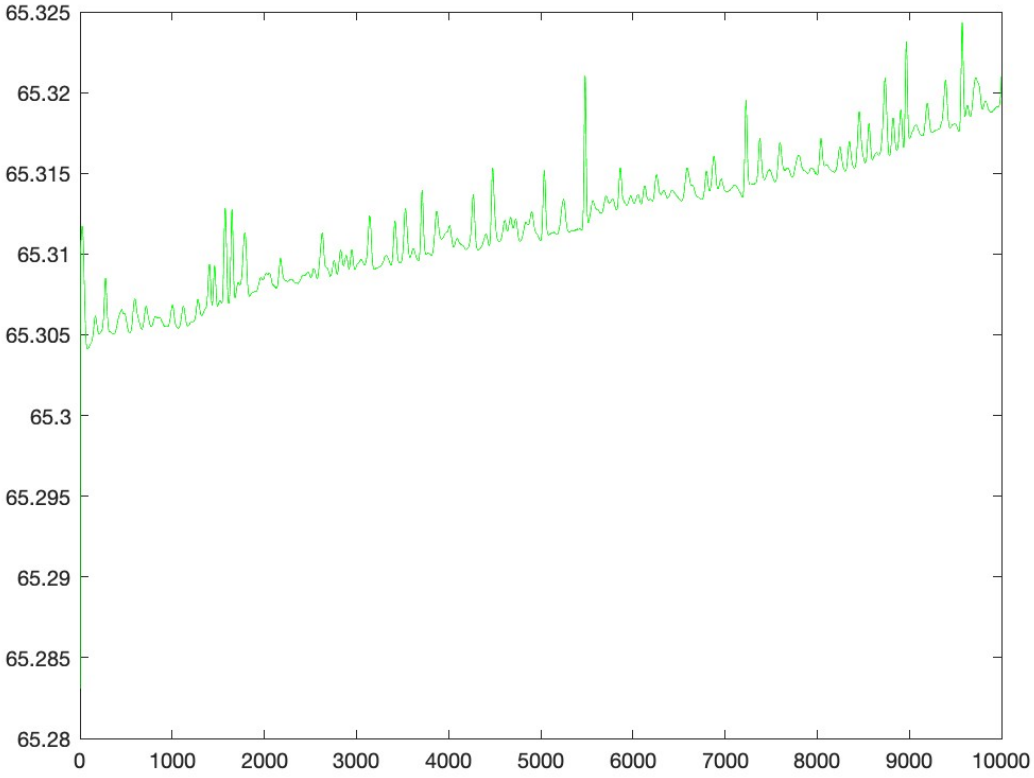
Particle 3

Question1

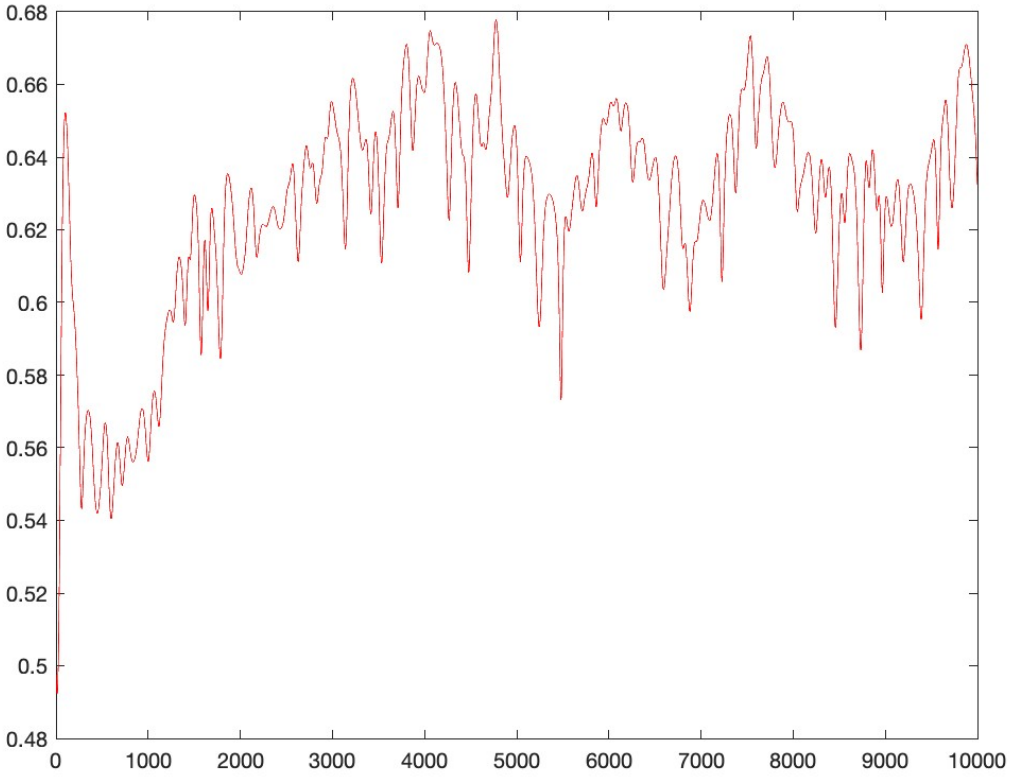
Not using thermostat in these simulations

Baseline (N = 100, v_inial = 0, dt = 0.001)

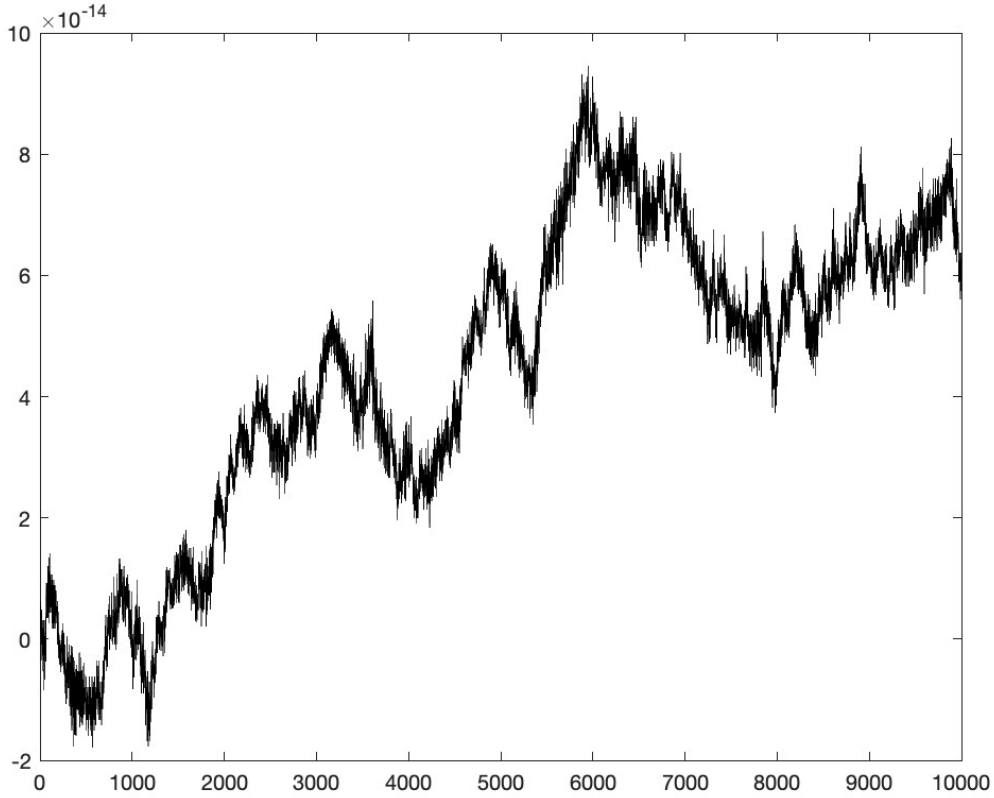
Total Energy



Total temperature



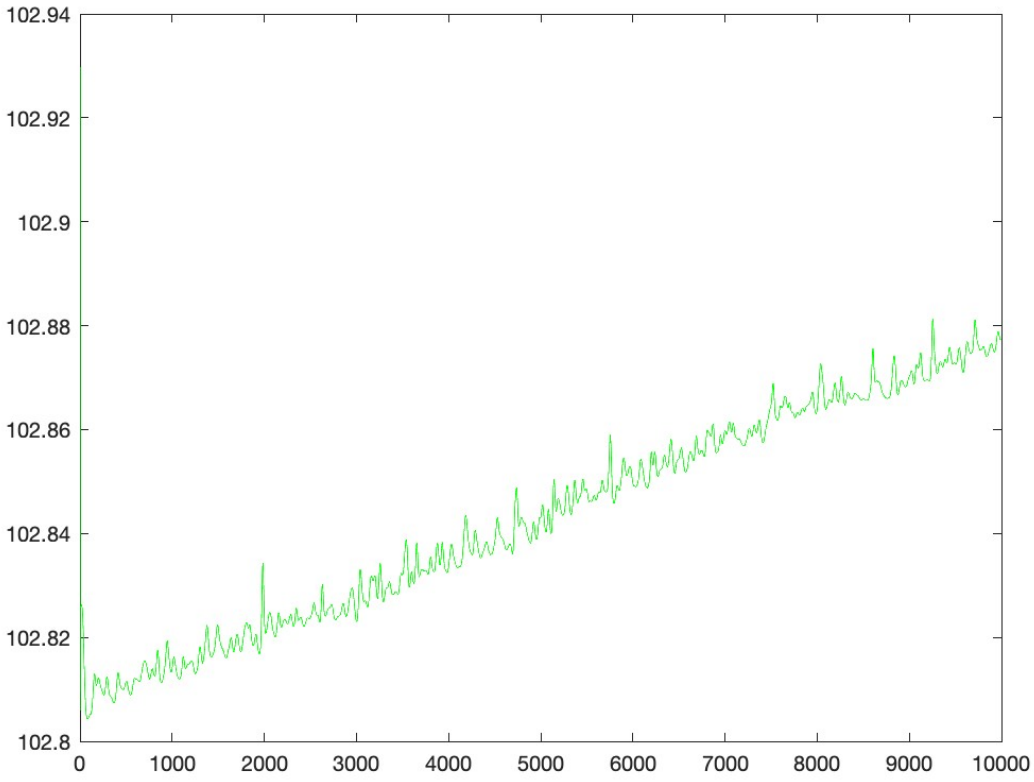
Total momentum



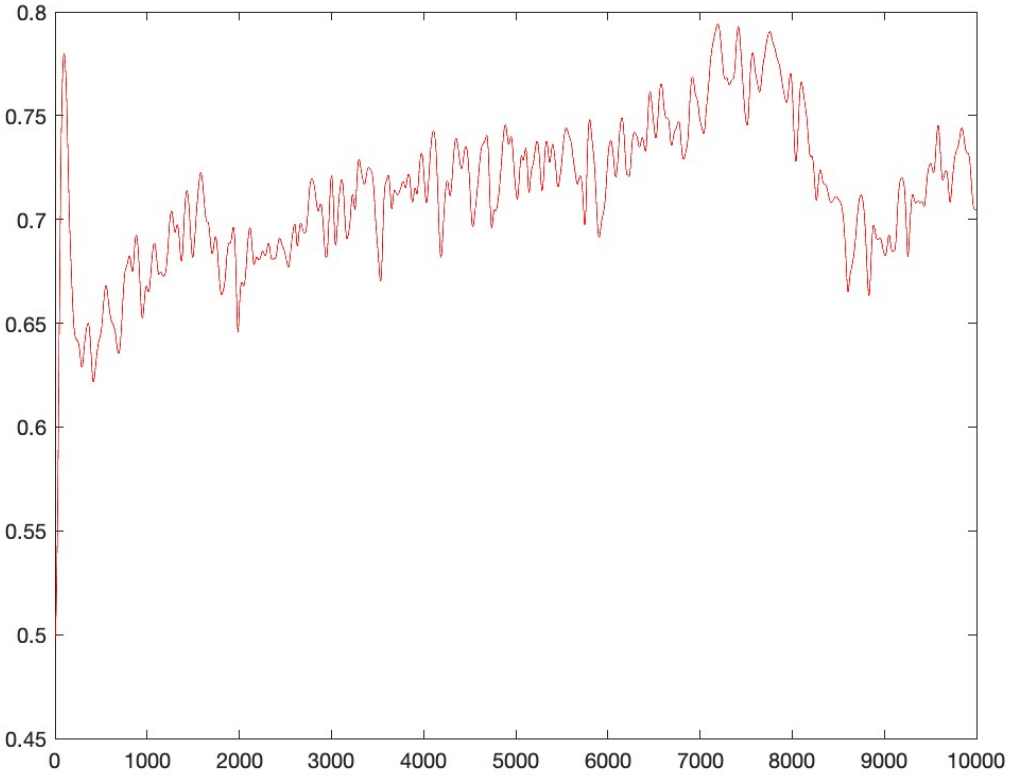
Overall, Total Energy and Total momentum are slowly increasing. The reason for this is that during the numerical calculation, there are truncation errors of Euler Methods or RK methods. So as the simulation time goes by, the error increase which results in the increasing of Total Energy and Total momentum. Also, Total temperature starts to increase and stabilizes with increasing time, fluctuating at a constant. Because as the simulation proceeds, the potential energy of the particles is converted into kinetic energy, after which the system reaches equilibrium. 3000 time steps are needed to reach equilibrium.

Change N (N = 200, v_inial = 0, dt = 0.001)

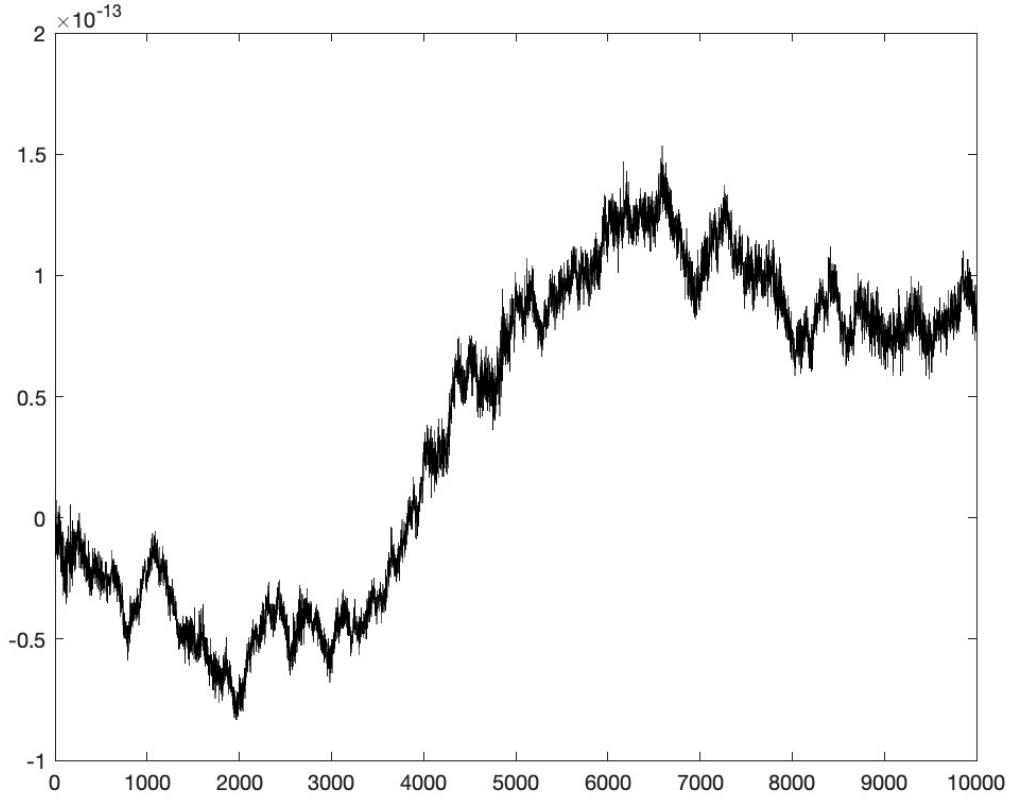
Total Energy



Total temperature



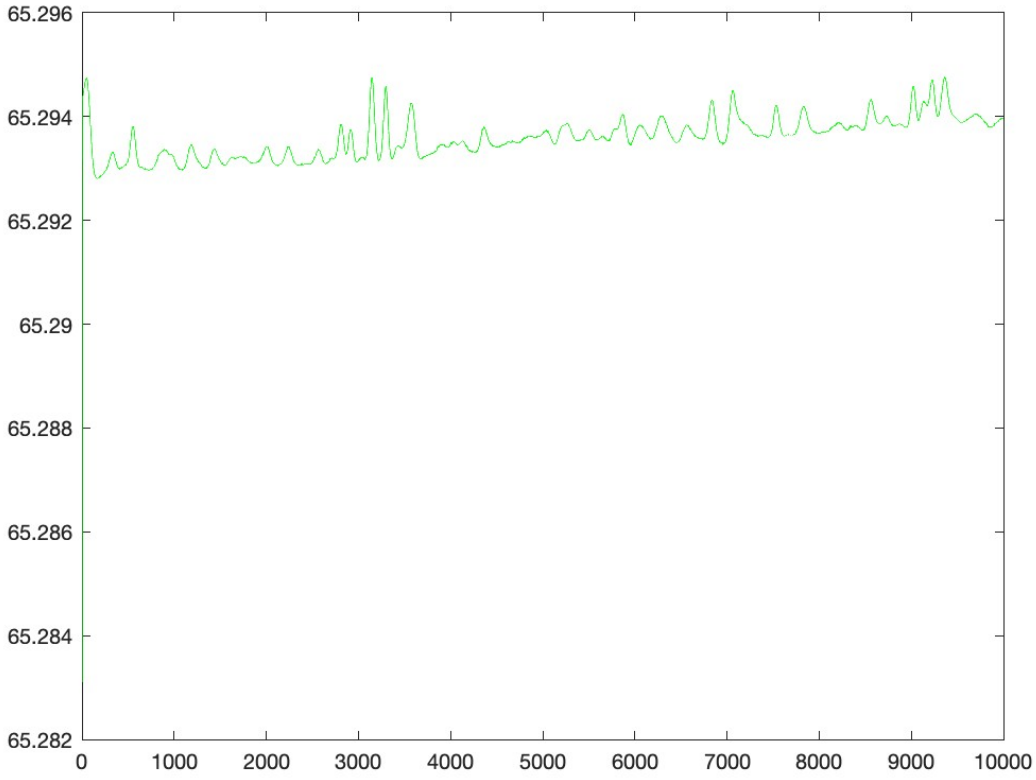
Total momentum



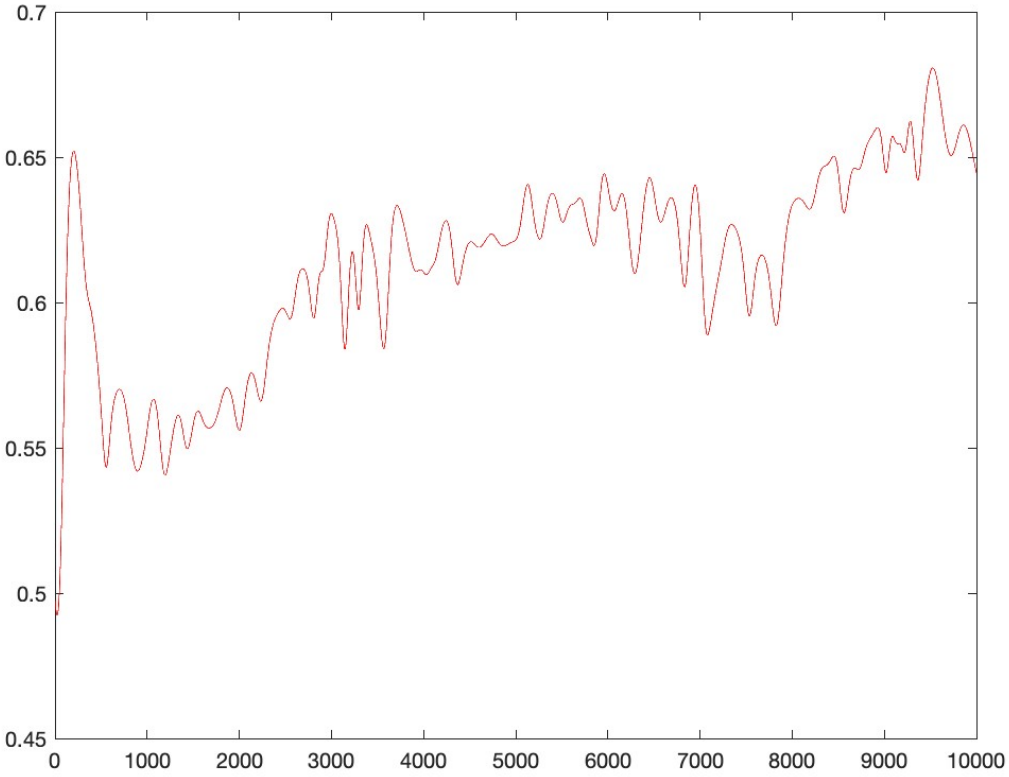
When N becomes 200, the total energy is doubled compared to baselin. And by the system temperature, I found that the system goes into equilibrium earlier when N=200. 2000 time steps are needed to reach equilibrium.

Change dt (N = 100, v_inial = 0, dt = 0.0005)

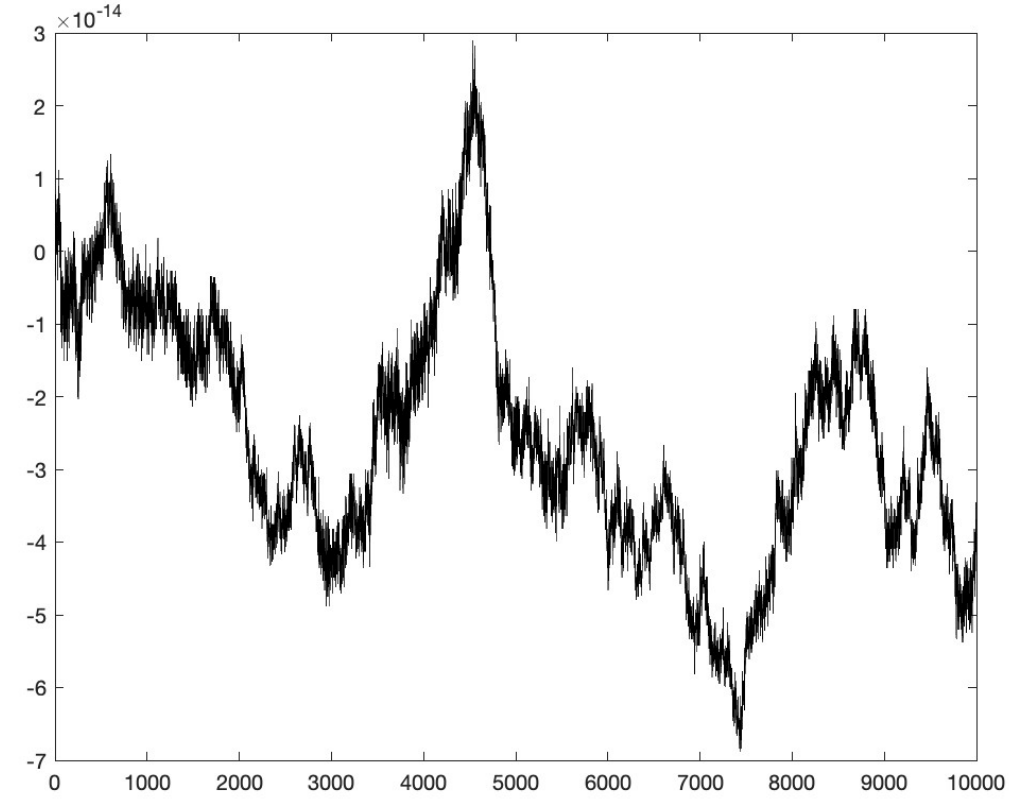
Total Energy



Total temperature



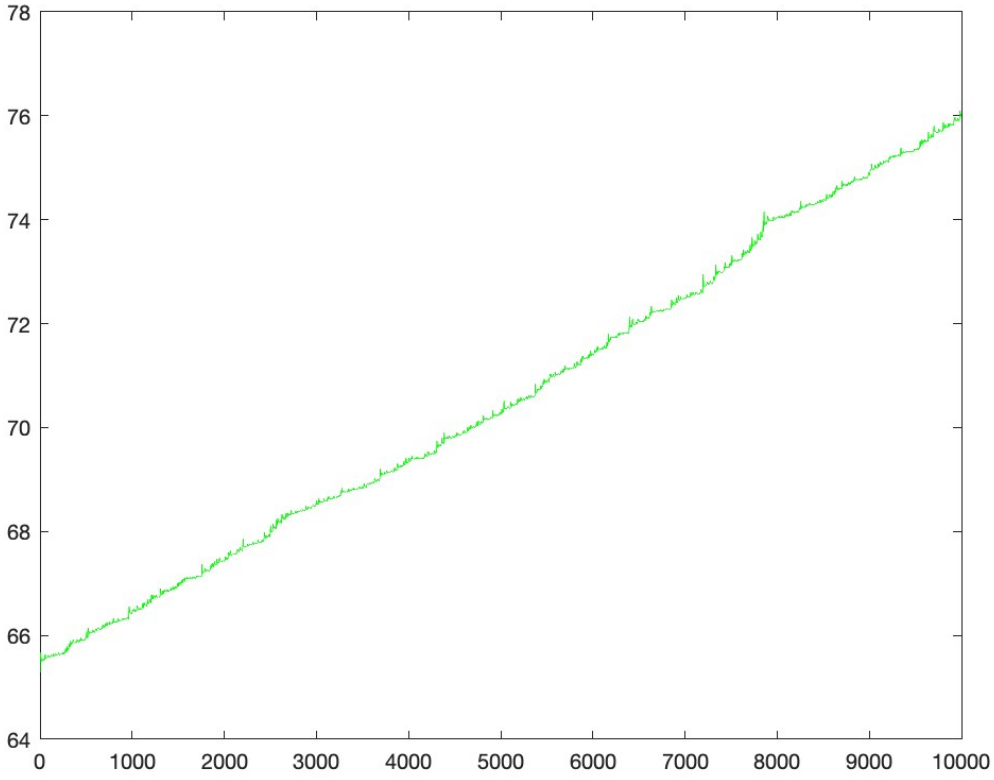
Total momentum



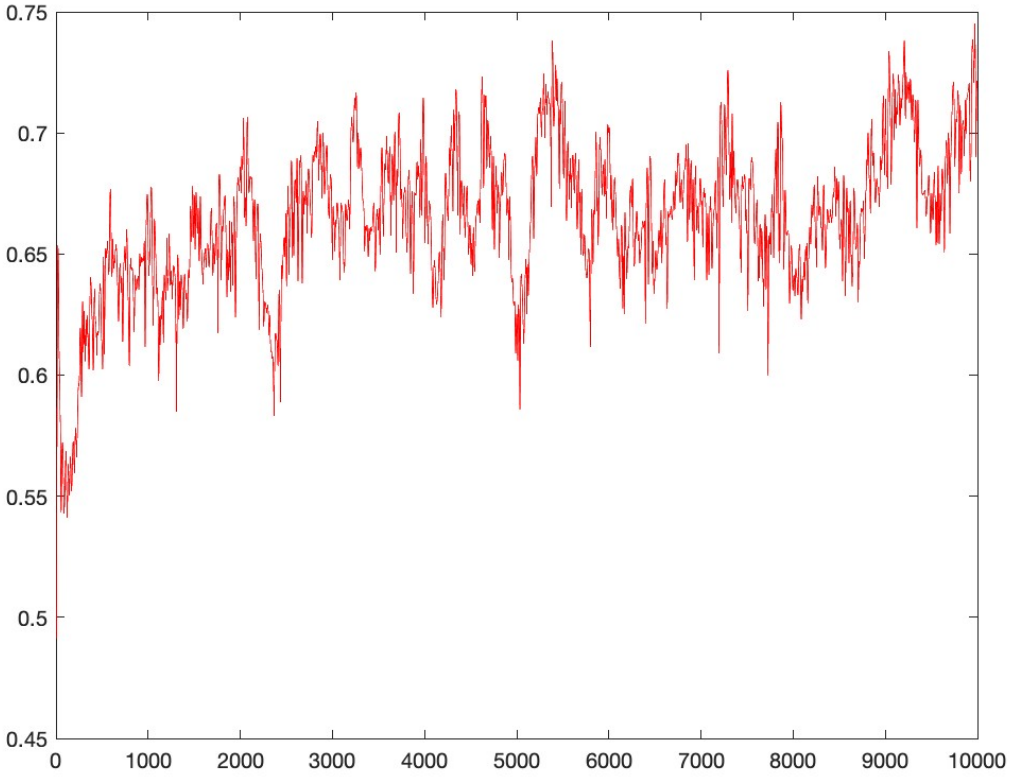
When dt becomes 0.0005, the total energy increases extremely slowly compared to baseline, and can even be seen as constant. total momentum also no longer increases all the time, but fluctuates at a constant value. This is because the error is reduced by reducing the step size in the numerical calculation. 3000 time steps are needed to reach equilibrium.

Change dt (N = 100, v_inial = 0, dt = 0.005)

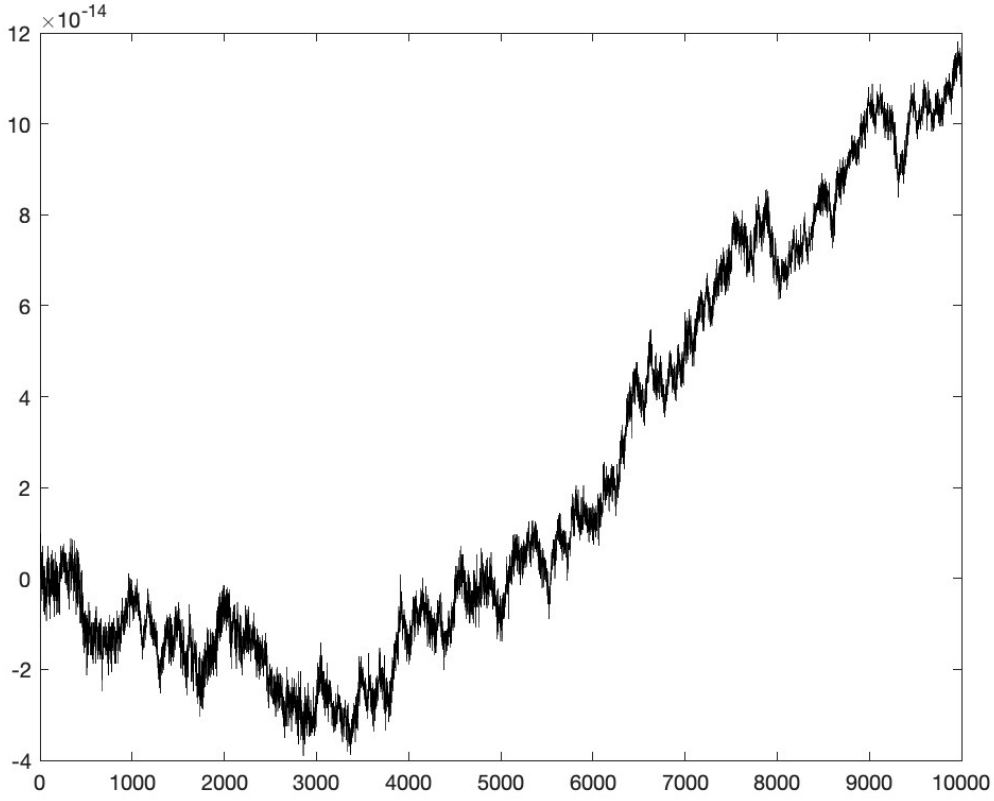
Total Energy



Total temperature



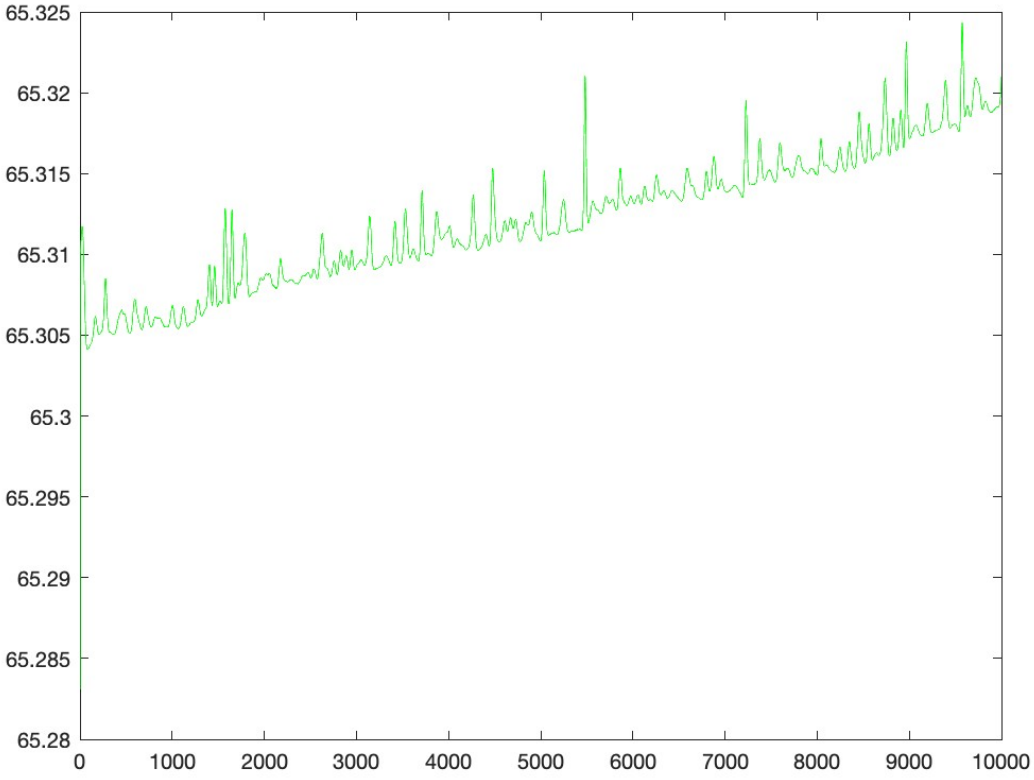
Total momentum



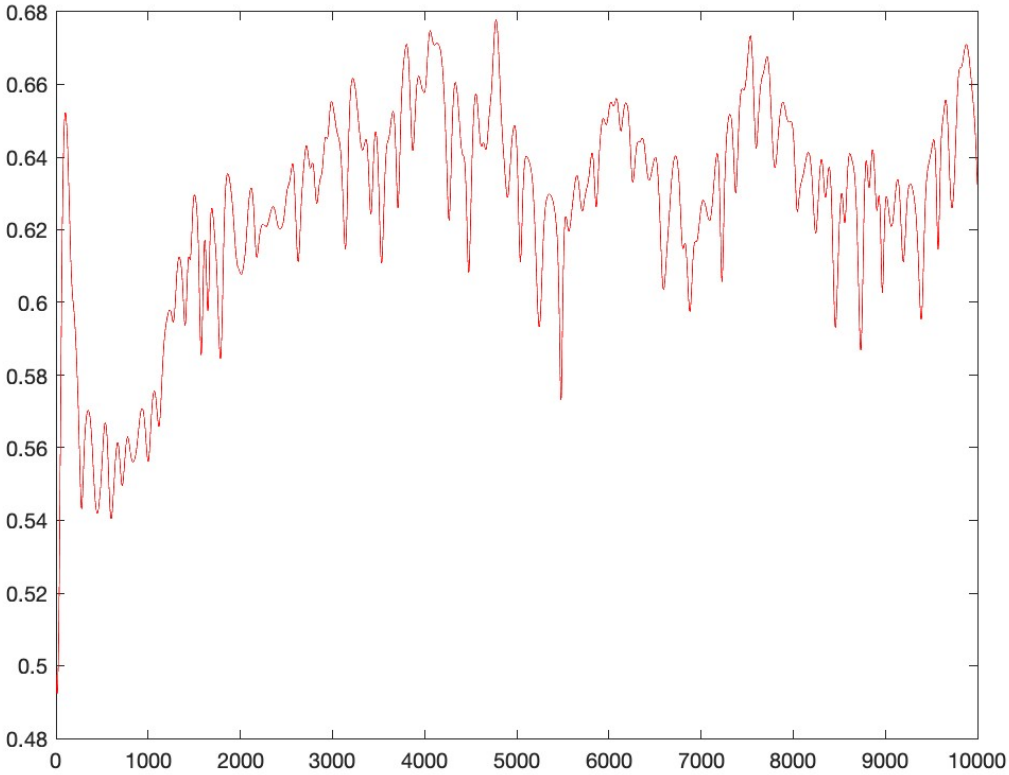
When dt becomes 0.005, the total energy and total momentum increase more rapidly compared to baseline. The magnitude and frequency of the total temperature fluctuations are greater. Because the error increases by increasing the step size in the numerical calculation. 3000 time steps are needed to reach equilibrium.

Change v_inial (N = 100, v_inial = 1, dt = 0.001)

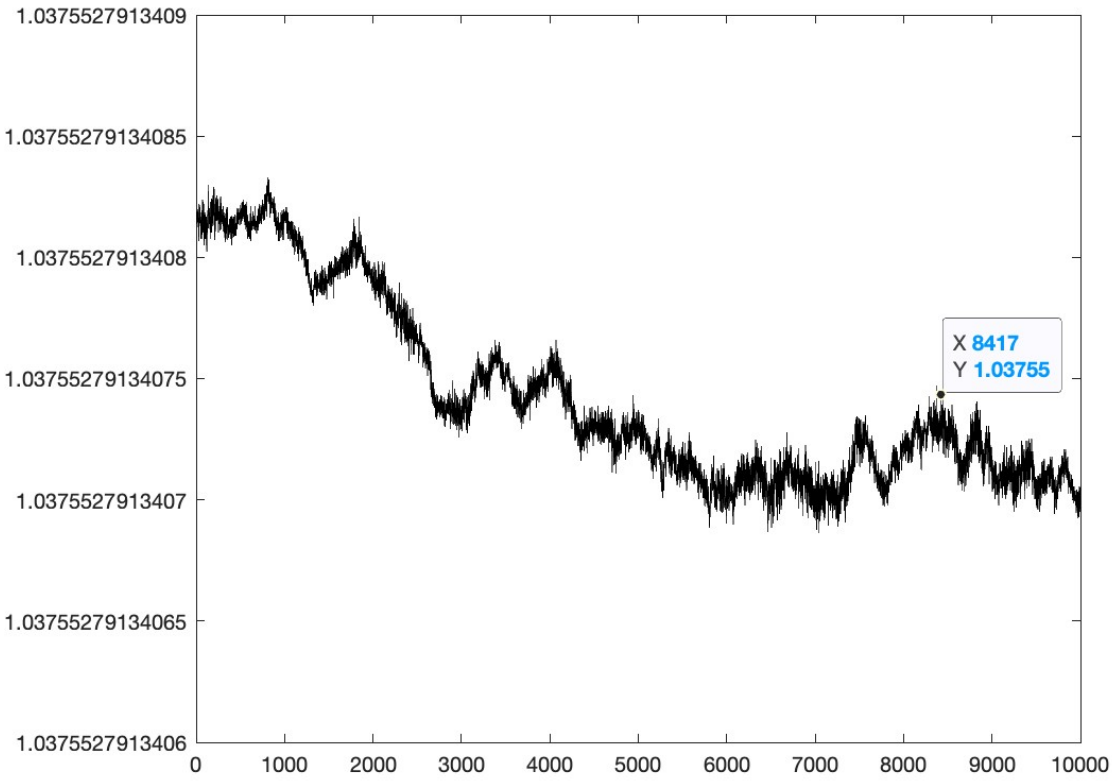
Total Energy



Total temperature



Total momentum



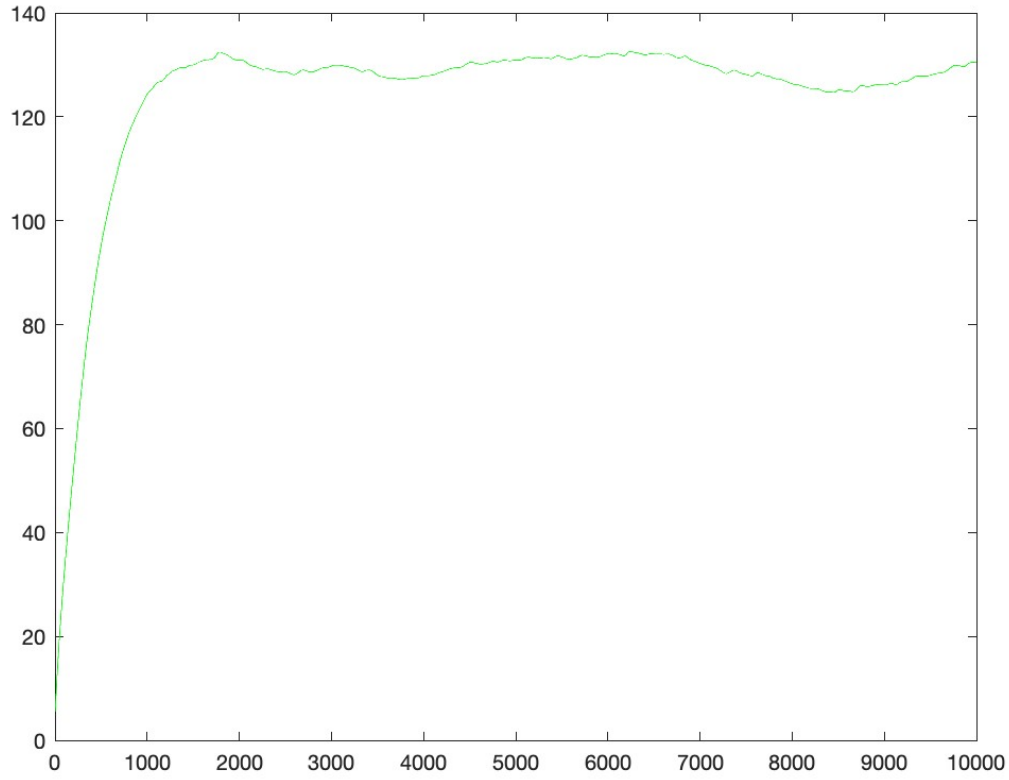
When changing the initial velocity, the total momentum at the beginning of the simulation is not zero. 3000 time steps are needed to reach equilibrium.

question 2

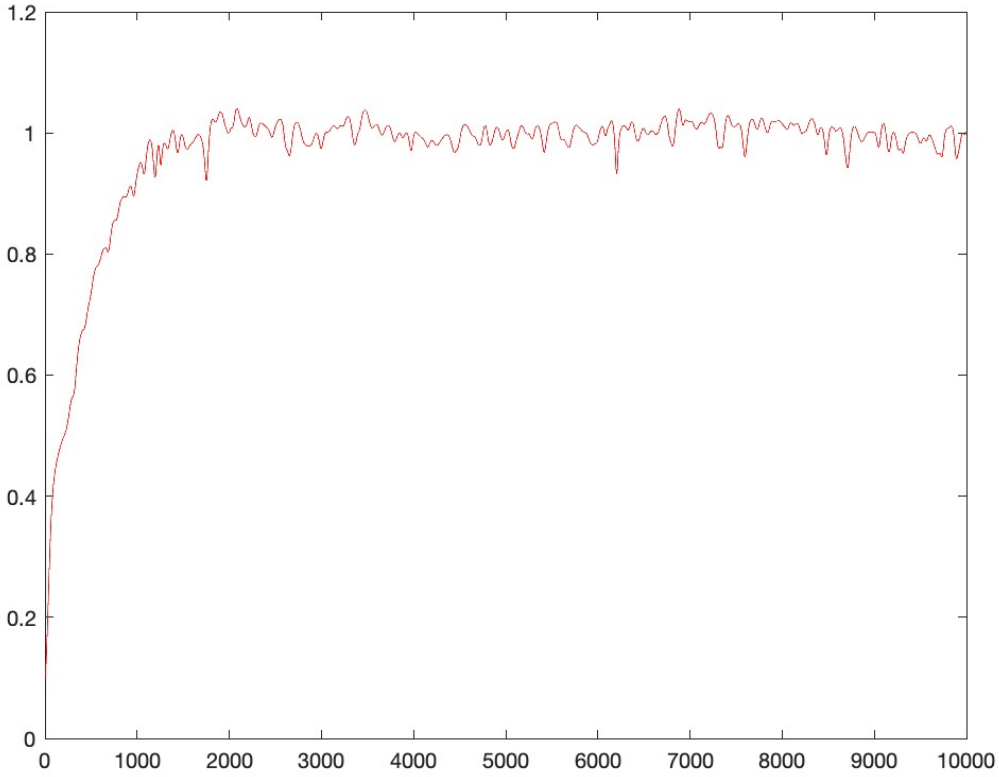
Using thermostat in these simulations

N = 100, T = 0.1

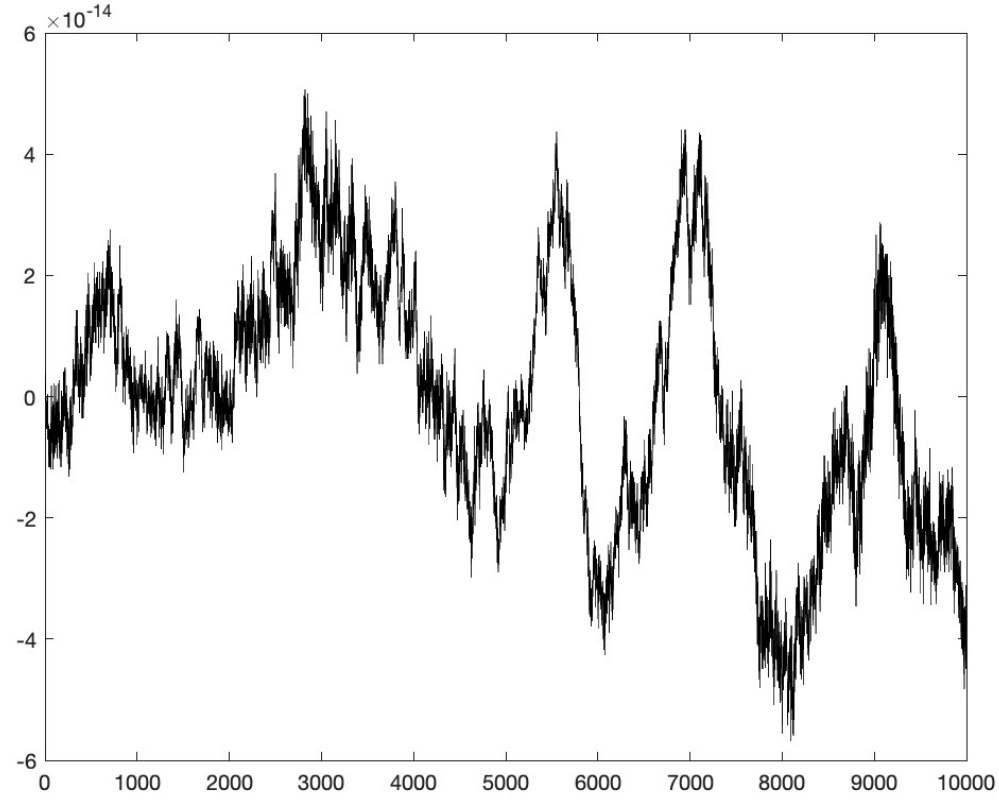
Total Energy



Total temperature



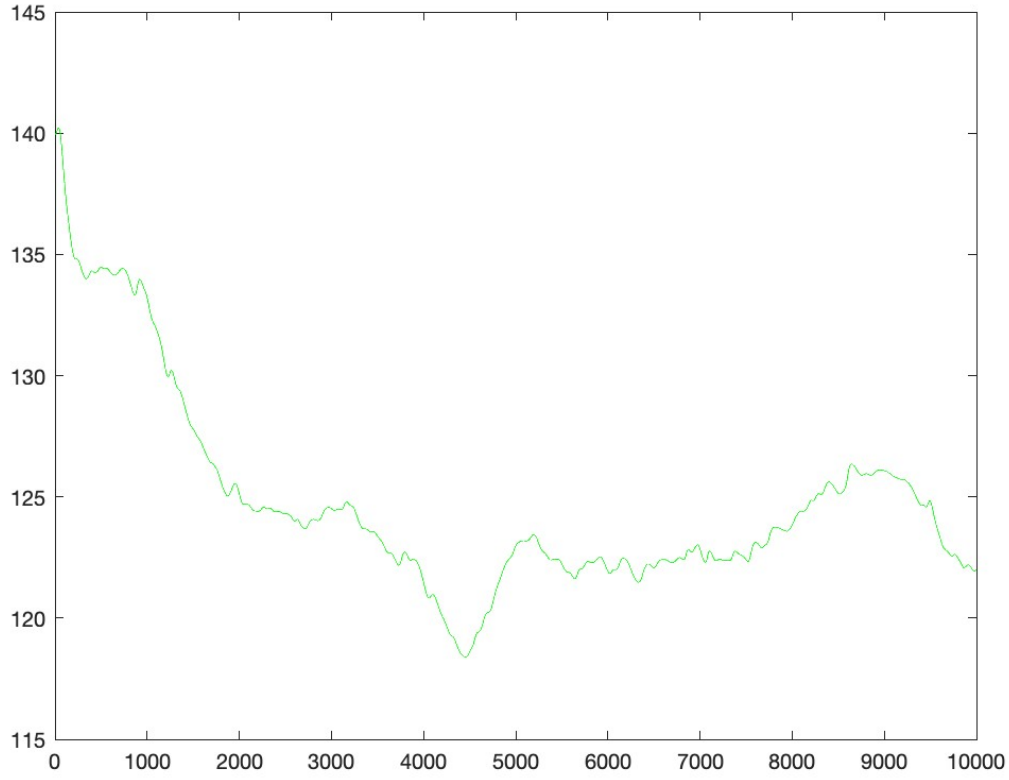
Total momentum



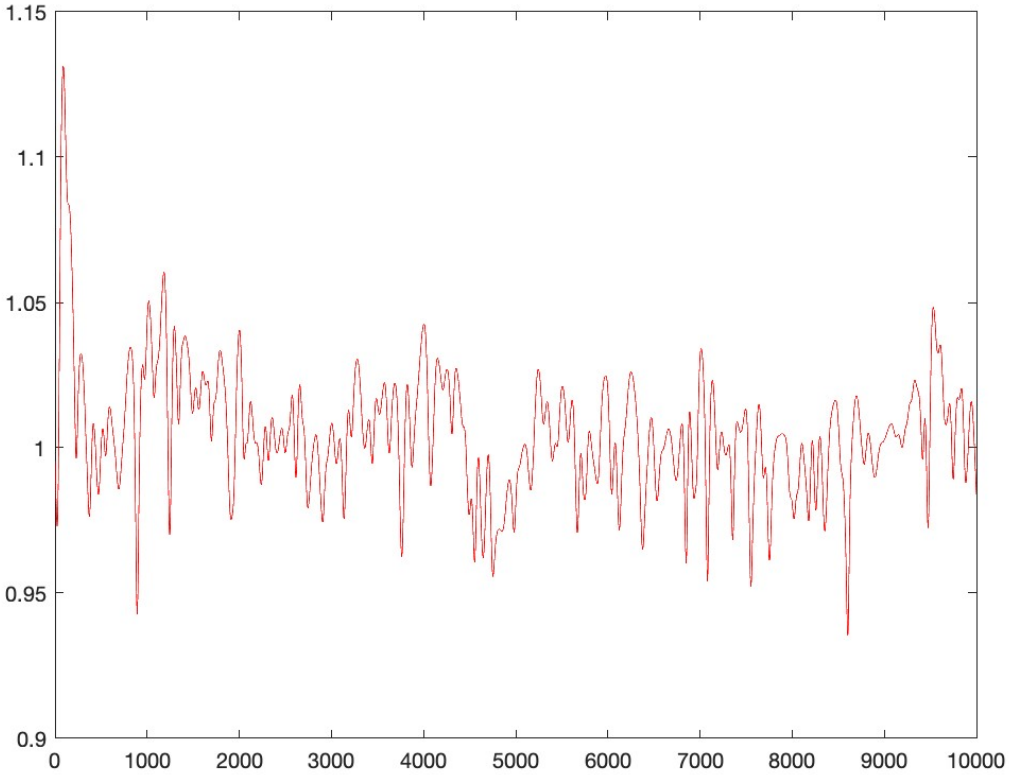
In molecular simulations, it is generally necessary to maintain the system temperature near a given value by means of a thermostat. The initial temperature is relatively low, so when the simulation starts. The total system temperature rises to approxiamte 1, because the potential energy of the particles is converted into kinetic energy . The momentem fluctuates at 0. 2000 time steps are needed to reach equilibrium.

N = 100, T = 1.0

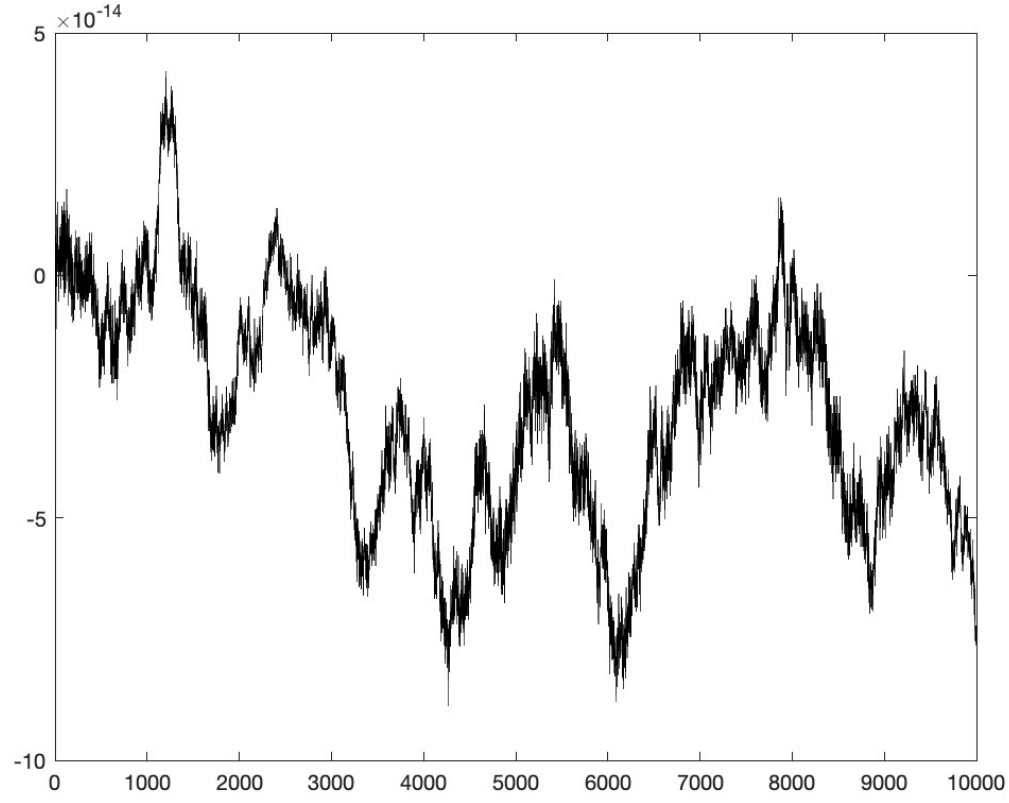
Total Energy



Total temperature



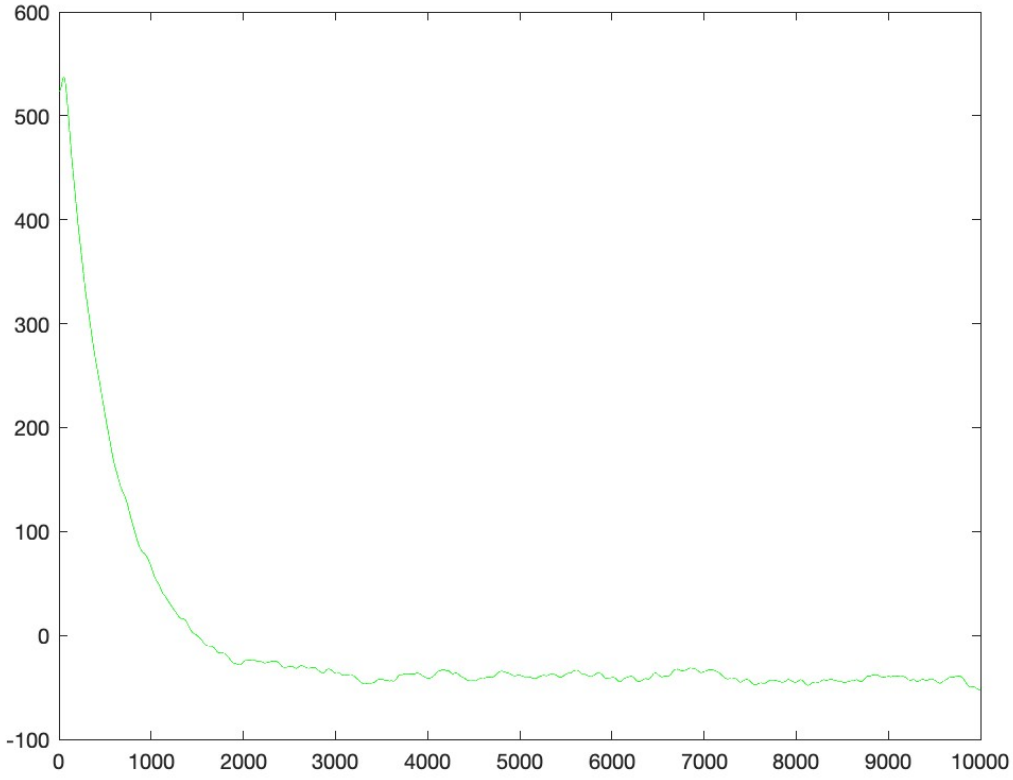
Total momentum



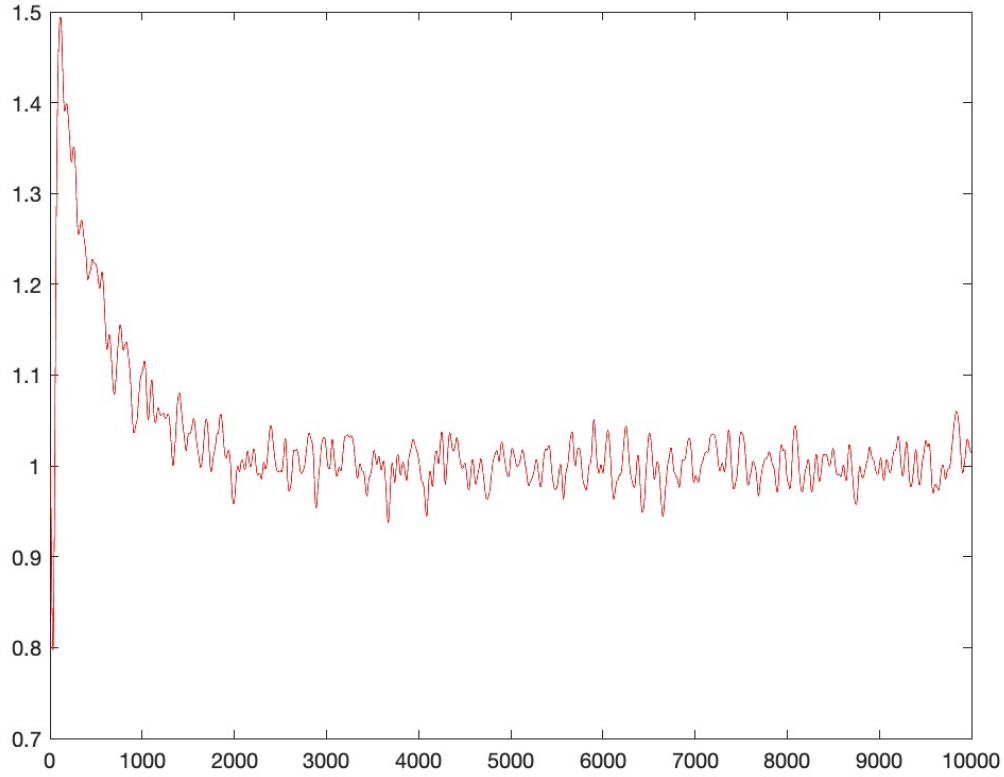
Samely, when the simulation starts, the potential energy of the particles is converted into kinetic energy. Thus, the temperature start increase a little bittle and decrease because of the thermostat. Also, the temperature decreases, which result in the decreasing of total energy. The momentem fluctuates at 0. 1000 time steps are needed to reach equilibrium.

N = 625, T = 1.0

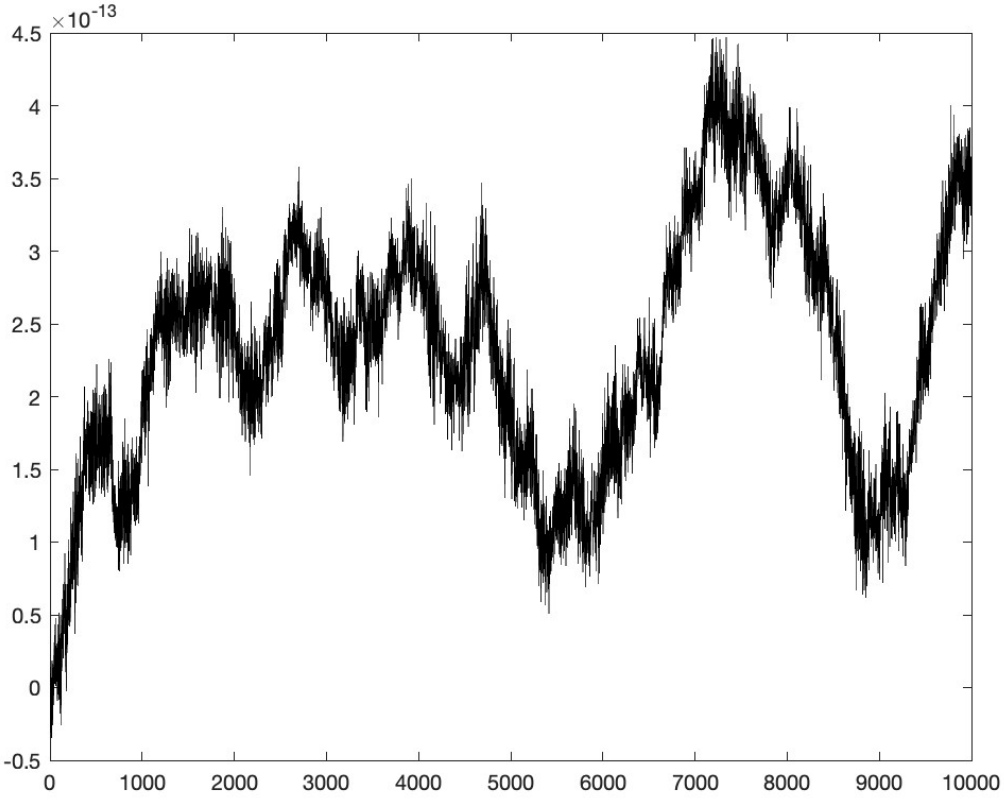
Total Energy



Total temperature



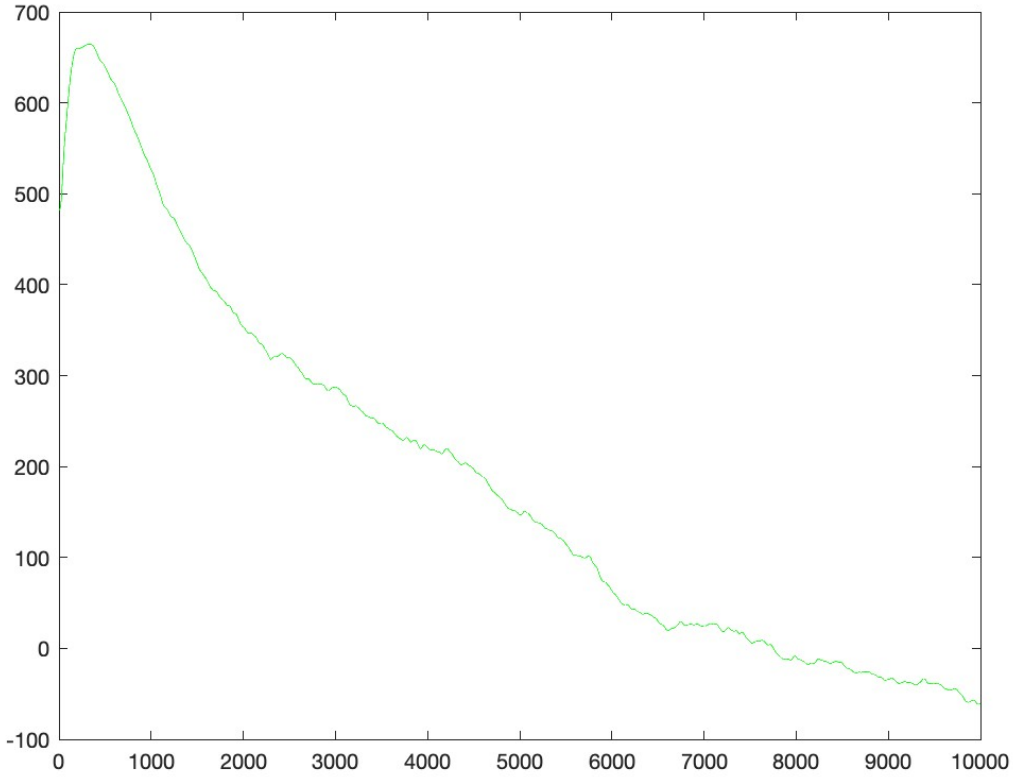
Total momentum



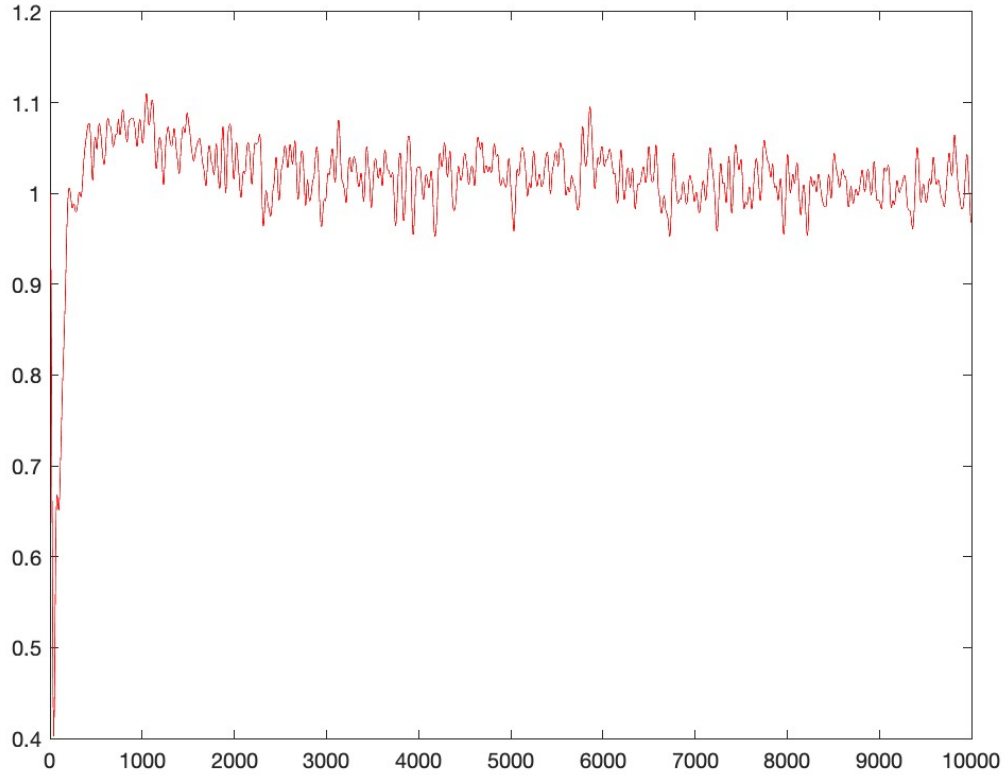
When the number of particles becomes 625, the amount of temperature transformed by the potential energy at the beginning of the simulation is much more than when N=100. So there is a large increase in temperature at the beginning, and then a slow drop. At the same time, the total energy decreases. 3000 time steps are needed to reach equilibrium.

N = 900, T = 1.0

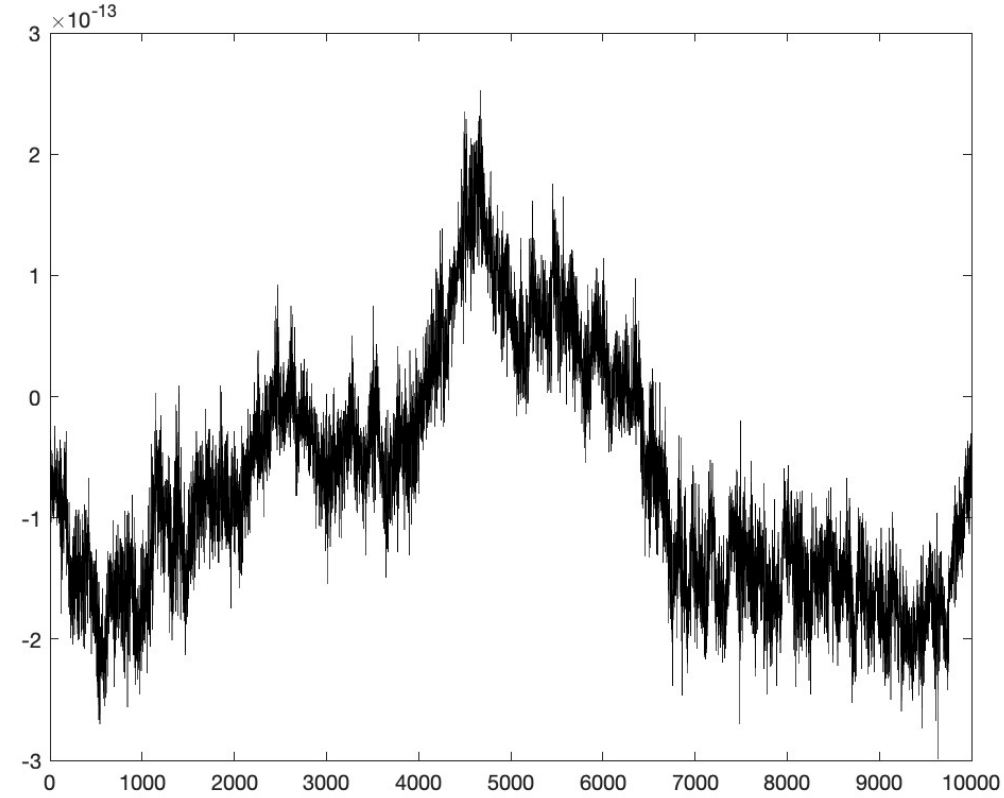
Total Energy



Total temperature



Total momentum



When the number of particles becomes 900, there are too many particles in the container. So the potential energy cannot be successfully converted into kinetic energy and thus into heat. So the system heat does not fluctuate much. But at the same time, there is energy exchange, so the total energy decreases slowly. 10000 time steps are needed to reach equilibrium.