Report for Exercise 10

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May 17, 2022

1 Task 1

In this exercises I adapted the code for the naive Verlet algorithm from task07 to simulate a micro-canonical ensemble using the nosé-hoover algorithm. The nosé-hoover-verlet code is in ”naive-nose-hoover-verlet.py”. In Figure 1 I compare the total energy of the system computed with the naive verelt method with the energy computed using the nosé-hoover-verlet with $Q = 10000000$. We can see that look similar(despite the small drop in the enerty of the naive-verlet). This show that the noseé-hoover-verlet indeed simulates the canonical ensemble for $Q \to \infty$.

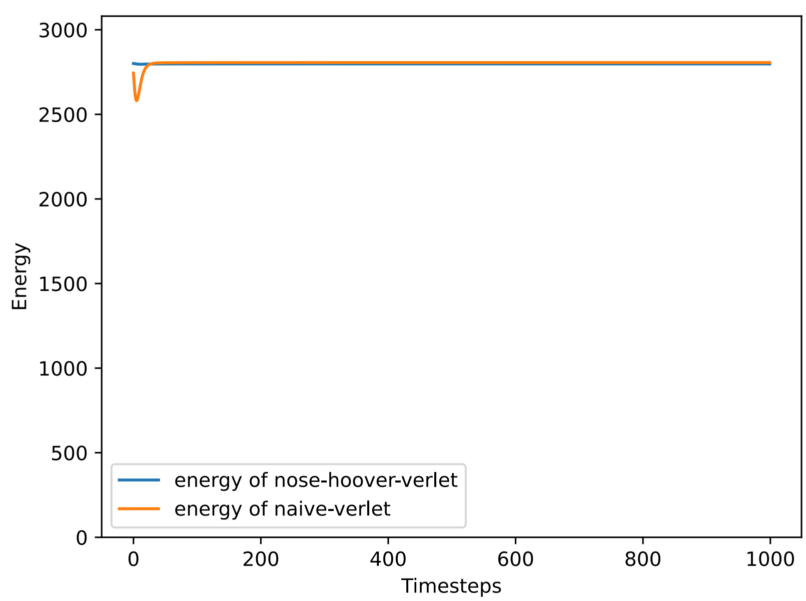

Figure 1: total energy of the system over time computed using the naive verlet and the nosé-hoover verlet for $Q = 10000000$.

2 Taks 2

For this task I observed the evolution of the instantaneous temperature for different values of Q as a function of time. I always simulated 60 particles in a box of size 10 coupled with a heat-batch of temperature $T = 1$. The results are shown in figure 2.

Looking at figure 2 one can see that for bigger values of Q the relaxation towards equilibrium

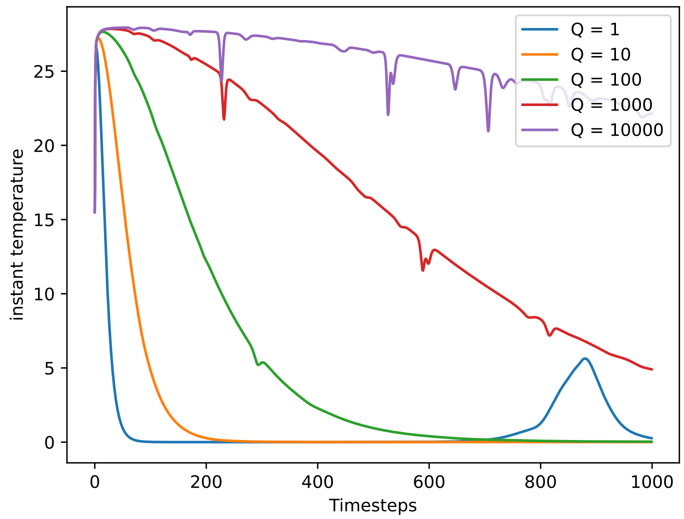

Figure 2: Instantaneous temperature over time obtained from nosé-hoover-verlet simulations for different thermal inertias Q.

takes longer then for smaller values of Q. This makes sense as for smaller Q the coupling to the heat bath is stronger and for bigger Q the coupling gets weaker and vanishes for $Q \to \infty$.

In figure 3, I again plotted the temperature over time for different values of Q but now most of the systems are already at equilibrium. One can see the temperatures fluctuate periodically over time and that for bigger Qs the frequency of the fluctuations gets smaller.

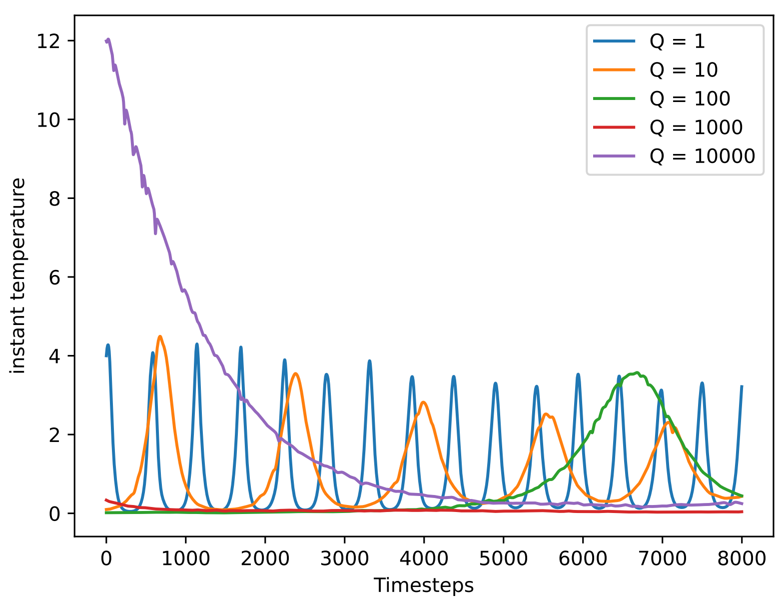

Figure 3: Instantaneous temperature over time obtained from nosé-hoover-verlet simulations for different thermal inertias Q where the system is already at equilibrium.

3 Task 3

In figure 4 on can see the total energy of the system with thermal inertial $Q = 10$.

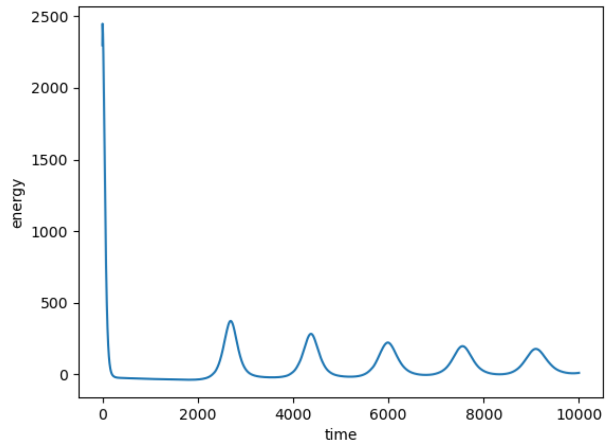

Figure 4: Total energy of the System

In figure 5 one can see the distribution of the sampled systems energy after it has reached equilibrium. I used $Q = 10$ for the Simulation.

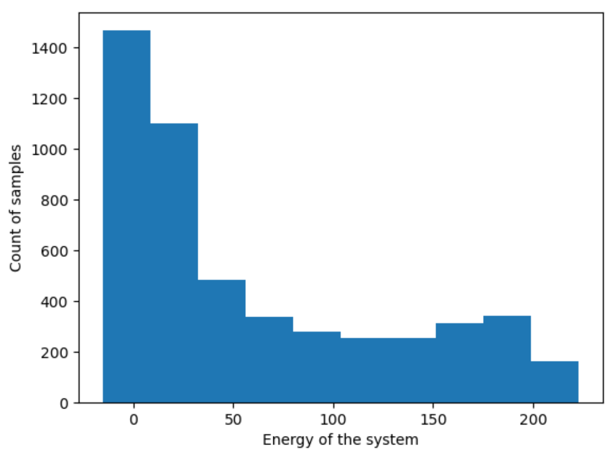

Figure 5: Distribution of the sampled energy of the system at equilibrium.

I think something is off here because I would expect the energy to be normally distributed and I am also not sure whats wrong. Maybe I would need to take bigger values for Q but also for $Q = 100$ I did not find a normal distribution.