Assignment 1

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Matthew Lazarus 100962142

Question 3: Enhancements

In this question, a number of electrons are randomly positioned within a set grid. With the system set to 300K, each electron is assigned velocity components based off of the Gaussian distribution. When an electron hits the top of the grid, it bounces back, and when it hits the side of the grid, it continues its trajectory from the opposite side of the grid. There is also a probability of scattering at each time step for each electron. Furthermore, two rectangular barriers were introduced into the system.

```
% Clear all previous variables, figures, etc, to ensure that the
 workspace
% is clean.
clear all
clearvars
clearvars -GLOBAL
close all

%Define constants that may need to be used later in the code.
global C
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.g = 9.80665; %metres (32.1740 ft) per sÂ²

%Thermal Velocity at 300K:
vth = sqrt(C.kb*300/(0.26*C.m_0));

%Find Mean Free Path
tmn = 0.2*10^-12;
freePath = tmn * vth;

% Set the number of electrons, time step and total time. Initialize
% matrices for the x and y positions, the x and y components of the
% velocity, and the temperature of the system. Column 1 of each
 matrice is
```

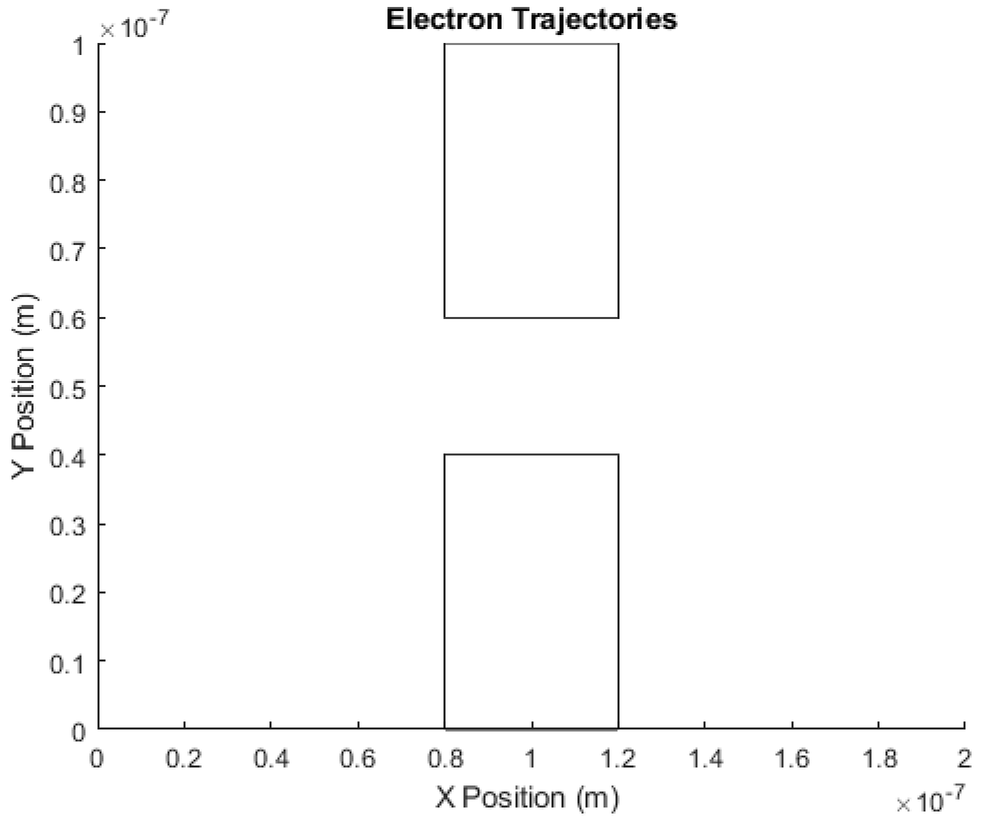
```
% the previous value, while column 2 is the current value.
numElectrons=20000;
dt = 4e-15; %seconds
nTime = 4e-12; %Simulation length
x = zeros(numElectrons,2); %Position (x)
y = zeros(numElectrons, 2); %Position (y)
vx = zeros(numElectrons, 2); %Velocity (x)
vy = zeros(numElectrons, 2); %Velocity (y)
vTotal = zeros(numElectrons, 2); %Velocity
temperature = zeros(numElectrons,2);

% Define two vectors to keep track of the time and distance since the
 last
% scatter, for each electron. Additionally initalize a counter for
 them.
distanceSinceLastScatter = zeros(numElectrons,1);
timeSinceLastScatter = zeros(numElectrons,1);
scatterCount = 0;
```

Now, randomly assign initial positions & velocities. Choose each velocity component based off of the Gaussian distribution. Divide by the square root of 2 as there are 2 degrees of freedom. This is derived from equating the acceleration of the electron to its kinetic energy, as seen by the equation below. Addditionally, ensure no electron is placed within one of the rectangular barriers.

$$(1/2)mv^2 = (2/2)kT$$

```
for electronCount = 1:numElectrons
    x(electronCount,2)=rand()*200e-9;
    if(x(electronCount,2)<1.2e-7 && x(electronCount,2)>0.8e-7)
        y(electronCount,2)=rand()*20e-9+0.4e-7;
    else
        y(electronCount,2)=rand()*100e-9;
    end

    vx(electronCount,2) = vth * randn()/sqrt(2);
    vy(electronCount,2) = vth * randn()/sqrt(2);
    vTotal(electronCount,2)=
 sqrt(vx(electronCount,1)^2+vy(electronCount,1)^2);
end

% Create a figure for the electron trajectories.
figure(1)
title('Electron Trajectories')
xlabel('X Position (m) ')
ylabel('Y Position (m)')
rectangle('Position', [0.8e-7 0 0.4e-7 0.4e-7])
rectangle('Position', [0.8e-7 0.6e-7 0.4e-7 0.4e-7])
axis([0 200e-9 0 100e-9]);


% Define a vector that will indicate whether an electron crosses a
 horizontal
% boundary. As only 5 electrons will be plotted, if the electron cross
 the
```

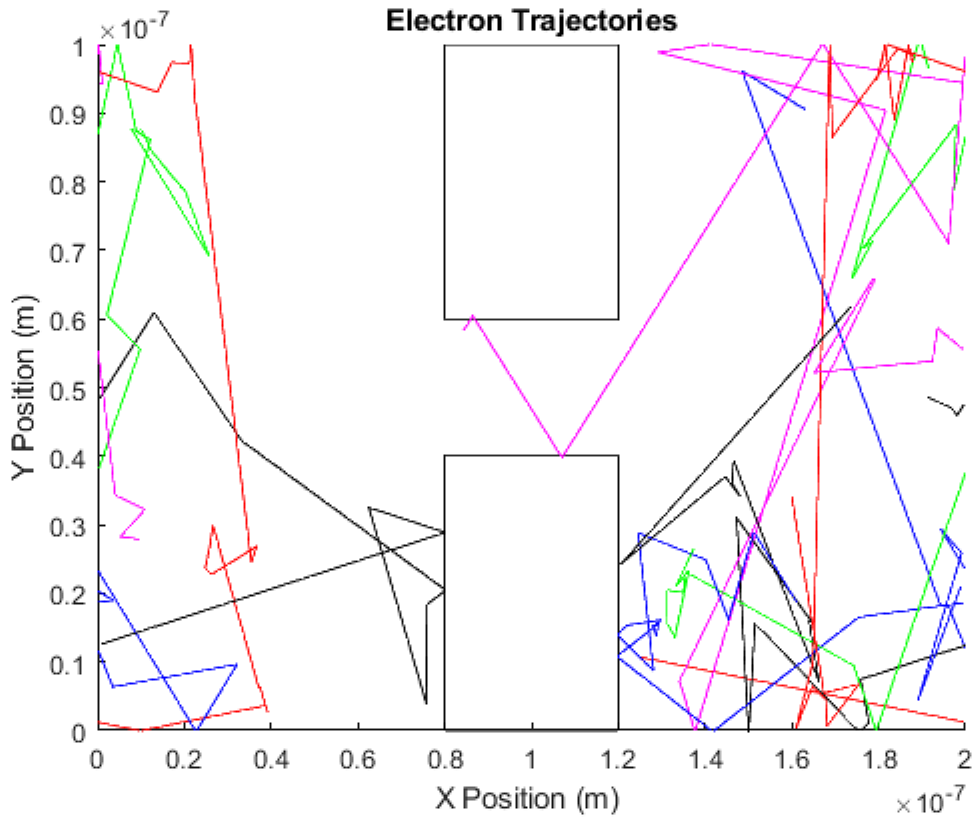
```
% boundary, a 1 will be set in the position of the vector that
 corresponds
% to the number of the electron (1-5).
xBreakpoint = zeros(5);
```



Electron Trajectories and Temperature

The following code is very similar to that used in Question 1 & 2. The main difference is the addition of the two rectangular barriers. If an electron hits one of the barriers, it will bounce off (same result as hitting the top or bottom of the grid).

```
% Run simulation over time.
for count =  1:ceil((nTime)/dt)
 % Run through each electron.
    for c = 1:numElectrons
        if(count~=1)
            % Calculate probability of scattering.
            Pscat = 1-exp(-dt/tmn);

            %  Update the previous positions and velocities.
            vx(c,1)=vx(c,2);
            vy(c,1)=vy(c,2);
            x(c,1)=x(c,2);
            y(c,1)=y(c,2);

            % Update the current position of the electron.
            x(c,2) = x(c,1) + vx(c, 2)*dt;
            y(c,2) = y(c,1) + vy(c, 2)*dt;

            %Update time and distance since the last scatter

 distanceSinceLastScatter(c)=distanceSinceLastScatter(c)+sqrt((x(c,2)-
x(c,1))^2+(y(c,2)-y(c,1))^2);
            timeSinceLastScatter(c)=timeSinceLastScatter(c)+dt;

            % Check to see if an electron hit a boundary. If it hit a
            % horizontal boundary, move it to the other side of the
 grid
            % (with the same velocity). If it hit a vertical boundary,
 it
            % should bounce off.
            if(x(c,2)>200e-9)
                x(c,2) = x(c,2)-200e-9;
                if(c<6 && c>0)
                    xBreakpoint(c)=1;
                end
            elseif(x(c,2)<0)
                x(c,2)=x(c,2)+200e-9;
                if(c<6 && c>0)
                   xBreakpoint(c)=1;
                end
            end
            if(y(c,2)>=100e-9)
                vy(c,2) = -vy(c,2);
            elseif(y(c,2)<=0)
                vy(c,2)=-vy(c,2);
            end

            % Check to see if an electron hit a barrier. If it hit, it
            % should bounce off.
            if(x(c,2)<1.2e-7 && x(c,2)>0.8e-7 &&(y(c,2)<0.4e-7 ||
 y(c,2)>0.6e-7))
                %Hit Box. Hit Sides if:
                if((y(c,2-1)<0.4e-7 || y(c,2-1)>0.6e-7))
                    vx(c,2)=-vx(c,2);
                else
                    vy(c,2)=-vy(c,2);
                end
            end

             %Check if the electron scatters
            r=rand();
            if(Pscat>r)
              %Scattering occurs. Update velocity components, then
 save
              % and clear scattering time and distance.
                vx(c,2) = vth * randn()/sqrt(2);
                vy(c,2) = vth * randn()/sqrt(2);

                scatterCount = scatterCount +1;
                scatterDistances(scatterCount) =
 distanceSinceLastScatter(c);
                scatterTimes(scatterCount)=timeSinceLastScatter(c);
                distanceSinceLastScatter(c)=0;
                timeSinceLastScatter(c)=0;
            end
        end
    end

    if(count>1)
        % Plot the displacement of the electrons in different colours.
        figure(1)
        hold on
        if(xBreakpoint(1)~=1)
            plot(x(1,1:2),y(1,1:2),'b')
        end
        if(xBreakpoint(2)~=1)
            plot(x(2,1:2),y(2,1:2),'r')
        end
        if(xBreakpoint(3)~=1)
            plot(x(3,1:2),y(3,1:2),'g')
        end
        if(xBreakpoint(4)~=1)
            plot(x(4,1:2),y(4,1:2),'k')
        end
        if(xBreakpoint(5)~=1)
            plot(x(5,1:2),y(5,1:2),'m')
        end
        hold off
    end

    % Reset xBreakpoint.
    xBreakpoint(:)=0;

    % Update the previous and current temperature values.
    temperature(:,1)=temperature(:,2);
    temperature(:,2) = (vx(:,2).^2 + vy(:,2).^2).*((0.26*C.m_0))./
C.kb;

    pause(0.000001)
end
```

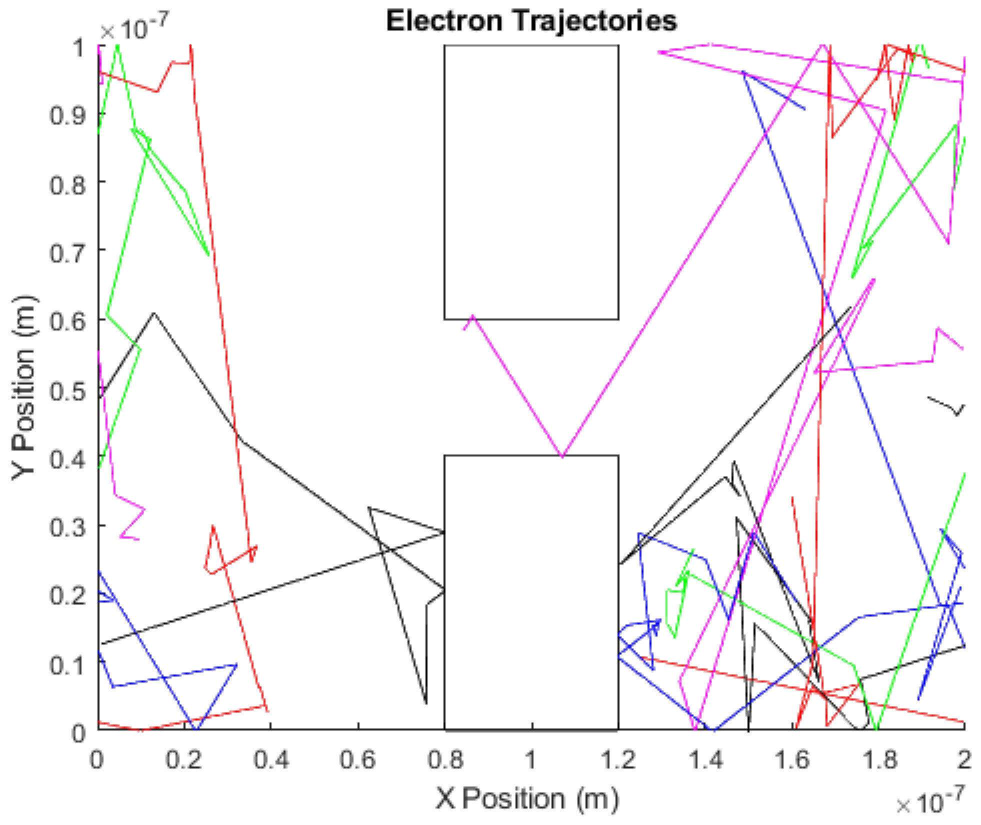


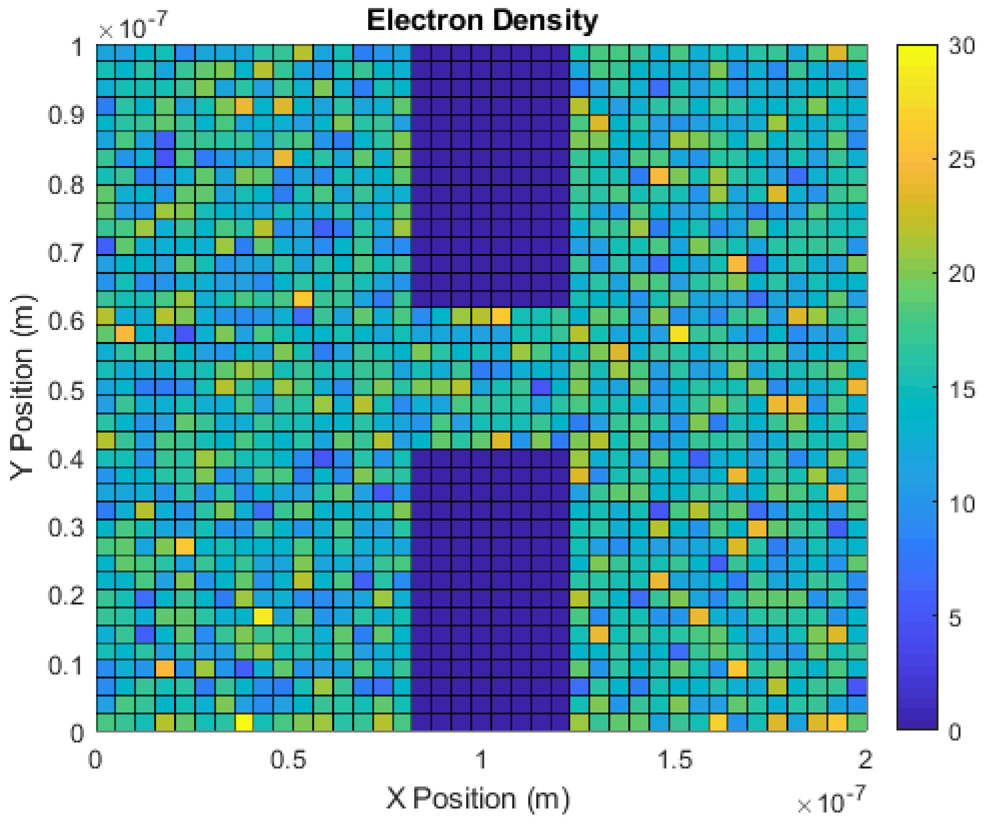
Electron Density and Temperature Map

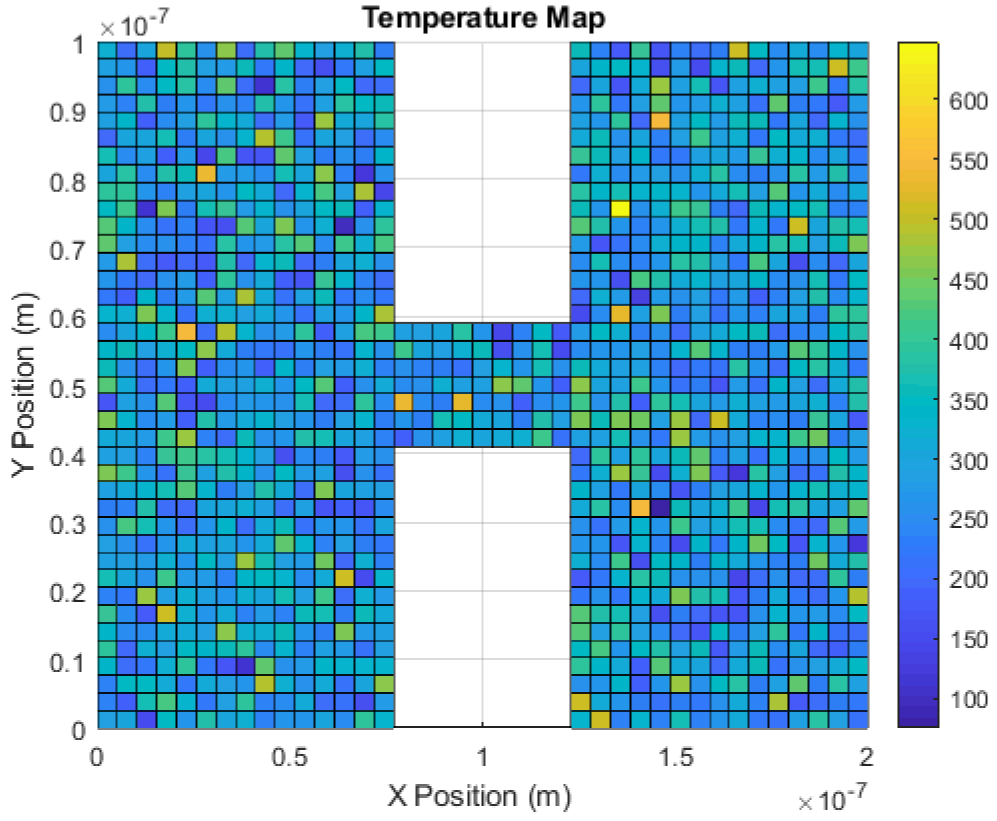
Divide the total grid into 40x40 grid for electron density and velocity (this will give 1600 "boxes"). For each electron, find its corresponding box and sum the number of electrons and total temperature for each box. Ensure no electrons are in the barrier regions.

```
electronCount=zeros(40,40);
electronTemperature=zeros(40,40);
for  eCount = 1:numElectrons
    % Find the box associated with the electron.
    xVal = ceil(40*x(eCount,2)/200e-9);
    yVal = ceil(40*y(eCount,2)/100e-9);
    if(xVal<1)
        xVal=1;
    end
    if(yVal<1)
        yVal =1;
    end
    if(xVal>40)
        xVal = 40;
    end
    if(yVal>40)
        yVal=40;
    end
    %Ensure no electron is within the barriers.
    if((yVal>24 || yVal<17)&&xVal>16&&xVal<25)
```

```
            if(xVal==24)
                xVal = 25;
            end
            if(xVal==17)
                xVal = 16;
            end
            if(xVal>17 && xVal <24)
                if(yVal>24)
                    yVal = 24;
                elseif(yVal<17)
                    yVal=17;
                end
            end
        end

        % Add to the total electron count and total temperature.
        electronCount(yVal,xVal) =electronCount(yVal,xVal)+1;
        electronTemperature(yVal, xVal) = electronTemperature(yVal, xVal)
     + temperature(eCount,2);
    end

    % Find the average temperature of each box.
    electronTemperature = electronTemperature ./ electronCount;

    % Plot the Electron Density and the Temperature Map
    figure(4)
    xAxis = linspace(0,200e-9,40);
    yAxis = linspace(0,100e-9,40);
    surf(xAxis,yAxis, electronCount);
    colorbar;
    view(2);
    title('Electron Density')
    xlabel('X Position (m) ')
    ylabel('Y Position (m)')

    figure(5)
    surf(xAxis,yAxis, electronTemperature);
    colorbar;
    view(2);
    title('Temperature Map')
    xlabel('X Position (m) ')
    ylabel('Y Position (m)')
```


Electron Trajectories
×10^-7
1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
Y Position (m)
0
0.2
0.4
0.6
0.8
1
1.2
1.4
1.6
1.8
2
X Position (m)
×10^-7


Electron Density
×10^-7
1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
Y Position (m)
0
0.5
1
1.5
2
X Position (m)
×10^-7
30
25
20
15
10
5
0



Mean Free Path and Time Between Collisions

```
%The actual mean free path is
actualMFP = mean(scatterDistances);

%The actual time between collisions is
actualTBC = mean(scatterTimes);
```

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