Assignment 1

Monte-Carlo Modeling of Electron Transport

Zachary St. Pierre

ELEC4700

02/06/2022

Carleton University

Part 1: Electron Modeling

The thermal velocity for the system can be calculated by rearranging the following equation:

$$v_{\text{th}} = \sqrt{\frac{2k_B T}{m_e}}$$

Where k_B is the Boltzmann constant, T is the initial temperature of the system, and m_e is the effective mass of the electron. Plugging in the values and solving gives:

$$v_{\text{th}} = 1.8704e + 05$$

The Mean Free Path can be found using the calculated thermal velocity and the given τ_{mn} value of 0.2ps.

$$MFP = v_{\text{th}} * \tau_{mn}$$

MFP = 37 nm

The number of electrons in the simulation can be varied based on desired amount by changing the N_e value in the MATLAB code. The number of plotted electrons can also be changed to any number lower than the number of electrons simulated. The following plot was generated with N_e = 1000 and 5 random particles selected to be plotted.

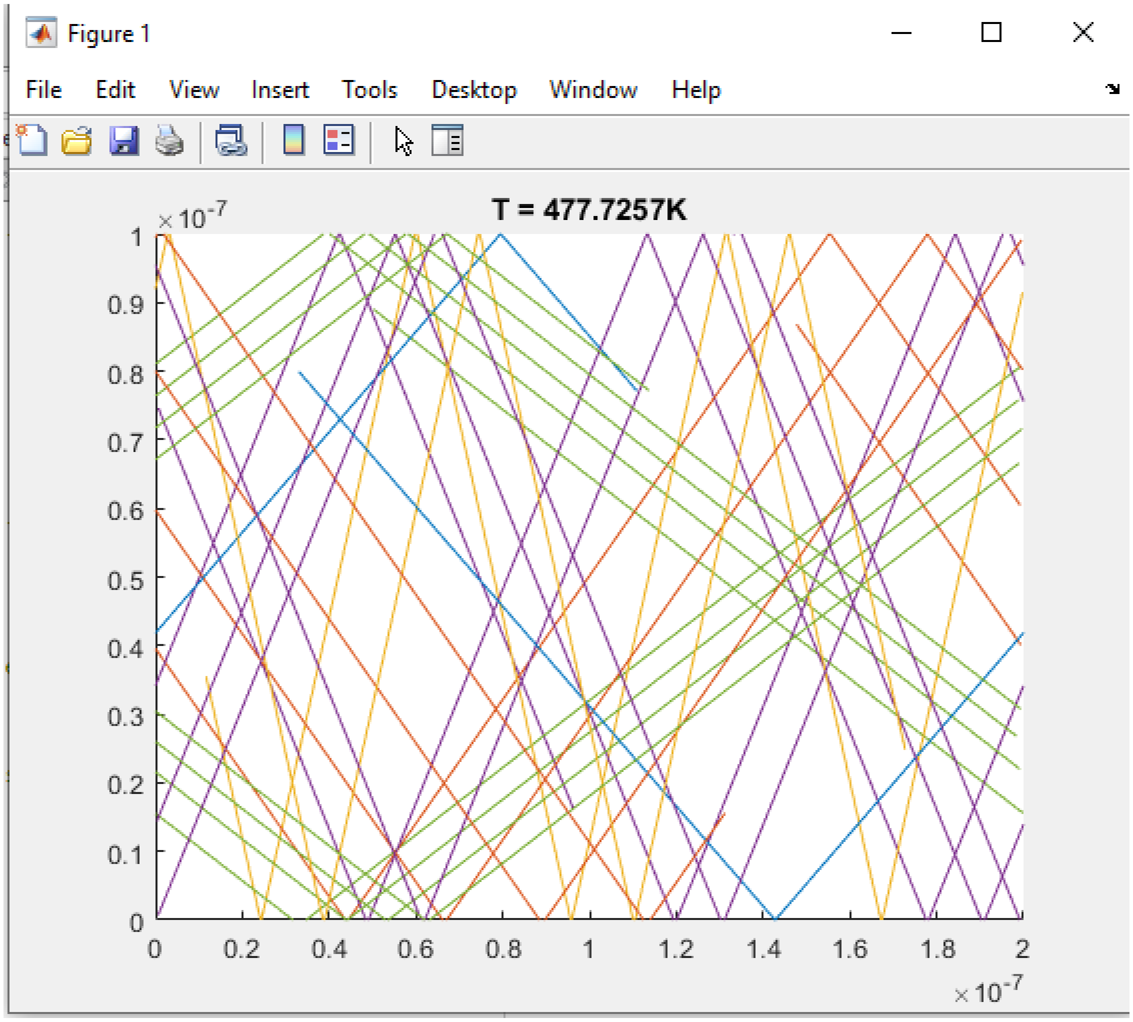

Figure 1: Simulated Travel of Electrons in a 200nm x100nm Silicon Plane

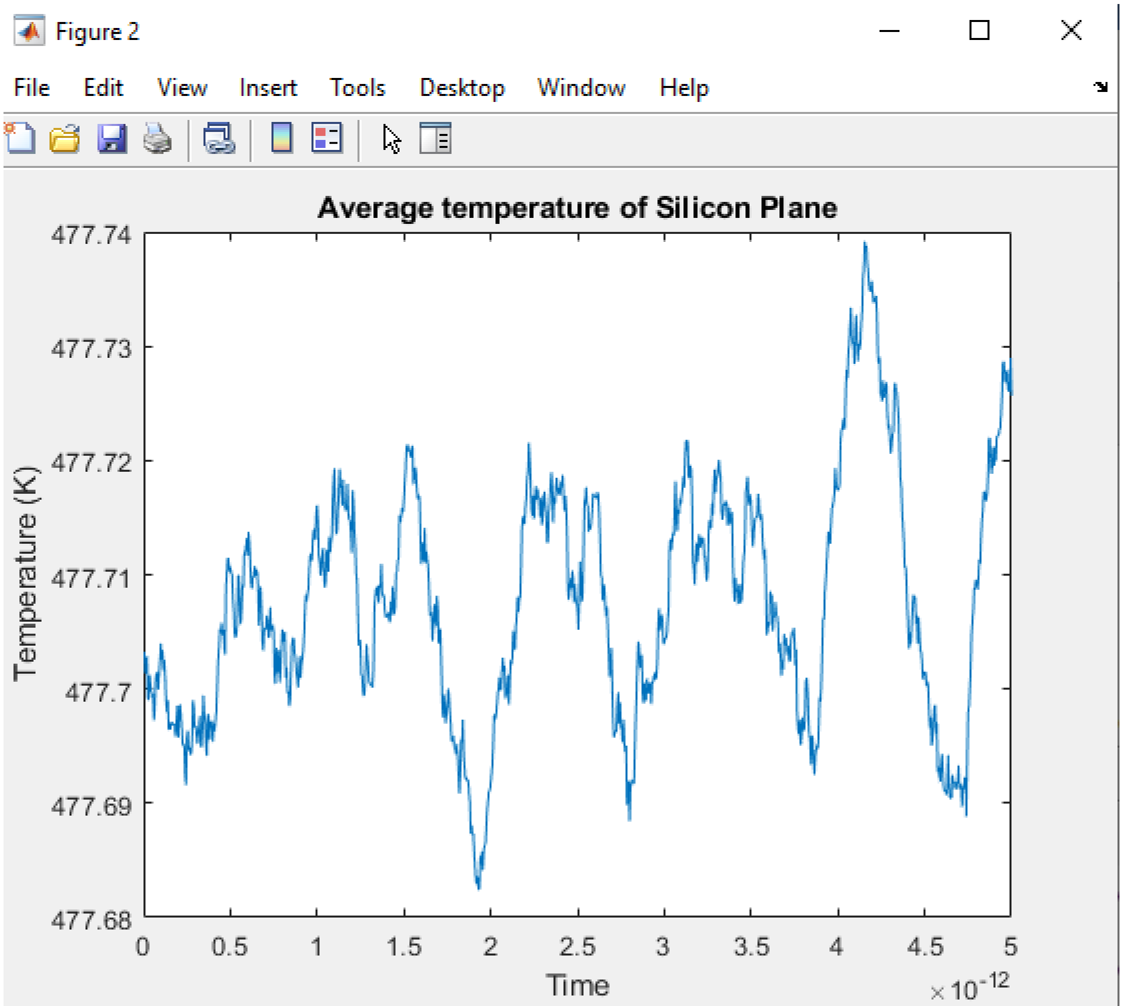

Figure 2: Average Temperature of the Silicon Plane

The average temperature of the silicone can be seen to be effectively constant, and this is due to the velocities of the particles remaining constant in the plane. I was unable to determine why the temperature was not roughly 300K which is what I expected the result for the plane to be.

Part 2: Collisions with Mean Free Path

The second part of the assignment is to add scattering and to add a Maxwell-Boltzmann distribution to the random velocities assigned to the x and y directions. The random velocities are assigned using the randn() function in MATLAB and multiplying each result by a deviation correlating to a Maxwell-Boltzmann distribution. The distribution of temperatures at the end of the simulation is shown by the following histogram:

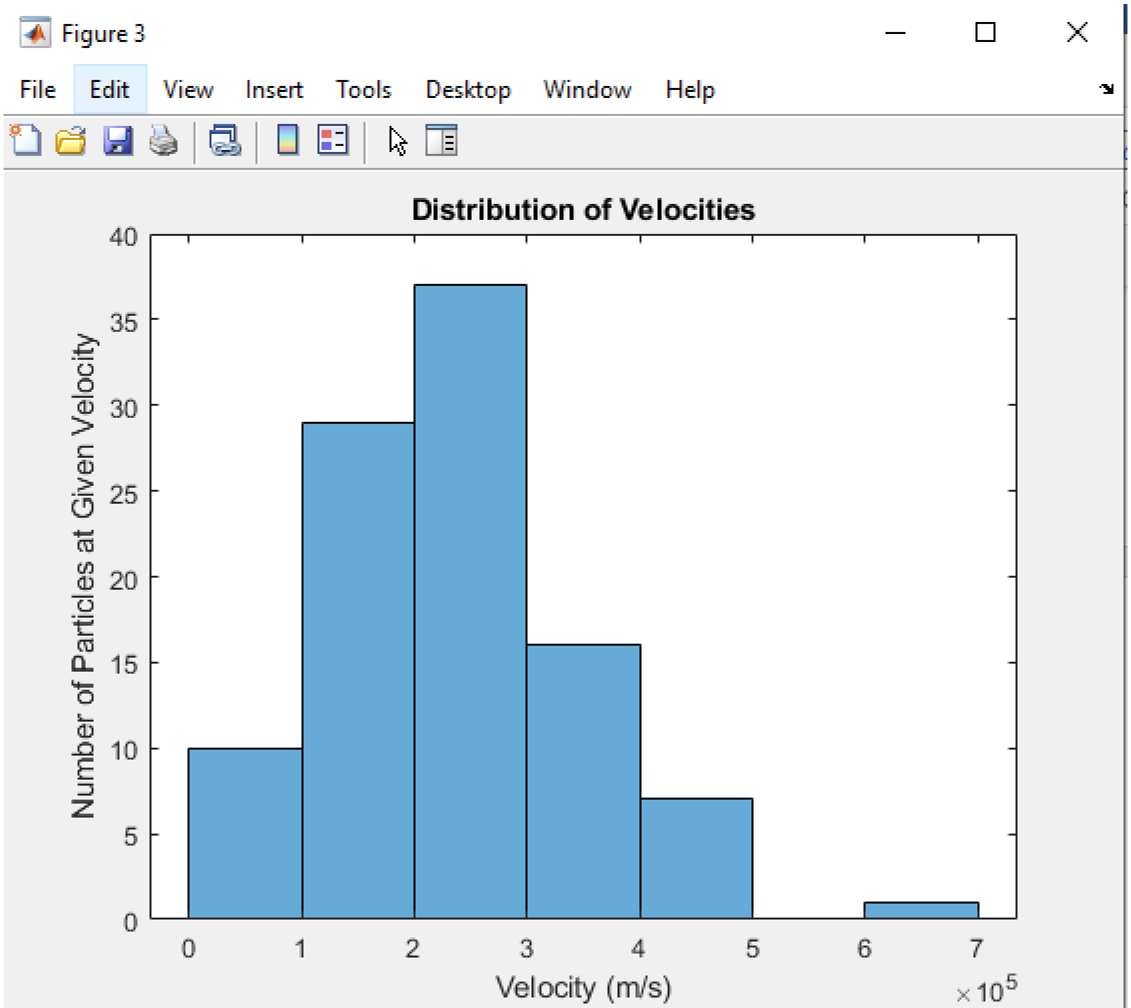

Figure 3: Distribution of Random Velocities

As shown in figure 3, the velocities are distributed roughly around the Vth calculated.

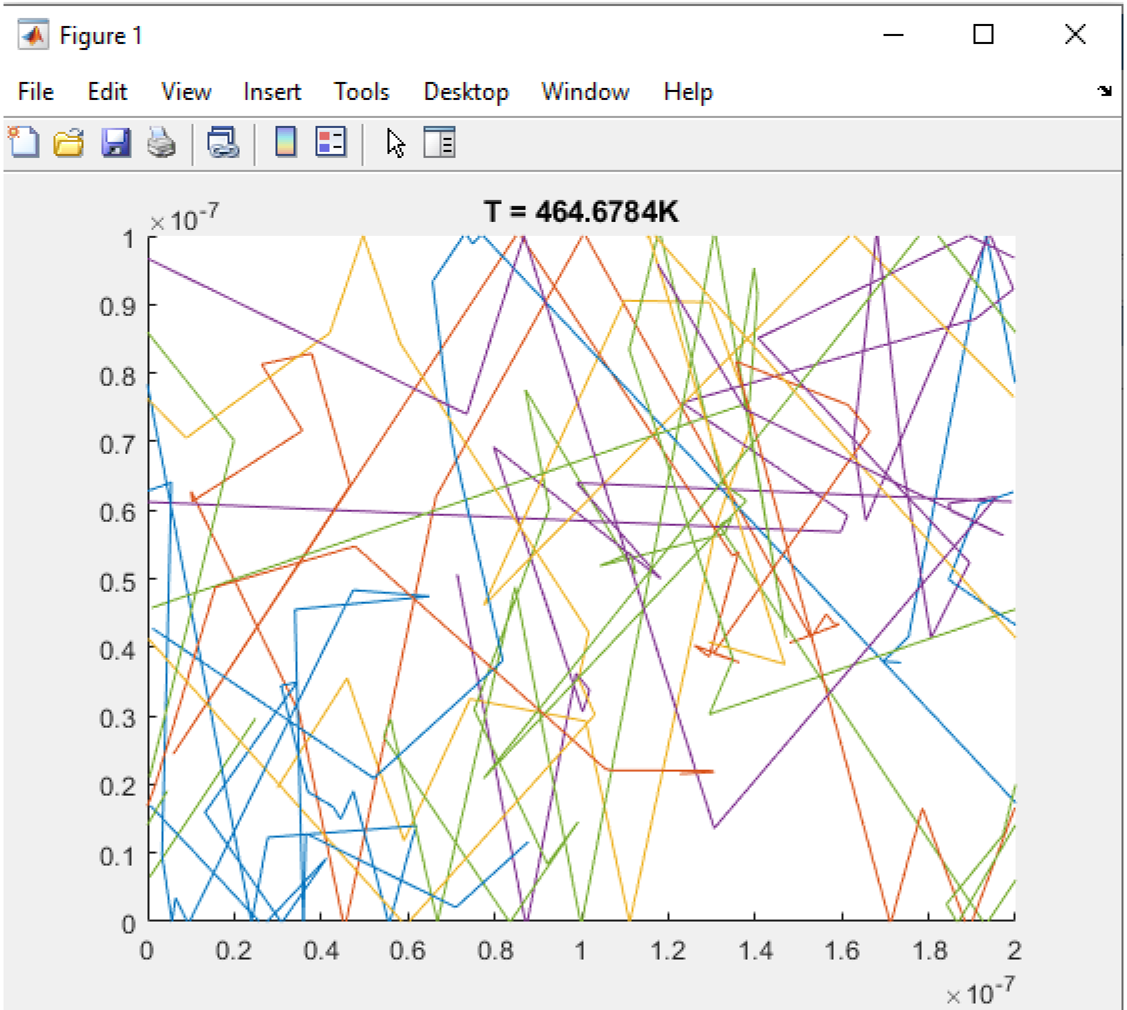

Figure 4: Simulation of Electrons Moving Through Silicon with Random Scattering Applied

Figure 4 shows the silicone plane with the electrons randomly scattering as well as reflecting specularly off the top and bottom boundaries. Since the velocities are now randomized the temperature plot varies greatly compared to the temperature in part 1.

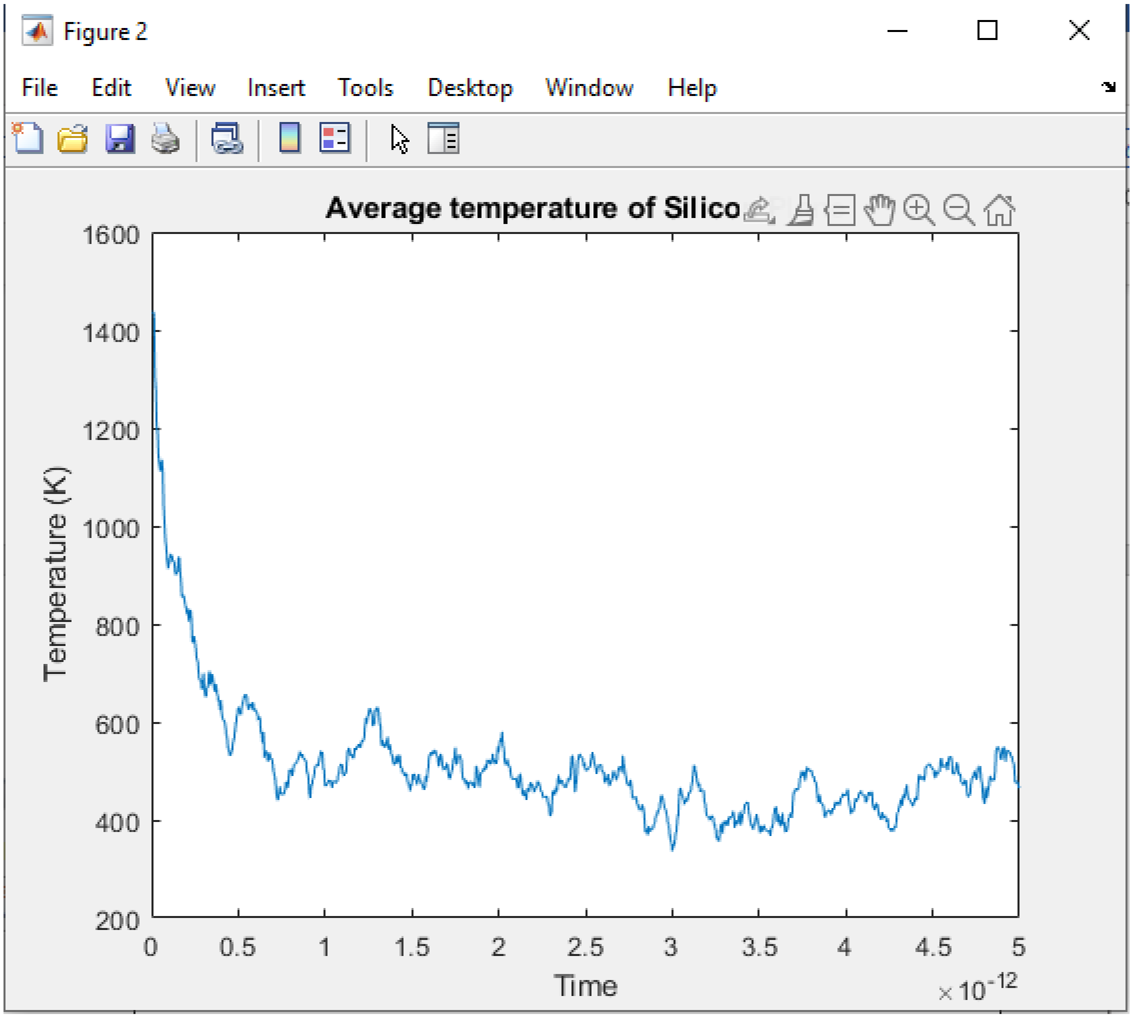

Figure 5: Temperature Plot of Randomly Scattering Electrons

As shown in figure 5, the temperature fluctuates roughly 200 degrees throughout the simulation.

Part 3: Enhancements

The third part of the assignment did not turn out as greatly as I had hoped. The objective of the 3rd part of the assignment was to add 2 boxes to the plane to act as a bottleneck for the electrons to bounce through. I was rather close to completing this section as I added the bottleneck but could not get the reflecting of the electrons off the bottleneck to work properly.

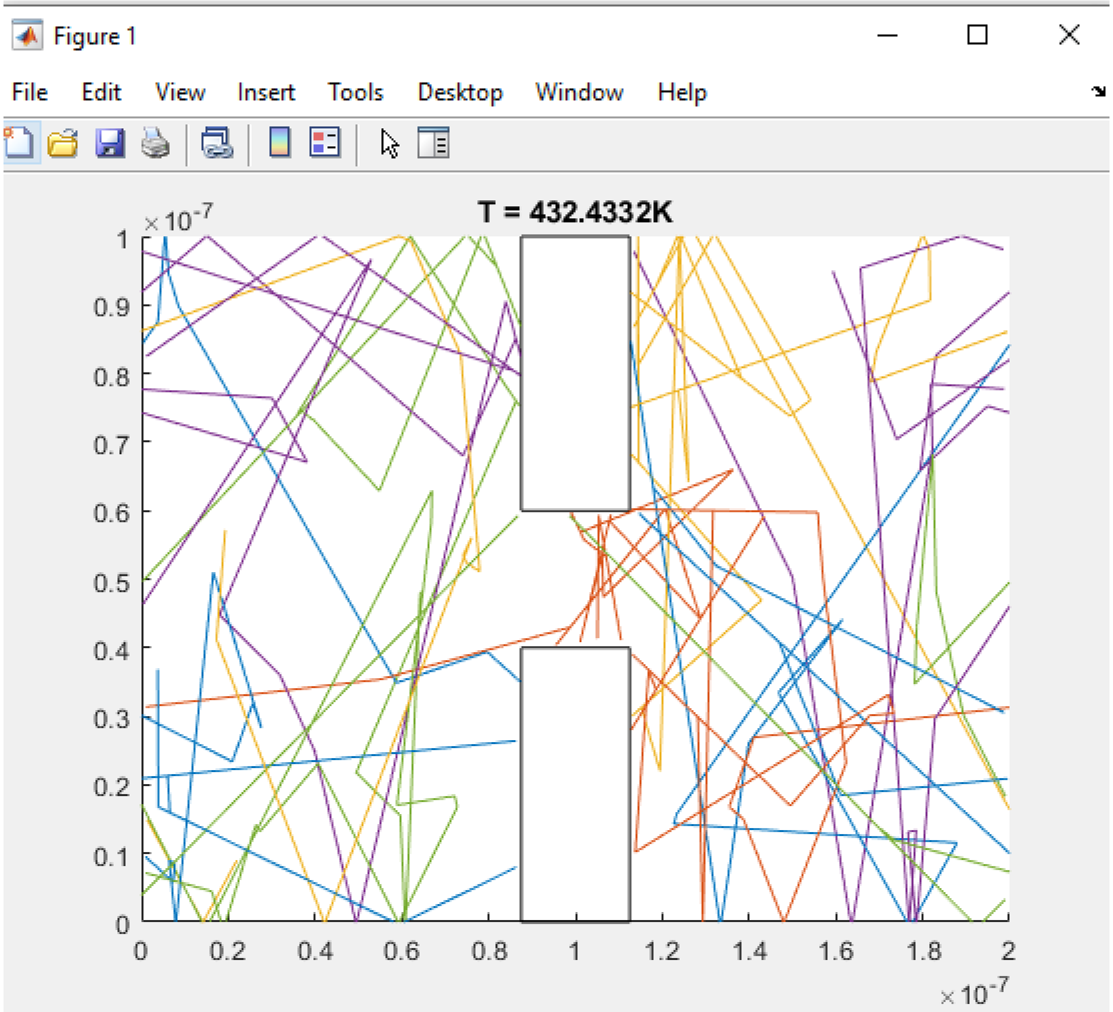

Figure 6: Electrons Scattering Through a Bottleneck

As shown in figure 6, the bottleneck is present, no electrons are in the boxes acting as the bottleneck, and electrons do reflect off of the boxes, but the electrons only reflect straight back instead of specularly through the bottleneck. I was unable to overcome this issue in before the assignment was due, but I plan on fixing it as soon as I can with assistance.

Since I was unable to complete the reflecting of the electrons properly, I never completed the electron density map or the temperature surface plot for the bottleneck section of the assignment. In place here is the average temperature of the silicone plane which is like that of part 2.

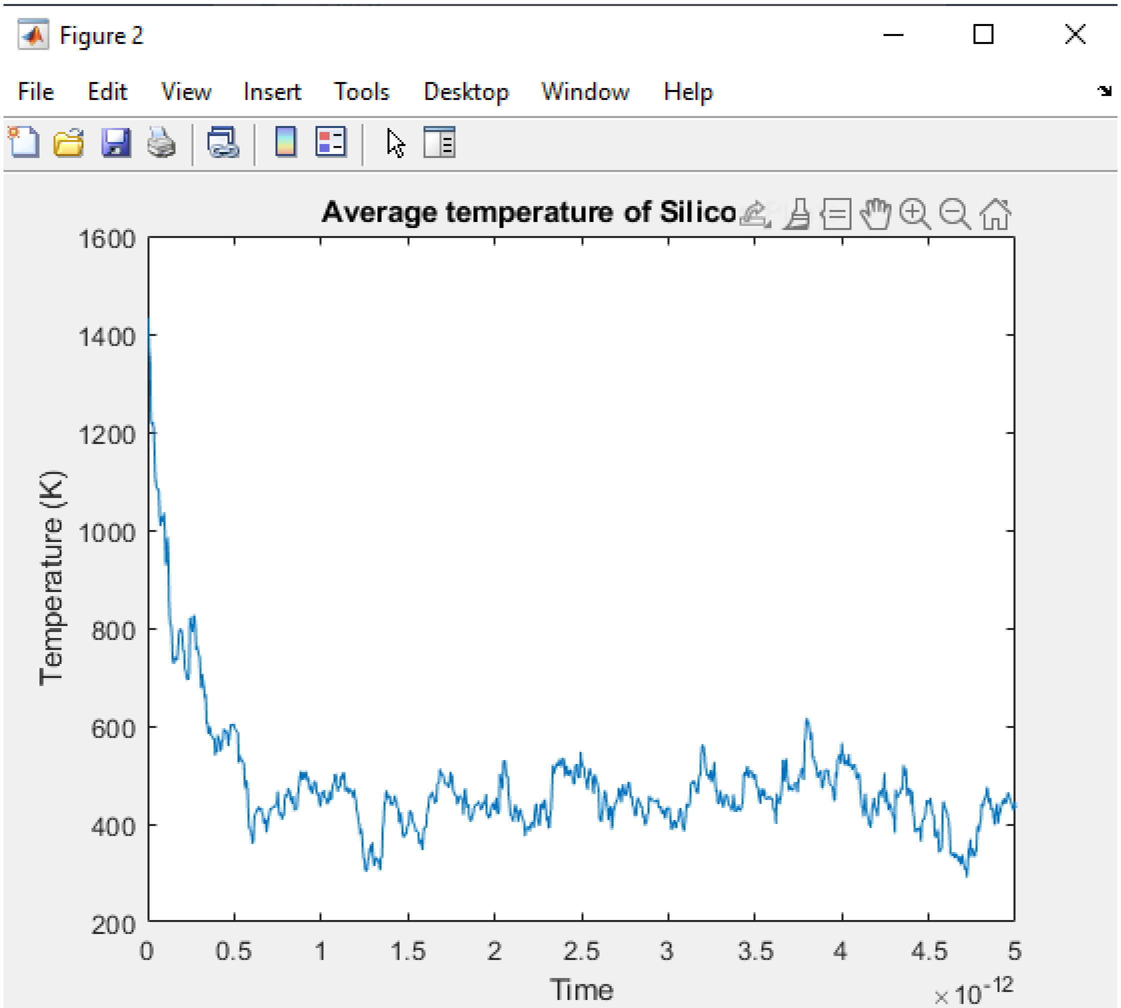

Figure 7: Average Temperature of Bottleneck Silicone Plane

Part 4: Curved Surface

Since I was unable to complete the reflecting and density maps for part 3, I only just started adding a curved surface for part 4. I was able to add a curved surface to the plane, and added logic to not let particles start in the circular boundary. I was working on calculating the angle of incidence against the normal to reflect to particles specularly off the circle. Figure 8 shows the plot of the electrons moving around the plane but going through the circle as the reflection off the boundary is not set up just yet, but in the code you can see the calculations added to compute the angle of incidence.

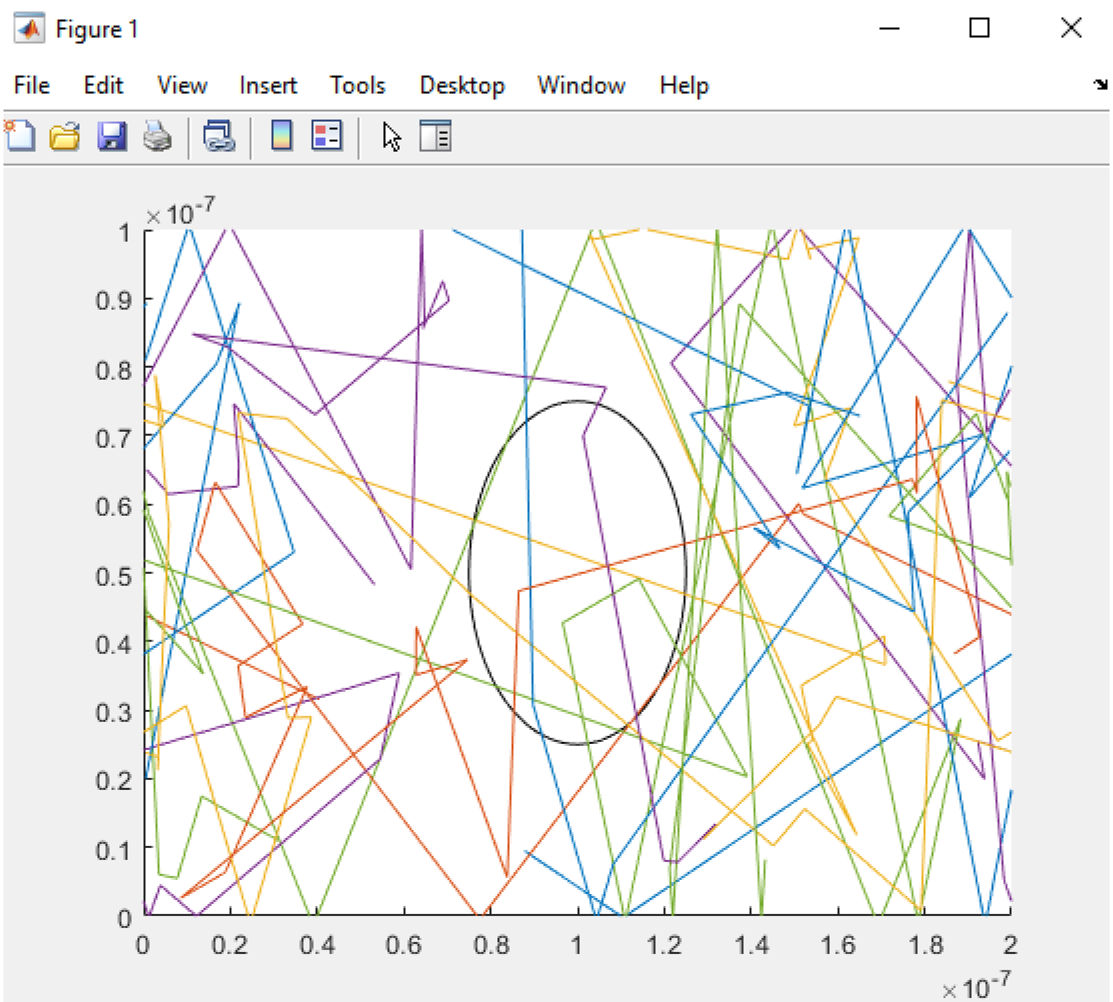

Figure 8: Attempt of Adding a Circular Object to the Silicone Plane