Carleton University

ELEC 4700 - Assignment #1

Monte-Carlo/Finite Difference Modeling of Electron Transport

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1 Question #1

Please refer to Question1.m for the code for this section. Note that a voltage of 1V was chosen rather than the recommended 0.1V to demonstrate the effect of the voltage perturbing the velocities of the electrons.

1.1 Part 1

The electric field can be expressed using the formula for a uniform electric field in a capacitor:

$$E = \frac{V}{d} \tag{1}$$

In the proposed geometry, the distance along the x direction is 200 nm and the voltage was chosen to be 1 V. The electric field across the geometry was calculated to be $5 \times 10^6 \frac{N}{C}$.

1.2 Part 2

The force on each electron is calculated by multiplying the electric field intensity by the elementary change.

$$\vec{F} = q\vec{E} \tag{2}$$

With the given electric field strength, the force on any given electron was calculated to be $8.010883 \times 10^{-13} N$.

1.3 Part 3

Using the mass of the electron, the electron acceleration can be calculated with following equation:

$$a = \frac{qV}{md} \tag{3}$$

The acceleration was calculated to be $8.7941 \times 10^{17} \frac{m}{s^2}$.

1.4 Part 4

The current in the given geometry was calculated by taking the following current density formula:

$$v = \frac{j}{nq} \tag{4}$$

In this case, j is the current density, v is the average thermal velocity of the electrons, n is the electron carrier density (chosen to be 1×10^{20}, and q is the elementary change. The current density can be converted to a current by multiplying by the area.

$$I = vnAq \tag{5}$$

The following diagram demonstrates the change in current of the system over a time period of 5 ps. The current increases as the particles travel in the electric field and as a result, the thermal velocity increases. The current continues to increases until a particle scatters off the background, which reduces the average thermal velocity of the system. Since there are so many particles and collisions that occur, the current converges to a balanced value where the thermal velocity remains relatively constant.

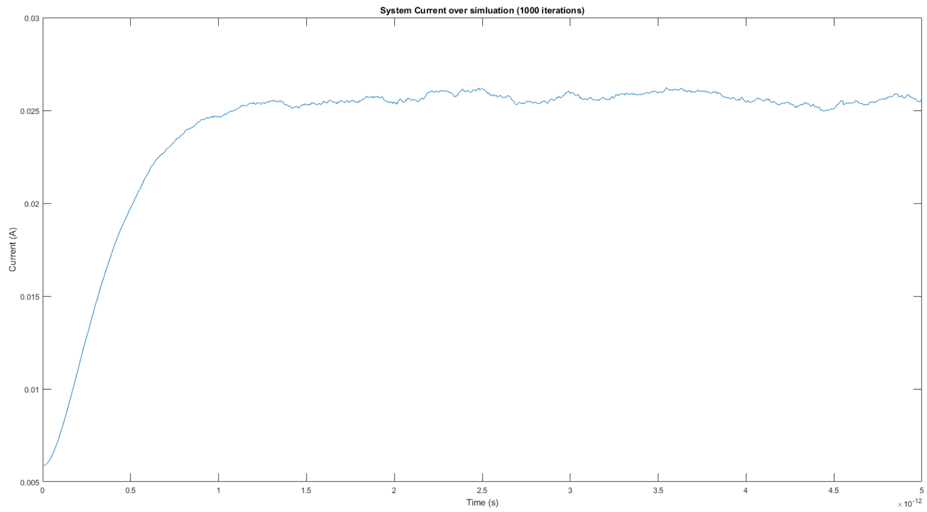

Figure 1: System Current Plot of 10 particles over 5 ps

1.5 Part 5

The following plot depict the electron density map and temperature of each particle in the system respectively.

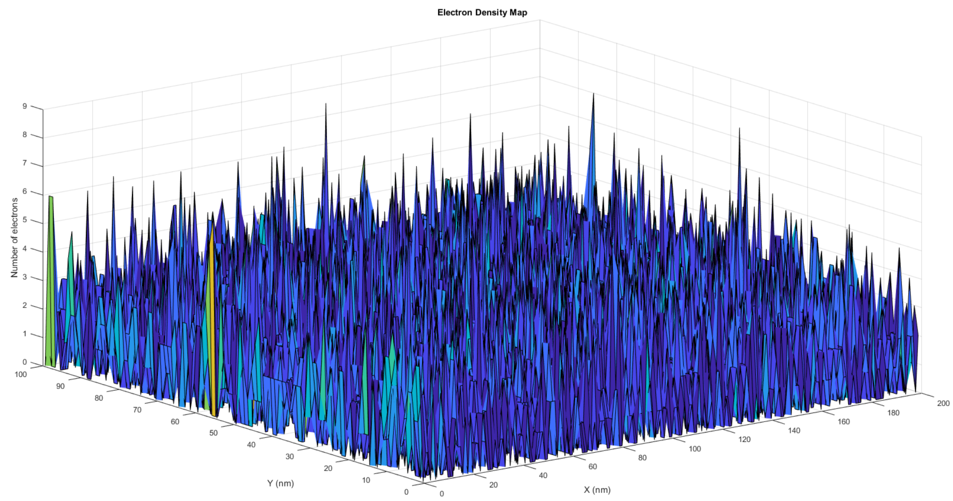

Figure 2: Electron Density Map of 30000 particles over 5 ps

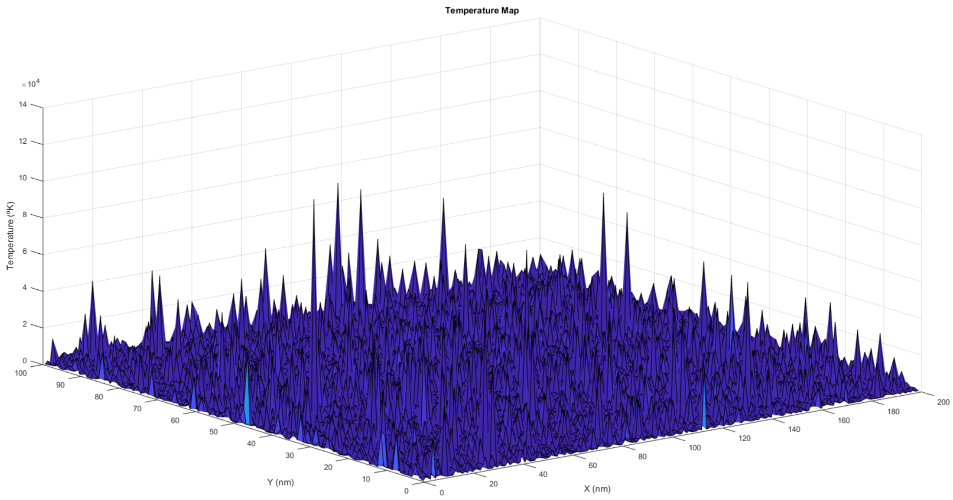

Figure 3: Temperature Map of 30000 particles over 5 ps

2 Question #2

Please refer to Question2.m for the code for this section.

2.1 Part 1

The two contact geometry that was evaluated in the previous assignment was used again. The system was 100 nm $\times$ 150 nm and consisted of two contacts that created a bottleneck that was 15 nm across. The following figures represent the voltage and electric field present in the described geometry.

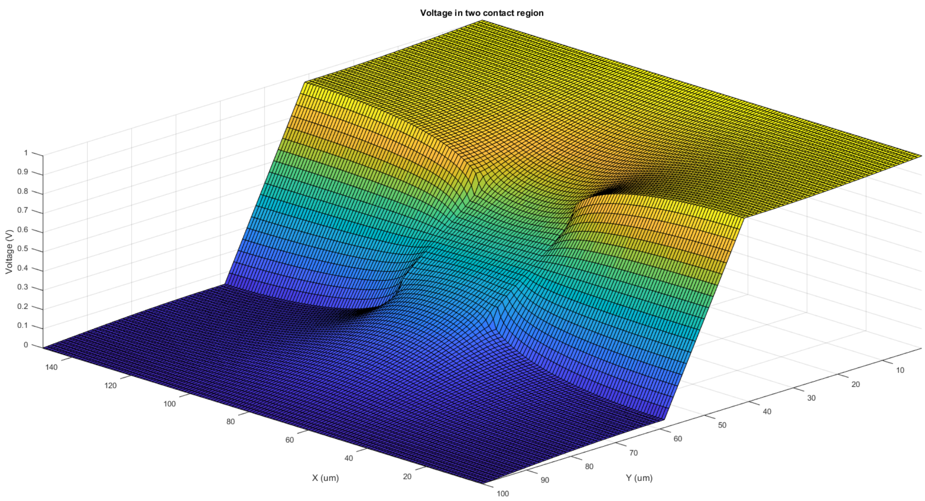

Figure 4: Electric Potential Map of the Bottleneck Geometry with a size of 100 nm $\times$ 150 nm

2.2 Part 2

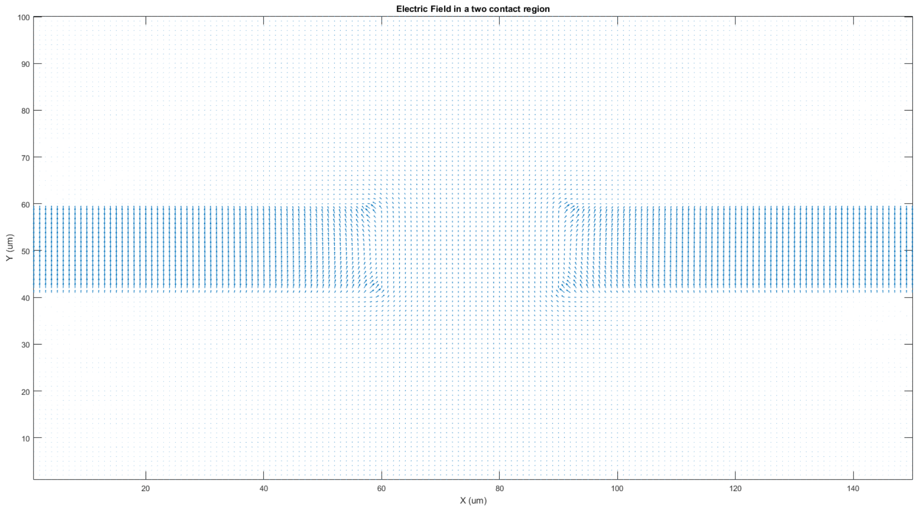

Figure 5: Electric Field Quiver Plot of the Bottleneck Geometry with a size of 100 nm $\times$ 150 nm

3 Question #3

Please refer to Question3.m for the code for this section.

The two previous questions were combined to simulate electron behaviour in the geometry described in part #2. The particles were perturbed with the electric field and the electric potential of the bottleneck geometry.

3.1 Part 1

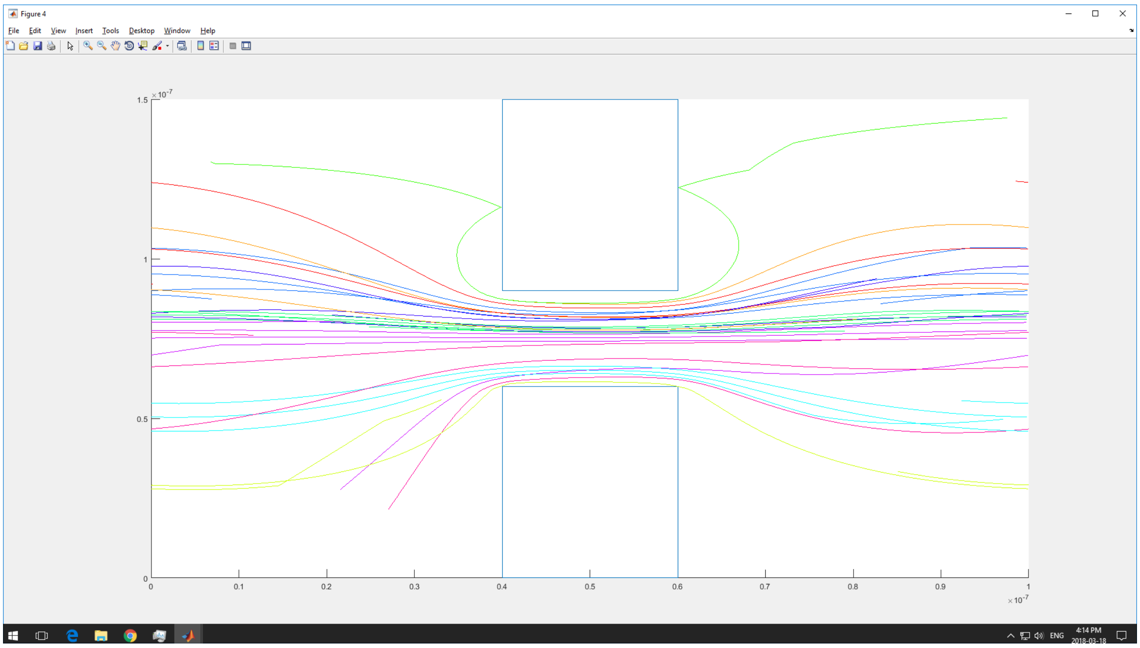

Figure 6: Particle Trajectory Plot of the Bottleneck Geometry with 10 Particles over 1000 Iterations

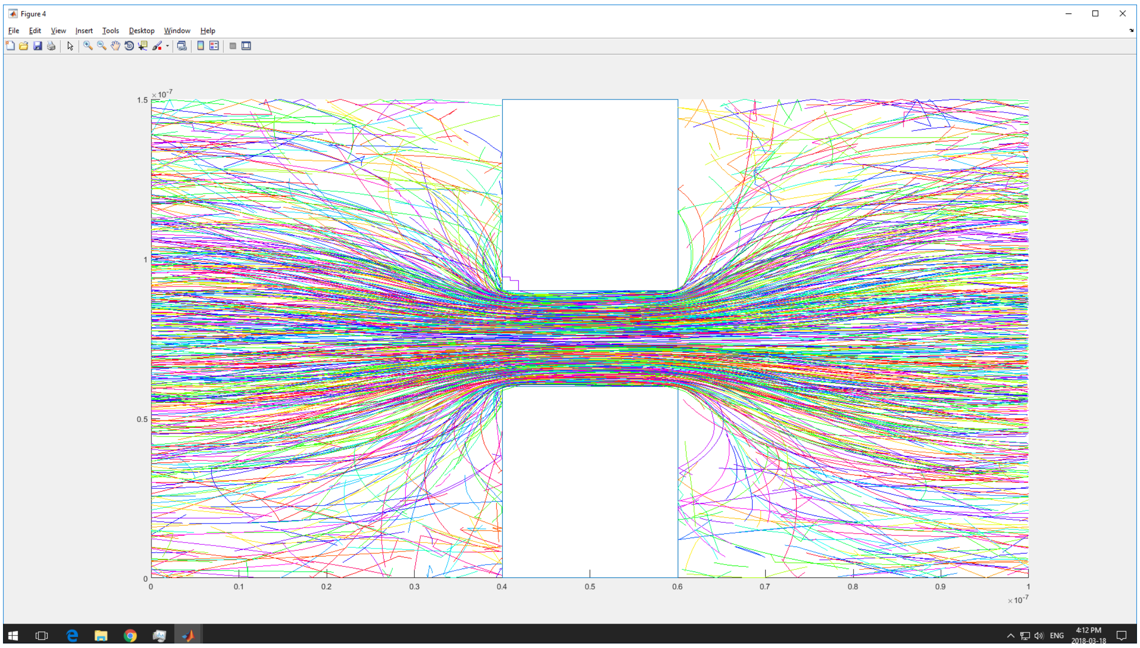

Figure 7: Particle Trajectory Plot of the Bottleneck Geometry with 1000 Particles over 1000 Iterations (20 % complete)

3.2 Part 2

Comment.

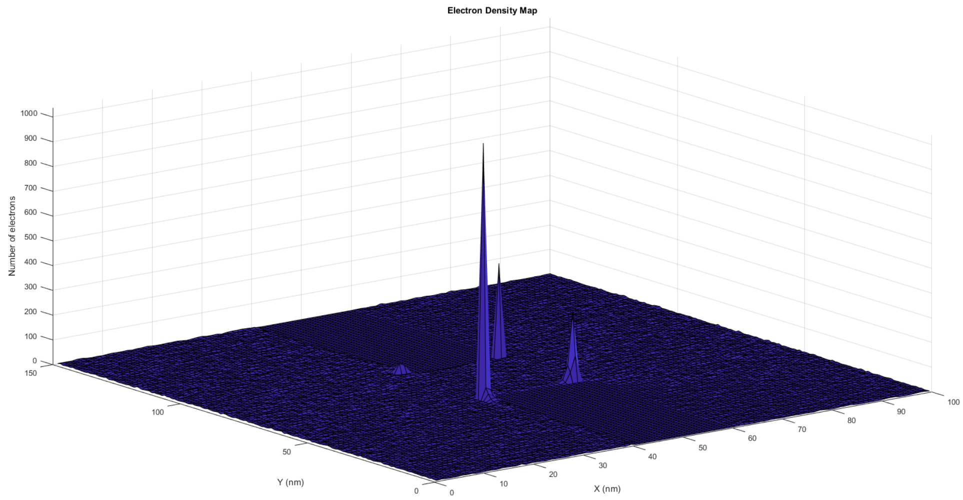

Figure 8: Electron Density Map of the Bottleneck Geometry with 30000 Particles over 1000 Iterations

3.3 Part 3

The system was rather accurate at emulating the behaviour of an electron in an electric field and electric potential. The values of the fields were adjusted to ensure that the effect of the field was noticeable and this skewed the current and temperature plots as can be seen in the following figures

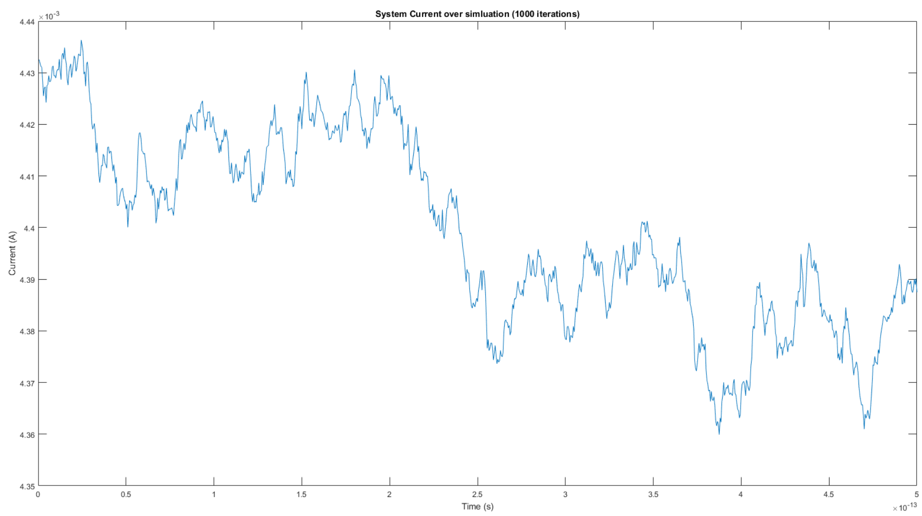

Figure 9: System Current Plot of the Bottleneck Geometry with 30000 Particles over 1000 Iterations

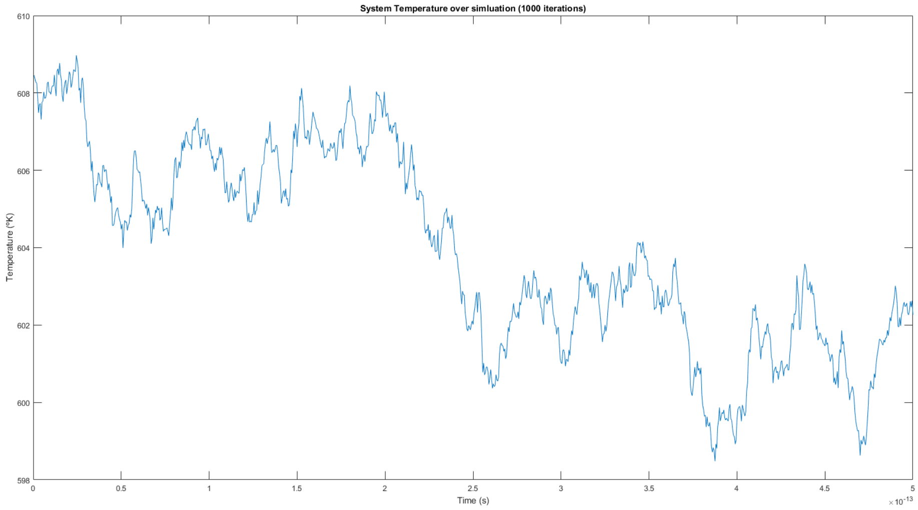

Figure 10: System Temperature Plot of the Bottleneck Geometry with 30000 Particles over 1000 Iterations

The temperature is low due to the electric field slowing down the particles after they have passed the bottleneck. If the current and temperature in the bottleneck were taken into account, the values would be much higher than they were in part #1 because of the added electric field.

Further modifications can be made to ensure that the particles do not go through the boxes. The 1000 particle simulation had particles that were moving so fast that they were penetrating the contact regions. An adjustment of the simulation time scale would ensure that the particles will not clip the contact regions.