

Chapter 1

Milestone 4

1.1 Force-Derivation from the Energy

```
[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

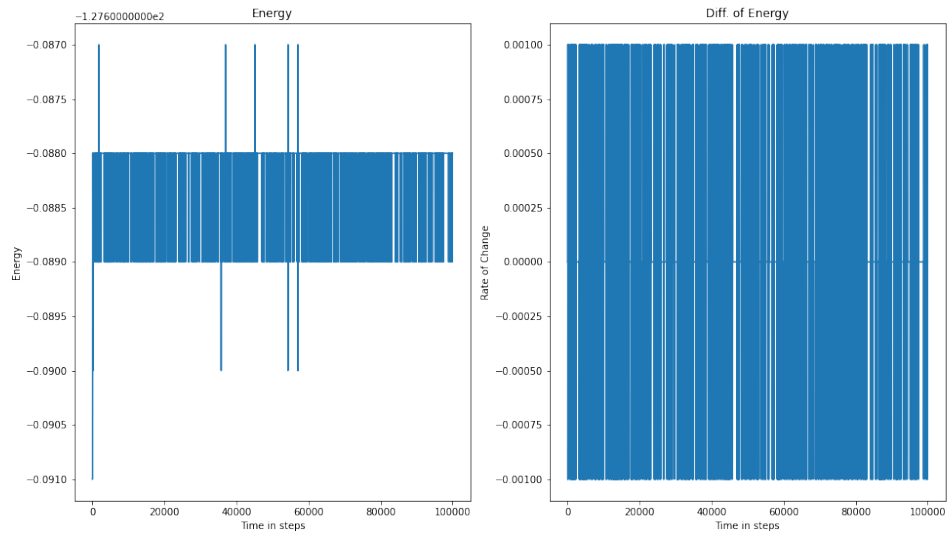


Figure 1.1: Simulation with a time step of 0.001

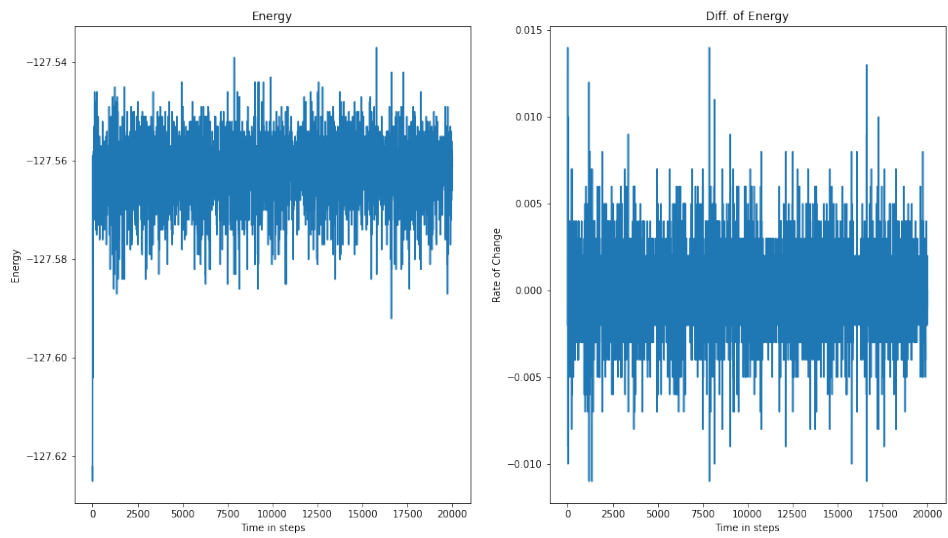


Figure 1.2: Simulation with a time step of 0.005

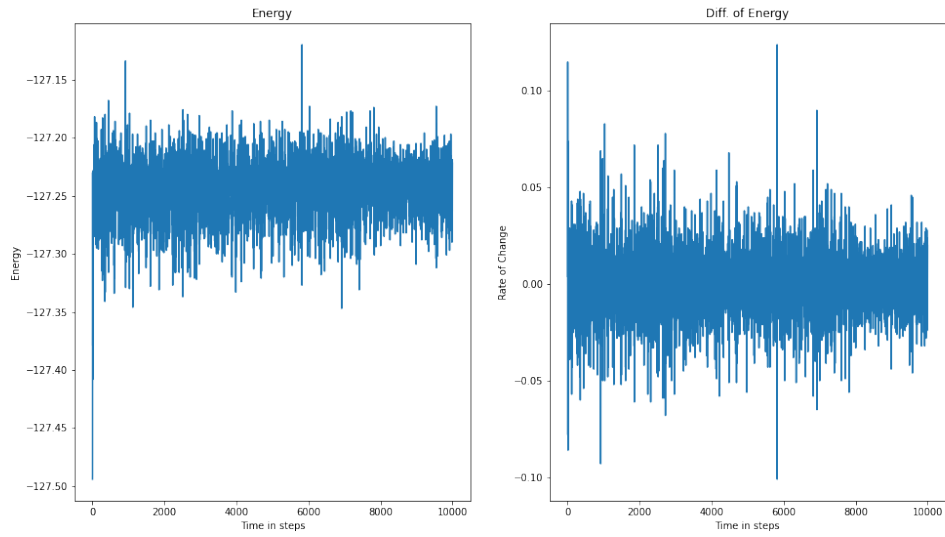


Figure 1.3: Simulation with a time step of 0.01

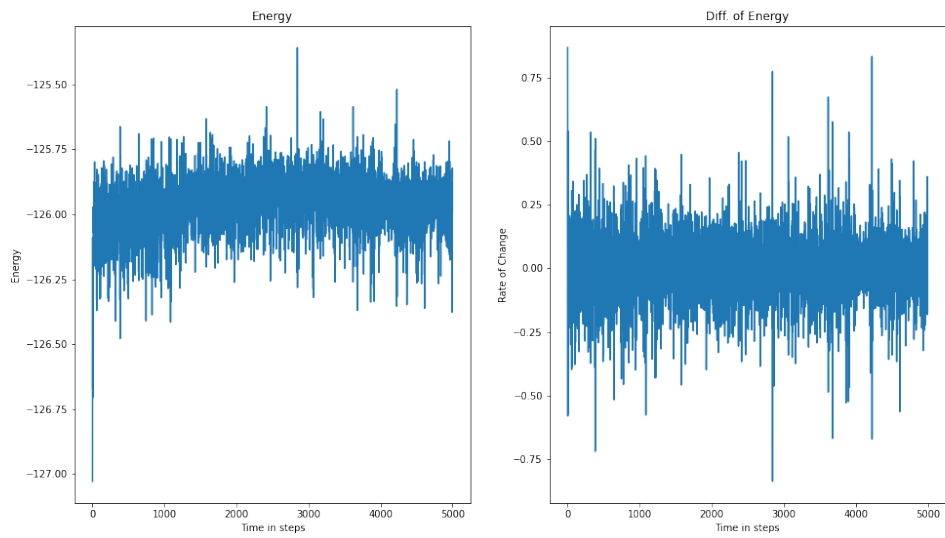


Figure 1.4: Simulation with a time step of 0.02

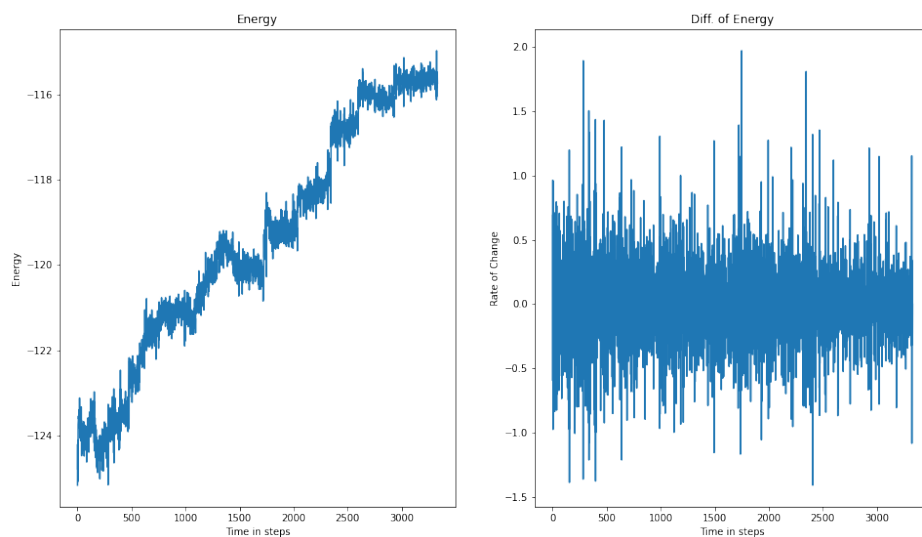


Figure 1.5: Simulation with a time step of 0.03

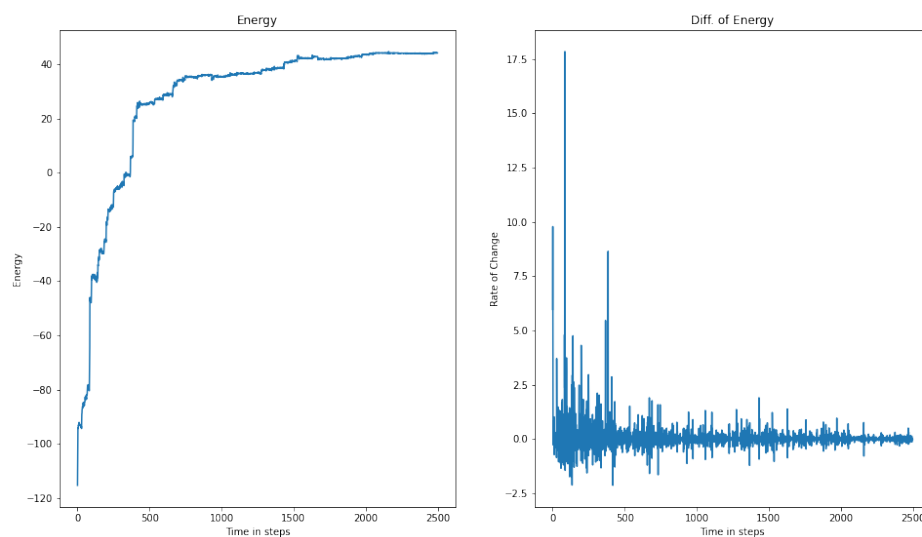


Figure 1.6: Simulation with a time step of 0.04



Figure 1.7: Simulation

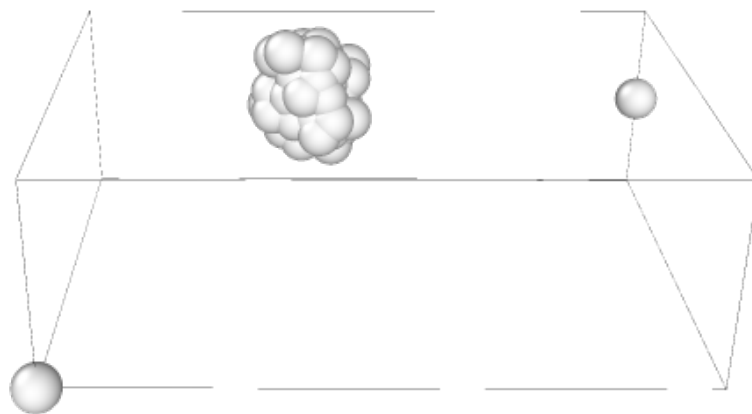


Figure 1.8: Simulation

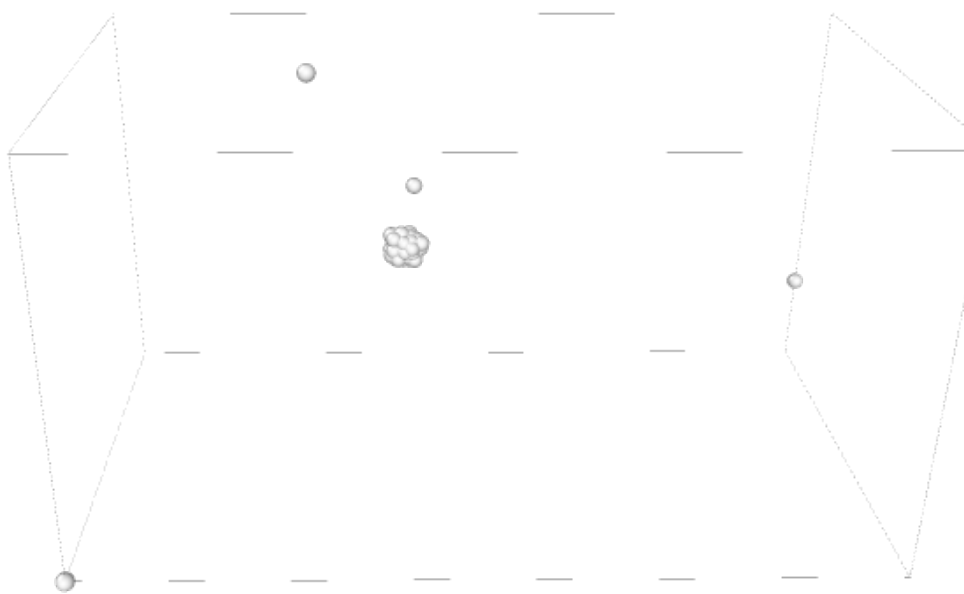


Figure 1.9: Simulation



Figure 1.10: Simulation

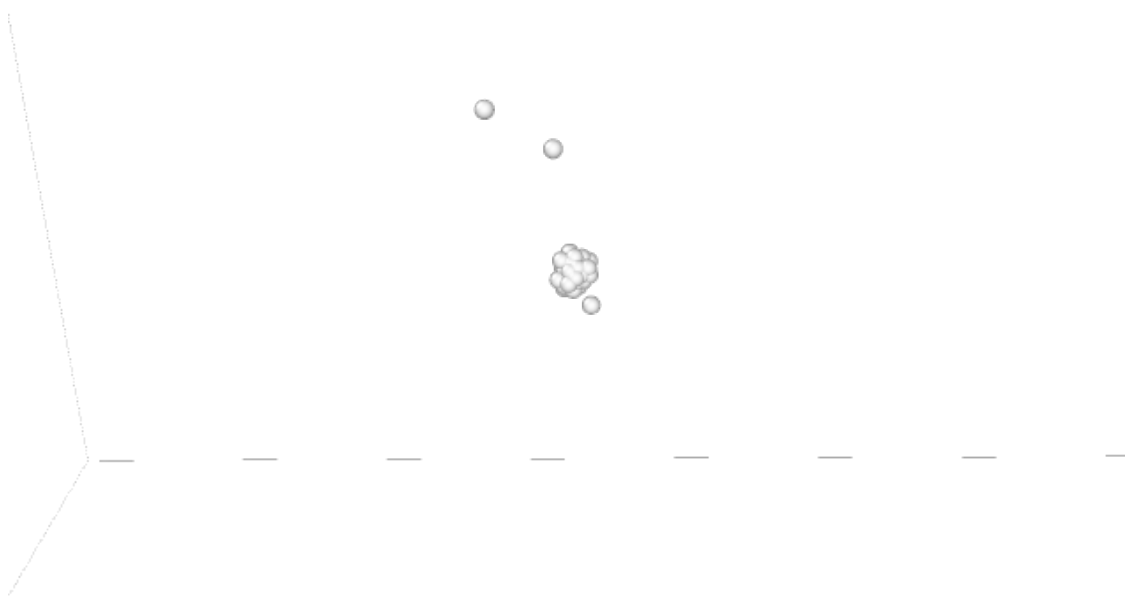


Figure 1.11: Simulation