

Sheet00

Computational Physics

12. Mai 2023

1 Solution

- a) As the first part of the exercise was to just implement the constructor we don't have anything to show for this part besides the code.
- b) In exercise part b we were supposed to write a measurement and equilibrate function that simulated the interaction between particles. Three different simulations were asked for. One with 16 particles, one with 64 and one with 256. After the system were in a rough equilibrium we measured the kinetic and potential energy of the system as well as the temperature. The resulting plots can be seen below.

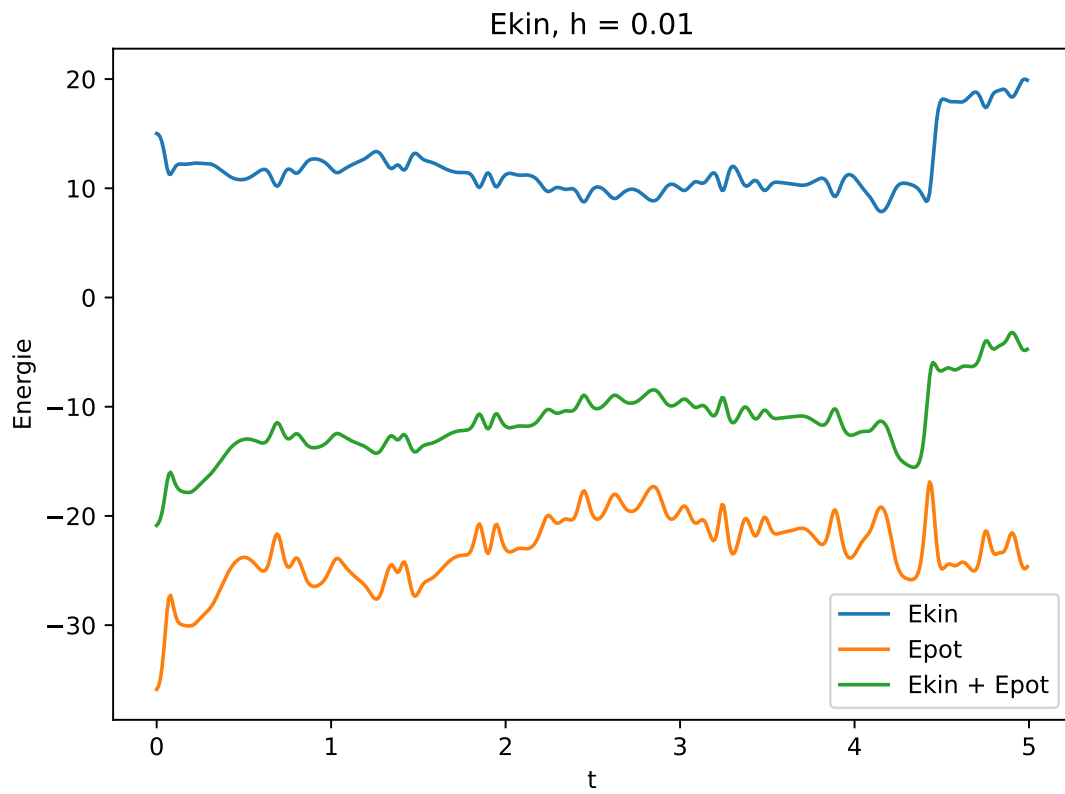


Abbildung 1: The energy of the 16 particle simulation over 5 seconds with a stepsize of 0.001.

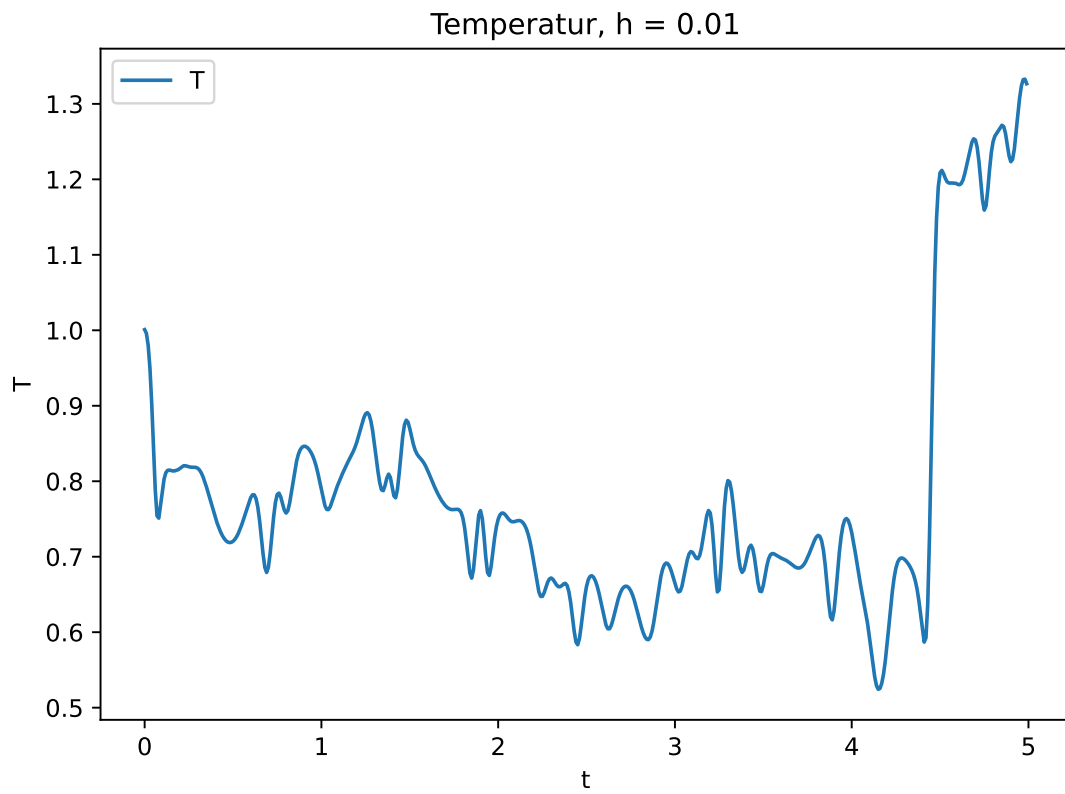


Abbildung 2: The temperature of the 16 particle simulation over 5 seconds with a stepsize of 0.001.

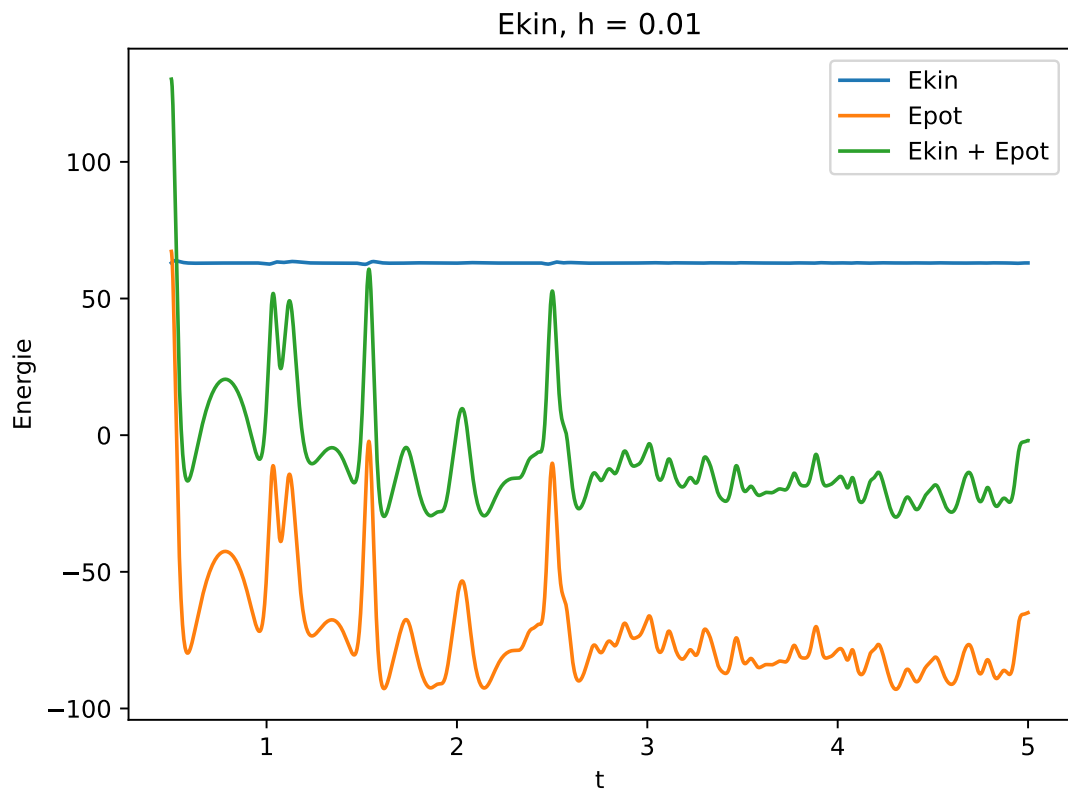


Abbildung 3: The energy of the 64 particle simulation over 5 seconds with a stepsize of 0.001.

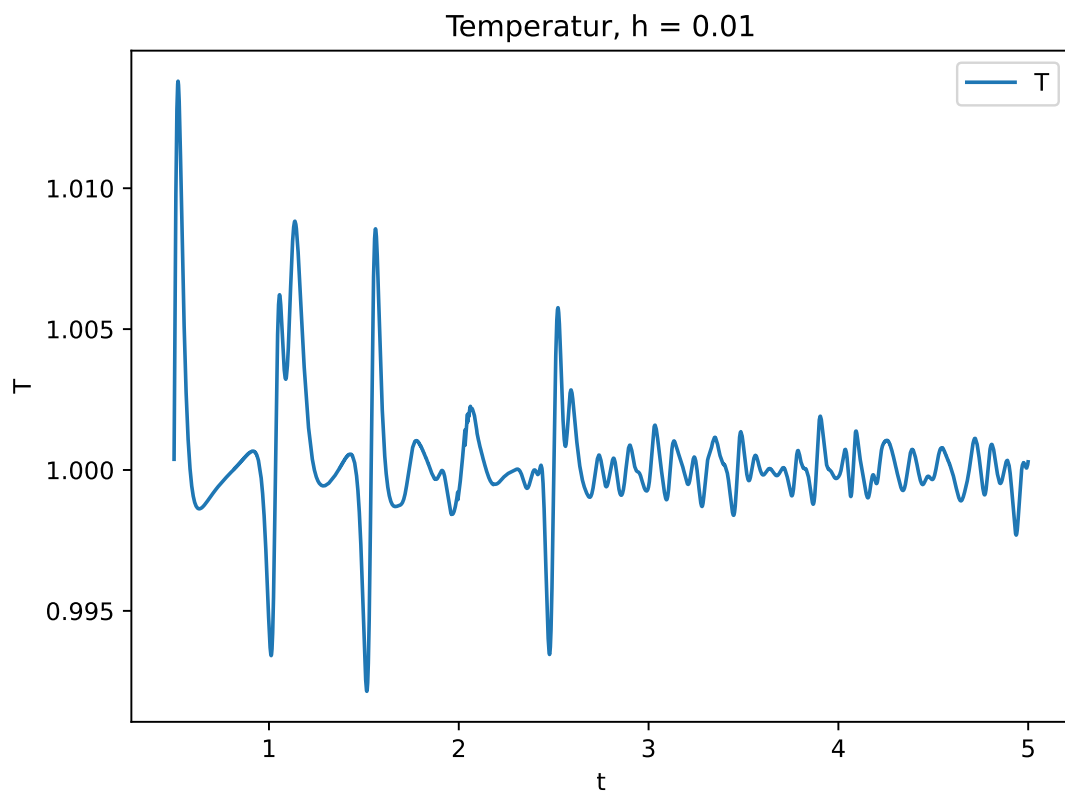


Abbildung 4: The temperature of the 64 particle simulation over 5 seconds with a stepsize of 0.001.

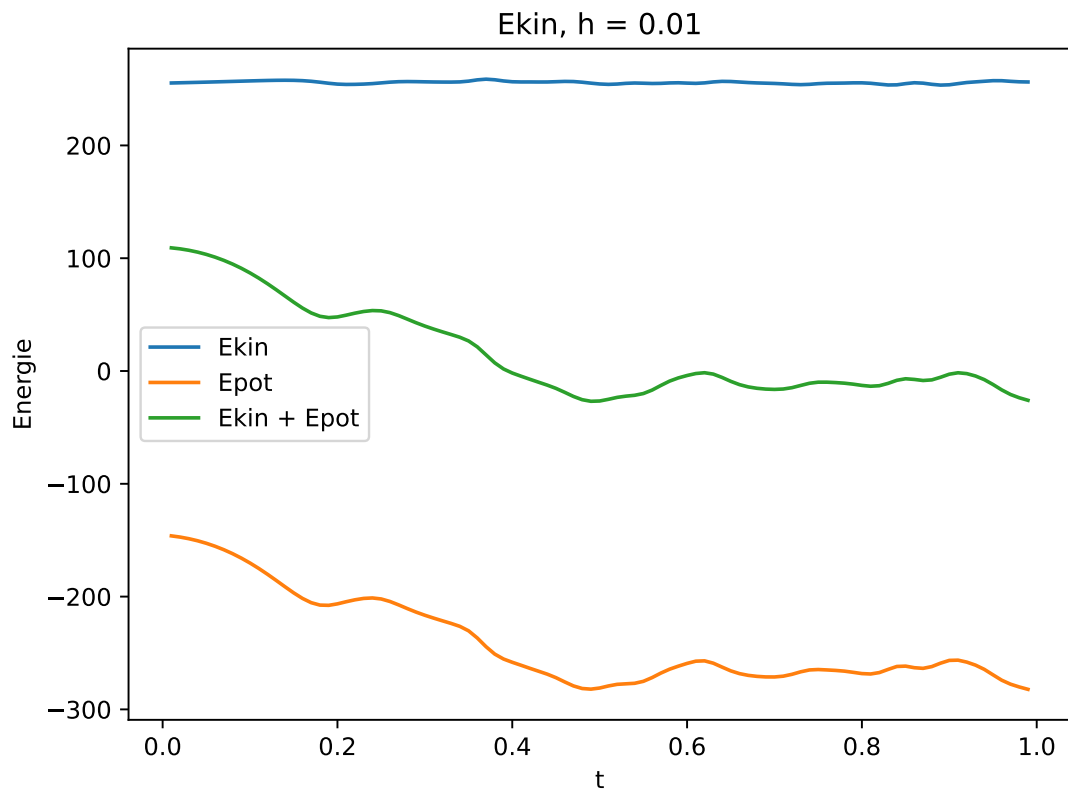


Abbildung 5: The energy of the 256 particle simulation over 5 seconds with a stepsize of 0.001.

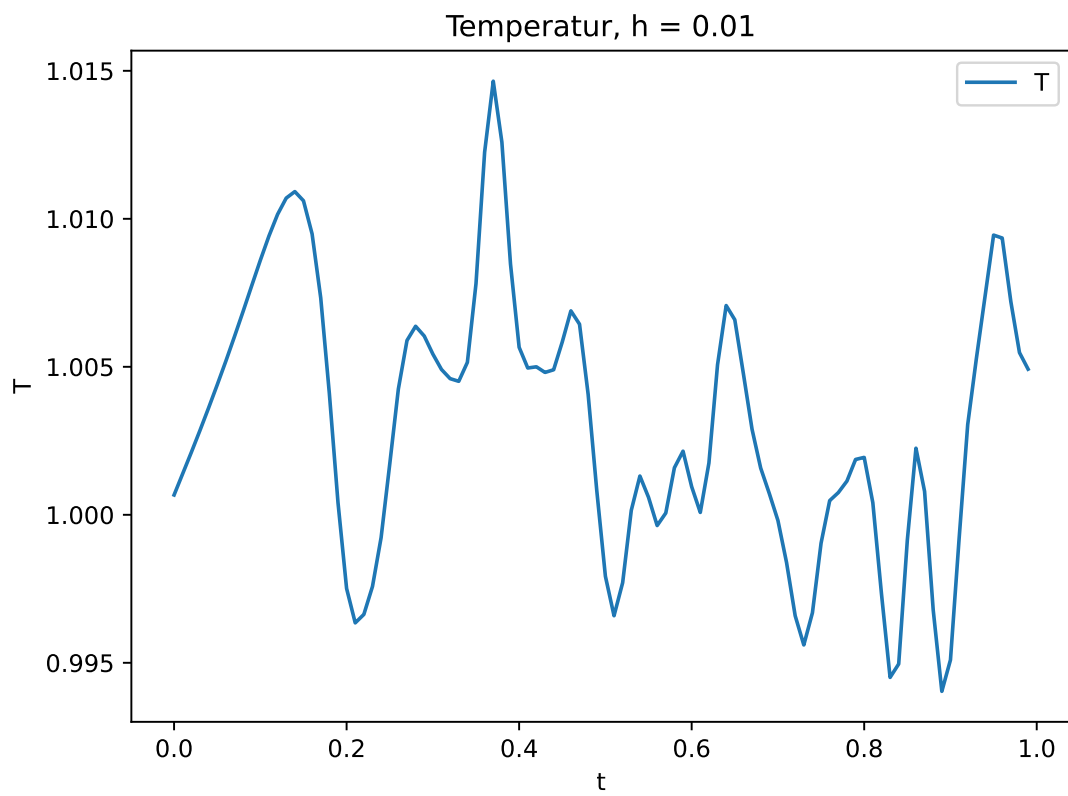


Abbildung 6: The temperature of the 256 particle simulation over 5 seconds with a stepsize of 0.001.

Overall we expected a smaller fluctuation in both energy in temperature. We also expected the potential Energy to be equal to the kinetic energy. However the potential energy is about twice as big. The kinetic energy also does some really weird stuff if we don't rescale it with the thermostat after every step. This is probably not intended, but we don't really have the time to find the bug. With more time we probably could have fixed that mistake.

- c) It is 20 minutes before midnight right now and our code just started working kind of like it should so I am not sure if the simulation is going to produce results soon enough. It's five minutes before midnight and the program is still running. So I guess this means we won't have plots on this part. Maybe I can append some plots after the due date.
- d) We implemented the isokinetic thermostat. However, we did not really have the time to test it out properly. But what probably happens is a condensed matter phase. So the particles we build something like a grid or semi stable system.
- e)
 - quantities that are kept constant are
 - * particle number
 - * Volumen of the box
 - * Basically the energy as well
 - So the simulation is modelling a microcanonical ensemble.
 - No the isokinetic thermostat is not physically accurate. A more accurate thermostat would be the Nose-Hoover Thermostat. This thermostat actually results in a Boltzmann-distribution for the energy.
 - First of all a chemical solution might be reactive. This could change the temperature over time. A chemical solution might also have particles of different mass. However this won't change the ensemble. Overall the most accurate ensemble would be the grand canonical ensemble as the chemical potential stays the same, but the particle number changes.