Carleton University

Department of Electronics

ELEC 4700 A

Assignment 1

Author:
Denis Shleifman
101001778

Professor:
Tom Smy

Date Submitted: February 2, 2020

Contents

1 Introduction

This assignment examined the random motion of particles within a box. Each question introduced a new degree of complexity into the simulation and therefore allowed for additional analysis. Question 1 comprised of the electrons in the box with simple boundary conditions. These boundary conditions included a wrap around in the x axis and reflections in the y axis. The analysis for this question can be found in Section 2 below. Question 2 added the effect of random scattering. The analysis for this question can be found in Section 3 below. Finally question 3 added a "bottle-neck" to the system. The analysis for this question can be found in Section 4 below.

2 Question 1

The analysis performed in this section include calculating the expected thermal velocity in Section 2.1 and the expected mean free path in Section 2.2. This is followed by plots of the particle trajectories and the temperature as it changes with time in Sections 2.3 and 2.4 respectively.

2.1 Thermal Velocity

This section contains the calculations necessary to obtain the expected thermal velocity of the particles. The expected thermal velocity of the particles can be calculated using Equation 1 below.

$$v_{th} = \sqrt{\frac{d_f T k_b}{m_{eff}}} \tag{1}$$

Where v_{th} is the thermal velocity, d_f is the number of degrees of freedom, T is the temperature in kelvin, k_b is Boltzmann's constant and m_{eff} is the effective mass of the particles. [2]

In this case the number of degrees of freedom is 2 because there are two axis in which the particles can move. The temperature of the board is set to $300k$, and finally the effective mass is taken as $0.26 \cdot m_e$ where m_e is mass of an electron. The calculation for the thermal velocity is therefore shown below.

$$v_{th} = \sqrt{\frac{2\,(300\text{k})\left(1.38 \cdot 10^{-23}\frac{\text{J}}{\text{k}}\right)}{0.26\,(9.11 \cdot 10^{-31})\,\text{kg})}}$$

The resulting thermal velocity is $v_{th} = 187\frac{\text{km}}{\text{s}}$.

2.2 Mean Free Path

This section contains the calculations necessary to obtain the mean free path. The mean free path is the average distance that a particle will travel before colliding with another particle. Since the average time between collisions is given at $\tau_{mn} = 0.2\text{ps}$, the equation for mean free path can therefore be written as shown below in Equation 2.

$$MFP = v_{av} \cdot \tau_{mn} \tag{2}$$

Where MFP is the mean free path, v_{av} is the average velocity of the particles and τ_{mn} is the average time between collisions.

In this case the thermal velocity is known, not the average. The equation to convert the thermal velocity to average velocity is shown in Equation 3 below.

$$v_{av} = v_{th} \cdot \frac{2}{\sqrt{\pi}} \tag{3}$$

Where v_{av} is the average velocity of the particles and v_{th} is the thermal velocity of the particles [2]. The calculation for the average velocity is shown below.

$$v_{av} = 187\frac{\text{km}}{\text{s}} \cdot \frac{2}{\sqrt{\pi}}$$

The resulting average velocity is $v_{av} = 166\frac{\text{km}}{\text{s}}$. Inserting this value into Equation 2 yields the calculation for the mean free path as shown below.

$$MFP = \left(187\frac{\text{km}}{\text{s}}\right)(0.2\text{ps})$$

The resulting estimated mean free path is $MFP = 33.1\text{nm}$.

2.3 Particle Trajectories

This section contains an analysis of the particle trajectories. Figure 1 below shows the trajectories of 7 out of the 10000 particles that were generated.

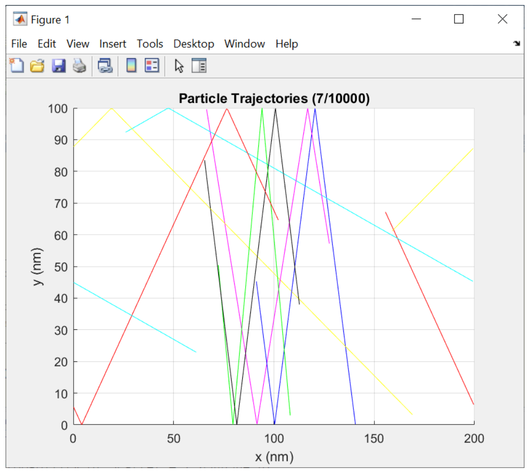

Figure 1: Particle Trajectories (7/10000)

In Figure 1, when particles reached either the bottom or the top of the box they can be seen to reflect, when they reach the left or right side they can be seen to wrap around. This is as expected.

2.4 Temperature Plot

This section contains an analysis of the system temperature. Figure 2 below shows the average temperature of the 10000 particles generated over time.

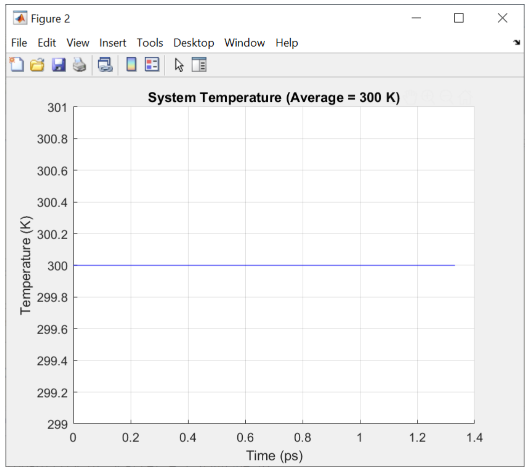

Figure 2: System Temperature over Time

In Figure 2, the temperature can be seen to remain constant at 300k. This is expected as the velocities of each particle was generated to ensure that its individual temperature remained at 300 k. Since the velocities never change (only the direction of the individual components), the temperature remains constant.

3 Question 2

The analysis performed in this section include examining the distribution of particle velocities in Section 3.1 followed by the plots of the particle trajectories and the temperature as it changes with time in Sections 2.3 and 2.4 respectively. Finally a comparison of the expected mean free path and time between collisions and the simulation values is found in Section 3.4.

3.1 Velocity Histogram

This section contains an analysis of the distribution of velocities of the system. Figure 3 below contains a histogram of the particle velocities at a simulation time of 5.34 ps.

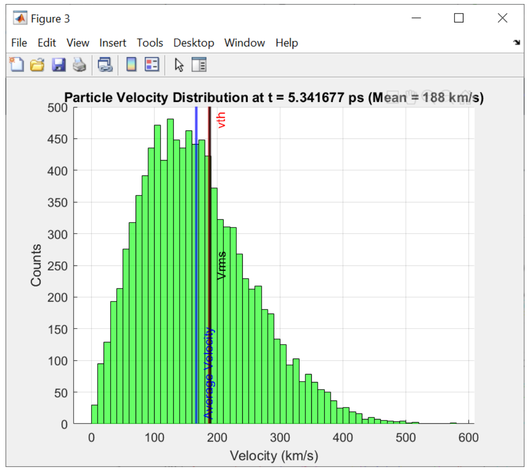

Figure 3: Velocity Distribution at t = 5.34 ps

As seen in Figure 3 the distribution of velocities follows the expected Maxwell-Boltzmann distribution. The average velocity of the particles does not coincide to the thermal velocity, however the Vrms does. This is as expected. Though Figure 3 only shows one instance, this same distribution and the same analysis and the same results will be obtained from analysing this plot at any other time.

3.2 Particle Trajectories

This section contains an analysis of the particle trajectories. Figure 4 below shows the trajectories of 7 out of the 10000 particles that were generated.

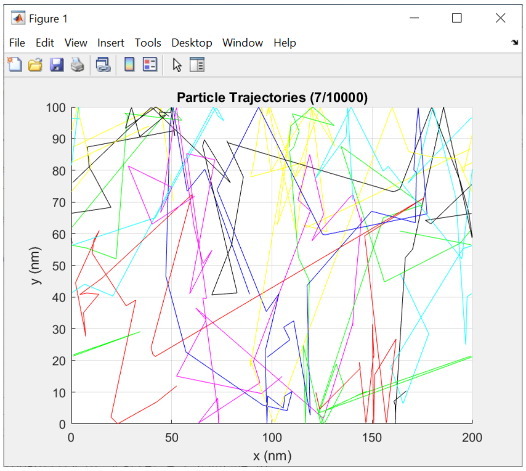

Figure 4: Particle Trajectories (7/10000)

In Figure 4, the addition of scattering can be noticed. This is evident as the particles can be seen to change direction seemingly randomly. This is as expected.

3.3 Temperature Plot

This section contains an analysis of the system temperature. Figure 2 below shows the average temperature of the 10000 particles generated over time.

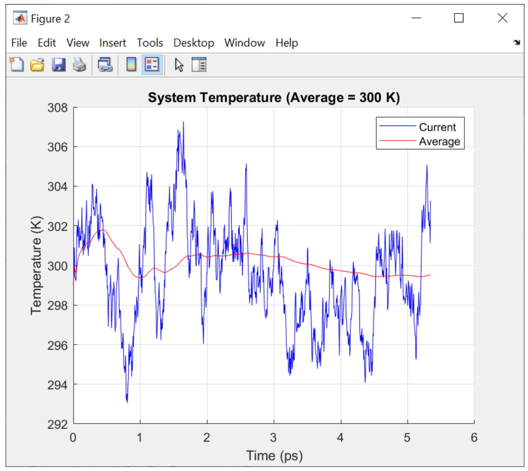

Figure 5: System Temperature over Time

In Figure 5, the temperature can be seen to fluctuate around 300k. Though the temperature fluctuates, the average temperature over time stabilizes to 300k. This is expected as the temperatures are assigned randomly.

3.4 Comparison of Mean Free Path and Time Between Collisions

The expected mean free path and time between collisions can be found in section 2.2. These values are MFP = 33.1nm and τ_{nm} = 0.2ps respectively. During the simulation, the average distance between collisions and the average time between collisions were collected. These values were 32.4 nm and 0.20 ps respectively. These values are very close to their expected counterparts.

4 Question 3

The analysis performed in this section include examining the plot of the particle trajectories in Section 4.1. This is followed by an examination of the particle location heatmap in Section 4.2 and the temperature heatmap in Section 4.3.

4.1 Particle Trajectories

This section contains an analysis of the particle trajectories. Figure 6 below shows the trajectories of 7 out of the 10000 particles that were generated.

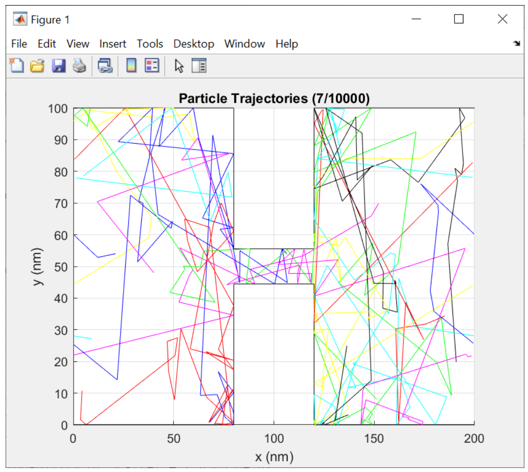

Figure 6: Particle Trajectories (7/10000)

In Figure 6, the addition of the "bottle-neck" as well as making particles scatter off boundaries can be noticed. This is evident as the particles never enter the forbidden regions and can be seen to randomly change directions when encountering any boundary. This is as expected.

4.2 Particle Location HeatMap

This section contains a heatmap showing the distribution of particle locations across the entire simulation. This is shown in Figure 7

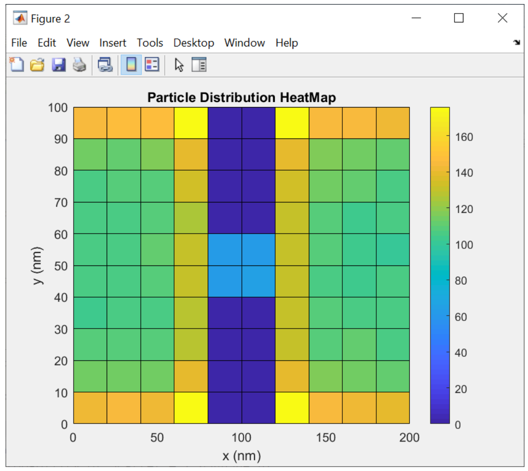

Figure 7: Particle Location HeatMap

As seen in Figure 7 ,particles are most likely to be located near boundaries, but are least likely to be located inside the "bottle-neck".

4.3 Temperature HeatMap

This section contains a heatmap showing the distribution of temperature across the entire simulation. This is shown in Figure 8

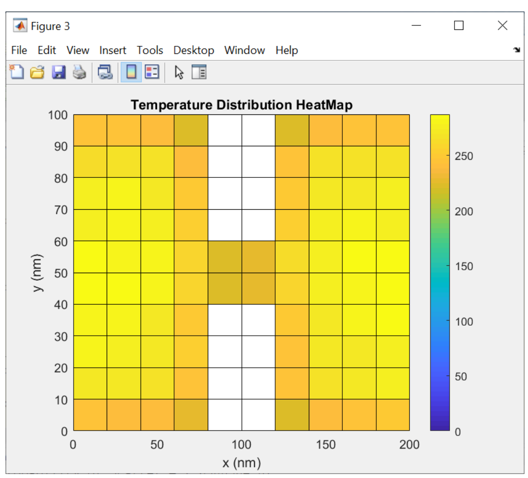

Figure 8: Temperature HeatMap

As seen in Figure 8 the hottest regions are located away from boundaries.

References

[1] *Society for Neuroscience, Ottawa Chapter* [Online] Available FTP: http://cdn.sfn-ottawa.ca Directory: images/misc File: cu-logo-vertical.png?1415290081

[2] “Kinetic Temperature,” *Hyper Physics.* [Online]. Available: http://hyperphysics.phy-astr.gsu.edu/hbase/Kinetic/kintem.html. [Accessed: 17-Jan-2020].