Table of Contents

ELEC 4700 Assignment 1: Monte-Carlo Modeling of Electron Transport

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```
clear all
clearvars
clearvars -GLOBAL
close all
% set(0,'DefaultFigureWindowStyle','docked')

global C L W

C.q_0 = 1.60217653e-19;             % electron charge
C.hb = 1.054571596e-34;             % Dirac constant
C.h = C.hb * 2 * pi;                % Planck constant
C.m_0 = 9.10938215e-31;             % electron mass
C.kb = 1.3806504e-23;               % Boltzmann constant
C.eps_0 = 8.854187817e-12;          % vacuum permittivity
C.mu_0 = 1.2566370614e-6;           % vacuum permeability
C.c = 299792458;                    % speed of light
C.m_n = 0.26*C.m_0;                 % effective mass of electrons

L = 200e-9;
W = 100e-9;

numElec = 8000;
numDispElec = 15;

Cols = hsv(numDispElec);
```

In this assignment, we will be modelling the movement of electrons through a semiconductor region. Specifically, we are modeling carriers as a population of electrons in an N-type Si semiconductor crystal. To do this we will be using $m_n = 0.26m_0$ as the effective mass of the electron and the size of the region will be 200 nm by 100 nm.

1 Electron Modeling

First, assuming the temperature of the system is 300 K, the thermal velocity of the electrons is: $v_{th} = \sqrt{\frac{kT}{m_n}}$

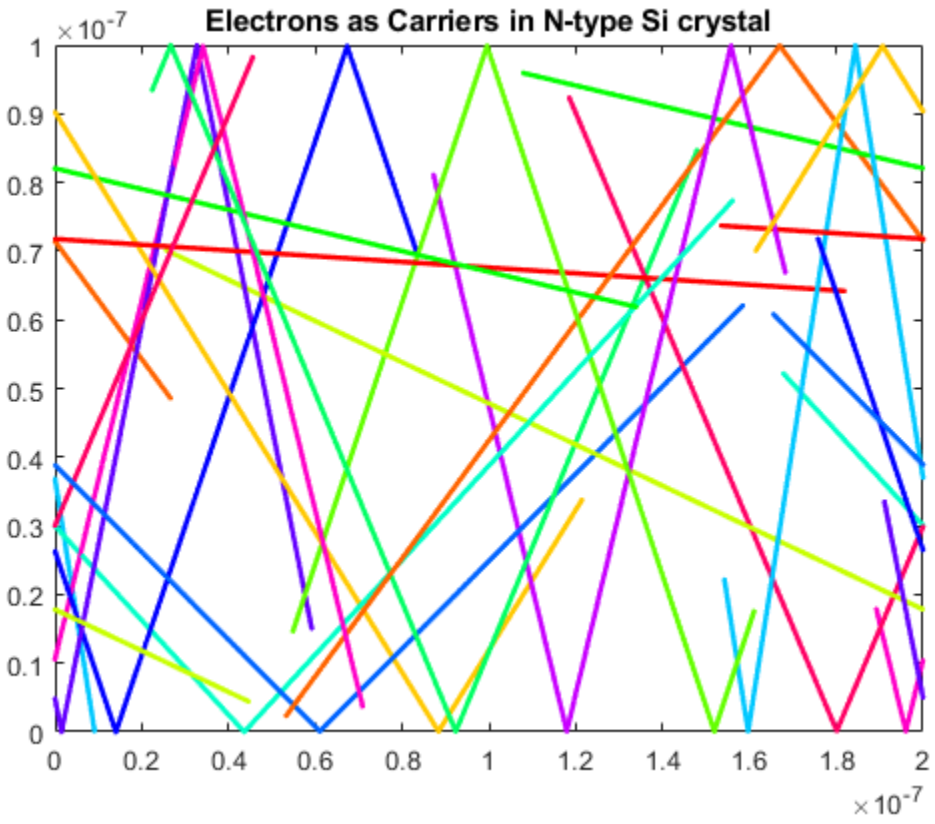
```
T = 300;
v_th = sqrt(3*C.kb * T/C.m_n);
```

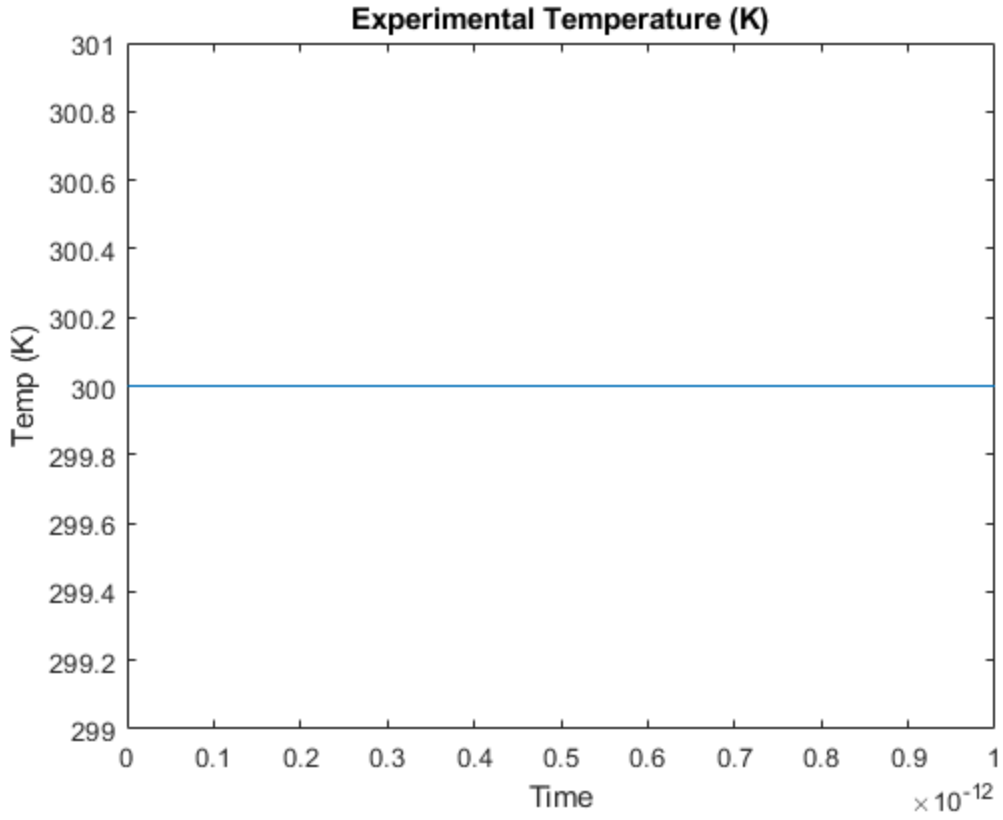
Given that the mean time between collisions is $\tau_{mn} = 0.2ps$, the mean free path can be calculated as: $L_n = \tau_{mn} * v_{th}$

```
t_mn = 0.2e-12;
L_n = t_mn * v_th;
```

With this information, we can create a simulation to visualize the trajectories of electrons through a region.

```
ElecModel;
```





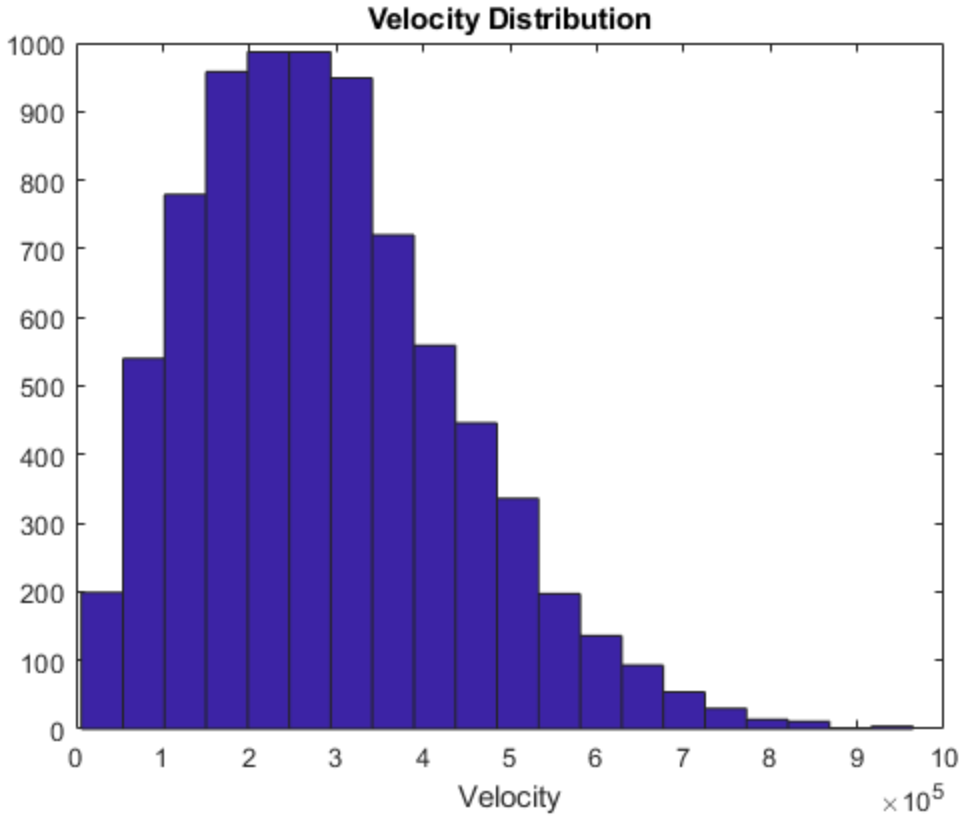
In the simulation plot, we see the trajectories of a sample of electrons. They are given an initial position in the plane along with an initial velocity - the magnitude is the thermal velocity for all electrons, but the direction is randomly assigned. As the simulation runs, the electrons position updates according to Newton's laws. The top and bottom of the plane - i.e. y = 0,W - are rigid and electrons bounce off of them. Meanwhile the x boundaries - i.e. x = 0,L - are periodic, so if an electron drifts off on one side, it'll reappear on the other side.

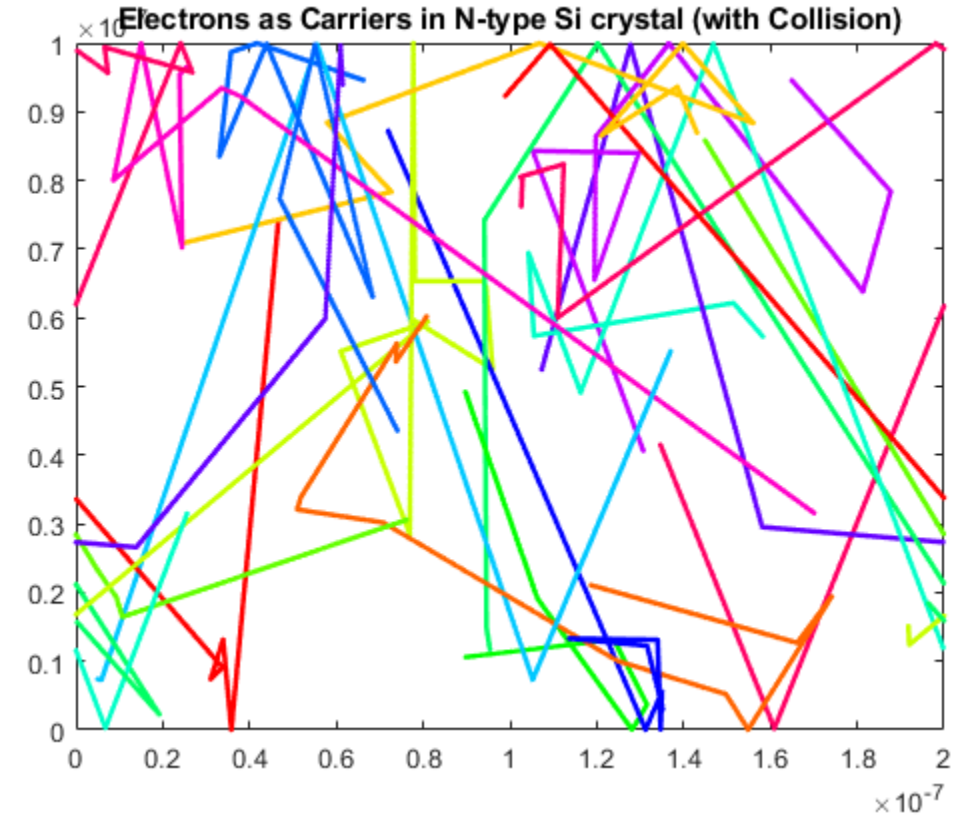
Plotting the average temperature of the system, we see that it's 300K. This makes sense as the magnitude of the velocity of all electrons is the thermal velocity which is based on the temperature of the system (which was set to 300K). The temperature is also constant over time as the magnitude of the velocity never changes.

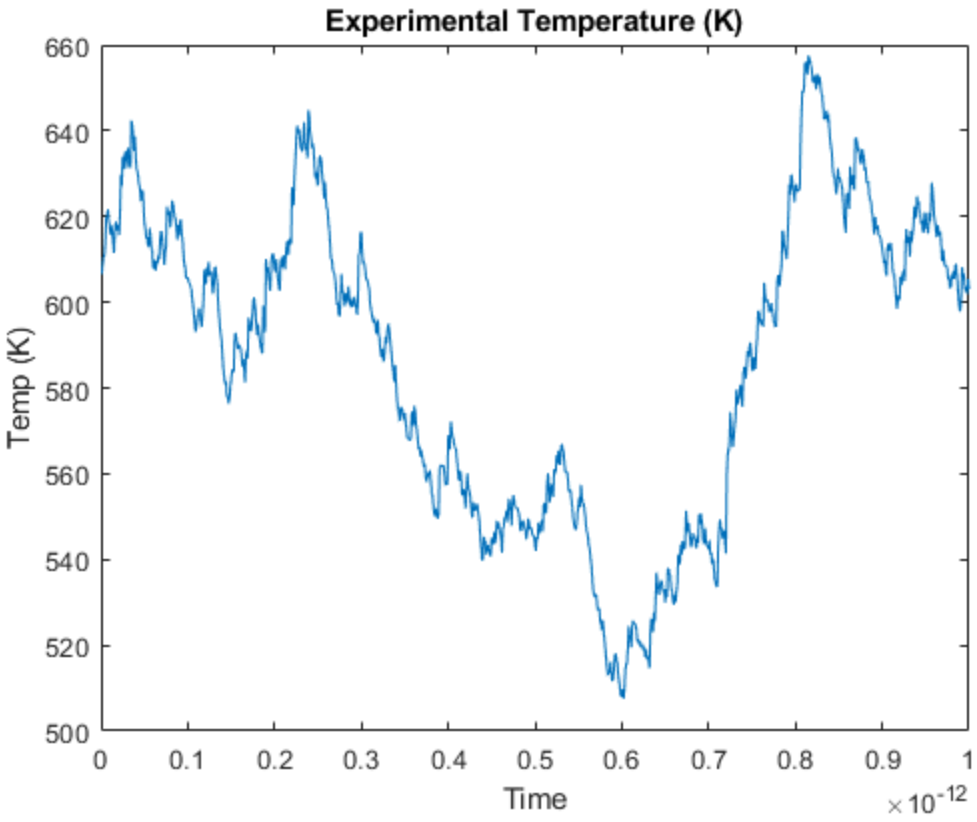
2 Collisions with Mean Free path (MFP)

In this part of the assignment, we will simulate electrons in a region similar to the previous part. However, now we will also add in the probability of electron collisions and velocities will now be chosen from the Maxwell-Boltzmann distribution.

```
CollwMFP;
```


Velocity Distribution
1000
900
800
700
600
500
400
300
200
100
0
0
1
2
3
4
5
6
7
8
9
10
Velocity
×10^5


Electrons as Carriers in N-type Si crystal (with Collision)
×10^-7
1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
0
0.2
0.4
0.6
0.8
1
1.2
1.4
1.6
1.8
2
×10^-7



This part adds on to the previous part as we add in scattering and assign electron velocities according to the Maxwell-Boltzmann Distribution. In Figure 3, a histogram shows the distribution of velocities. The shape of the distribution confirms that the velocity distribution is the Maxwell-Boltzmann Distribution. This was accomplished by obtaining the directional velocities from a Gaussian Distribution with a standard deviation of the thermal velocity.

Since the velocities of each electron are a lot more varried, it's unsurprising to see that the temperature of the system overtime varies quite a bit. It should also be noted that the temperature varies around 600K rather than 300K. Because each velocity direction is based on the thermal velocity (rather than the magnitude) we see that the temperature is essentially double that of the previous part.

From the simulation, we calculate the mean time between collisions to be about 0.13 ps, slightly less than the expected 0.2 ps, and the Mean Free Path is calculated as about 42.8 nm which is also slightly below the expected 45.8 nm.

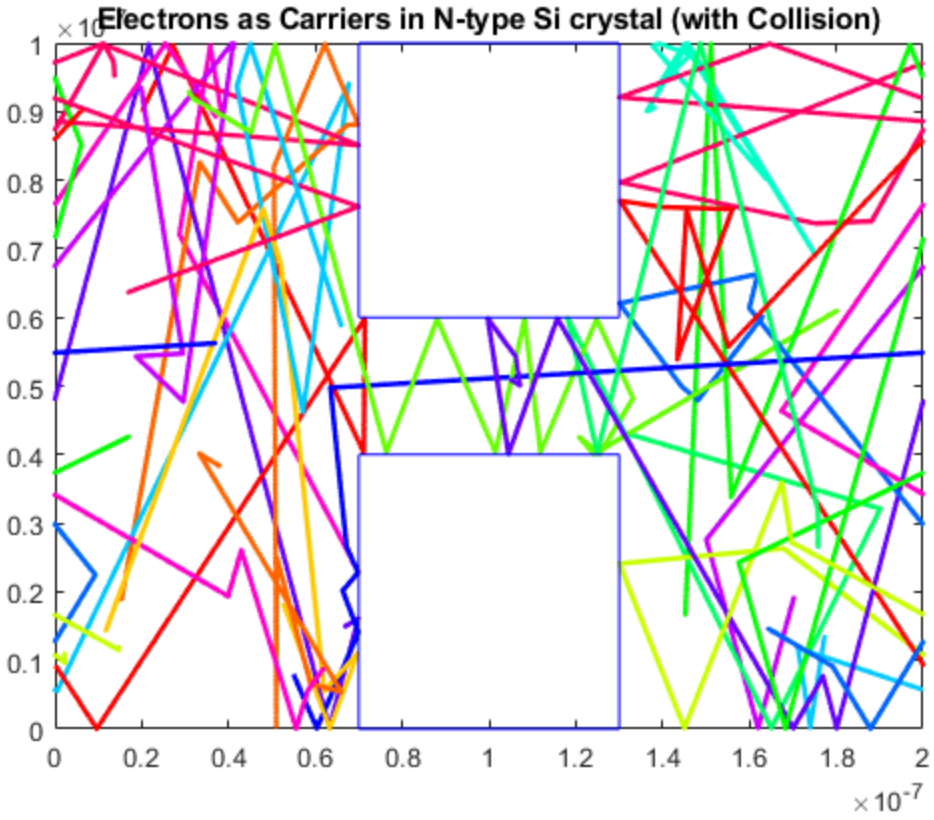
3 Enhancements

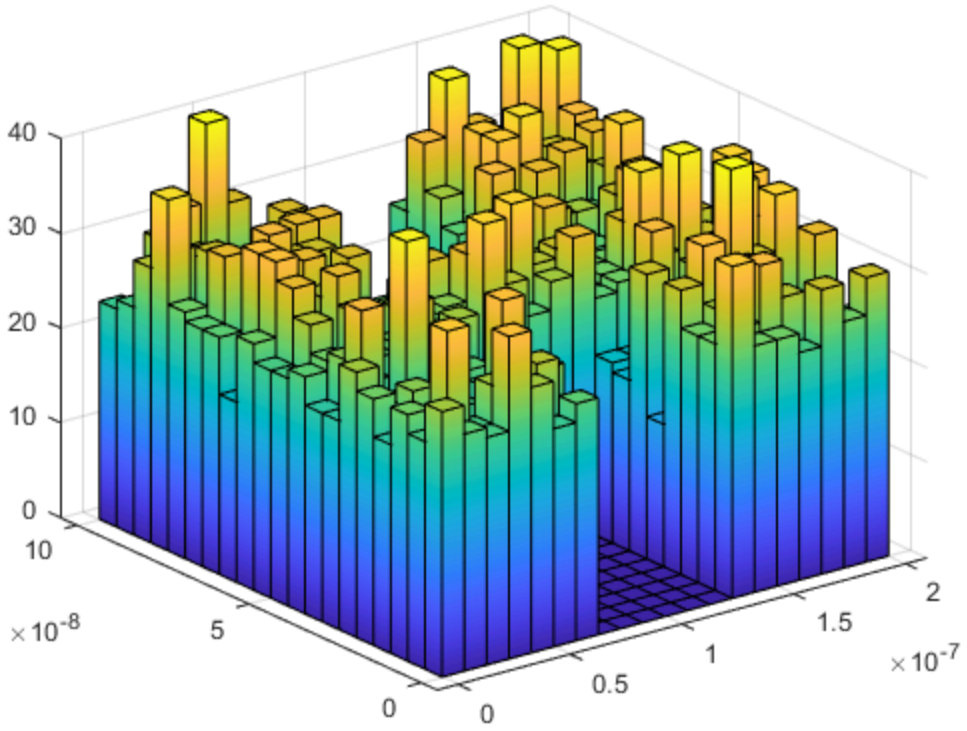
In this last part we will add some boxes into the region to create a bottle-neck. These boxes may be either specular or diffusive - for the purpose of the report, the boxes have been left as diffusive.

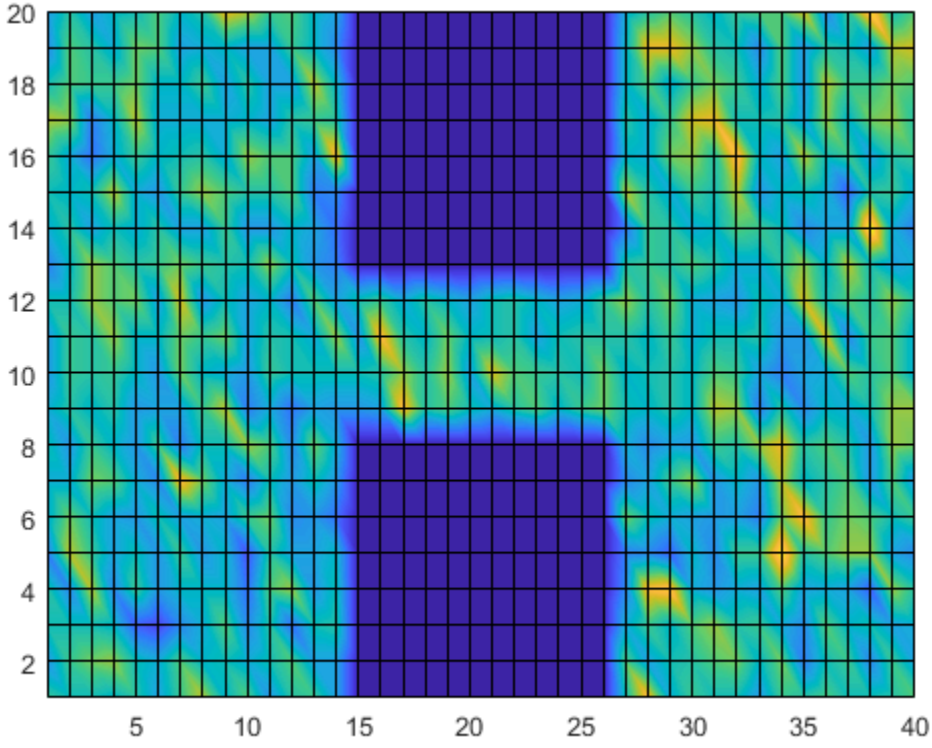
```
Enhancements;
```

```
s =

  Surface with properties:
```

```
      EdgeColor: [0 0 0]
      LineStyle: '-'
      FaceColor: 'flat'
  FaceLighting: 'flat'
      FaceAlpha: 1
          XData: [1×40 double]
          YData: [20×1 double]
          ZData: [20×40 double]
          CData: [20×40 double]

Use GET to show all properties
```




40
30
20
10
0
10
5
0
×10^-8
0
0.5
1
1.5
2
×10^-7


20
18
16
14
12
10
8
6
4
2
5
10
15
20
25
30
35
40

Because of the boxes, the electrons are a bit more restricted in where their initial position can be set to and where they can travel. So, when the simulation first starts, we see a lot of electrons appear to the sides of the boxes, with maybe a few in the bottle-neck area. Then, depending on the scattering, some other electrons may find their way into the bottle-neck.

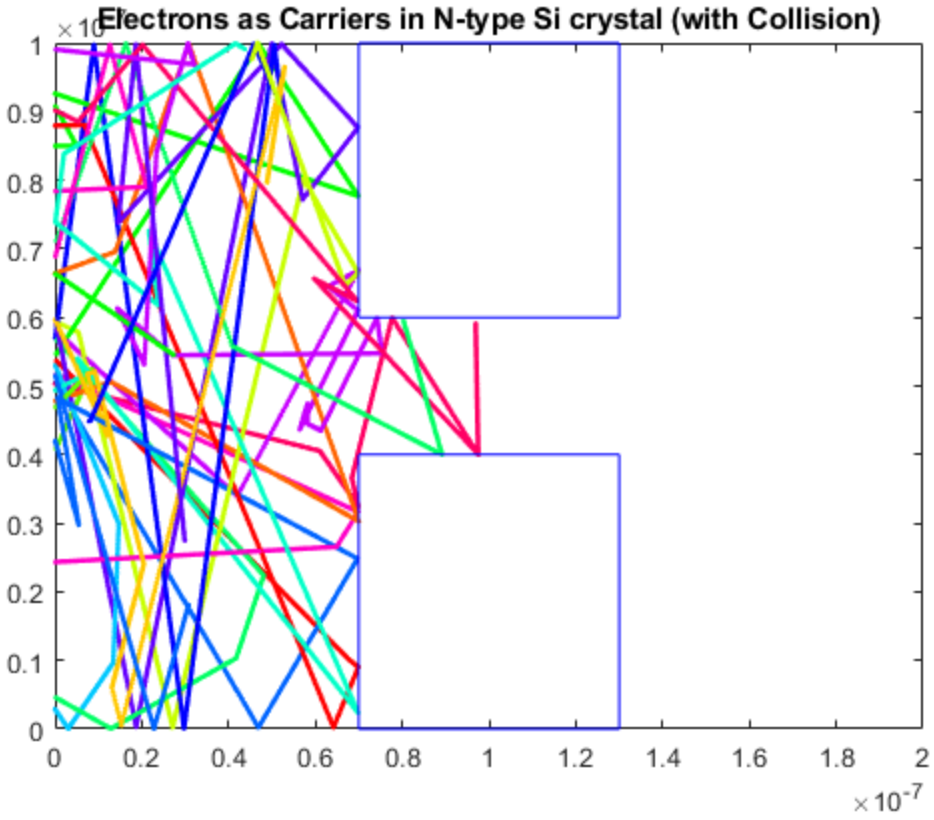
Creating a density map to observe the distribution of the electrons in the region confirms our original observation of many more elctrons being located towards the sides of the boxes.

In the distribution plot, we see that the highest densities are located in the regions to the left and right of the boxes. This makes sense as there is a higher probability of an electron with an initial position in the larger open areas rather than the smaller bottle-neck. Additionally, with the probability of scattering it is possible for an electron to not find itself inside the bottle neck.

These results are also reflected in the temperature map (as electron density effects the temperature of the material). We see higher temperatures on the sides of the material as they have a higher density of electrons.

Making some small adjustments to the previous simulation, we can simulate and injection of negative charge carriers into the system.

```
InjectionMod;
```



Not too much to note here, but we see that with scattering, it can take a while for electrons to start going through the bottle-neck and towards the otherside of the region.

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