Carleton University

ELEC 4700 - Assignment #1

Monte-Carlo Modeling of Electron Transport

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supervised by

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1 Question #1

Please refer to Assignment1.m for the code for this section.

1.1 Part 1

The thermal velocity in two dimensions is defined by the following equation:

$$v_{th} = \sqrt{\frac{2k_BT}{m_e}} \tag{1}$$

Where k_B is Boltzmann's constant, T is the temperature in kelvin and m_e is the mass of the electron. The following equation was implemented in code in the following manner:

```
%Assign velocity
std0 = sqrt(2 * C.kb * Temp / C.m_0); %Thermal Velocity
Vx(1:nPart) = std0 * randn(1, nPart);
Vy(1:nPart) = std0 * randn(1, nPart);
```

To ensure that the velocity for each particle is in a random direction, the normal random variable is used. V_x and V_y are column vectors that store the velocity of particles $1 : nPart$.

1.2 Part 2

The mean free path can be defined by multiplying the mean collision time with the thermal velocity:

$$\lambda_{mn} = v_{th} \times \tau_{mn} \tag{2}$$

This is done in code with the following snippet:

```
%Calculate mean free path
mfp = tmn .* sqrt(Vx.^2+Vy.^2);
```

Since the velocity is in two dimensions, the magnitude of the velocity vector is calculated and multiplied by the mean collision time.

1.3 Part 3

Electron transport in two dimensions was simulated with the random thermal velocities in a box measuring 200 nm by 100 nm. Over 1000 iterations, the following 2-D particle trajectory plot was produced:

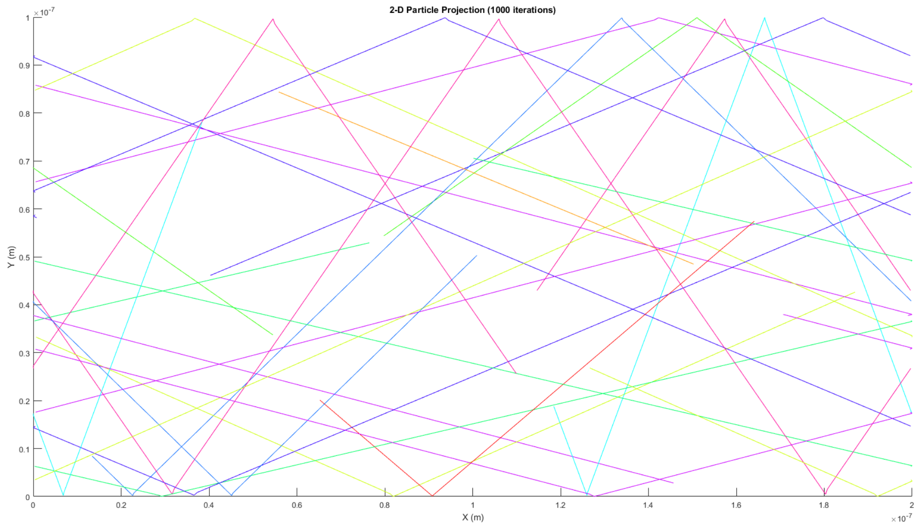

Figure 1: 2-D particle trajectory plot of 10 particles over 5 ps

The temperature of the simulation was calculated using the following code snippet:

```
%Calculating Temperature
vth = sum(Vx.^2+Vy.^2)/10;
T(1,c) = (vth*C.m_0)/(2*C.kb);
```

The temperature is calculated by reversing the equation (1) and solving for T. Because of the random variable that is added to the system, the temperature will not be 300°K as it was when setting the velocities. The following plot is the temperature of the system during the simulation:

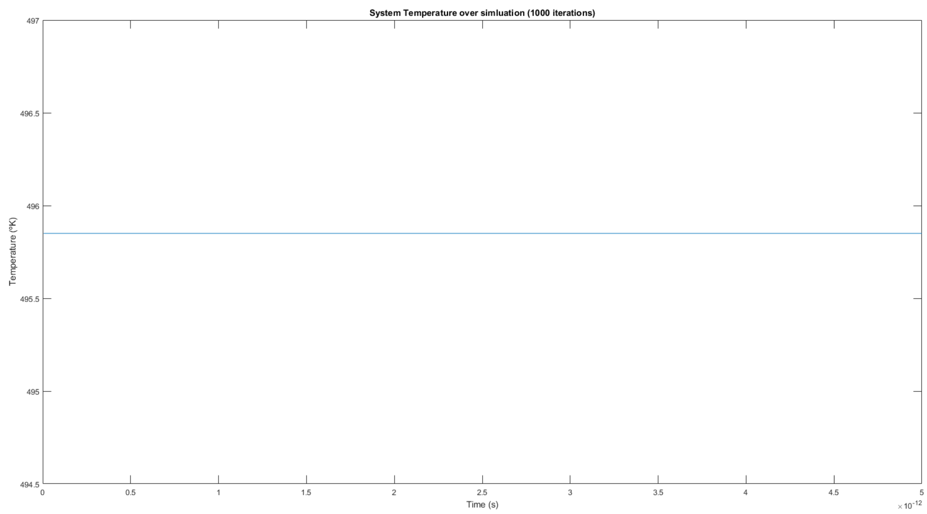

Figure 2: Temperature of the particle trajectory simulation

2 Question #2

Please refer to Assignment2.m for the code for this section.

2.1 Part 1

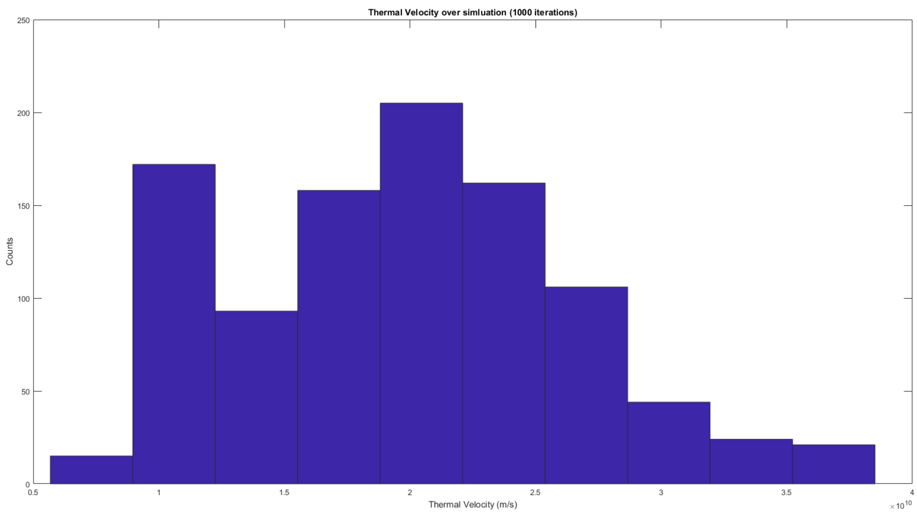

Figure 3: Histogram of thermal velocities

2.2 Part 2

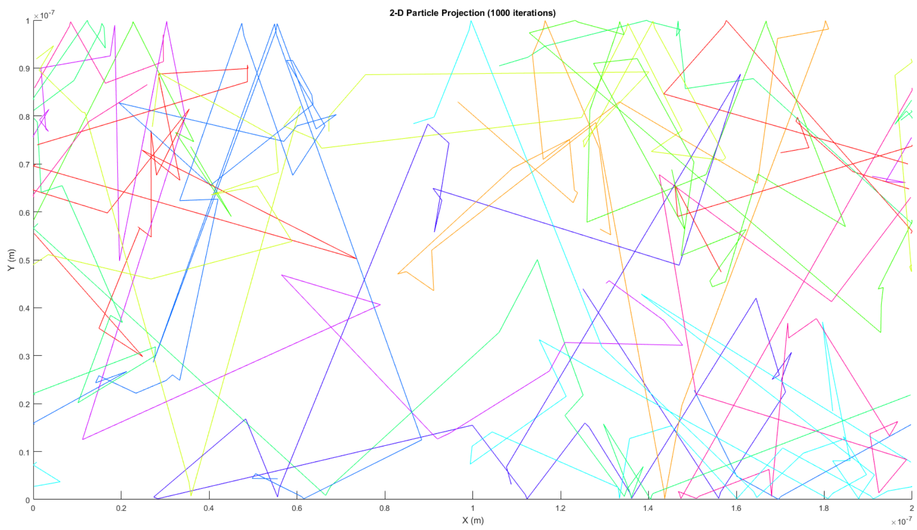

Figure 4: 2-D particle trajectory plot of 10 particles over 5 ps with scattering

2.3 Part 3

One can observe that the temperature of the system fluctuates with each collision that takes place. The following graph demonstrates the changes in temperature over the course of the simulation:

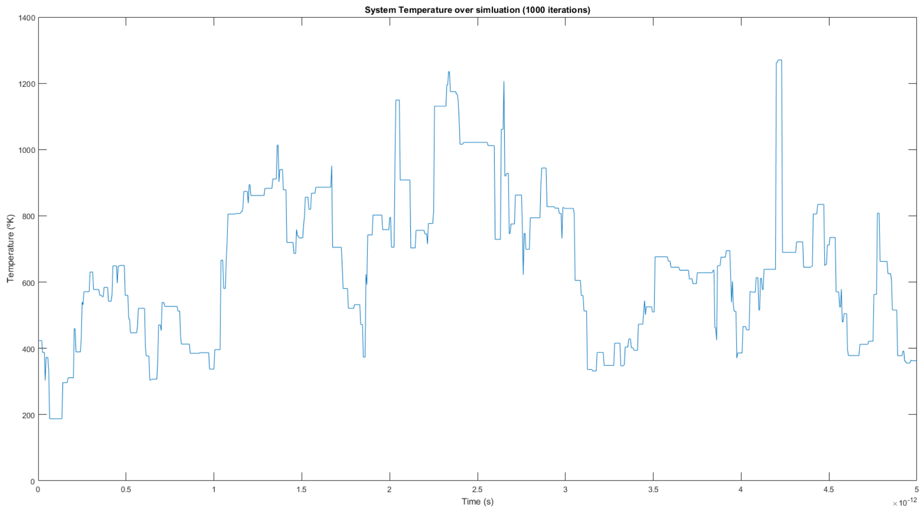

Figure 5: Temperature of the particle trajectory simulation

2.4 Part 4

The average mean free path (mfp) and mean collision time of each particle in the system was calculated within the main loop of the code:

```
%Calculating Temperature
vth(1,c) = sum(Vx.^2+Vy.^2)/nPart;
T(1,c) = (vth(1,c)*C.m_0)/(2*C.kb);

%Calculate mean free path
mfp(1,c) = tmn*vth(1,c);
```

At the end of the simulation, the mfp and mean collision time calculations are performed and displayed in the command window:

```
%Output minor calculations
format long
fprintf('Mean free path was calculated to be %f m\n',sum(mfp)/c)
fprintf('Mean collision time is %e s\n',nx/(sum(vth)/c))

Mean free path was calculated to be 0.003735 m
Mean collision time was calculated to be 1.070853e-17 s
```

The mean free path calculation appears to be large at first glance. Recall that the probability of scattering was calculated with the following equation:

$$P_{scat} = 1 - e^{-\frac{dt}{\tau_{mn}}} \tag{3}$$

Using $dt = 5 \times 10^{-15}s$ and $0.2 \times 10^{-12}s$, the probability was calculated to be $P_{scat} = 0.024690087971667$. If the average thermal velocity is of the order of $10^{10}m/s$, then this mean free path appears to be reasonable given the relatively low probability of scattering.

One can observe that the mean collision time is quite smaller than the $0.2 \times 10^{-12}s$ that was initially used for calculation. This is partly due to the arbitrary time set of $dt = 5 \times 10^{-15}s$ used to make the simulation appear to run smoothly.

3 Question #3

Please refer to Assignment3.m for the code for this section.

3.1 Part 1

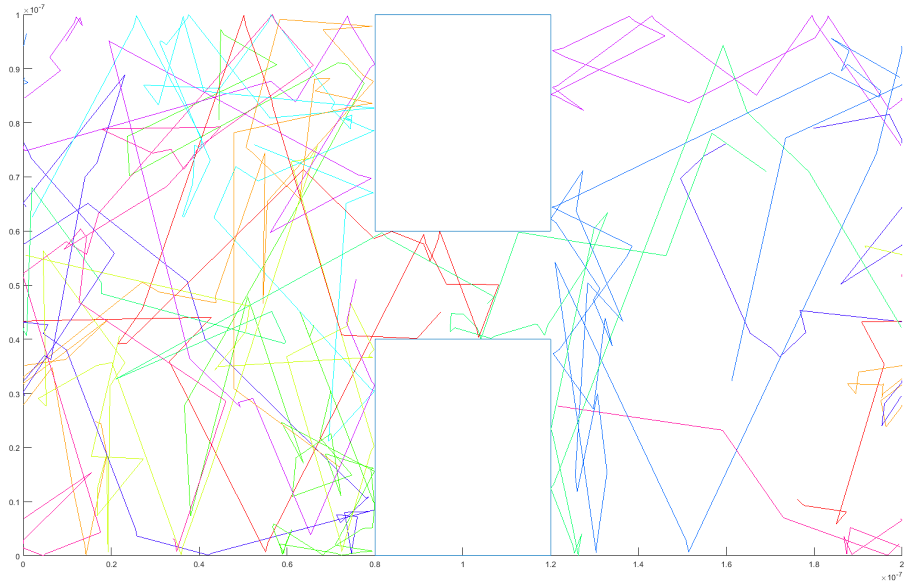

Figure 6: 2-D particle trajectory plot of 10 particles over 5 ps with scattering and barrier

3.2 Part 3

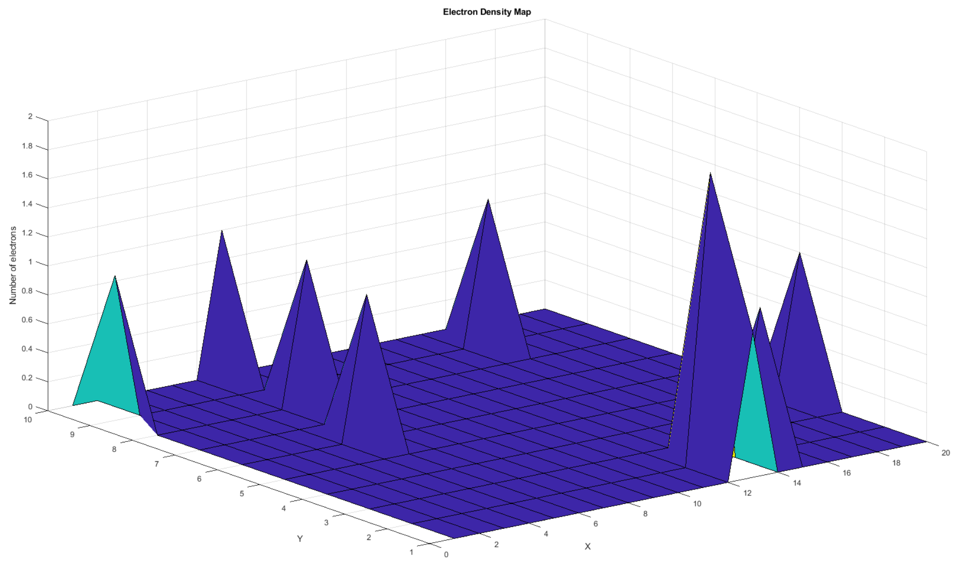

Figure 7: Electron Density Map

3.3 Part 4

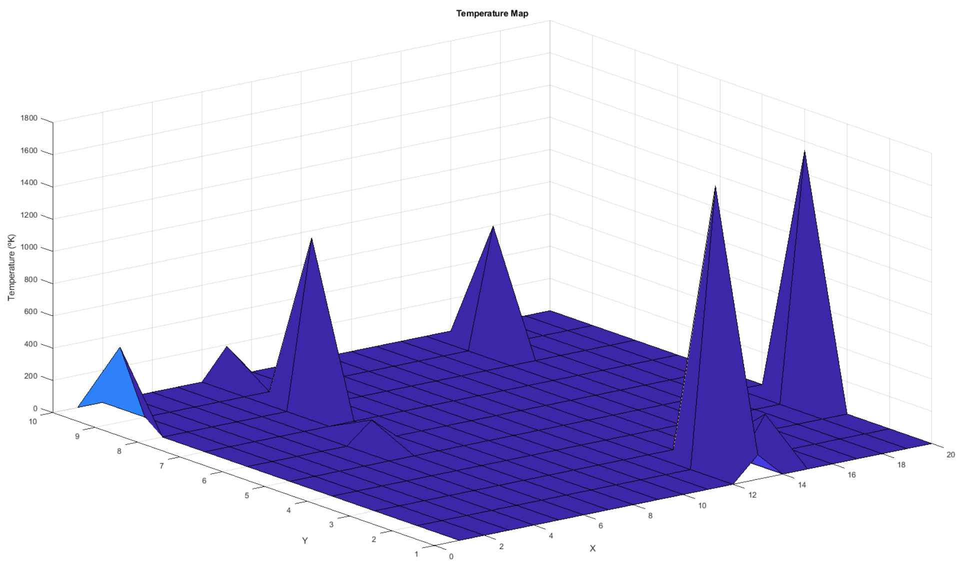

Figure 8: Temperature Map