ELEC 4700

Assignment 3

Monte-Carlo/Finite Difference Method

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March 21st, 2021
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Part 1: Assignment 1 without Bottle-Neck

The purpose of this part was to extend Assignment 1's solution, without the bottleneck, to incorporate an applied voltage across the region.

With the addition of this applied voltage, the voltage introduces an electric field which affects the electrons within the region. Since the region is free of obstructions (due to no bottle-neck), it is assumed this electric field is constant over the region. The formula below can be used to calculate the electric field, for any constant electric field:

$$\Delta V = Ed \rightarrow E = \frac{\Delta V}{d} = \frac{V_{applied}}{regionLength} \text{ [V/m]}$$

Note: ΔV represents the applied voltage since GND = 0V is used as a reference, and d is the region's length because it is assumed the applied voltage is across the x-dimension, following Assignment 2's requirements.

With this equation, and an applied voltage of 0.1V, the electric field is:

$$E = \frac{0.8V}{200nm} = \mathbf{500k\ V/m}$$

The electric field introduces a force on the electrons within the region. Due to the constant electric field, this force will also be constant. However, regardless of this, the force is calculated with the following formula:

$$F = qE$$

where q is the charge of an electron, and E is the electric field.

The force is calculated as:

$$F = (1.60217662x10^{-19})(500kV/m) = \mathbf{8.0108x10^{-14}\ N}$$

Next, by Newton's laws of motion, this force provides an acceleration to all electrons within the region. This is defined by the following equation:

$$F = ma \rightarrow a = \frac{F}{m}$$

The acceleration is calculated as:

$$a = \frac{8.0108x10^{-14}}{0.26(9.10938356x10^{-31})} = \mathbf{3.3823x10^{17}\ m/s^2}$$

Due to the acceleration, ultimately from the applied voltage, the velocity and position calculations must change. In assignment 1, there was no applied voltage, so the velocity was entirely dependent on the thermal velocity due to the temperature of the system. Now, the new velocities are not only dependent on the temperature of the system, but also the acceleration. From kinematics, these is calculated with the following equations:

$$v_o = v_{th}$$

$$v_f = v_i + a * dt \rightarrow v_f = v_i + a * dt$$

Similarly, the position can also be calculated as follows:

$$x_f = x_i + v * dt + \frac{1}{2}at^2$$

With these equations, the solution from Assignment 1 can be modified and re-simulated. These results are shown in Figure 1.

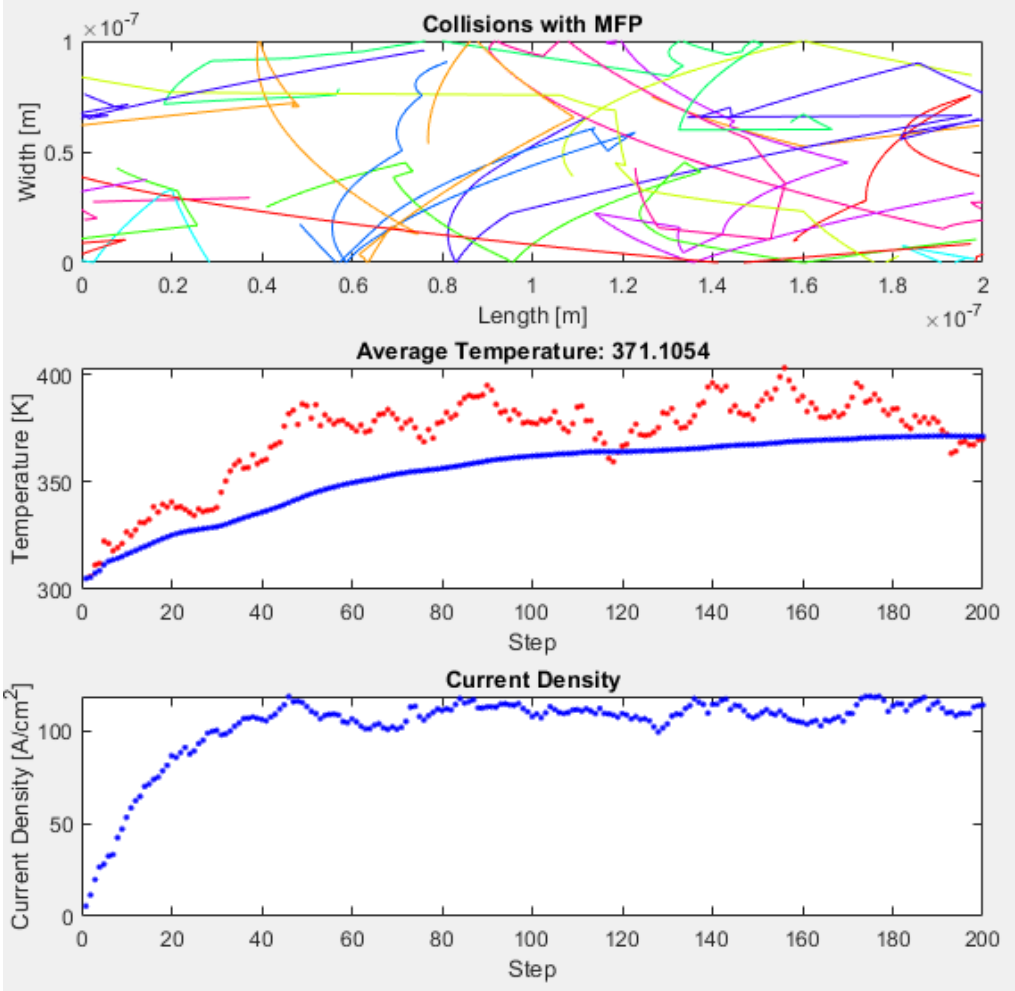

Figure 1: Assignment 1 Solution with Added Voltage

Figure 1 shows the simulations for the particle trajectories, temperature, and current density. As can be seen in the figure, due to the applied voltage, there is now an electric field (constant, in this case), that also produces a force and acceleration which interacts with the electrons. Due to this acceleration, the velocity now increases linearly through time (until the electron randomly scatters, and the velocity "resets"), and the position changes quadratically. This is evident in the particle trajectories. In addition, since the velocity increases, the total, and average, velocity is now a function of the thermal velocity as well as the velocity due to acceleration. As seen in Assignment 1, a faster velocity increases the temperature of the lattice, and this is also seen in the second subplot.

Finally, also due to the voltage and electric field, there is also a current found within the region. This current represents the electron drift current density and it can be related to the average carrier velocity (or v_x, since the applied voltage is in the x-direction) with the following equation:

$$J_x = envv_x$$

where J_x is the current density, e is the charge of the electron, n is the concentration, and v_{th} is the thermal velocity.

Therefore, since the velocity increases over time, except for when the particle scatters, the current will also increase over time. This current, along with the velocity, are the reason behind the lattice temperature increase. In this case, the average temperature is approximately 371K, rather than 300K as before. Also note that both the temperature and current will average to a constant as time approaches infinity, due to the scattering of the electrons. These results align with expectations.

Next, the electron density map was plotted to provide insight into the final locations of the electrons. This result is shown in Figure 2.

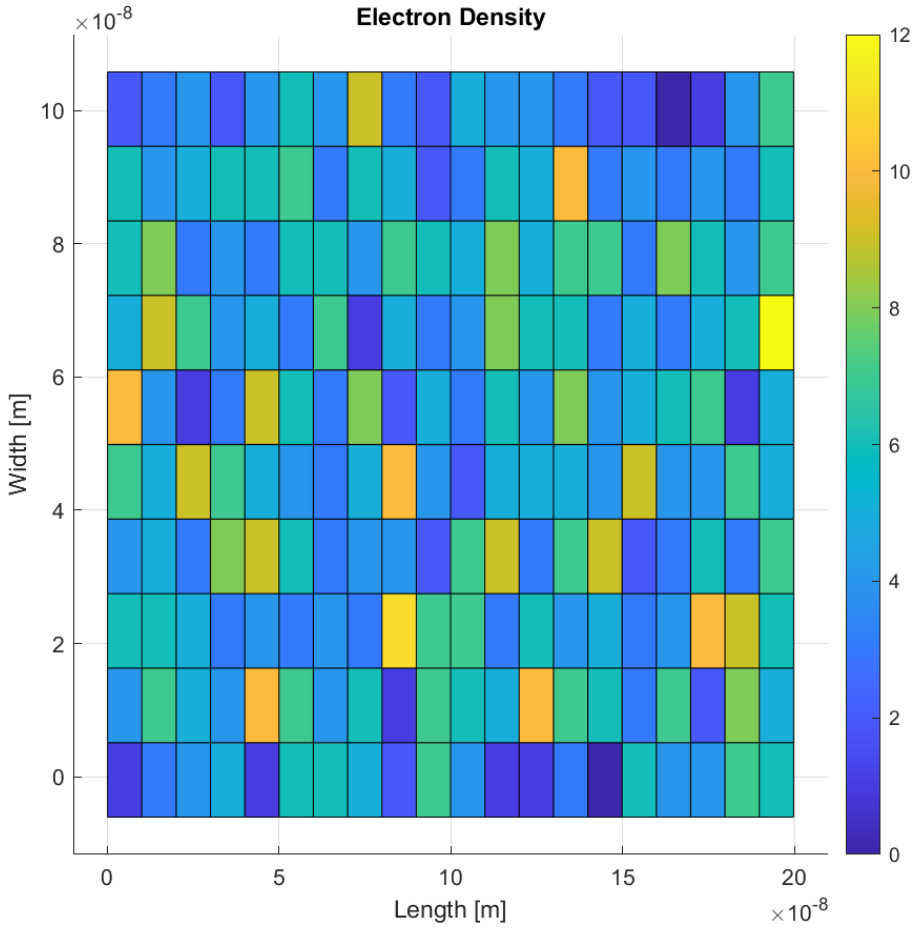

Figure 2: Electron Density Map

As seen in Figure 2, the locations of the electrons appear random, with high and low peaks throughout the region. This is expected since there are no obstructions to block the electrons' final positions and they can move in the region freely.

Finally, a temperature distribution was plotted to observe the temperature throughout the lattice. This result is shown in Figure 3.

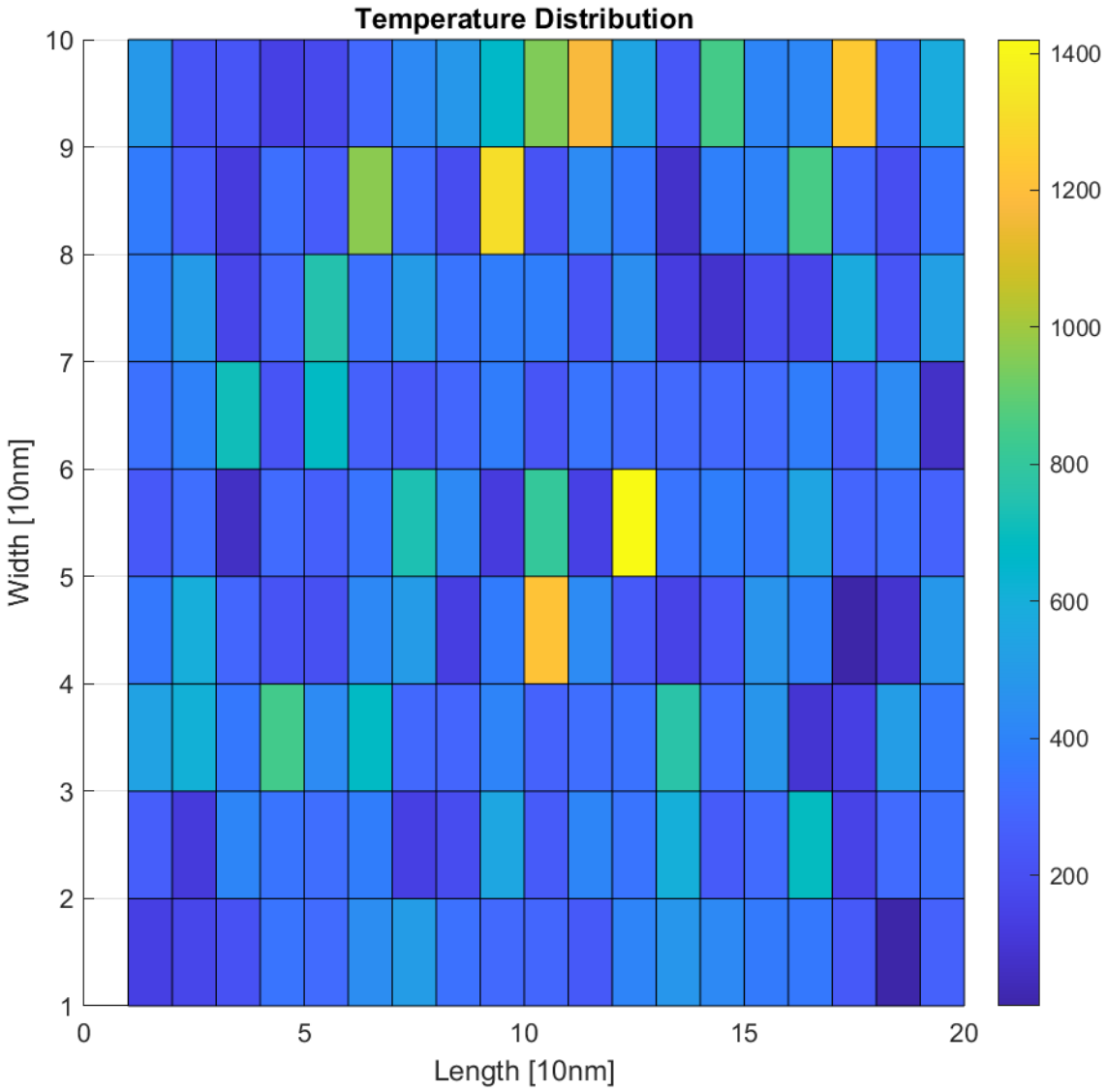

Figure 3: Temperature Distribution

As seen in Figure 3, the temperature also appears random throughout the region. In some bins, there does appear to be hotter temperatures, but this may be due to a large number of fast-moving electrons in the same region. However, the randomness should be accurate due to no obstructions within the region.

Part 2: Use Assignment 2 to Calculate E-field with Bottleneck

The purpose of this part was to use Assignment 2's finite difference method solution to solve for the voltage within the region, with the bottlenecks in place. This is necessary because the bottlenecks are assumed to have 0 conductivity, and thus affects the electric field within the larger region. Since these bottlenecks affect the electric field, the electric field is no longer constant within the region, and the

previous equation no longer applies. Instead, the voltage of the region can be found by the FDM of Assignment 2. The voltage distribution, with the bottleneck in place, is shown in Figure 4. Note that Assignment 2's conductivity values were used, but Assignment 3's voltage was used. Specifically, the voltage applied to the left boundary was 0.1V, the conductivity inside the boxes was 0.01 Ω^{-1}, and the conductivity in the larger region was 1 Ω^{-1}.

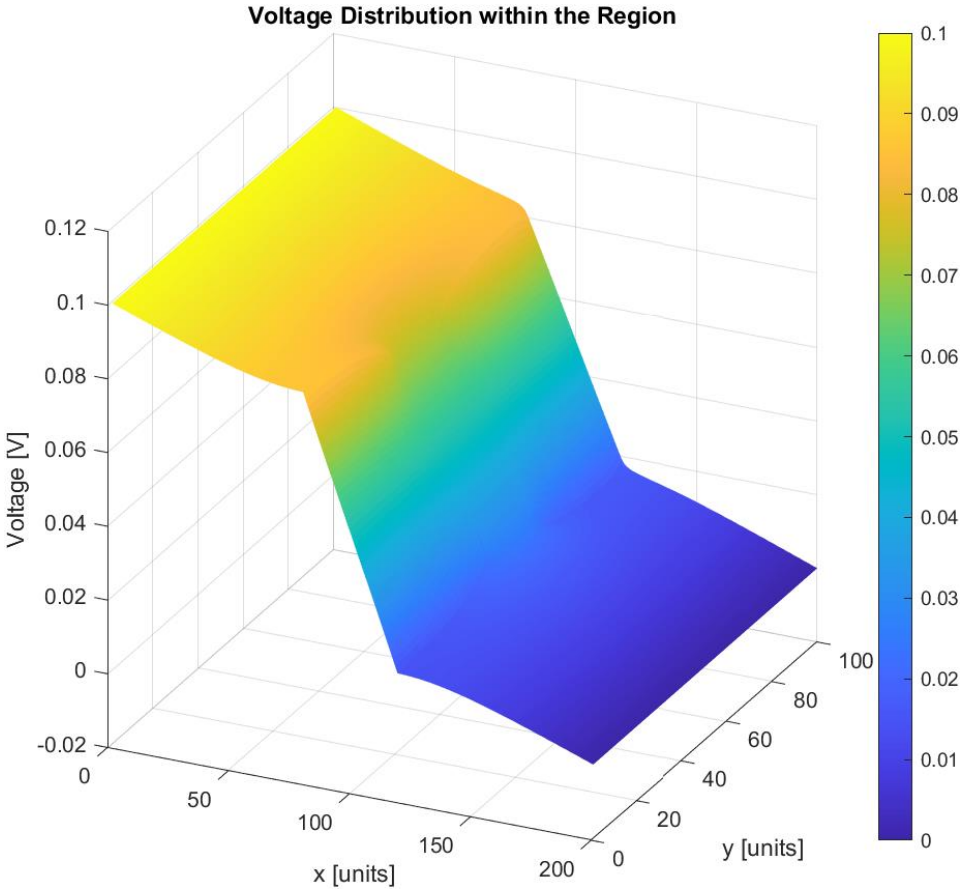

Figure 4: Bottleneck Voltage Distribution

As can be seen in the figure, the results align with the previous assignment, but with the exception of a different voltage boundary. Specifically, due to the larger conductivity outside the of the region, there is a smaller resistivity outside the boxes than inside the boxes. This is why the voltage drop inside the boxes is considerably larger, but still note that the boundary is kept to 0.1V, rather than 1V.

The electric field can then be calculated with the following equation:

$$\vec{E} = -\nabla V$$

Note that the electric field will be a matrix because the voltage distribution is a matrix.

The electric field within the region is shown in Figure 5.

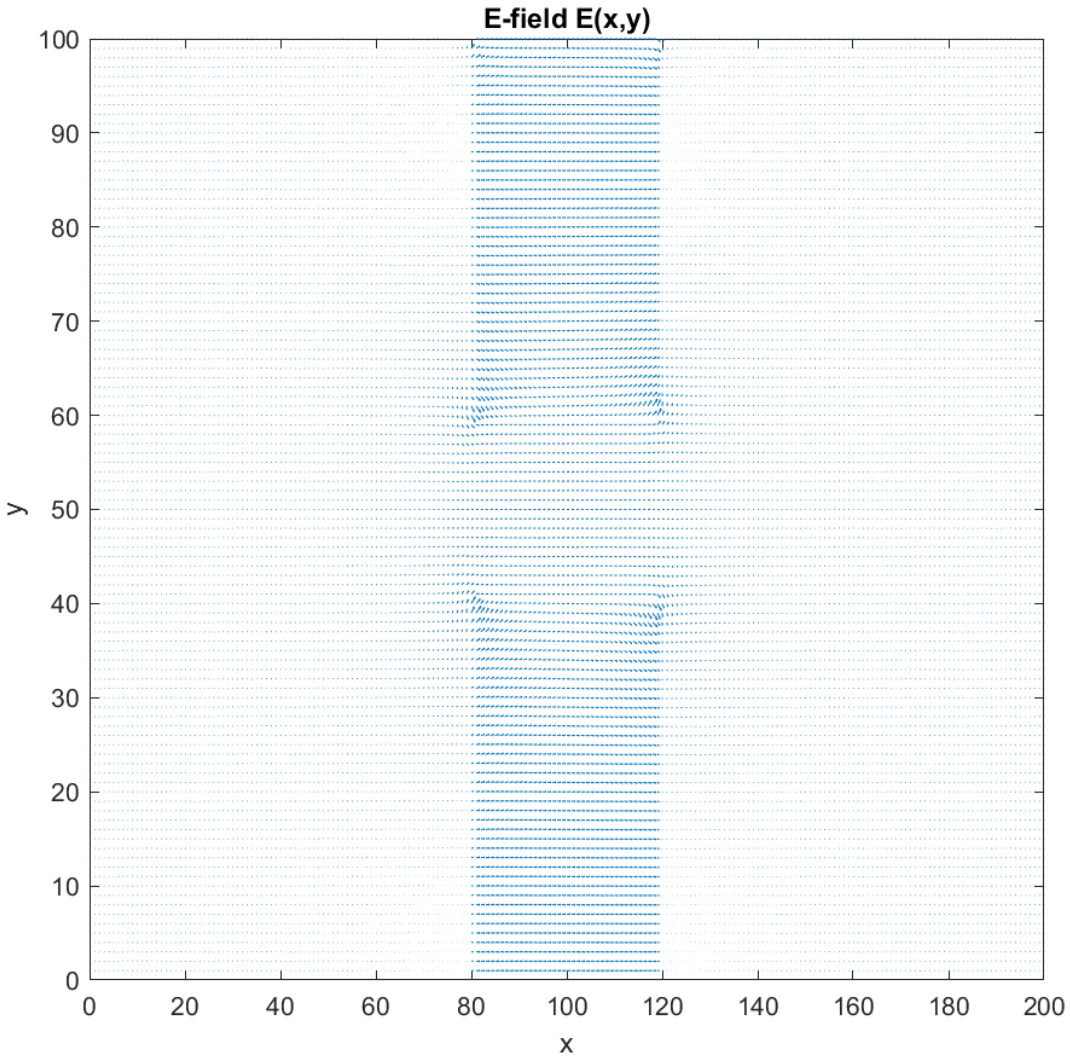

Figure 5: Electric Field with Bottleneck

As seen in the figure, the results also align with Assignment 2. Due to the smaller conductivity of the boxes, and consequently larger resistivity and voltage drop, the electric field within the boxes is larger than outside. Numerically, the electric field inside the boxes was calculated to be approximately 0.0018V/m, and outside the boxes was approximately 0.000234V/m. Note that the electric field is considerably smaller than the simple case (without bottlenecks) in Part 1: max of 0.0018V/m vs. 500kV/m.

Then, as before, the force and acceleration can be re-calculated, noting that neither of these properties will be constant throughout the region since the electric field is not constant. Once the acceleration is re-calculated, the simulation can be re-done to simulate electron behaviour and current with the bottleneck present. This result is shown in Figure 6.

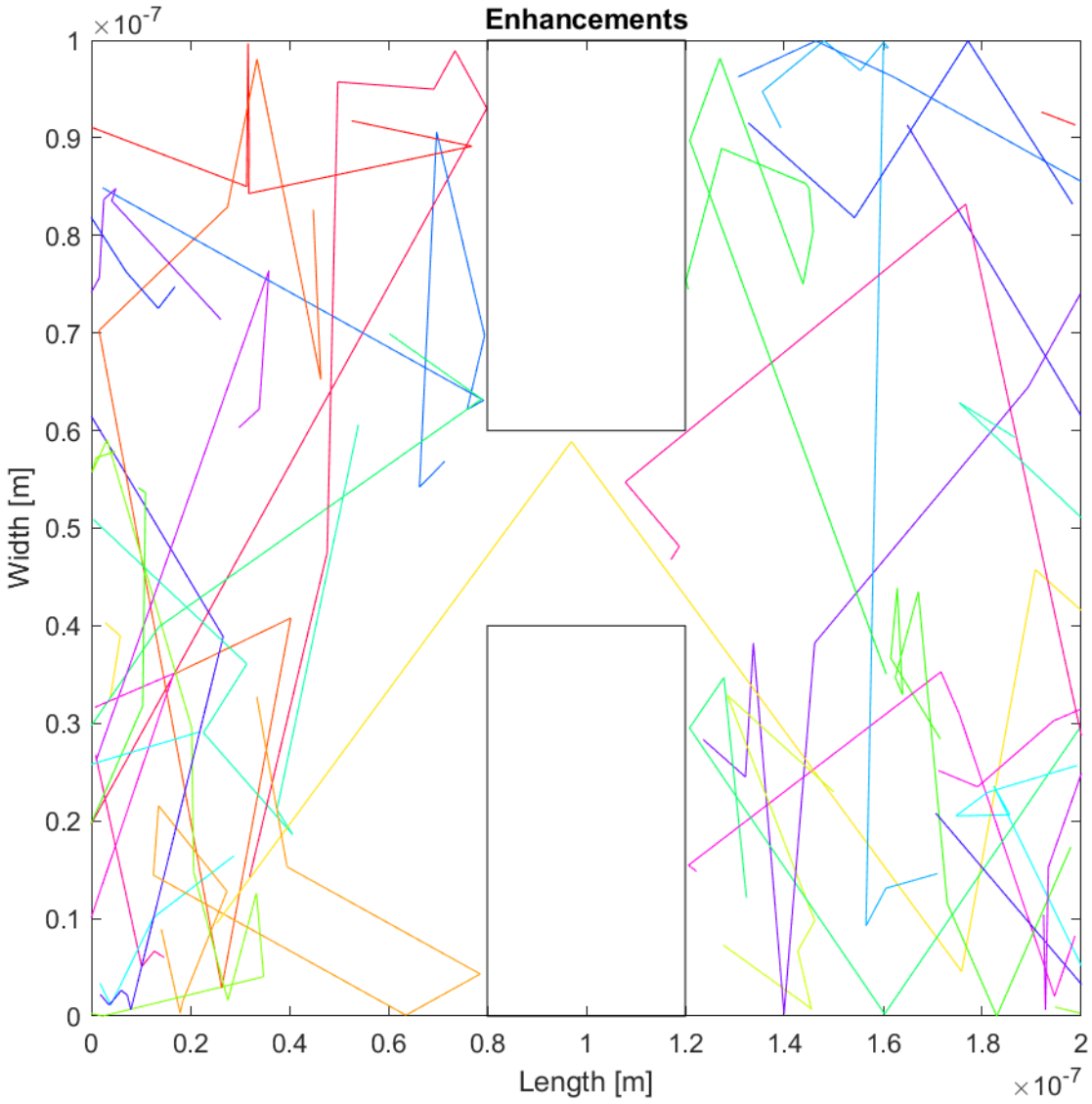

Figure 6: Particle Trajectories for Part 2

This result is very similar to the last part of Assignment 1 where the bottlenecks were introduced. While there is an applied voltage, the electric field, force, and acceleration are too small to be able to notice the quadratic behaviour, so the linear velocity dominates. In addition, this means the net velocity will be approximately equal to the thermal velocity, and so the drift velocity will be nearly zero. This concept is evident in the results since the electrons seem to be moving randomly within the region – which implies little drift current.

Note that only 20 electrons were plotted and 500 simulated, rather than 1000 and 1000, as stated in the report. This is because, due to the way the solution was programmed, the simulation was very slow with large numbers of electrons. Therefore, 20 electrons were used to show the general behaviour of the 500 electrons, and each of the 500 electrons could represent 2 electrons for the requirement's sake. As this is just modelling, the overall behaviour should be the same.

For the next part, the applied voltage will be increased, but this is explained further in the report.

Part 3: Coupled Simulations

The purpose of this part of the assignment was to couple the two simulations (voltage/electric field simulation and the molecular dynamics simulation) together to investigate current flow with the varying widths of the bottleneck obstruction.

The first step was to couple the simulations and run the simulation with the bottleneck as found in Assignment 1 – the default case. The same steps as before were followed: set the voltage boundary, find the voltage distribution by FDM, calculate the electric field, calculate the force, calculate the acceleration, and then apply the acceleration to the velocity and position of the electrons.

For this step, the assignment suggested an applied voltage of 0.8V. However, since the time step, dt, was set to a value such that the electrons only travelled 1/100 of the region's length, the time step was very small. Specifically, the time step was:

$$dt = \frac{regionLength}{100(v_{th})} = \frac{200nm}{100(1.8702x10^5)} = 1.0694x10^{-14}$$

So, since the position calculation has a $(dt)^2$ term, if the acceleration is not large enough, the squared term will not be large enough, and the linear term will dominate. Therefore, to compensate this very small time step, 1 gigavolt was used for simulations to provide a larger electric field, force, and acceleration – especially since the electric field outside of the bottlenecked region was already very small. The result of this applied voltage and the bottleneck within the region is shown in Figure 7.

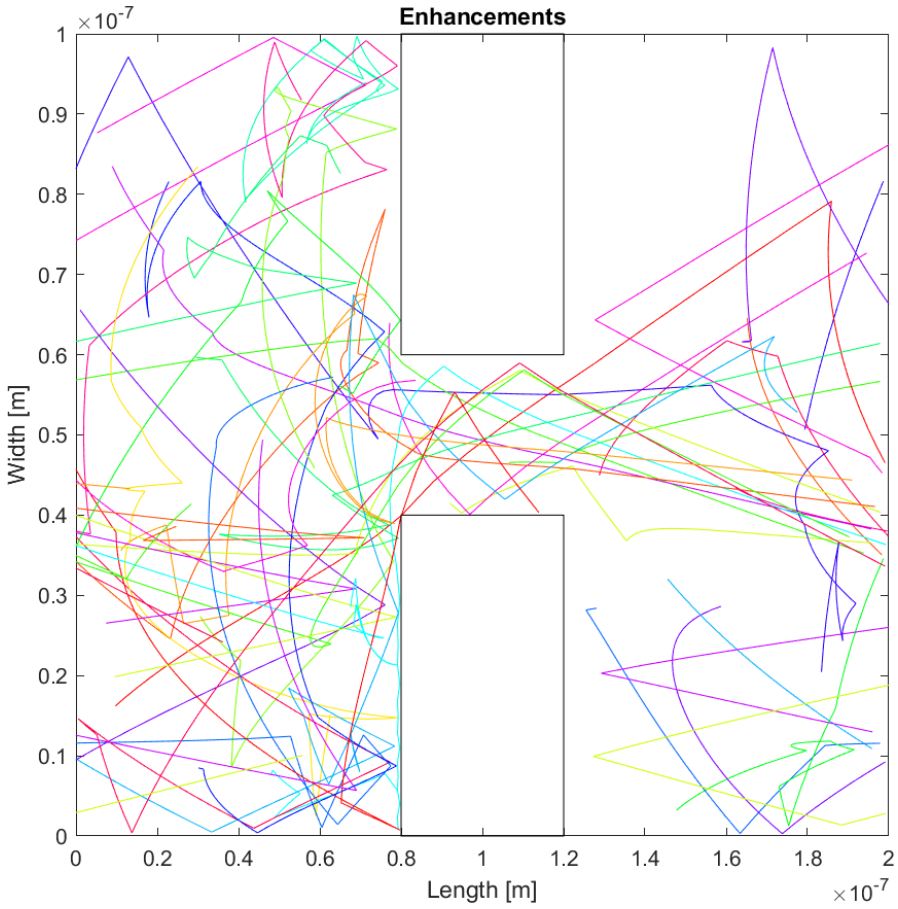

Figure 7: Part 3a Particle Trajectories

As can be seen in the solutions, the particle trajectories have a quadratic path, as expected. At 0.8V, the acceleration was not large enough to produce a quadratic path. In any case, it can clearly be seen that this voltage creates a current in the positive-x direction (because the left BC is 1GV and the right BC is 0V). However, due to the bottleneck, the electrons are restricted on the left side since there is only a small opening to get to the right side. Even when they do the through the bottleneck, the right side brings them back to the left side. Ultimately, most electrons get trapped on the left side. The reason this occurs is that the acceleration is large enough to reduce all negative-x travelling electrons and increase their velocity to push them right.

This can be clearly seen in a density map, which is shown in Figure 8.

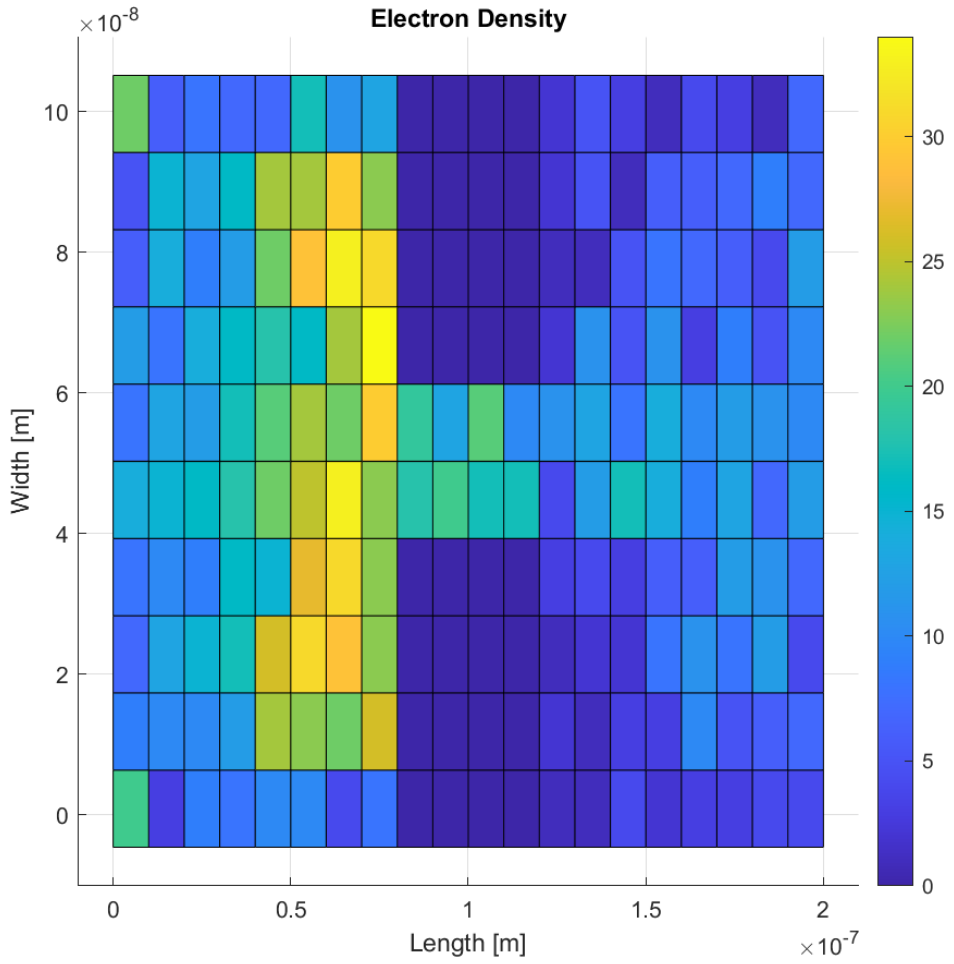

Figure 8: Part 3 Electron Density Map

As can be seen in this figure, the majority of electrons are confined within the left side of the region. Therefore, the bottleneck is acting like a resistance – it allows electrons to pass through (small densities on the right side), but the barrier is stopping most from doing so. This also implies that the current is limited since the most of the confined electrons may eventually be truly trapped, and their net velocity may approach zero.

With this result and observation, the next step is to investigate the current vs. bottleneck width. While the same simulation can be run, all that needs to change is to set heights of the boxes differently. Since the default case is 20% open, two test cases were chosen: 40% open and 60% open. These results are shown in Figure 9.

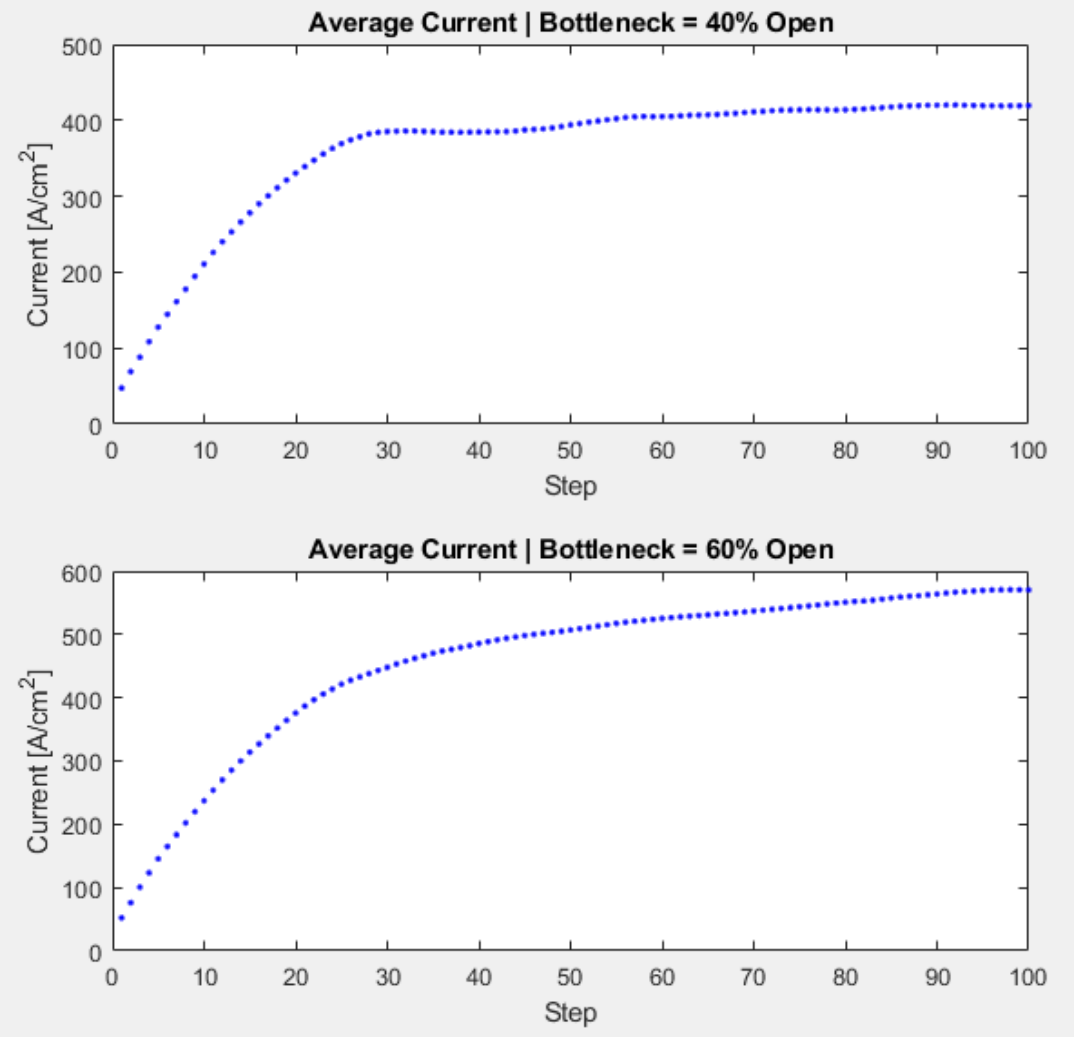

Figure 9: Current vs. Bottleneck Investigation

As can be seen in the figure, the results align with expectations once again. That is, as the bottleneck increases/decreases, the current gets smaller/larger. While both eventually tend to remain constant as time progresses, 60% open had a current density approaching 600mA/cm^2 whereas 40% open restricts the current down to approximately 450mA/cm^2. Therefore, as the bottleneck narrows, its effective resistance increases and limits/lowers the current (limit is done by scattering, but it does lower).

The final to make this simulation be more accurate would be to make the region or scenario more realistic. This may be achieved in several ways, with a few examples as follows:

1. **Add collision behaviour between electrons.** This example would follow the Molecular Dynamics topic, but has not been implemented in this assignment. Currently, the program only deals with boundary conditions (whether it's the region's boundary or a box's boundary) and scattering involves a random probability. Given the confined space, and for example, 5000 electrons, the probability of scattering may even be much less the event of two electrons colliding, and therefore, scattering. Therefore, the simulation could be more accurate with collision behaviour.

2. **Add more-realistic boundary conditions.** Due to the confined region, there are lots of opportunities for the electrons to interact with a boundary. Therefore, the simulation could be more accurate with more-realistic boundary conditions. Currently, most boundaries deal with a specular or diffusive nature. However, since these boundaries would realistically define regions of different materials, energy from the electrons should be taken into consideration where some energy may be transmitted into the material, as an example, rather than simply switching directions or generating a random new velocity. Note that this applies to both the top/bottom walls, as well as the boxes, since there will implicitly be different mediums in these locations.
3. **Add more-realistic region behaviour.** In the real-world, at a microscopic level, materials always have imperfections/non-idealities associated with the internal material. That is, a constant behaviour is (likely) rarely present. Therefore, to better model the real-world, the conductivity of the internal region could be changed to vary around a value to provide a "tolerance" to the material. This can be done through a Monte Carlo simulation, where each mesh element could have a randomized conductivity between $\sigma(1 \pm x)\%$. This way, Assignment 2's FDM can still be used to calculate the voltage across the region (noting that this time, there would be more fluctuations within the "constant" region), and the electric field, force, and acceleration would follow. Ultimately, this introduces a simulation in each mesh element affects the electrons differently, thereby modelling the real-world imperfections more accurately.