Exploration of particles in confined spaces: using numerical methods

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The goal of this project is to explore numerically how gasses behave and how it might relate to statistical mechanics.

I. METHOD

The implementation of a verlet algorithm to simulate a two dimensional gas inside a rectangular box. Each particle has a position and velocity which is updated according to

$$\vec{\boldsymbol{r}}_i(t+\Delta t) = \vec{\boldsymbol{r}}_i(t) + \vec{\boldsymbol{v}}_i(t)\Delta t + \frac{1}{2}\frac{\vec{\boldsymbol{f}}_i(t)}{m}\Delta t^2 \quad (1)$$

$$\vec{\boldsymbol{v}}_i(t+\Delta t) = \vec{\boldsymbol{v}}_i(t) + \frac{\vec{\boldsymbol{f}}_i(t) + \vec{\boldsymbol{f}}_i(t+\Delta t)}{2m}\Delta t \quad (2)$$

where the force

$$\vec{\boldsymbol{f}}_i = -\frac{\partial V_w}{\partial \vec{\boldsymbol{r}}_i} - \sum_{j\neq i}\frac{\partial V(r_{ij})}{\partial \vec{\boldsymbol{r}}_i} \quad (3)$$

is given by the wall potential $V_w = V_x + V_y$ and the particle-particle potential $V(r_{ij})$

$$V(r_{ij}) = \epsilon\left[\left(\frac{a}{r_{ij}}\right)^{12} - 2\left(\frac{a}{r_{ij}}\right)^{6}\right] \quad (4)$$

$$V_x(\vec{\boldsymbol{r}}_i) = \begin{cases} \frac{K}{2}(x_i - L_x)^2 & \text{if } x > L_x \\ \frac{K}{2}x_i^2 & \text{if } x < 0 \end{cases} \quad (5)$$

$$V_y(\vec{\boldsymbol{r}}_i) = \begin{cases} \frac{K}{2}(y_i - L_y)^2 & \text{if } y > L_y \\ \frac{K}{2}y_i^2 & \text{if } y < 0 \end{cases} \quad (6)$$

where ϵ is the interaction parameter for the particles, L_x and L_y are the side length of the box, K is the parameter which determines the "softness" of the walls and a is the point where the switch between repulsive and attractive force between particles change, if the distance between the two particles $r_{ij} = a$ then we can say the two particles touch, so a can be seen as the diameter of the particles. In order to make implementation easier $a = 1$. Now the force between particles is

$$\frac{\partial V(r_{ij})}{\partial \vec{\boldsymbol{r}}_i} = 12\epsilon\left[-\left(\frac{1}{r_{ij}}\right)^{13} + \left(\frac{1}{r_{ij}}\right)^{7}\right]. \quad (7)$$

The force from the walls is

$$\frac{\partial V_x(x_i)}{\partial x_i} = \begin{cases} K(x_i - L_x) & \text{if } x > L_x \\ Kx_i & \text{if } x < 0 \end{cases} \quad (8)$$

with the same in the y direction. We also choose the mass $m = 1$ so the force becomes equal to the acceleration. This is also done to simplify the implementation. The program is written in fortran and the different states and simulations are set by editing an input file, the results should be able to be recreated by using the same inputs.

II. ONE PARTICLE

In order to simulate a gas first the system must be calibrated to one particle. First we can run different simulations with different time-steps to see how the particles behave. The box size is 10×10, the time is set to 10. In figure 1 the paths of 4 particles is traced over the same time but with different time steps, here we can see that a time step of $\Delta t = 0.01$ gives a decent trajectory. Time-steps above this results in a deteriorated path. In figure 2 the different energies for the paths in figure 1 is plotted over time. Here we can also see that the energy drift with a time-step of $\Delta t = 0.01$ is not too bad, this is thus a candidate for the highest time-step that gives a stable simulation.

III. MULTIPLE PARTICLES

For all the simulations beyond 1 particle the time step is set to $\Delta t = 0.001$, this is because of the stability it provides and the short run time for even very large systems, in tests of time at 40 and particles above 100 the run time does not exceed a few seconds. In the case of two particles the start positions and velocities are chosen, but in larger systems this is done randomly with the velocities such that each particle starts with a kinetic energy of the EPP value. The box size is also increased to 40×40. Before we can simulate gases we check that the system handles collisions of particles. The EPP value is set to 30.

In figures 3, 4, 5 and 6 paths and energy drift as collisions happen is plotted. As we can see, the energy is very well conserved over short time spans. So we can pretty confidently expand the system. We now expand the box to 50×50 and the time to 200.

In figure 7 the path of one particle is plotted as it explores the box. This might suggest that

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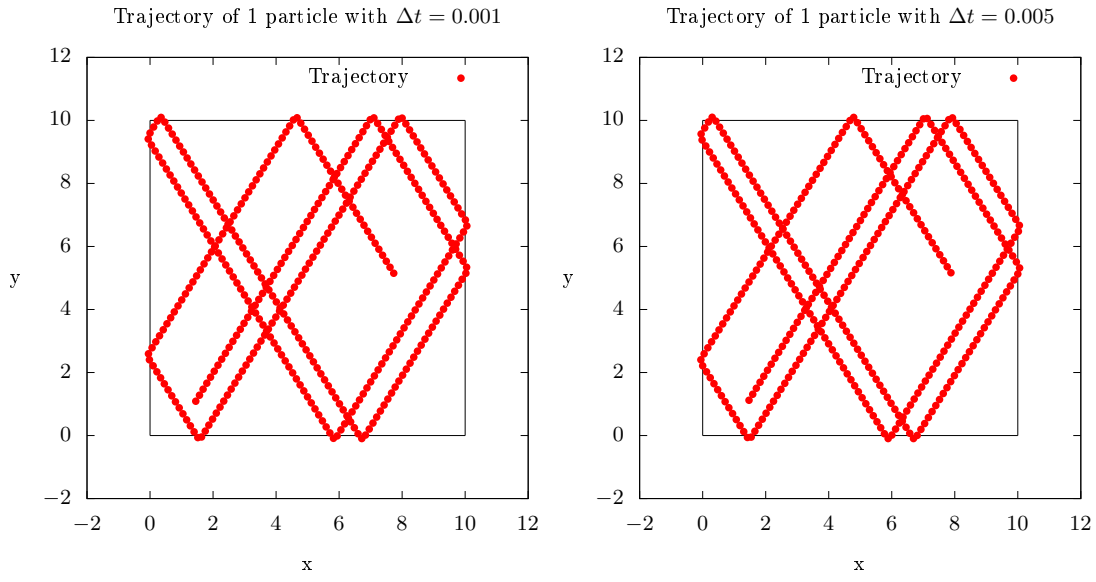
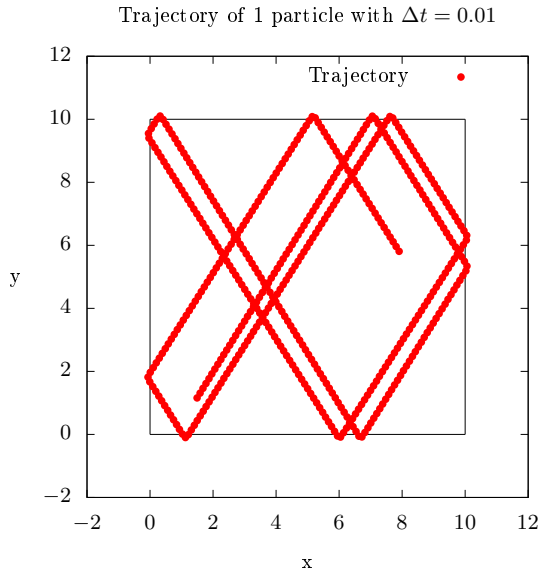
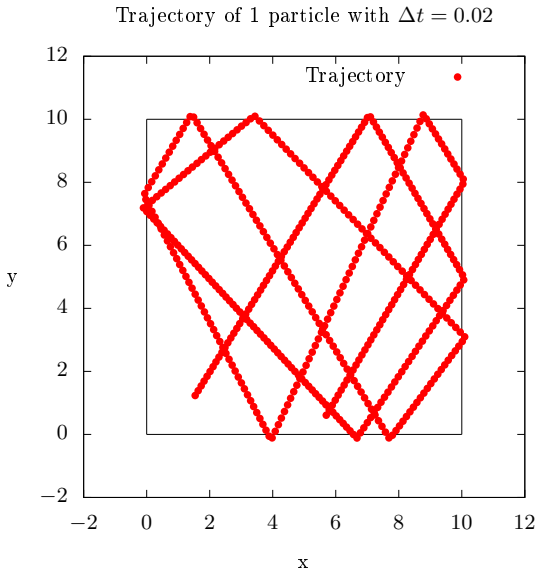


(a) Path of one particle with $\Delta t = 0.001$

(b) Path of one particle with $\Delta t = 0.005$



(c) Path of one particle with $\Delta t = 0.01$



(d) Path of one particle with $\Delta t = 0.02$

FIG. 1: Path of one particle with different values of time step Δt the wall constant $K = 6000$

in gasses with low density the particles eventually explores all of the box.

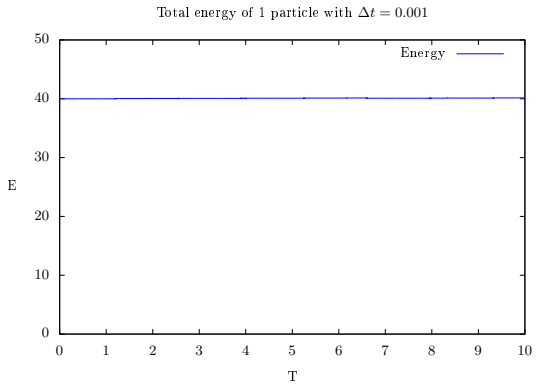
In order to find out how the energy of the particles is distributed over time, all the energy might be given to a chosen number of particles by editing the "distr" parameter in the input file of the program. A system of 50×50 is chosen with 10 particles and the system is let go for a long time.

in figure 8 the energy is plotted as it is distributed among the particles, an animation of this can also be seen at this link

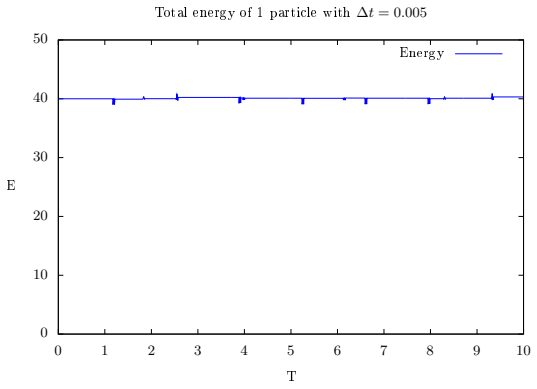
In order to numerically calculate the probability distribution, 100 particles was simulated in a box with lengths 50 over a time of 1000 and an EPP of 10, larger EPP is unstable over very long times. In figure 9 the numerical and theoretical probability distributing is plotted for velocity in the x direction

IV. SOLIDS

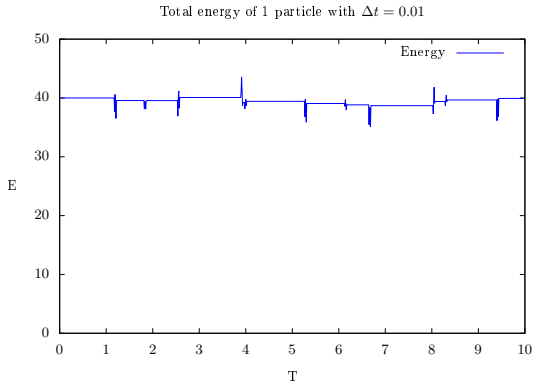
We now want to explore how the system behaves when the kinetic energy is close to ϵ this is done by setting the EPP to around 1 and the hcp parameter to 1 to override most of the other parameters. The initial case is 19 particles in an hexagonal pattern. The initial state is shown in figure 10. In figure 11 the end state with different initial energies i shown,



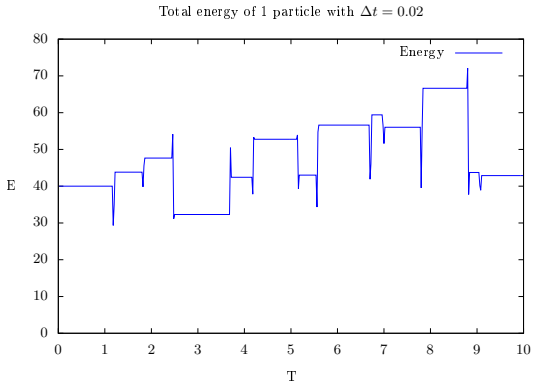
(a) Energy drift of one particle with $\Delta t = 0.001$



(b) Energy drift of one particle with $\Delta t = 0.005$

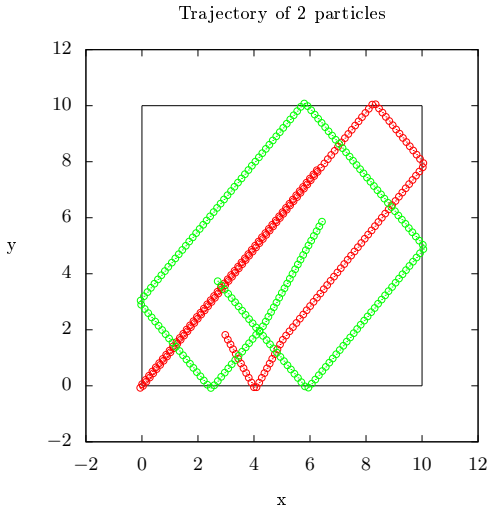


(c) Energy drift of one particle with $\Delta t = 0.01$

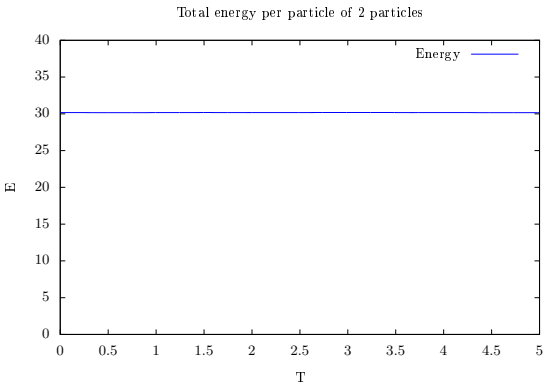


(d) Energy drift of one particle with $\Delta t = 0.02$

FIG. 2: Energy drift of one particle with different values of time step dt, the initial energy is set to 40



(a) Path of two particles, with collisions



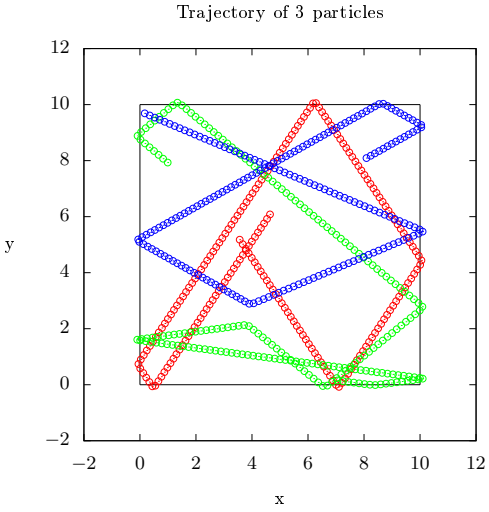
(b) Total energy per particle of the two particles as the collisions happen

FIG. 3: Two particles over a short time scale

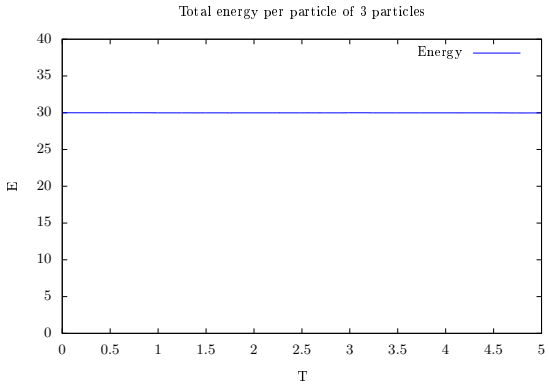
in figure 11d the initial energy is chosen such that the total energy is around 0.

ACKNOWLEDGMENTS

The author would like to thank Mathilde Hirsum and Paul Gunnar Dommersnes for answering all questions raised during the implementation of the

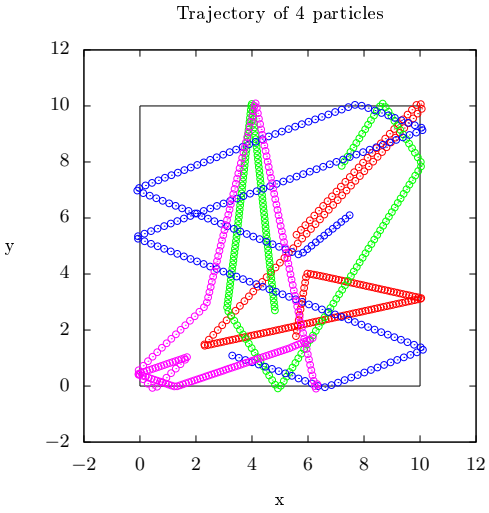


(a) Path of three particles, with collisions

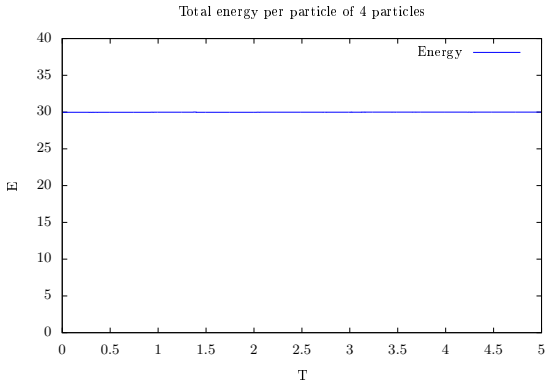


(b) Total energy per particle of the three particles as the collisions happen

FIG. 4: Three particles over a short time scale



(a) Path of four particles, with collisions



(b) Total energy per particle of the four particles as the collisions happen

FIG. 5: Four particles over a short time scale

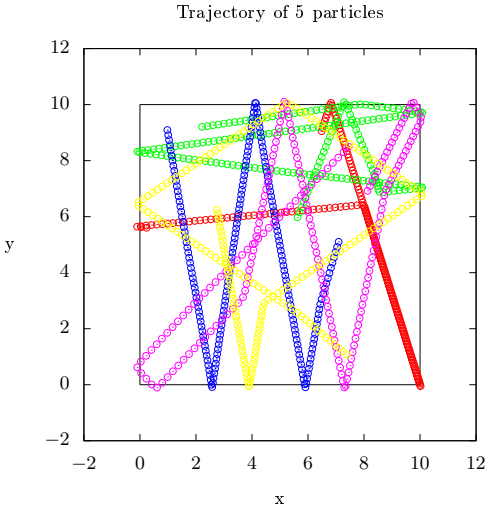
program.

Appendix A: Source code

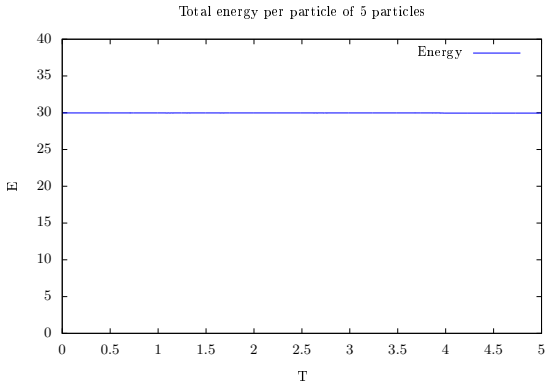
The source code may have been given to you along with this text, if it wasnt the source code along with the source for this text and raw data can be found at https://github.com/Mannen-I-Skogen/TFY4230-Numerical

Appendix B: Animations

Some of the systems in this text are animated and can be found Here

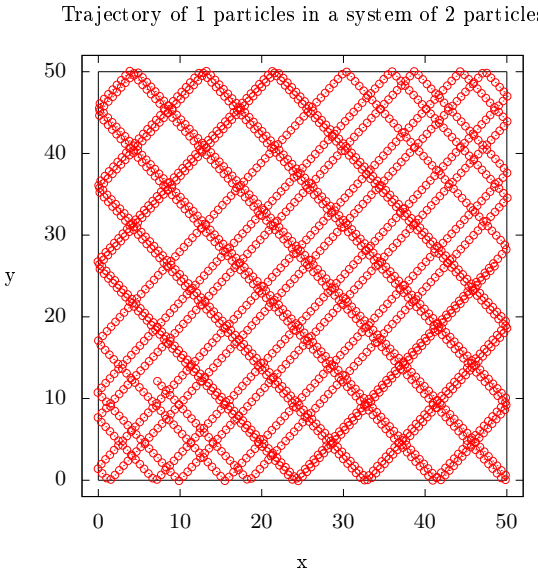


(a) Path of five particles, with collisions

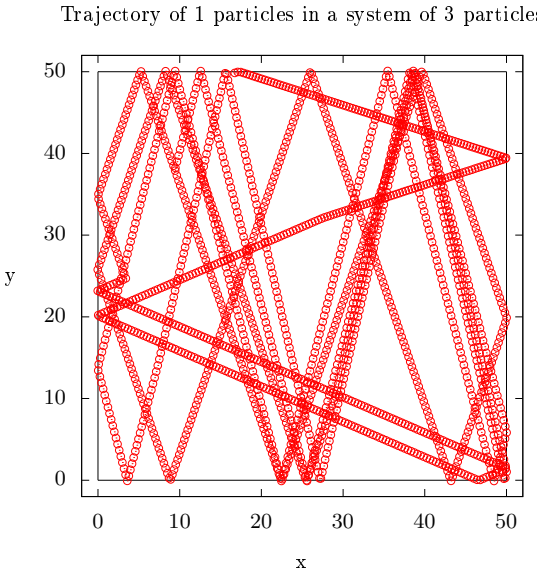


(b) Total energy per particle of the five particles as the collisions happen

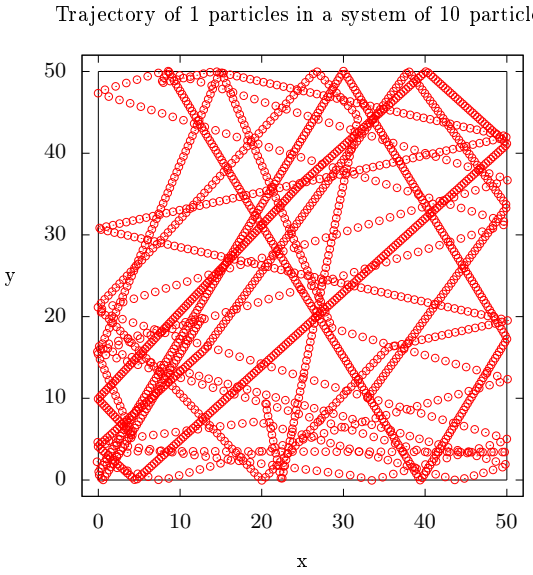
FIG. 6: Five particles over a short time scale



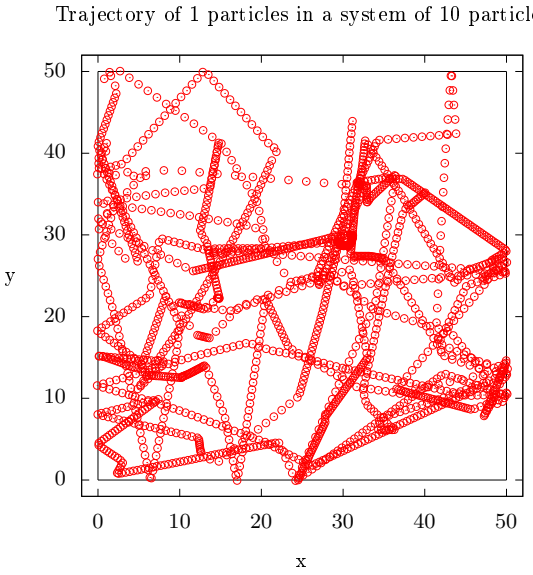
(a) Path of one particle in a system with 2 particles



(b) Path of one particle in a system with 3 particles

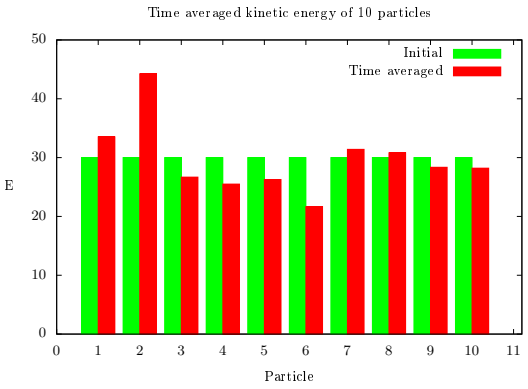


(c) Path of one particle in a system with 10 particles

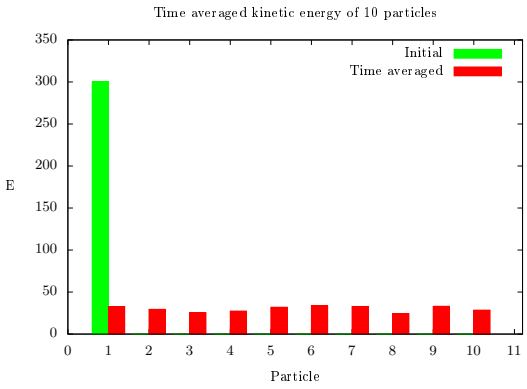


(d) Path of one particle in a system with 100 particles

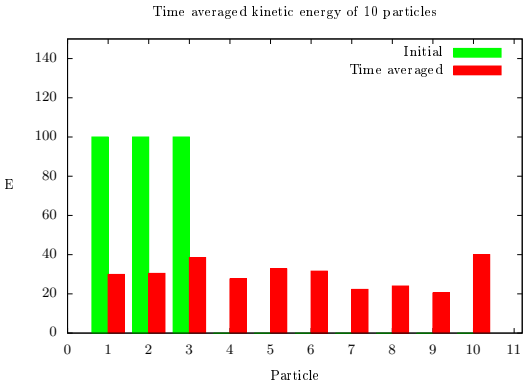
FIG. 7: Path of one particle in large system



(a) Kinetic energy for 10 particles at the start and the average kinetic energy with the energy evenly distributed at the start



(b) Kinetic energy for 10 particles at the start and the average kinetic energy with the all the energy given to one particle at the start



(c) Kinetic energy for 10 particles at the start and the average kinetic energy with the energy evenly distributed among just 3 particles at the start

FIG. 8: Path of one particle with different values of time step dt

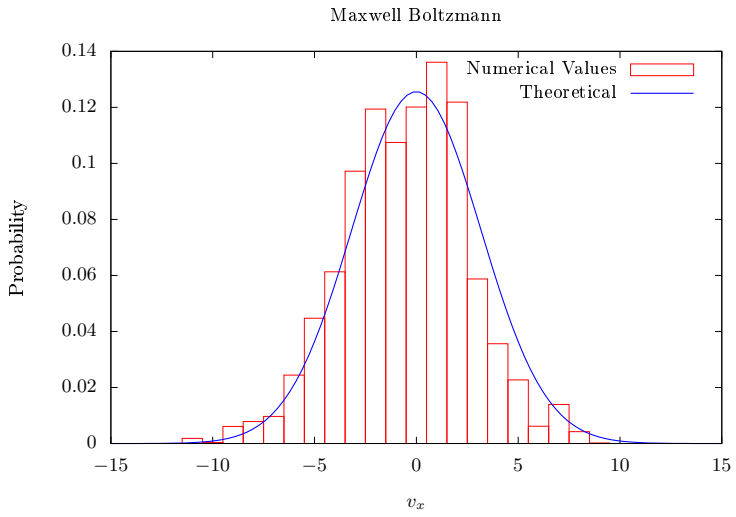


FIG. 9: Probability distribution of velocity of one particle

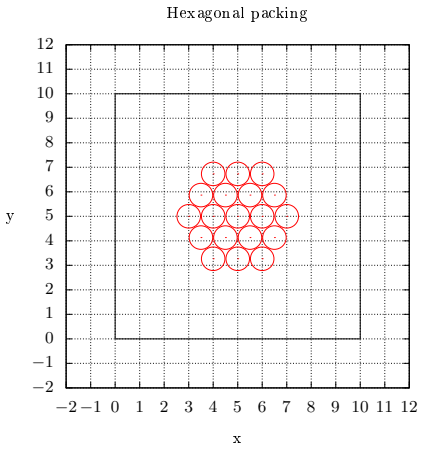
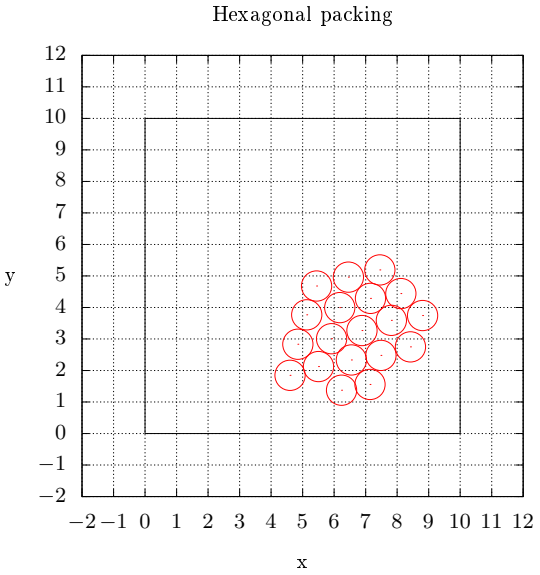
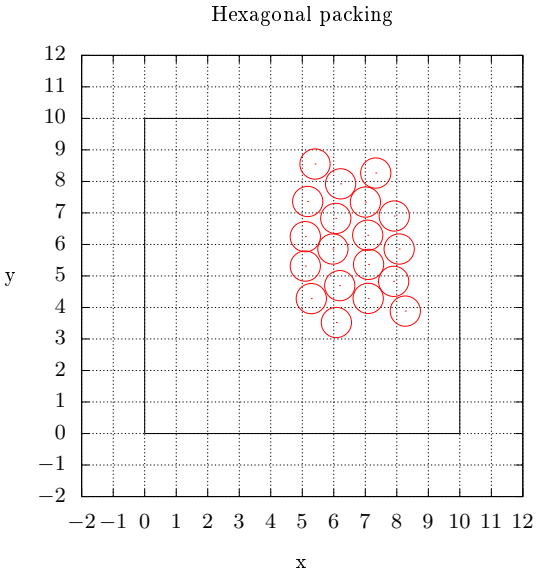


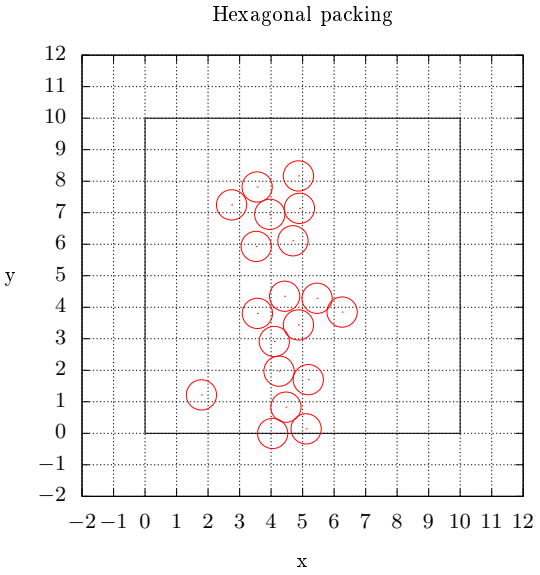
FIG. 10: The initial state of the solid, 19 particles packed in a hexagonal formation.



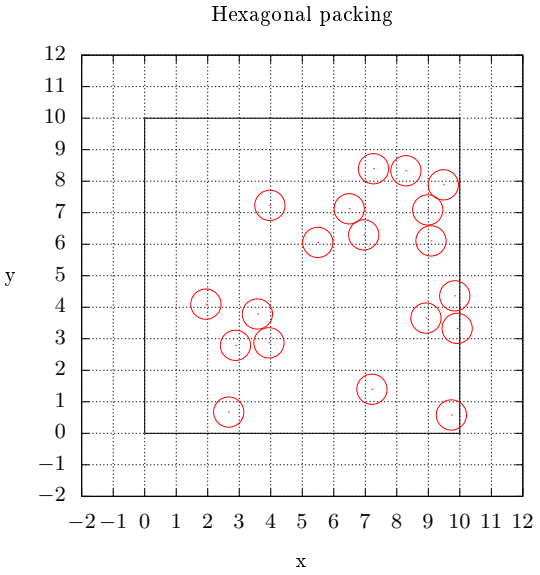
(a) The state of a solid after time evolution with an initial kinetic energy of 0.5



(b) The state of a solid after time evolution with an initial kinetic energy of 1.0



(c) The state of a solid after time evolution with an initial kinetic energy of 2.0



(d) The state of a solid after time evolution with an initial kinetic energy of 2.4

FIG. 11: Path of one particle with different values of time step dt