Assigment 1 - Monte-Carlo Modeling of Electron Transport

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Simulation 1- Basic Electron Modelling

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The purpose of Simulation 1 is to place electrons randomly inside the designated area. They will all have the same relative velocity but travel in random directions. When they make contact with the top or bottom boundary, they will "bounce" off them and travel in the opposite direction. When they encounter side walls, the electron will "teleport" from one side to the other to maintain the electron density in the designated area.

S1 Initialization of individual electron values

S1 vth and MFP

```
Thermal Velocity = 1.870193e+05 m/s
Mean free path = 3.740385e-08
```

S1 Electrons position and velocity arrays

```
% Plotting Area
wArea = 200e-9;
1Area = 100e-9;
numElec = 1000;
                              %Number of simulated Electrons
numEPlot = 10;
                             %Number of plotted Electrons
dt = (lArea*wArea);
                             %Typically 1/100 of region size
stepsTot = 200;
                             %Total amount of steps (1000 was a long simulation)
tTot= stepsTot*dt;
                             %Total Simulation time
x = zeros(1,numElec);
                             %Inital X matrix
y = zeros(1,numElec);
                             %Inital y matrix
vx = zeros(1,numElec);
                             %Inital velocity x matrix
vy = zeros(1,numElec);
                             %Inital velocity y matrix
vtot = zeros(1,numElec);
                             %Inital velocity matrix
colors = rand(numElec,3);
                              %Color assignment for each electron
```

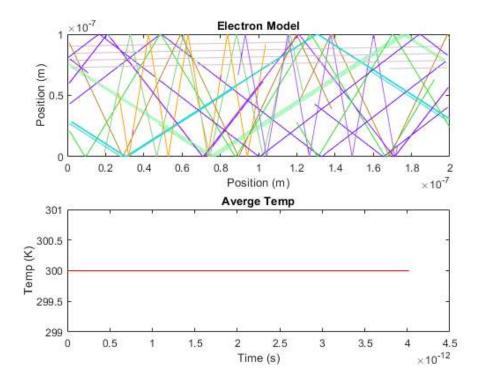
S1 Electron Random Assignments

```
for cnt = 1:numElec
    x(cnt)=rand()*wArea;
    y(cnt)=rand()*lArea;
    angle = (2*pi*rand());
    vx(cnt)=vt*cos(angle);  % velocity * random direction
    vy(cnt)=vt*sin(angle);  % velocity * random direction
    vtot(cnt)= sqrt (vx(cnt)^2)+(vy(cnt)^2);
end
```

S1 Main Loop

```
t=0;
 intCNT = 2;
 eTemp(1) = Temp;
while t < tTot
                           t = t + dt;
                             %Store old position
                             oldx = x;
                             oldy = y;
                             %Update to new position
                             x(1:numElec) = x(1:numElec) + (vx(1:numElec).*dt);
                             y(1:numElec) = y(1:numElec) + (vy(1:numElec).*dt);
                             vtot(1:numElec)= sqrt((vx(1:numElec).^2)+(vy(1:numElec).^2));
                              %Apply boundary conditions
                              for check = 1:numElec
                                                           %If bottom contact, bounce off in opposite direction
                                                           if (y(check)<=0)</pre>
                                                                                        y(check) = 0;
                                                                                        vy(check) = -vy(check);
                                                           %If top contact, bounce off in opposite directio
                                                           if (y(check)>=lArea)
                                                                                        y(check) = lArea;
                                                                                        vy(check) = -vy(check);
                                                           end
                                                           % if left side of box, come out right side % \left( 1\right) =\left( 1\right) \left( 
                                                           if(x(check)<=0)</pre>
                                                                                x(check) = x(check) + wArea;
                                                           %if right side of box, come out left side \,
                                                           if(x(check)>=wArea)
                                                                         x(check) = x(check) - wArea;
```

```
end
    end
    %Plot Boundary and map some electrons
    for Eplot = 1:numEPlot
        subplot (2,1,1)
        %if the electron went out of sides and back on other side, do not
        %draw line
        if abs(oldx(Eplot)-x(Eplot))<(wArea/2)</pre>
            p = plot([oldx(Eplot),x(Eplot)],[oldy(Eplot),y(Eplot)]);
        end
        p.Color=colors(Eplot,:);
        axis([0,wArea,0,lArea]);
        title('Electron Model'), xlabel('Position (m)', 'FontSize', 10), ylabel('Position (m)', 'FontSize', 10);
        hold on;
    end
    pause(0.01);
   %Plot Averge Temprature in the system
    subplot (2,1,2)
   Time(:,intCNT) = t;
    allT = ((vtot(:).^2).*mn)./(2*kb);
   eTemp(:,intCNT) = mean(allT);
   plot(Time,eTemp,"r");
   title('Averge Temp'),xlabel('Time (s)', 'FontSize', 10), ylabel('Temp (K)', 'FontSize', 10),ylim([299,301]);
    hold on;
    intCNT = intCNT +1;
end
```



Simulation 2 - Collisions with Mean Free Path (MFP)

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The purpose of this simulation is to allow the electrons to scatter as if making contact with another electron. This is done by randomizing the velocity in x and y when a randomly generated value is less then the probability of scattering. The temperature of the systems is monitored over time as the velocities of the particles will undergo net change. This change is over a normal distribution so the net temperature should equal the set temperature. The Mean free path and mean time between collisions is also tracked (about the same metric but one is distance and the other is time). A histogram is produced to show the distribution of the velocities.

```
clc
clear all
close all
%Initial
m0 = 9.10938215e-31;
                             % electron mass
mn = 0.26*m0;
                              % Effective mass
                             % Inital Temp (K)
Temp = 300;
kb = 1.3806504e-23;
                             % Boltzmann constant
tmn = 0.2e-12;
                             % Mean time between collision
% Region Area
wArea = 200e-9;
1Area = 100e-9;
%Thermal Velocity (Question 1.A)
vt=sqrt((2*kb*Temp)/mn);
                              % Sim in 2D so (2*kb*Temp), 3D is (3*kb*Temp)
%Electrons position and velocity arrays
numElec = 1000;
                              %Number of simulated Electrons
numEPlot = 20;
                             %Number of plotted Electrons
dt = (lArea*wArea);
                             %Typically 1/100 of region size
stepsTot = 200;
                             %Total amount of steps (1000 was a long simulation)
tTot= stepsTot*dt;
                             %Total Simulation time
x = zeros(1,numElec);
                             %Inital X matrix
                             %Inital y matrix
y = zeros(1,numElec);
vx = zeros(1,numElec);
                             %Inital velocity x matrix
vy = zeros(1,numElec);
                             %Inital velocity y matrix
vtot = zeros(1,numElec);
                             %Inital velocity matrix
avgTemp=0;
                               %Set average Temp to 0
%Probability of Scatter
                               %Turn Scatter on (1) or off(0)
scatOn = 1;
Pscatter = 1-exp(-dt/tmn);
                             %Scatter Equation with tmn
tScatter = zeros(1, numElec); %track scatter for each particle
%Electron Graph initial
for cnt = 1:numElec
    x(cnt)=rand()*wArea;
   y(cnt)=rand()*lArea;
    vx(cnt)=(vt/sqrt(2))*randn(); % velocity * Gaussian dist
    vy(cnt)=(vt/sqrt(2))*randn(); % velocity * Gaussian dist
    Varience = sqrt(kT/m) - Do we use this?
    vtot(cnt)= sqrt (vx(cnt)^2)+(vy(cnt)^2);
                             %Random Color for each electron
    colors= rand(numElec,3);
end
```

S2 Main Loop

```
t=0;
intCNT = 1; %Counter with time
while t < tTot
    t = t + dt;

%Store old position
    oldx = x;
    oldy = y;

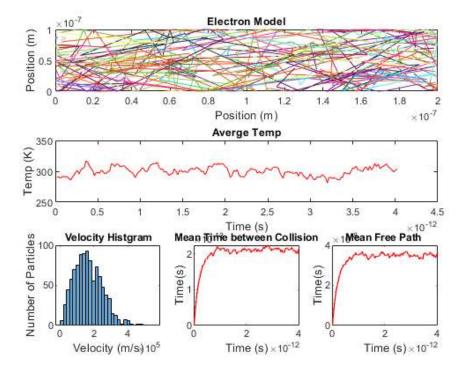
%Update to new position
    x(1:numElec) = x(1:numElec) + (vx(1:numElec).*dt);
    y(1:numElec) = y(1:numElec) + (vy(1:numElec).*dt);

vtot(1:numElec) = sqrt ((vx(1:numElec).^2)+(vy(1:numElec).^2));</pre>
```

```
for check = 1:numElec
    %Scatter
    if scatOn==1
        if Pscatter > rand()
            vx(check)=(vt/sqrt(2))*randn();
            vy(check)=(vt/sqrt(2))*randn();
            tScatter(check)= 0; %If collision, time goes to 0
            tScatter(check) = tScatter(check) + dt; %track time increaing while no collision
        end
    end
    %Apply boundary conditions
    %If bottom contact, bounce off in opposite direction
    if (y(check)<=0)</pre>
        y(check) = 0;
        vy(check) = -vy(check);
    %If top contact, bounce off in opposite directio
    if (y(check)>=lArea)
       y(check) = lArea;
        vy(check) = -vy(check);
    %if left side of box, come out right side
    if(x(check)<=0)</pre>
       x(check) = x(check) + wArea;
    %if right side of box, come out left side
    if(x(check)>=wArea)
      x(check) = x(check) - wArea;
    end
end
%Plot Boundary and map some electrons
for Eplot = 1:numEPlot
    figure(1)
    subplot (3,1,1)
    %if the electron went out of sides and back on other side, do not
    if abs(oldx(Eplot)-x(Eplot))<(wArea/2)</pre>
        p = plot([oldx(Eplot),x(Eplot)],[oldy(Eplot),y(Eplot)]);
    p.Color=colors(Eplot,:);
    axis([0,wArea,0,lArea]);
    title('Electron Model'), xlabel('Position (m)', 'FontSize', 10), ylabel('Position (m)', 'FontSize', 10);
    hold on;
end
pause(0.01);
%Calc Average Temp for all t and Plot
subplot (3,1,2)
Time(:,intCNT) = t;
allT = ((vtot(:).^2).*mn)./(2*kb);
avgTemp(:,intCNT) = mean(allT);
plot(Time,avgTemp,"r");
title('Averge Temp'),xlabel('Time (s)', 'FontSize', 10), ylabel('Temp (K)', 'FontSize', 10), ylim([250,350]);
hold on;
intCNT = intCNT +1;
%Histogram of velocities over time
if intCNT > (stepsTot-5)
    subplot(3,3,7)
    histogram([vtot(:)],30)
    title('Velocity Histgram'), xlabel('Velocity (m/s)', 'FontSize', 10), ylabel('Number of Particles', 'FontSize', 10);
%Mean time between collision
```

```
Time(:,intCNT) = t;
allScat(:,intCNT) = mean(tScatter(tScatter>0));
subplot(3,3,8)
plot(Time,allScat,'r');
title('Mean Time between Collision'),xlabel('Time (s)', 'FontSize', 10), ylabel('Time(s)', 'FontSize', 10);
hold on;

%Mean Free Path over time
Time(:,intCNT) = t;
mfp(:,intCNT) = mean(tScatter(tScatter>0))*mean(vtot(tScatter>0));
subplot(3,3,9)
plot(Time,mfp,'r');
title('Mean Free Path '),xlabel('Time (s)', 'FontSize', 10), ylabel('Time(s)', 'FontSize', 10);
hold on;
end
```



From the results, the average temprature remains the same over time because the xy velocities of a single electron is randomized over a normal distribution therefore the average velocity and temprature over all electron will be around the same values set (300K and 1.87e-5 m/s)

The average mean free path over time increases to the appriximate value calculated in Simulation 1 of 3.74e-8. The mean time between collision is about the same value as set for the probability of scattering as tmn = 0.2e-12.

Simulation 3 - Enhancements

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Simulation 3 adds solid blocks into the area and the electons will "bounce" off the walls when making contact. The electrons will continue to scatter. There should be some type of re-thermalization for the electrons which make contact with the boxes so a value is added to reduce the velocity therefore reducing temprature when contact is make (vloss). An electron density map and temprature map is displayed. (Some initial values may be changed to reduce simulation time. To improve in the future, use linear indexing). Some bleeding or error does exsist looking at the density map.

S3 Initialization of electron values

```
clc
clear all
close all
%Initial
```

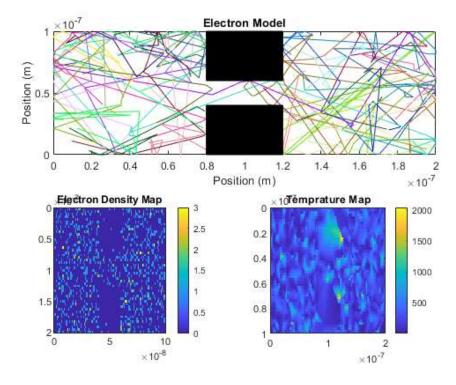
```
% electron mass
m0 = 9.10938215e-31;
mn = 0.26*m0;
                             % Effective mass
Temp = 300;
                             % Inital Temp (K)
kb = 1.3806504e-23;
                            % Boltzmann constant
tmn = 0.2e-12;
                             % Mean time between collision
% Region Area
wArea = 200e-9;
lArea = 100e-9;
%Thermal Velocity (Question 1.A)
vt=sqrt((2*kb*Temp)/mn);
                             % Sim in 2D so (2*kb*Temp), 3D is (3*kb*Temp)
%Electron motion
numElec = 1000;
                               %Number of simulated Electrons
numEPlot = 40;
                             %Number of plotted Electrons
                          %Typically 1/100 of region size
dt = (lArea*wArea);
stepsTot = 60;
                            %Total amount of steps (1000 was a long simulation)
tTot= stepsTot*dt;
                             %Total Simulation time
x = zeros(1,numElec);
                             %Inital X matrix
y = zeros(1,numElec);
                             %Inital y matrix
vx = zeros(1,numElec);
                             %Inital velocity x matrix
vy = zeros(1,numElec);
                             %Inital velocity y matrix
vtot = zeros(1,numElec);
                             %Inital velocity matrix
%Probability of Scatter
                               %Turn Scatter on (1) or off(0)
scatOn = 1;
Pscatter = 1-exp(-dt/tmn);
                               %Scatter Equation
tScatter = zeros(1,numElec);
%Bottle Neck Boundary reduced to prevent bleeding
% X limit (no particle between X1 and X2 - Cosider Y limits)
boxX1=80e-9:
boxX2=120e-9;
% Y Limit (no particles between 0 and Y1 and Y2 to Y limit)
boxY1 = 40e-9;
boxY2 = 60e-9;
%Electron Graph
for cnt = 1:numElec
   x(cnt)=rand()*wArea;
   y(cnt)=rand()*lArea;
   %If the electrons are place in the box, re-roll position
    while (x(cnt)>=boxX1 && x(cnt)<=boxX2 && (y(cnt)<=boxY1 || y(cnt>=boxY2))) %Relocate them if in boundary
       x(cnt)=rand()*wArea;
       y(cnt)=rand()*lArea;
    end
    vx(cnt)=(vt/sqrt(2))*randn(); % velocity * Gaussian dist
    vy(cnt)=(vt/sqrt(2))*randn(); % velocity * Gaussian dist
   %Varience = sqrt(kT/m) - Do we use this?
   vtot(cnt)= sqrt (vx(cnt)^2)+(vy(cnt)^2);
    colors= rand(numElec,3);
end
%Boundary Energy/Velocity loss coefficient (reduction in velocity =
%reduction in temprature)
vloss = 0.95;
```

S3 Main Loop

```
t=0;
while t < tTot
    t = t + dt;
    %Store old position
    oldx = x;
    oldy = y;
```

```
%Update to new position
x(1:numElec) = x(1:numElec) + (vx(1:numElec).*dt);
y(1:numElec) = y(1:numElec) + (vy(1:numElec).*dt);
vtot(1:numElec)= sqrt ((vx(1:numElec).^2)+(vy(1:numElec).^2));
for check = 1:numElec
    %Scatter
    if scat0n==1
        if Pscatter > rand()
            vx(check)=(vt/sqrt(2))*randn();
            vy(check)=(vt/sqrt(2))*randn();
            tScatter(check)= 0; %If collision, time goes to 0
            tScatter(check) = tScatter(check) + dt; %track time increaing while no collision
        end
    end
    %Apply Boundary Conditions
    %If bottom contact, bounce off in opposite direction
    if (y(check)<=0)</pre>
        y(check) = 0;
        vy(check) = -vy(check);
    %If top contact, bounce off in opposite directio
    if (y(check)>=lArea)
        y(check) = lArea;
        vy(check) = -vy(check);
    %if left side of box, come out right side
    if(x(check)<=0)</pre>
       x(check) = 0;
       vx(check) = -vx(check);
    %if right side of box, come out left side
    if(x(check)>=wArea)
       x(check) = wArea;
       vx(check) = -vx(check);
    end
    %Apply bottle neck conditions
    %If contact on left walls of boundary (not in Gap)
    if (oldx(check)<boxX1 && x(check)>=boxX1 && (y(check)<= boxY1 || y(check)>= boxY2))
        x(check)=boxX1;
        vx(check) = -(vx(check)*vloss);
    %If contact on right walls of boundary (not in Gap)
    if (oldx(check)>boxX2 \& x(check)<=boxX2 \& (y(check)<=boxY1 || y(check)>= boxY2))
        x(check)=boxX2;
        vx(check) = -(vx(check)*vloss);
    %If contact with bottom boundary in gap
    if (x(check)>boxX1 && x(check)< boxX2 && oldy(check)>boxY1 && y(check)<= boxY1)</pre>
        y(check)= boxY1;
        vy(check) = -(vy(check)*vloss);
    %If contact with top boundary in gap
    if (x(check)>boxX1 && x(check)< boxX2 && oldy(check)<boxY2 && y(check)>=boxY2)
        y(check)=boxY2;
        vy(check) = -(vy(check)*vloss);
    end
%Plot Boundary and map some electrons
for Eplot = 1:numEPlot
    figure(1)
    subplot (2,1,1)
    %if the electron went out of sides and back on other side, do not
```

```
%draw line
        if abs(oldx(Eplot)-x(Eplot))<(wArea/2)</pre>
            p = plot([oldx(Eplot),x(Eplot)],[oldy(Eplot),y(Eplot)]);
        rectangle('Position',[boxX1 0 (boxX2-boxX1) boxY1],'FaceColor',[0 0 0])
        rectangle('Position',[boxX1 boxY2 (boxX2-boxX1) (lArea-boxY2)],'FaceColor',[0 0 0])
        p.Color=colors(Eplot,:);
        axis([0,wArea,0,lArea]);
        title('Electron Model'), xlabel('Position (m)', 'FontSize', 10), ylabel('Position (m)', 'FontSize', 10);
    end
    %Electron Density Map
    eMapX=linspace(0, wArea, 100);
    eMapY=linspace(0, lArea, 50);
    EDM=histcounts2(y,x,eMapY,eMapX);
    subplot(2,2,3)
    imagesc(eMapY,eMapX,EDM),colorbar,title('Electron Density Map');
   %Electron Temprature Map
    allT = ((vtot(:).^2).*mn)./(2*kb);
    xv = linspace(min(x), max(x), 100);
    yv = linspace(min(y), max(y), 50);
    [X,Y] = meshgrid(xv,yv);
    ETM=griddata(x,y,allT,X,Y);
    subplot(2,2,4);
    imagesc(xv,yv,ETM),colorbar,title("Temprature Map")
    axis([0, wArea, 0 lArea]);
end
```



Simulation 4 - Enhancements - Injection

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Section 3-2 has the electrons injected from one point and another box is added compared to simulation 3. The injection is done from the left side of the area. The velocity from injection point is influenced to travel in the right direction towards the gap (as if forceing them into the material). Once they are injected, they continue to scatter. (Some value are changed or reduced to decrease simulation times)

S4 Initialization of individual electron values

```
clc
clear all
close all
m0 = 9.10938215e-31;
                             % electron mass
mn = 0.26*m0;
                             % Effective mass
                             % Inital Temp (K)
Temp = 300;
                             % Boltzmann constant
kb = 1.3806504e-23;
                             % Mean time between collision
tmn = 0.2e-12;
% Region Area
wArea = 200e-9;
lArea = 100e-9;
%Thermal Velocity (Question 1.A)
vt=sqrt((2*kb*Temp)/mn);
                          % Sim in 2D so (2*kb*Temp), 3D is (3*kb*Temp)
```

S4 Electrons position and velocity arrays

```
numElec = 50;
                         %Number of simulated Electrons
avgTemp=0;
                         %Set average Temp to 0
%Electron color assignment
for cnt = 1:numElec
   colors= rand(numElec,3);
   y(cnt) = 50e-9;
end
%Probability of Scatter
                         %Turn Scatter on (1) or off(0)
scatOn = 1;
Pscatter = 1-exp(-dt/tmn);
                        %Scatter Equation
tScatter = zeros(1,numElec);
```

S4 Bottle Neck Boundary

X limit (no particle between X1 and X2 - Cosider Y limits)

```
boxX1=80e-9;
boxX2=120e-9;
% Y Limit (no particles between 0 and Y1 and Y2 to Y limit)
boxY1 = 40e-9;
boxY2 = 60e-9;

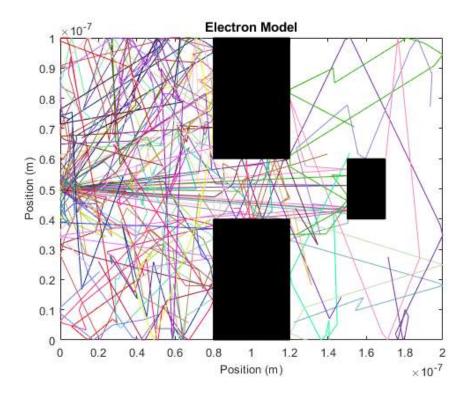
%New Box
boxX3 = 150e-9;
boxX4 = 170e-9;
boxY3 = 40e-9;
boxY4 = 60e-9;

%Boundary Energy/Velocity loss coefficient, when hitting wall, increase
%velocity = increase temp, decrease velocity = decrease temp
vloss = 0.95;
```

S4 Main loop

```
t=0;
intCNT = 1; %Counter with time
while t < tTot
   t = t + dt;
    %Store old position
    oldx = x;
    oldy = y;
    %Inject one elctron for each loop iteration
    if intCNT <= numElec</pre>
        %Add a velocity for injected electron but have it dominate in the y
        %direction to go towards the gap
        vx(intCNT)=0.9*(vt/sqrt(2))*abs(randn());  % velocity * Gaussian dist
        vy(intCNT)=0.1*(vt/sqrt(2))*randn(); % velocity * Gaussian dist
        vtot(intCNT)= sqrt (vx(intCNT)^2)+(vy(intCNT)^2);
    %Update to new position
    x(1:numElec) = x(1:numElec) + (vx(1:numElec).*dt);
   y(1:numElec) = y(1:numElec) + (vy(1:numElec).*dt);
    vtot(1:numElec)= sqrt ((vx(1:numElec).^2)+(vy(1:numElec).^2));
    for check = 1:numElec
        %Scatter
        if scatOn==1
            if Pscatter > rand()
                if vx ~= 0
                vx(check)=(vt/sqrt(2))*randn();
                vy(check)=(vt/sqrt(2))*randn();
            end
        end
        %Apply Boundary Conditions
        %If bottom contact, bounce off in opposite direction
        if (y(check)<=0)</pre>
            y(check) = 0;
            vy(check) = -vy(check);
        end
        %If top contact, bounce off in opposite directio
        if (y(check)>=lArea)
            y(check) = lArea;
            vy(check) = -vy(check);
        %if left side of box, come out right side
        if(x(check)<=0)</pre>
           x(check) = 0;
           vx(check) = -vx(check);
        %if right side of box, come out left side
        if(x(check)>=wArea)
           x(check) = wArea;
           vx(check) = -vx(check);
        end
        %Apply bottle neck conditions
        %If contact on left walls of boundary (not in Gap)
        if (oldx(check) < boxX1 \& x(check) > = boxX1 \& (y(check) < = boxY1 || y(check) > = boxY2))
            x(check)=boxX1;
            vx(check) = -(vx(check)*vloss);
        %If contact on right walls of boundary (not in Gap)
        if (oldx(check)>boxX2 \& x(check)<=boxX2 \& (y(check)<=boxY1 || y(check)>= boxY2))
            x(check)=boxX2;
            vx(check) = -(vx(check)*vloss);
        end
        %If contact with bottom boundary in gap
        if (x(check)>boxX1 && x(check)< boxX2 && oldy(check)>boxY1 && y(check)<= boxY1)</pre>
```

```
y(check)= boxY1;
            vy(check) = -(vy(check)*vloss);
        %If contact with top boundary in gap
        if (x(check)>boxX1 && x(check)< boxX2 && oldy(check)<boxY2 && y(check)>=boxY2)
            y(check)=boxY2;
            vy(check) = -(vy(check)*vloss);
        %Apply bottle neck conditions for new box
        %If contact with left wall
        if (oldx(check)<boxX3 && x(check)>=boxX3 && y(check)>= boxY3 && y(check)<= boxY4)
            x(check)=boxX3;
            vx(check) = -(vx(check)*vloss);
        %If contact on right walls of boundary
        if (oldx(check)>boxX4 && x(check)<=boxX4 && y(check)>= boxY3 && y(check)<= boxY4)
            x(check)=boxX4;
            vx(check) = -(vx(check)*vloss);
        %If contact with bottom boundary in gap
        if (x(check)>boxX3 && x(check)< boxX4 && oldy(check)>boxY4 && y(check)<= boxY4)
           y(check)= boxY4;
            vy(check) = -(vy(check)*vloss);
        %If contact with top boundary in gap
        if (x(check)>boxX3 && x(check)< boxX4 && oldy(check)<boxY3 && y(check)>=boxY3)
           y(check)=boxY3;
            vy(check) = -(vy(check)*vloss);
        end
    end
    %Plot Boundary and map some electrons
    for Eplot = 1:numEPlot
        figure(1)
       %if the electron went out of sides and back on other side, do not
        if abs(oldx(Eplot)-x(Eplot))<(wArea/2)</pre>
            p = plot([oldx(Eplot),x(Eplot)],[oldy(Eplot),y(Eplot)]);
        rectangle('Position',[boxX1 0 (boxX2-boxX1) boxY1],'FaceColor',[0 0 0])
        rectangle('Position',[boxX1 boxY2 (boxX2-boxX1) (lArea-boxY2)], 'FaceColor',[0 0 0])
        rectangle('Position',[boxX3 boxY3 (boxX4-boxX3) (boxY4-boxY3)],'FaceColor',[0 0 0])
        p.Color=colors(Eplot,:);
        axis([0,wArea,0,lArea]);
        title('Electron Model'), xlabel('Position (m)', 'FontSize', 10), ylabel('Position (m)', 'FontSize', 10);
        hold on;
    end
    intCNT = intCNT + 1;
end
```



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