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

Contents

1 - Electron Modelling

a) Since we are doing a 2D simulation of the electrons, there are 2 degrees of freedom. Since $1/2mv^2$ of energy is attibuted to each degree of freedom, and since 1/2kT is associated with each degree of freedom, then for our 2D system:

$$\frac{1}{2}mv_{th}^2 = k_BT$$

Solving for v_{th}, using the fact that the effective mass of an electron m_n is 0.26 the rest mass m_o:

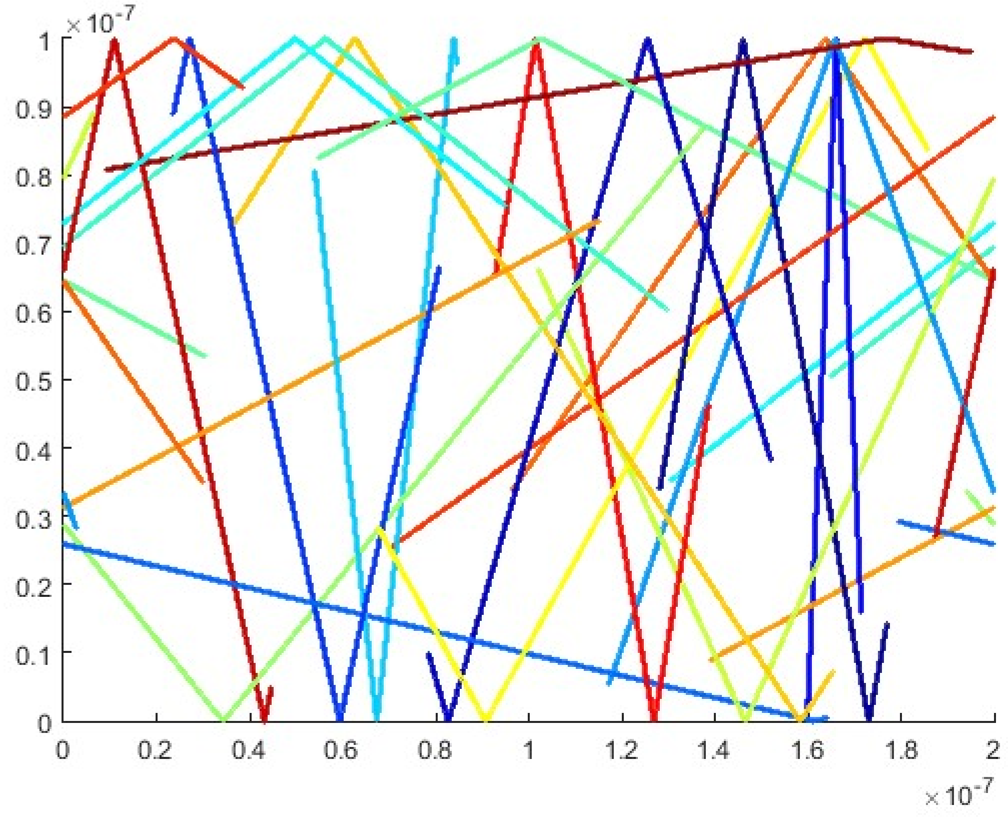
$$v_{th} = 1.870 \times 10^5 m/s$$

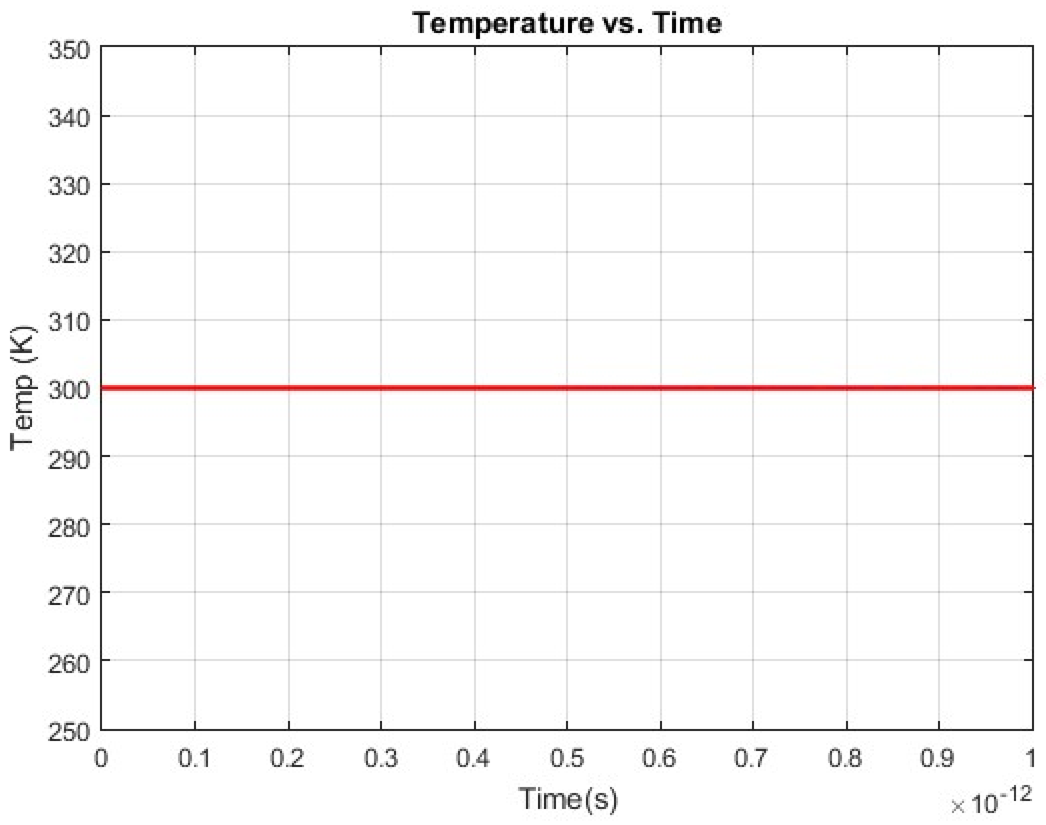
b) $MFP = (v_{th})(\tau_{mn}) = (1.870 \times 10^5 m/s)(0.2ps) = 37.4nm$

Following is the code for part 1:

```
clearvars
clearvars -GLOBAL
close all

C.m_0 = 9.10938215e-31;             % electron mass
C.kb = 1.3806504e-23;               % Boltzmann constant

nElectrons = 10000;
nPlot=20; % number of electrons to actually plot
T = 300;
L = 200e-9;
W = 100e-9;
dt = 1e-15; % since 1/100 of 200nm is 2nm, smallest step allowed is 2nm/vth ~= 1e-14s
TStop = 1e-12; % 1000 timesteps
Vth = sqrt(2*C.kb*T/(C.m_0*0.26)); % using 2 degrees of freedom
time = 0;
Temp = T; % temperature variable that updates in TempCalc
taumn = 0.2e-12; % average time between collisions
cc = jet(nPlot); % colorscale used to plot different electron colors

x = rand(1, nElectrons)*L; % assigning random initial particle positions
y = rand(1, nElectrons)*W;
```

```
Theta = rand(1, nElectrons)*2*pi; % random velocity direction
Vx = cos(Theta)*Vth;
Vy = sin(Theta)*Vth;

figure(1)
hFig1 = figure(1);
set(hFig1, 'Position', [500 0 600 1000])

for i=0:dt:TStop
    time = i;

    subplot(2,1,1); % plotting electron positions
    hold on
    for j=1:nPlot
        plot(x(j), y(j), 'o','markers', 1, 'Color', cc(j,:));
    end
    axis([0 L 0 W]);

    V2tot=Vx.*Vx+Vy.*Vy; % calculated temp based on total velocities
    KE = mean(V2tot)*0.5*(C.m_0*0.26);
    Temp = KE/C.kb;

    subplot(2,1,2); % plotting temp vs. time
    plot(time,Temp, 'ro', 'markers',1,'MarkerFaceColor', 'b');
    hold on
    axis([0 TStop 250 350]);
    xlabel('Time(s)');
    ylabel('Temp (K)');
    grid on
    title('Temperature vs. Time');

    x = x - dt * Vx; % moving the particles in one time step
    y = y - dt * Vy;

    for j=1:nElectrons % specular and periodic boundaries
        if x(j) > L
            x(j) = x(j) - L;
        elseif x(j) < 0
            x(j) = x(j) + L;
        end

         if y(j) > W
             Vy(j) = -Vy(j);
         elseif y(j) < 0
             Vy(j) = -Vy(j);
         end
    end

    pause(0.001)

end
```


×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


Temperature vs. Time
Temp (K)
350
340
330
320
310
300
290
280
270
260
250
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
Time(s)
×10^-12

Part 1 Discussion

As shown in the temperature vs. time plot, the temperature does indeed remain at 300K, since the velocities of the electrons remains constant the entire time. As will be seen in the next sections, rethermalization of the electrons alters the velocities, and thus the temperature will fluctuate accordingly.

2 - Collisions with MFP

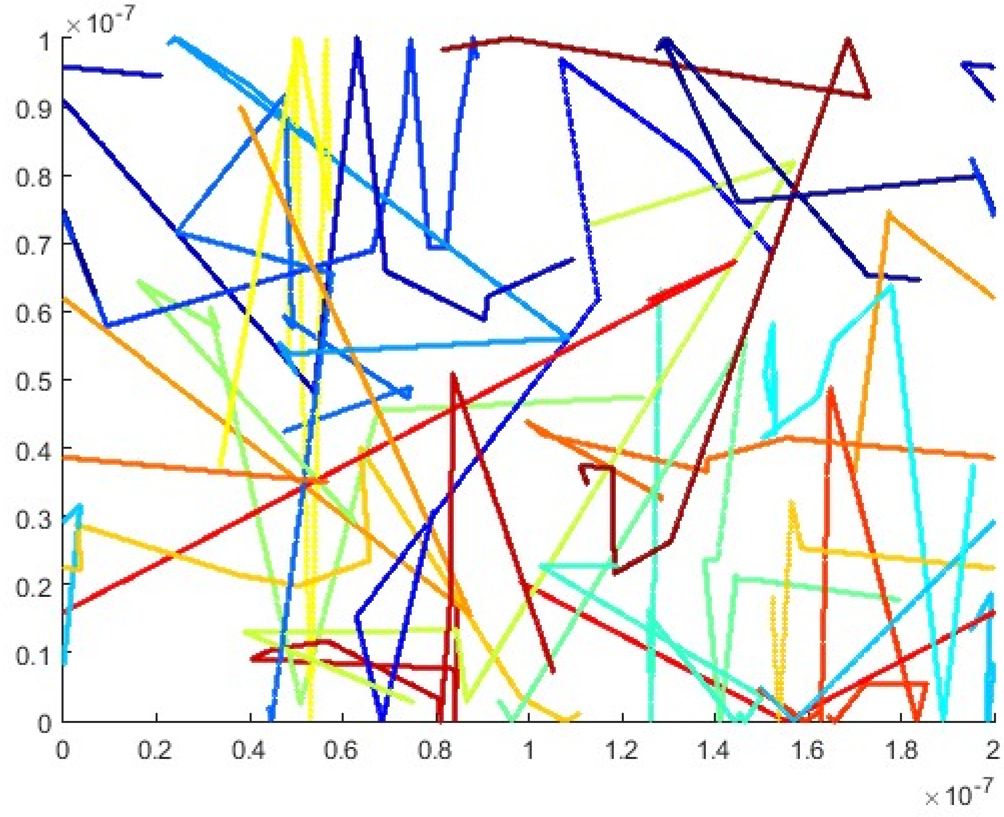
As mentioned in slideshow "3-MonteCarlo" on slide 16, the velocity for each direction (x, y) can be given by a gaussian distribution centered around the thermal velocity v_{th}, with a standard deviation of $(\frac{k_b T}{m})^{0.5}$. This method was used to determine the velocity components for the simulation, but clearly this resulted in an issue as the average temperature for the system becomes ~450K even with the initial thermal velocity being calculated with 300K. The Maxwell-Boltzman distribution would have been used to find the individual velocity components, but it was unclear how to do so in Matlab. Due to this issue, calculated values of average thermal velocity, mean free path, and average time between collisions are all incorrect. However, the methods used to calculate these parameters still appear valid.

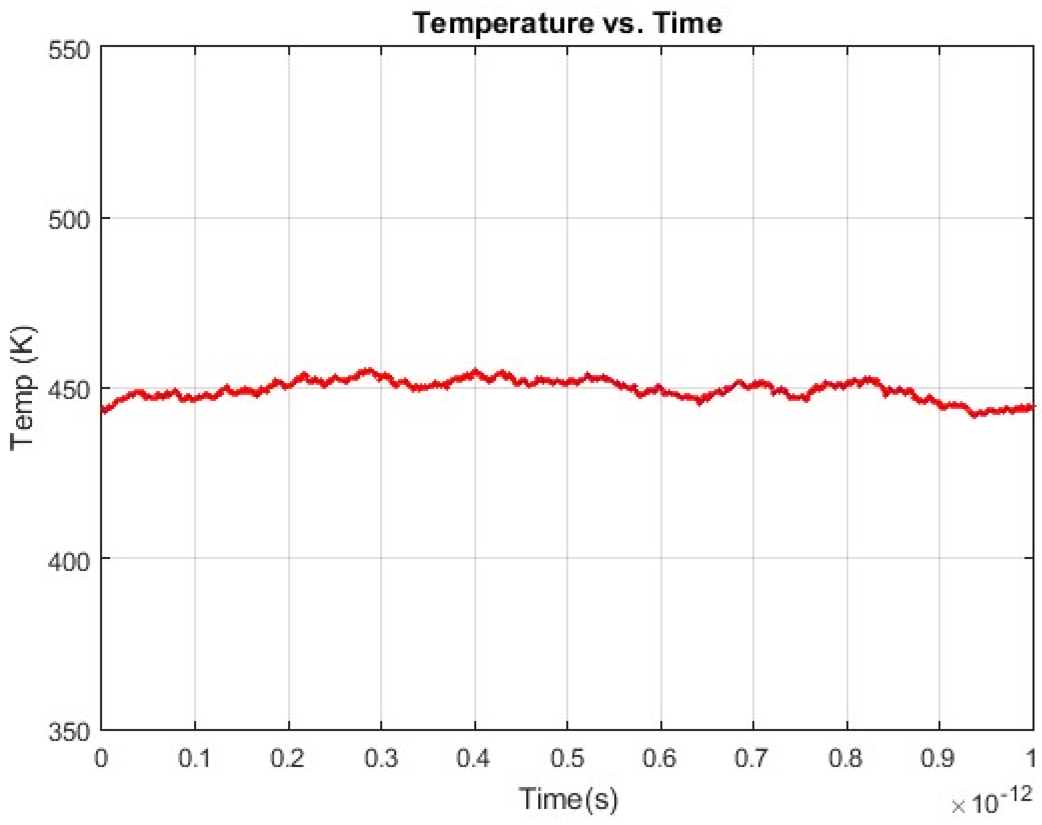
Following is the code for part 2:

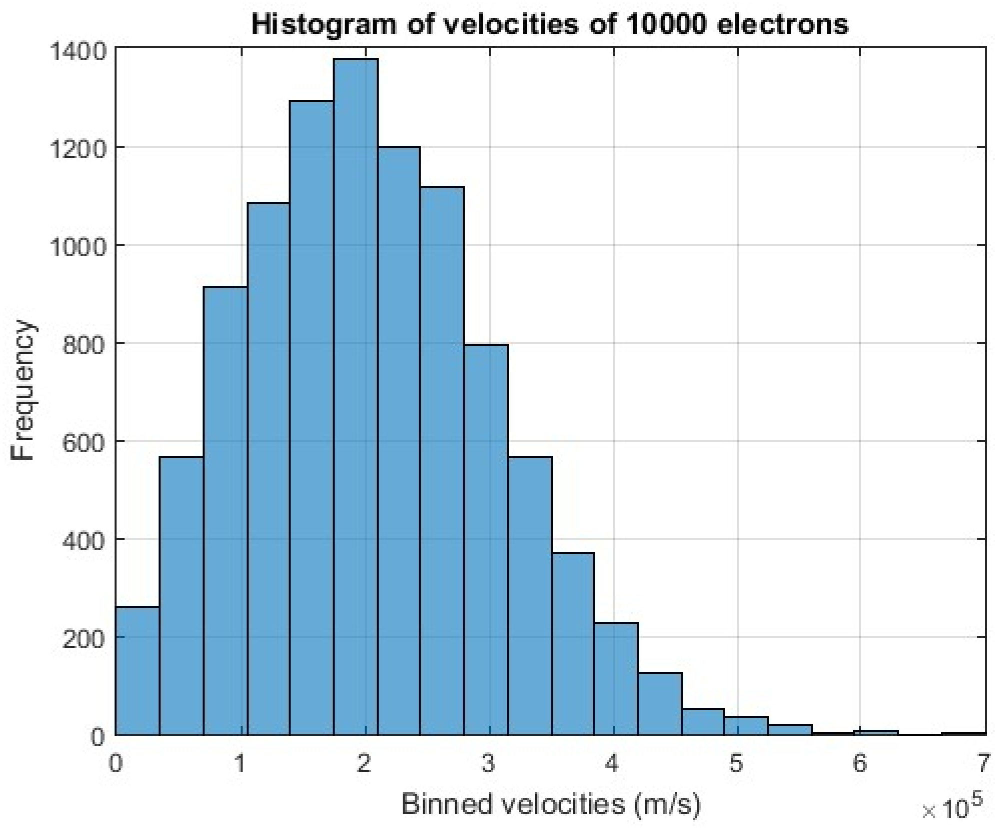
```
C.m_0 = 9.10938215e-31;              % electron mass
C.kb = 1.3806504e-23;                % Boltzmann constant

nElectrons = 10000;
nPlot=20; % number of electrons to actually plot
T = 300;
L = 200e-9;
W = 100e-9;
dt = 1e-15; % since 1/100 of 200nm is 2nm, smallest step allowed is 2nm/vth ~= 1e-14s
TStop = 1e-12; % 1000 timesteps
Vth = sqrt(2*C.kb*T/(C.m_0*0.26)); % using 2 degrees of freedom
time = 0;
Temp = T; % temperature variable that updates in TempCalc
taumn = 0.2e-12; % average time between collisions
sigmaMB = sqrt(C.kb*T/(C.m_0*0.26)); % standard deviation on vth
cc = jet(nPlot); % colorscale used to plot different electron colors

collisionT = zeros(200,nElectrons); % matrices for tracking collision time and velocities
collisionV = zeros(200,nElectrons);
collisionIndex = ones(1,nElectrons);
collisions = 0;

x = rand(1, nElectrons)*L; % assigning random initial particle positions
y = rand(1, nElectrons)*W;

Theta = rand(1, nElectrons)*2*pi; % selecting Vx and Vy from Gaussian centered at vth
Vx = cos(Theta).*(Vth + sigmaMB*randn(1, nElectrons));
Vy = sin(Theta).*(Vth + sigmaMB*randn(1, nElectrons));

avgV = sum(sqrt(Vx.^2+Vy.^2))/nElectrons % calculation of initial average velocity

figure(2)
hFig2 = figure(2);
set(hFig2, 'Position', [500 0 600 1000])

for i=0:dt:TStop
    time = i;
    subplot(2,1,1); % plotting electron positions
    hold on
    for j=1:nPlot
        plot(x(j), y(j), 'o','markers', 1, 'Color', cc(j,:));
    end
    axis([0 L 0 W]);

    V2tot=Vx.*Vx+Vy.*Vy; % calculated temp based on total velocities
    KE = mean(V2tot)*0.5*(C.m_0*0.26);
    Temp = KE/C.kb;

    subplot(2,1,2); % plotting temp vs. time
    plot(time,Temp, 'ro', 'markers',1,'MarkerFaceColor', 'b');
    hold on
    axis([0 TStop 350 550]);
    xlabel('Time(s)');
    ylabel('Temp (K)');
    grid on
    title('Temperature vs. Time');

    x = x - dt * Vx; % moving the particles in one time step
    y = y - dt * Vy;

    for j=1:nElectrons % specular and periodic boundaries
        if x(j) > L
            x(j) = x(j) - L;
        elseif x(j) < 0
            x(j) = x(j) + L;
        end

         if y(j) > W
             Vy(j) = -Vy(j);
         elseif y(j) < 0
             Vy(j) = -Vy(j);
         end
    end

    for j=1:nElectrons % collision, mfp, and mean time between collisions tracking
        if (1-exp(-dt/taumn)) > rand()
            collisions = collisions+1;
            collisionT(collisionIndex(j)+1,j) = time;
            collisionV(collisionIndex(j)+1,j) = sqrt(Vx(j)^2+Vy(j)^2);
            collisionIndex(j)=collisionIndex(j)+1;

            Theta = rand(1, 1)*2*pi; % rethermalizing after collision
            Vx(j) = cos(Theta)*(Vth + sigmaMB*randn(1, 1));
            Vy(j) = sin(Theta)*(Vth + sigmaMB*randn(1, 1));
        end
    end

    pause(0.000001)

end

figure(3) % histogram of final velocity distribution
```

```
histogram(sqrt(Vx.^2+Vy.^2), 20);
hold on
xlabel('Binned velocities (m/s)');
ylabel('Frequency');
grid on
title('Histogram of velocities of 10000 electrons');
hold off

MFP=0;
TBC=0;

for i=1:nElectrons % calculation of time between collisions (TBC) and mean free path (MFP)
    for j=1:collisionIndex(i)
        if j ~= 1
            TBC = TBC + collisionT(j,i)-collisionT(j-1,i);
            MFP = MFP + (collisionT(j,i)-collisionT(j-1,i))*(collisionV(j,i)-collisionV(j-1,i));
        end
    end
end

TBC = TBC/collisions
MFP = MFP/collisions
```

```
avgV =

   2.0423e+05


TBC =

   1.6015e-13


MFP =

   7.8686e-09
```


×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


Temperature vs. Time
550
500
450
400
350
Temp (K)
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
Time(s)
×10^-12



Part 2 Discussion

As shown in the histogram of velocities, even though the individual components were selected from Gaussian distributions, it appears that the overal velocity distribution is similar to the Maxwell-Boltzman distribution. As seen from the particle trajectories they are clearly exhibiting scattering in random directions at random intervals. The temperature vs. time plot shows that although the temperature exhibits minor fluctuations over time, it remains centered around ~450K. If the correct distributions were used, it would be assumed that this central temperature would be 300K instead. Comparing the TBC and MPF found in part 1 and the ones calculated in this code, there is clearly a discrepancy. As mentioned before, this is likely due to the average thermal velocity being larger than it should be, due the way velocities were selected from Gaussian distributions.

3 - Enhancements

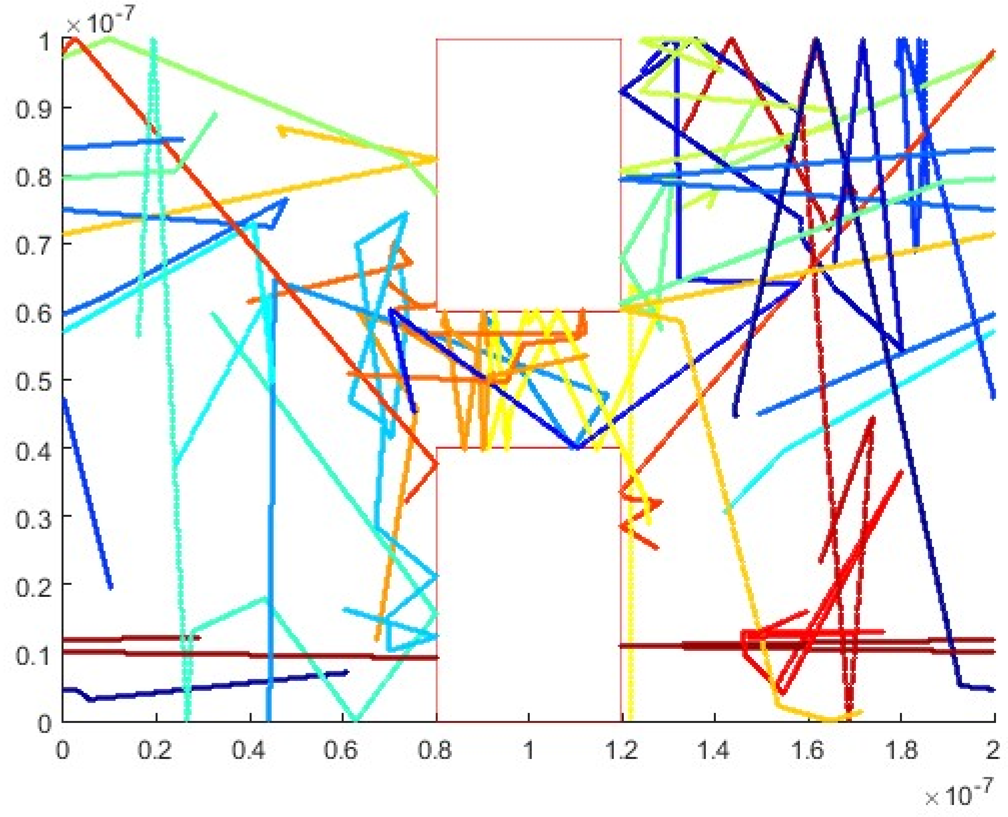
Following is the code for part 3:

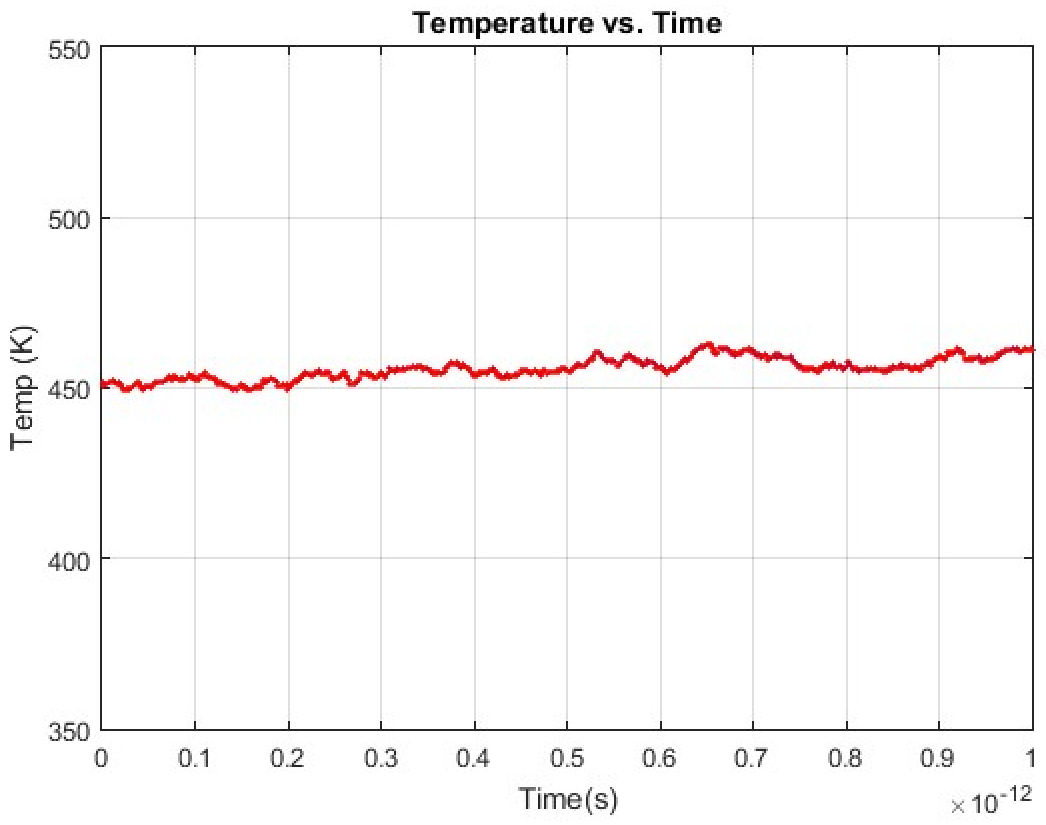
```
C.m_0 = 9.10938215e-31;             % electron mass
C.kb = 1.3806504e-23;               % Boltzmann constant

nElectrons = 10000;
nPlot=20; % number of electrons to actually plot
T = 300;
L = 200e-9;
W = 100e-9;
dt = 1e-15; % since 1/100 of 200nm is 2nm, smallest step allowed is 2nm/vth ~= 1e-14s
TStop = 1e-12; % 1000 timesteps
Vth = sqrt(2*C.kb*T/(C.m_0*0.26)); % using 2 degrees of freedom
time = 0;
Temp = T; % temperature variable that updates in TempCalc
taumn = 0.2e-12; % average time between collisions
sigmaMB = sqrt(C.kb*T/(C.m_0*0.26)); % standard deviation on vth
```

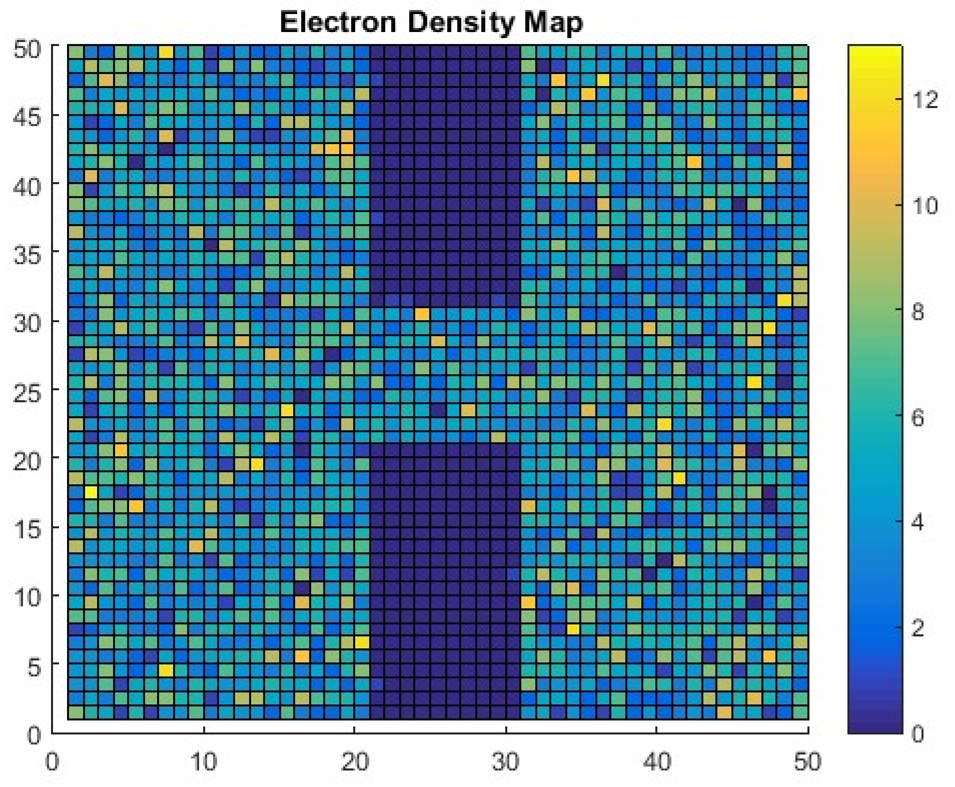
```
cc = jet(nPlot); % colorscale used to plot different electron colors

collisionT = zeros(200,nElectrons); % matrices for tracking collision time and velocities
collisionV = zeros(200,nElectrons);
collisionIndex = ones(1,nElectrons);
collisions = 0;

x = rand(1, nElectrons)*L; % assigning random initial particle positions
y = rand(1, nElectrons)*W;

for i=1:nElectrons % ensuring particles do not start in boxed boundaries
   while(1)
      if ( x(i)<1.2e-7 && x(i)>0.8e-7 && (y(i)<0.4e-7 || y(i)>0.6e-7))
          x(i) = rand*L;
          y(i) = rand*W;
      else
        break
      end
   end
end

Theta = rand(1, nElectrons)*2*pi; % selecting Vx and Vy from Gaussian centered at vth
Vx = cos(Theta).*(Vth + sigmaMB*randn(1, nElectrons));
Vy = sin(Theta).*(Vth + sigmaMB*randn(1, nElectrons));

avgV = sum(sqrt(Vx.^2+Vy.^2))/nElectrons

figure(4)
hFig4 = figure(4);
set(hFig4, 'Position', [500 0 600 1000])

subplot(2,1,1); % plotting lines of box boundaries
hold on
plot([0.8,0.8]*1e-7,[0,0.4]*1e-7, 'r-')
plot([0.8,0.8]*1e-7,[0.6,1]*1e-7, 'r-')
plot([1.2,1.2]*1e-7,[0,0.4]*1e-7, 'r-')
plot([1.2,1.2]*1e-7,[0.6,1]*1e-7, 'r-')
plot([0.8,1.2]*1e-7,[0,0]*1e-7, 'r-')
plot([0.8,1.2]*1e-7,[0.4,0.4]*1e-7, 'r-')
plot([0.8,1.2]*1e-7,[0.6,0.6]*1e-7, 'r-')
plot([0.8,1.2]*1e-7,[1,1]*1e-7, 'r-')

for i=0:dt:TStop
    time = i;

    subplot(2,1,1); % plotting electron positions
    hold on
    for j=1:nPlot
        plot(x(j), y(j), 'o','markers', 1, 'Color', cc(j,:));
    end
    axis([0 L 0 W]);

    V2tot=Vx.*Vx+Vy.*Vy; % calculated temp based on total velocities
    KE = mean(V2tot)*0.5*(C.m_0*0.26);
    Temp = KE/C.kb;
    subplot(2,1,2); % plotting temp vs. time
    plot(time,Temp, 'ro', 'markers',1,'MarkerFaceColor', 'b');
    hold on
    axis([0 TStop 350 550]);
    xlabel('Time(s)');
    ylabel('Temp (K)');
    grid on
    title('Temperature vs. Time');

    x = x - dt * Vx; % moving the particles in one time step
    y = y - dt * Vy;

    for j=1:nElectrons % specular and periodic boundaries
        if x(j) > L
            x(j) = x(j) - L;
        elseif x(j) < 0
            x(j) = x(j) + L;
        end

         if y(j) > W
             Vy(j) = -Vy(j);
         elseif y(j) < 0
             Vy(j) = -Vy(j);
         end
    end

    for j=1:nElectrons % collision, mfp, and mean time between collisions tracking
        if (1-exp(-dt/taumn)) > rand()
            collisions = collisions+1;
            collisionT(collisionIndex(j)+1,j) = time;
            collisionV(collisionIndex(j)+1,j) = sqrt(Vx(j)^2+Vy(j)^2);
            collisionIndex(j)=collisionIndex(j)+1;

            Theta = rand(1, 1)*2*pi; % rethermalizing after collision
            Vx(j) = cos(Theta)*(Vth + sigmaMB*randn(1, 1));
            Vy(j) = sin(Theta)*(Vth + sigmaMB*randn(1, 1));
        end
    end

    % the following code is uncommented if diffusive boundaries are desired
    %%%%%%%%% BlockBordersDiffusive Begin %%%%%%%%%%%

%     for i=1:nElectrons % rethermalized when hit boundary, theta defines scattering angle so it
%         if Vy(i)<0 && y(i)>0.6e-7 && y(i)<0.61e-7 && x(i)<1.2e-7 && x(i)>0.8e-7
%             Theta = rand*pi;
%             Vx(i) = cos(Theta)*(Vth + sigmaMB*randn(1, 1));
%             Vy(i) = sin(Theta)*(Vth + sigmaMB*randn(1, 1));
%         elseif Vy(i)>0 && y(i)<0.4e-7 && y(i)>0.39e-7 && x(i)<1.2e-7 && x(i)>0.8e-7
%             Theta = rand*pi+pi;
%             Vx(i) = cos(Theta)*(Vth + sigmaMB*randn(1, 1));
%             Vy(i) = sin(Theta)*(Vth + sigmaMB*randn(1, 1));
%         elseif Vx(i)<0 && x(i)>0.8e-7 && x(i)<0.81e-7 && (y(i)<0.4e-7 || y(i)>0.6e-7)
%             Theta = rand*pi-pi/2;
%             Vx(i) = cos(Theta)*(Vth + sigmaMB*randn(1, 1));
%             Vy(i) = sin(Theta)*(Vth + sigmaMB*randn(1, 1));
%         elseif Vx(i)>0 && x(i)<1.2e-7 && x(i)>1.19e-7 && (y(i)<0.4e-7 || y(i)>0.6e-7)
%              Theta = rand*pi+pi/2;
%              Vx(i) = cos(Theta)*(Vth + sigmaMB*randn(1, 1));
%              Vy(i) = sin(Theta)*(Vth + sigmaMB*randn(1, 1));
%          end
%      end

    %%%%%%%%% BlockBordersDiffusive End %%%%%%%%%%%


    % the following code is uncommented if specular boundaries are desired
    %%%%%%%%% BlockBorders Begin %%%%%%%%%%%

    for i=1:nElectrons % conditions for meeting a boundary, specular reflection by inverting x c
        if Vy(i)<0 && y(i)>0.6e-7 && y(i)<0.61e-7 && x(i)<1.2e-7 && x(i)>0.8e-7
            Vy(i)=-Vy(i);
        elseif Vy(i)>0 && y(i)<0.4e-7 && y(i)>0.39e-7 && x(i)<1.2e-7 && x(i)>0.8e-7
            Vy(i)=-Vy(i);
        elseif Vx(i)<0 && x(i)>0.8e-7 && x(i)<0.81e-7 && (y(i)<0.4e-7 || y(i)>0.6e-7)
            Vx(i)=-Vx(i);
        elseif Vx(i)>0 && x(i)<1.2e-7 && x(i)>1.19e-7 && (y(i)<0.4e-7 || y(i)>0.6e-7)
            Vx(i)=-Vx(i);
        end
    end

    %%%%%%%%% BlockBorders End %%%%%%%%%%%

    pause(0.001)

end

MFP=0;
TBC=0;

for i=1:nElectrons % calculation of time between collisions (TBC) and mean free path (MFP)
    for j=1:collisionIndex(i)
        if j ~= 1
            TBC = TBC + collisionT(j,i)-collisionT(j-1,i);
            MFP = MFP + (collisionT(j,i)-collisionT(j-1,i))*(collisionV(j,i)-collisionV(j-1,i));
        end
    end
end

TBC = TBC/collisions
MFP = MFP/collisions

figure(5) % plotting electron density map in a 50x50 grid
hold on
n=hist3([x',y'],[50 50]);
pcolor(n');
colorbar;
title('Electron Density Map');
hold off

V5050 = zeros(50);

for h=1:nElectrons % calculating velocities for temperature calculation
```

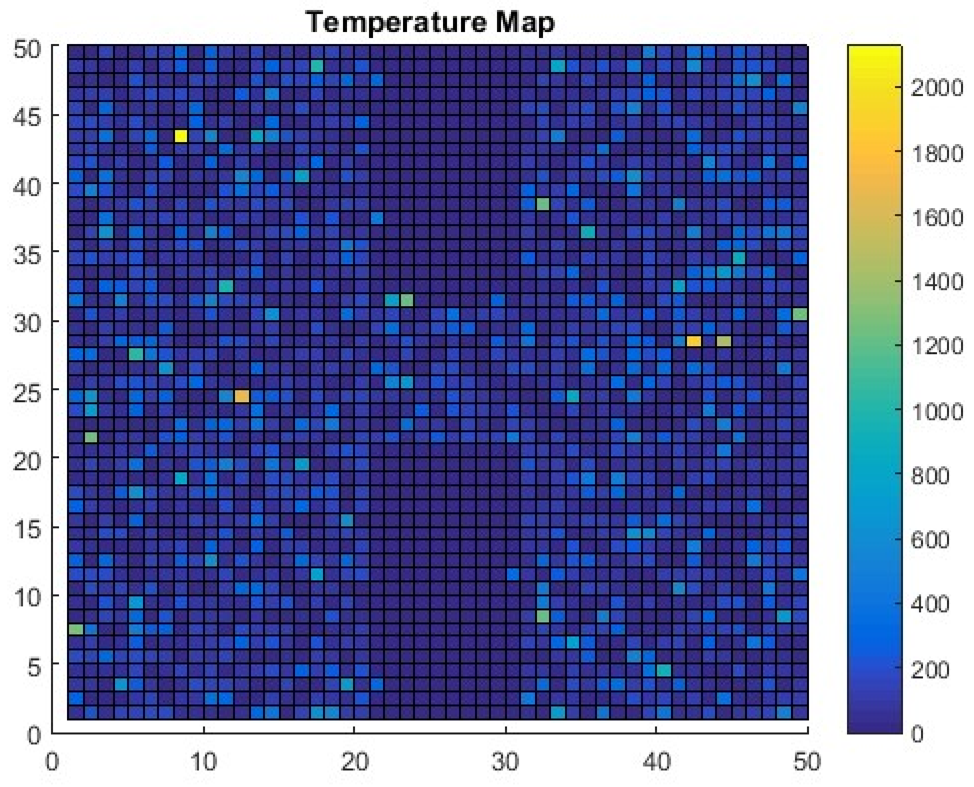
```
    for i=1:50
        for j=1:50
            if x(h)>((i-1)/50*L) && x(h)<(i/50*L) && y(h)>((j-1)/50*W) && y(h)<(j/50*W)
                V5050(i,j)=Vx(h)^2+Vy(h)^2;
            end
        end
    end
end

for i=1:50 % taking average velocity per cell
    for j=1:50
       if n(i,j)~=0
          V5050(i,j) = V5050(i,j)/n(i,j);
       else
          V5050(i,j) = 0;
       end
    end
end

figure(6) % plotting temperature density
hold on
m=V5050.*0.5*0.26*C.m_0/C.kb;
pcolor(m');
colorbar;
title('Temperature Map');
hold off
```

```
avgV =

   2.0582e+05


TBC =

   1.6062e-13


MFP =

   8.0319e-09
```


×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


Temperature vs. Time
550
500
450
400
350
Temp (K)
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
Time(s)
×10⁻¹²





Part 3 Discussion

As shown in the trajectories plot, all of the electrons begin outside of the boundaries and also scatter off of the boundaries when encountered. The specular scattering is observed in this plot, but to enable diffuse scattering the labelled code in the section above would need to be uncommented, and the specular code would need to be commented. The maps of electron density and temperature appear to show some electrons in the boundaries, but that is only due to the histogram having bins that include the borders of the boundaries.

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