Plasma Build-Up in Vacuum Discharges

via Particle-in-Cell simulations

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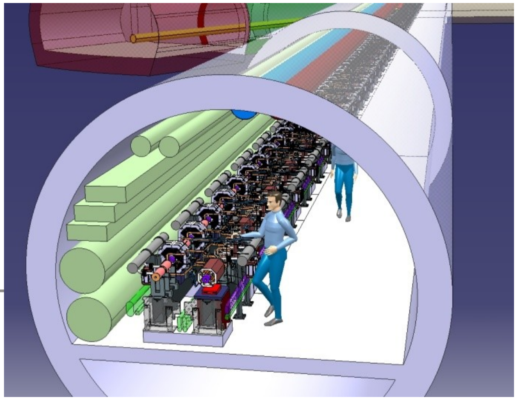
Outline

- Introduction: Why and how to model plasma build-up in vacuum discharges?
- A new tool for discharge simulation
  - 2D Arc-PIC code description
- Physical discharge model
  - Crucial assumptions and special aspects
- An example simulation

Introduction

Main concern: Vacuum discharges in CLIC

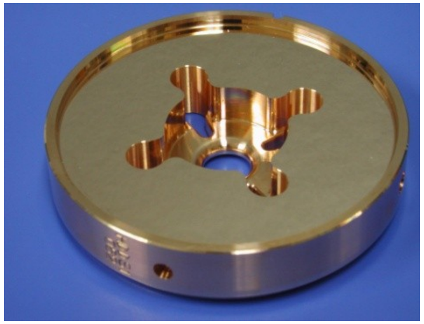


- Why to study vacuum discharges?

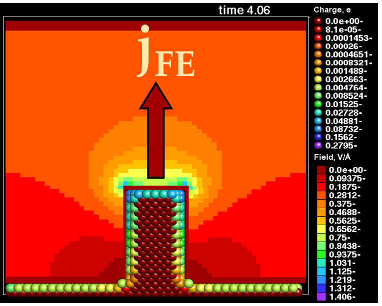
1. Going to the limits of conventional acceleration techniques → *highest possible gradient*
2. Estimated power consumption: **415 MW** (LHC: 120 MW) → *cost reduction by efficiency optimisation*

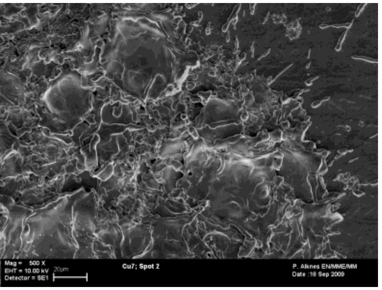
- Knowing how to lower breakdown rate is a key issue in points (1) and (2)

Detail of a CLIC accelerating structure, working at 100 MV/m

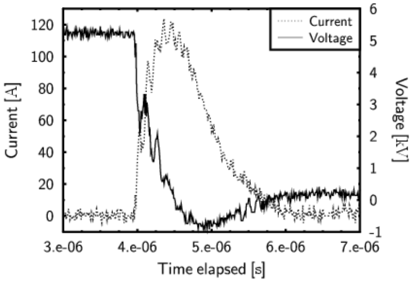


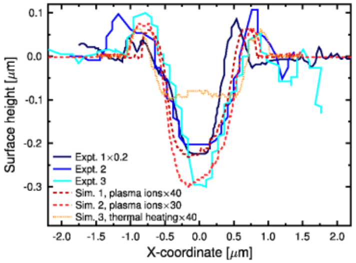
Why to model plasma build-up in vacuum discharges?

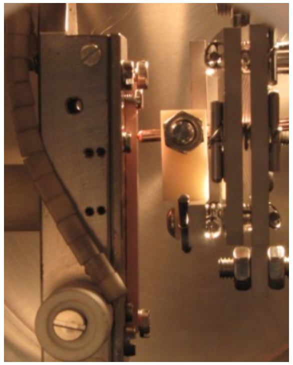




- Isn't it already 'too late' once the plasma has formed?
- As a part of our multi-scale model, plasma simulations provide us with a **link between**
  1. Micro- & macroscopic surface processes: Triggering (nano-scale) → plasma → crater formation (visible effect)
  2. Theory & experiments: Using reasonable physical assumptions (theory), the aim is to predict the evolution of measurable quantities (experiment)







How to model plasma build-up in vacuum discharges?

- The particle-in-cell method is probably the most suitable for discharge modelling since it provides us with a
  - Kinetic description of the plasma necessary for collisionless plasmas, that are far from a Maxwell-Boltzmann distribution
  - Self-consistent electrostatic(-magnetic) field description, crucial for this high-current phenomenon close to an absorbing wall, giving rise to a plasma sheath
- However, vacuum discharges are *non-linear* and *stochastic* in their nature
  - Poses a challenge to any numerical method – with each of them having their limitations

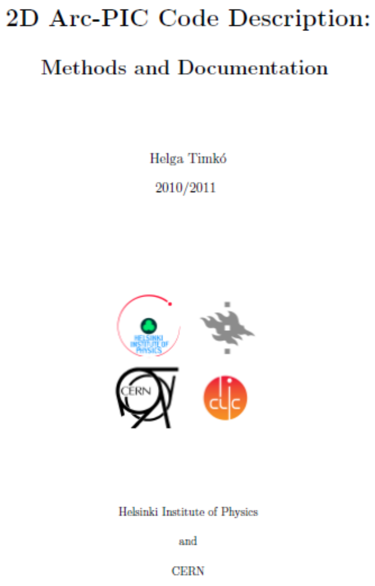
Particles:
Continuous Lagrangian phase space

Fields:
Discrete Eulerian grid points

Part I: 2D Arc-PIC Code Description

2D Arc-PIC code

- The new 2D Arc-PIC code has been developed and benchmarked last year
- Serial 2d3v electrostatic particle-in-cell code
  - Cylindrical symmetry
  - Monte-Carlo Collision routines adapted from *K. Matyash, IPP*
  - Optional external magnetic field
- Several options for *potential boundary conditions* and *particle injection schemes*
  - Simple options to carry out different tests
  - Discharge option (physics model described in Part II)
- Will be accessible for CERN and HIP
  - Automatic analysis scripts
  - Extensive code documentation to be published as a CLIC note



2D Arc-PIC Code Description:

Methods and Documentation

Helga Timkó

2010/2011

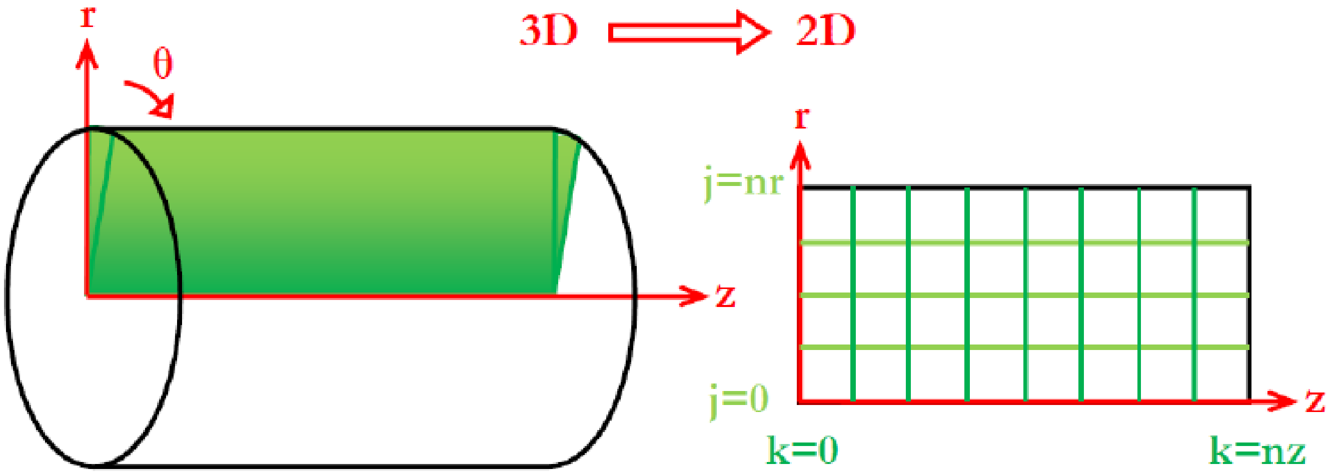
Helsinki Institute of Physics

and

CERN

What does 2d3v mean?

- Particles have 2 coordinate and 3 velocity components
  - Collisions are 3D
  - Movements are 2D: Particles are projected into a 2D-slice of a cylinder
- Difference from 3D: In 2D, no turbulent phenomena and associated transport/diffusion can occur



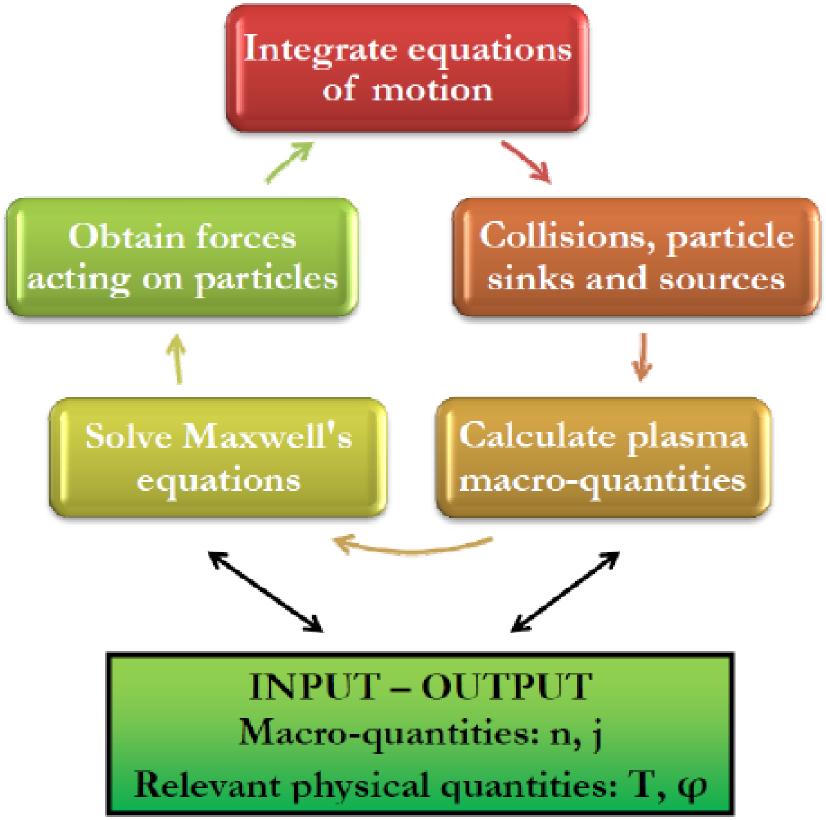
Assumptions embodied in the numerical model

- Dimensionality: 2D, cylindrical symmetry
- Electrostatic phenomenon: Even for high currents, electrostatic forces exceed magnetic confinement effects

∴ A 3D, electromagnetic picture of the problem would be a *higher order correction* to the solution

$$\left(\frac{\partial^2}{\partial r^2}+\frac{1}{r}\frac{1}{\partial r}+\frac{\partial^2}{\partial z^2}\right)\varphi=-\frac{e}{\varepsilon_0}n_e$$

The PIC method and its limitations



Integrate equations of motion

Collisions, particle sinks and sources

Calculate plasma macro-quantities

Solve Maxwell's equations

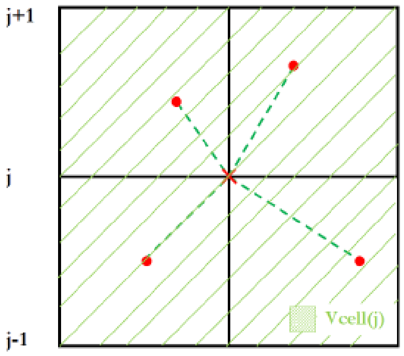
Obtain forces acting on particles

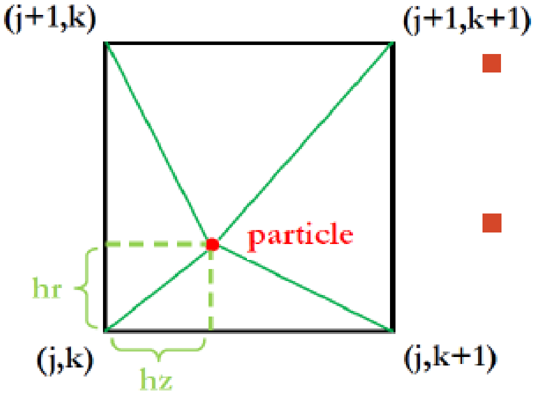
INPUT – OUTPUT
Macro-quantities: n, j
Relevant physical quantities: T, φ

Why discharge modelling is so hard:

- Stability requirements $\Delta x < 3.4\lambda_{Db},\quad \Delta t \leq 0.2\omega_{pe}^{-1},$
  - Non-linear problem, while discretisation is linear ⇒ prone to numerical instabilities
  - Stability diagnostics is built-in
- Limited dynamic range
  - Can’t cover 1 nA – 100 A
- Memory-heavy simulations
  - High density only in a few simulation cells, while memory allocation is homogeneous

2D Arc-PIC: An efficient code



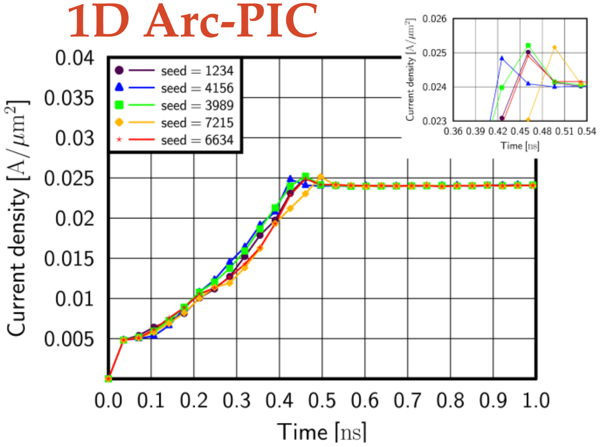


Some details for those who are familiar with PIC…

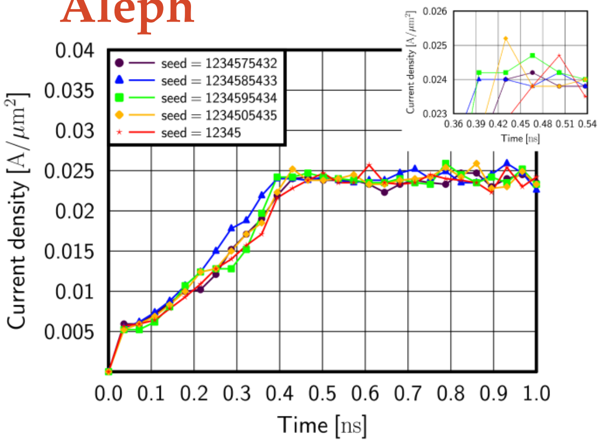
- Efficient: All variables are dimensionless
  - No unnecessary multiplications
- A well-optimised *finite difference method* Poisson solver
  - Using the 'SuperLU' lower-upper triangular matrix factorisation and inversion package
- An accurate implicit particle mover using the *Boris method*
- Charge assignment and field interpolation: Via 1st order *cloud-in-cell scheme*
  - Guarantees momentum conservation on a uniform grid

Benchmarking via code-to-code comparisons

1D Arc-PIC



Aleph



- Codes are usually tested via simple test problems that have a known analytic solution
- If the code is then run in a non-linear regime as in the case of breakdowns, subtle, earlier undiscovered flaws may lead to a wrong solution of the problem, and we wouldn't even necessarily notice it!
- Code-to-code comparisons are essential for such problems
  - A collaboration on this with Sandia National Labs is ongoing since 1.5 years now;
  - Obtained good agreement with a simple 1D discharge model

Part II: The Discharge Model

Phenomena taken into account – Three species: e^-, Cu, Cu^+

Initial
Cu, e^-

- Cu evaporation, enhanced electron field emission from a field emitter tip (Fowler-Nordheim eq)

$$j_{FE} = a_{FN} \frac{(eE_{LOC})^2}{\phi t(y)^2} e^{-b_{FN} \frac{\phi^{3/2} v(y)^2}{eE_{loc}}}, \quad \text{where } E_{loc} = \beta \cdot E$$

$$t(y) = 1,\ v(y) = 0.956 - 1.062 y^2 \quad \text{where y=} \sqrt{\frac{e^3 E_{LOC}}{4\pi\varepsilon_0 \phi^2}}$$

- Electron field emission also from the flat cathode surface

Create ions

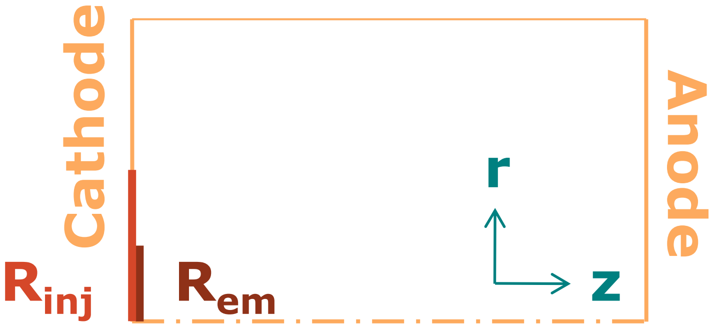
- Collisions, esp. ionisation collisions

More e^- and
Cu

- Sputtering of Cu neutrals at the walls, enhanced MD yield at the cathode above a certain ion flux
- Secondary electron yield due to ion bombardment at the cathode

How the FE tip is modelled…

- We simulate a FE tip placed into the middle of the system; geometrically, the tip itself is not resolved
  - Emission radius: Assumed FE radius; used to calculate erosion, melting, and current density to current conversion
  - Injection radius: In practice, particles are injected within this radius

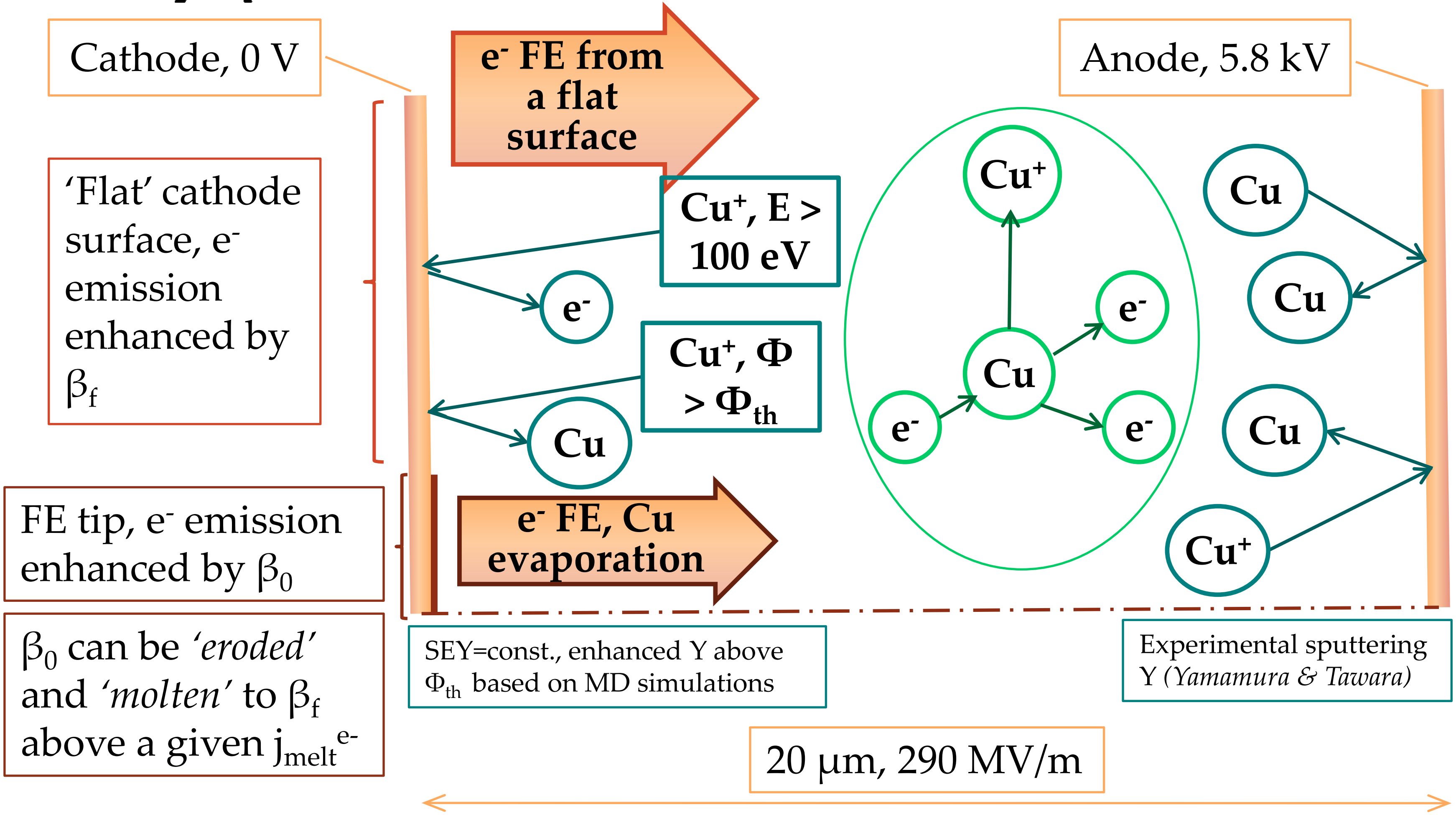


FE tip is source of

- Enhanced FN electron emission, limited to 12 GV/m
- Neutral evaporation in a fixed ratio $r_{Cu/e}$ (compared to FE)

Grid resolution high (note: limited memory, no. of jobs)

Overview of vacuum discharge boundary conditions



Cathode, 0 V

Anode, 5.8 kV

‘Flat’ cathode surface, e^- emission enhanced by β_f

FE tip, e^- emission enhanced by β_0

β_0 can be *‘eroded’* and *‘molten’* to β_f above a given j_{melt}^{e-}

e^- FE from a flat surface

Cu^+, E > 100 eV

Cu^+, $\Phi > \Phi_{th}$

e^- FE, Cu evaporation

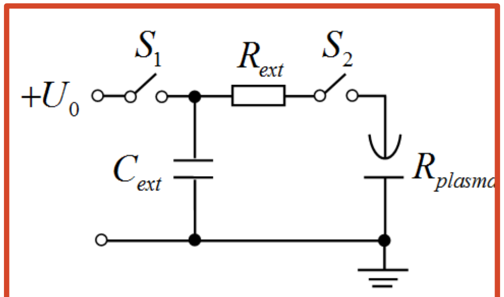
SEY=const., enhanced Y above Φ_{th} based on MD simulations

Experimental sputtering Y *(Yamamura & Tawara)*

20 μm, 290 MV/m

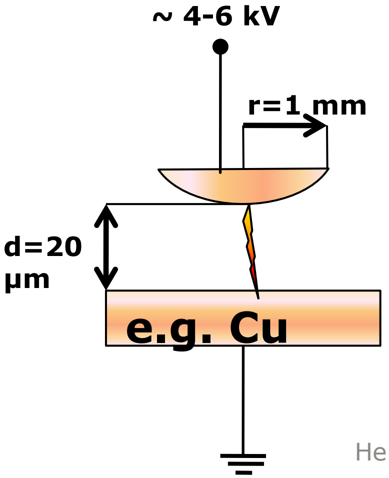
Circuit model –
Inspired by the DC setup

EXPERIMENT



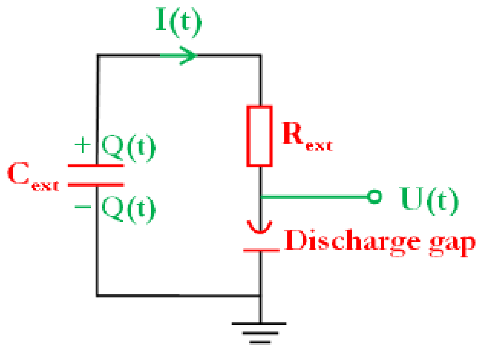
$R_{ext} = 30\Omega$

$C_{ext} = 0.1 - 27.5nF$



- A vacuum arc in steady-state has typically a burning voltage of 10 V, we apply 5 – 6 kV over 20 µm! Isn‘t this a contradiction?
- No: The energy available for a breakdown is finite, will be eventually consumed ⇒ during the plasma build-up, the external potential will drop
  - A vacuum discharge is a transient phenomenon; and one thing we would like to predict is how it's current-voltage characteristic looks like

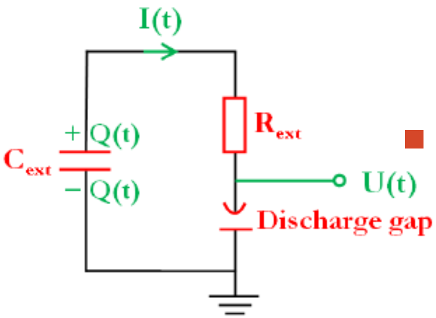
SIMULATION



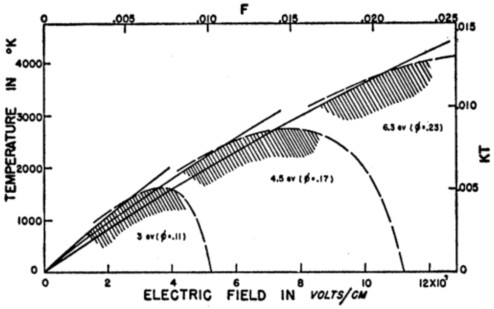
$$Q(t_{i+1}) = Q(t_i) - I(t_i)\,\Delta t,$$

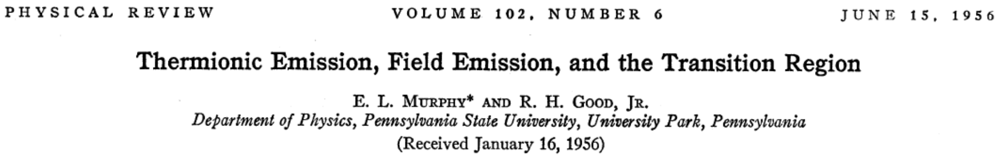
$$U(t_{i+1}) = \frac{Q(t_{i+1})}{C_{ext}} - R_{ext} I(t_i),$$

Circuit model – Where does the charge come from?



- Another fact: Vacuum arcs carry **10 – 100 A** current at a maximum; what is the physics behind charge depletion and how to implement it?
- We simulate an idealistic 'pool' of charges that is immediately accessible, but much can happen in a fraction of a ns! (see Part III)
  - One may interpret the capacitance as the capacitance of the discharge gap itself
  - Charge depletion is modelled implicitly via a reasonable electron FE current cut-off (corresponding to 12 GV/m, which is the range of applicability of pure field emission)





PHYSICAL REVIEW VOLUME 102, NUMBER 6 JUNE 15, 1956

Thermionic Emission, Field Emission, and the Transition Region

E. L. MURPHY* AND R. H. GOOD, JR.
Department of Physics, Pennsylvania State University, University Park, Pennsylvania

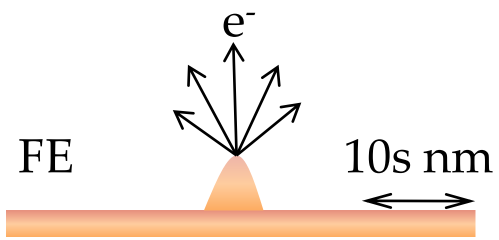
(Received January 16, 1956)

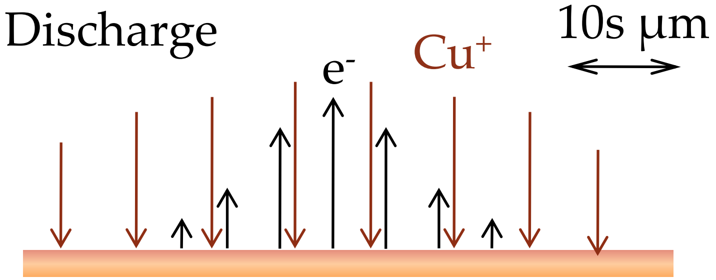
From FE to discharge currents – In practice

- In real life we can observe the full dynamic range of a vacuum discharge:
  - > 10s pA in 'weak' FE phase
  - Space charge limited 'strong' FE phase, typically ~ nA – μA
  - Discharge current, up to 10 – 100 A
- At the same time, the involved area changes:
  - Typically $10^{-20} - 10^{-14}$ m^2 for weak FE ⇒ R_{em} ~ 0.1 – 100 nm
  - During the discharge, the bombarded area has R ~ 10 – 100 μm

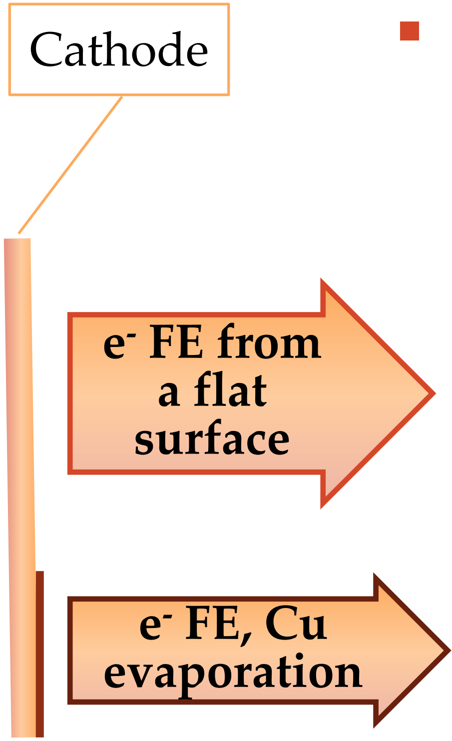
Up to 12 orders of magnitude difference

Up to 12 orders of magnitude difference





From FE to discharge currents – In theory

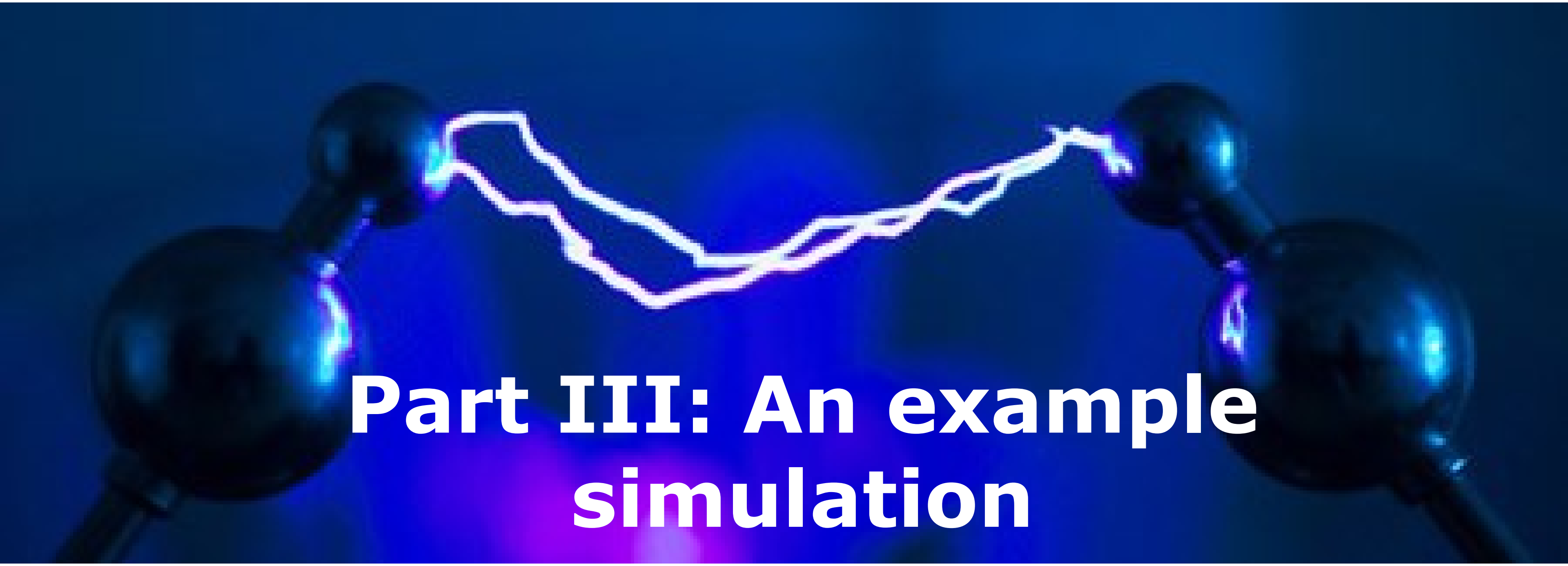


Cathode

e^- FE from a flat surface

e^- FE, Cu evaporation

- How can we model this with a method that can cover 3 – 4 orders of magnitude dynamic range at the most?
  - Start from strong FE (0.01 – 0.1 A)
  - Option 1: Increase by hand the emission radius
    - Would require a dynamic re-weighting of super-particles; non-trivial task because energy and momentum cannot be conserved at the same time
  - Option 2: Try to model the expansion of the spot through reasonable physical assumptions
    - The region outside the FE tip can be involved in field emitting electrons through a combination of $\beta_f \sim 10 - 15$ and a sheath
    - Motivation: We never measured $\beta < 10 - 15$; also a ‘flat’ surface will have asperities that can lead to a spreading FE

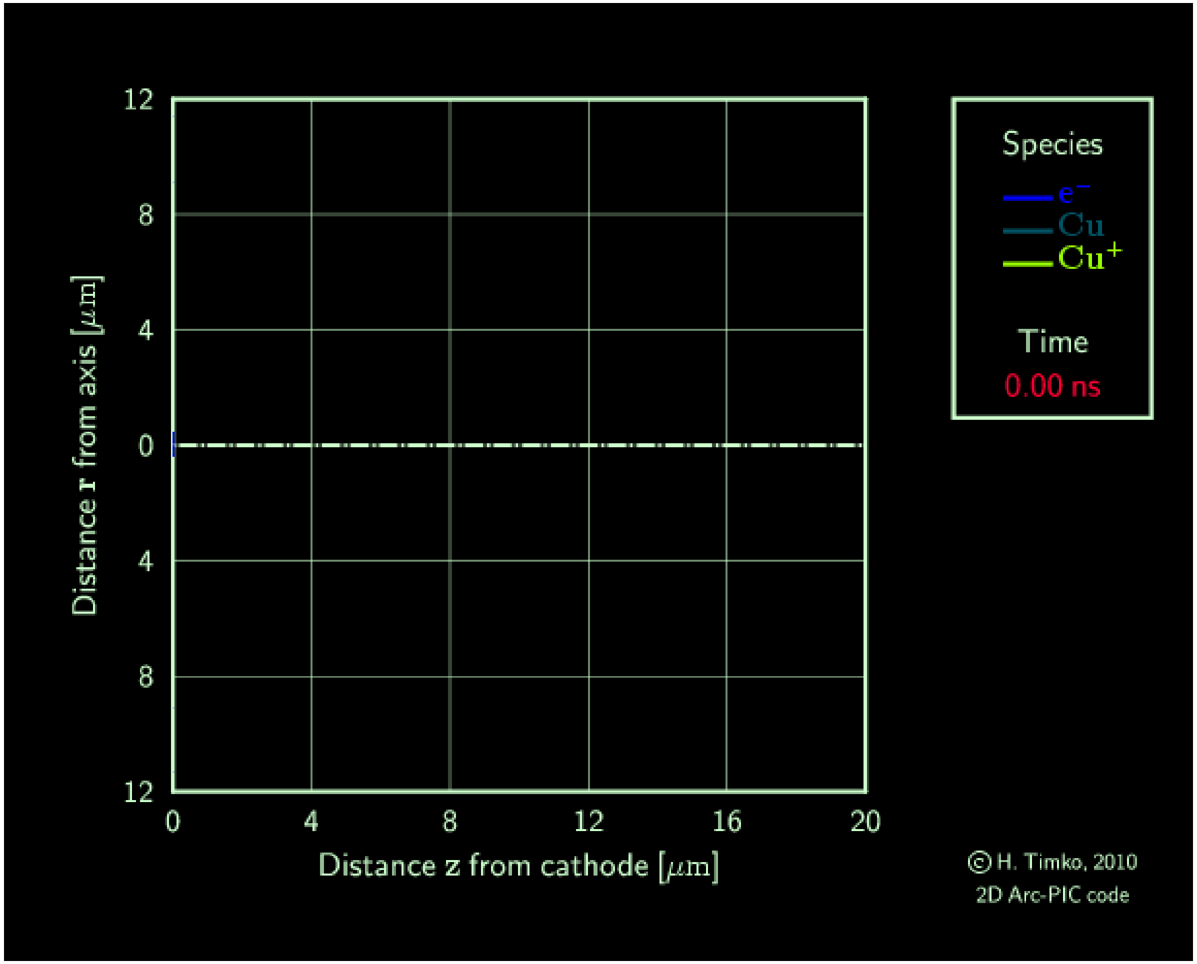


Part III: An example simulation

Input parameters

- R_{em} = 1 dz = 0.1 μm
- R_{inj} = 4 dz = 0.4 μm
- N_{Db} = 1000, $r_{Cu/e}$ = 0.015
- $j_{melt} = 50*10^8$ A/cm^2 (upper limit)
- $\beta_0 = 35$, $\beta_f = 10$
- External circuit: C = 0.01 nF, R = 25 Ω
- Initial voltage across the gap: 5.8 kV
- System size: 120 by 200 dz (12 by 20 μm)
- Gaussian injection; except for
  - Evaporated neutrals: v_r, v_t suppressed by **10**
  - FE electrons **fully Gaussian**

Movie


12
8
4
0
4
8
12
Distance r from axis [μm]
0
4
8
12
16
20
Distance z from cathode [μm]
Species
e^-
Cu
Cu^+
Time
0.00 ns
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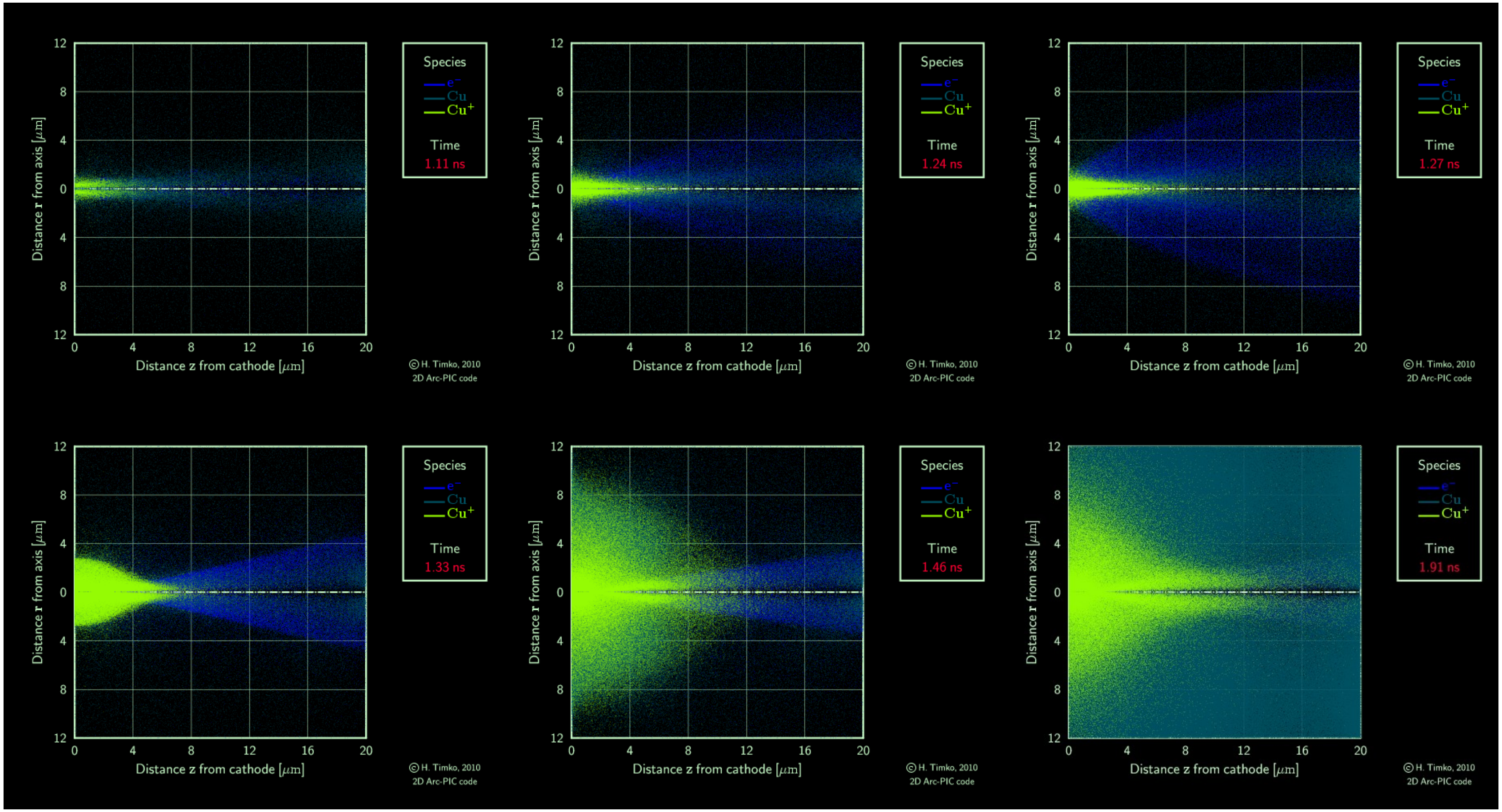
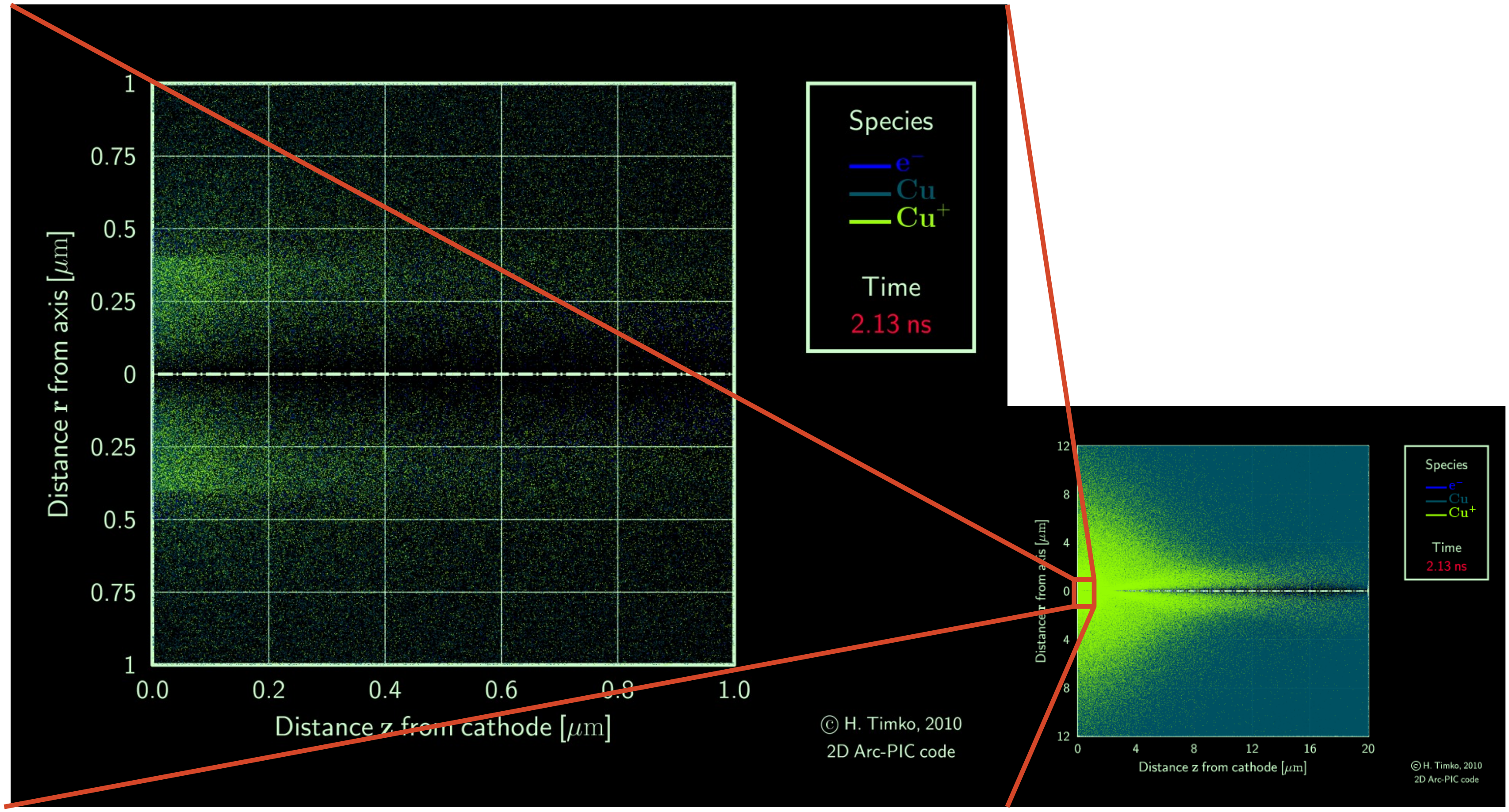
2D Arc-PIC code

Coordinates



Coordinates – zoomed in



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2D Arc-PIC code

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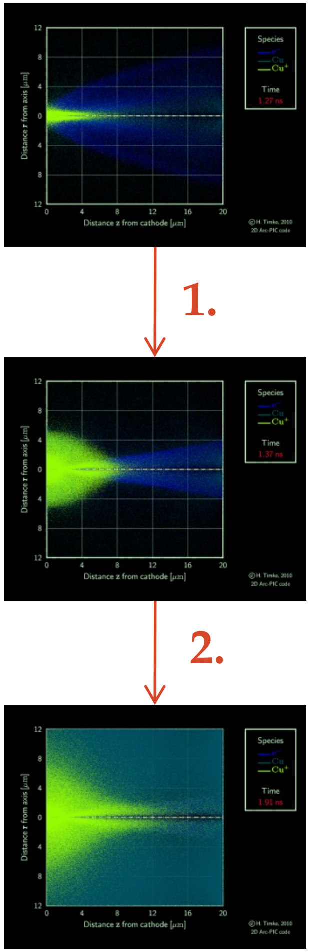
2D Arc-PIC code

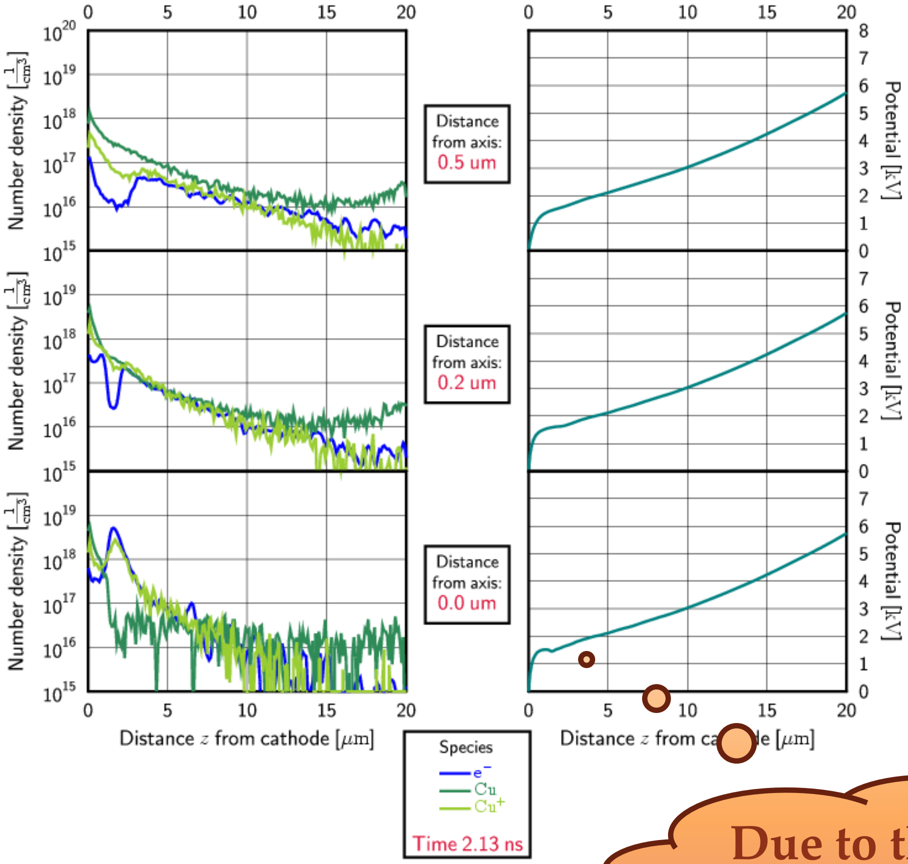
Observations

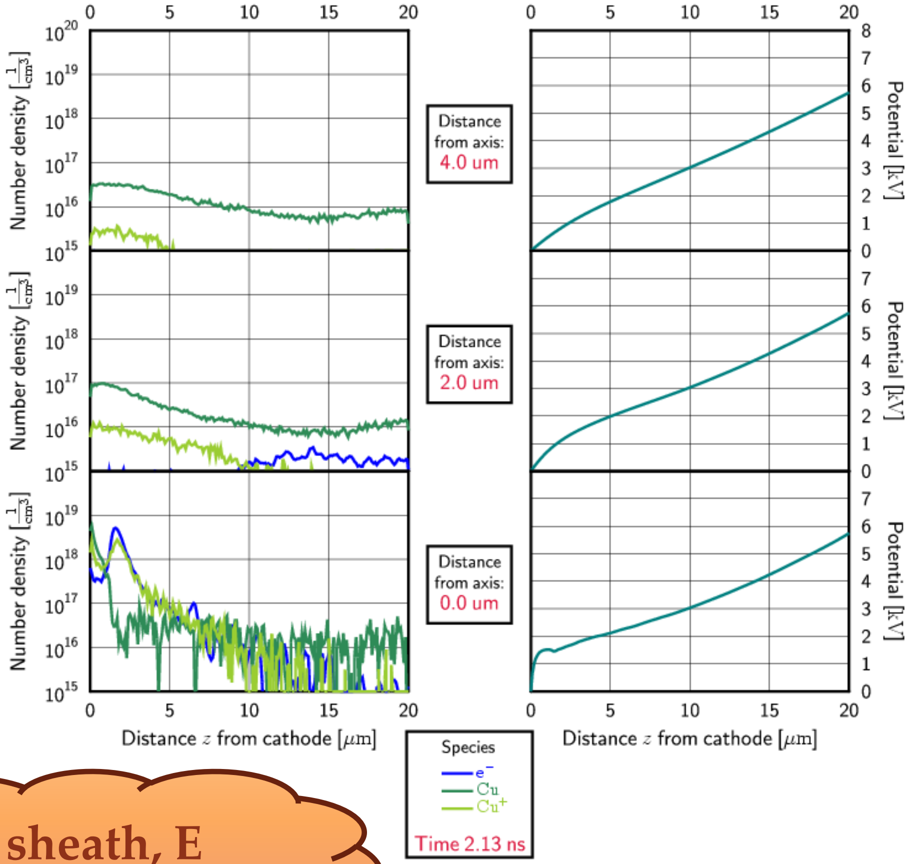


- Fully cathode dominated phenomenon
- Although FE starts from a small area, the discharge plasma can involve a macroscopic area on the cathode
- Transitions seen:

1. Transition from strong FE to a small discharge plasma
   - Sudden ionisation avalanche
   - A plasma sheath forms, the plasma becomes quasi-neutral
   - Focusing effect
2. Transition from a surface-defined phase to a volume-defined phase
   - When neutrals fill the whole system
   - Self-maintaining
   - Macroscopic damage

Potential & densities

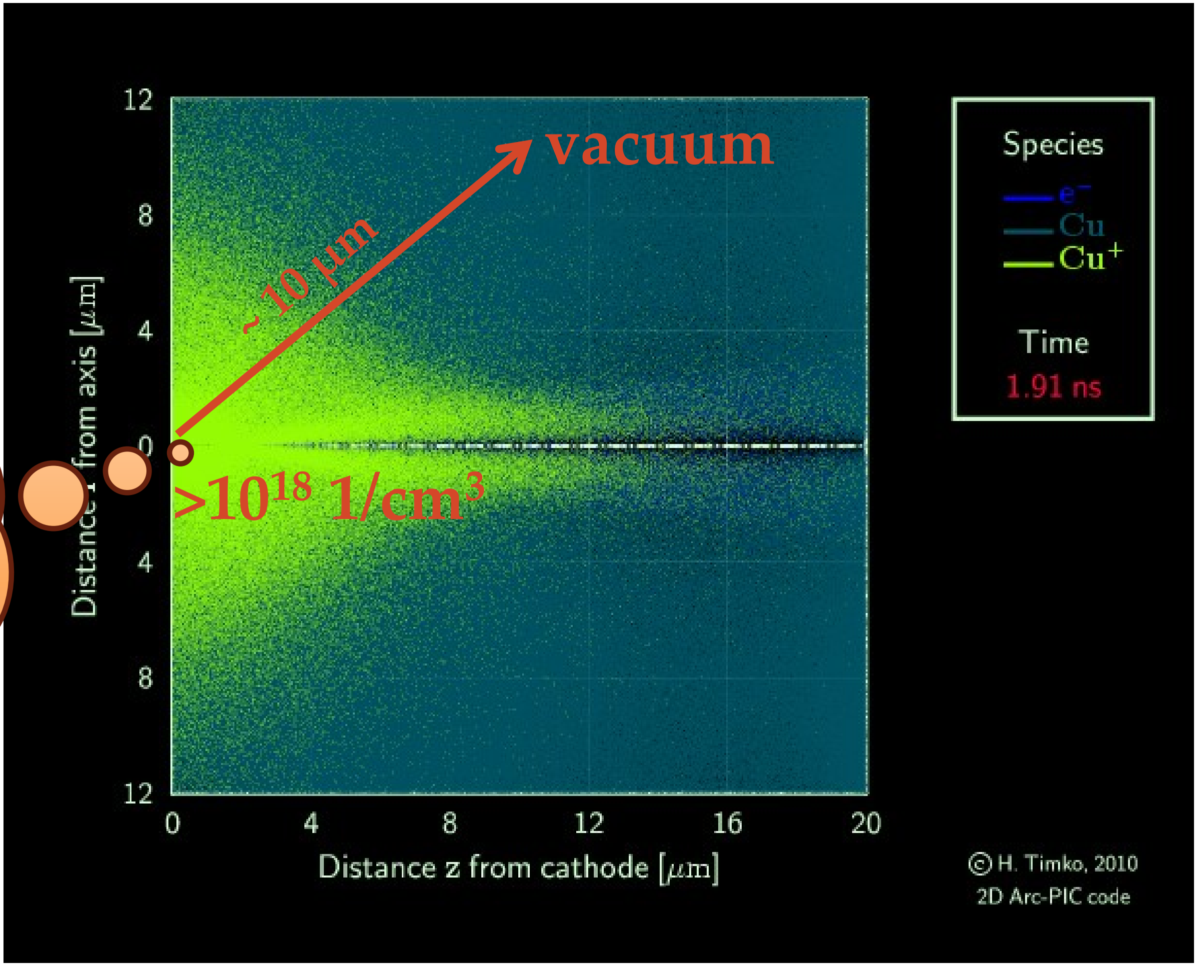




Due to the sheath, E ~ 6-7 GV/m!

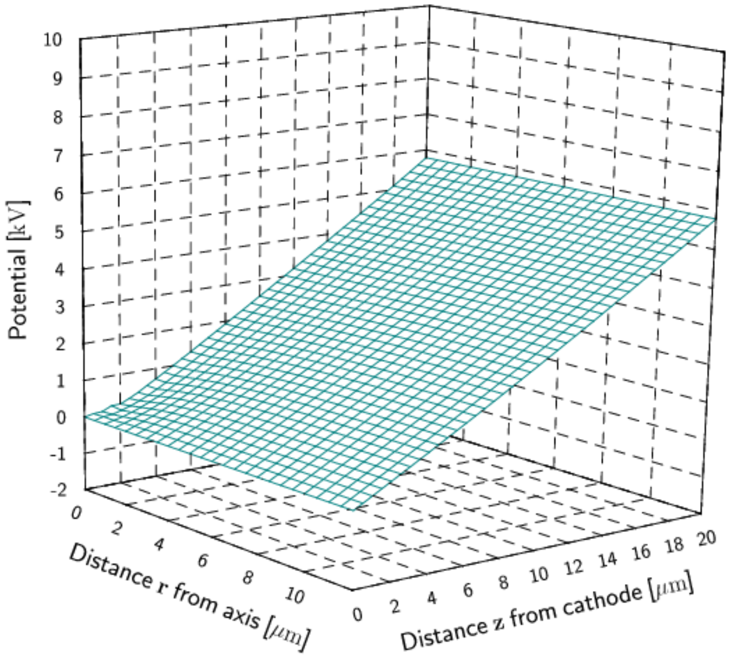
Steep gradients

Sheath enhances FE only in a small region!

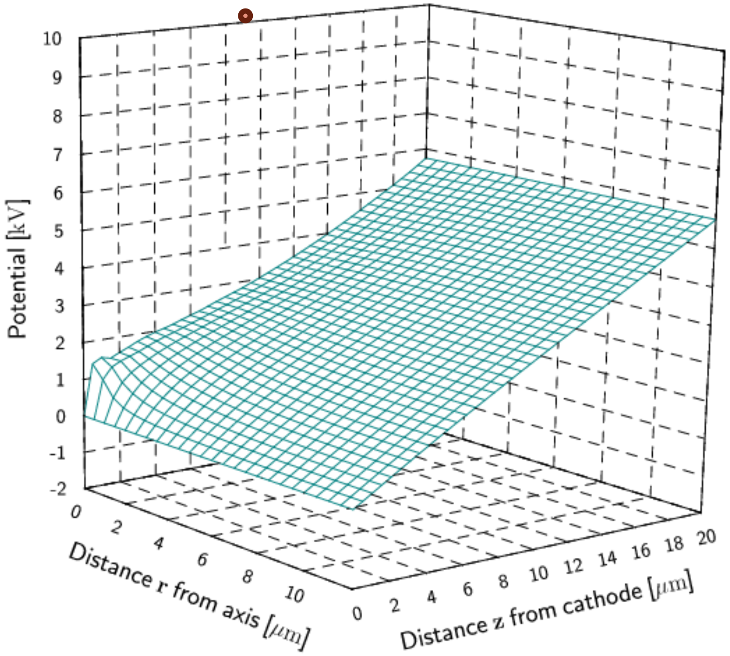


Full 2D potential

Plasma: Sheath



Time 1.26 ns

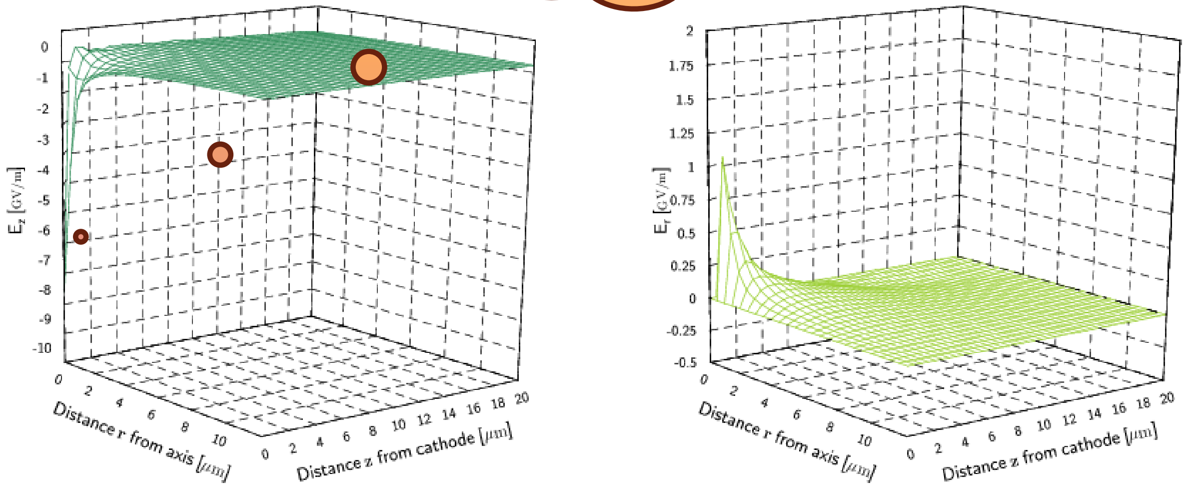


Time 2.13 ns

FE: Space charge

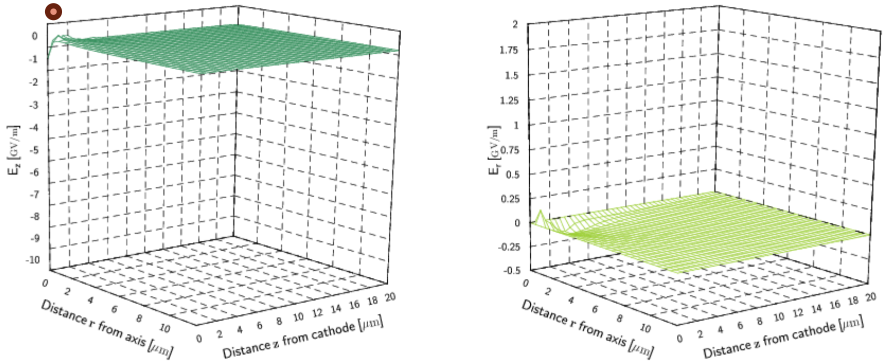
Full 2D E-field

Plasma: Sheath



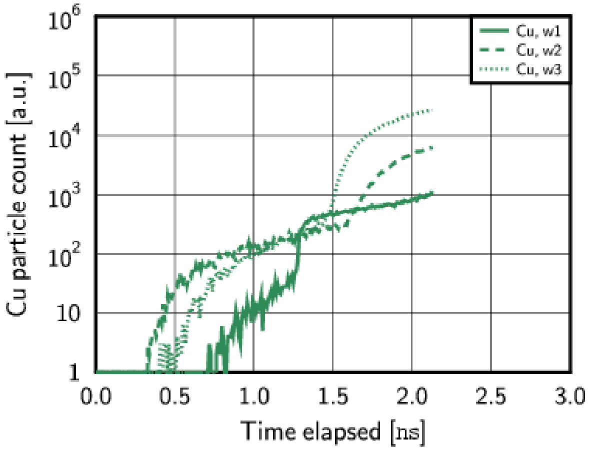
Time 2.13 ns

FE: Space charge

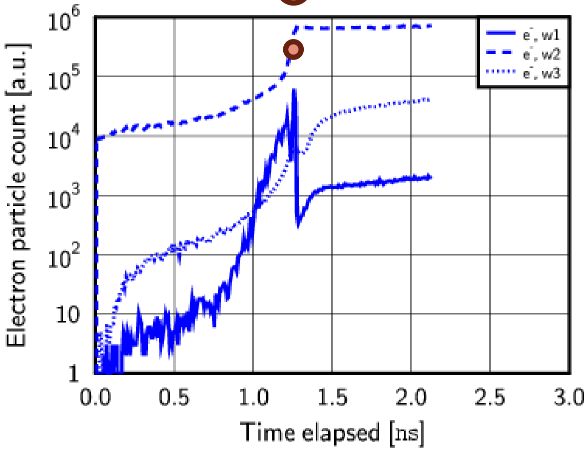


Time 1.26 ns

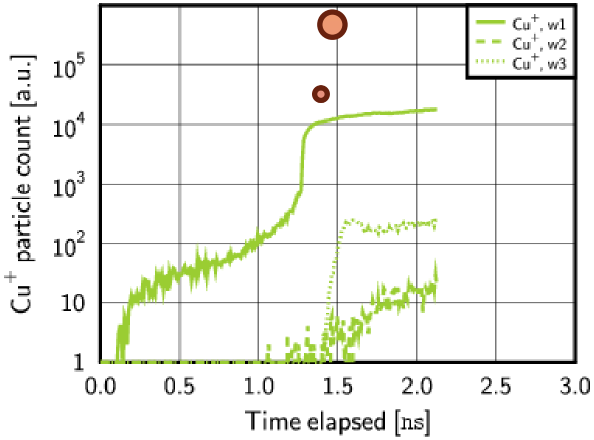
Absorbed particle counts



Breakdown
⇒ becomes
conductive

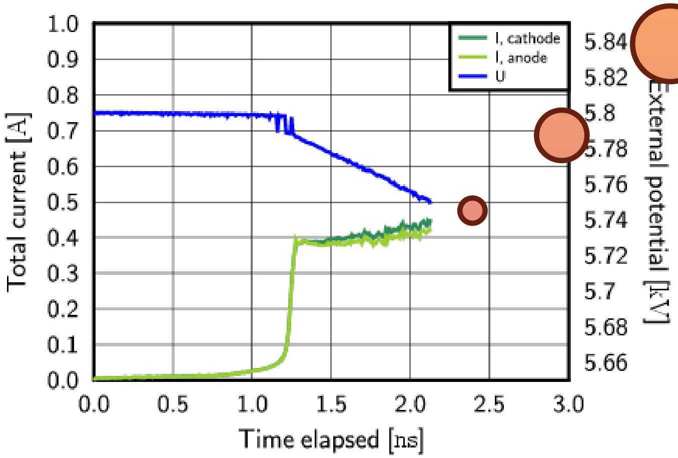


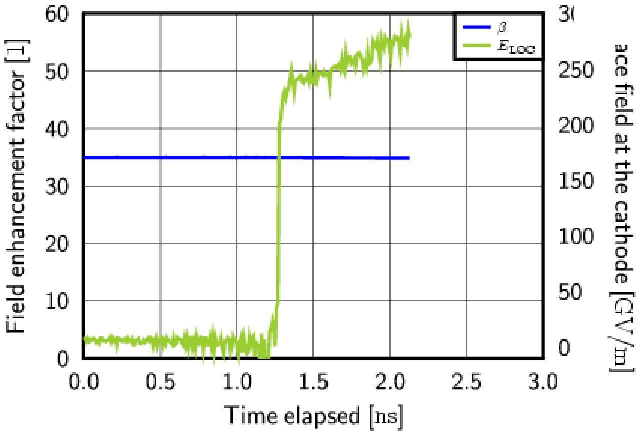
Cu^+ follows
the Cu curve

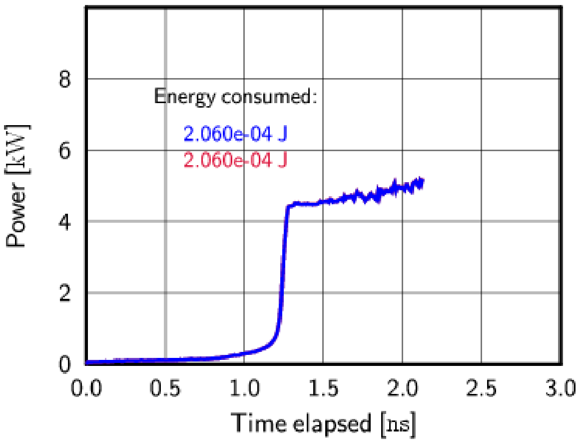


Other diagnostics

Limited FN: imitates current depletion! Growing current: expanding spot







Conclusions

- The 2D Arc-PIC code has been developed and its simulations give us new type of insight into the physics of breakdown plasmas

- The code is available for CERN and HIP, but obtaining reliable results is an art of itself
  - Extremely time-consuming, because the result is highly sensitive to input parameters (exponential dependencies)
  - Requires a deep knowledge of the PIC method, in order to filter out unphysical effects

Outlook

- Personally, I am about to finish my PhD work by completing the above last study on 2D discharge plasmas
  - DC/RF comparison planned
  - Perhaps even a study of an external magnetic field effect

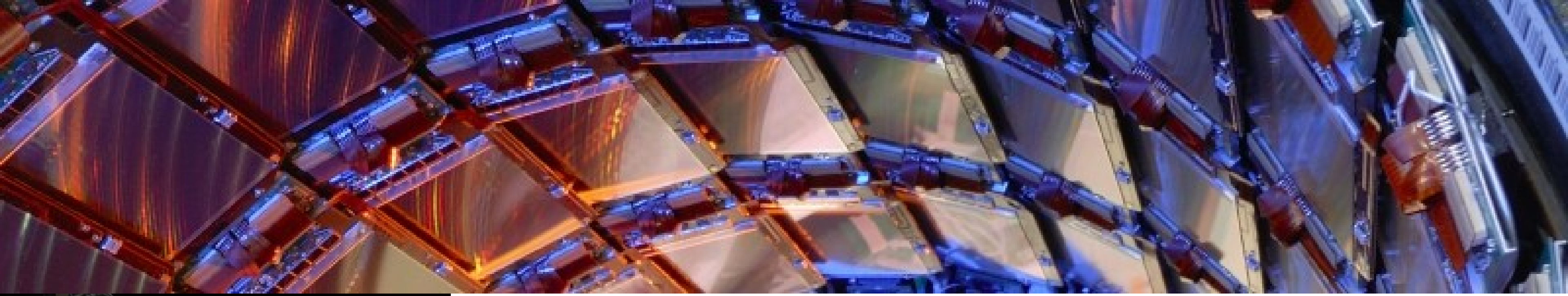
- It is uncertain yet how long I will continue as a PhD Student at CERN, but HIP has plans to place another PhD Student to CERN sometime in the future

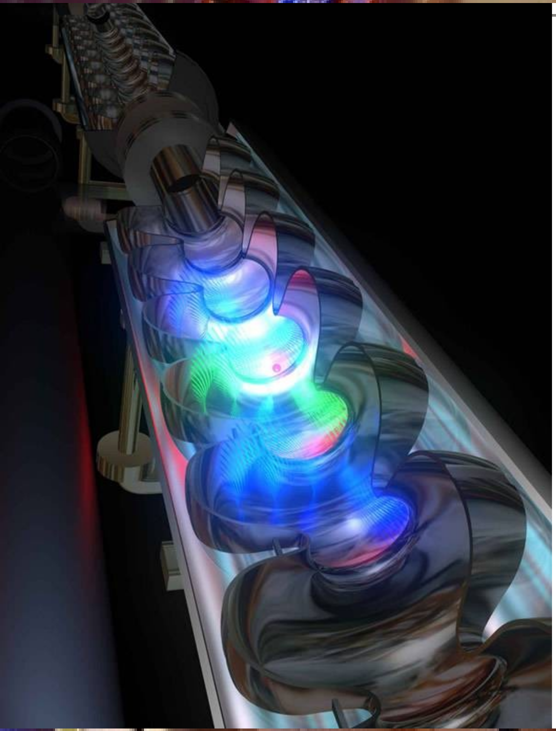
My special thanks to…

… our collaborators at the Max-Planck-Institut für Plasmaphysik, in Greifswald, Germany,

Ralf Schneider and *Konstantin Matyash*,

who taught me the PIC method, showed me all important tricks, and advised me how to write my own code.





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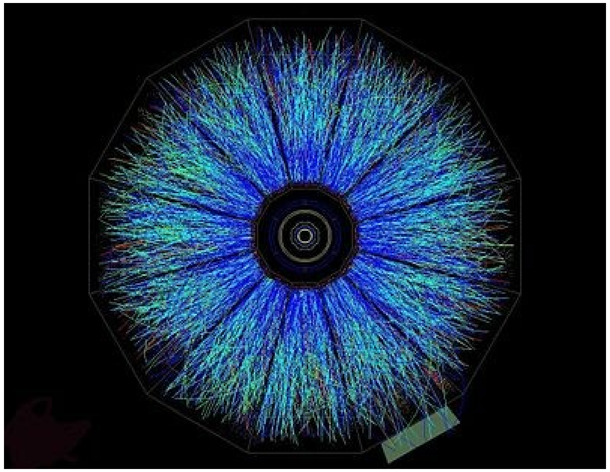

Thank you!