Final report

# Analysis of 2D Arc-PIC simulations

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## 1 Field emission

There had seemed to be some problems with the current density being a bit lower than expected from the Fowler-Nordheim (FN) equation. I tested this with the `FlexFN2_ring` model (which only injects electron), with a 6 $\mu$m emitter radius and the local field set to 12 GV/m (with circuit model `FixedVoltage`, parameter `UNz` set to about 2.37). I was able to reproduce the problem, but for me it was due to a simple mistake in calculating the FN current density. I had used $d_{gap} = 20.0$ $\mu$m instead of the actual value 20.0058872585 $\mu$m. The 0.03 % error in the gap distance resulted in $\sim 0.3$ % error in the current density.

Before finding my error I also rederived some of the equations in the code concerning field emission. I found no errors in them.

In the file `arcbound_original.cpp` (and similarly in other arcbound-files) the local field at the emitter is calculated:

```
field = - 2.69036254e-10*dz/SQU(Omega_pe)*sqrt(T_ref*n_ref)*Ez[i]*beta;
```

after which the current density is calculated with FN equation:

```
double I_FN = 4.7133e9 * SQU(field) * exp(-62.338/field);
```

and finally converted into number of superparticles injected:

```
//Rescale to units (#Superparticles / omega_pe^-1) / lambda_Db^2
I_FN *= Ndb/(6.7192539e-12*n_ref*sqrt(T_ref));
//Area factor
I_FN *= alpha;
// [#superparticles]
I_FN *= PI*(SQU(R2*dz)-SQU(R1*dz))*(e2inj_step*Omega_pe);
```

Everything seemed to be correct and derived from original and accurate expressions. For example, the derivations were done with

$$\lambda_{DB} = \sqrt{\frac{\epsilon_0 T_e}{e^2 n_e}} \approx \sqrt{\frac{552635 \cdot T_e}{n_e}} \text{ [cm]},$$

instead of

$$\lambda_{DB} \approx 7.43 \cdot 10^2 \sqrt{T_e / n_e}.$$

The less accurate form was found elsewhere in the code, at least in the files `init.cpp` (line 139) and `initialParticles.cpp` (line 104), but to my understanding (and experimenting) these do not affect the field emission.

# 2 Space charge

After looking at the field emission, I switched space charge and particle collisions back on and investigated how emitter size and the external field affect the current density. The simulations were again run with `FlexFN2_ring`, which only injects electrons, with emitter radii of 6.0, 3.0, 0.5 and 0.1 $\mu$m. The potential was set using circuit model `FixedVoltage` and input variable `UNz [Te]`. `UNz [Te]` was scanned from 0.4 to 2.0 `Te` in steps of 0.1, although some points of interested were scanned with more precision. The reference electron temperature `Te` was 2900. The local field at the emitter (without space charge) was calculated with:

$$E_{loc} = \frac{\beta \cdot \mathrm{UNz} \cdot \mathrm{T_e}}{d_{gap}} = 5.0735065 \ \mathrm{T_e} \text{ [GV/m]},$$

where the gap distance $\mathrm{d_{gap}} = 20.0058873$ $\mu$m, field enhancement factor $\beta = 35$ and the electron reference temperature $\mathrm{T_e} = 2900$ V. The results can be seen in Figure 1 and Figure 2.

Each simulation was 10 000 timesteps ($\sim \ 1.8 \cdot 10^{-2}$ ns). The current density always started at the FN value, but quickly decreased as the electrons filled the gap. There was usually some oscillation as the current density settled at its space charge limited value (see Figure 3). The mean current density (from the cathode) of the last 5000 timesteps was chosen as the final value of the current density.

Because the emitted current density ranged many orders of magnitude, it was necessary to change the particle weighting accordingly. This I did by trial and error, making sure that there was a sufficient amount of particles in the system for an accurate space charge effect, while keeping the simulation time and size small. The corresponding parameter `Particles in a Debye cube Ndb` ranged from $\sim 10$ to $\sim 10^7$.

I checked if the current density changed significantly, when the number of super particles was changed (in either direction). Based on these tests I am quite confident that the data points in Fig. 1 and Fig. 2 do not have significant error bars. However, if a more rigorous analysis of the space charge effect is needed (e.g. for code-to-code comparisons), it would be better to run the simulations

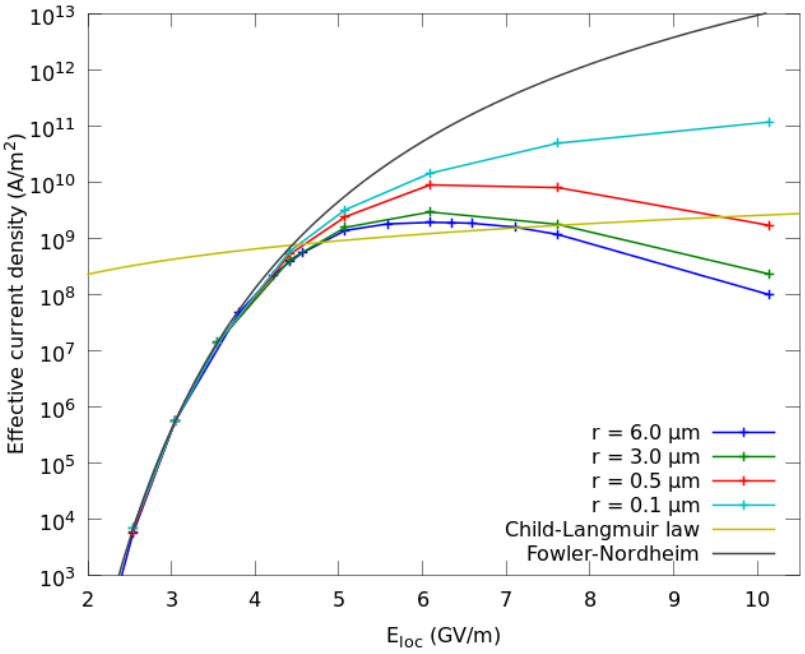



Figure 1: Space charge limited current density. The local field $E_{loc}$ is calculated from the external field (no space charge).

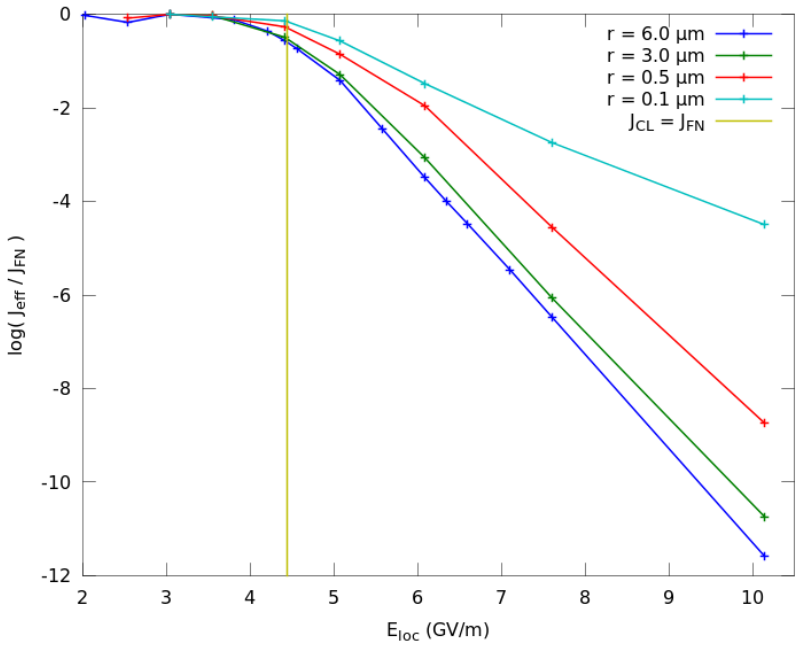



Figure 2: The ratio of space charge limited current density to the Fowler-Nordheim current density, showing the relative effect of space charge. The yellow line shows the point where FN emission reaches CL law.

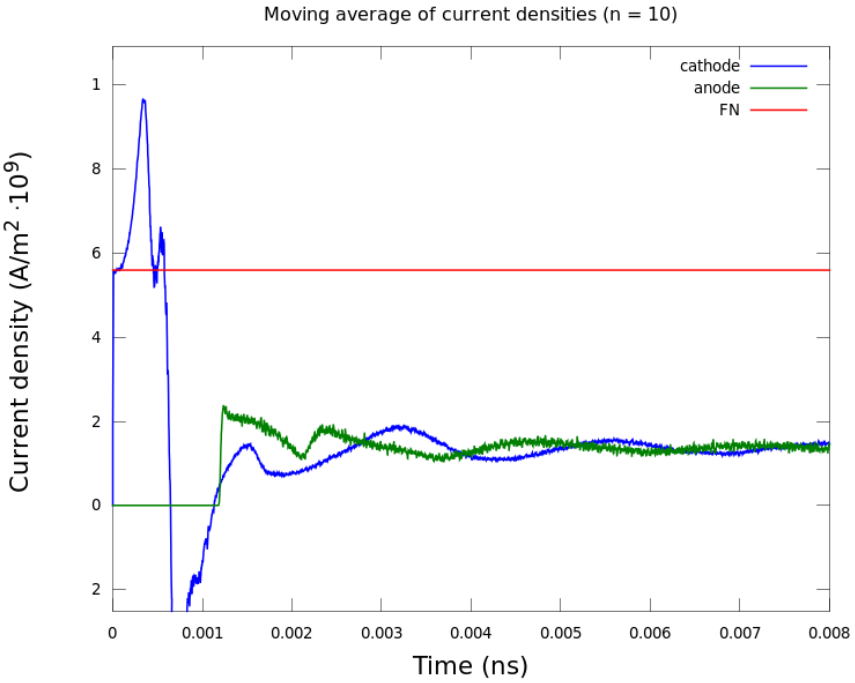



Figure 3: Space charge limited current density settling to its final value. This figure covers the first 5000 timesteps.

again, treating the super particle ratio more consistently. For example, keeping the number of particles in the steady state approximately constant.

From the results, we can see that with a low external field the effective current density is very close to that given by the FN equation. At around 4 GV/m the space charge begins to significantly limit the current, reducing it by several orders of magnitude. The limiting effect is greater the bigger the emitter is. The big emitters also seem to reach their maximum current density at some point, after which strengthening the external field only lowers the average current. It's not clear if emitters of all sizes reach their maximum at some point.

To further investigate the space charge effect, I compared it to the Child-Langmuir (CL) Law[1] (also known as Child's Law or the Three Halves Power Law)

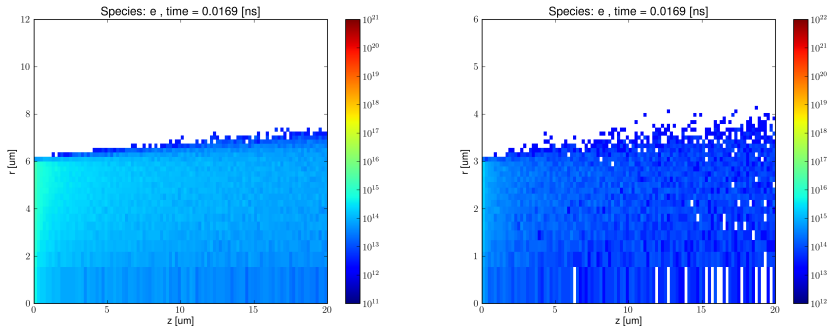
$$J_{CL} = \frac{4\epsilon_0}{9}\sqrt{2e/m_e}\frac{V^{3/2}}{d^2},$$

where $V$ is the voltage between the electrodes and $d$ is the gap distance. In our simulations (with $d = 20.005887$ $\mu$m) the equation can also be written:

$$J_{CL} = 1.65011 \cdot 10^{10} E^{3/2} \text{ [A/m}^2\text{]},$$

where $E$ is the external field ($E = E_{loc}/\beta = E_{loc}/35$).

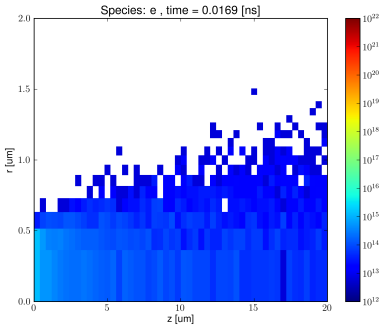
[1] http://en.wikipedia.org/wiki/Space_charge#Child.27s_Law



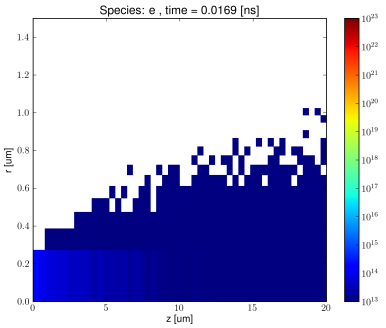

6.0 $\mu$m




3.0 $\mu$m




0.5 $\mu$m




0.1 $\mu$m

Figure 4: Distribution of electrons in a steady state of space charge limited field emission.

The CL equation gives the maximum current density, in a situation where:

1. The electrodes are planar, parallel, equipotential surfaces of infinite dimensions.
2. Electrons travel ballistically between electrodes (i.e., no scattering).
3. The electrons have zero velocity at the cathode surface.
4. In the interelectrode region, only electrons are present.
5. The current is space-charge limited.
6. The anode voltage remains constant for a sufficiently long time so that the anode current is steady.

In these simulations, all but the 1st and 2nd conditions are met. However, after running a few simulations with space charge switched off but collisions switched on, as well as space charge on but collision off, it was clear that the scattering of electrons through collisions was insignificant. Therefore, one of the main reasons

for the discrepancy between the CL equation and the simulations could be that the emitter radius wasn't infinite. As the gap distance remained constant, the ratio $R_{emission}/d_{gap}$ was higher for bigger emitters, which is why they followed CL Law more closely. This could also be seen by the amount of dispersion. With 6.0 and 3.0 $\mu$m emitters the radius of the electron flux grew about 15 % (very rough estimate), with 0.5 $\mu$m $\sim$ 150 % and with 0.1 $\mu$m $\sim$ 1000 % (Figure 4). The discretization from the PIC method could also contribute to the discrepancy.

Although CL Law doesn't fully apply in the simulations, it tells us when the space charge begins to have an effect on current density. This roughly at the point where $J_{FN} = J_{CL}$, or $E_{loc} \approx 4.44$ GV/m and UNz $\approx 0.86$. So in this sense, the space charge in the simulation is in agreement with theory.

# 3 Gridsize analysis

I briefly investigated how changing the gridsize affects simulation results. I ran the simulations with default settings. The simulation model was `ArcOriginal`, circuit name `TwoCapacitors` (with `UNz` set to 2.0), 1500 particles in a Debye cube (`Ndb`) and electron reference temperature `Te` 2900 eV. I changed only the number of grid cells and the size of a cell and the emitter, so that the physical size of the system remained the same. The cellsize was changed by increasing or decreasing the parameter `Grid size dz in Debyes` in the input-file. For the emitter, both the radius of injection (`Remission`) and the radius used for current calculation (`Remission_theor`) were changed.

The two main differences in the simulation results were the time of breakdown and the oscillations in the current (Figure 5). In all cases, the smaller the gridsize was the faster breakdown occurred. However, with smaller gridsizes there was significantly more oscillations in the current, both in short and long timescales. On short timescales the period of the oscillations was about the same and very sinusoidal, but on longer timescales the oscillations were more sporadic.

Gridsizes larger than 120x200 were prone to having very large current (and particle emission) spikes at the moment of breakdown, leading to very long simulation times and, at some point, an unresolved error that terminated the simulation.

Most of these effects may simply be due to the changing ratio of particles per cell (at a steady state), and could have been avoided by changing the particle weighting accordingly. For example, if the gridsize was changed from 120x200 to 240x200, the number of super particles should be quadrupled. However, according to earlier tests by Lotta Mether and Kyrre Sjøbæk, the correlation between gridsize and time-to-breakdown persists even when the super particle ratio is accounted for.

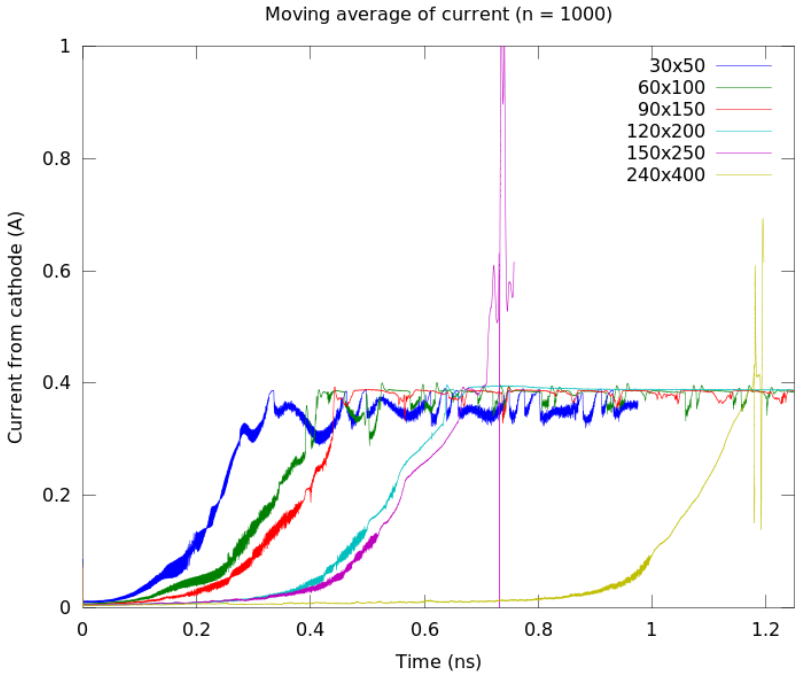



Figure 5: Current from cathode with different gridsizes. The current is calculated as a moving average of the neighbouring 1000 timesteps.

# 4 Initial distribution of neutrals

First, I ran simulations with the default settings (see the beginning of previous section), adding only the initial distribution of neutrals. As should be expected, adding the neutrals made the breakdown occur faster. Otherwise, the simulation results were roughly the same, although there was some indication that increasing the particle density of the distribution could lower the peak of the number of $Cu^+$ ions and electrons (see Figure 7 and Figure 8).

Distributing the same amount of neutrals in a smaller area near the emitter also made the breakdown occur faster (Fig. 10 and Fig. 11). An interesting exception is when the neutrals were distributed in the entire area. That case didn't actually take the longest for a breakdown to occur, but the peak of the number of $Cu^+$ ions and electrons was clearly lower than in other cases.

Next I tried to see if sputtering alone could cause a breakdown to occur. Again, I used the original settings, but set the ratio of emitted neutrals per emitted electrons (`r_Cu_e`) to zero. I used distribution sizes from 1$\mu$m x 1$\mu$m to 20$\mu$m x 20$\mu$m, and number of initial neutrals from $3.9 \cdot 10^5$ to $9.4 \cdot 10^6$. The neutral injection temperature was 300 eV.

I found that breakdown current could in fact be reached, but only very briefly. As expected, increasing the number of electrons increased the current overall, however, the breakdown curret always remained the same. Only the neutrals right next to the emitter caused significant ionization. An optimal distribution size was roughly 2 $\mu$m x 2 $\mu$m, which is smaller than the emitter radius (4$\mu$m). Because I used the original settings, the radius used for calculating the FN current density was actually only 1 $\mu$m, but the electrons were emitted from an area with 4 $\mu$m.

Classical sputtering alone cannot maintain a self-sustaining arc, because at the energy of $\sim$ 300 eV the sputtering yield is less than one[2]. Nevertheless, there seems to also be at least some heat spike sputtering in the simulations, because in some cases the total number of Cu and $Cu^+$ increased in the beginning (Fig. 15 and Fig. 16), meaning the sputtering yield should be $> 1$.

I tried increasing the injection temperature, which perhaps could increase the amount of heat spike sputtering. I didn't have time to run many simulations or do a thorough analysis, but increasing the injection temperature definitely increased ionization and the current (not the breakdown current), as can be seen in Figure 17.

[2] Yamamura & Tawara. Atom Data Nucl. Data 62 (1996) 149

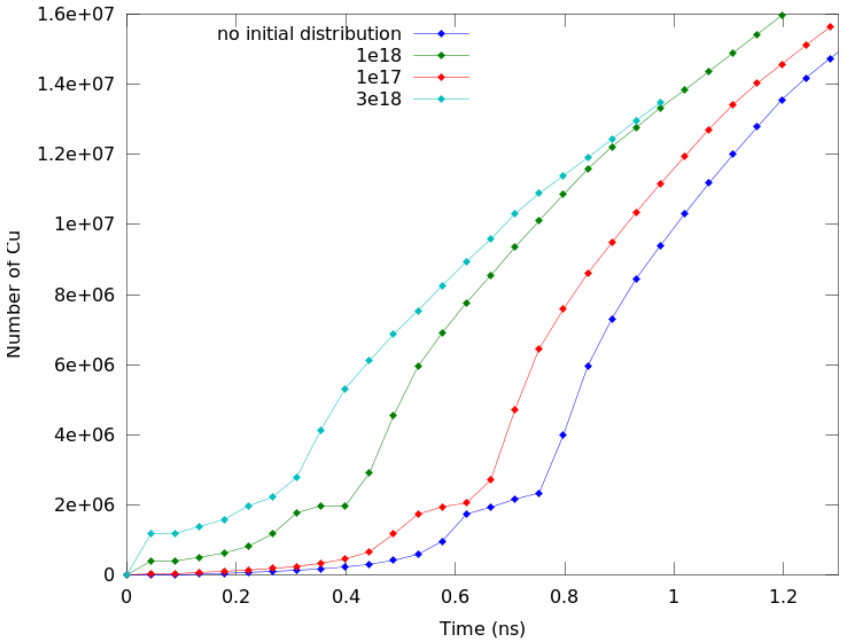



Figure 6: The number of neutrals in simulations with different initial neutral densities. The densities are in [1/cm$^3$] and the area of distribution is 5 $\mu$m x 5 $\mu$m.

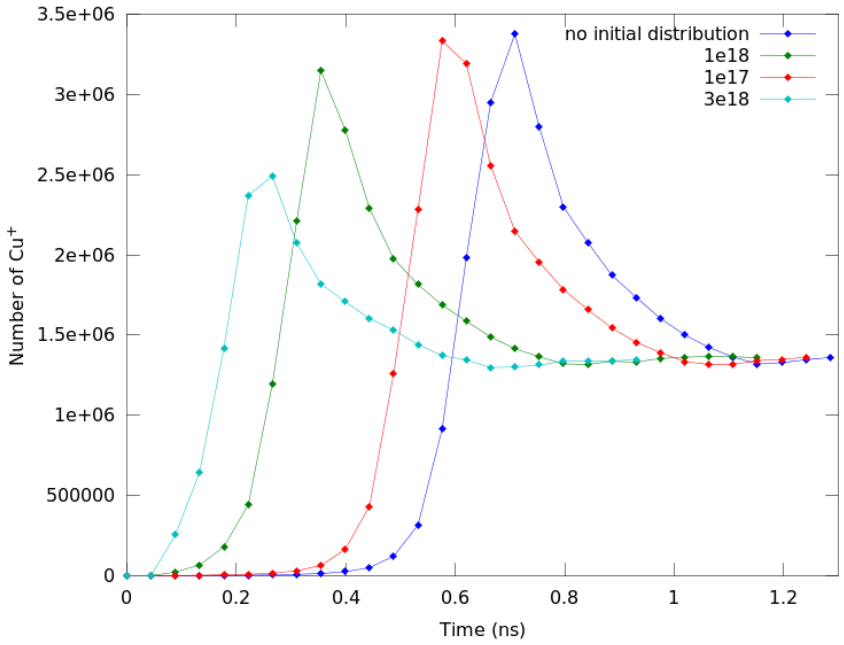



Figure 7: The number of $Cu^+$ ions in simulations with different initial neutral densities. The densities are in [1/cm$^3$] and the area of distribution is 5 $\mu$m x 5 $\mu$m.

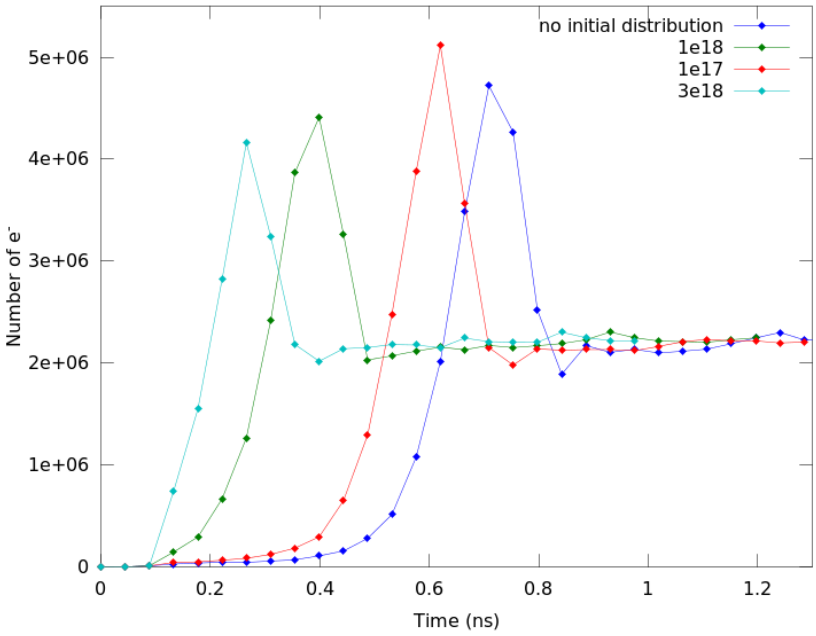



Figure 8: The number of electrons in simulations with different initial neutral densities. The densities are in [1/cm$^3$] and the area of distribution is 5 $\mu$m x 5 $\mu$m.

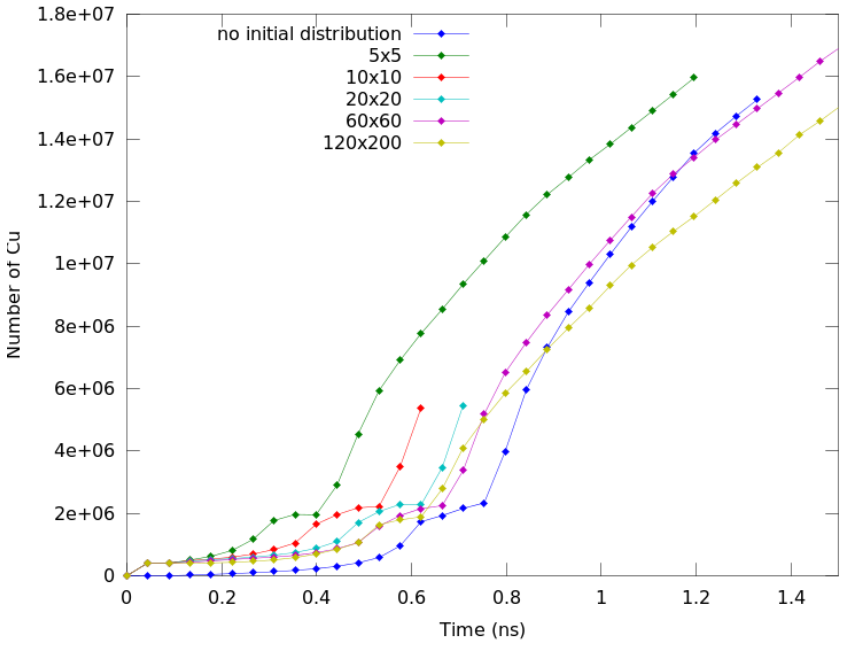



Figure 9: The number of neutrals in simulations with different areas of distribution. The number of particles in the initial distribution is always $3.93 \cdot 10^8$

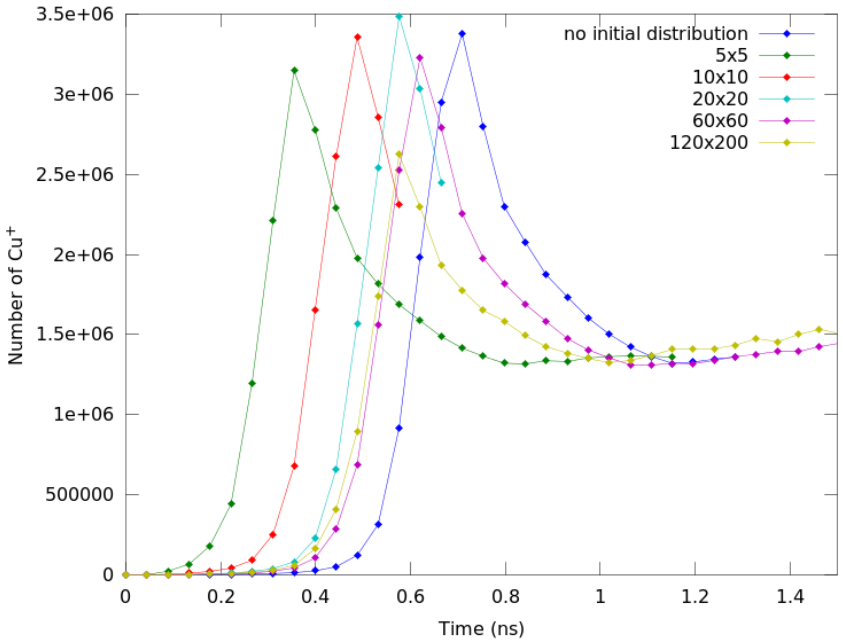



Figure 10: The number of $Cu^+$ ions in simulations with different areas of distribution. The number of particles in the initial distribution is always $3.93 \cdot 10^8$

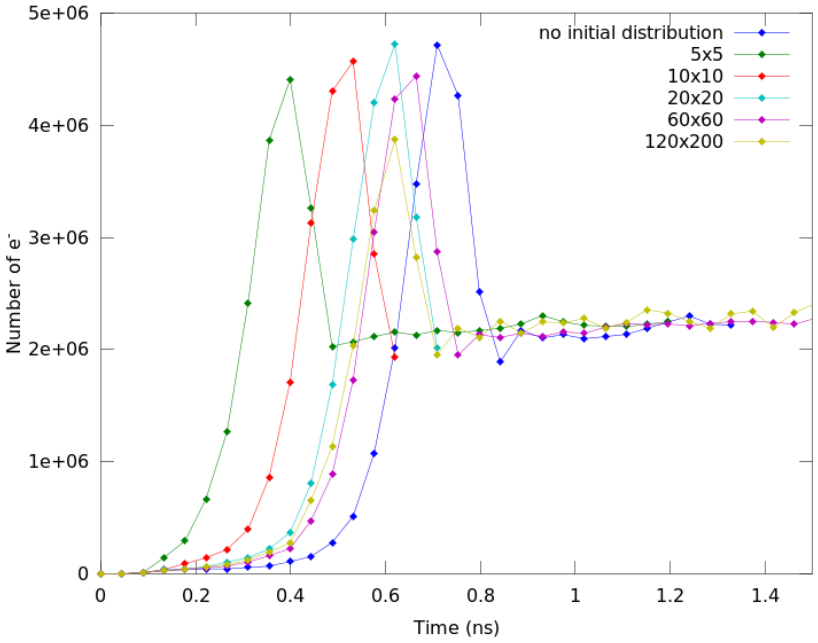



Figure 11: The number of electrons in simulations with different areas of distribution. The number of particles in the initial distribution is always $3.93 \cdot 10^8$

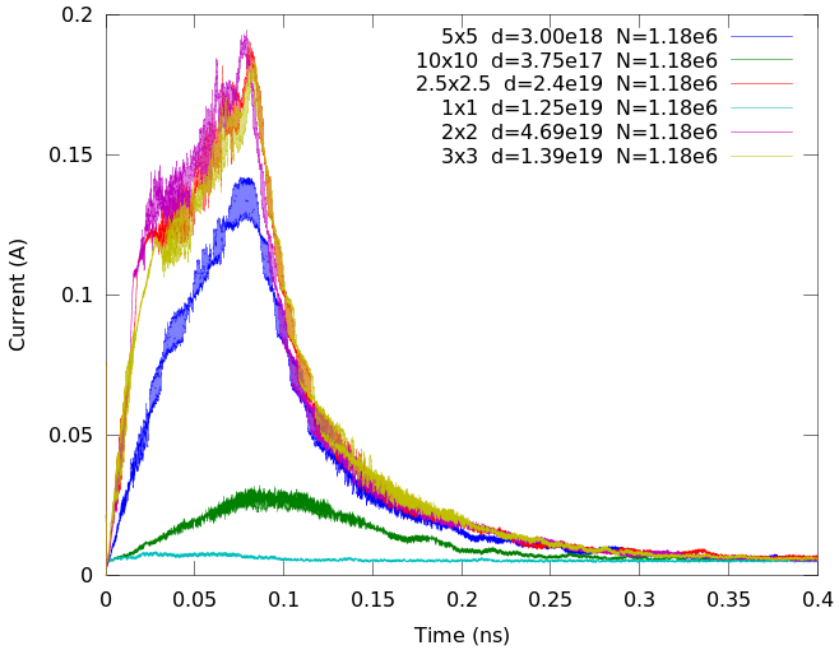



Figure 12: Currents from simulations with a fixed number of initial neutrals and no evaporation of neutrals.. The area of distribution is in [$\mu$m] and the corresponding density in [1/cm$^3$]. The current is calculated as a moving average of the neighbouring 1000 timesteps.

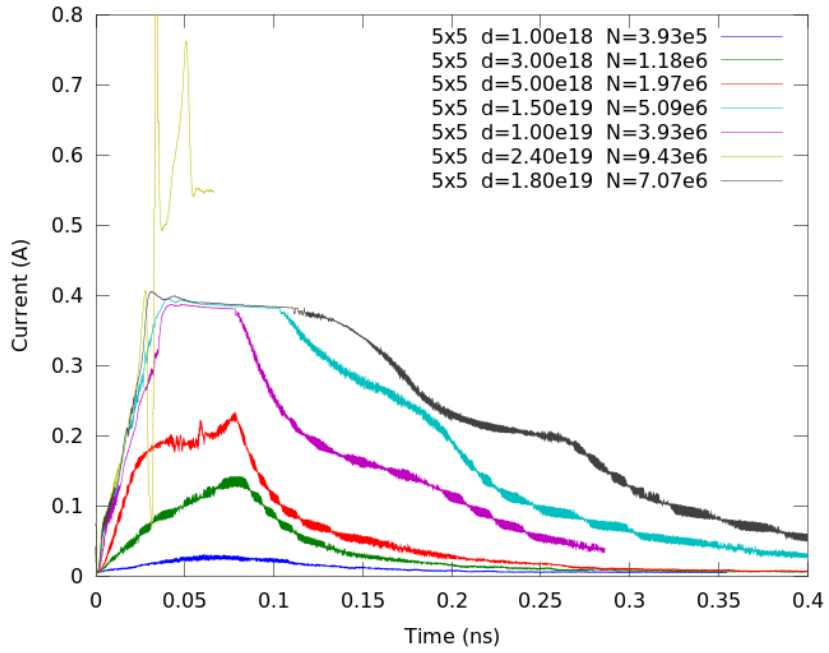



Figure 13: Currents from simulations with a fixed area of distribution and no evaporation of neutrals. The area of distribution is in [$\mu$m] and the corresponding density in [1/cm$^3$]. The current is calculated as a moving average of the neighbouring 1000 timesteps.

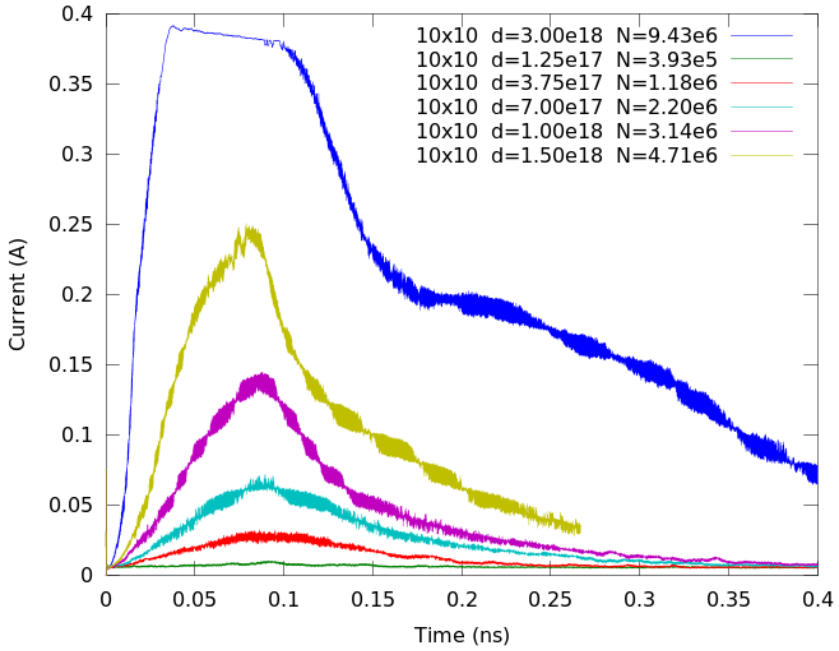



Figure 14: Currents from simulations with a fixed area of distribution and no evaporation of neutrals. The area of distribution is in [$\mu$m] and the corresponding density in [1/cm$^3$]. The current is calculated as a moving average of the neighbouring 1000 timesteps.

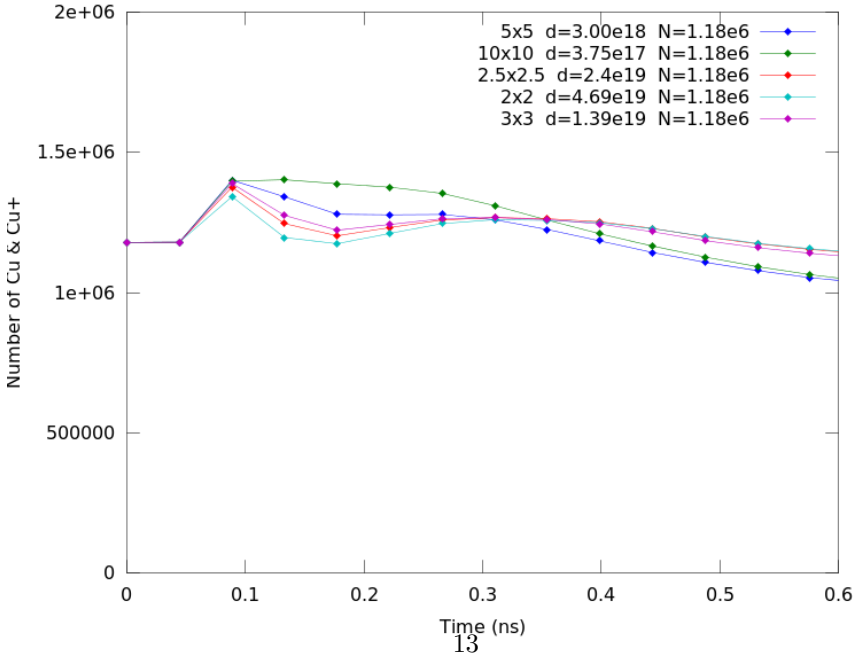





Figure 15: The total number of neutrals and $Cu^+$ ions in simulations with no evaporation of neutrals. The area of the initial distribution is in [$\mu$m] and the corresponding particle density in [1/cm$^3$].

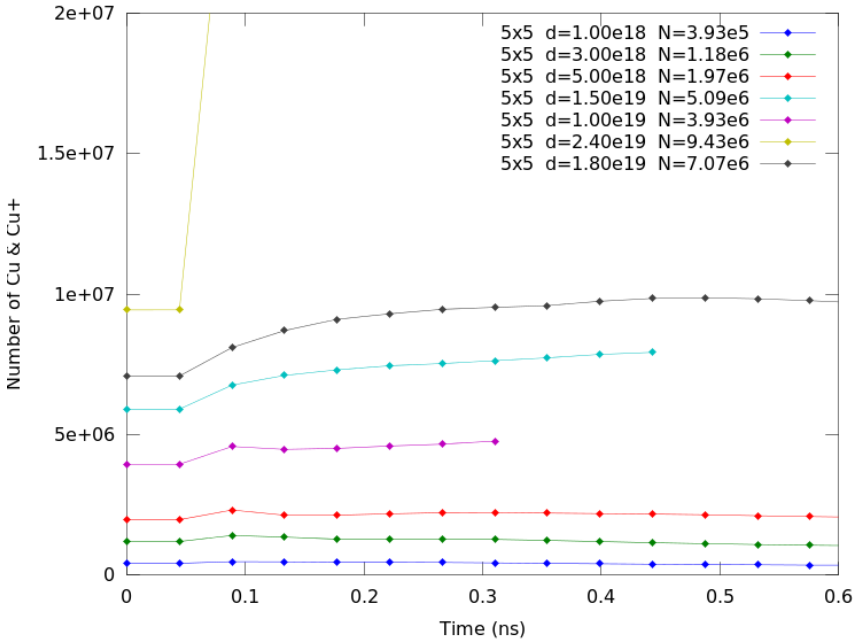



Figure 16: The total number of neutrals and $Cu^+$ ions in simulations with no evaporation of neutrals. The area of the initial distribution is in [$\mu$m] and the corresponding particle density in [1/cm$^3$].

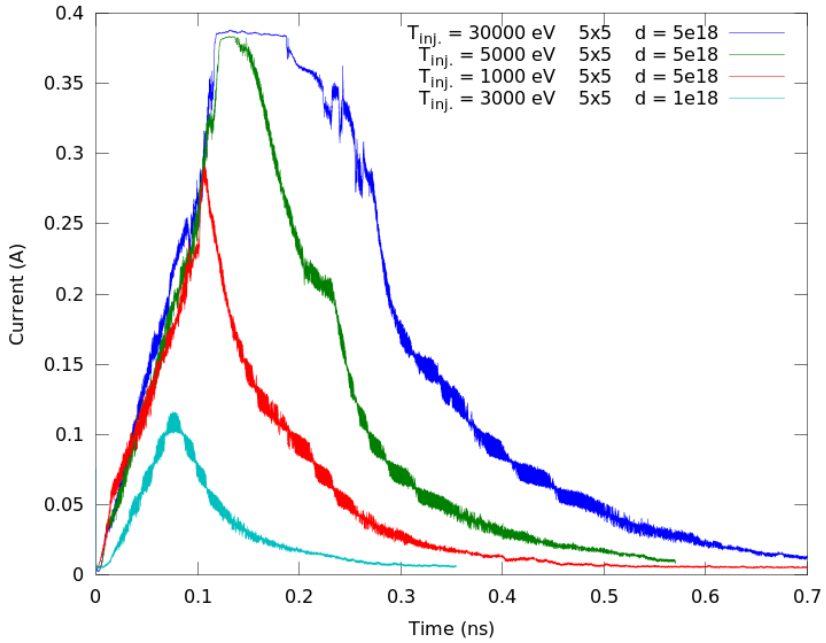



Figure 17: Currents from simulations with varying injection temperature of neutrals. The currents are calculated as a moving average of the neighbouring 1000 timesteps.