ELEC 4700 Assignment 3 - Monte-Carlo/Finite Difference Method

Contents

1 - Monte-Carlo Simluation

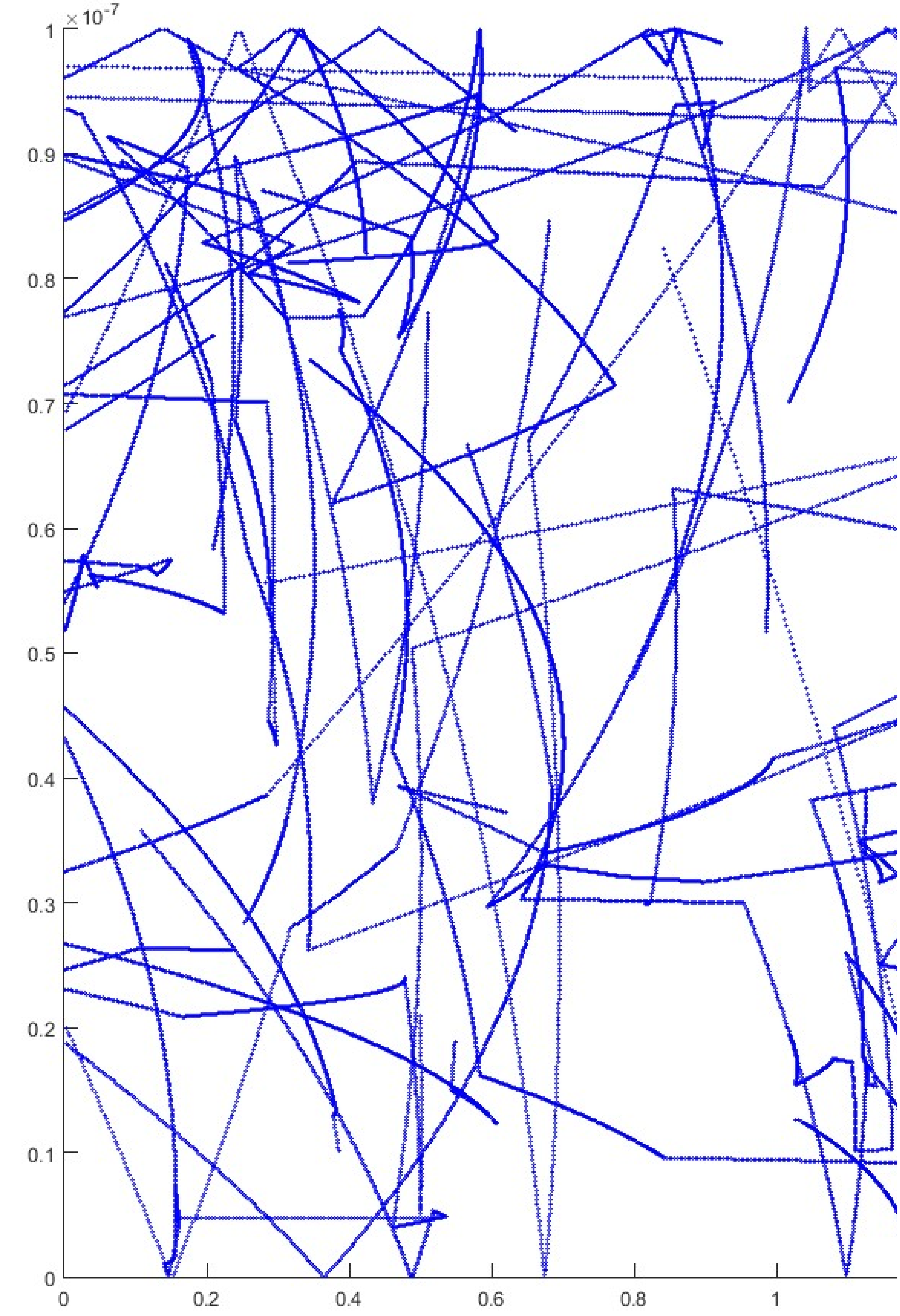
Below is the code to simulate electron motion under the influence of an external electric field.

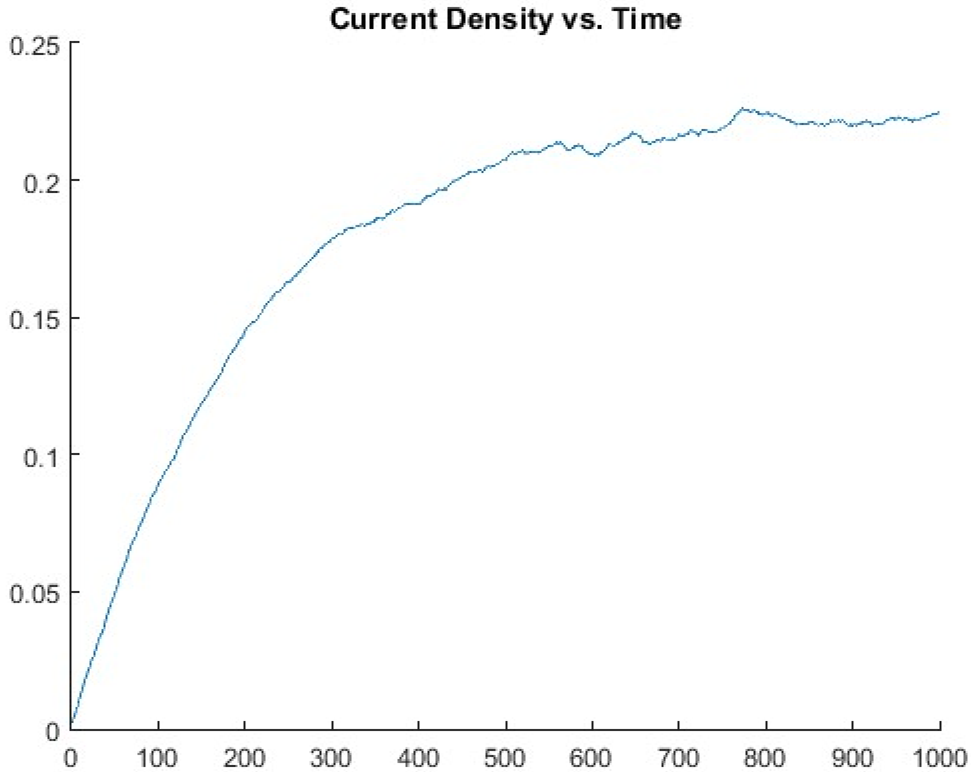
```
C.m_0 = 9.10938215e-31;            % electron mass
C.kb = 1.3806504e-23;              % Boltzmann constant
C.q_0 = 1.60217653e-19;            % electron charge

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

delVx = 0.8; % voltage difference in x direction
delVy = 0;

Ex = delVx/L;
Ey = delVy/W;

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
```

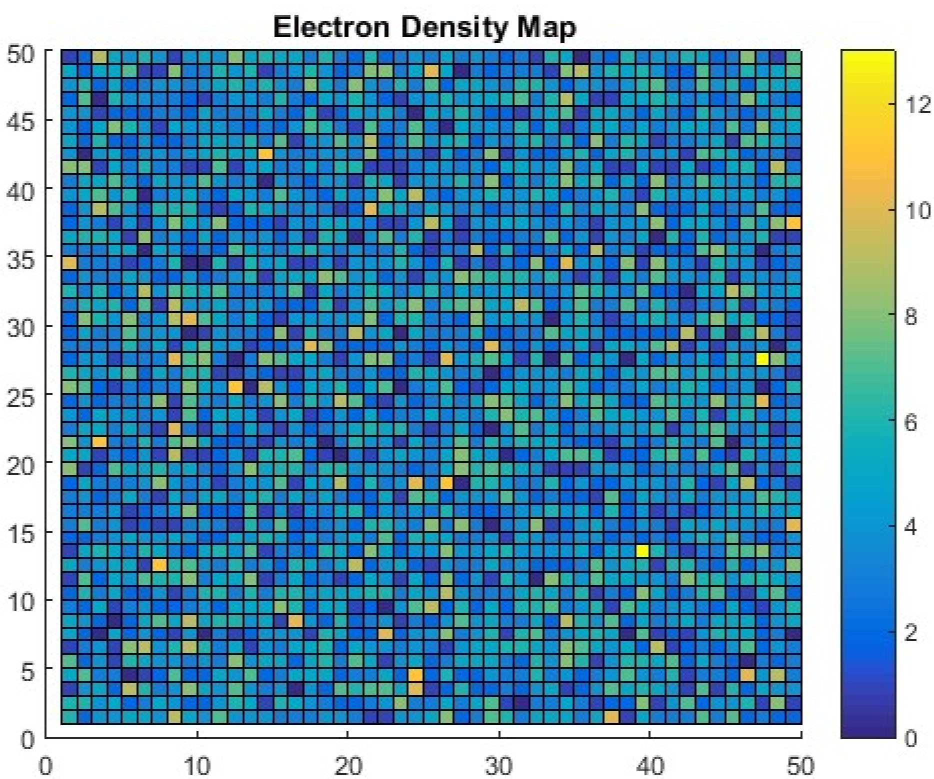
```
currentD = zeros(1,1000);
currentDTime = linspace(1,1000,1000);

figure(2)
hFig2 = figure(2);
set(hFig2, 'Position', [0 0 1200 1000])

q=0;

for i=0:dt:TStop
    time = i;
    q=q+1;

    hold on

    plot(x(1:30), y(1:30), 'bo','markers', 1);
    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;

    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

    Vx = Vx + Ex*C.q_0/C.m_0*dt; % second term is acceleration x time
    Vy = Vy + Ey*C.q_0/C.m_0*dt;

    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

    currentD(q) = 10^15*C.q_0*mean(Vx)*10^(-2); % j-nev, 10^-2 is to convert everything to cm
```

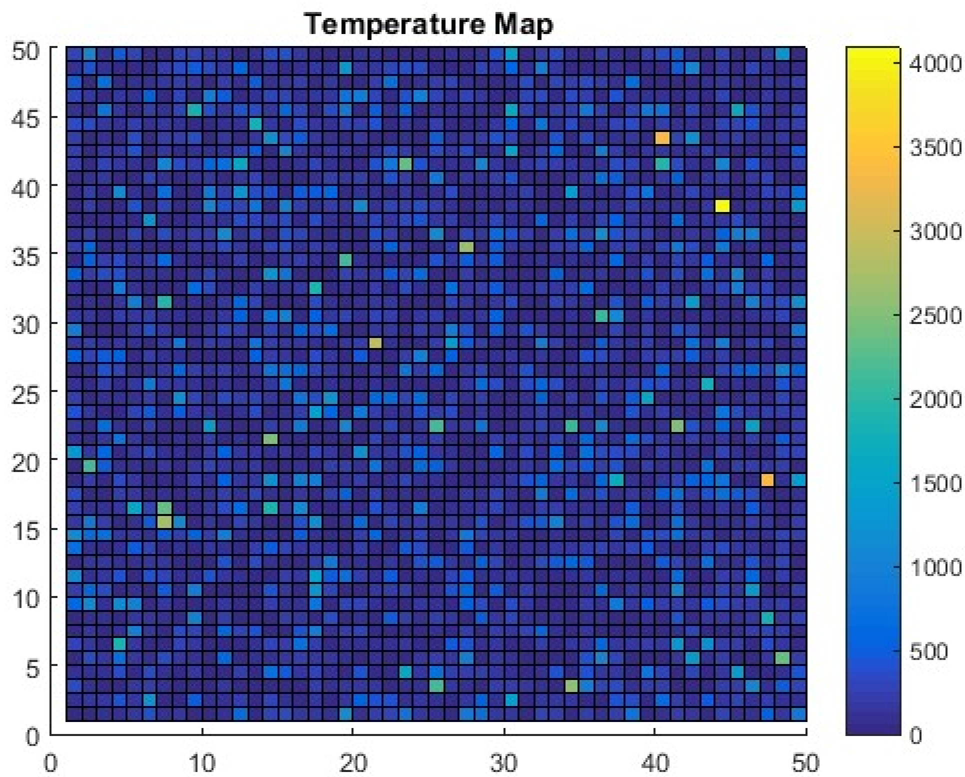
```
    pause(0.000001)

end

figure(1) % plotting current density vs time
hold on
plot(currentDTime(1:1000), currentD(1:1000))
title('Current Density vs. Time');
hold off

figure(3) % 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(4) % 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 =

   2.0731e+05
```


$\times 10^{-7}$
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


Current Density vs. Time
0.25
0.2
0.15
0.1
0.05
0
0
100
200
300
400
500
600
700
800
900
1000


Electron Density Map
50
45
40
35
30
25
20
15
10
5
0
0
10
20
30
40
50
12
10
8
6
4
2
0



1 - Monte-Carlo Simluation Discussion

1a) Since the electric field is just the voltage divided by the distance over which it is applied, the electric field for a 0.1V difference over a distance of 200nm would be 0.1V/200nm = 500,000V/m.

1b) The force on an electron is given by F = qE where q is the charge on the electron, and E is the electric field. For electrons in a 0.1V difference over a distance of 200nm, electrons would experience a force of F = (500,000V/m)(1.6 x 10^{-19}C) = 80 pN

1c) Done in code

1d) The relationship between electron drift current density and average carrier velocity is given by the equation j=nev, where j is the current density, n is the electron concentration, e is the elementary charge, and v is the average carrier velocity. The current plot is generated by the above code. As seen, the current density increases over time. This is due to the fact that the electrons are continually being sped up by the electric field and there is no boundary to slow them down.

1e) Done in code

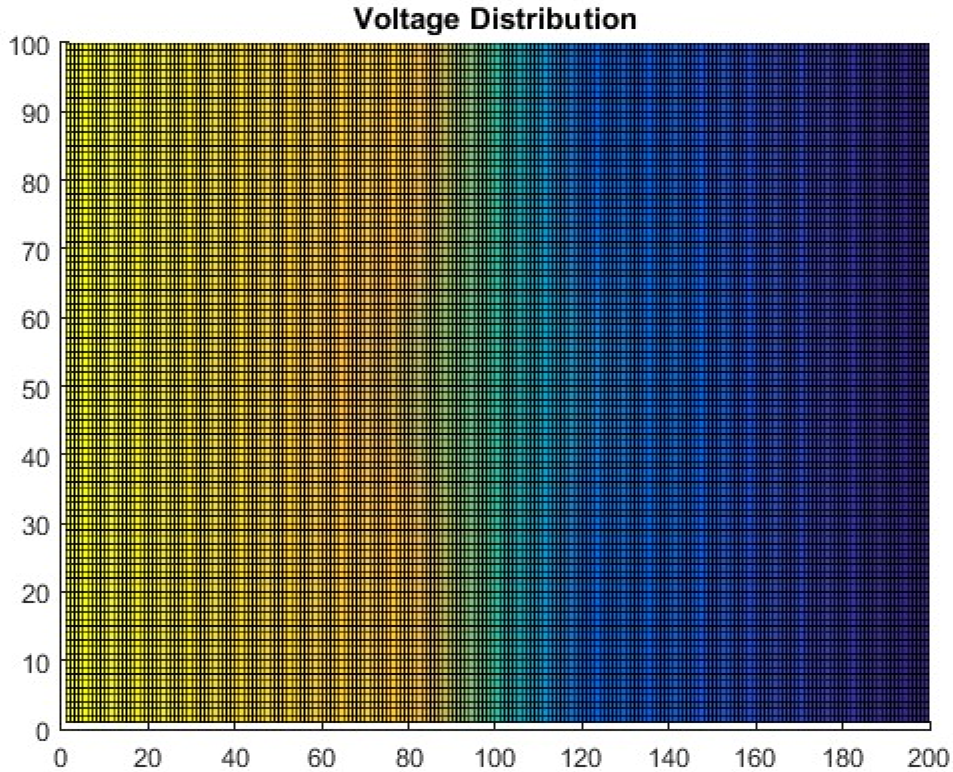
2 - Finite Difference Method

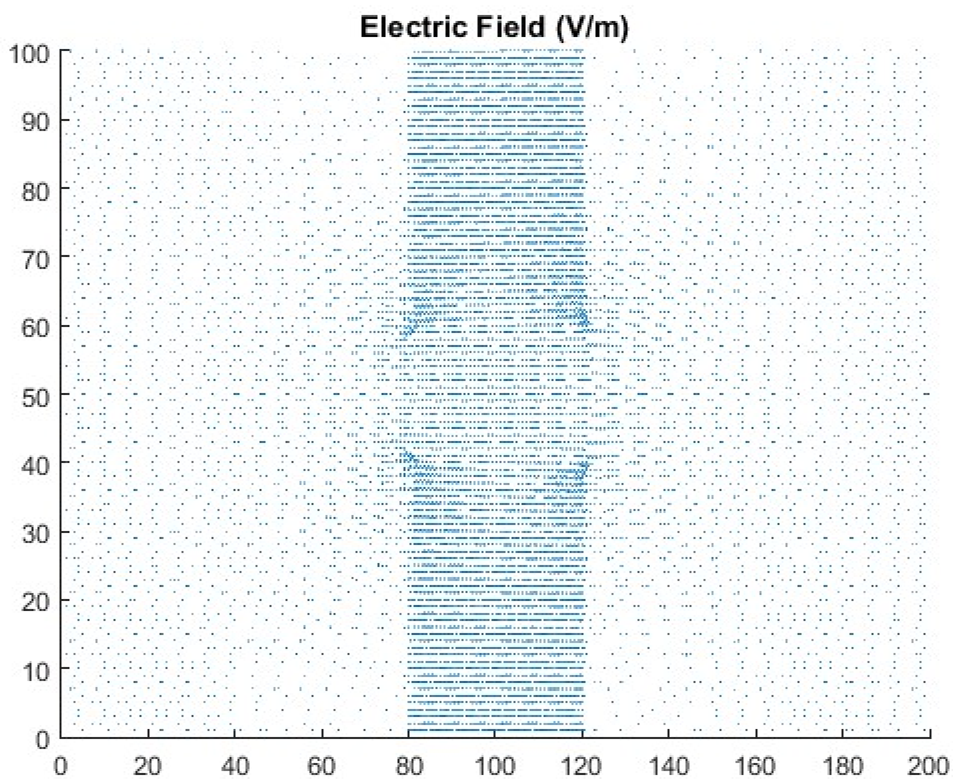
Below is the code to calculate the electric field using the finite difference method.

```
clearvars
clearvars -GLOBAL
close all

L = 200;
W = 100;
Lb = 40;
Wb = 40;
```

```
Vo = 1;
maxI = 200;
delta = 1;

Sigma = ones(W,L);

for i=1:Wb
    for j=round(L/2-Lb/2):round(L/2+Lb/2)
        Sigma(i,j) = 0.01;
    end
end
for i=round(W-Wb):W
    for j=round(L/2-Lb/2):round(L/2+Lb/2)
        Sigma(i,j) = 0.01;
    end
end

G = sparse(L*W,L*W);
B = zeros(1,L*W);

for i=1:W
    for j=1:L
        n = j + (i-1)*L;

         if j==1
            G(n,:) = 0;
            G(n,n) = 1;
            B(n) = Vo;
        elseif j==L
            G(n,:) = 0;
            G(n,n) = 1;
        elseif j==1 && i==1
            G(n,:) = 0;
            G(n,n) = -(Sigma(i+1,j) + Sigma(i,j+1));
            G(n,n+1) = Sigma(i,j+1);
            G(n,n+L) = Sigma(i+1,j);
        elseif j==L && i==1
            G(n,:) = 0;
            G(n,n) = -(Sigma(i+1,j) + Sigma(i,j-1));
            G(n,n-1) = Sigma(i,j-1);
            G(n,n+L) = Sigma(i+1,j);
        elseif j==1 && i==W
            G(n,:) = 0;
            G(n,n) = -(Sigma(i-1,j) + Sigma(i,j+1));
            G(n,n+1) = Sigma(i,j+1);
            G(n,n-L) = Sigma(i-1,j);
        elseif j==L && i==W
            G(n,:) = 0;
            G(n,n) = -(Sigma(i-1,j) + Sigma(i,j-1));
            G(n,n-1) = Sigma(i,j-1);
            G(n,n-L) = Sigma(i-1,j);
        elseif i==1
            G(n,:) = 0;
            G(n,n) = -(Sigma(i+1,j) + Sigma(i,j+1) + ...
                Sigma(i,j-1));
            G(n,n+1) = Sigma(i,j+1);
```

```
            G(n,n+L) = Sigma(i+1,j);
            G(n,n-1) = Sigma(i,j-1);
        elseif i==W
            G(n,:) = 0;
            G(n,n) = -(Sigma(i,j+1) + Sigma(i,j-1) + ...
                Sigma(i-1,j));
            G(n,n-1) = Sigma(i,j-1);
            G(n,n+1) = Sigma(i,j+1);
            G(n,n-L) = Sigma(i-1,j);
        else
            G(n,:) = 0;
            G(n,n) = -(Sigma(i,j+1) + Sigma(i,j-1) + ...
                Sigma(i-1,j) + Sigma(i+1,j));
            G(n,n-1) = Sigma(i,j-1);
            G(n,n+1) = Sigma(i,j+1);
            G(n,n-L) = Sigma(i-1,j);
            G(n,n+L) = Sigma(i+1,j);
        end

    end
end

F=G\B';

Vmap = zeros(W,L);

for i=1:W
    for j=1:L
        n = j + (i-1)*L;
        Vmap(i,j) = F(n);
    end
end

figure(1)
hold on
surf(Vmap);
title('Voltage Distribution')
hold off
pause(0.001);

[Ex,Ey]=gradient(-Vmap);

figure(2)
hold on
quiver(Ex,Ey);
axis([0 L 0 W])
title('Electric Field (V/m)')
hold off
pause(0.001);
```





3 - Combination

Below is the code that implements the electron motion from part 1 under the influence of the electric field from part 2, with the bottle-neck included.

```
clearvars
clearvars -GLOBAL
close all

L = 200;
W = 100;
Lb = 40;
Wb = 40;
Vo = 10;
maxI = 200;
delta = 1;

Sigma = ones(W,L);

for i=1:Wb
    for j=round(L/2-Lb/2):round(L/2+Lb/2)
        Sigma(i,j) = 0.01;
    end
end
for i=round(W-Wb):W
    for j=round(L/2-Lb/2):round(L/2+Lb/2)
        Sigma(i,j) = 0.01;
    end
end

G = sparse(L*W,L*W);
B = zeros(1,L*W);

for i=1:W
    for j=1:L
        n = j + (i-1)*L;

         if j==1
            G(n,:) = 0;
            G(n,n) = 1;
            B(n) = Vo;
        elseif j==L
            G(n,:) = 0;
            G(n,n) = 1;
        elseif j==1 && i==1
            G(n,:) = 0;
            G(n,n) = -(Sigma(i+1,j) + Sigma(i,j+1));
            G(n,n+1) = Sigma(i,j+1);
            G(n,n+L) = Sigma(i+1,j);
        elseif j==L && i==1
            G(n,:) = 0;
            G(n,n) = -(Sigma(i+1,j) + Sigma(i,j-1));
            G(n,n-1) = Sigma(i,j-1);
            G(n,n+L) = Sigma(i+1,j);
        elseif j==1 && i==W
            G(n,:) = 0;
            G(n,n) = -(Sigma(i-1,j) + Sigma(i,j+1));
            G(n,n+1) = Sigma(i,j+1);
            G(n,n-L) = Sigma(i-1,j);
        elseif j==L && i==W
```

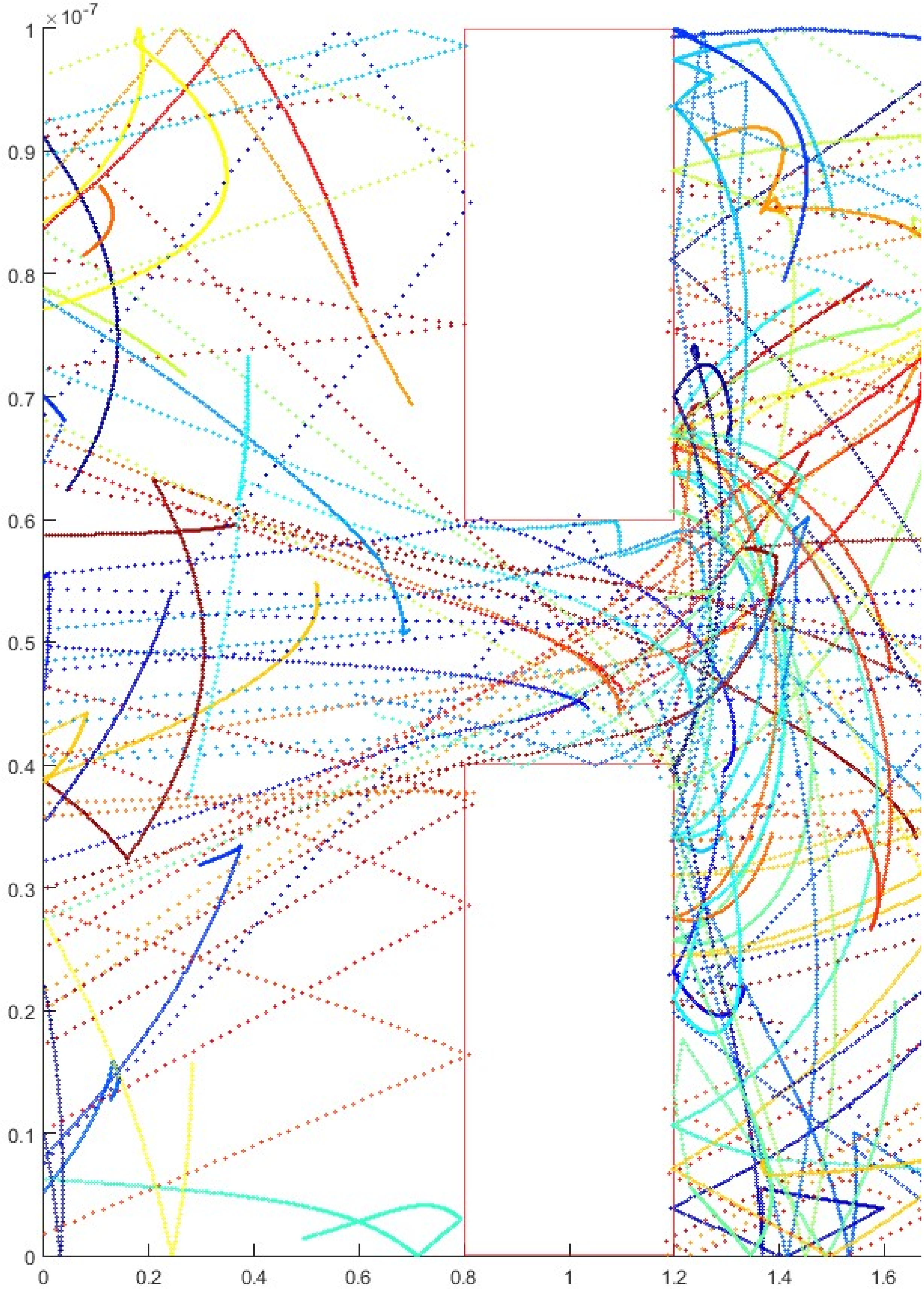
```
            G(n,:) = 0;
            G(n,n) = -(Sigma(i-1,j) + Sigma(i,j-1));
            G(n,n-1) = Sigma(i,j-1);
            G(n,n-L) = Sigma(i-1,j);
        elseif i==1
            G(n,:) = 0;
            G(n,n) = -(Sigma(i+1,j) + Sigma(i,j+1) + ...
                Sigma(i,j-1));
            G(n,n+1) = Sigma(i,j+1);
            G(n,n+L) = Sigma(i+1,j);
            G(n,n-1) = Sigma(i,j-1);
        elseif i==W
            G(n,:) = 0;
            G(n,n) = -(Sigma(i,j+1) + Sigma(i,j-1) + ...
                Sigma(i-1,j));
            G(n,n-1) = Sigma(i,j-1);
            G(n,n+1) = Sigma(i,j+1);
            G(n,n-L) = Sigma(i-1,j);
        else
            G(n,:) = 0;
            G(n,n) = -(Sigma(i,j+1) + Sigma(i,j-1) + ...
                Sigma(i-1,j) + Sigma(i+1,j));
            G(n,n-1) = Sigma(i,j-1);
            G(n,n+1) = Sigma(i,j+1);
            G(n,n-L) = Sigma(i-1,j);
            G(n,n+L) = Sigma(i+1,j);
        end

    end
end

F=G\B';

Vmap = zeros(W,L);

for i=1:W
    for j=1:L
        n = j + (i-1)*L;
        Vmap(i,j) = F(n);
    end
end

% figure(1)
% hold on
% surf(Vmap);
% title('Voltage Distribution')
% hold off
% pause(0.001);

[Ex,Ey]=gradient(-Vmap);

% figure(2)
% hold on
% quiver(Ex,Ey);
% axis([0 L 0 W])
% title('Electric Field (V/m)')
```

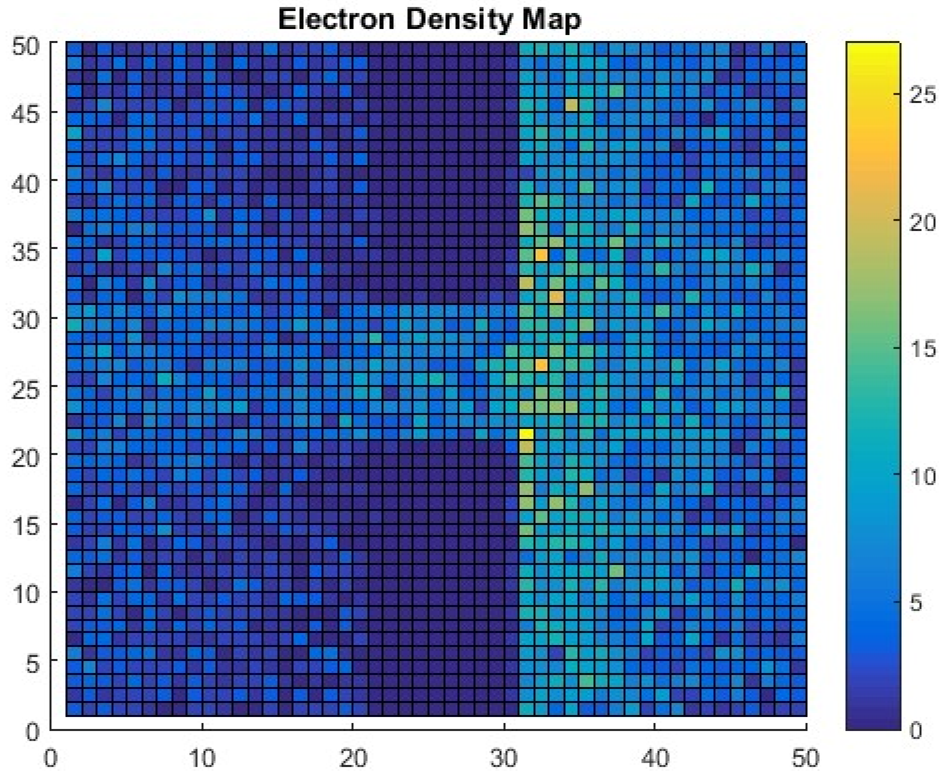
```
% hold off
% pause(0.001);

Ex=Ex'/(1e-9);
Ey=Ey'/(1e-9);

%%%%%%%%%%%%%%%%%%%%

C.m_0 = 9.10938215e-31;             % electron mass
C.kb = 1.3806504e-23;               % Boltzmann constant
C.q_0 = 1.60217653e-19;             % electron charge

nElectrons = 10000;
nPlot=20; % number of electrons to actually plot
T = 300;
Lp = L*1e-9;
Wp = W*1e-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)*Lp; % assigning random initial particle positions
y = rand(1, nElectrons)*Wp;

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*Lp;
          y(i) = rand*Wp;
      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', [200 0 900 1000])

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-')

axis([0 Lp 0 Wp]);

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

    for j=1:nPlot
        plot(x(j), y(j), 'o','markers', 1, 'Color', cc(j,:));
    end


    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;

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

    for i=1:length(Vx)
        xE = round((x(i)*1e9+1)*200/201);
        yE = round((y(i)*1e9+1)*100/101);
        if xE>L
            xE=Lp;
        end
        if yE>W
            yE=Wp;
        end
        if xE<1
            xE=1;
        end
        if yE<1
            yE=1;
        end
        Vx(i) = Vx(i) + Ex(xE,yE)*C.q_0/C.m_0*dt;
        Vy(i) = Vy(i) + Ey(xE,yE)*C.q_0/C.m_0*dt;
    end

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

         if y(j) > Wp
             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

        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)<0.63e-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)>0.37e-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)<0.85e-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)>1.15e-7 && (y(i)<0.4e-7 || y(i)>0.6e-7)
                Vx(i)=-Vx(i);
            end
        end

        pause(0.001)

    end

    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
```

```
avgV =

   2.0617e+05
```


$\times 10^{-7}$
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



3 - Combination Discussion

1a) Done in code

1b) As shown from the density plot, there are a large number of electrons collected on one side of the barrier. This is a result of the periodic boundary conditions that send electrons that go off the left side of the box into the right side of the box. If the electron goes through the gap with some y velocity, eventually after enough times of crossing the box it will end up blocked by the boundary. The random collisions add a layer of randomness to this process, so particles are also able to escape from being stuck on that side of the bottle-neck. However, as shown they tend to end up there more than anywhere else.

1c) Next steps to make this simulation more accurate would be to allow a certain amount of electrons with certain velocities to penetrate the bottle-neck based on the conductivity defined for that region. As the conductivity increases we expect that electrons would be able to pass through more easily, so defining this in-simluation would be useful.

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