Carleton University

Department of Electronics

ELEC4700

Assignment 3 - Monte-Carlo/Finite Difference Method

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Date of Submission: March 21, 2021

Contents

1 Introduction

The purpose of this assignment is to explore how Monte-Carlo and the Finite Difference methods can be used together to create complex field simulations.

2 Part 1 - Without Bottleneck

2.1 Electric Field

The electric field across the x dimension of the semiconductor when there is a potential difference of 0.1V can be calculated using the following equation:

$$E = \frac{\Delta V}{d} = \frac{0.1V}{200nm} = 5 \times 10^5 V/m \tag{1}$$

Where E is the electric field, ΔV is the potential difference and d is the displacement between the potential difference (left and right).

2.2 Force on each electron

Using the electric field calculated above, the force on each electron can be calculated as follows:

$$F = qE = 1.602 \times 10^{-19} C * 5 \times 10^5 V/m = 1.602 \times 10^{-19} C * 5 \times 10^5 N/C = 8.01 \times 10^{-14} N \tag{2}$$

Where F is the force on the electron, q is the charge of the electron and E is the electric field.

2.3 Acceleration

Now using the force calculated above the acceleration of each electron can be determined as follows:

$$F = m_{eff} a => a = \frac{F}{m_{eff}} = \frac{8.01 \times 10^{-14} N}{0.26 * 9.11 \times 10^{-31} kg} = 3.382 \times 10^{17} m/s^2 \tag{3}$$

Where m_{eff} is the effective mass of the electron, a is the acceleration of the electron and F is the force on the electron from the electric field.

This acceleration can then be added to the velocity of the particle when updating the position using the following equations:

$$v = \frac{dx}{dt} => dx = vdt => \Delta x = v\Delta t \tag{4}$$

$$a = \frac{dv}{dt} => dv = adt => \Delta v_a = a\Delta t \tag{5}$$

$$v = v_o + \Delta v_a => v = v_o + a\Delta t \tag{6}$$

$$P = P + \Delta x => P = P + v\Delta t => P = P + (v + \Delta V_a)\Delta t => P = P + (v + a * \Delta t)\Delta t \tag{7}$$

Where P is the position (x or y), V is the velocity (x or y), a is the acceleration and Δt is the time step of the simulation.

Using this equation and the Monte-Carlo simulator from Assignment-1 without the bottle-neck and a potential difference of 0.1V, the following 2D plot of particle trajectories was produced:

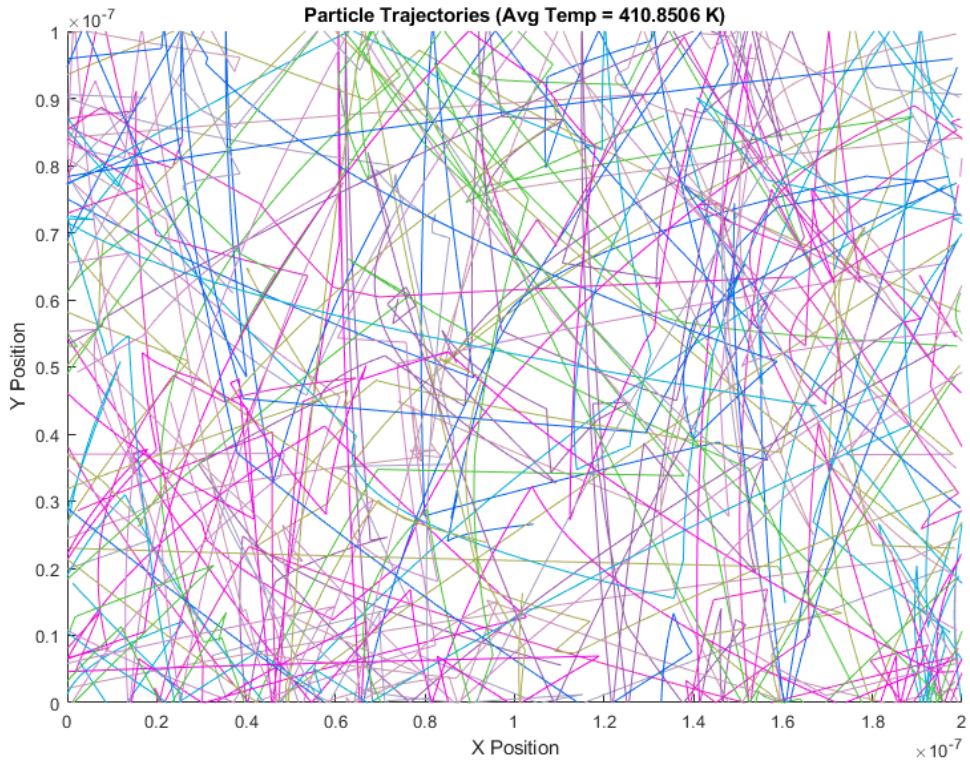

Figure 1: Particle Trajectories

Notice in this figure that the trajectories curve to the right due to the electric field created by the potential difference between the left and right sides of the plot.

2.4 Current

Electron drift current density and average carrier velocity are related through the following equation [2]:

$$J_x(t) = envd_x(t) \tag{8}$$

Where e is the charge of the particle, n is the number of electrons per unit volume, v_{dx} is the average drift velocity and J_x is the electron drift current density. To get the average drift velocity in the x direction all the x-velocity components of each particle were averaged.

The following figure shows the current density as a function of time:

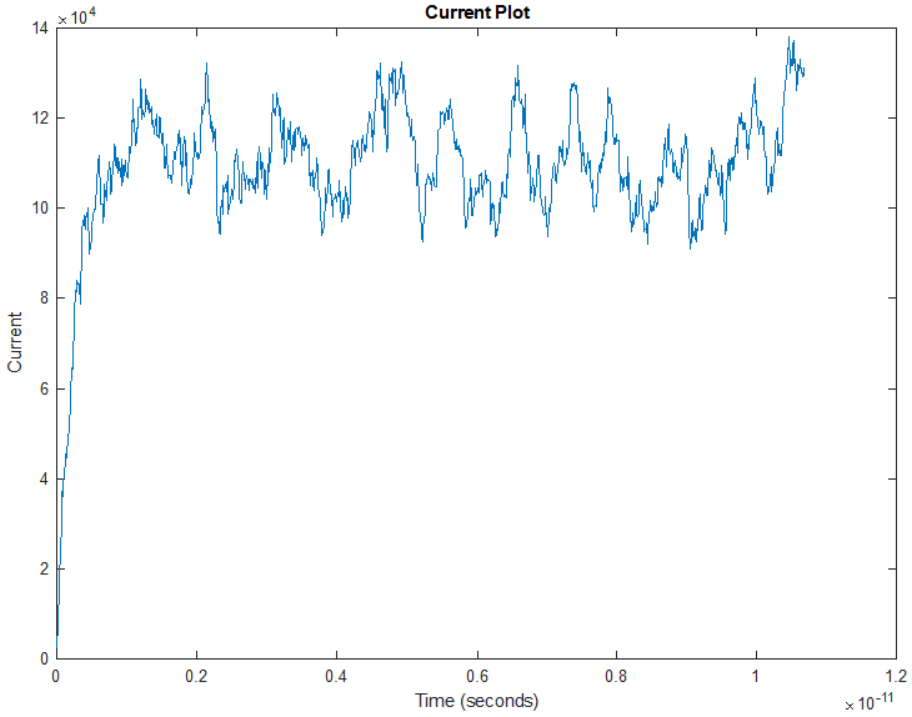

Figure 2: Current

From this figure it can be seen that some time after the particles have accelerated from rest, the current steady's around $11 \times 10^4 A/m^2$. This is because the particles must accelerate for there to be a drift velocity as they originally are going in random directions.

2.5 Density and Temperature Maps

The density and temperature maps associated with this simulation can be seen in the following figures:

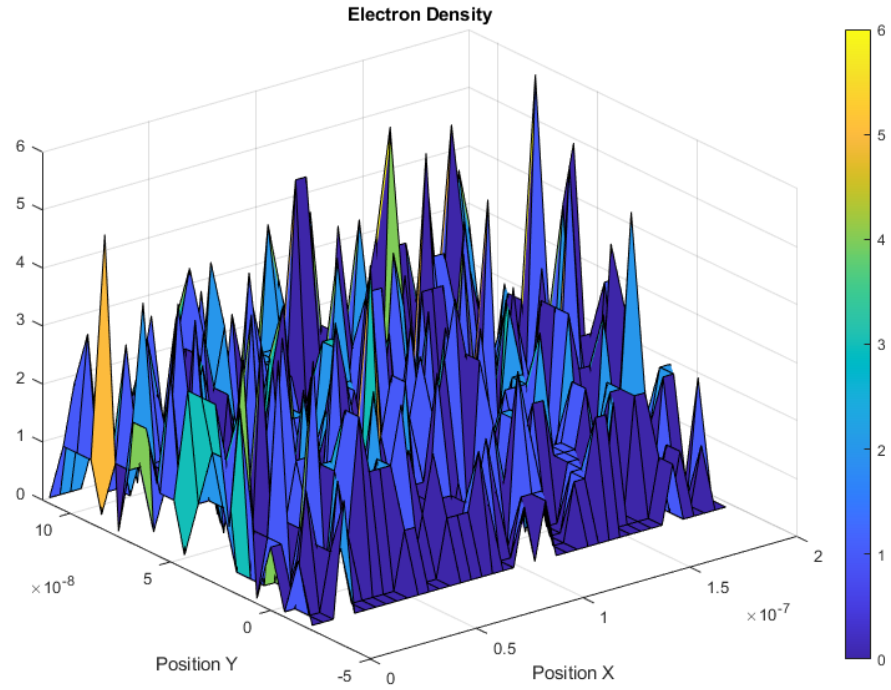

Figure 3: Density Map

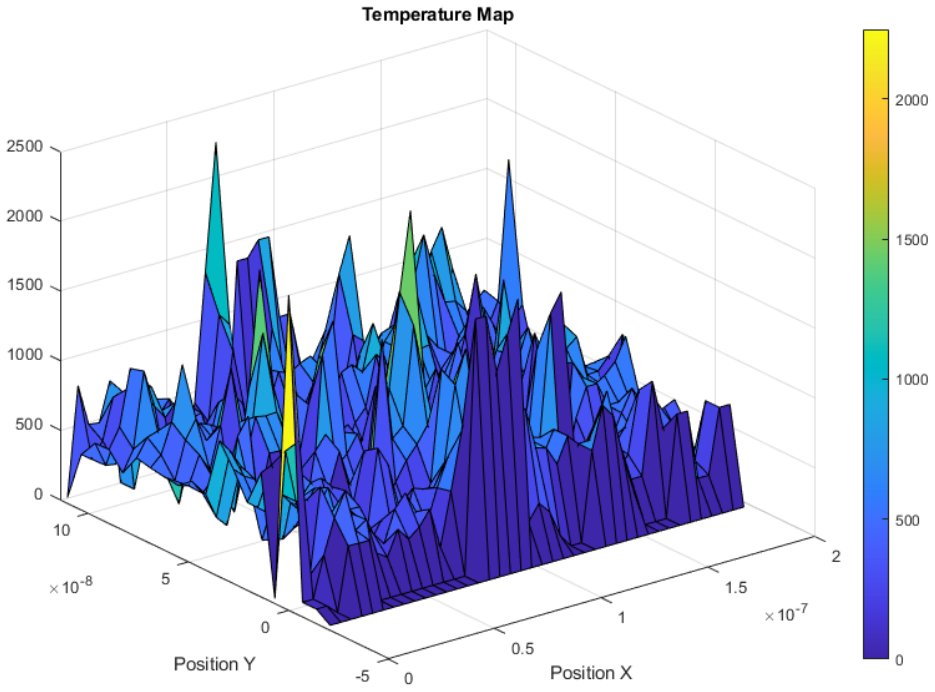

Figure 4: Temperature Map

NOTE TO TA: This temperature map is a corrected version of assignment 1 where I originally lost marks for a bad temperature map.

3 Part 2 - With Bottleneck

3.1 Potential Gradient

The potential gradient was calculated in assignment-2 using the finite difference method. A 2D and 3D representation of the potential gradient for a potential difference of 0.8V can be seen in the figures below:

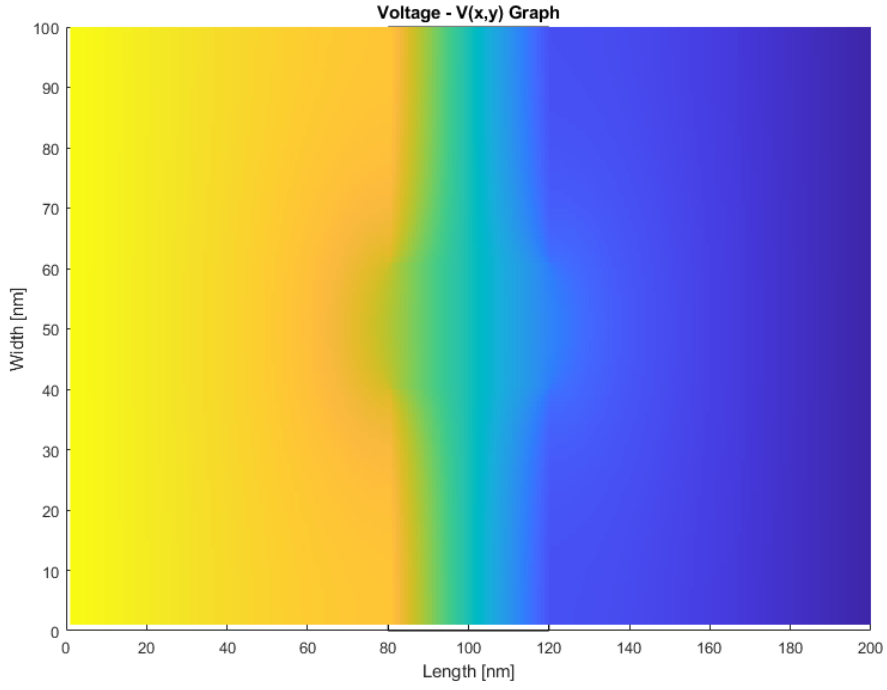

Figure 5: 2D Potential Gradient

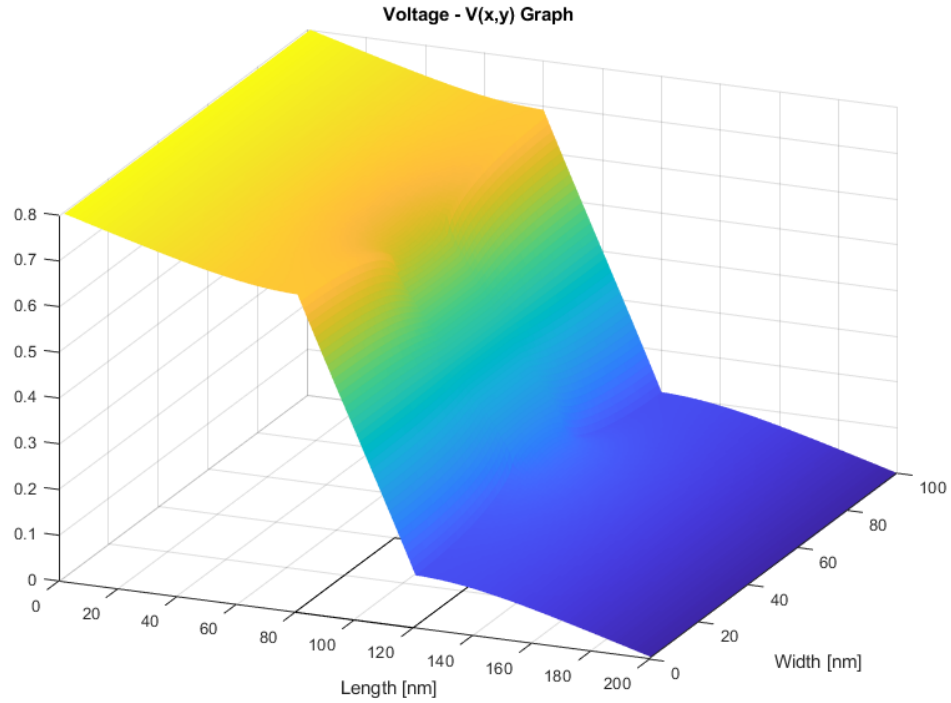

Figure 6: 3D Potential Gradient

3.2 Electric Field

The electric field generated using assignment-2 for a 0.8 potential difference can be seen in the figures below:

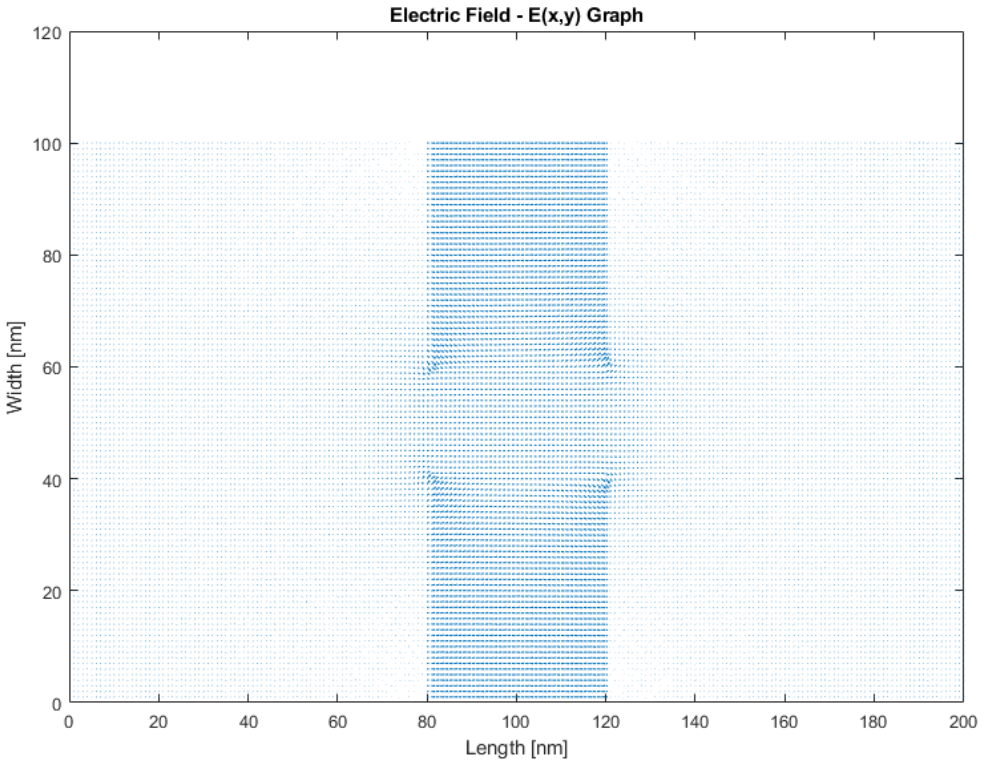

Figure 7: Electric Field

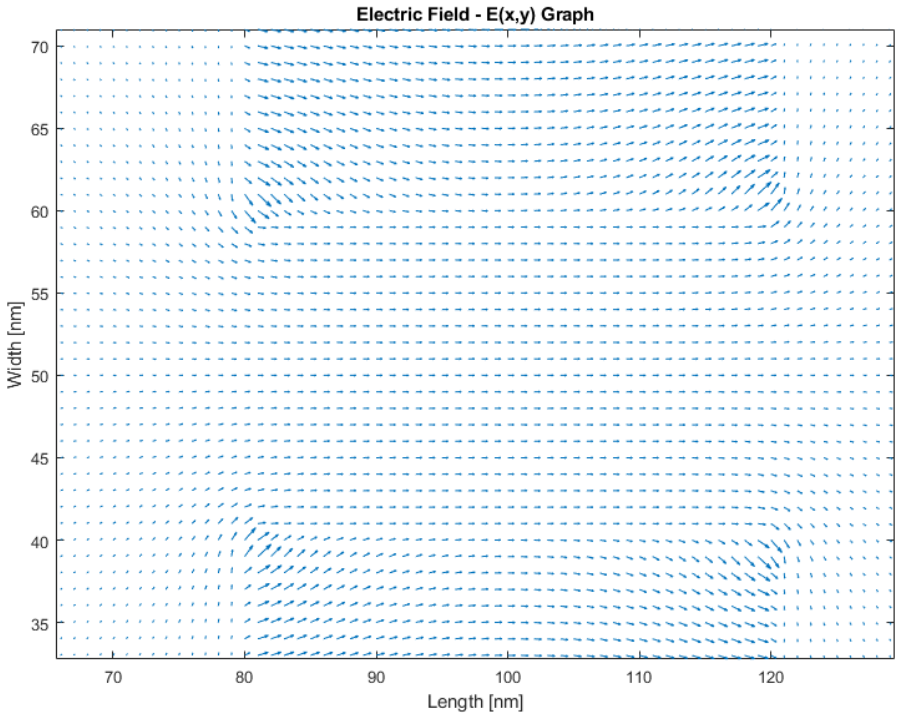

Figure 8: Electric Field (Zoomed)

Note that the electric field arrows point toward the barrier gap.

3.3 Trajectories

Using the electric field gradient above and the Monte Carlo simulation from assignment-1, the trajectories under this field can be seen in the figure below:

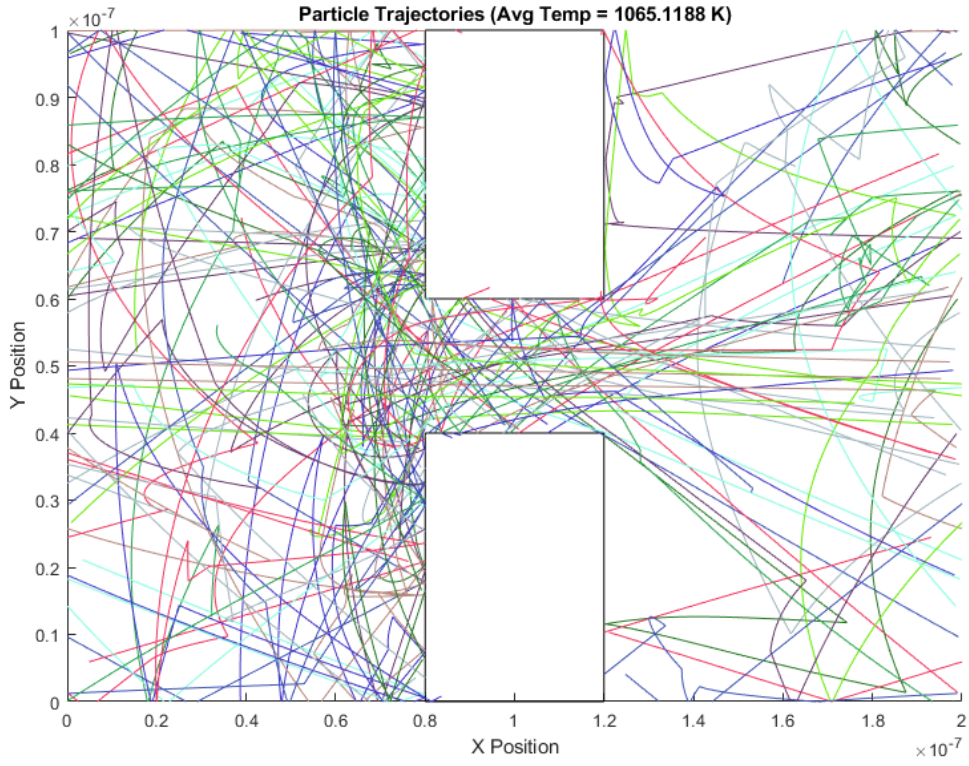

Figure 9: Particle Trajectories

At high speeds I have some random bugs where very occasionally particles will enter the corners of the barriers. I discussed this with Professor Smy and he said that this is acceptable for the scope of this assignment.

4 Part 3 - Coupled Simulations Investigation

4.1 Density

The density map of the particles for the coupled simulation with a 20nm gap and a 0.8V potential difference is as follows:

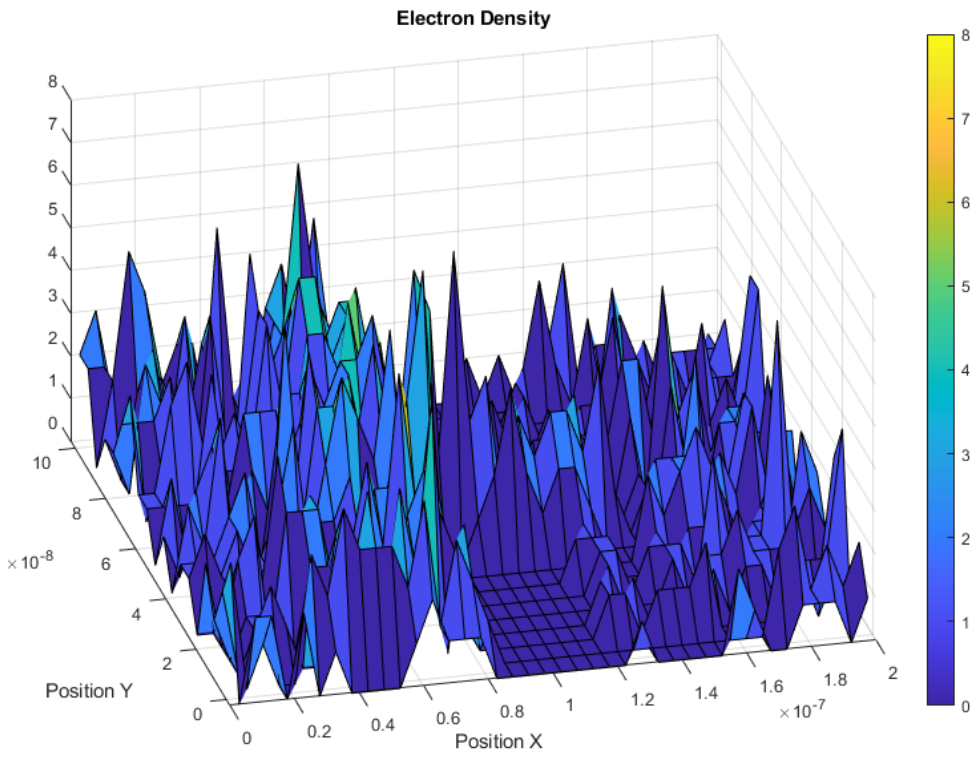

Figure 10: Density Map

From this map it can be seen that particles build-up on the left side of the barrier. This is because the electric field pulls the particles from left to right causing the particles on the right to teleport to the left and get stuck against the barrier. It should be noted however that the electric field does pull the particles around the corners through the gap however this is not enough to prevent this buildup.

4.2 Current of Varying Bottleneck Widths

The average current across all the time steps of bottlenecks varying from 30nm to 10nm is as follows:

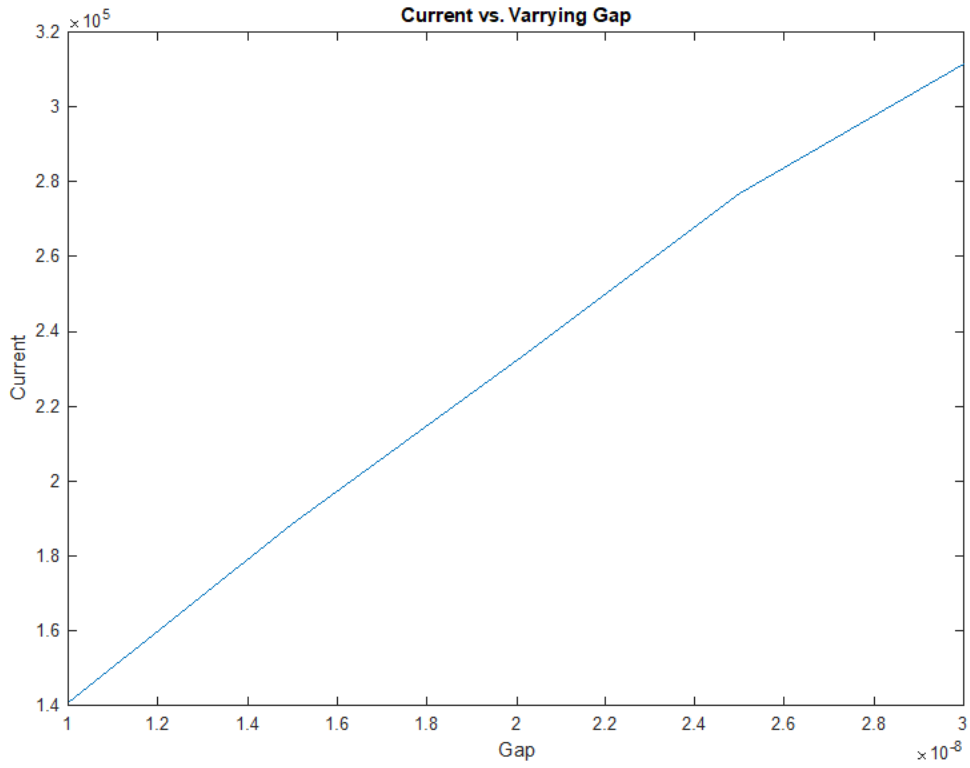

Figure 11: Current Density vs. Barrier Gap

As expected, the current increases as the gap gets larger.

4.3 Next Steps

To make this simulation more accurate and function at larger electric fields, one next step that I propose is adjusting the time step based on the velocity of the particle. Since the particles accelerate depending on the potential difference applied, the velocity of a particle can become very large causing the time step to jump the particle a significant distance across the simulation area and through corners of the barrier. By varying the time step to be a fraction of each particles velocity, the step could be small enough to negate this issue.

References

[1] T. Smy, "ELEC 4700 Assignment - 3 Monte-Carlo/Finite Difference Method." March 21, 2021

[2] T. Smy, "Transport, Continuity Equations and Simulation" March 21, 2021