Assignment 1 Report
ELEC 4700

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Submitted: Sunday February 2^{nd}, 2019

1 Part 1: Electron Modelling

1.1 Thermal Velocity

The thermal velocity can be modeled by the equation,

$$v_{th} = \sqrt{\frac{3k_BT}{m_e}} \tag{1}$$

where k_B is the boltzmann's constant [1.380649e-23 $\frac{m^2kg}{s^2K}$], T is the temperature in Kelvin, and m is the effective mass of the particle. There is term of 3 in the numerator due to the 3 degrees of freedom for the movement of a particle. The effective mass of the particle is equal to the rest mass of an electron (9.1093837015e-31 kg) multiplied by a factor of 0.26. Assuming a temperature of 300 Kelvin, the thermal velocity would be,

$$v_{th} = \sqrt{\frac{3(1.380649e-23\frac{m^2kg}{s^2K})(300K)}{2.36843976239000e-31kg}}$$

$$v_{th} = 2.290507532173916 \times 10^5 m/s$$

1.2 Mean Free Path

The mean free path can be modelled by,

$$MFP = v_{th} \times t_{mn} \tag{2}$$

where v_{th} is the thermal velocity and t_{mn} is the mean time between collisions. The given mean time between collisions is 0.2ps. The mean free path would then be,

$$MFP = (2.290507532173916e+05\frac{m}{s})(0.2e-12s)$$

$$MFP = 4.58101506434783 \times 10^{-8}[m]$$

1.3 2-D Plot of Particle Trajectories

The trajectories of the particles travelling at the same speed but random direction are plotted and shown in Figure 1.

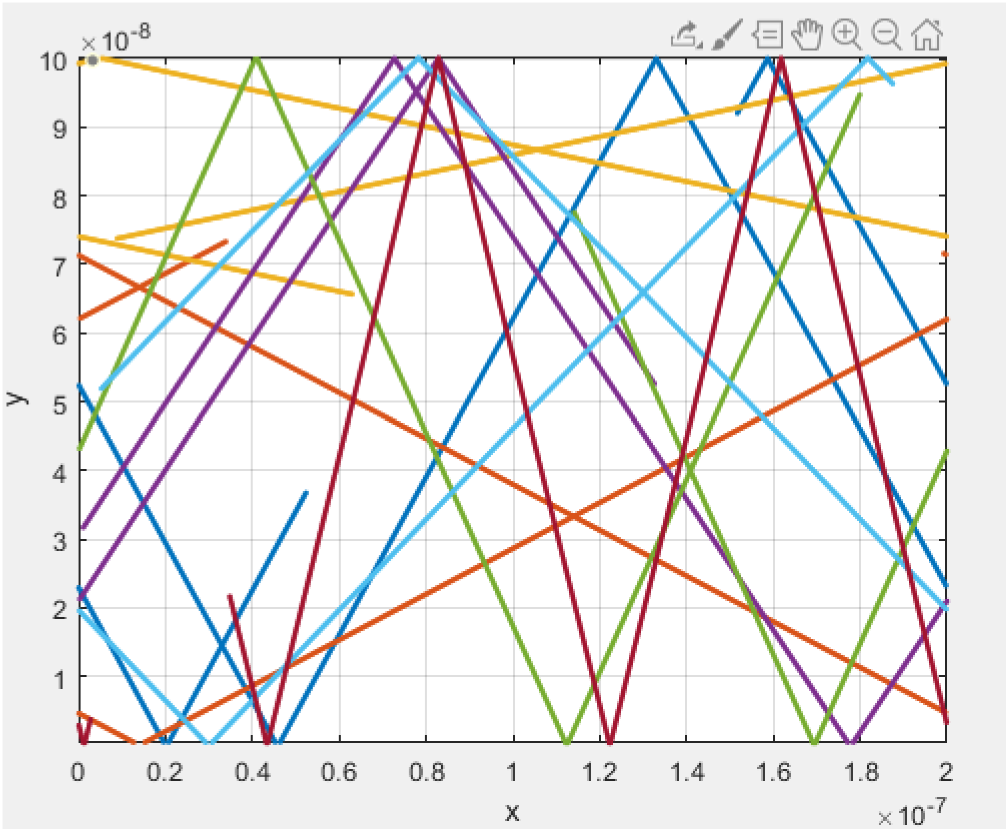

Figure 1: 2-D plot of 7 particle trajectories

1.4 Temperature Plot

The semiconductor temperature could be calculated by using the following equation,

$$[\frac{1}{2}mv^2]_{av} = \frac{3}{2}k_BT \tag{3}$$

where $[\frac{1}{2}mv^2]_{av}$ is the average kinetic energy of the particles in the box, including their mass and velocity. k_B and T are once again Boltzmann's constant and temperature. Rearranging this equation for temperature the temperature at each time-step can be calculated using,

$$T = (\frac{2}{3})(\frac{1}{k_B})(\frac{1}{2})(m)\frac{\sum^p(V_x^2 + V_y^2)}{p} \tag{4}$$

where V_x and V_y are the velocities in the x and y directions, and p is the number of particles. A temperature plot is created from the calculated temperatures in Figure 2. The temperature should stay constant since the average velocity of all the particles should be the thermal velocity.

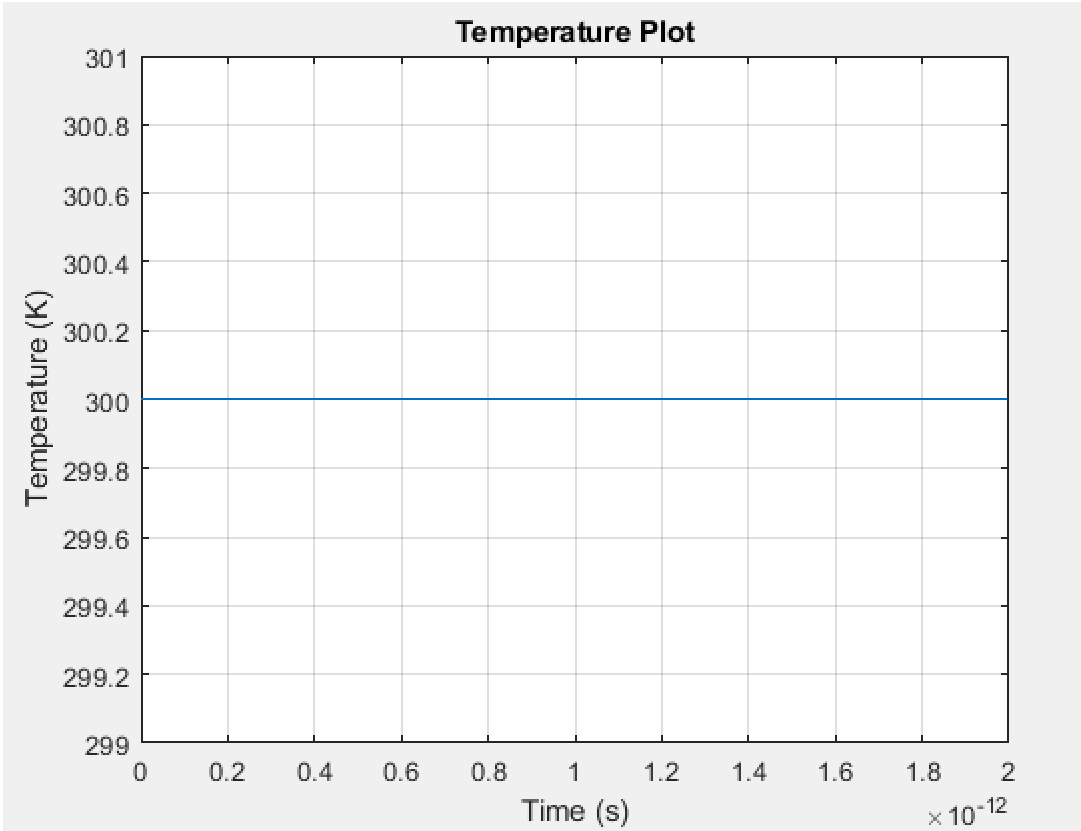

Figure 2: semiconductor temperature on a plot to verify that it stays constant

2 Part 2: Collisions with Mean Free Path

2.1 Histogram

The velocities of each particle are randomized in the x and y direction using the random function for a normal distribution. The velocity of each particle based on their direction x and y can be found using,

$$V = \sqrt{V_x^2 + V_y^2}$$

where the each particle velocity ’V’ can be plotted on a histogram. The histogram shown in Figure 3 features 100 bins for 10000 particles. The resulting distribution of particle velocities appears as a maxwell-boltzmann distribution.

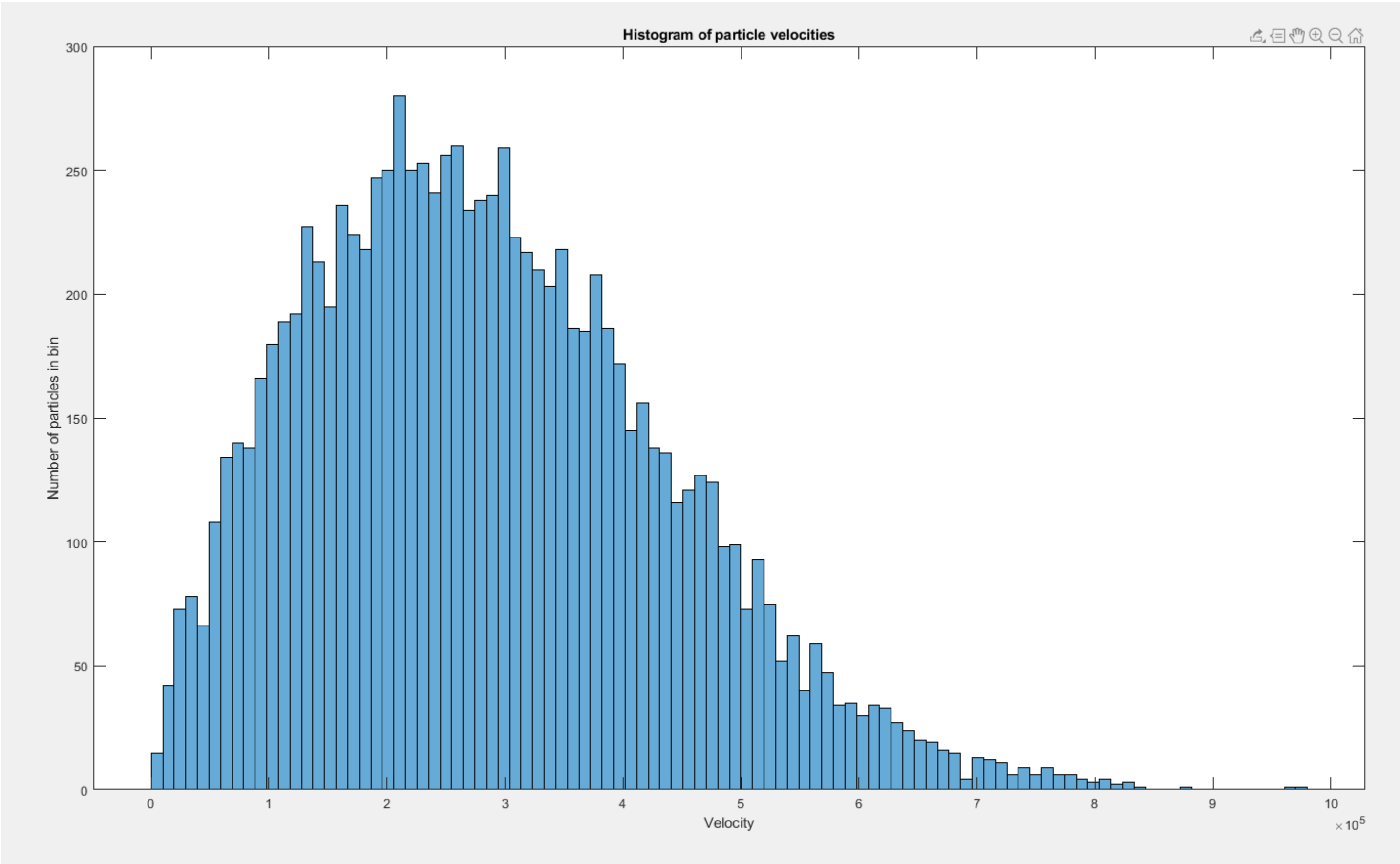

Figure 3: Histogram of particle velocities showing a Maxwell-Boltzmann distribution (100 bins, 10000 particles)

2.2 2-D plot of Particle Trajectories

Below in Figure 4 a 2-D plot using the new random scattering rules. Velocities often increase (dotted lines) and decrease (bolder lines) every time time they scatter and change direction. This is based on the exponential scattering rule,

$$P_{scatter} = 1 - e^{-\frac{dt}{\tau_{mn}}}$$

using the random function to get random values [0,1], a scatter will occur if $P_{scatter} > rand$. When a particle scatters, it's speed and direction are randomly re-assigned.

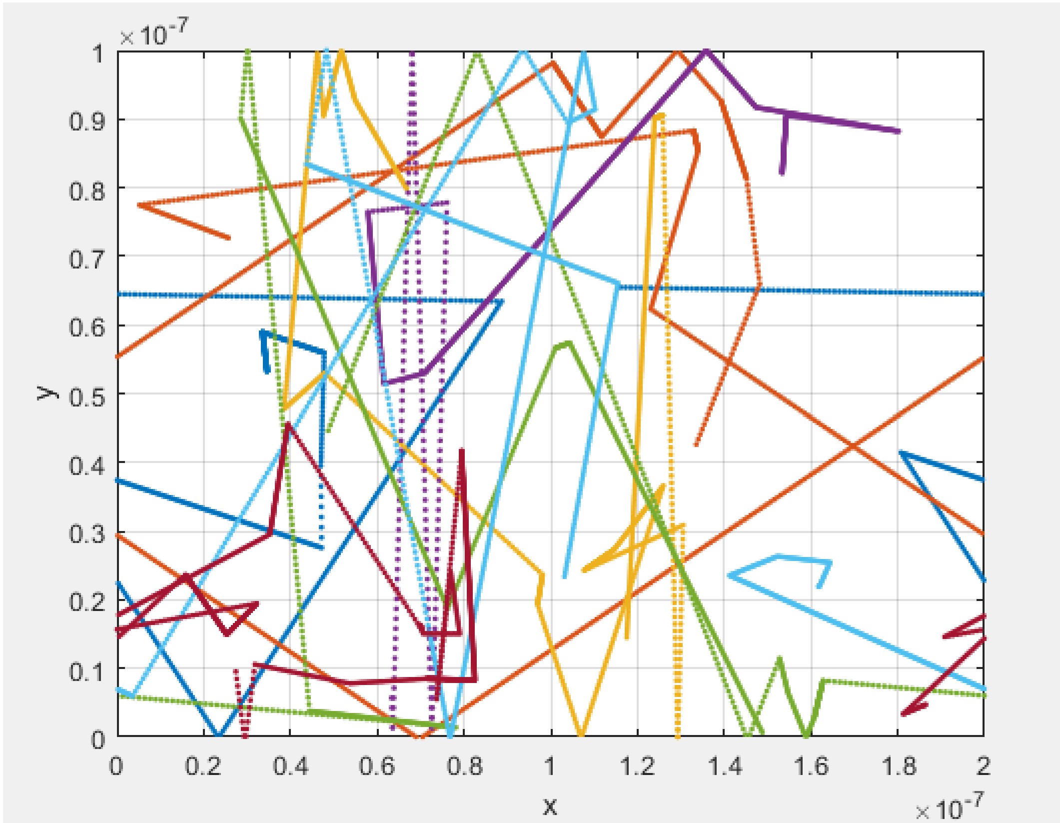

Figure 4: Particle trajectories with a scattering probability

2.3 Temperature Plot

The temperature plot is then graphed again to show the average temperature over time in Figure 5. In this case the scattered particles cause the temperature to rise and fall. This is probably due to the total velocity increasing and decreasing randomly for all the particles every time they scatter.

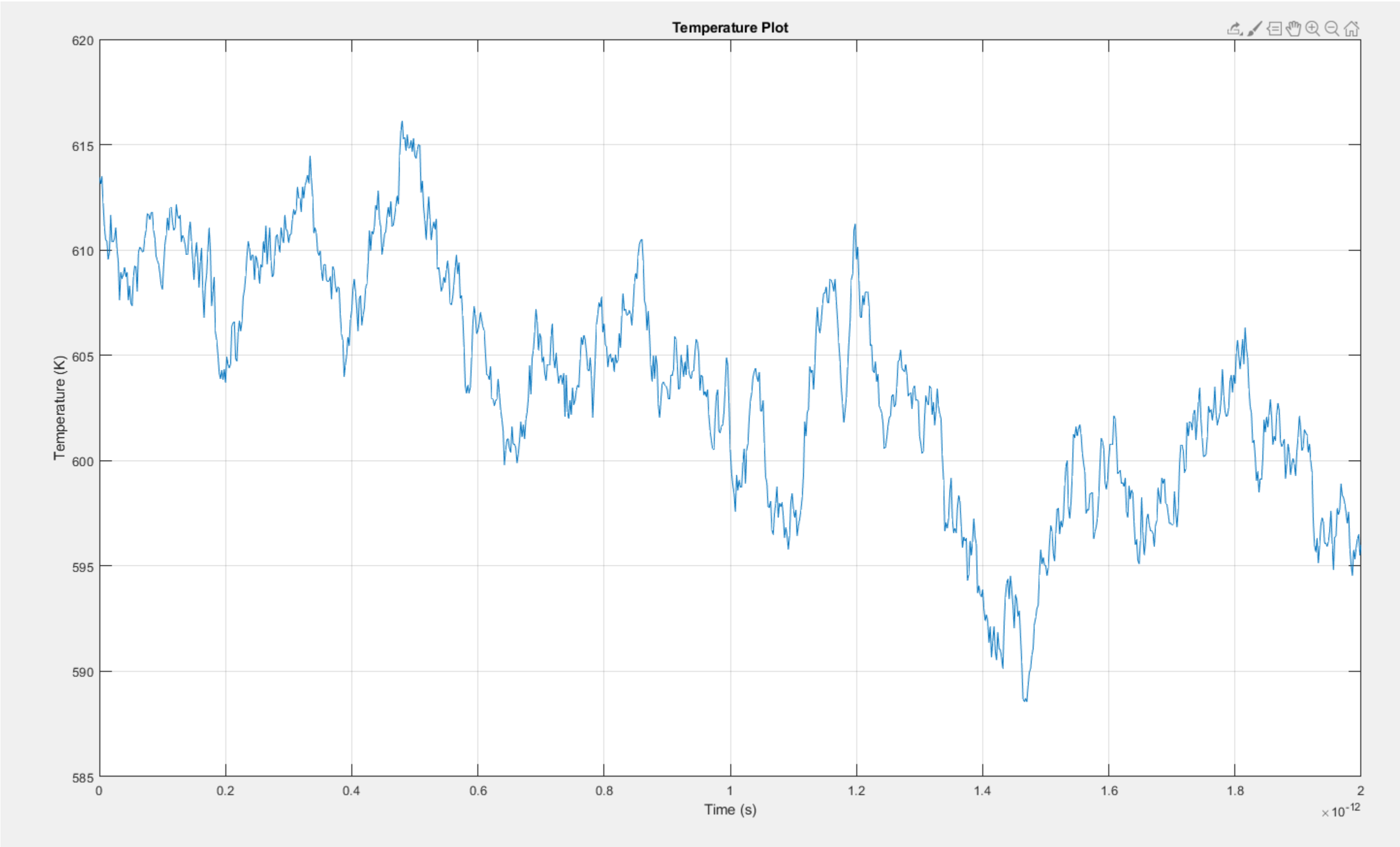

Figure 5: Temperature plot when particles change velocities from scattering

2.4 Mean Free Path and Mean Time between collisions (τ_{mn})

The mean free path and mean time between collisions can be measured experimentally. By taking the time in between each scatter for each particle and divided by the number of collisions you can get the mean time between collisions for each particle.

$$A = \frac{1}{\#collisions} \sum^{collisions} \Delta t_{collisions}$$

The mean time between each scatter for each particle can be added together and then divided by the amount of particles to get the final mean time between collisions,

$$t_{mn} = \frac{\sum A}{particles}$$

To get the mean free path, the distance each particle travels before scattering must be found. This can be found by finding the velocity of the particle before it scatters and multiplying it by the mean time between the collisions. The resulting mean time between collisions and mean free path vary for each simulation but are usually around,

$$t_{mn} = \ 4.078978693894408e - 14[s]$$

$$MFP = \ 1.153114624654788e - 08[m]$$

Comparing this to the calculated t$_{mn}$ ($2{\times}10^{-13}$) and mean free path ($MFP = 4.58101506434783 \times 10^{-8}[m]$) the model isn't great but somewhat close to the expected values.

3 Part 3: Enhancements

3.1 2-D plot of particle trajectories

2 boundary boxes are added to the plot for the particles to bounce off of. The boxes are created to create a specular or diffusive reflection. The specular reflection acts like the y-boundaries of the box and reflects a particle by reversing its direction depending on which side of the box it hits. A diffusive reflection creates a scatter type effect which causes the particle to bounce of in a random direction when hitting the box. Figure 6 shows the boxes when given specular reflection. Figure 7 shows the scatter off the boxes when given a diffusive reflection.

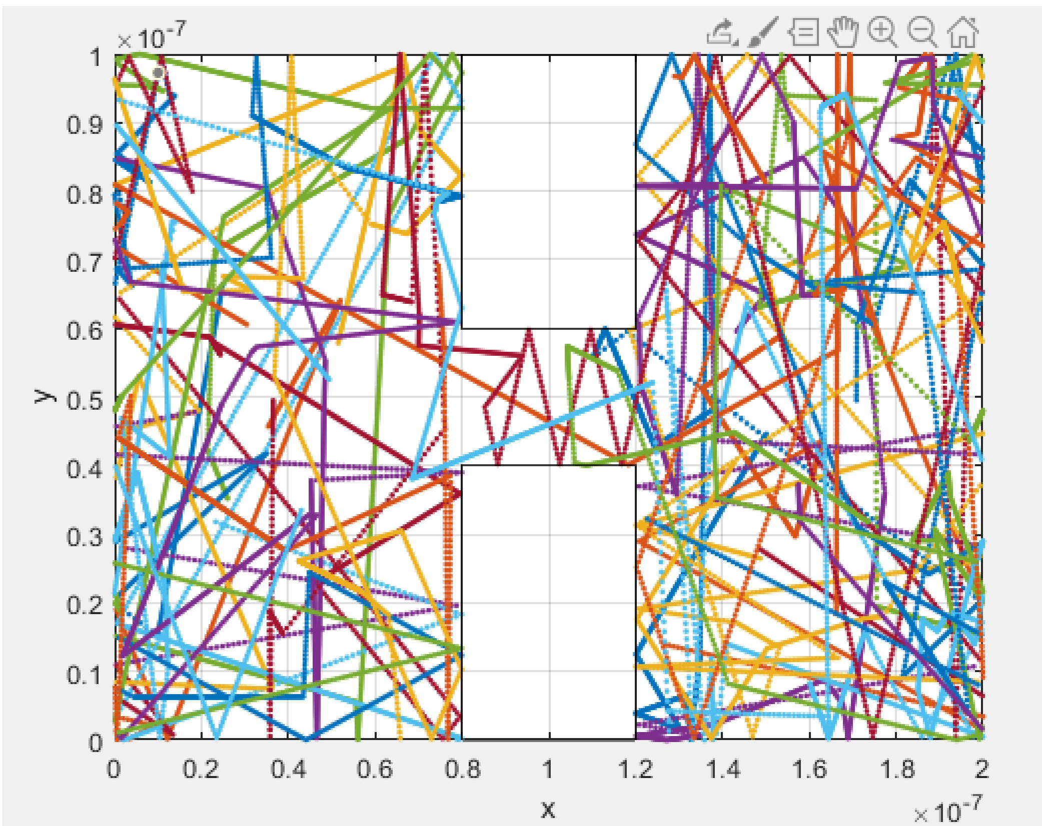

Figure 6: Particle trajectories with box boundaries and specular reflection off the boxes

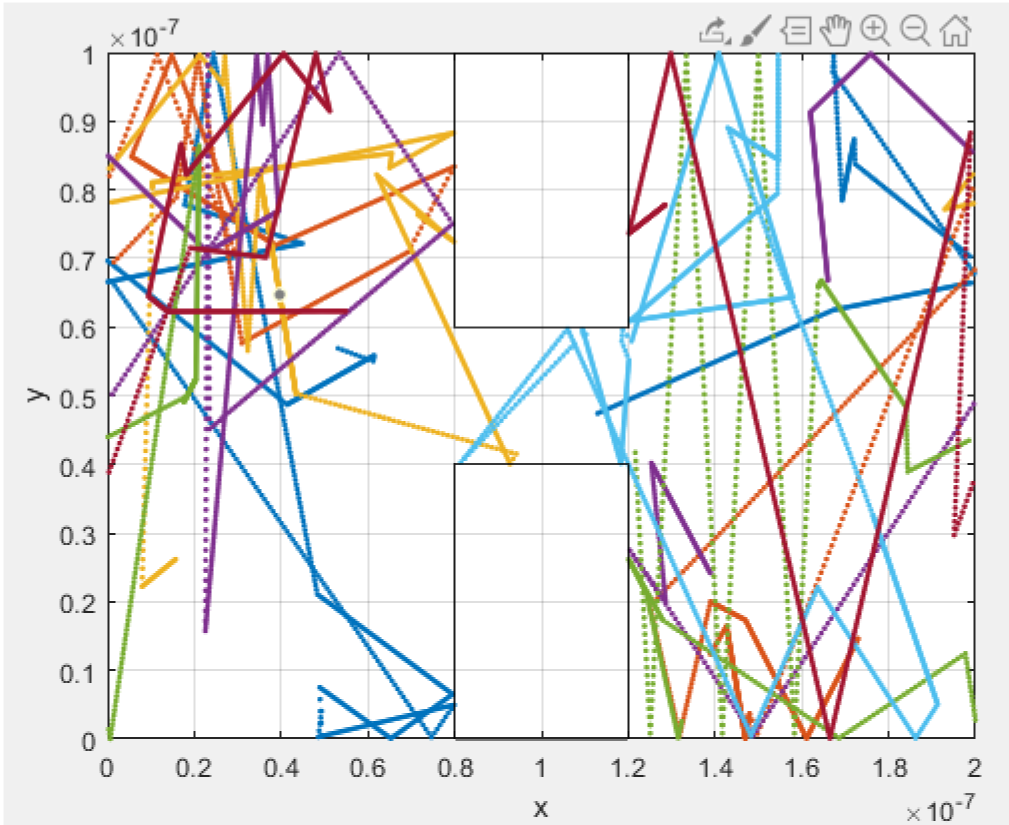

Figure 7: Particle trajectories with box boundaries and diffusive reflection off the boxes

3.2 Electron Density Map

An electron density map is made which shows the location of all the particles after the simulation is complete. In Figure 8 there are 10 000 particles in the simulation and the final density plot shows the empty spots where the boxes would be. I expected the electrons to be more dense in the bottle-neck between the two boxes but it seems in specular reflection the particles don't have much difficulty leaving the space.

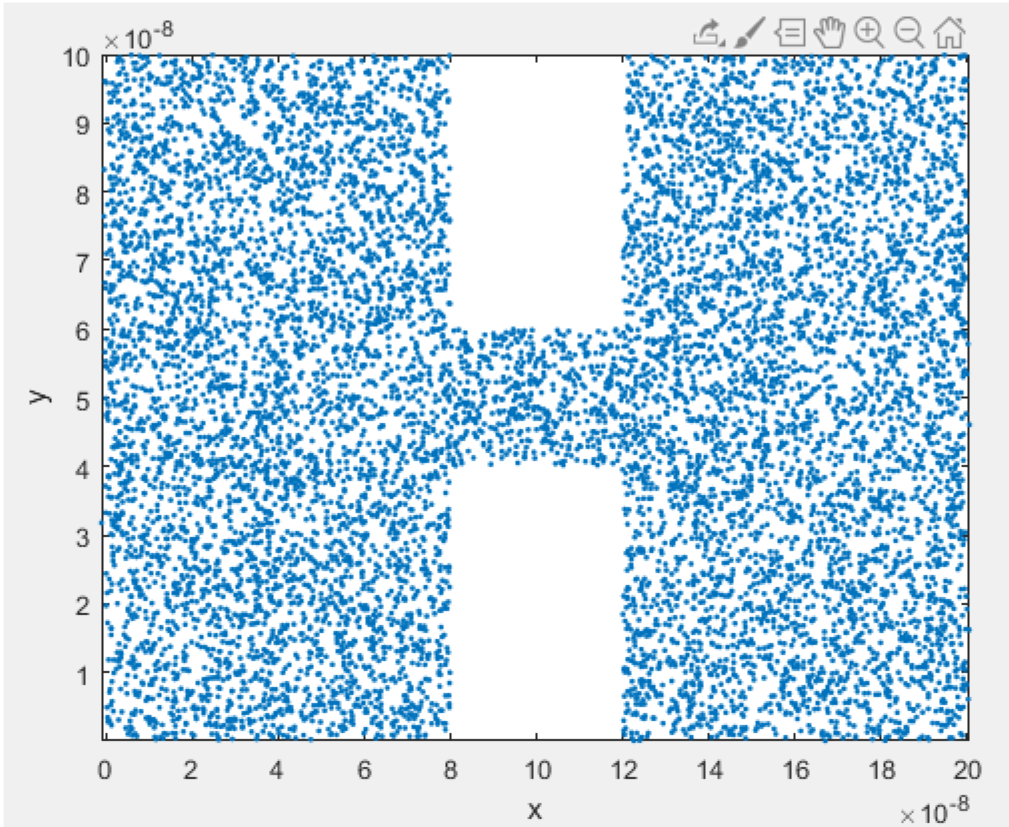

Figure 8: Electron density map of 10 000 particles at the end of simulation

3.3 Temperature Map