

Computational physics - Statistical Physics

Martin Johnsrud

March 13, 2020

Introduction

By numerically integrating Newton's equation of motion of many particles, confined to a box and interacting via the Leonard-Jones potential, it is possible to see the emergence of statistical behavior like the Maxwell-Boltzmann distribution. In this exercise, we explore this behavior, and ... (more to come)

Single particle

A single particle with position $\vec{x} = (x_1, x_2)$ in a box is modeled in a potential

$$V_w(\vec{x}) = \begin{cases} \frac{1}{2}K(r - R)^2, & r > R \\ 0, & r < R, \end{cases}$$

where $r = |\vec{x}|$. This leads to a force

$$\vec{F}_w(\vec{x}) = -\nabla V_w(\vec{x}) = \begin{cases} -K(r - R)\hat{x}, & r > R \\ 0, & r < R. \end{cases}$$

This equation can be numerically integrated to simulate the trajectory of the particle. This project is done using verlet integration,

$$\begin{aligned} \vec{x}(t + \Delta t) &= \vec{x}(t) + \dot{\vec{x}}(t)\Delta t + \frac{1}{2}\vec{F}(\vec{x}(t))\Delta t^2 \\ \dot{\vec{x}}(t + \Delta t) &= \dot{\vec{x}}(t) + \frac{1}{2}\left[\vec{F}(\vec{x}(t)) + \vec{F}(\vec{x}(t + \Delta t))\right]\Delta t \end{aligned}$$

Everything is done in units defined by the parameters K, R and ϵ , so that mass of the particle disappears from the equations.

Figure 1 shows simulation series of one particle in a box, using different step lengths. The energy of the particle can be used to assess the accuracy of the simulation. As there are no dissipative forces, energy is conserved. Accurate simulations should then have very small changes in energy, $\delta E - E(0)$, relative to the starting energy $E(0)$. This is plotted to the right in figure 1. $\Delta t = 0.01$ seems to yield sufficient accuracy, and will be used throughout this exercise.

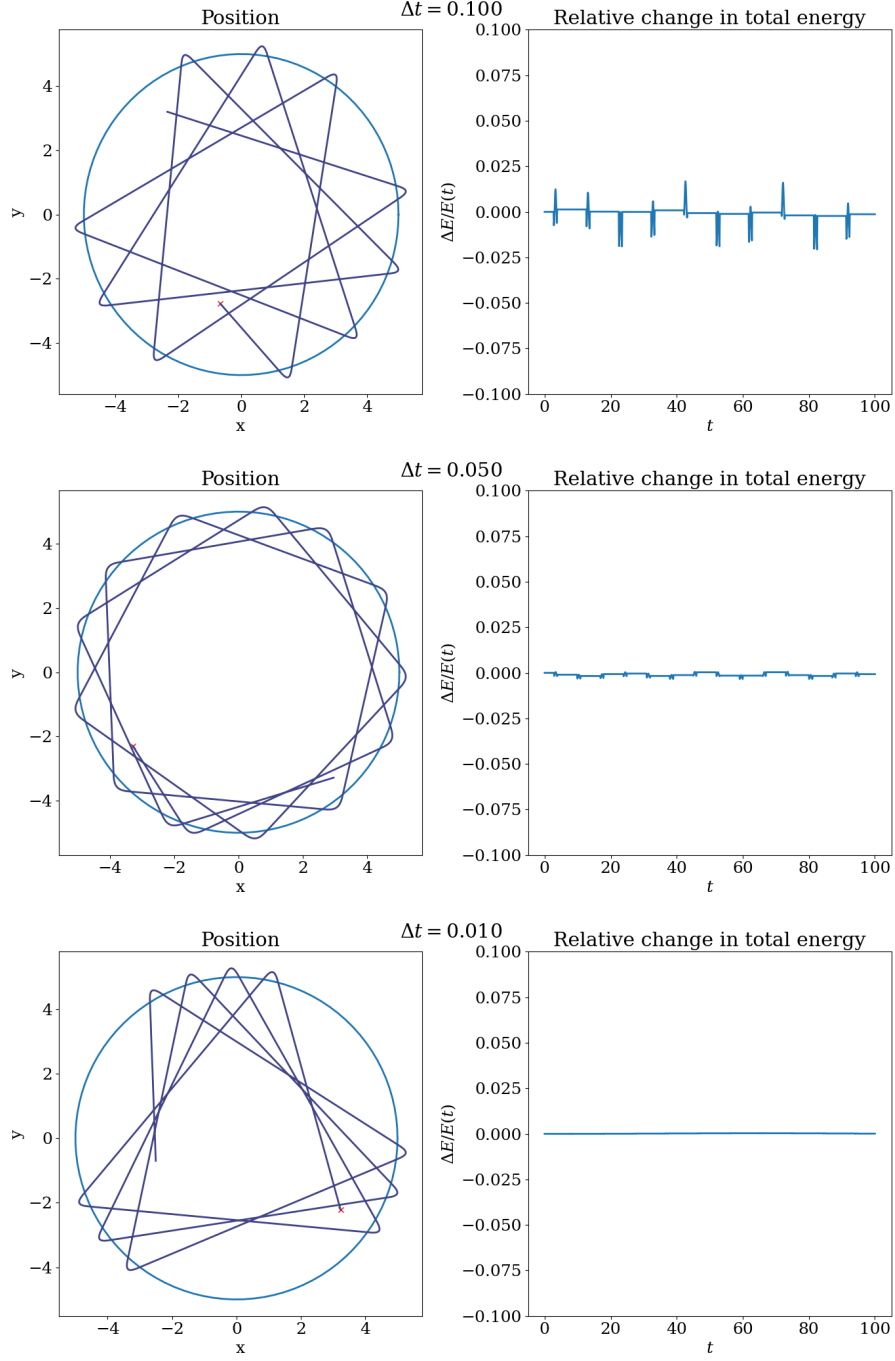


Figure 1: The figure shows the path of a particle in the potential described in the text, integrated using different steplengths. The right side shows the relative change in energy of the particle, as a function of time. The red x marks the starting position of the particle.

N particles

When modeling N particles $\{\vec{x}_k\} = \{(x_1^{(k)}, x_2^{(k)})\}$, each one of them is subject to the force from the potential $V_w(\vec{x}_k)$, as well as a modified Leonard-Jones potential the interaction potential. The potential felt by particle k is then

$$V_k(\vec{x}_j) = \sum_{r_{kj} < a} \epsilon \left[\left(\frac{a}{r_{kj}} \right)^{12} - 2 \left(\frac{a}{r_{kj}} \right)^6 + 1 \right]$$

Here, $r_{kj} = |\vec{x}_k - \vec{x}_j|$. The force on particle k by this potential is

$$F_k(\vec{x}_j) = -\nabla_k V(\vec{x}_j) = \sum_{r_{kj} < a} 12\epsilon \left[\left(\frac{a}{r_{kj}} \right)^{12} - \left(\frac{a}{r_{kj}} \right)^6 \right] \frac{\hat{x}_{kj}}{r_{kj}},$$

where $\hat{x}_{kj} = (\vec{x}_k - \vec{x}_j)/r_{kj}$. This is, like in the case with one particle, simulated using verlet integration, only now using the force.

$$\Sigma \vec{F}_k = -\nabla_k (V_w(\vec{x}_k) + V_w(\vec{x}_j)).$$

Figure 2 shows the simulation of particles with interactions implemented, as well as how the relative shifts in total energy in the total energy. It is evident that the system immediately becomes chaotic, and the ergodic hypothesis seems much more plausible. This becomes even clearer in figure 3, showing a scatter plot of the position of 50 particles over a time $T = 1000$.

Even if only one particle is given velocity, and the rest is still at $t = 0$, the system quickly reaches equilibrium. This is showcased in figure 4.

Even though with only $N = 50$, the statistical properties of the system become evident. Considering the system as a canonical ensemble, with temperature defined as

$$T = 1/2 \langle \vec{x}^2 \rangle,$$

a single particle will follow the Maxwell-Boltzmann velocity distribution

$$P(x_i) = \sqrt{\frac{1}{2\pi T}} \exp \left[-\frac{\dot{x}_i^2}{2T} \right].$$

This is shown in figure 5

Lastly, the pressure on the wall is given By

$$P = \sum_k \vec{F}_w^k \cdot \hat{e}_r / 2\pi R = \sum_{r_k > R} K(r_k - R) / 2\pi R$$

And ideal gas would fulfill

$$\frac{p2\pi R}{NT} = 1$$

Figure 6 shows this ratio for different simulation runs with different parameters, all of which have an average within 50% of 1. The ideal gas law can thus be used as a rough estimate for the system, but the radius of the particles ($a = 0.8$) cannot be completely neglected.

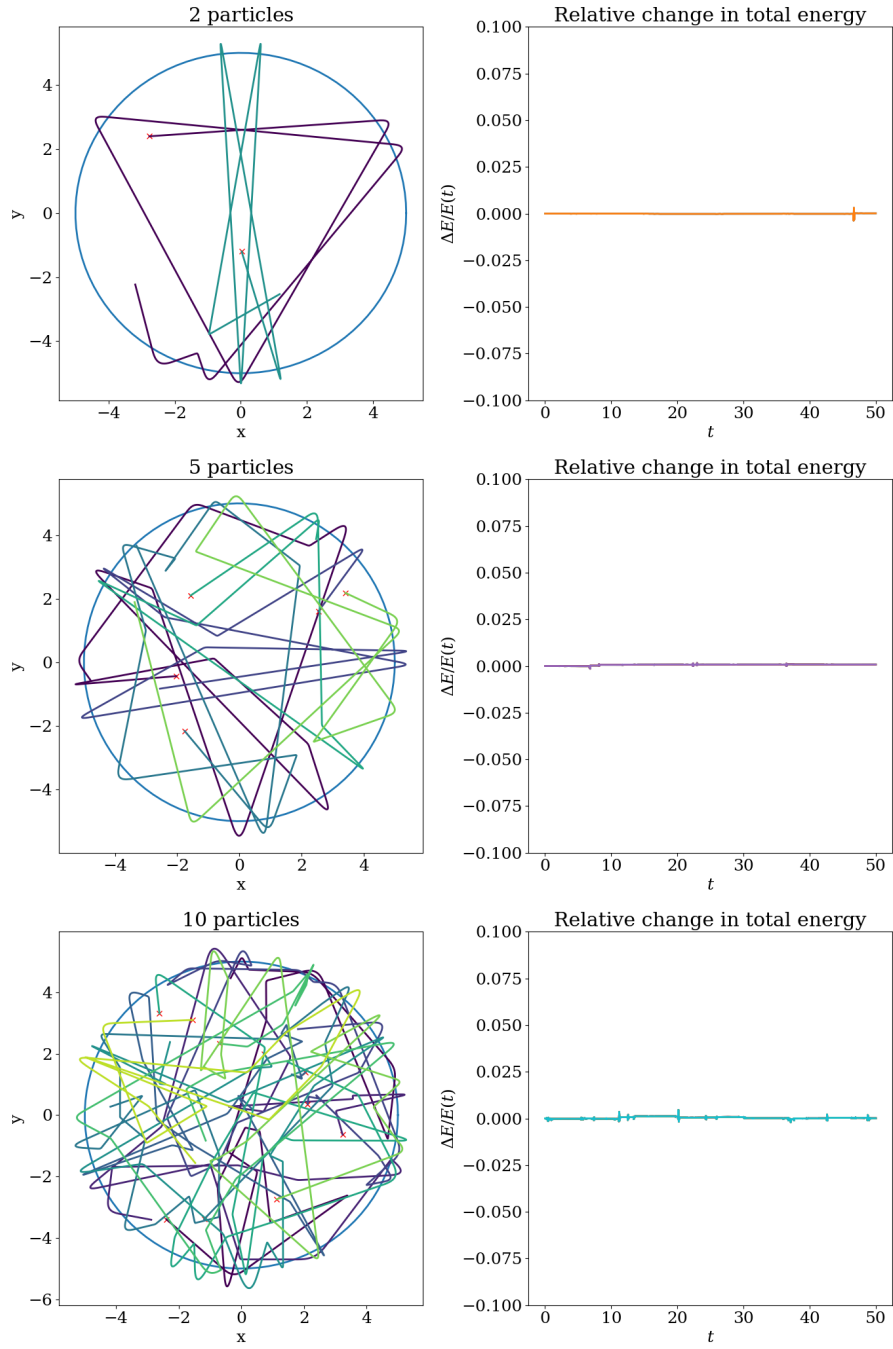


Figure 2: On the left, the path of different numbers of particles are shown. On the right, though there are some jumps in total energy, it is very close to conserved, giving confidence to the model.

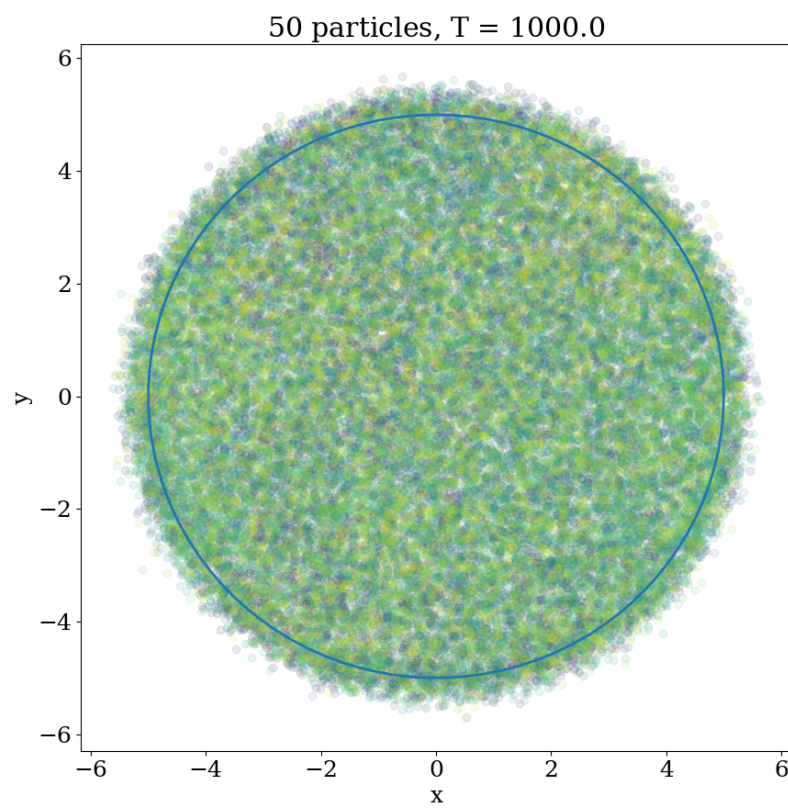


Figure 3: A scatter plot of the position of 50 particles, each with 1000 datapoints shown. Different particles have different color, showing that the particles get mixed.

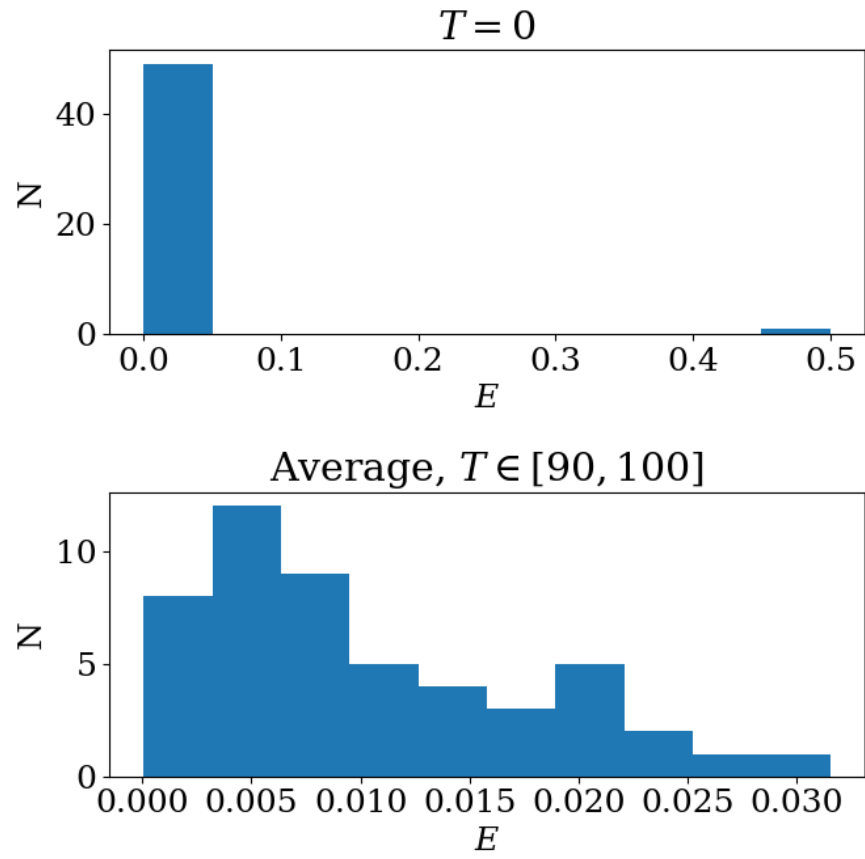


Figure 4: The velocity distribution at the start and at the end of the simulation. The kinetic energy has diffused throughout the system

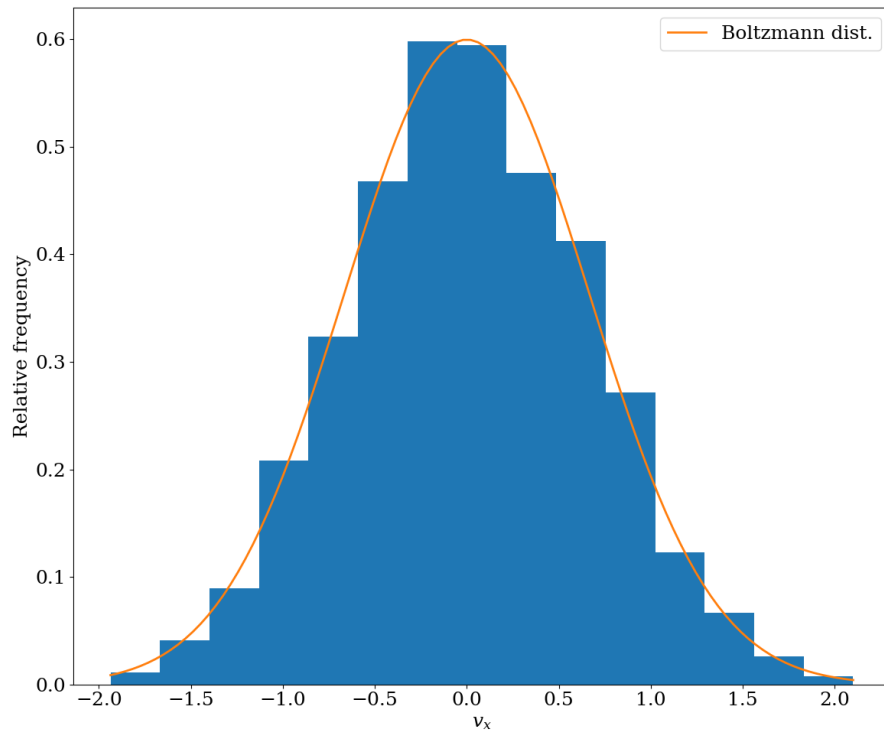


Figure 5: The nornalized velocity distribution of the velocity distribution of one particle in a simulation with $N = 50$. The orange line is the Boltzmann distribution of the ensamble.

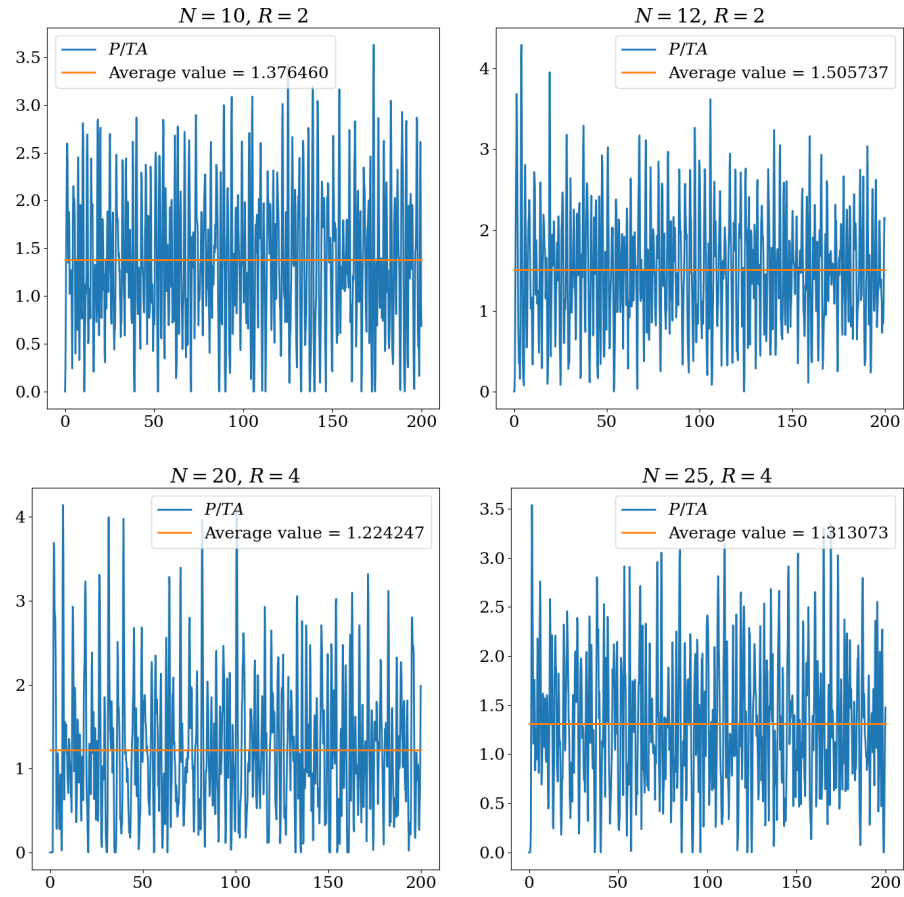


Figure 6: Pressure divided by temperature and area, for different values of N and R . The average of this value is close to 1 for all simulations.