Computatonal physics - Statistical Physics

Martin Johnsrud

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Introduction

By numerically integrating Newtons equation of motion og many particles, confined to a box and interacting via the Leonard-Jones potential, it is possible to see the emergence of statistical behvior This exercise uses verlet integration to simulated particles in a circular potential and investigates the accuracy of the numericall scheme, and emergent fenomena like ergodicity, the Maxwell-Boltzmann distribution and the ideal gas law.

Single particel

A single particel 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 equiation can be numerically integrated to simulate the trajectory of the particle. This project is done using verlet integration,

$$\vec{x}(t+\Delta t) = \vec{x}(t) + \dot{\vec{x}}(t)\Delta t + \frac{1}{2}\Sigma F\big(\vec{x}(t)\big)\Delta t$$
$$\dot{\vec{x}}(t+\Delta t) = \dot{\vec{x}}(t) + \frac{1}{2}\Big[\Sigma\vec{F}\big(\vec{x}(t)\big) + \Sigma\vec{F}\big(\vec{x}(t+\Delta t)\big)\Big]\Delta t^2$$

Everything is done in units defined by the parametres K, R, k_b and ϵ, so that constantsats dissapears from the equations.

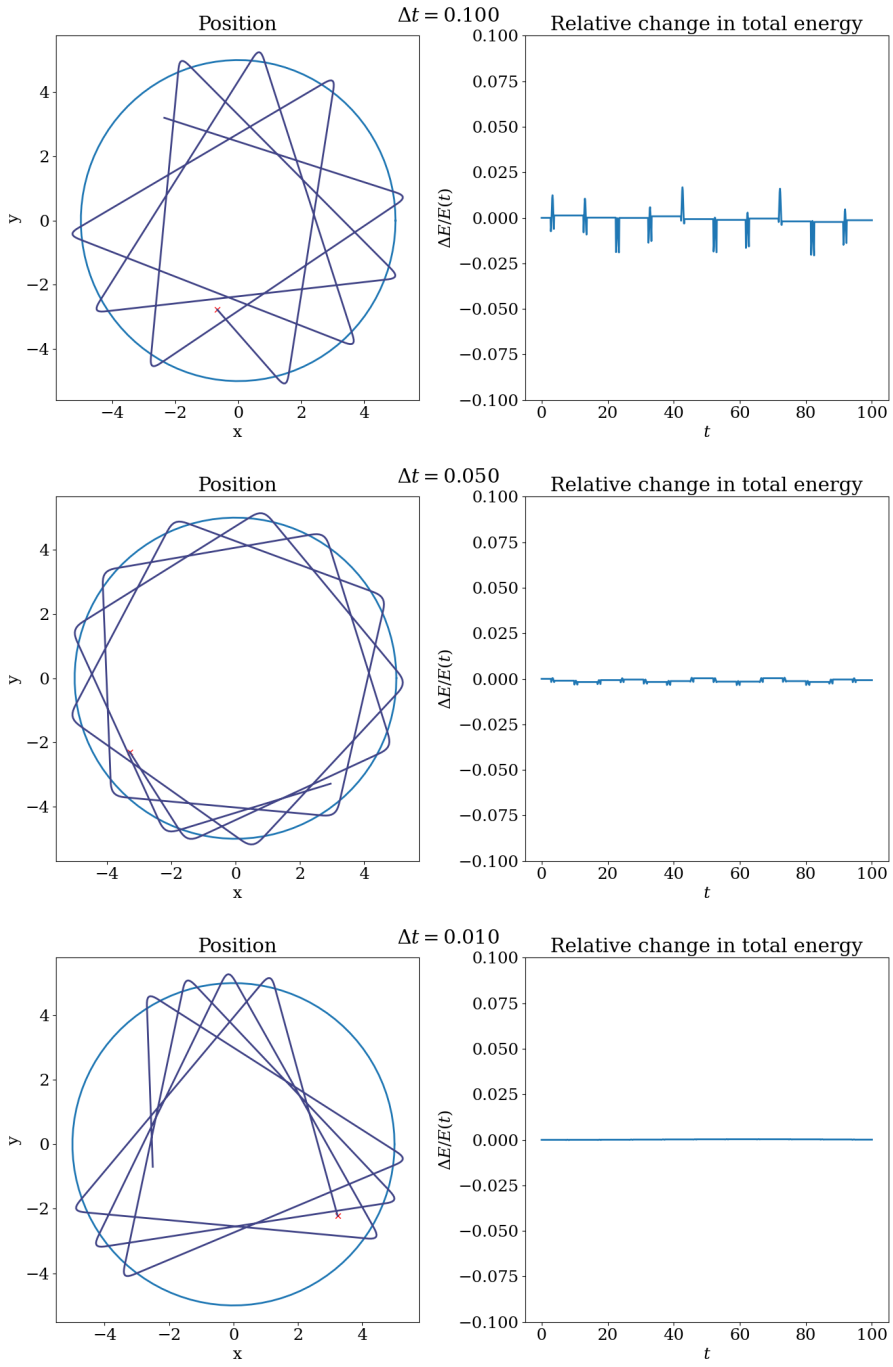

Figure 1: The figure shows the path of a particle in the potential described in the text, integrated using different steplengths. The right side shows the relative change in energy of the particle, as a function of time. The red x marks the starting position of the particle.

Figure 1 shows simulation series of one particle in a box, using different steplengths. The energy of the particle can be used to assess the accuracy of the particle. As there are noe dissipative forces, energy is conserved. Accurate simulations should then have very small changes in energy, $\Delta E = E(t) - E(0)$, relative the starting energy $E(0)$. This is plotted to the right in figure 1. $\Delta t = 0.01$ seems to yield sufficient accuracy, and wil be used throughout this exercise.

When simulation only one particle, the system is not ergodic. Though the middle of the system is a valid spot for the particle to be, it will never reach it. By inspection of the figures, we see the probability distribution of the different points within the circle, where velocity will be constant, is not constant, and thus breaking the ergodic hypothesis.

N particles

When moddeling 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 as an interaction potential. The potential felt by particle k is

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

Here, $r_{kj} = |\vec{x}_k - \vec{x}_j|$. The force on particel 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.

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

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 becom evident. Considering the system as a canonical ensamble, with temperature defined as

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

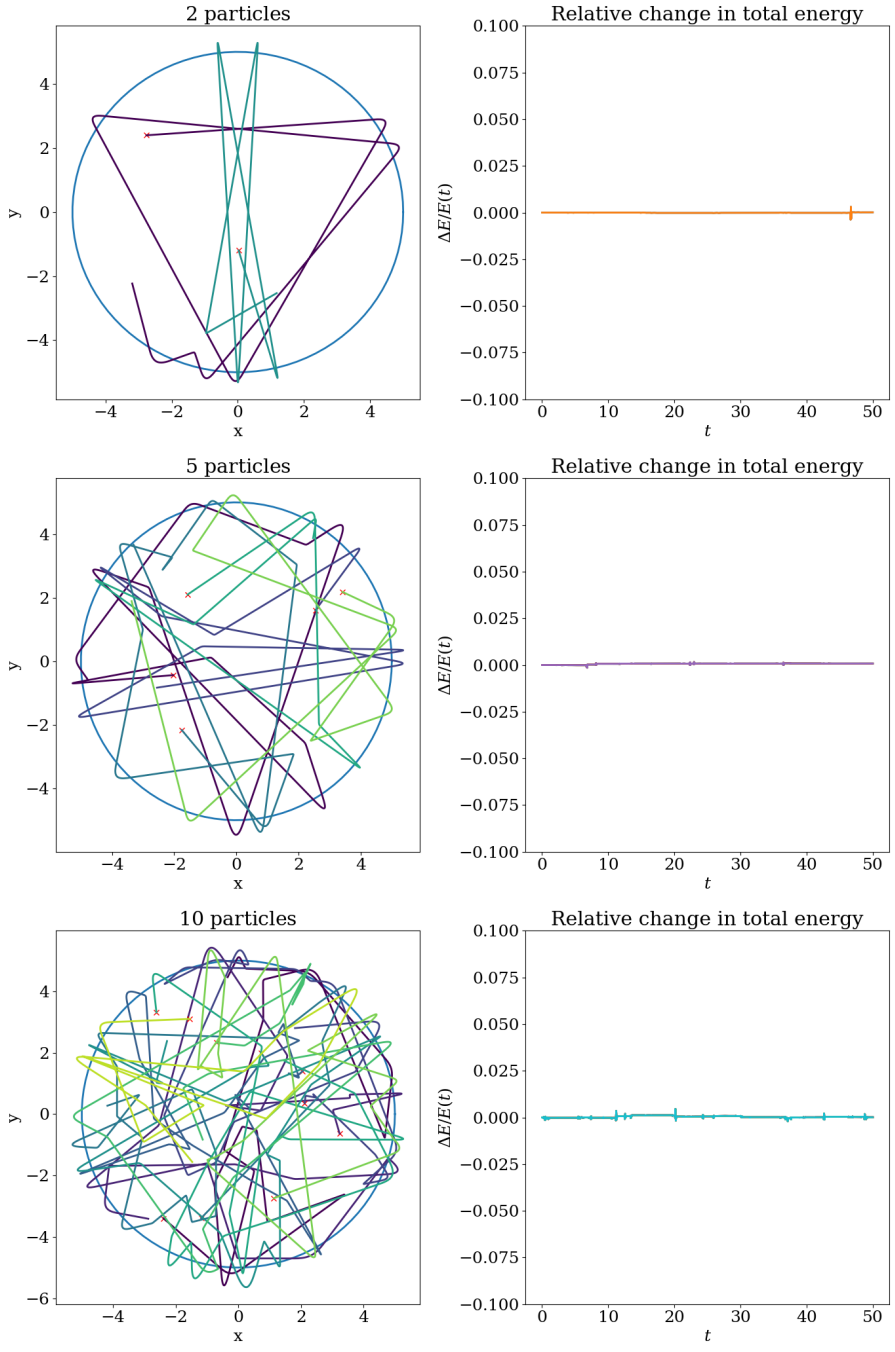

Figure 2: On the left, the path of different numbers of particles are shown. Though there are some jumps in total energy, it is very close to conserved, giving confidence to the model.

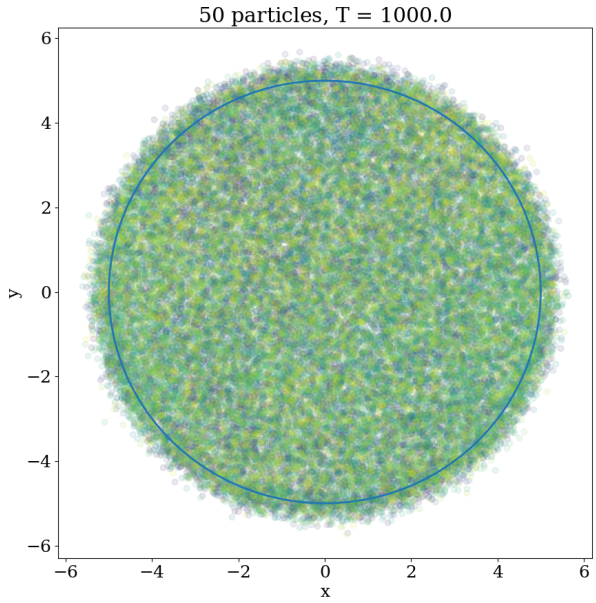

Figure 3: A scatter plot of the position of 50 particles, each with 1000 datapoints shown. Different particles have different collor, showing that the particles get mixed.

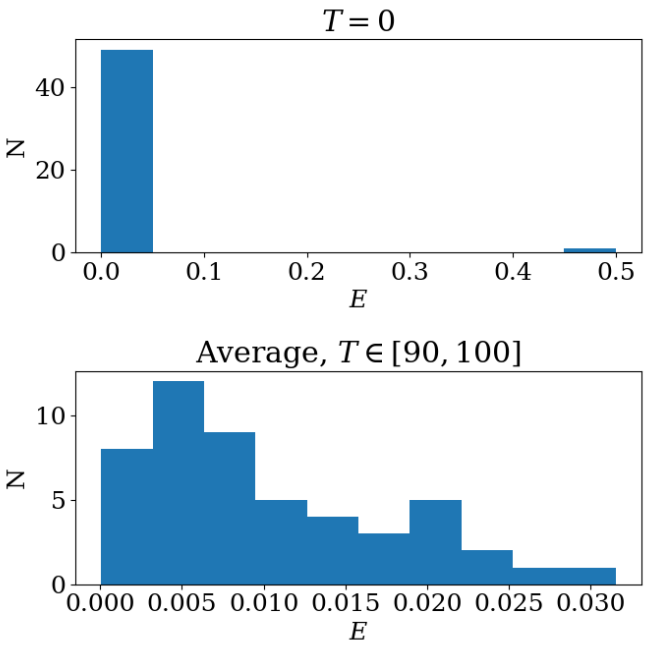

Figure 4: The velocity distribution at the start and at the end of the simulation. The kinetic energy has diffused throughout the system

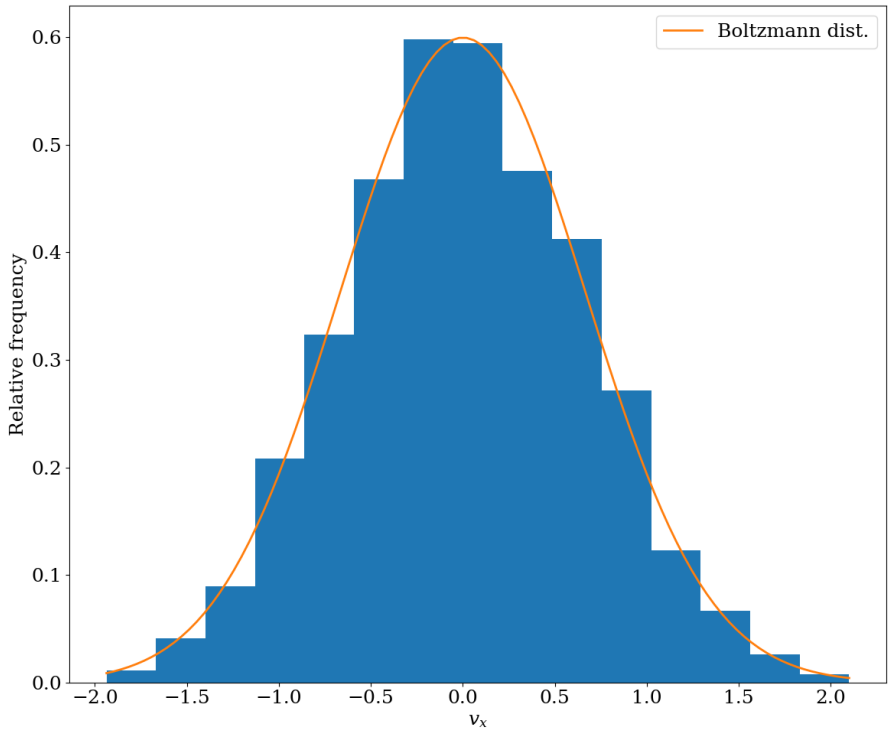

Figure 5: The noralized velocity distribution of the velocity distribution of one particle in a simulation with $N = 50$. The orange line is the Boltzmann distribution of the ensamble.

a single particle will follow the Maxwell-Boltzmann velocity distribution

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

This is shown in figur 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

$$\frac{p 2\pi R}{NT} = 1$$

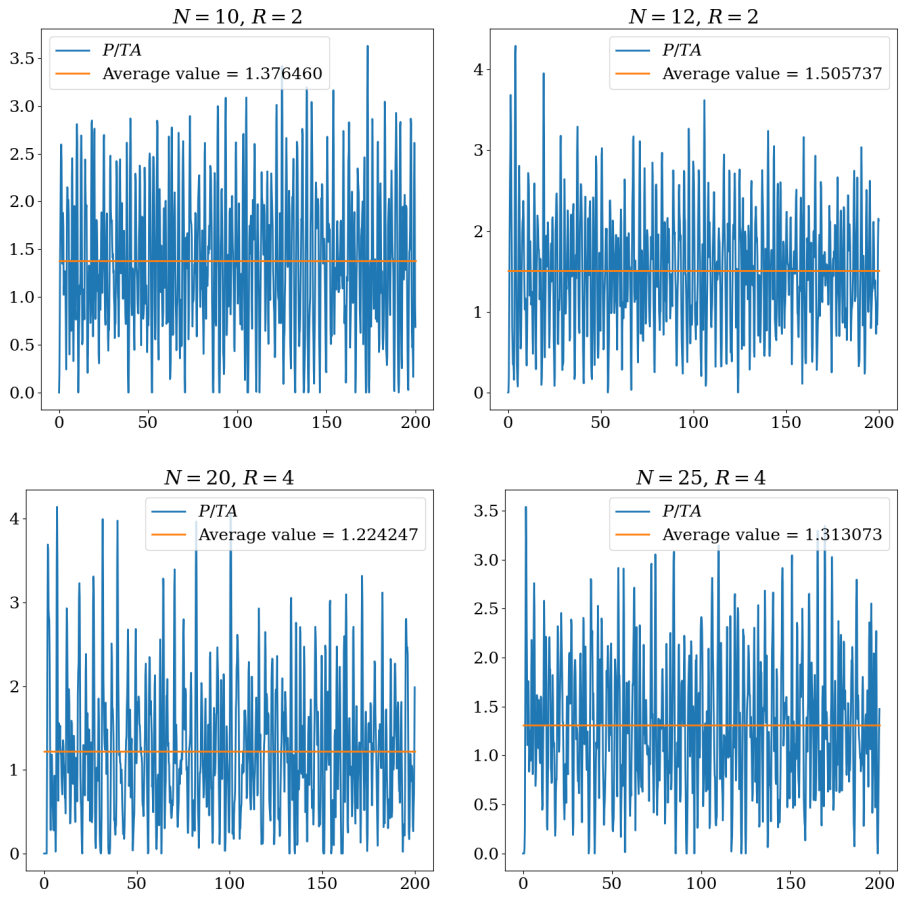

Figure 6: Pressure divided by temperature and area, for differeent values of N and R. The average of this value is close to 1 for all simuations.

Figure 6 shows this ratio for different simulation runs with different parameters, all of witch has 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 completly neglected.