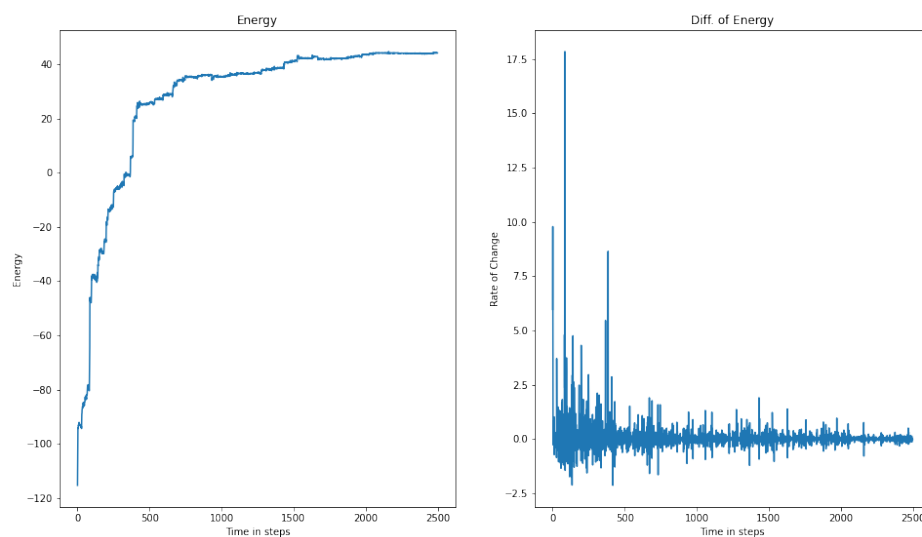


Figure 1.6: Simulation with a time step of 0.04



Figure 1.7: Simulation

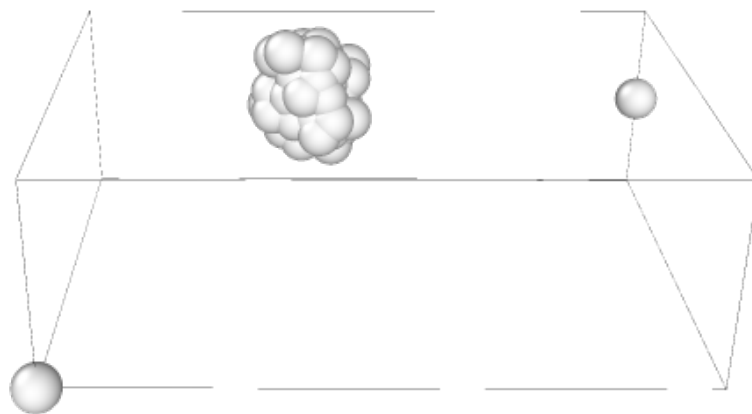


Figure 1.8: Simulation



Figure 1.9: Simulation



Figure 1.10: Simulation

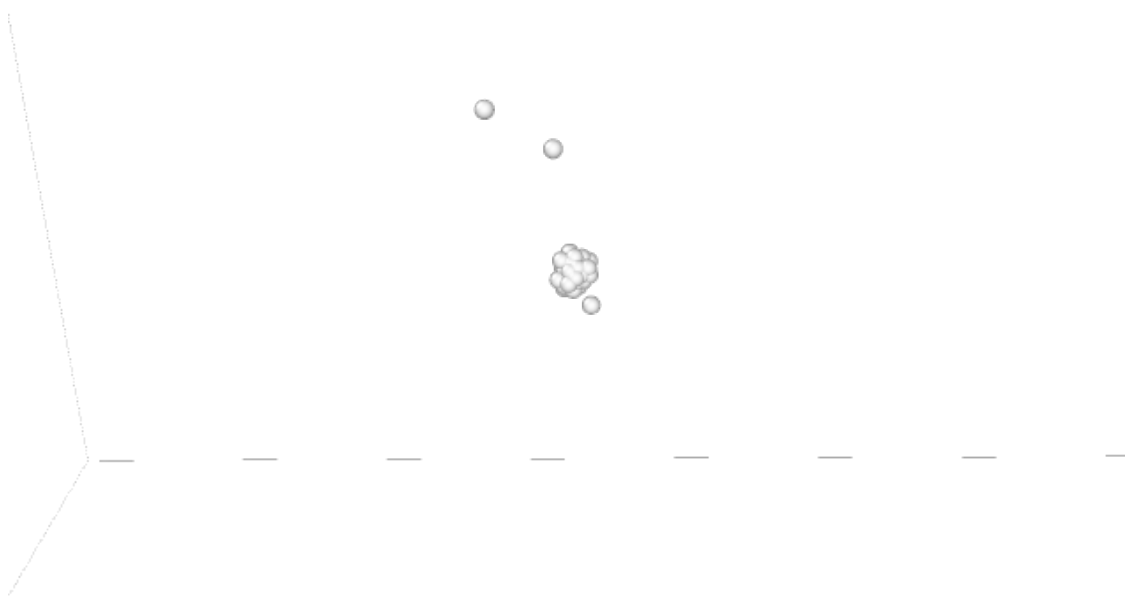


Figure 1.11: Simulation

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

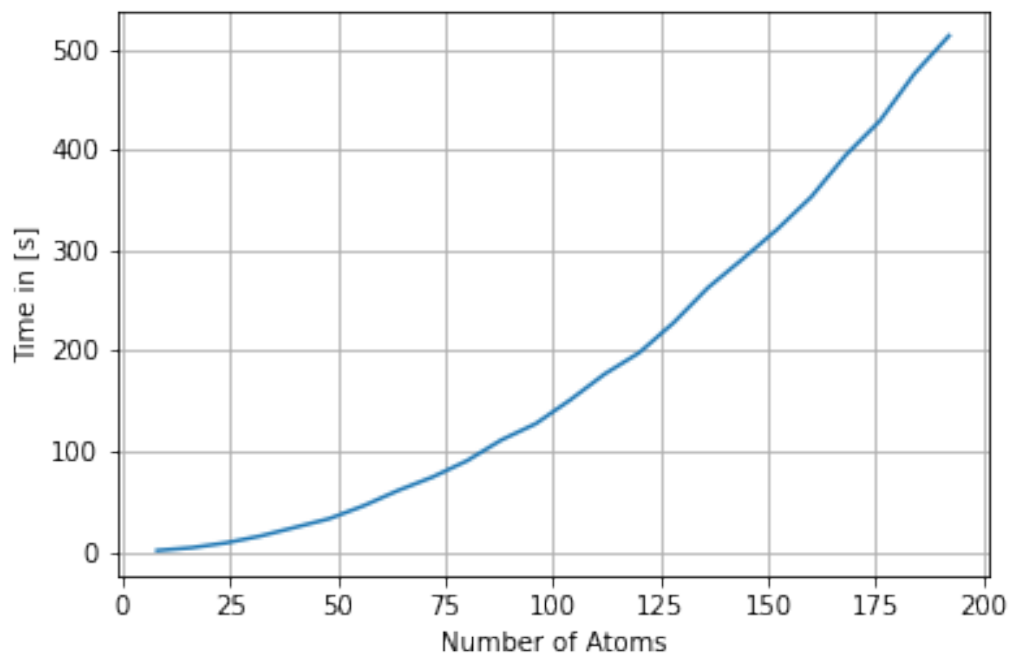


Figure 2.1: Simulationtime from 8 to 192 Atoms