ELEC 4700 Assignment 3: Monte Carlo and Finite Difference Method

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March 15, 2020

1 Part 1: Adding Electric field to Monte-Carlo

1. By applying a voltage, the electric field is;

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

Where V is the applied voltage and d is the distance. If a voltage of 0.1 V is applied in the x-direction over a region of length 200 nm;

$$E_x = \frac{0.1\ V}{200\ nm}$$

$$\boxed{E_x = 5 \times 10^5\ \ V/m}$$

2. The force on each electron can be calculated as;

$$F = Eq \tag{2}$$

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

$$\boxed{F_x = 8.0109 \times 10^{-14}\ \ N}$$

3. The acceleration on electrons is calculated as;

$$a = \frac{F}{m} \tag{3}$$

where m is the effective mass of an electron. This evaluates as;

$$\boxed{a_x = 3.3823 \times 10^{17}\ \ m/s^2}$$

To update the velocity with each time step, the following equation was added;

$$V_x = V_x + a_x \Delta t;$$

A plot of the electron trajectories with an applied voltage in the x-direction of 0.1 V for a subset of 25 electrons over 50 time steps is shown in Figure 1;

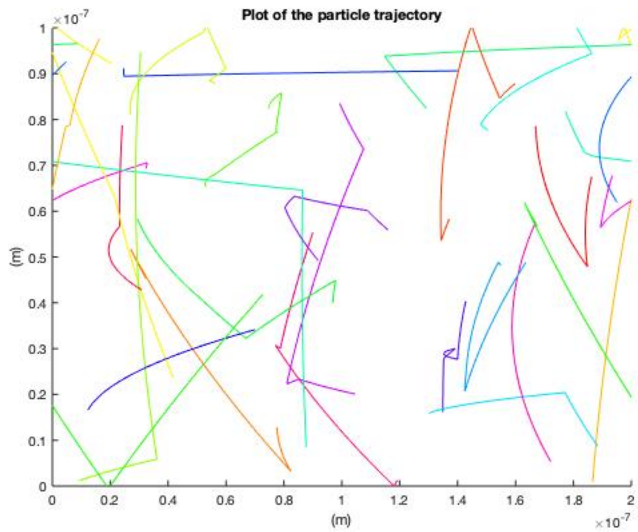

Figure 1: Trajectory of 20 electrons

4. The the relationship between the electron drift current density and average carrier velocity is;

$$J = -qnV \tag{4}$$

where J is the current density (A/m), n is the electron concentration and V is the average carrier velocity (1). A plot of the current density over time is;

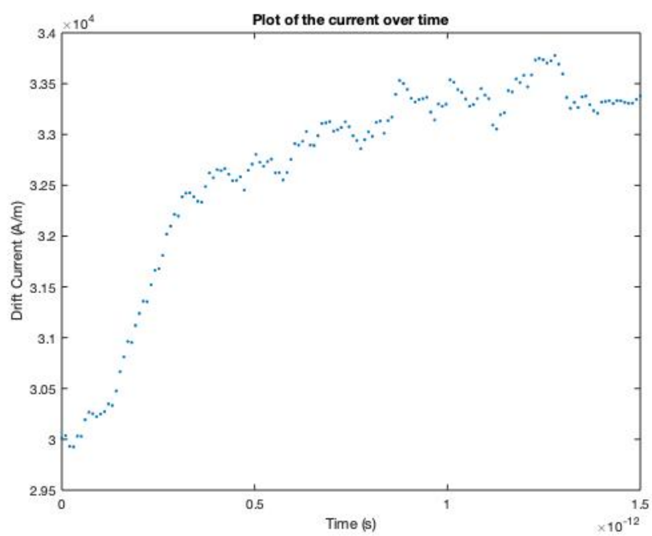

Figure 2: Current behaviour of 3000 electrons over time

At the beginning of the simulation, the current increases until it remains relatively constant. The increase in current is explained by the velocity initialization at the first time step. Each particle is initially assigned a random velocity from the Maxwell-Boltzmann distribution. As the time steps increase, the particle is accelerated according to the electric field at the particles position. Due to the acceleration caused by the applied electric field, the current density increases and then remains relatively constant.

5. The normalized density map of the electrons is;

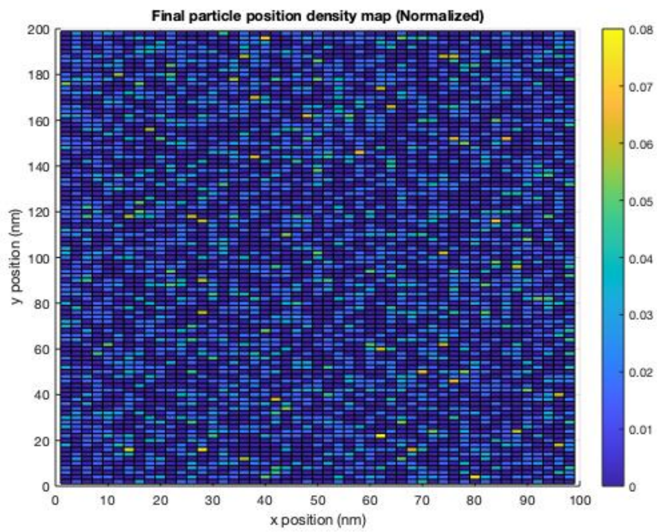

Figure 3: Normalized density of 3000 electrons

The density map of the electrons is;

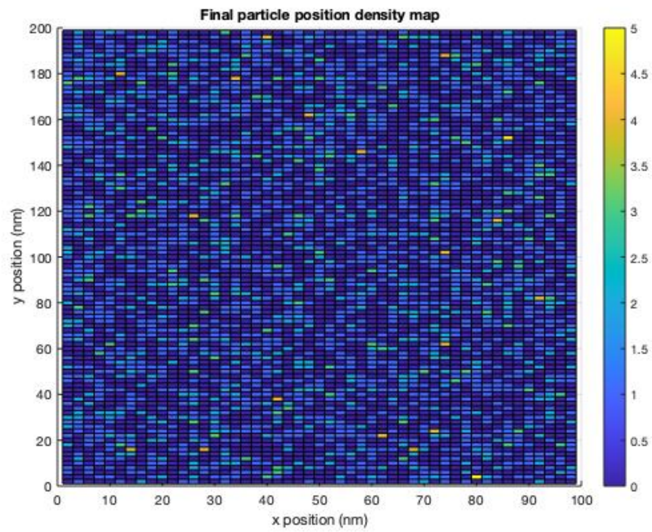

Figure 4: Density of 3000 electrons

The temperature map of electrons is;

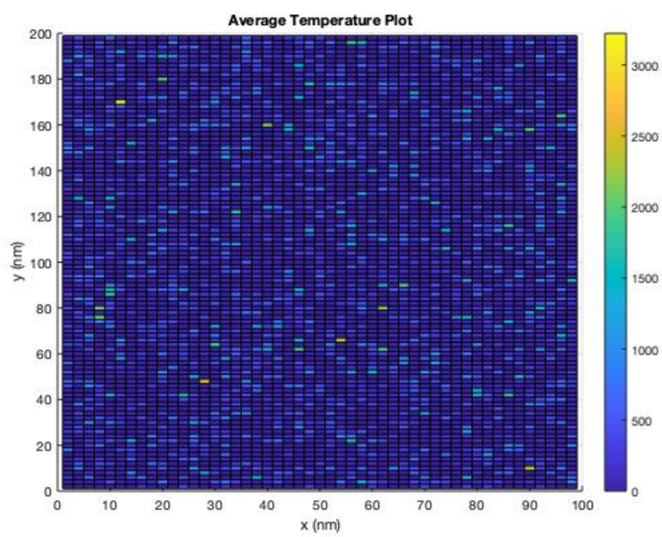

Figure 5: Temperature of 30000 electrons over time

The temperature and density distribution is uniform throughout the entire region.

2 Part 2: Finite Difference and Monte-Carlo Integration

1. The finite difference method code was used to calculate the potential with a bottleneck. A surface plot is shown below;

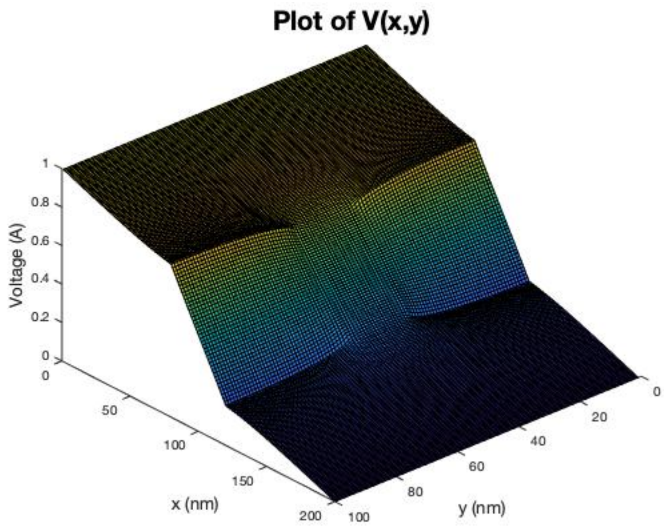

Figure 6: Voltage surface plot of a region with bottleneck

2. A plot of the electric field is shown below;

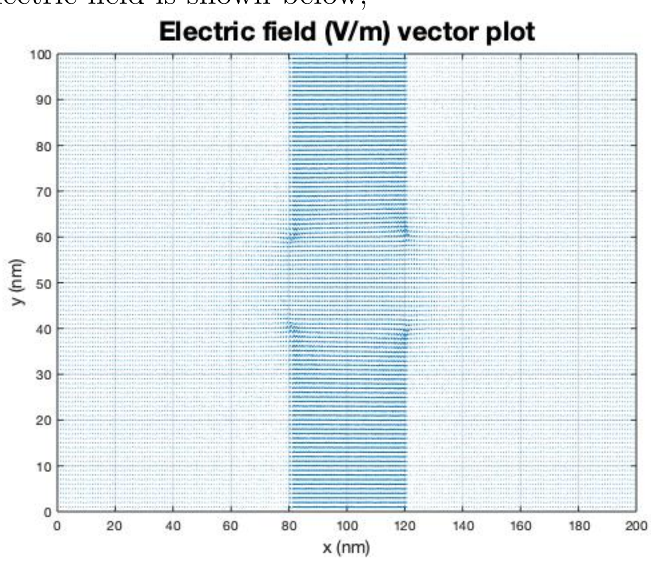

Figure 7: Two-dimensional plot of the electric field of a region with bottleneck

As expected, the electric field is largest in the region of high conductivity. Additionally, the field is large between the bottleneck.

3. A plot of the particle trajectories for a subset of 50 particles over 50 time steps is shown below;

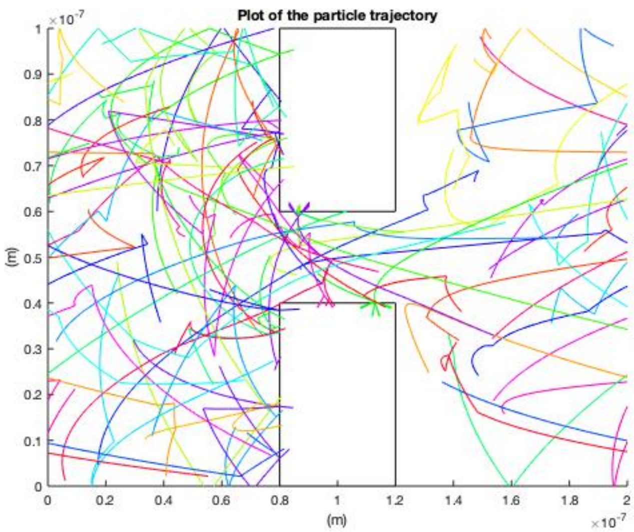

Figure 8: Two-dimensional plot of particle trajectories

A plot of the particle trajectories for a subset of 50 particles over 1,000 time steps is shown below;

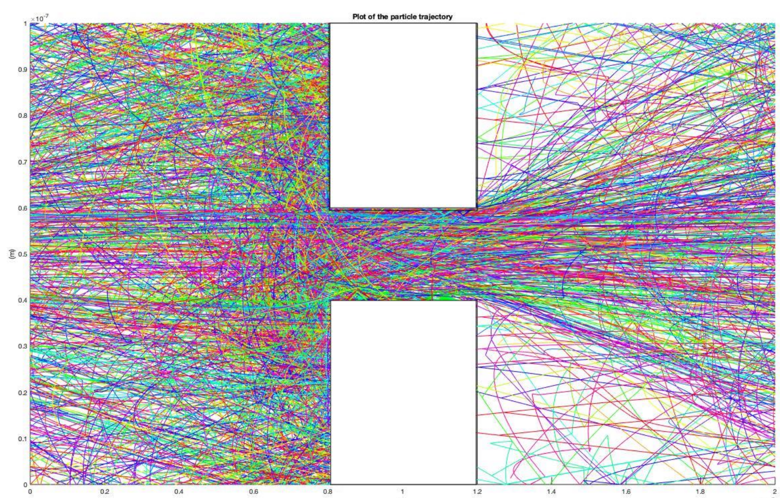

Figure 9: Two-dimensional plot of particle trajectories after 1,000 timestpes

The trajectory of the particles is as expected due to acceleration from the electric field. The field is large between the two bottleneck regions. Consequently, the particles are accelerated through that region.

3 Part 3: Coupled Simulations

1. A normalized density map of the 30,000 particles after 1,000 timesteps is shown below;

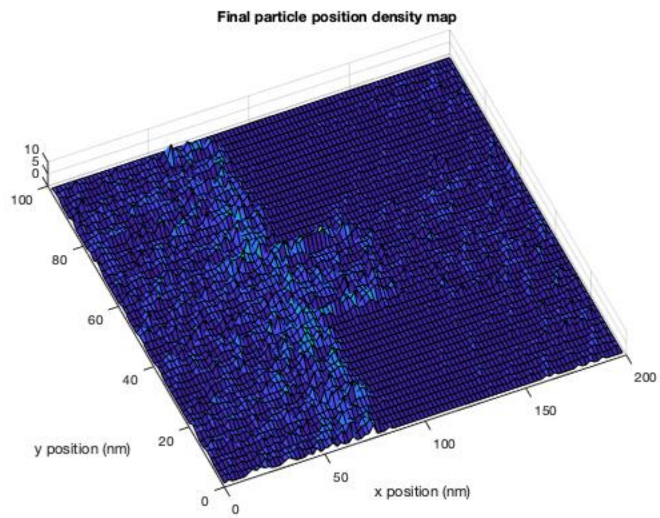

Figure 10: Normalized density map of particle location

As seen in the Figure, there are regions with a higher concentration of particles. This can be explained by the higher electric field in the bottleneck region and between the regions.

2. The current density was calculated for bottleneck widths varying from 5 nm to 50 nm. The average current density of 50 steps was plotted against the bottleneck width as shown in Figure 11;

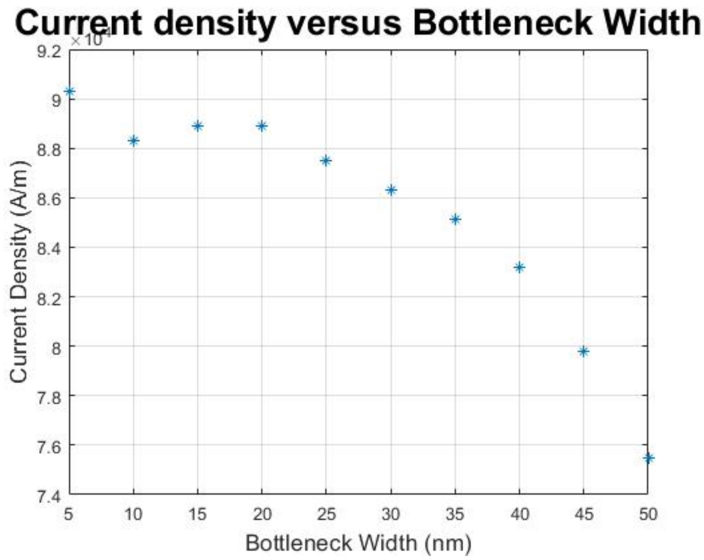

Figure 11: Plot of average calculated current density for various bottleneck widths

A plot of the calculated current from the finite difference method is shown below;

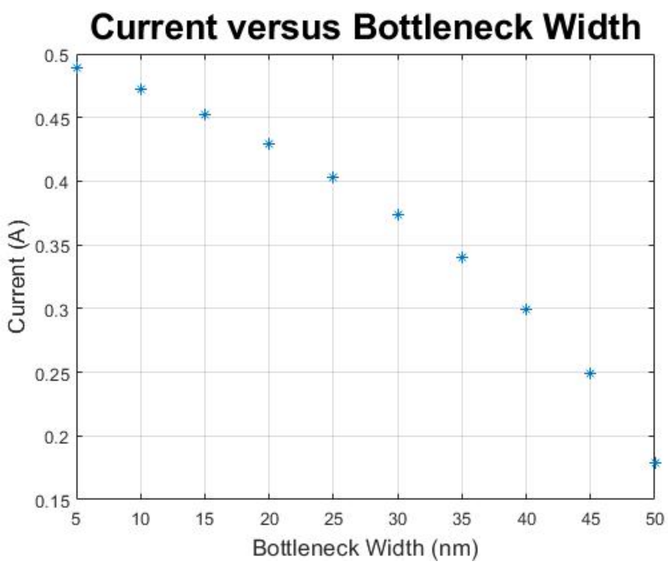

Figure 12: Plot of calculated current for various bottleneck widths

The conductivity map for the cases with a bottleneck width of 5nm and of 45 nm are shown in Figures 13 and 14, respectively;

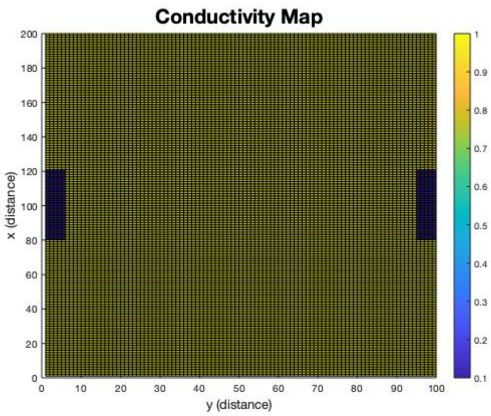

Figure 13: 5 nm Bottleneck width

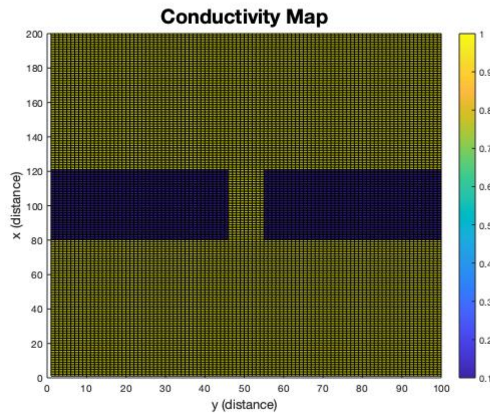

Figure 14: 45 nm Bottleneck width

3. To make the simulation more accurate, next steps would be to;

   - Decrease the mesh size
   - Decrease the time step
   - Increase the number of particles in simulation
   - Increase the number of steps
   - Account for elastic scattering, inelastic interactions and back scattering of electrons

   Ultimately, this simulation is optimal for rudimentary problems with simple geometries. Improvements aim to generate a better and more accurate approach for simple problems.

A References

[1] "Chapter 2:Semiconductor Fundamentals." Carrier Transport, ecee.colorado.edu/ bart/-book/book/chapter2/ch2_7.htm.