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

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1. Electron Modelling

a) Thermal Velocity (vth)

Assuming T = 300 K, and using the equation below, the thermal velocity was determined to be 1.8702×10^5 m/s.

```
vth = ((2*kB*T)/mn)^0.5
```

vth 1.8702e+05

b) Mean Free Path (mfp)

Assuming $\tau mn = 0.2$ ps, and using the equation below, the mean free path was determined to be 3.7404×10^{-8} m.

```
mfp = vth*tmn
```

mfp 3.7404e-08

c) i) 2-D Plot of Particle Trajectories

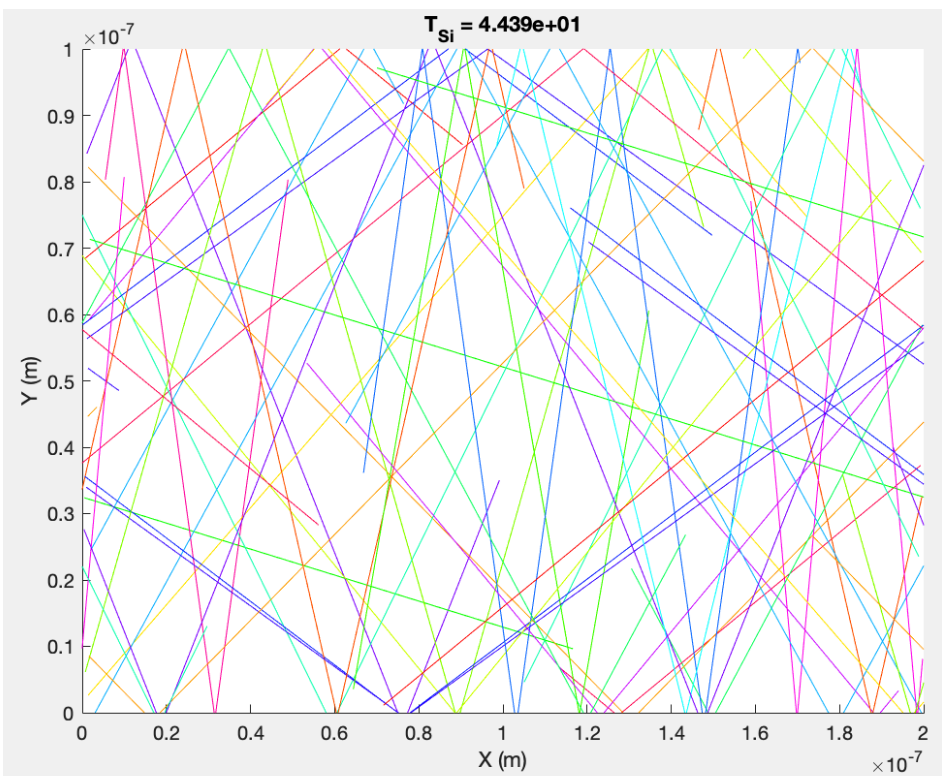

Figure 1: Sample electron trajectories.

ii) Temperature Plot

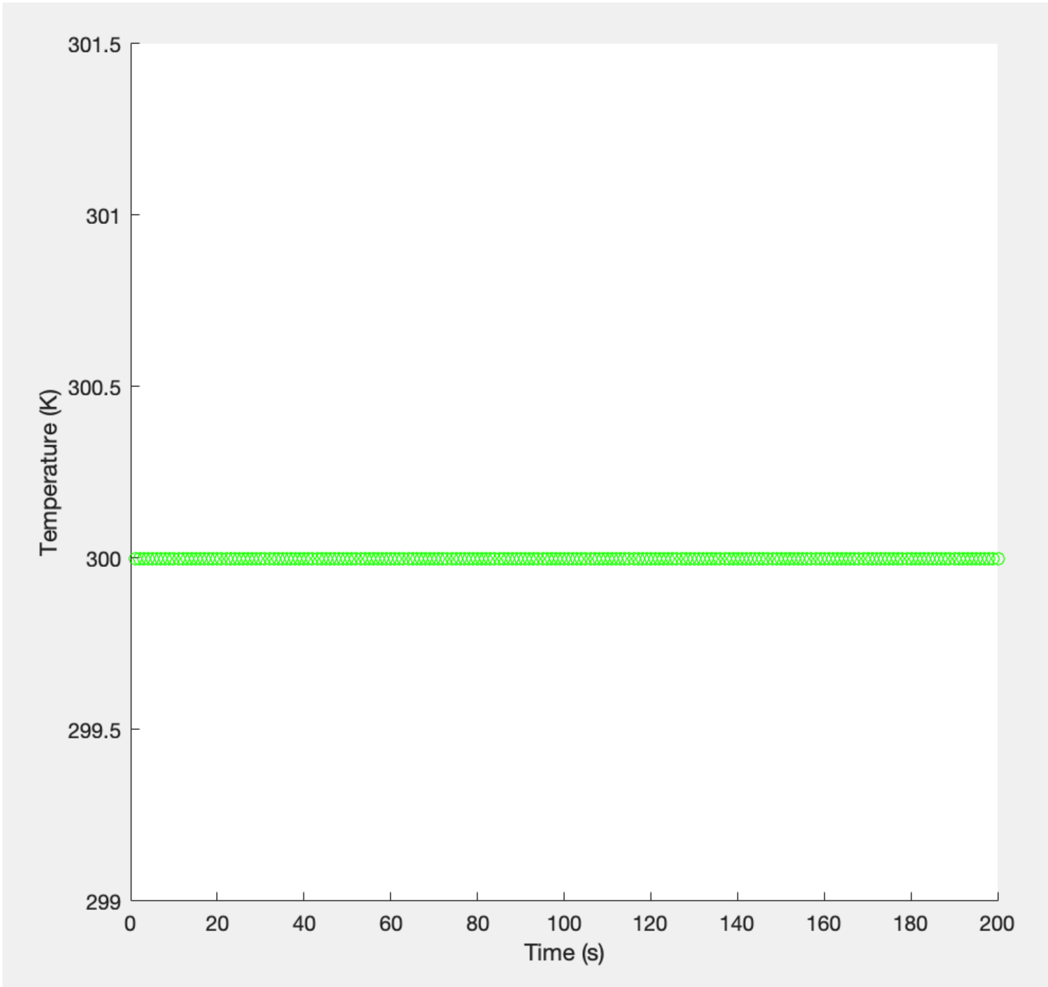

Figure 2: Temperature plot over time without scattering.

The plot above makes sense (for without scattering and with specular reflection) since the particles shouldn't be losing any kinetic energy and therefore, the temperature of the system should remain constant.

Note: ~~When I switched my velocity distributions from rand to randn the temperature values were a bit more normal (on the order of 100s of K), but every time I used rand it would give very low temperatures as shown above.~~

Note 2: Changed Vx to `Vx = sqrt((V^2)-(Vy.^2));` which gave the correct temperature value of 300 K.

2. Collisions with Mean Free Path

a) Histogram

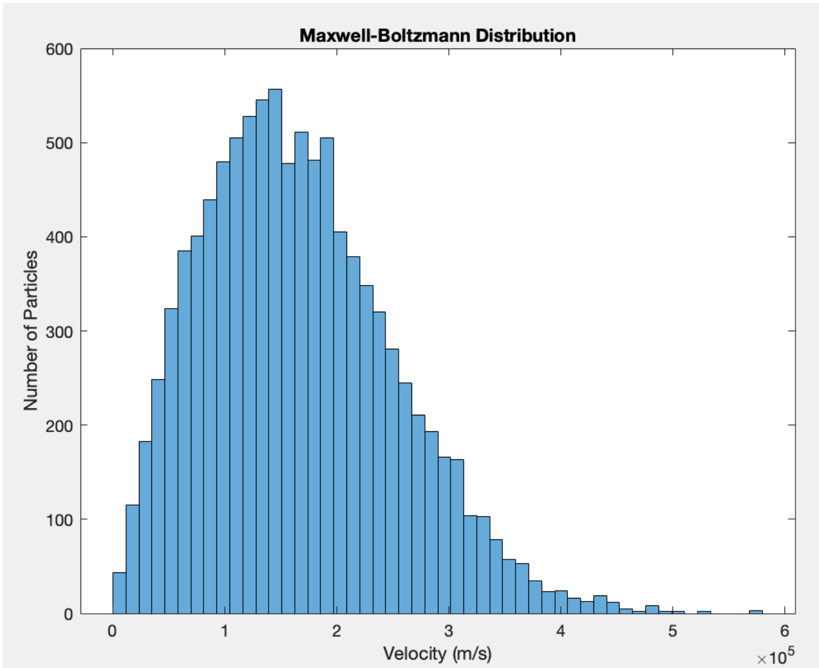

Figure 3: Histogram for the Maxwell-Boltzmann Distribution of electron velocities.

b) 2-D Plot of Particle Trajectories

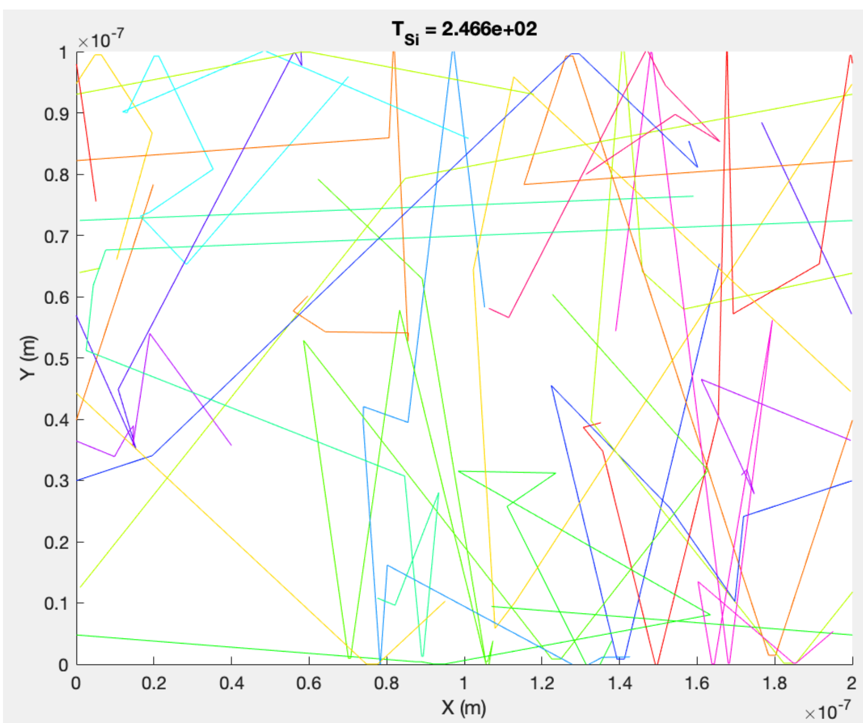

Figure 4: Sample electron trajectories with scattering.

c) Temperature Plot

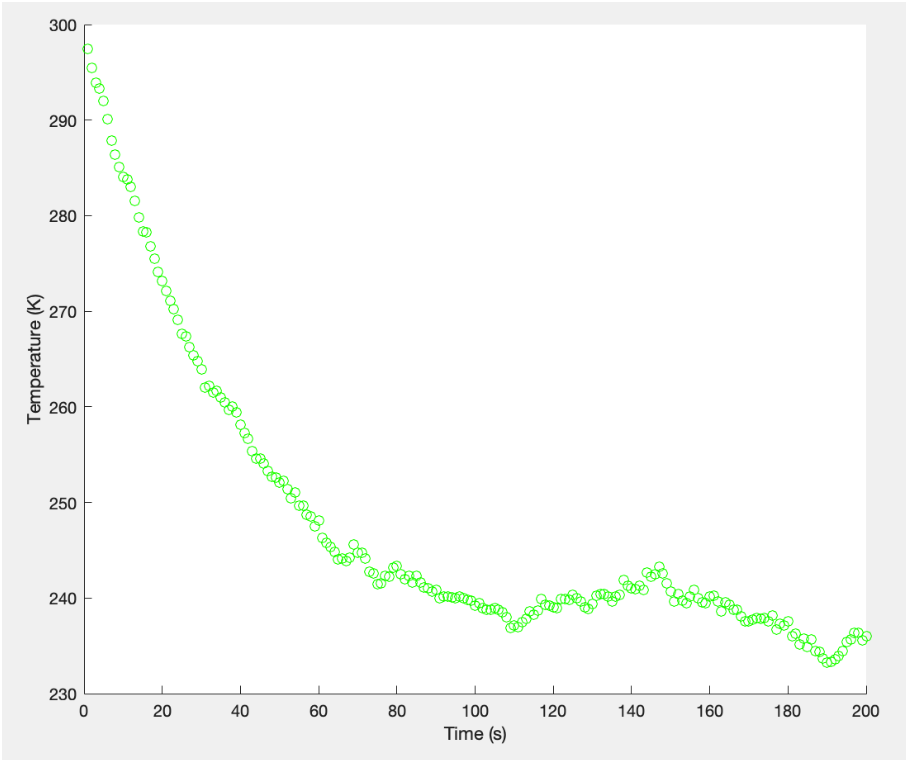

Figure 5: Temperature plot over time with scattering.

What happens to the average temperature over time?

As time goes on and the electrons scatter more and more, the temperature (average kinetic energy of the particles) continues to drop, until it reaches a steady state. This occurs due to the electrons losing kinetic energy each time they scatter inelastically (overall energy isn’t conserved since the new velocities are random). This results in the net kinetic energy decreasing up to a point.

d) MFP and τmn

mfp	3.7404e-08	m
avgmfp	5.1375e-08	m
tmn1	2.0000e-13	s
tmn2	2.7471e-13	s

The simulated MFP and τmn (avgmfp, tmn2) were found to be fairly similar to the ones calculated in Part 1 (mfp, tmn1).

3. Enhancements

All of the part 3 code has been done with the option to turn on and off: injection (no electrons present at the start, electrons being injected from the left), boundary conditions, scattering and boxes.
Part 1 uses injection OFF, boundary conditions ON, scattering ON and boxes ON.

1.

a) 2-D Plot of Particle Trajectories

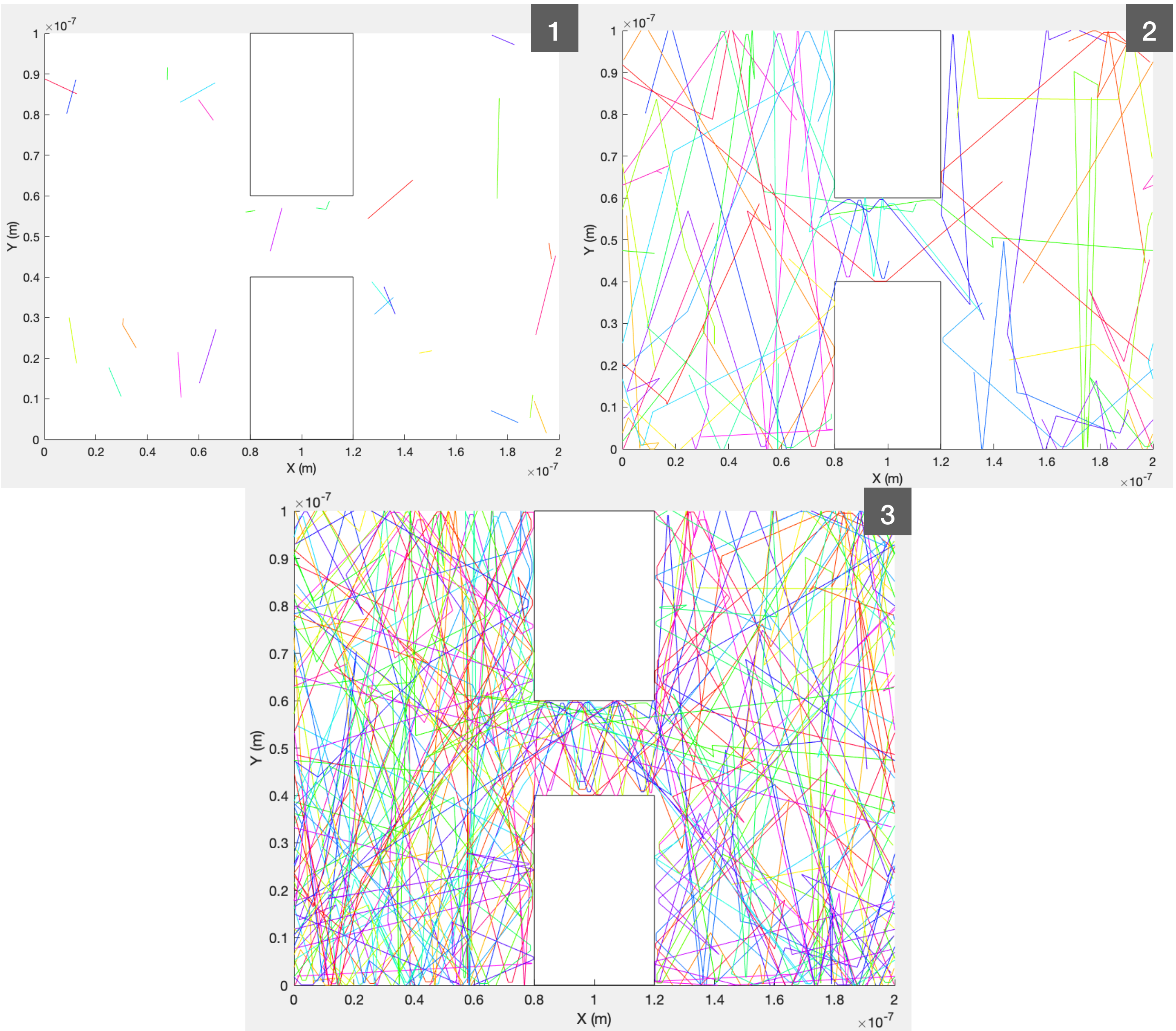

Figure 6: Sample electron trajectories with the “bottle-neck” effect at 3 different time points.

b) Electron Density Map

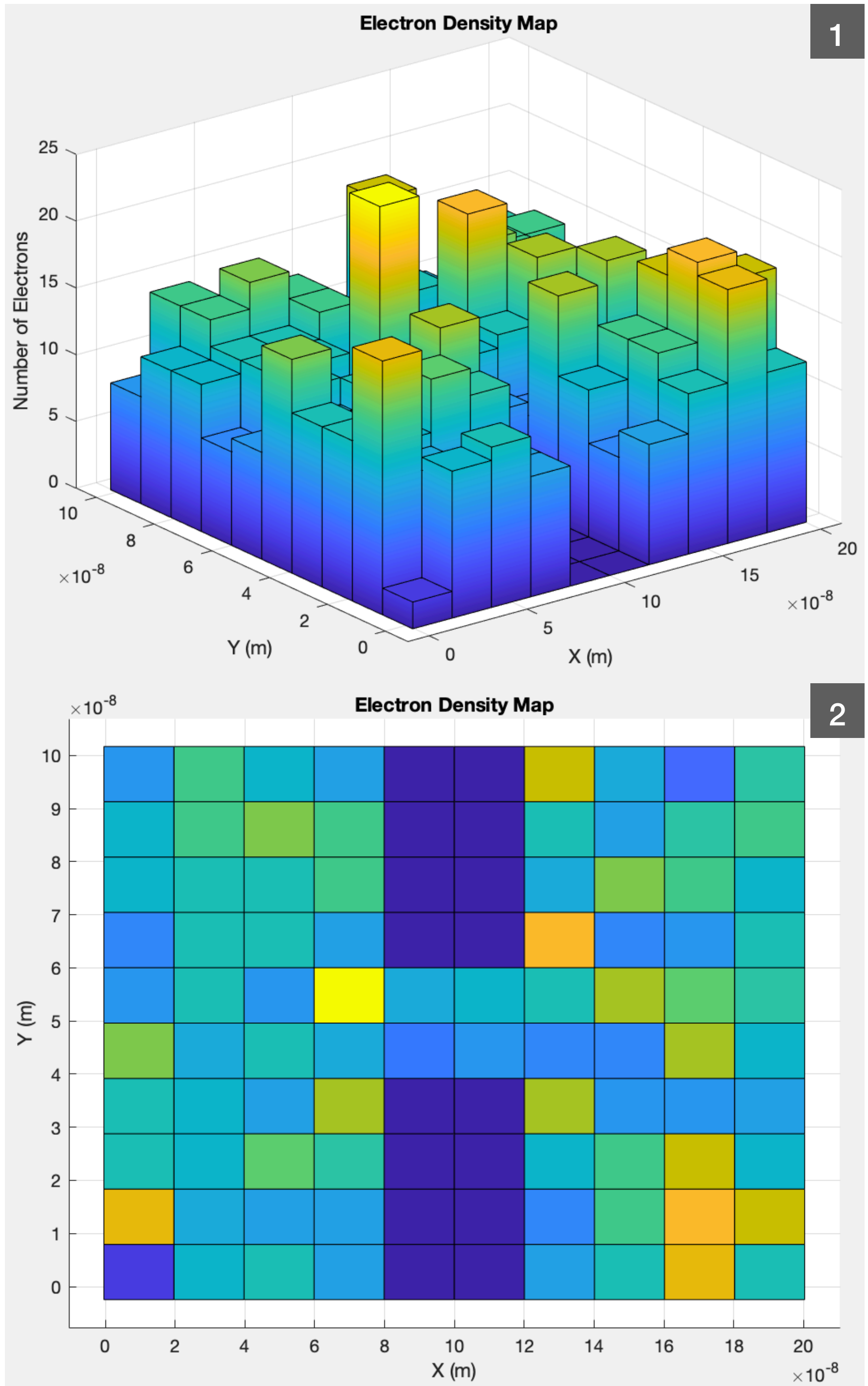

Figure 7: Electron density map viewed from the side (1) and above (2).

c) Temperature Map

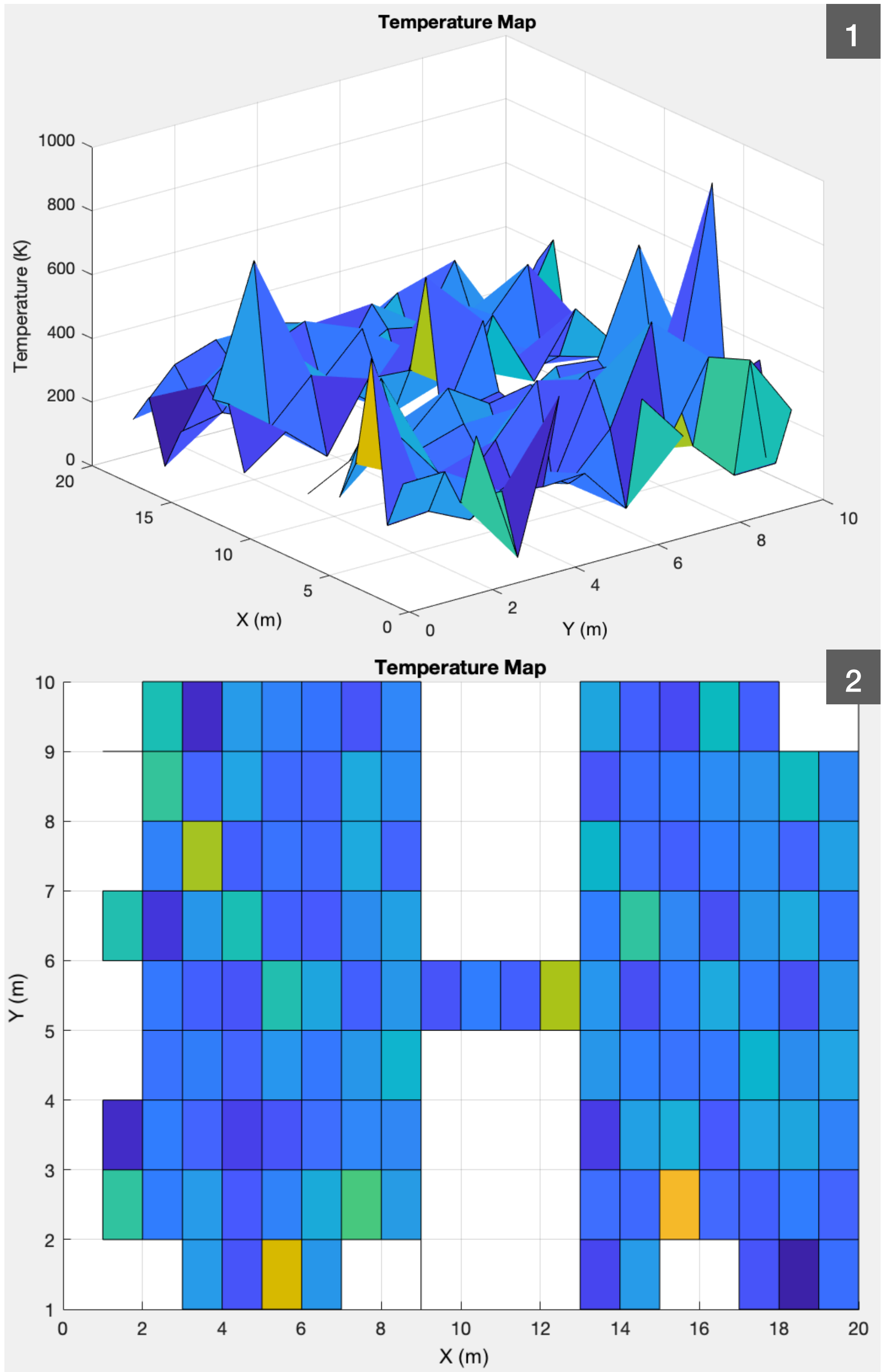

Figure 8: Temperature map viewed from the side (1) and above (2).

2. b)
The part 3.2 enhancements were done following the 2b) Injection model.
Part 2 uses injection ON, boundary conditions OFF, scattering ON and boxes ON.

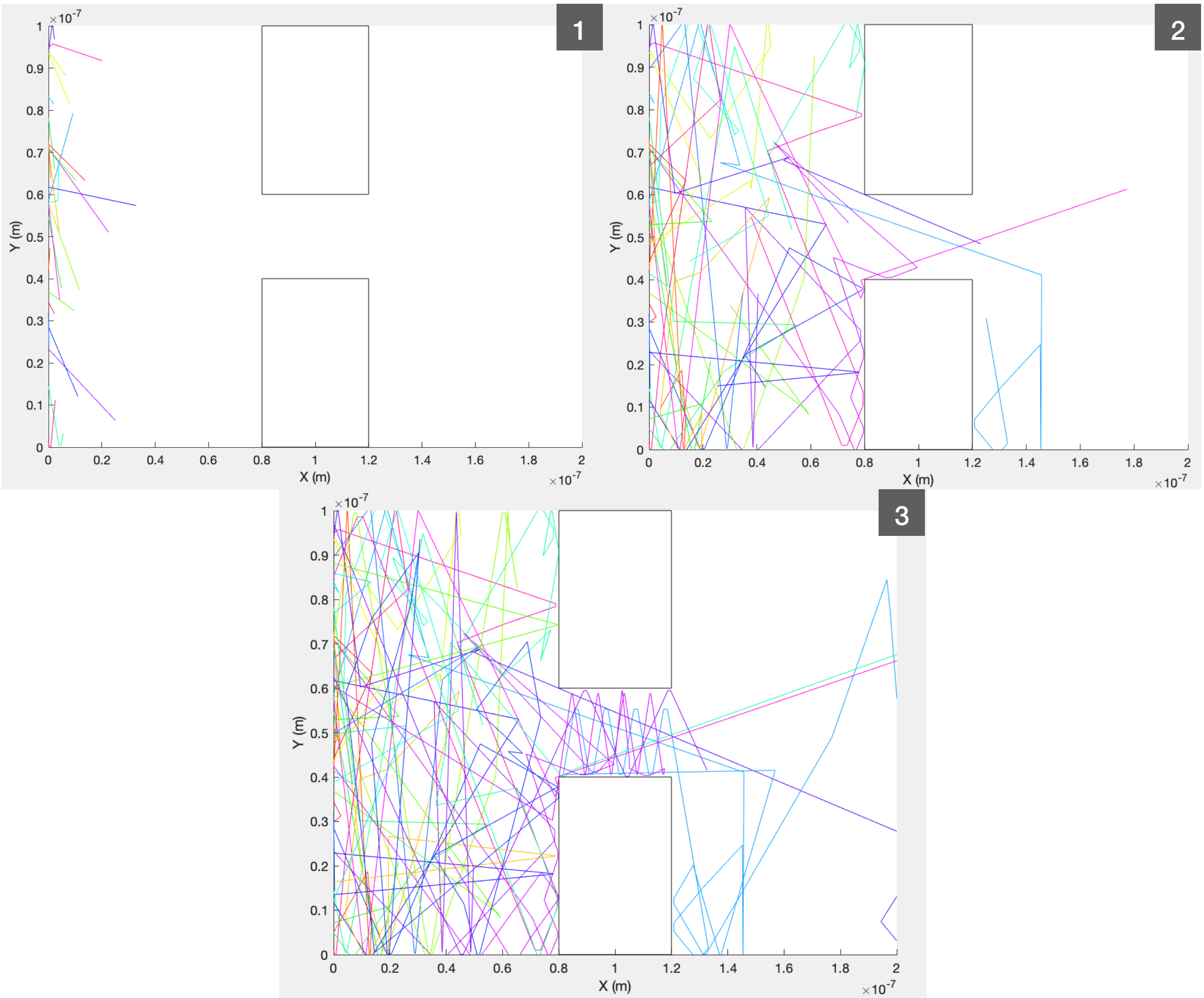

Figure 9: Sample electron injection from the left side at 3 different time points.