ELEC 4700-ASSIGNMENT1

Monte-Carlo Modeling of Electron Transport

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Part 1: Electron Modelling

To calculate the thermal energy, it is noted that there are two degrees of freedom for the electrons. UsingMaxwell's principle of equipartition of energy,

$$\overline{KE} = \frac{1}{2}kT = 2(\frac{1}{2}m\overline{v^2}) \Rightarrow \overline{v^2} = \frac{2kT}{m}$$

```
clear all
close all
m0 = 9.10938356e-31;m
= 0.26*m0;
T = 300;
k = 1.38064852e-23;
vth = sqrt(2*k*T/m)
```

vth =1.8702e+05

Or 187 km/s. The mean free path, l, is simply

```
l = vth*0.2e-12
```

l =3.7404e-08

Thus, the mean free path is about 37.4 nm.

Here are some variables to control the simulations:

```
height = 100e-9;
length = 200e-9;
population_size = 3000;
plot_population = 10; time_step
= height/vth/100;iterations =
1000;
```

```
show_movie = 0;
```

For the simulations, these arrays will hold information about the state of the system, including the positions,velocities, and temperatures.

```
% Each row corresponds to an electron with the positions andvelocities
% [x y vx vy]
state = zeros(population_size, 4);
trajectories = zeros(iterations, plot_population*2);temperature =
zeros(iterations,1);
```

Generate an initial population with constant speeds

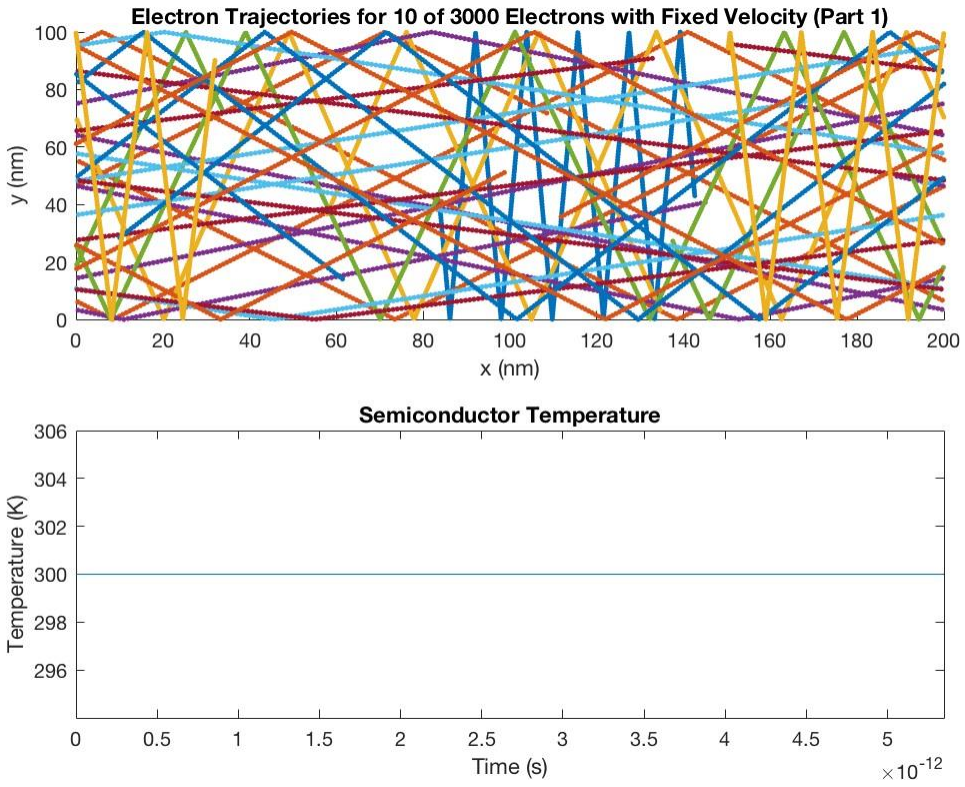
```
for i = 1:population_sizeangle
      = rand*2*pi;
      state(i,:) = [length*rand height*rand vth*cos(angle)
  vth*sin(angle)];
end
```

Iterate over time and update the positions, while plotting the state.

```
for i = 1:iterations
      state(:,1:2) = state(:,1:2) + time_step.*state(:,3:4);

      % Look for collisions with the boundariesj =
      state(:,1) > length;
      state(j,1) = state(j,1) - length;

      j = state(:,1) < 0;
      state(j,1) = state(j,1) + length;

      j = state(:,2) > height;
      state(j,2) = 2*height - state(j,2);state(j,4) =
      -state(j,4);

      j = state(:,2) < 0; state(j,2) = -
      state(j,2);
      state(j,4) = -state(j,4);

      temperature(i) = (sum(state(:,3).^2) + sum(state(:,4).^2))*m/k/2/population_size;

      % Record the trajectoriesfor
      j=1:plot_population
            trajectories(i, (2*j):(2*j+1)) = state(j, 1:2);
      end

      % Update the movie every 5 iterationsif
      show_movie && mod(i,5) == 0
            figure(1);
            subplot(2,1,1);
```

```
            hold off;
            plot(state(1:plot_population,1)./1e-9,
state(1:plot_population,2)./1e-9, 'o');
            axis([0 length/1e-9 0 height/1e-9]);
```

```
            title(sprintf('Trajectories for %d of %d Electrons with FixedVelocity (Part
 1)',...
            plot_population, population_size));xlabel('x
            (nm)');
            ylabel('y (nm)');if i >
            1
                subplot(2,1,2);
                hold off;
                plot(time_step*(0:i-1), temperature(1:i));
                axis([0 time_step*iterations min(temperature)*0.98
 max(temperature)*1.02]);
                title('Semiconductor Temperature');
                xlabel('Time (s)'); ylabel('Temperature
                (K)');
            end
            pause(0.05);
        end
end


% Show trajectories after the movie is overfigure(1);
subplot(2,1,1);
title(sprintf('Electron Trajectories for %d of %d Electrons with FixedVelocity (Part
 1)',...
        plot_population, population_size));xlabel('x
(nm)');
ylabel('y (nm)');
axis([0 length/1e-9 0 height/1e-9]);hold on;
for i=1:plot_population
        plot(trajectories(:,i*2)./1e-9, trajectories(:,i*2+1)./1e-9, '.');
end

if(~show_movie)
        subplot(2,1,2);
        hold off;
        plot(time_step*(0:iterations-1), temperature); axis([0
        time_step*iterations min(temperature)*0.98
 max(temperature)*1.02]); title('Semiconductor
        Temperature');xlabel('Time (s)');
        ylabel('Temperature (K)');
end
```



Part 2: Collisions with Mean Free Path

For the second simulation, the initial velocities are assigned based on a Maxwell-Boltzmann distribution, and scattering is modelled. First, calculate the scattering probability in one time step:

```
p_scat = 1 - exp(-time_step/0.2e-12)
```

p_scat =

0.0264

The distribution of velocities in x and y is Gaussian, with a standard deviation of $\sqrt{kT/m}$. This results in an overall Maxwell-Boltzmann velocity distribution at temperature T

```
v_pdf = makedist('Normal', 'mu', 0, 'sigma', sqrt(k*T/m));
```

The initial population is generated using this distribution:

```
for i = 1:population_sizeangle
      = rand*2*pi;
```

```
        state(i,:) = [length*rand height*rand random(v_pdf)
  random(v_pdf)];
end
```

The average velocity should be calculated to be correct:

```
avg_v = sqrt(sum(state(:,3).^2)/population_size + ...
      sum(state(:,4).^2)/population_size)
```

avg_v =

1.8836e+05

This returns a velocity of about 187 km/s, which is correct. This varies a little bit, since the initial velocitiesare random with a MB distribution.

The second simulation loop follows:

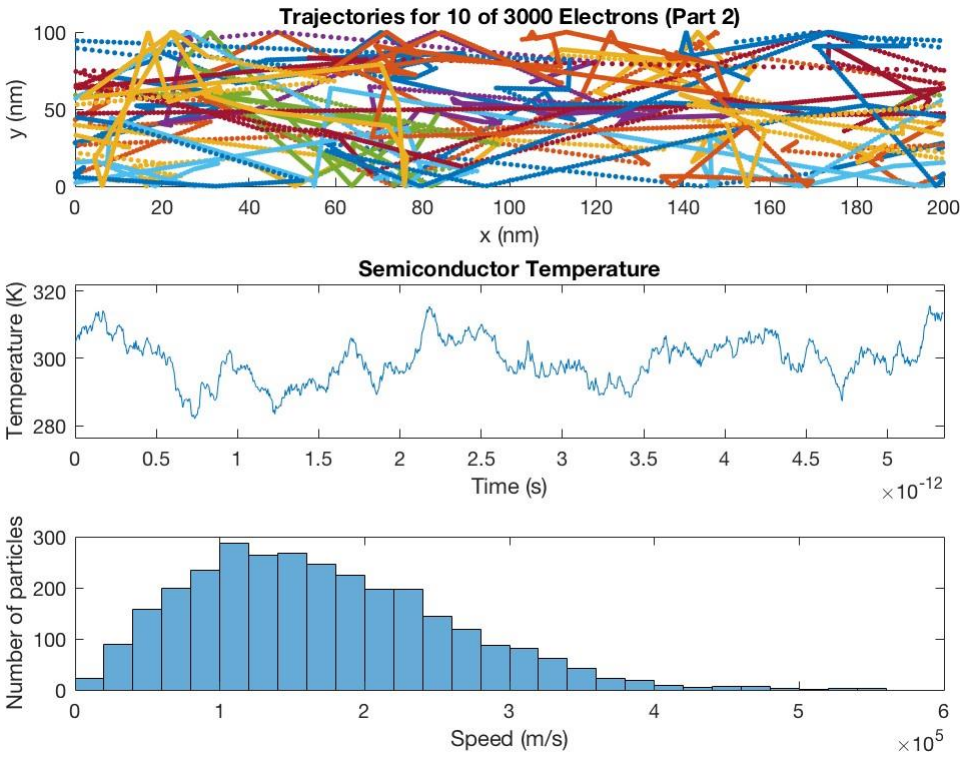
```
for i = 1:iterations
      %Update positions
      state(:,1:2) = state(:,1:2) + time_step.*state(:,3:4);

      j = state(:,1) > length; state(j,1) =
      state(j,1) - length;

      j = state(:,1) < 0;
      state(j,1) = state(j,1) + length;

      j = state(:,2) > height;
      state(j,2) = 2*height - state(j,2);state(j,4) =
      -state(j,4);

      j = state(:,2) < 0; state(j,2) = -
      state(j,2);
      state(j,4) = -state(j,4);

      % Scatter particles
      j = rand(population_size, 1) < p_scat; state(j,3:4) =
      random(v_pdf, [sum(j),2]);

      % Record the temperature
      temperature(i) = (sum(state(:,3).^2) + sum(state(:,4).^2))*m/k/2/population_size;

      % Record positions for subset of particles that will be graphedfor
      j=1:plot_population
            trajectories(i, (2*j):(2*j+1)) = state(j, 1:2);
      end

      % Update the movie every 5 iterationsif
      show_movie && mod(i,5) == 0
            figure(2);
            subplot(3,1,1);
```

```
            hold off;
            plot(state(1:plot_population,1)./1e-9,
state(1:plot_population,2)./1e-9, 'o');
            axis([0 length/1e-9 0 height/1e-9]); title(sprintf('Trajectories for %d
            of %d Electrons (Part
2)',...
```

```
            plot_population, population_size));xlabel('x
            (nm)');
            ylabel('y (nm)');if i >
            1
                subplot(3,1,2);
                hold off;
                plot(time_step*(0:i-1), temperature(1:i));
                axis([0 time_step*iterations min(temperature)*0.98
 max(temperature)*1.02]);
                title('Semiconductor Temperature');
                xlabel('Time (s)'); ylabel('Temperature
                (K)');
            end

            % Show histogram of speeds
            subplot(3,1,3);
            v = sqrt(state(:,3).^2 + state(:,4).^2);
            title('Histogram of Electron Speeds');
            histogram(v);
            xlabel('Speed (m/s)');
            ylabel('Number of particles');


            pause(0.05);
        end
end



% Show trajectories after the movie is overfigure(2);
subplot(3,1,1);
title(sprintf('Trajectories for %d of %d Electrons (Part 2)',...plot_population,
        population_size));
xlabel('x (nm)');
ylabel('y (nm)');
axis([0 length/1e-9 0 height/1e-9]);hold on;
for i=1:plot_population
        plot(trajectories(:,i*2)./1e-9, trajectories(:,i*2+1)./1e-9, '.');
end

% Show temperature plot over time
if(~show_movie)
        subplot(3,1,2);
        hold off;
        plot(time_step*(0:iterations-1), temperature); axis([0
        time_step*iterations min(temperature)*0.98
 max(temperature)*1.02]); title('Semiconductor
        Temperature');xlabel('Time (s)');
        ylabel('Temperature (K)');
```

```
end

% Show speed histogram
subplot(3,1,3);
v = sqrt(state(:,3).^2 + state(:,4).^2);
```

```
title('Histogram of Electron Speeds');
histogram(v);
xlabel('Speed (m/s)');
ylabel('Number of particles');
```



This second simulation shows that the average temperature fluctuates over time due to the scattering, but it has an average of 300K over time.

Part 3: Enhancements

Here, the boundaries can be set to be specular or diffusive. If they are diffusive, the electrons bounce offat a random angle rather than one symmetrical about the normal with the boundary.

The non-periodic top and bottom boundaries can be set to be either specular (1) or diffusive (0) with thefollowing parameters:

```
top_specular = 0;
bottom_specular = 0;
```

This simulation also includes boxes (obstacles) Also, each box can seperately be set to be specular (1)or diffusive (0)

```
% The values are [xmin xmax ymin ymax] for each boxboxes =
1e-9.*[80 120 0 40; 80 120 60 100];
```

```
boxes_specular = [0 1];

% Generate an initial population
```

```
for i = 1:population_sizeangle
      = rand*2*pi;
      state(i,:) = [length*rand height*rand random(v_pdf)
 random(v_pdf)];

      % Make sure no particles start in a box
      while(in_box(state(i,1:2), boxes))
            state(i,1:2) = [length*rand height*rand];
      end
end
```

Run through the third simulation:

```
for i = 1:iterations
      state(:,1:2) = state(:,1:2) + time_step.*state(:,3:4);

      j = state(:,1) > length; state(j,1) =
      state(j,1) - length;

      j = state(:,1) < 0;
      state(j,1) = state(j,1) + length;j =

      state(:,2) > height;

      if(top_specular)
            state(j,2) = 2*height - state(j,2);state(j,4) =
            -state(j,4);
      else % Diffusive
            % The electron bounces off at a random anglestate(j,2)
            = height;
            v = sqrt(state(j,3).^2 + state(j,4).^2);angle =
            rand([sum(j),1])*2*pi; state(j,3) = v.*cos(angle);
            state(j,4) = -abs(v.*sin(angle));
      end

      j = state(:,2) < 0;

      if(bottom_specular)
            state(j,2) = -state(j,2);
            state(j,4) = -state(j,4);else %
      Diffusive
            % The electron bounces off at a random anglestate(j,2)
            = 0;
            v = sqrt(state(j,3).^2 + state(j,4).^2);angle =
            rand([sum(j),1])*2*pi; state(j,3) = v.*cos(angle);
            state(j,4) = abs(v.*sin(angle));
      end
```

```
% Look for particles that have "entered" a box and move them to
% where they should be.for
j=1:population_size
      box_num = in_box(state(j,1:2), boxes);
```

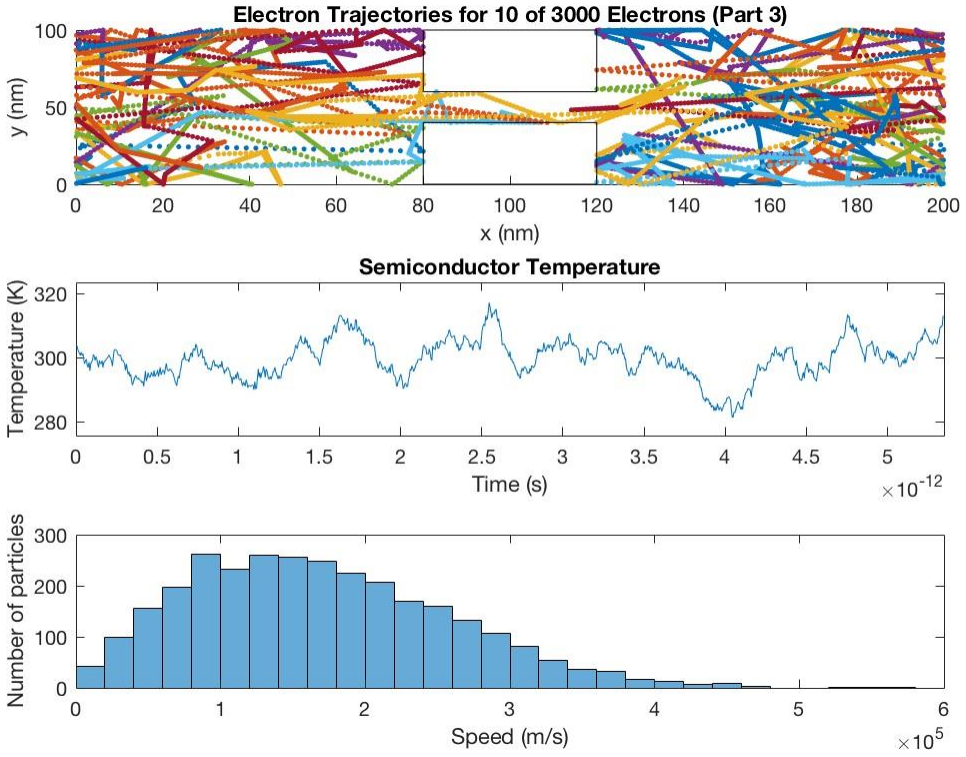
```
while(box_num ~= 0)
    % To see which side the electron collided with,
    % find which one it's closer tox_dist =
    0;
    new_x = 0;
    if(state(j,3) > 0)
        x_dist = state(j,1) - boxes(box_num,1);new_x =
        boxes(box_num,1);
    else
        x_dist = boxes(box_num,2) - state(j,1);new_x =
        boxes(box_num,2);
    end


    y_dist = 0;
    new_y = 0;
    if(state(j,4) > 0)
        y_dist = state(j,2) - boxes(box_num, 3);new_y =
        boxes(box_num, 3);
    else
        y_dist = boxes(box_num, 4) - state(j,2);new_y =
        boxes(box_num, 4);
    end


    if(x_dist < y_dist) state(j,1)
        = new_x;
        if(~boxes_specular(box_num))sgn
            = -sign(state(j,3));
            v = sqrt(state(j,3).^2 + state(j,4).^2);angle =
            rand()*2*pi;
            state(j,3) = sgn.*abs(v.*cos(angle));state(j,4)
            = v.*sin(angle);
        else % Specular
            state(j,3) = -state(j,3);
        end
    else
        state(j,2) = new_y;
        if(~boxes_specular(box_num))
            sgn = -sign(state(j,4));
            v = sqrt(state(j,3).^2 + state(j,4).^2);angle =
            rand()*2*pi;
            state(j,3) = v.*cos(angle); state(j,4) =
            sgn.*abs(v.*sin(angle));
        else % Specular
            state(j,4) = -state(j,4);
```

```
            end
        end

        box_num = in_box(state(j,1:2), boxes);
    end
end


% Scatter particles
j = rand(population_size, 1) < p_scat;
```

```
    state(j,3:4) = random(v_pdf, [sum(j),2]);

    % Record the temperature
    temperature(i) = (sum(state(:,3).^2) + sum(state(:,4).^2))*m/k/2/population_size;

    % Record positions for subset of particles that will be graphedfor
    j=1:plot_population
        trajectories(i, (2*j):(2*j+1)) = state(j, 1:2);
    end

    % Update the movie every 5 iterationsif
    show_movie && mod(i,5) == 0
        figure(3);
        subplot(3,1,1);
        hold off;
        plot(state(1:plot_population,1)./1e-9,
state(1:plot_population,2)./1e-9, 'o');
        hold on;

        % Plot the boxes
        for j=1:size(boxes,1)
            plot([boxes(j, 1) boxes(j, 1) boxes(j, 2) boxes(j, 2)
boxes(j, 1)]./1e-9,...
                [boxes(j, 3) boxes(j, 4) boxes(j, 4) boxes(j, 3)
boxes(j, 3)]./1e-9, 'k-');end

        axis([0 length/1e-9 0 height/1e-9]); title(sprintf('Trajectories for %d
        of %d Electrons (Part
3)',...
        plot_population, population_size));xlabel('x
        (nm)');
        ylabel('y (nm)');
        if i > 1
            subplot(3,1,2);
            hold off;
            plot(time_step*(0:i-1), temperature(1:i));
            axis([0 time_step*iterations min(temperature(1:i))*0.98
max(temperature)*1.02]);
            title('Semiconductor Temperature');
            xlabel('Time (s)'); ylabel('Temperature
            (K)');
        end

        subplot(3,1,3);
        v = sqrt(state(:,3).^2 + state(:,4).^2);
        title('Histogram of Electron Speeds');
        histogram(v);
```

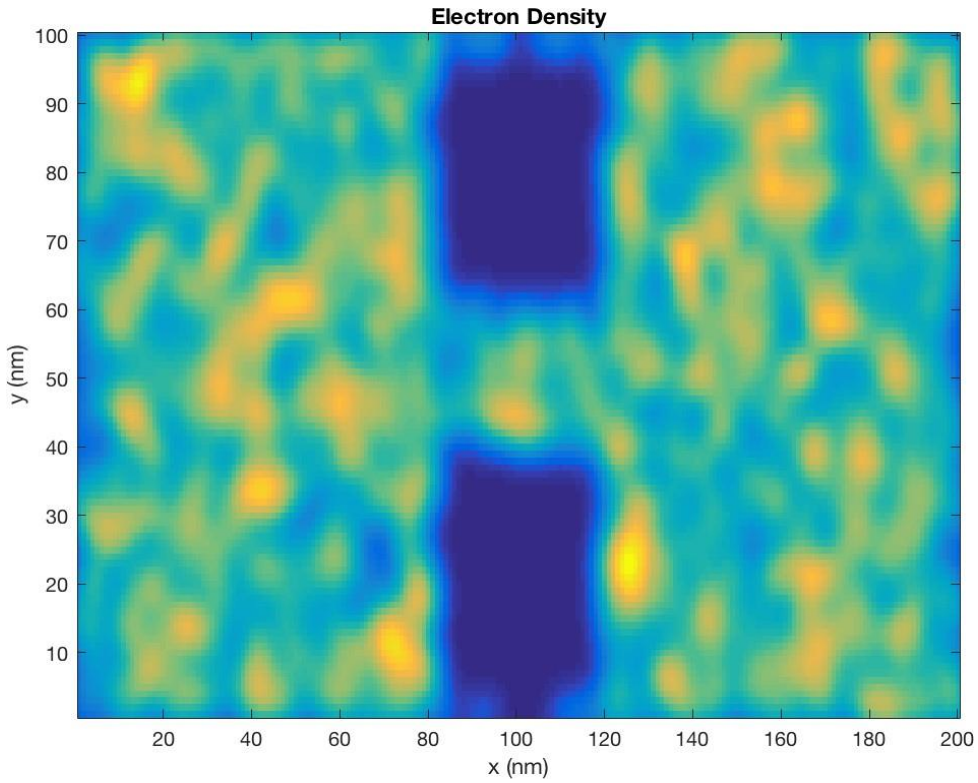
```
    xlabel('Speed (m/s)');
    ylabel('Number of particles');

    pause(0.05);
end
```

```
end

% Show trajectories after the movie is overfigure(3);
subplot(3,1,1);
title(sprintf('Electron Trajectories for %d of %d Electrons (Part3)',...
      plot_population, population_size));xlabel('x
(nm)');
ylabel('y (nm)');
axis([0 length/1e-9 0 height/1e-9]);hold on;
for i=1:plot_population
      plot(trajectories(:,i*2)./1e-9, trajectories(:,i*2+1)./1e-9, '.');

end

% Plot the boxes
for j=1:size(boxes,1)
    plot([boxes(j, 1) boxes(j, 1) boxes(j, 2) boxes(j, 2) boxes(j,1)]./1e-9,...
          [boxes(j, 3) boxes(j, 4) boxes(j, 4) boxes(j, 3) boxes(j,3)]./1e-9, 'k-');
end

% Plot temperature
if(~show_movie)
      subplot(3,1,2);
      hold off;
      plot(time_step*(0:iterations-1), temperature); axis([0
      time_step*iterations min(temperature)*0.98
 max(temperature)*1.02]); title('Semiconductor
      Temperature');xlabel('Time (s)');
      ylabel('Temperature (K)');
end

subplot(3,1,3);
v = sqrt(state(:,3).^2 + state(:,4).^2);
title('Histogram of Electron Speeds');
histogram(v);
xlabel('Speed (m/s)');
ylabel('Number of particles');
```



For the final simulation, an electron density map is created, by creating a 2D histogram over space:

```
density = hist3(state(:,1:2),[200 100])';

% Smooth out the electron density mapN =
20;
sigma = 3;
[x y]=meshgrid(round(-N/2):round(N/2), round(-N/2):round(N/2));f=exp(-
x.^2/(2*sigma^2)-y.^2/(2*sigma^2));
f=f./sum(f(:));
figure(4);
imagesc(conv2(density,f,'same'));
set(gca,'YDir','normal'); title('Electron
Density'); xlabel('x (nm)');
ylabel('y (nm)');
```



The temperature map is created using a similar procudure. The electron velocities are put into bins overspace to calculate the temperature at different points:

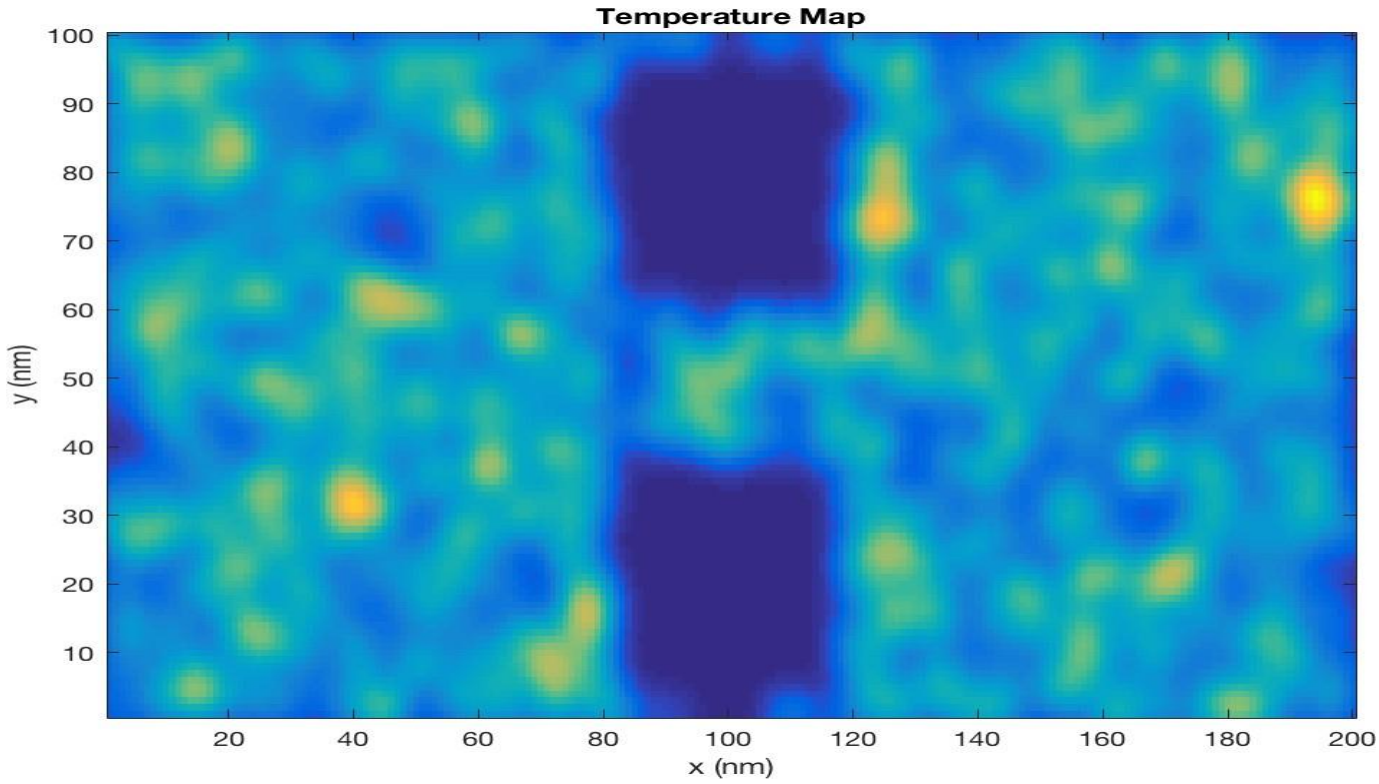
```
temp_sum_x = zeros(ceil(length/1e-9),ceil(height/1e-9));temp_sum_y
=       zeros(ceil(length/1e-9),ceil(height/1e-9));      temp_num      =
zeros(ceil(length/1e-9),ceil(height/1e-9));

% Look at velocities of all the particlesfor
i=1:population_size
    % Find which "bin" it belongs in:x =
    floor(state(i,1)/1e-9);
    y = floor(state(i,2)/1e-9);if(x==0)
        x = 1;
    end
    if(y==0)
        y= 1;
    end

    % Add its velocity components to the cumulative count:
    temp_sum_y(x,y) = temp_sum_y(x,y) + state(i,3)^2;
    temp_sum_x(x,y) = temp_sum_x(x,y) + state(i,4)^2;
    temp_num(x,y) = temp_num(x,y) + 1;
end
```

Now, with the velocities added up, calculate the temperatures:

```
temp = (temp_sum_x + temp_sum_y).*m./k./2./temp_num;
temp(isnan(temp)) = 0;
temp = temp';
```

Like with the density map, perform some smoothing:

```
N = 20;
sigma = 3;
[x y]=meshgrid(round(-N/2):round(N/2), round(-N/2):round(N/2));f=exp(-
x.^2/(2*sigma^2)-y.^2/(2*sigma^2));
f=f./sum(f(:));
figure(5);
imagesc(conv2(temp,f,'same'));
set(gca,'YDir','normal');
title('Temperature Map'); xlabel('x
(nm)');
ylabel('y (nm)');
```



The relationship between the temperature map and the electron density map is very noticable. However,some the of the electrons have considerably higher speeds, and this can be seen on the temperature map.