Project 3 – SI1336 Simulation and modeling

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3.1. Estimate the volume of a 10-dimensional unit sphere using the midpoint method and the hit-and-miss MC method. Study the integration error.

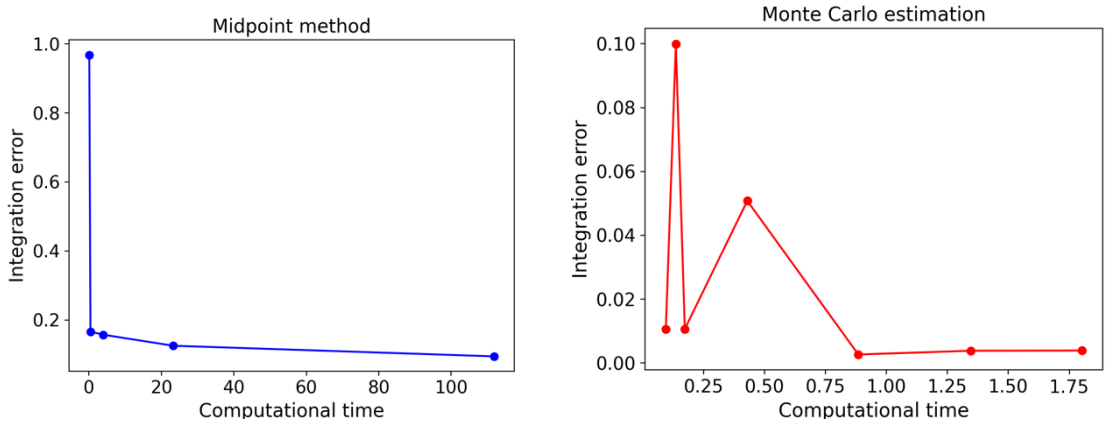


Figure 1

The plots above illustrate the time dependence on the integration error for the midpoint method and the Monte Carlo method respectively.

To calculate the integration error, the absolute value of the difference between the analytical value and the numerical value were implemented for both the Midpoint method and the Monte Carlo method. The numerical value for the Monte Carlo method was derived by calculating the mean value of 100 iterations with points ranging from 5000 to 100000.

Due to the fact that the Monte-Carlo method gives values that varies a lot, a better way to estimate the integration error is to calculate the standard deviation. If you plot the computational time against the standard deviation, you get:

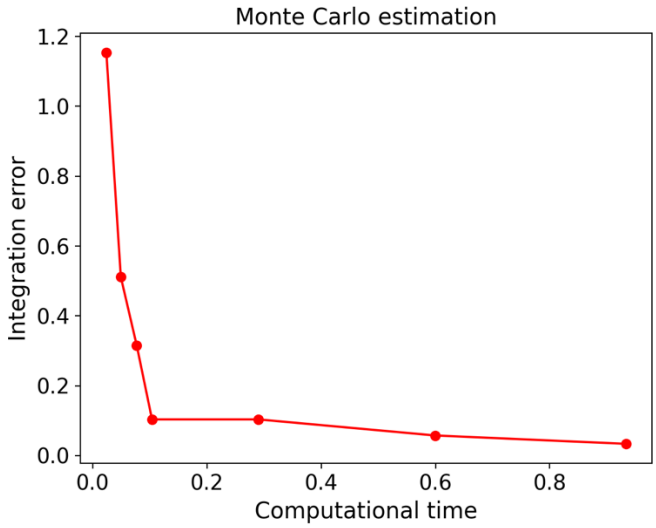


Figure 2

It can be concluded by comparing figure 1 and 2 that the time for the integration error to reach 0, i.e. get an accurate numerical value, is much smaller for the Monte Carlo method compared to the Midpoint method.

3.2a. Implement LJ potential with $\sigma = \varepsilon = T = 1$. Study the quality of the integration by monitoring the total energy for different time steps.

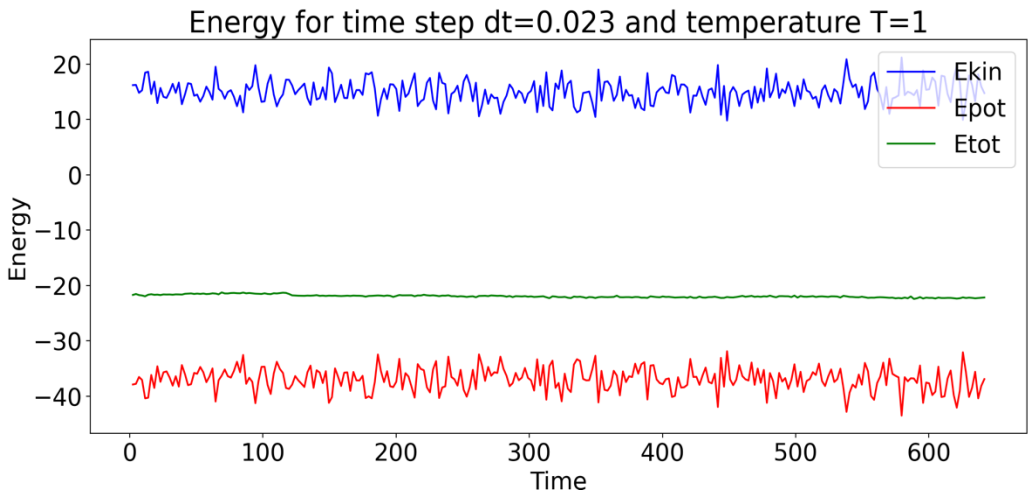


Figure 3

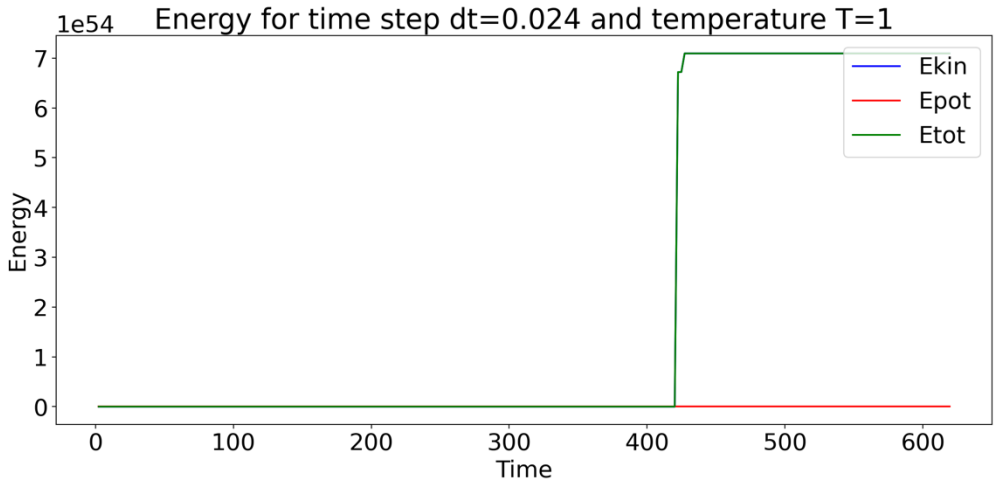
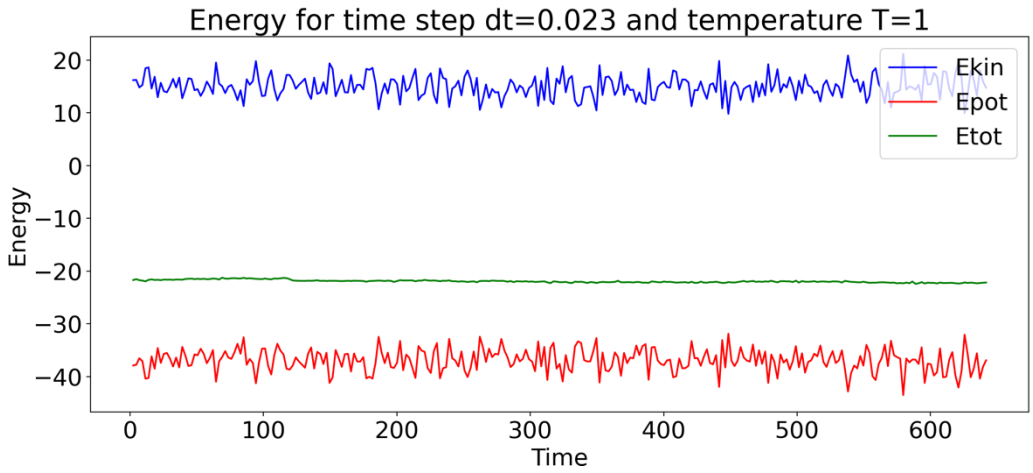
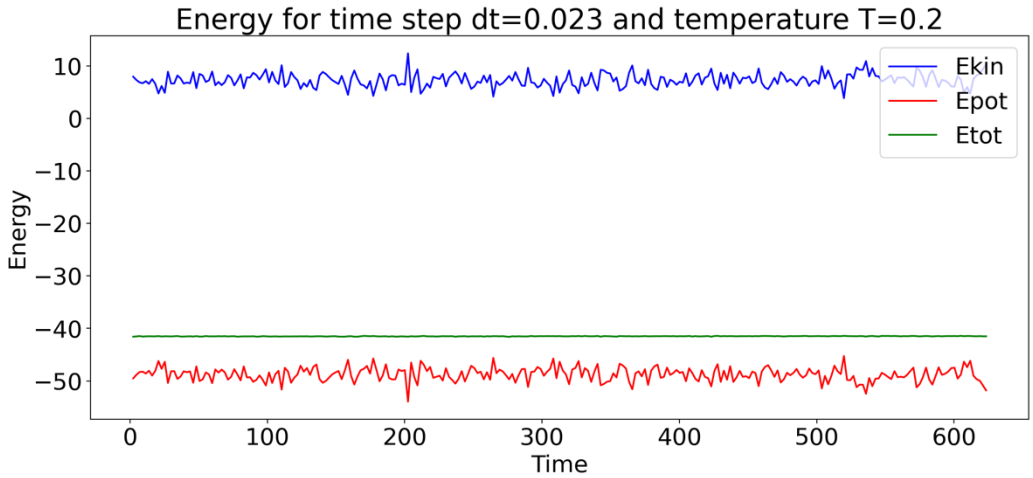


Figure 4

From figure 3, it can be observed that the MD is energy conserving for time step $dt = 0.023$. However, as the time step increases the conservation of energy does not longer hold up as the value of the kinetic energy shoots up to a factor of 10^{54} after a longer time (see figure 4).

3.2b. Let $T = 0.2$. What happens with the kinetic and potential energy?





From the plots above it can be observed that a decrease in temperature resulted in a decrease in both the kinetic and potential energy. It can also be observed that the energies fluctuate less for $T = 0.2$, resulting in a better energy conservation.

When running the simulation, less particle movement could be noticed with the decreased temperature, which is exactly what is expected in reality as well.

3.2c. Implement an Andersen thermostat and run for $T = 1, 0.2$. What are the differences at long times? Can you explain physically what you see?

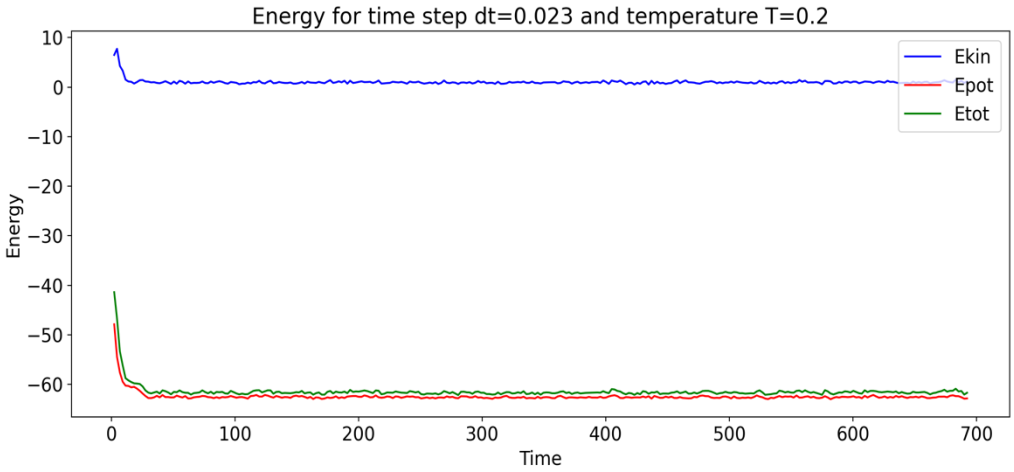


Figure 5

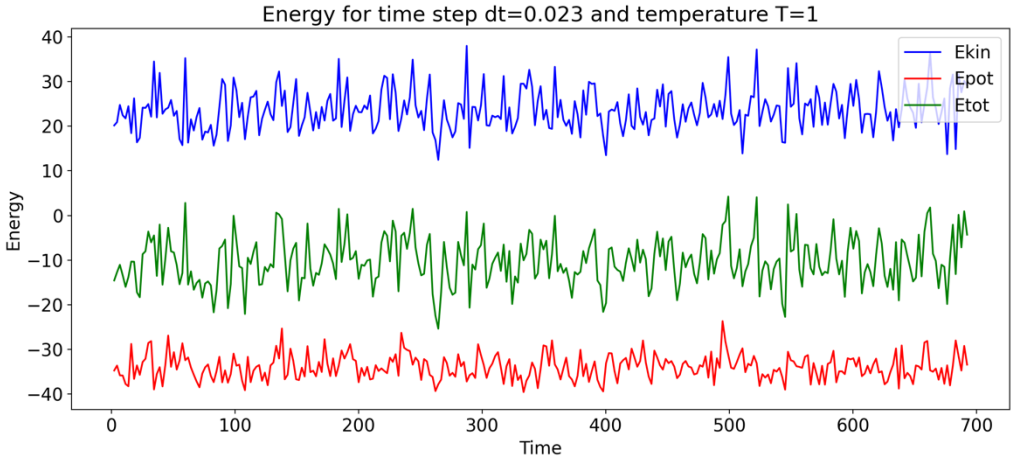


Figure 6

As expected, the Andersen thermostat disrupted the dynamics (not in a negative way necessarily). By implementing the thermostat with step size 1000, the particles became more sensitive to temperature changes as the oscillations were damped significantly for $T = 0.2$ (figure 5). It can be observed that the kinetic energy reached a small value close to 0, as the total energy curve almost collapsed with the potential energy curve.

The physical interpretation of the results can be explained as a phase transition. When T is small, the particles aligned in a structured pattern when running the simulation, representing a solid material. Thus, as the T increased, the kinetic energy increased concurrently resulting in higher particle movement and triggering a more chaotic behavior (represented by the oscillations in figure 6).

3.2d. Use MD with thermostat to calculate the average energy and heat capacity between $T \in [0.2, 1]$. Can you explain the behavior of the heat capacity by looking at the sampled configurations of the particles?

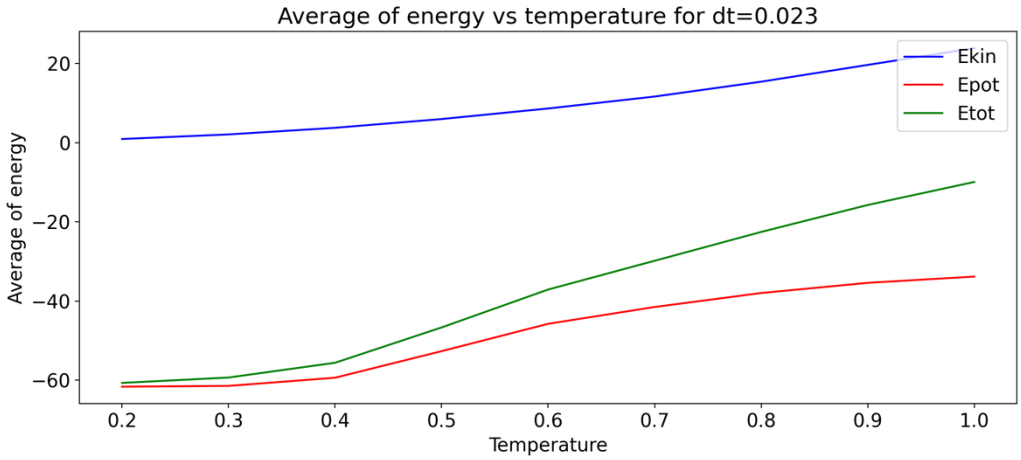


Figure 7

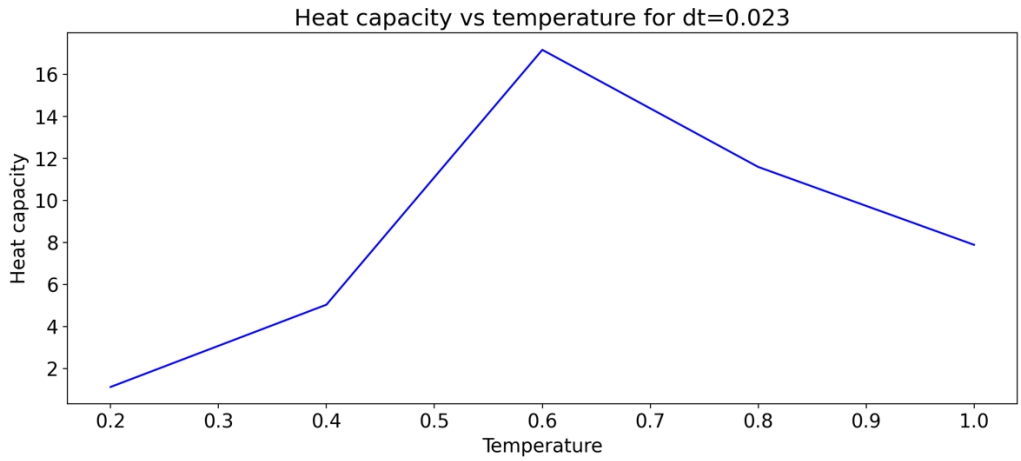


Figure 8: The heat capacity with Etot for different values of T

Heat capacity is defined according to:

$$C_v = \frac{\delta E}{\delta T} = \frac{(\Delta E)^2}{k_B T^2} = \frac{\langle E^2 \rangle - \langle E \rangle^2}{k_B T^2}$$

The heat capacity measures how much energy is needed to achieve a certain temperature change per kilogram. As observed from figure 8 the heat capacity keeps increasing until T=0.6 where a clear spike can be seen, after which it starts to decrease. The result can be described as a phase transition, where in the mixed phase, the temperature does not increase with added energy, resulting in a very large heat capacity.

The phase transition can also be verified via the animation that shows the configurations of particles, where they are organized in a structured pattern for small energies and start to move as the energy increases.