# ELEC 4700 Modelling of Integrated Devices

## Assignment 3: Monte Carlo/Finite Difference Method

Due: March 15, 2020

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**Introduction**

This report will show how the first two assignments can be combined to show the effect that a voltage distribution will have over a plate, and how electrons will act in the plate. Using the same parameters as before, the simulations are run, and the behavior of the systems will be explained in each of the sections of this report. First the basic empty cell will be used and then it will be made more complex as more features are added.

**Part 1: Electric Force on Electrons with Scattering**

The first problem that needed to be solved was to combine the basic functions of the first two assignments. To do this,

When a 0.1 Volt bias is applied to one boundary of the simulation box, in particular the left side boundary which is defined by (X = L) in the simulation. The distribution of this field should be uniform in an ideal case, but the way the MATLAB code solves the numerical Laplace has inherent error, so there is some variation across the length and width of the simulation. For simplicity the average of the electric field was found using MATLAB. Equation 1 shows how the electric field is calculated for a 1D solution that is known to be uniform over the plate.

$$E = -\frac{dV}{dx} \quad \text{(Eq. 1)}$$

$$E = -\frac{0.1\,V - 0\,V}{200\,nm - 0\,nm} = -500\,000\ (N/C)$$

Once the electric field has been calculated, it is very easy to find the force on the electrons in the simulation using Equation 2.

$$F = QE = -qE = ma \quad \text{(Eq. 2)}$$

$$F = -qE = -(1.602e-19\,C)(-500\,000\,N/C) = 8.01 * 10^{-14}\,N$$

Now that the force on each of the particles is found using a uniform electric field, the mass of the particle is known, and the acceleration can be calculated. Using Equation 3, the acceleration can be calculated.

$$a = \frac{F}{m_e} \quad \text{(Eq. 3)}$$

$$a = \frac{F}{m_e} = \frac{-qE}{m_0 * 0.26} = -\frac{(1.602e-19\,C)\left(-8.01 * 10^{-14}\frac{N}{C}\right)}{(9.11e-31\,kg)(0.26)} = 3.3817 * 10^{17}\ (m/s^2)$$

Now that the acceleration of each of the particles has been calculated. The electrons can be mapped as a function of time with the velocity being updated at each step. The second version of assignment 1 will be used where the electrons populate an open plate of 100 nm by 200 nm. They will all be given a random initial velocity and direction with scattering occurring randomly

just like before. When the electrons experience scattering the simulation will act as if the energy is lost and the acceleration will be reset, while particles that do not scatter will continue to speed up as the velocity will increase until scattering occurs. The velocities will be updated at each step and Figure 1 shows the simulation after 100 time steps with 50 electrons.

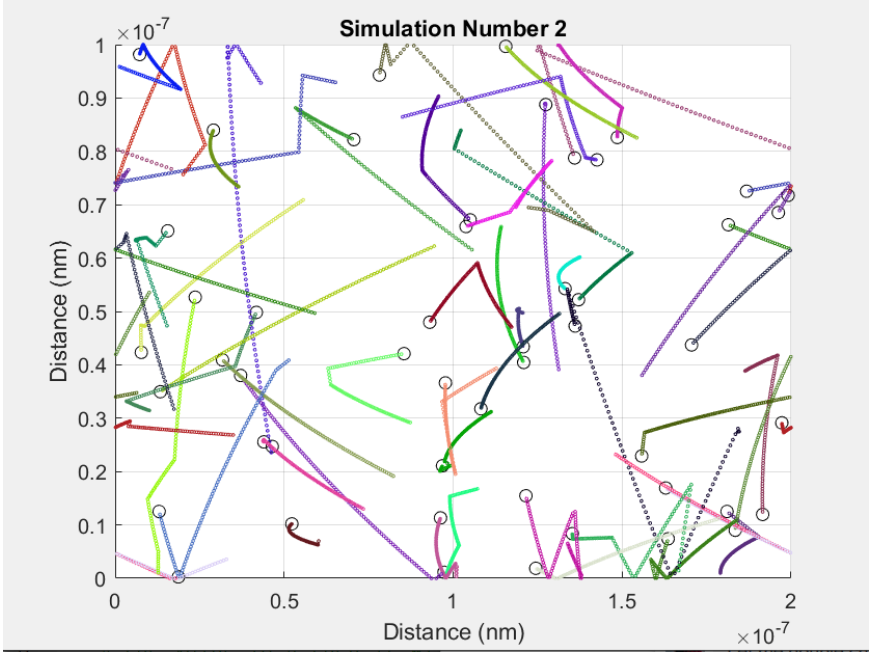


Figure 1: 2D Particle Trajectory Plot

Due to the constant acceleration in this problem which arises from the uniform electric field, the formulas used to calculate the new velocities and new positions were simple compared to a non-uniform field. The electron density can be found for the end of the simulation as well as the temperature map for the electrons. I have decided to make these two slightly different from the ones provided in the assignment manual as I find they do not convey much meaningful information. A histogram plot for the electron density and a colour coded heat map are instead created with examples shown below from the same simulation as Figure 1. Figure 2 and 3 show the electron density and heat map respectively.

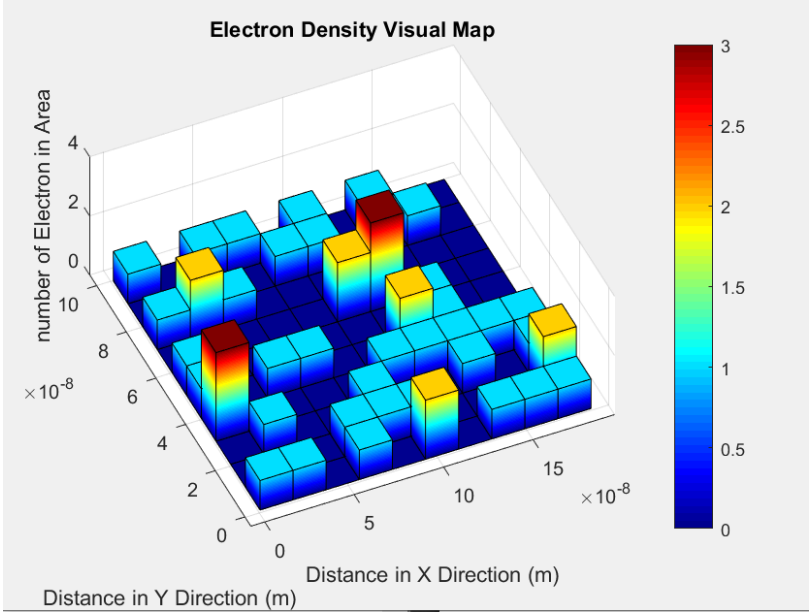


Figure 2: Electron Density Map

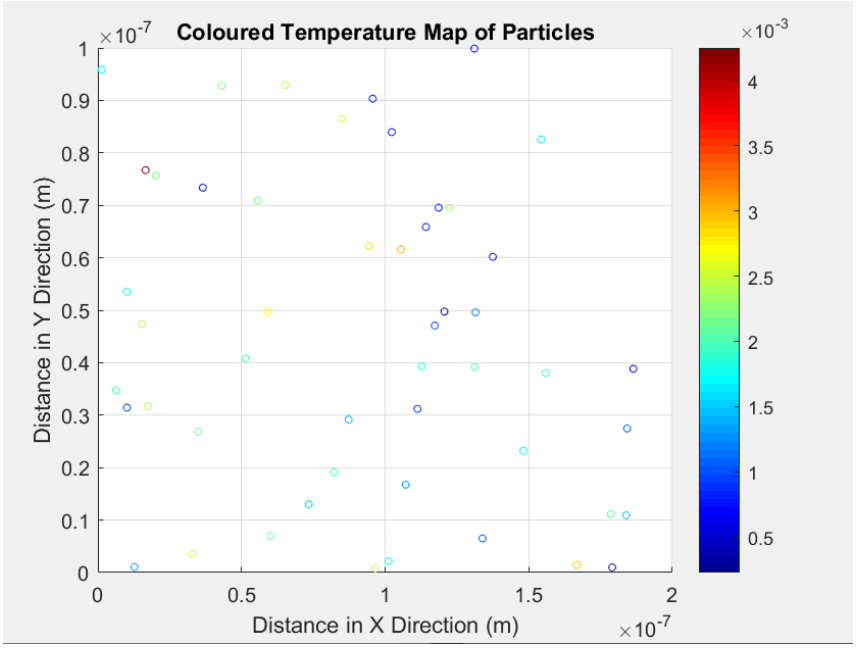


Figure 3: Electron Heat Map

These two convey meaningful information about how the electrons may gather into a certain region or how the temperature shows up as a function of position. Another simulation was run with 5000 particles over 100 timesteps to show how these may change with a larger number of particles. Figure 4 and 5 show the new electron density and heat maps respectively.

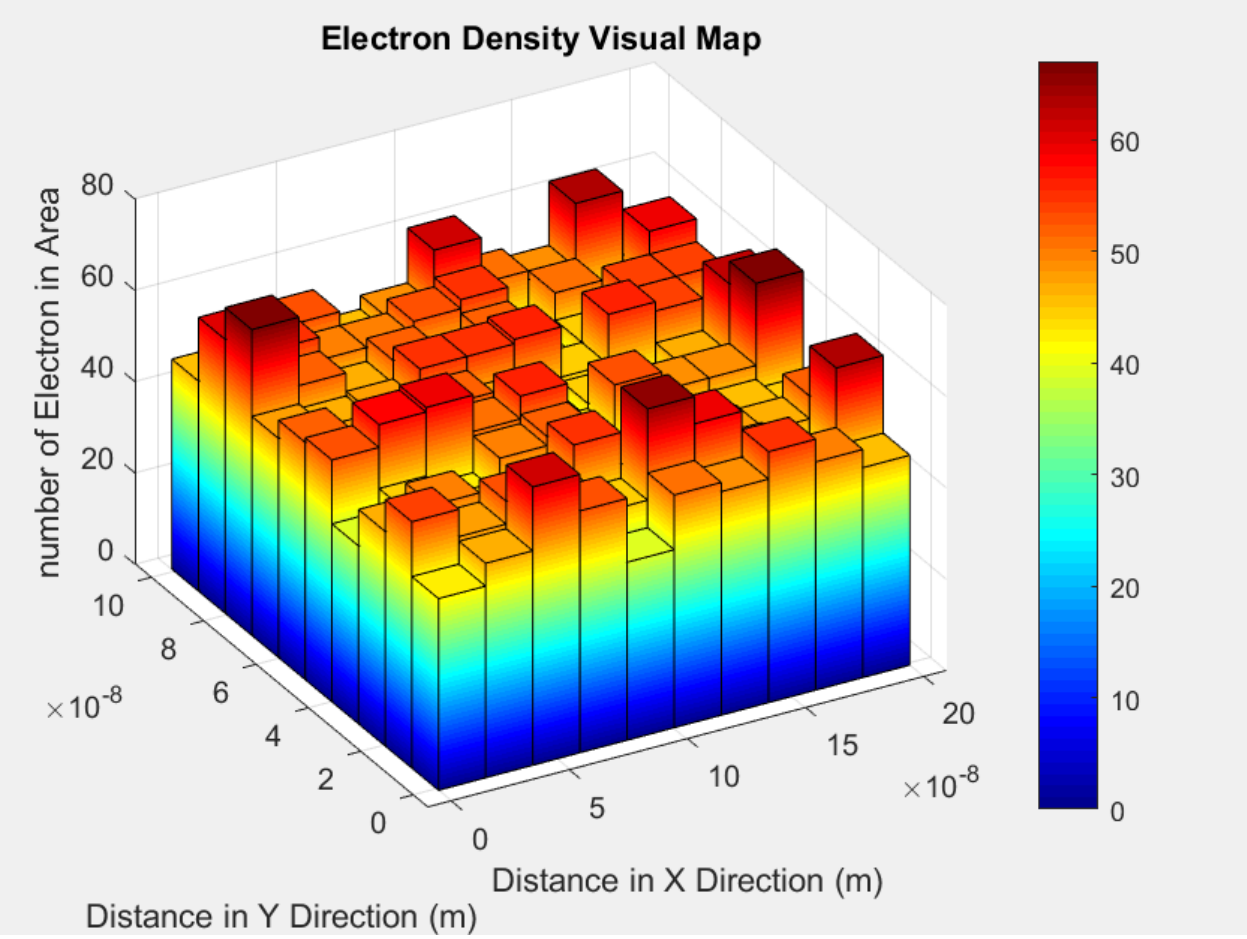


Figure 4: New Electron Density Map

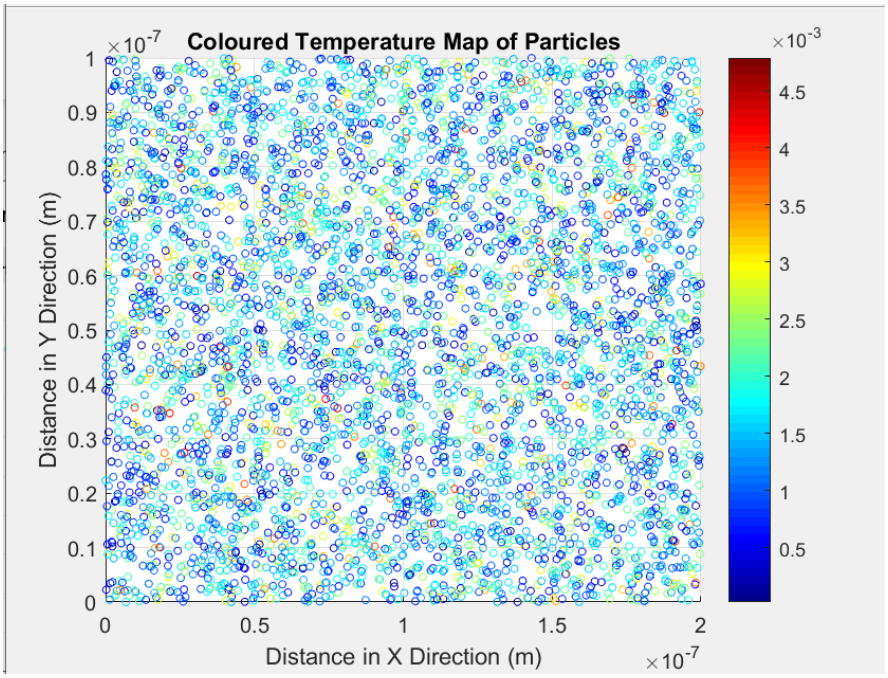

Figure 5: New Electron Heat Map

From these plots, it can be seen that the distribution of the electrons at the end of the simulation is reasonably uniform over the surface, the number of bins can be changed for a more accurate picture of the simulation. The heat map also does not seem to show a bias to any particular part of the simulation region.

**Part 2: Bottleneck Region**

Now that the basic simulation has been setup with a constant acceleration of the E field applied. A more sophisticated one with varying E fields can be simulated to see the effect a bottleneck with different conduction values has on the system. The same voltage of 0.1 V is applied to one end of the plate while the other is held to ground. The bottleneck region is centred in the middle of the simulation and covers half of the simulation region in the x direction and the tunnel region will only be 20 % of the height of the simulation. This can be seen from the conduction map shown in Figure 6.

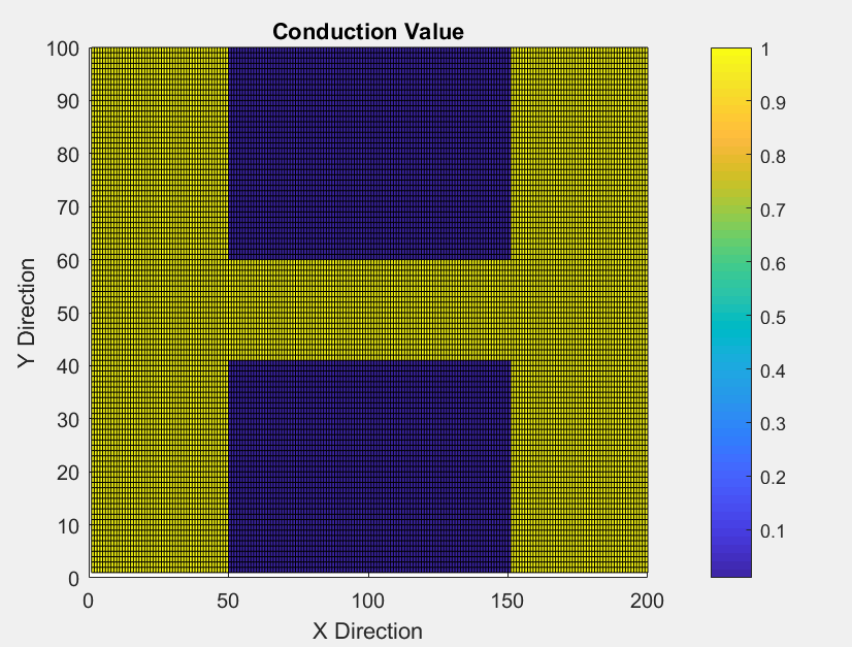


Figure 6: Conduction Map for Bottleneck Region

Figure 7 shows the voltage over the plate with 0.1 V held at one end, and Figure 8 shows the electric field which is calculated from the voltage information.

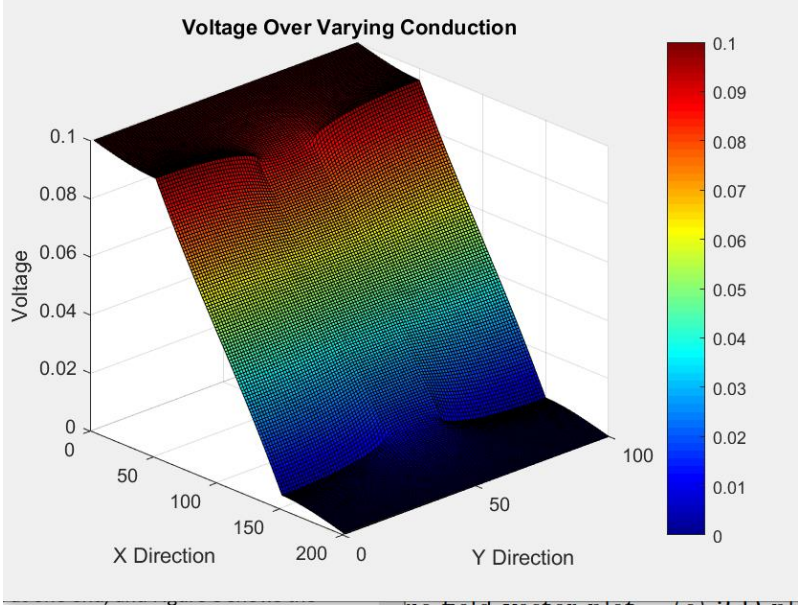


Figure 7: Voltage Over the Bottleneck Region

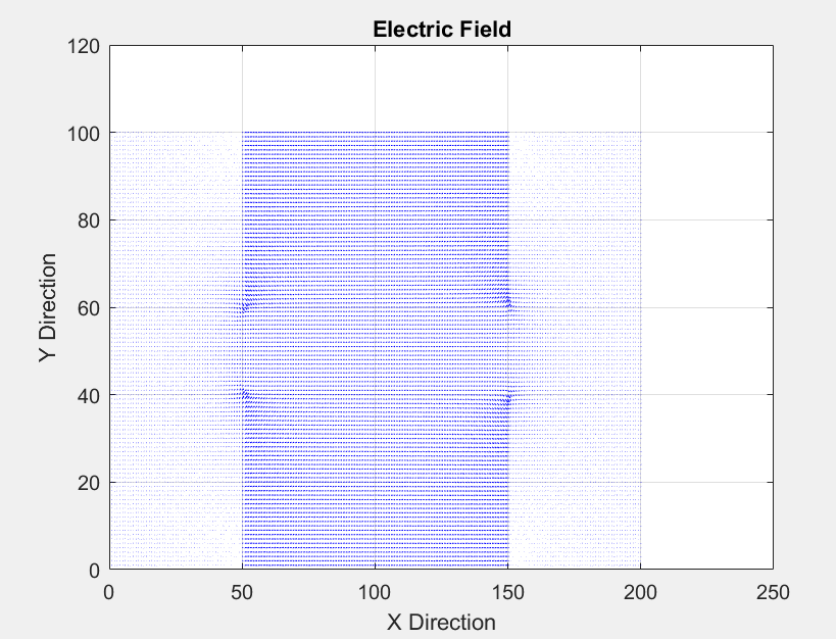


Figure 8: Electric Field over the Bottleneck Region

Using the information generated by these plots and calculations, the behavior of electrons within this field can be simulated to see their effect on how the particles behave. The following code in Figure 9 shows how a loop is used to cycle through all of the particles in the simulation space at each step to find the electric field in the X and Y direction. This allows the velocities to be updated for each of the particles in the differing levels of E field.

```
for count = 1:e_num
    X = ceil((10^9)*new_xposition(count))
    Y = ceil((10^9)*new_yposition(count))
    EX = (10^9)*Ex(Y,X)
    EY = (10^9)*Ey(Y,X)
    FX = -q*EX
    FY = -q*EY
    AX = FX/me
    AY = FY/me
    new_xvelocity(count) = new_xvelocity(count) + AX*timestep
    new_yvelocity(count) = new_yvelocity(count) + AY*timestep
end
```

Figure 9: Code for Updating Velocities Due to E Field

When this was used in the simulation for 1000 particles over 1000 timesteps, the result can be seen in figure 10.

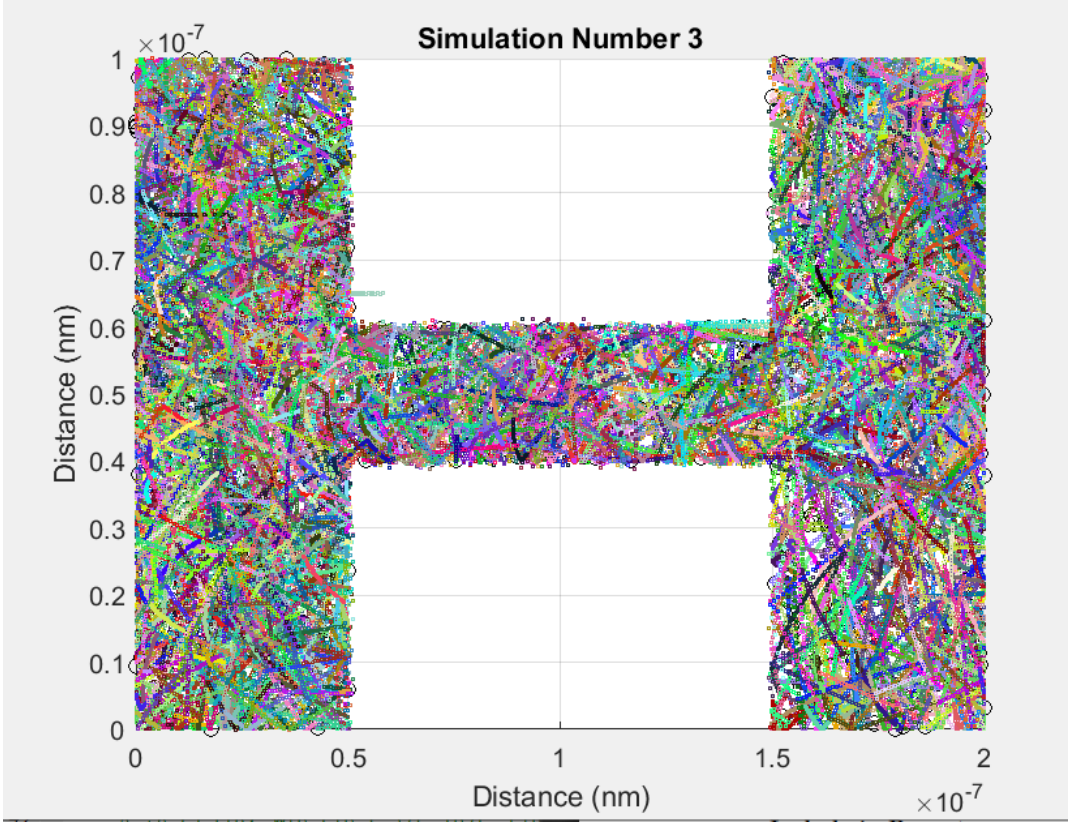


Figure 10: Particle Trajectories

**Part 3: Investigate Device Parameters**

When the bottleneck is added and simulated for a reasonable length of time, the effect of the bottleneck mixed with the electric field can be seen. Using the final positions of the particles in an electron density map, the effect of the bottleneck can be compared. Figure 11 shows the electron density map at the beginning of the simulation and at the end of the simulation after 400 timesteps. The number of particles used was 5000 particles and the voltage bias is 0.1 Volts.

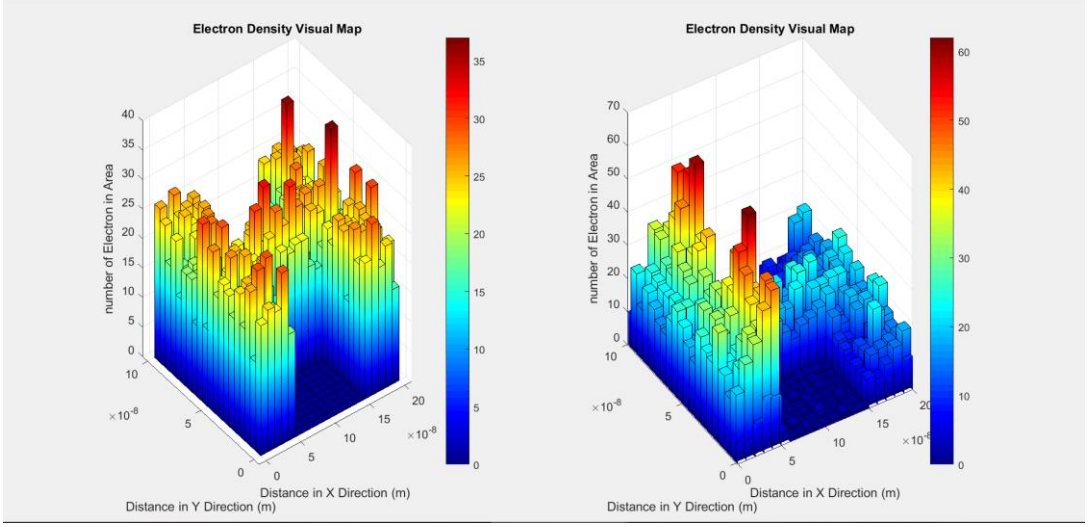


Figure 11: Electron Density Before and After Simulation for 0.1 Volts

Changing the potential will change the effect on the simulation, this time 0.8 Volts was used as the bias and Figure 12 is the resulting plot using all the same parameters as before.

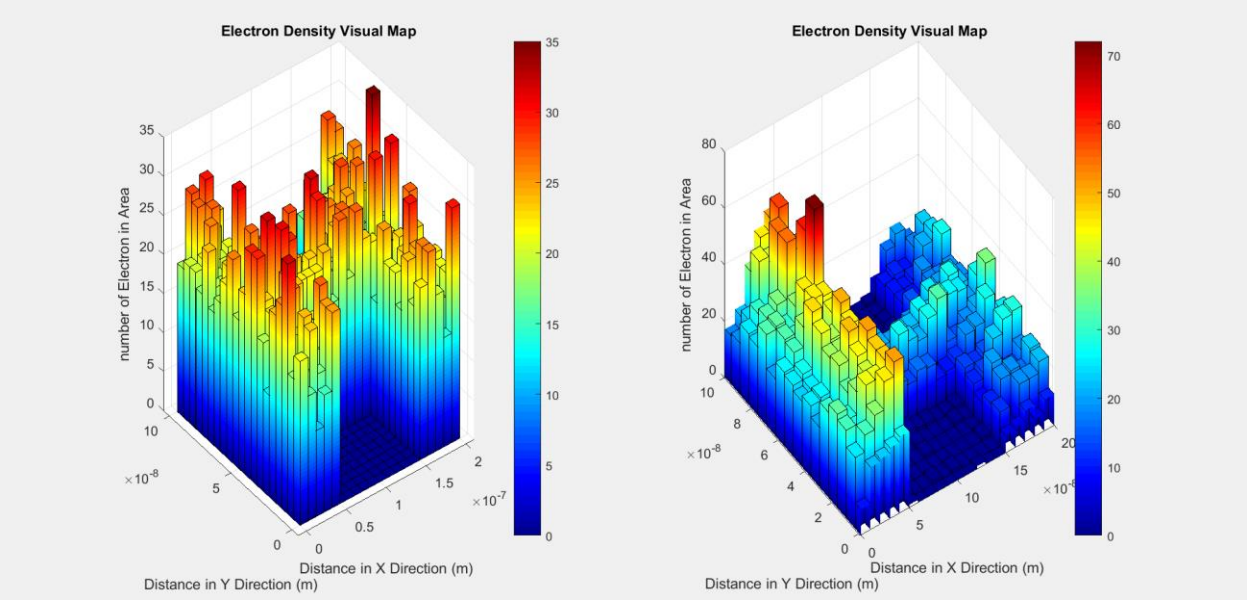


Figure 12: Electron Density Before and After Simulation for 0.8 Volts

Figure 13 shows the same simulation with a voltage bias of 3 Volts so that a very clear picture can be acquired of the effect raising the voltage has on the simulation.

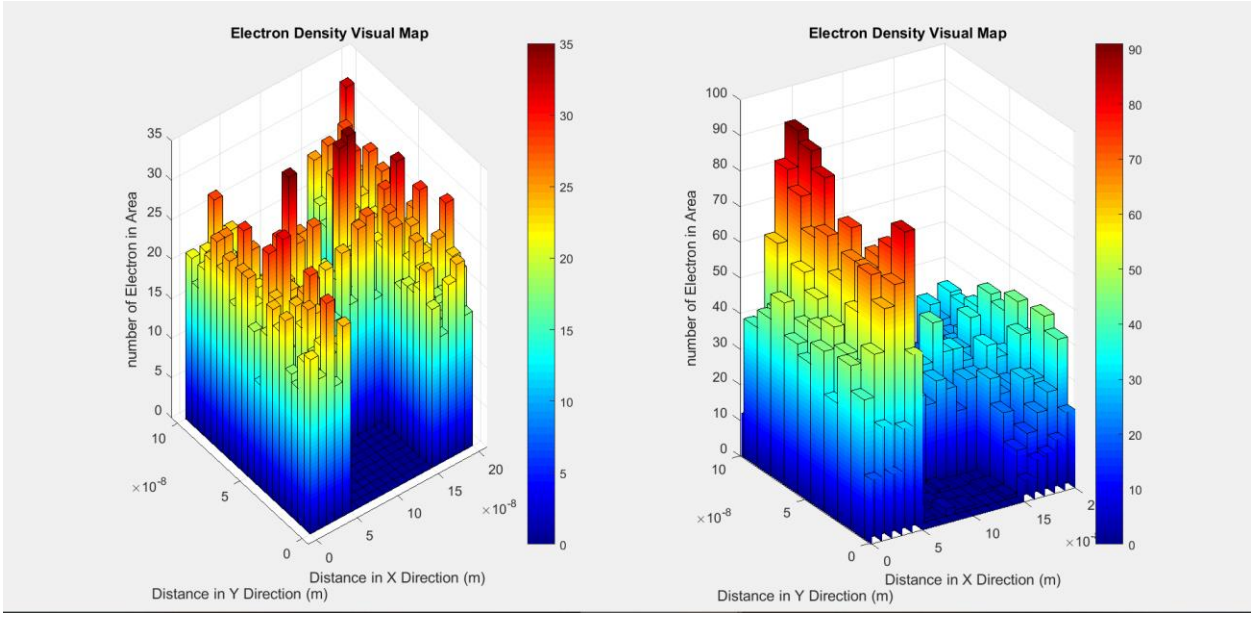


Figure 13: Electron Density Before and After Simulation for 3 Volts

From these plots it seems that the particles have hard time getting through the bottleneck region and they get stuck on the one side of the bottleneck. Effect can be seen in real life where there exists problem, especially at high frequency in waveguiding at corners and bottlenecks.

One way to make this simulation more accurate to real life is to fix the scattering to make it more realistic. When a scatter occurs, energy is transferred between particles and then they each change velocities. In our simulation we had the assumption that when scattering occurred, the electron would just choose another random velocity and go off in that direction. This could be improved by some calculations that determined a more likely angle and velocity based off of mass transfer and charge difference. This can incorporate the force on the particle due to the other electrons in the simulation space in the form of a coulomb force. This would make the like particles reflect from one another during their trajectories.