Simulating early-stage vacuum arc plasmas

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Thanks to Helga Timkó and Walter Wuench

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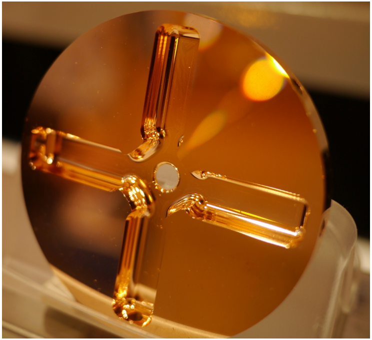
Outline

Motivation

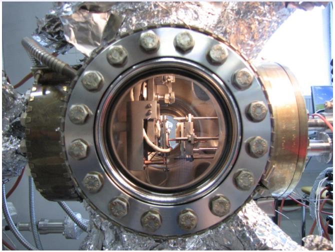
- Want to build high-gradient ($E_{\mathrm{acc}} \geq 100\mathrm{MV/m}$) particle accelerators
- Highest gradient achieved in normal-conducting structures
- Gradient limited by arcs
- Understand arc ignition!

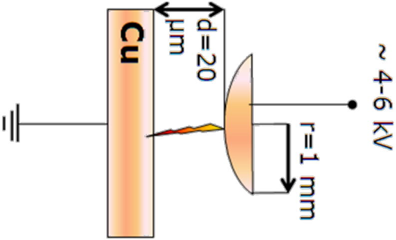
→ Design structures more resistant to arcing

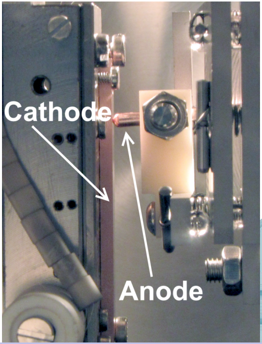


Experimental comparison: DC spark experiment

- High-voltage DC pulses on spark gap in ultra high vacuum
- Understand basic behavior of vacuum arc breakdowns
- Measure gap voltage & current through the breakdown



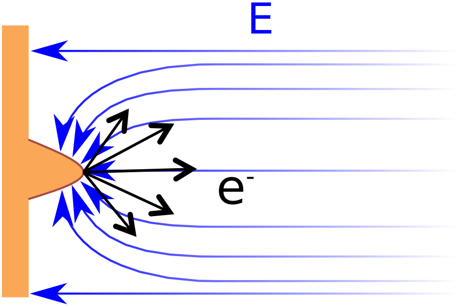




Evolution of a early-stage vacuum arc

Stages:

1. Field emission
2. Ionization cascade
3. Expansion



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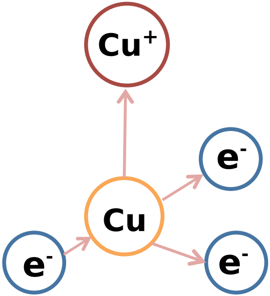
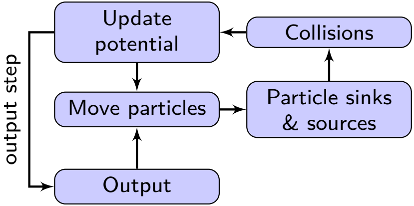


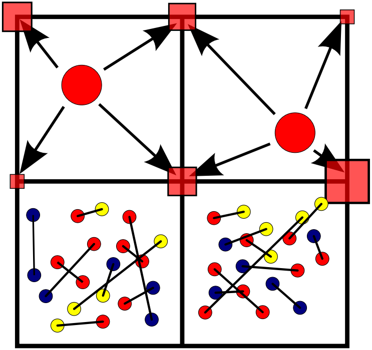
Particle in cell (PIC) + Monte Carlo Collisions (MCC)

- Volume divided into grid
  - Field solver
  - Proximity for collisions
- Macro-particles moves in continuous phase-space

Main loop:



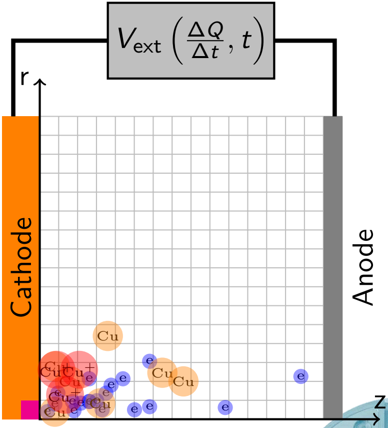
Distribute charges to grid points



Collide random pairs of particles in each cell

ArcPic2D

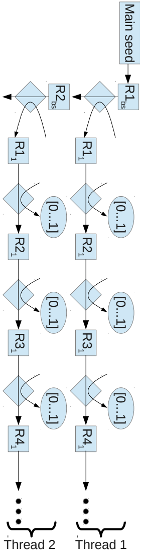
- 2d3v electrostatic particle-in-cell (PIC) + MCC
  - cylindrical symmetry
  - uniform grid
  - finite-difference field solver
  - Monte-Carlo collisions
- Planar electrode geometry
- Particles: e^-, Cu^+, Cu
- Physics (***modular part***):
  - ***External circuit***
  - ***Particle emission***
  - Collisions (el./inel.)
  - Electrostatic interaction
- C++, partly OO for modularity
  - Test physics models
- Supports parallel execution



Code originally developed by Helga Timkó

ArcPic2D parallelism

- OpenMP multithreading
  - Shared memory
  - Requiring few code changes
- Multi-stream RNG
- Parallel neutral-neutral collisions
- Load balancing
- Test case:
  - 1.8 M neutral particles
  - 5x5 µm cylinder
  - T=300 eV, $\rho = 10^{17}/\mathrm{cm}^3$
- Quite good scaling
  - Almost linear
  - Slower than ideal due to serial sections



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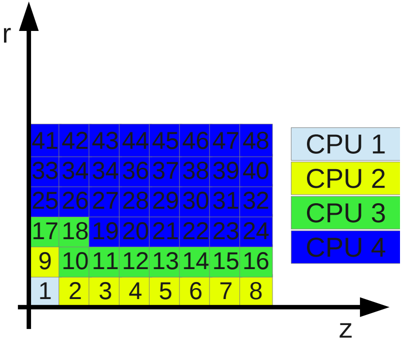

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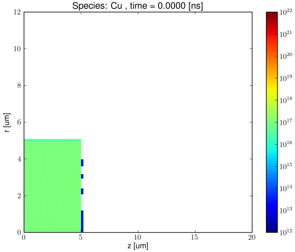

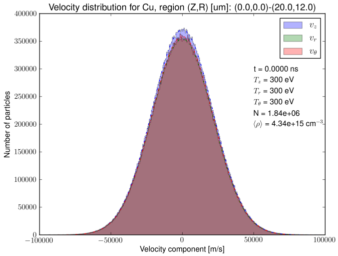

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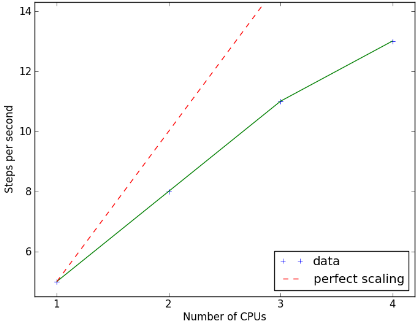
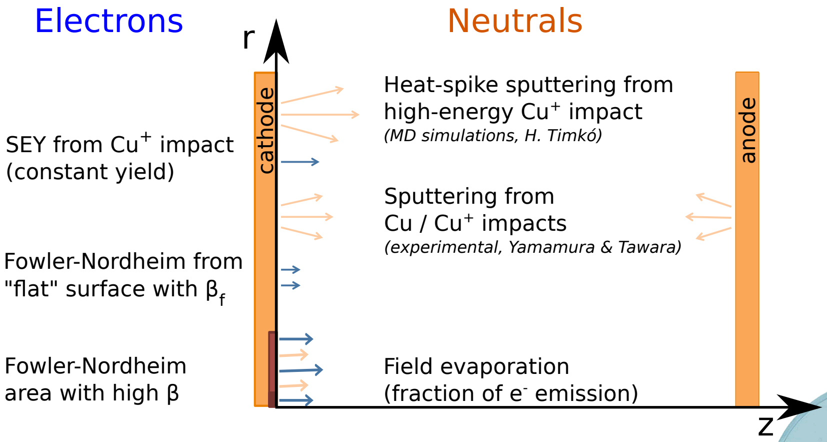
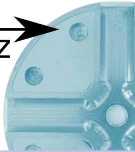


Emission model





Main simulation parameters

Emission:

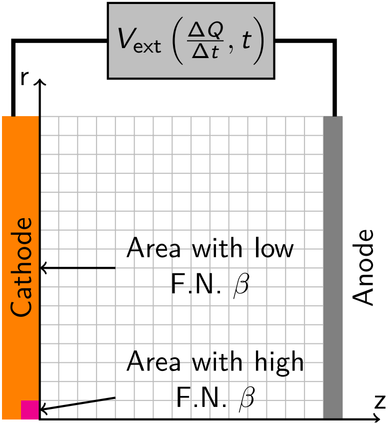
$$\beta_{\text{tip}} = 35.0$$
$$\beta_{\text{flat}} = 2.0$$
$$R_{\text{tip}} \approx 56\ \text{nm}$$
$$R_{\text{inj.}}(e^-) = 400\ \text{nm}$$
$$\frac{\#\ \text{Cu evap.}}{\#\ \text{e}^-\ \text{emitted}} = 0.075$$
$$R_{\text{inj.}}(Cu) = 2\ \mu\text{m}$$

Field:

$$E_z = 0.29\ \text{GV/m}$$

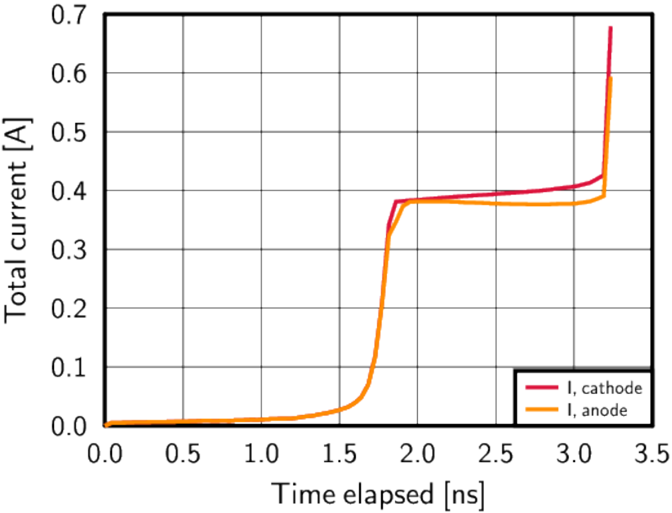
Mesh/domain:

$$R \times Z = 12 \times 20\ \mu\text{m}$$
$$\Delta Z = \Delta R = 0.1\ \mu\text{m}$$
$$\Delta t = 1.77\ \text{fs}$$
$$w_{\text{sp}} \approx 21.3$$

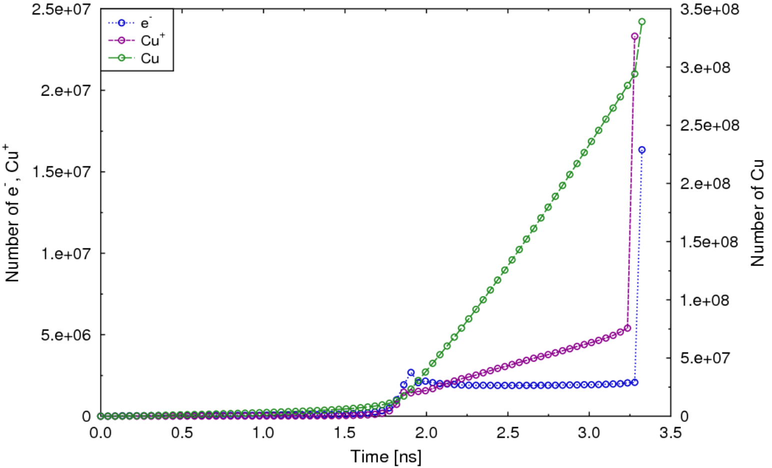


Main difference wrt. typical run:
More Cu, in larger area

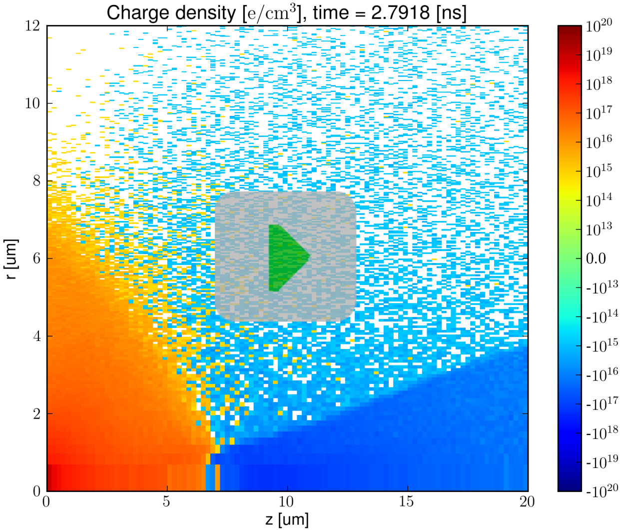
Current


0.7
0.6
0.5
0.4
0.3
0.2
0.1
0.0
Total current [A]
0.0
0.5
1.0
1.5
2.0
2.5
3.0
3.5
Time elapsed [ns]
I, cathode
I, anode

Particle count



Charge density



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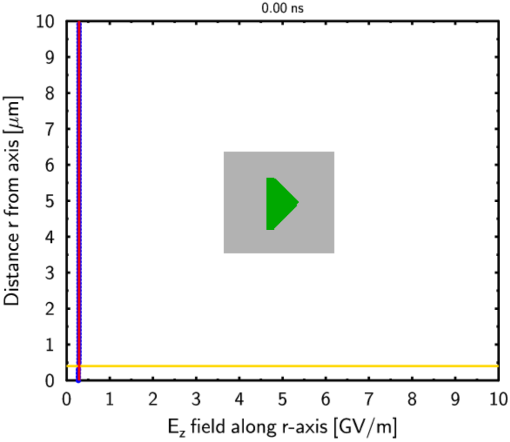
Field on cathode



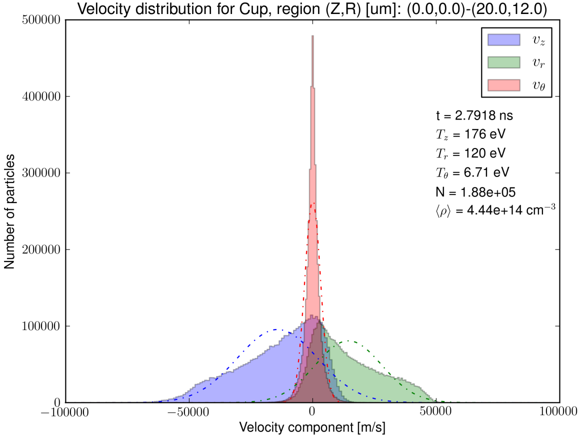
Last two frames

Fowler-Nordheim

On web

Velocity distribution

- Plasma far from equilibrium
- Hard to define a temperature
- Different velocity components and species have different distributions
- Some spatial separation



Conclusion

- Initial ignition
  - → Increasing neutral population
  - → Increasing Cu^+ population

⇒ Higher field on cathode
  - → activation of flat surface field emission
  - → rapid expansion of arc

Challenges

- Simulation speed with high particle numbers / dynamic range
  - Separate simulations for different regimes
  - Dynamic particle weighting
- Simplified surface model
  - Not taking surface state into account
  - Simplified heat spike sputtering model
  - High-field electron emission
  - Modeling of initial tip using only $E_z(r = 0)$

Summary

- ArcPic2D: 2d3v PIC/MCC simulation of vacuum arcs
- Breakdown spreading when E_z rises such that flat surface starts emitting
- Need to revisit surface models

System description

System
Electrons, ions and neutral atoms,
inside gap with metal ends,
with high electric field,
biased by external circuit

Description
Maxwells equations,
Newtonian mechanics,
Scattering & ionization crossections,
Surface physics model,
Circuit model

Wanted
Currents and particle densities
as function of space and time

Simulation
Plasma dynamics by PIC with Monte-Carlo collisions,
boundary conditions from surface & circuit models

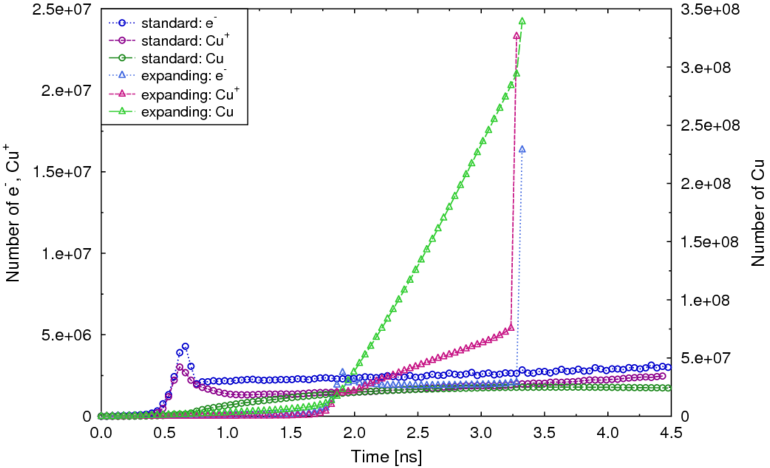
Monte-Carlo collisions

- Particles inside same cell
  are considered “close enough” to collide
- For each collision type, create random particle pairs
- Implemented collisions:
  - Coulomb scattering (e^-,e^-), (Cu^+,Cu^+), (Cu^+, e^-)
  - Elastic collisions (e^-,Cu), (Cu, Cu)
  - Charge exchange/momentum transfer (Cu^+,Cu)
  - Impact ionization $e^- + Cu \rightarrow 2\ e^- + Cu^+$

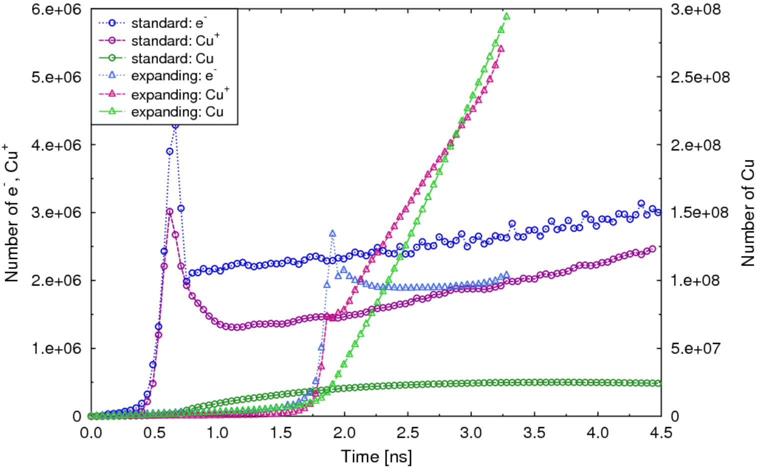
Results

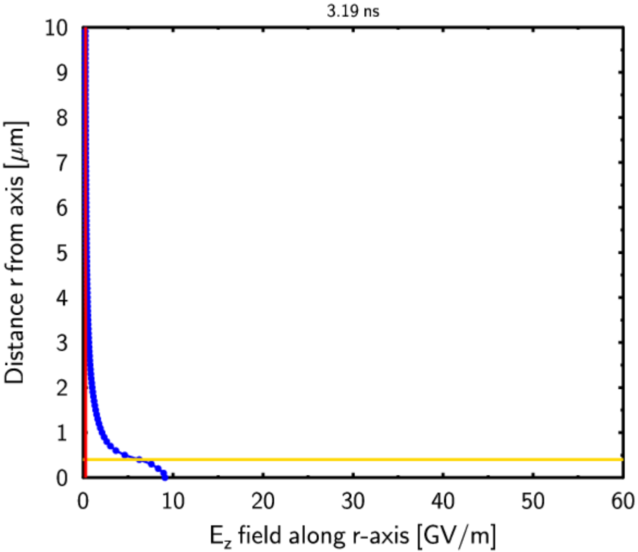
- Wanted: Set of parameters allowing arc ignition and growth
  - . . . while keeping within model validity boundaries
- Parameters studied:
  - Numerical convergence
    - Particle weigthing
    - Grid size
    - Time step
  - Electron injection
    - Special center-cell
    - All cells treated equal
    - Fowler-Nordheim β (tip/flat)
    - Tip melting current or time
  - Cu injection
    - Evaporation ratios
    - Evaporation area
    - Pre-injection

Particle w. comparison

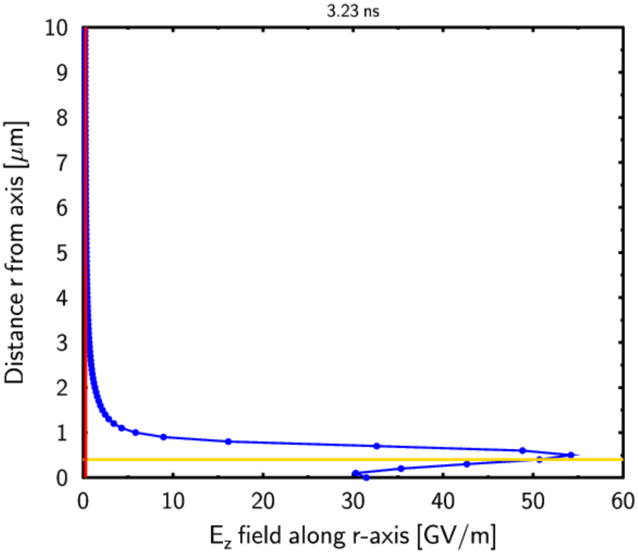


Particle w. comparison (zoom)





Back to field animation



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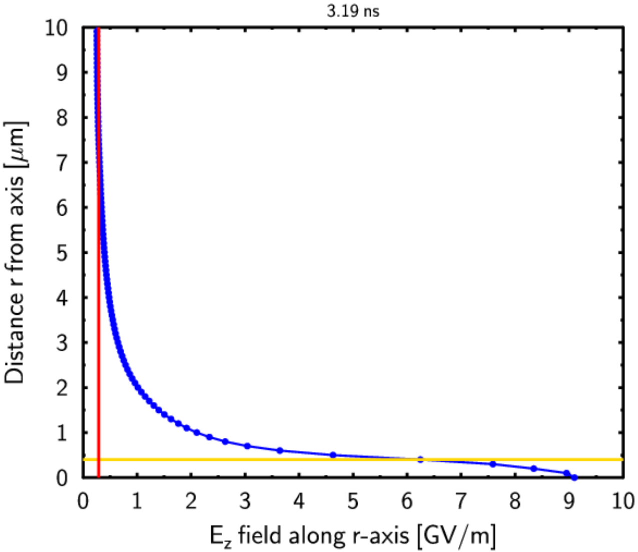
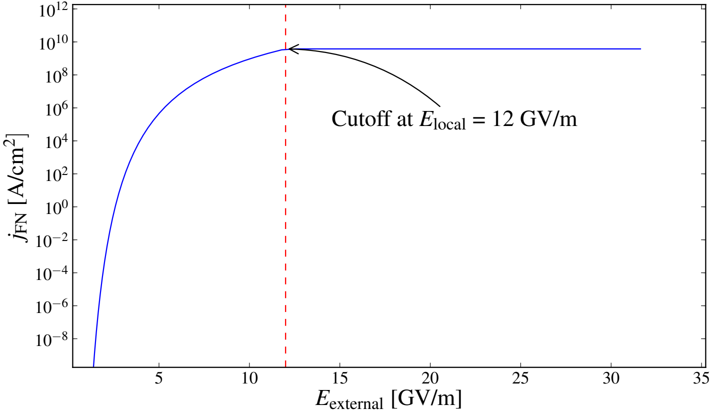
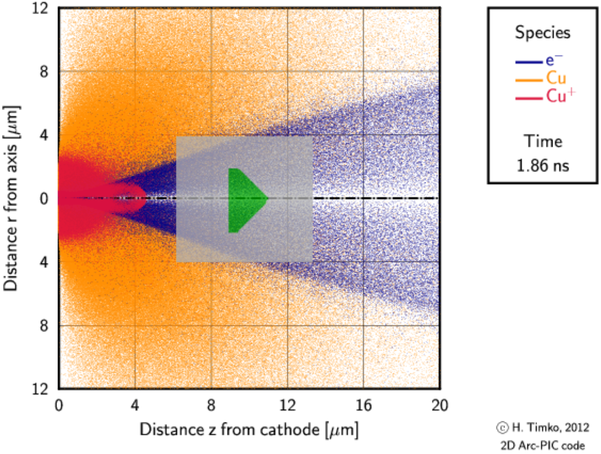


Back to field animation



Back to field animation

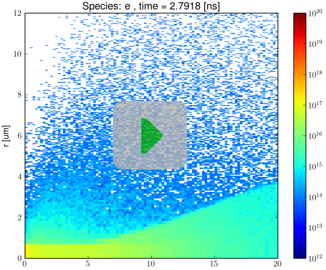
Particle plot

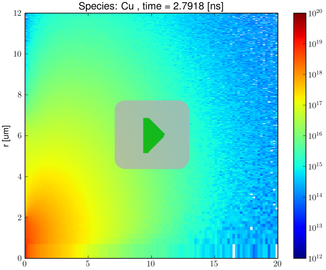


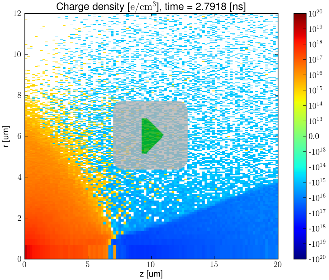
▸ Particle densities

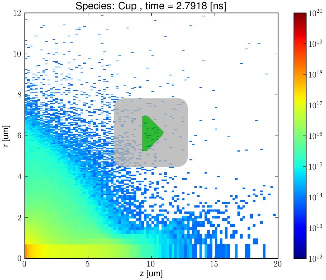
▸ On web

Density animations [cm^{-3}]









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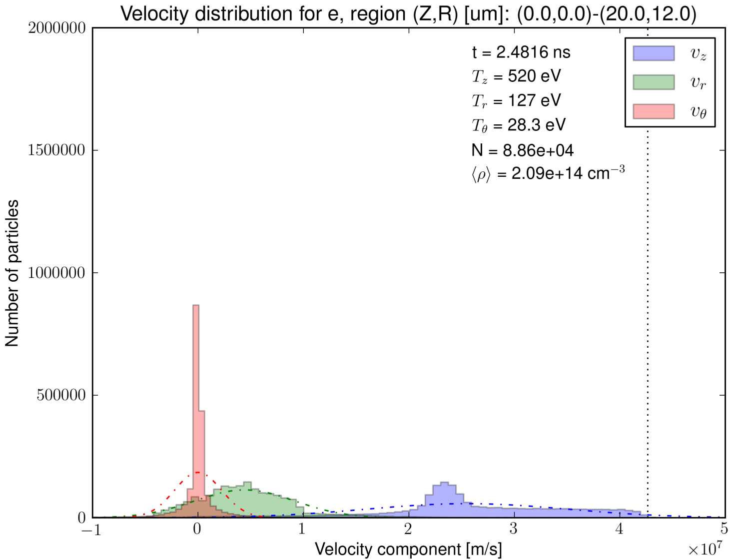
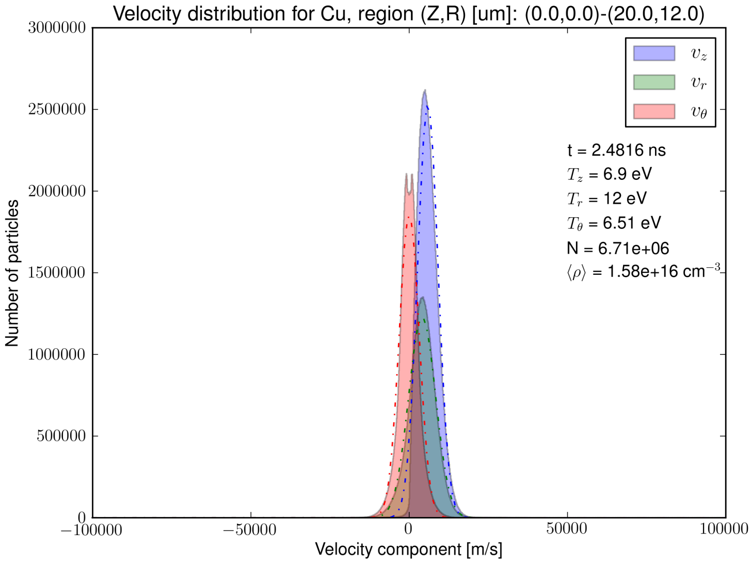

Velocity distribution for e, region (Z,R) [um]: (0.0,0.0)-(20.0,12.0)
t = 2.4816 ns
T_z = 520 eV
T_r = 127 eV
T_θ = 28.3 eV
N = 8.86e+04
$\langle\rho\rangle$ = 2.09e+14 cm^{-3}
v_z
v_r
v_θ
Number of particles
2000000
1500000
1000000
500000
0
−1
0
1
2
3
4
5
Velocity component [m/s]
$\times 10^7$


Velocity distribution for Cu, region (Z,R) [um]: (0.0,0.0)-(20.0,12.0)
Number of particles
Velocity component [m/s]
3000000
2500000
2000000
1500000
1000000
500000
0
−100000
−50000
0
50000
100000
v_z
v_r
v_θ
t = 2.4816 ns
T_z = 6.9 eV
T_r = 12 eV
T_θ = 6.51 eV
N = 6.71e+06
$\langle\rho\rangle$ = 1.58e+16 cm^{-3}