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HIP

Dynamic coupling between particle-in-cell and atomistic simulations

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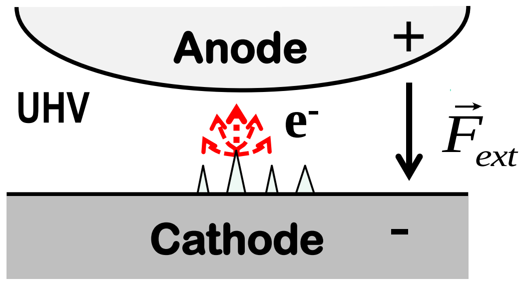
Outline

- The plasma onset stage of vacuum BD and its importance for BD mitigation
- Two schools of thought:
  “explosive emission” vs “thermal evaporation”
- Concurrent ED-MD simulations on nanotips
- The thermal runaway process
- Integrating with PIC simulations
- Results
- Conclusions

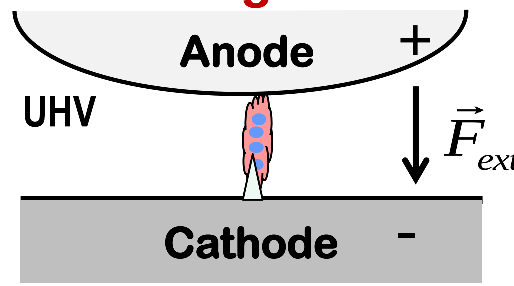
Vacuum breakdown stages

Stage 1



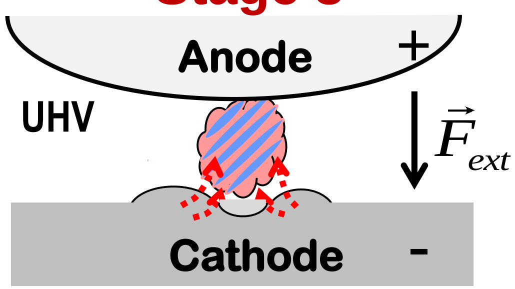
Sharp tips on surface, field enhancement, electron emission

Stage 2



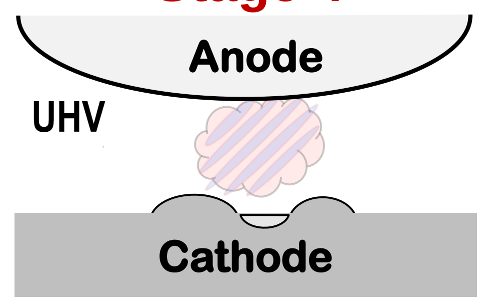
Plasma onset: thermal runaway, neutral evaporation

Stage 3



Ionization, plasma formation-expansion, high current, voltage collapse

Stage 4

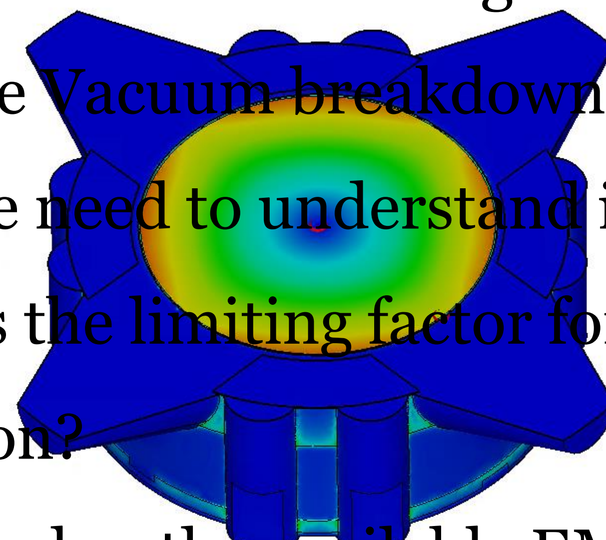


Extinction of energy, plasma cools-recombines, crater remains

Importance of stages 2,3: power flow limits

- Can we use this as a design way to mitigate Vacuum breakdown?
- First we need to understand it
- What is the limiting factor for BD initiation?
- What makes the available EM power to be sufficient in some cases, while insufficient in other?

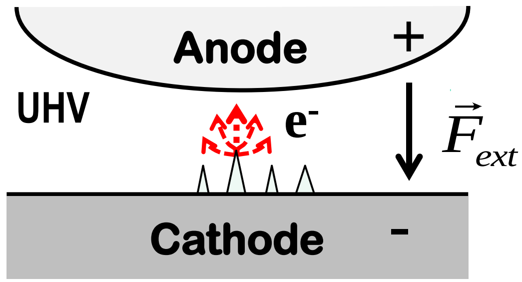
Soft Cu electrode,
Anton Saressalo



Calculated S_c @ 100 MHz
Jan Paszkiewicz

Vacuum breakdown stages

Stage 1



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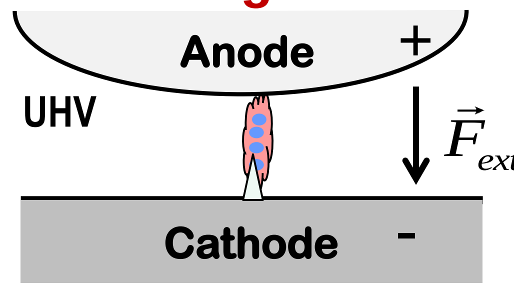

Plasma onset: thermal runaway, neutral evaporation

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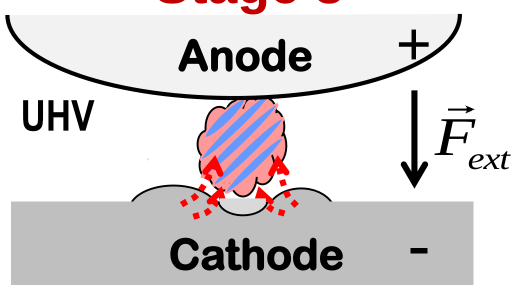

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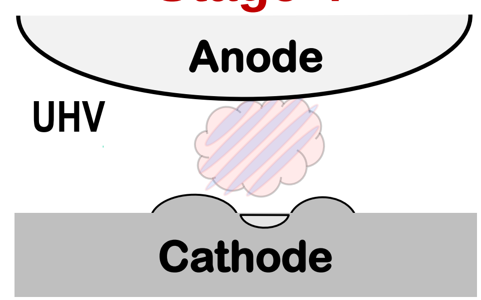


Extinction of energy, plasma cools-recombines, crater remains

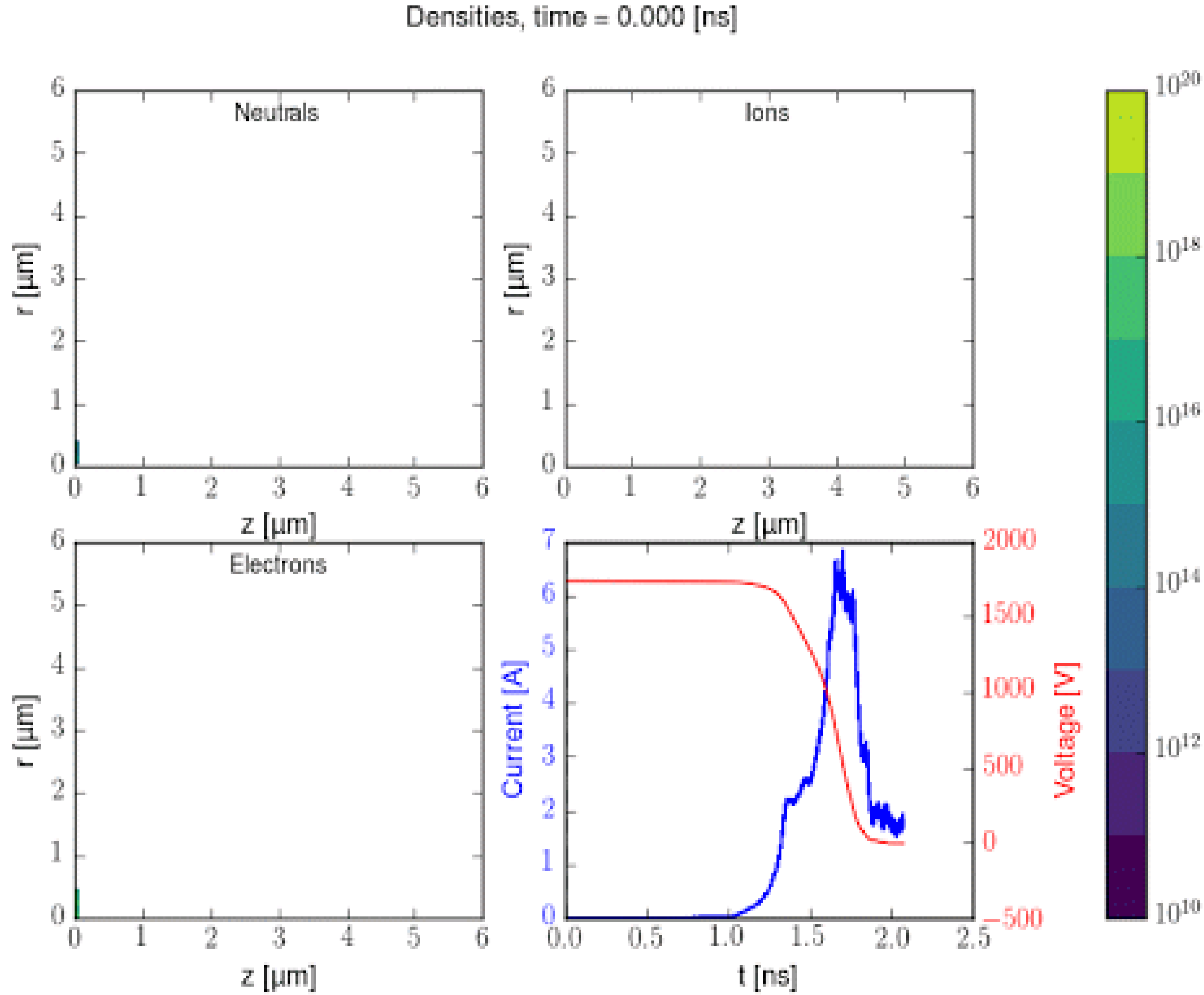
Plasma ignition: schools of thought

- **Explosive emission (ECTON model):**
  - ✓ Tip heats up by Joule heating (FE current)
  - ✓ The heat accumulates while the shape stays constant
  - ✓ Extreme temperatures
  - ✓ Direct phase transition from metal to plasma

- **Thermal runaway - evaporation:**
  - ✓ Tip heats by Nottingham & Joule and melts on top
  - ✓ Maxwell stress pulls and sharpens it
  - ✓ Molten material at high temperatures emits vapor
  - ✓ Vapor ionizes by e collisions (and field ionization)
  - ✓ Ions sputter out more vapor
  - ✓ Plasma gradually builds up

ArcPIC results

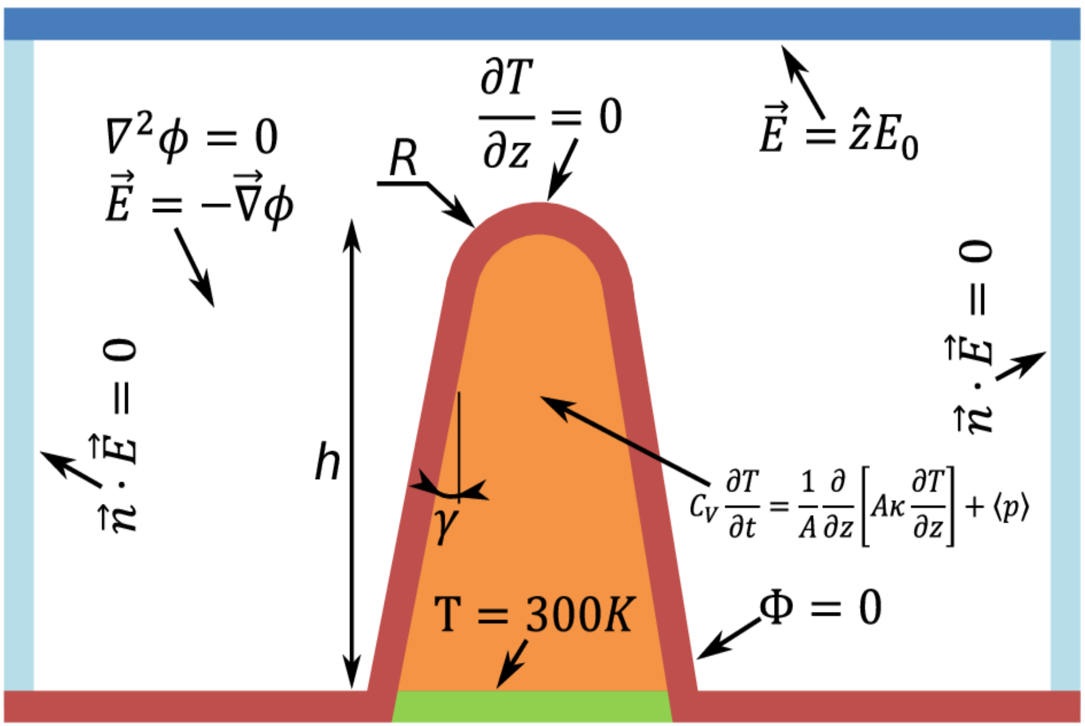
- Plasma can ignite emitter assuming a small tip that:
  - Emits e with an enhancement β>35
  - Releases >15 evaporated neutrals per 1000 e.
- What is the origin of those neutrals?
- What are the mechanisms in **Stage 2** that produce the necessary vapor?

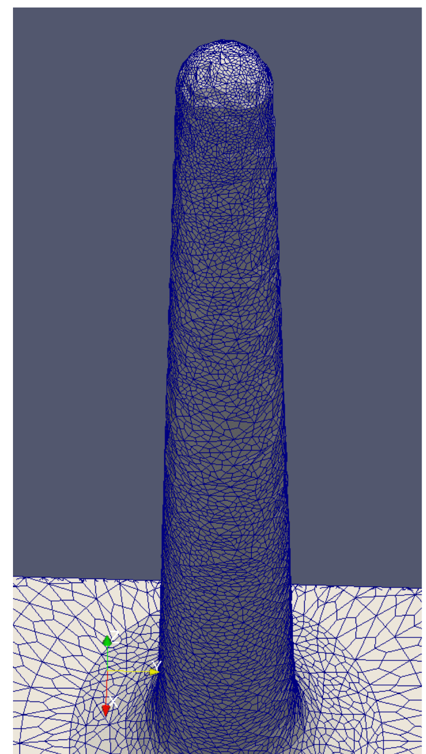


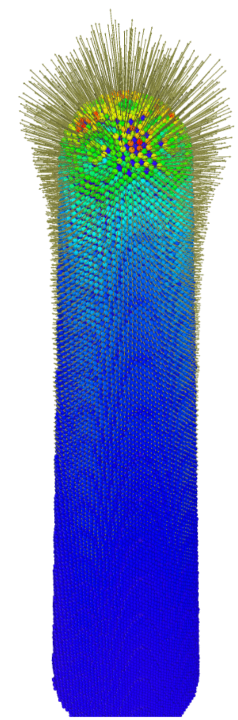
H. Timko et. al., Contrib. Plasma. Phys. 4, 229 (2015).
Animation by K. Sjobaek

Hybrid MD-ED-Emission-Heat

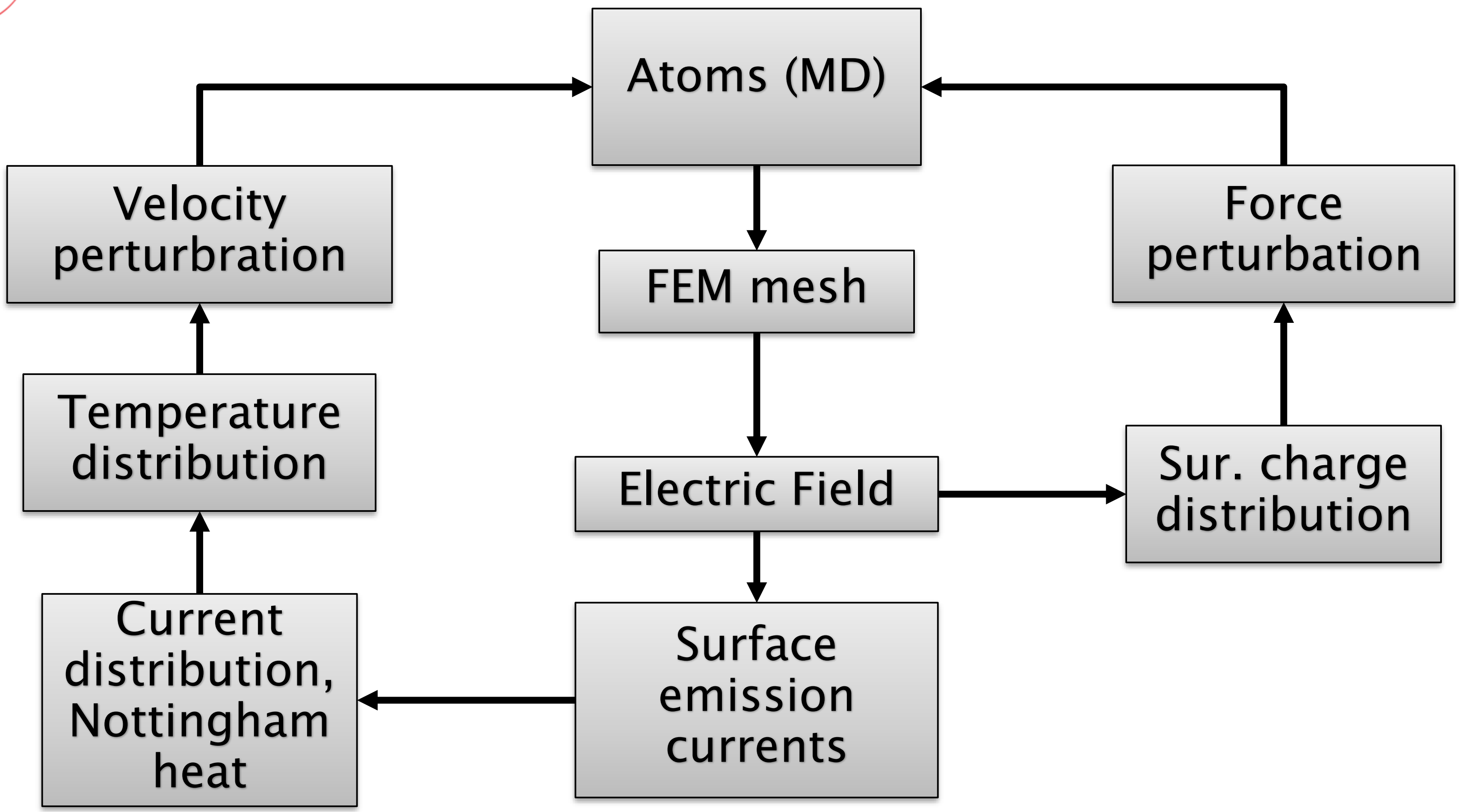
- ❖ Thermal runaway: complex process that involves various phenomena that have to be taken into account in the calculations



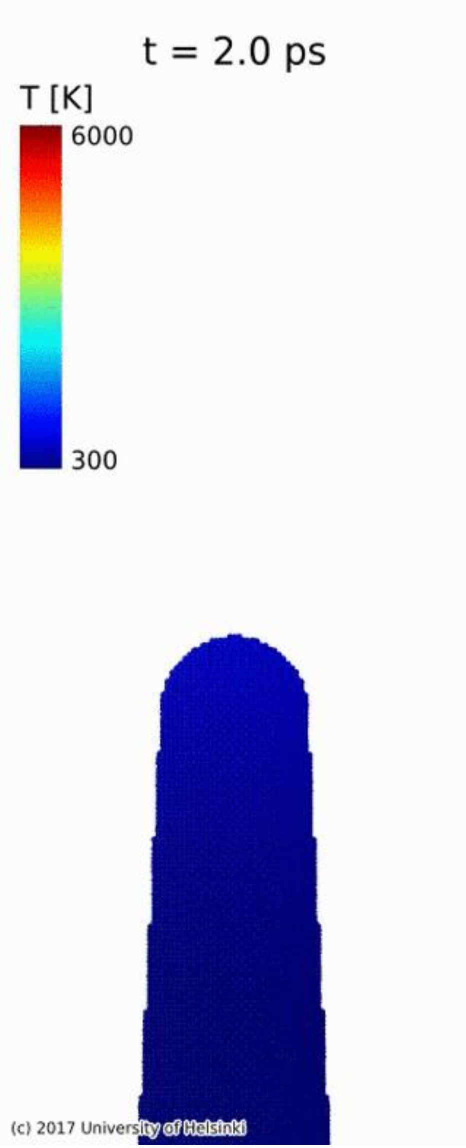




The concurrent algorithm



Thermal runaway



- E_{appl}=0.8GV/m
- Mean evaporation rate (first to last evaporation events) r_{Cu}= 75±11 atoms/ps
- Mean current r_e = 2807±153 e/ps
- $r_{Cu/e}$= 0.025±0.003 atoms/e
- The assumption of the ArcPIC simulations (0.015 atoms/e) was not unrealistic at all

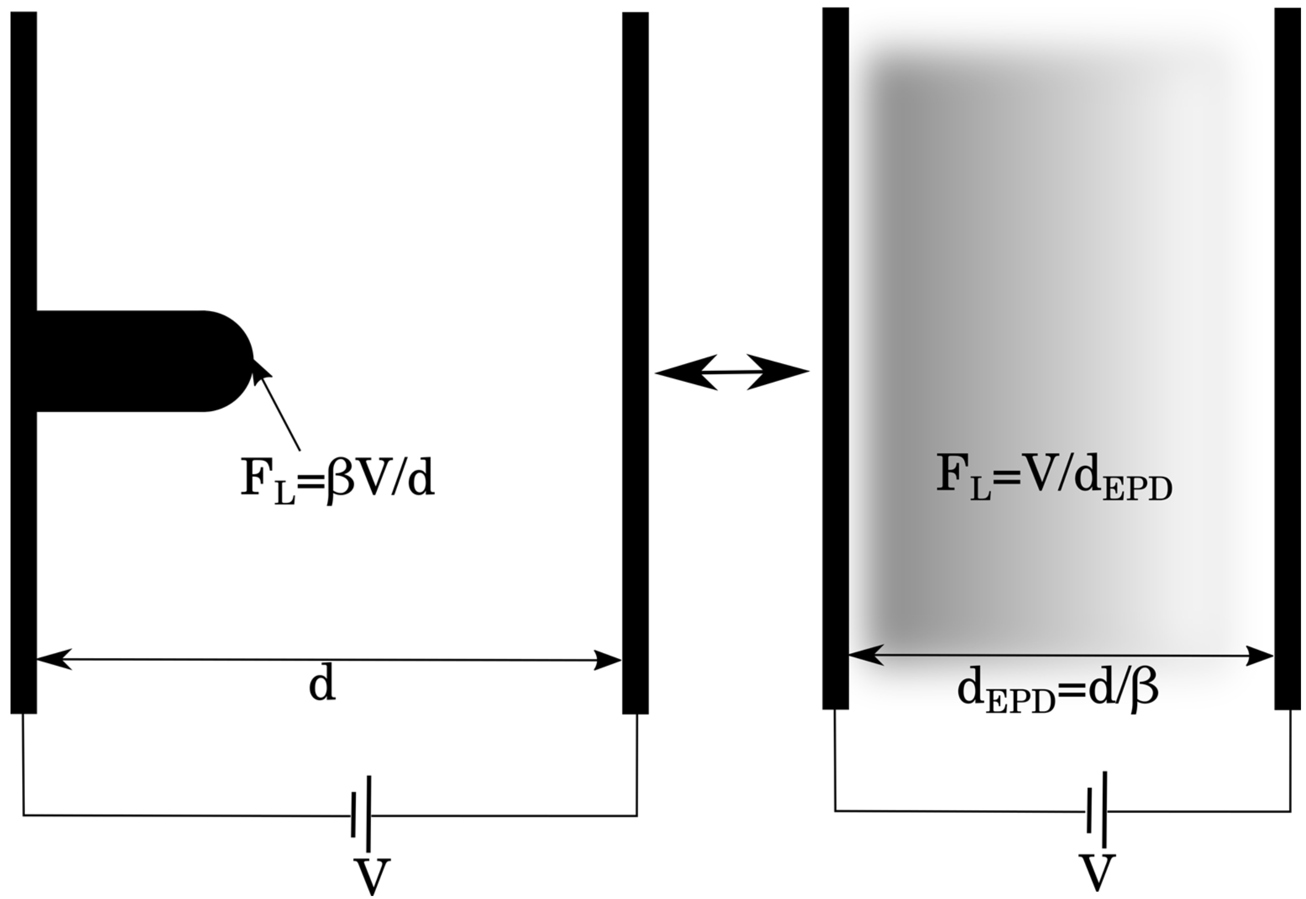
A. Kyritsakis et. al, J. Phys. D: Appl. Phys. 51, 225203 (2018)

Problem 1: Space-charge limited Field Emission in 3D

- In reality, no field emitter is flat and the 1D model is inadequate
- Standard treatment: Equivalent Planar Diode (EPD) model to correct for the field enhancement factor

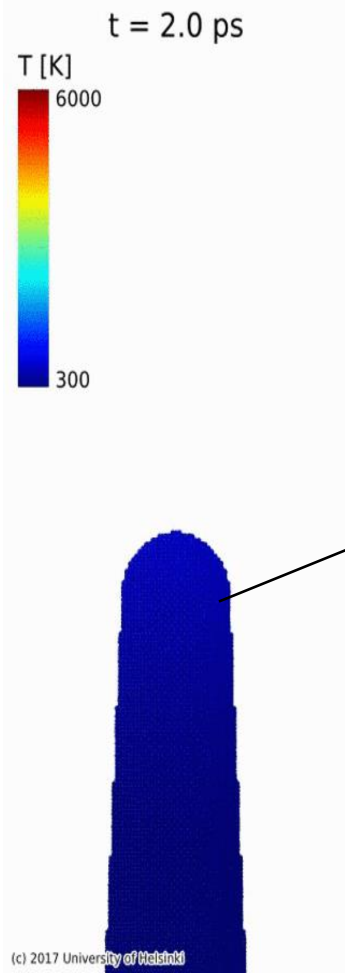
➢ EPD fails for a simple reason: The electron beam **spreads** and J is **not constant** as in the 1D case

➢ NEED for **PIC simulations**

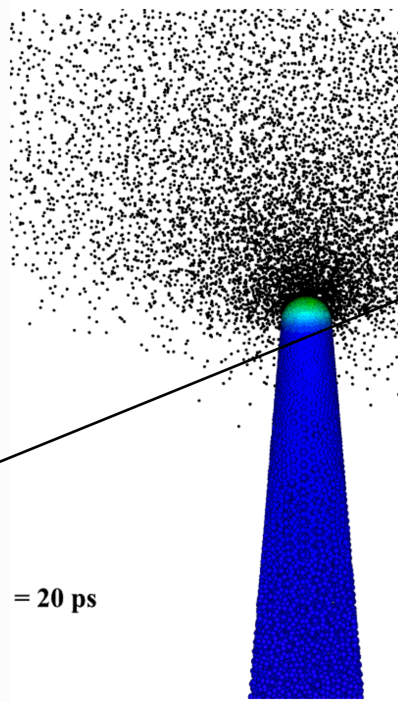


Problem 2: connecting stages 2 and 3

Stage 2 (runaway)

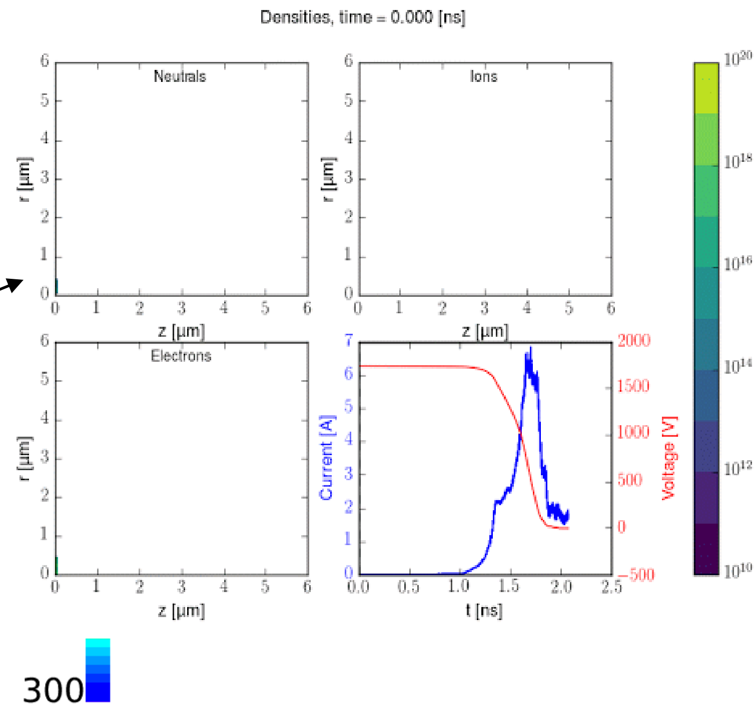


Stage 2&3 (multi-scale)



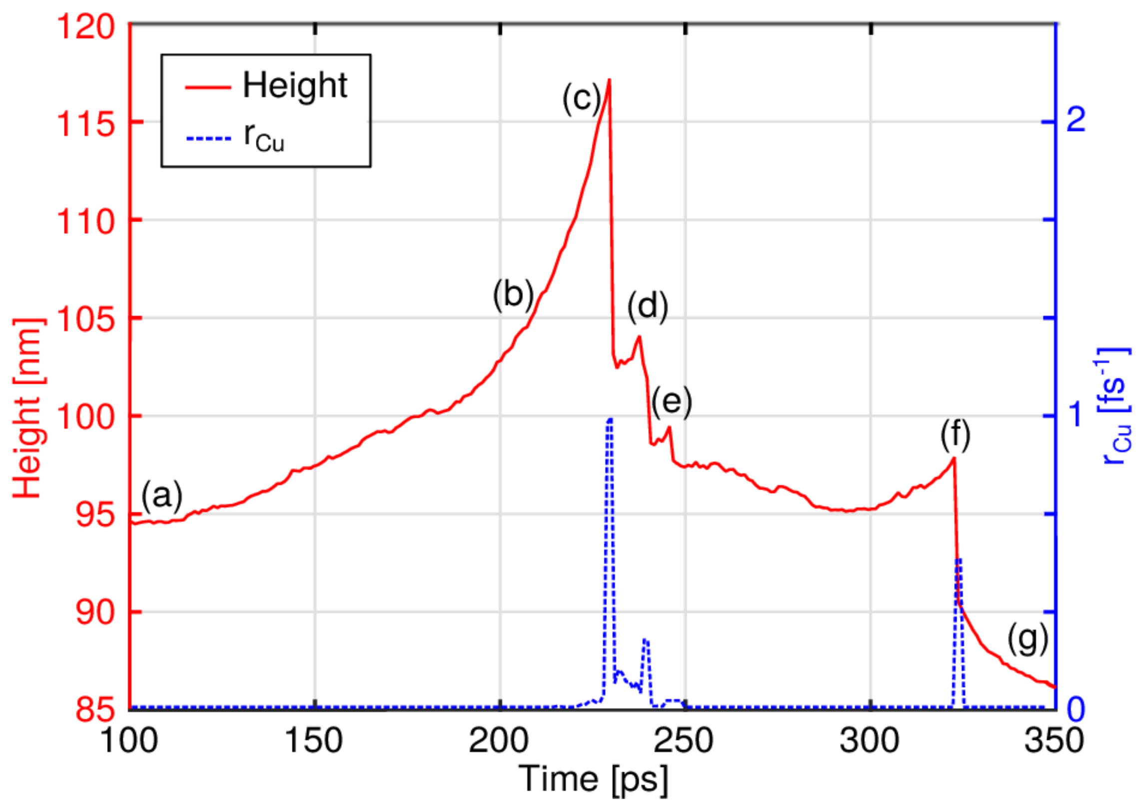
= 20 ps

Stage 3 (Plasma onset)

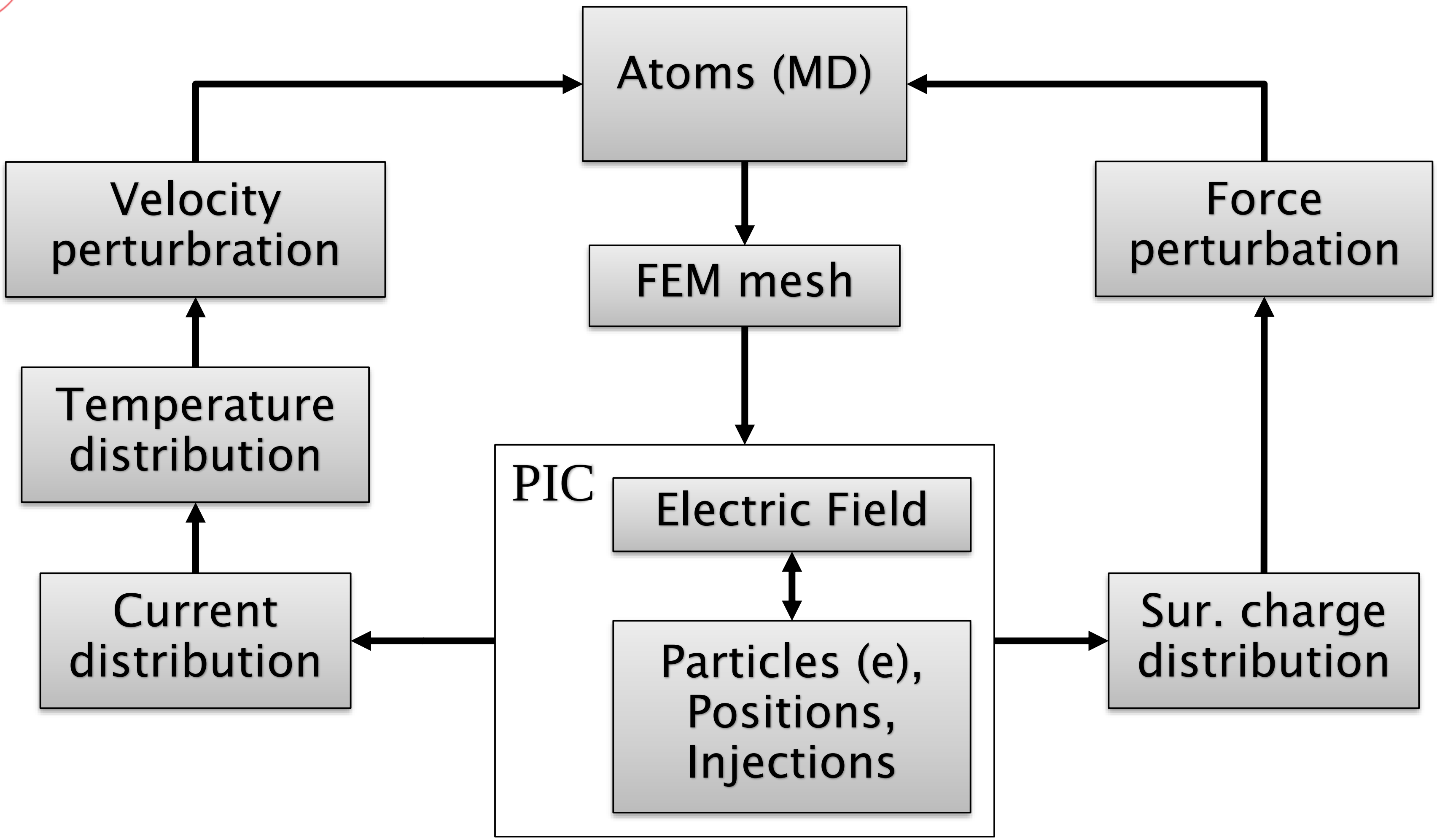


Problem 3: Does the runaway stop?

- What happens if we continue?
- Does the process continue providing necessary evaporation for a sufficient time to ignite plasma?

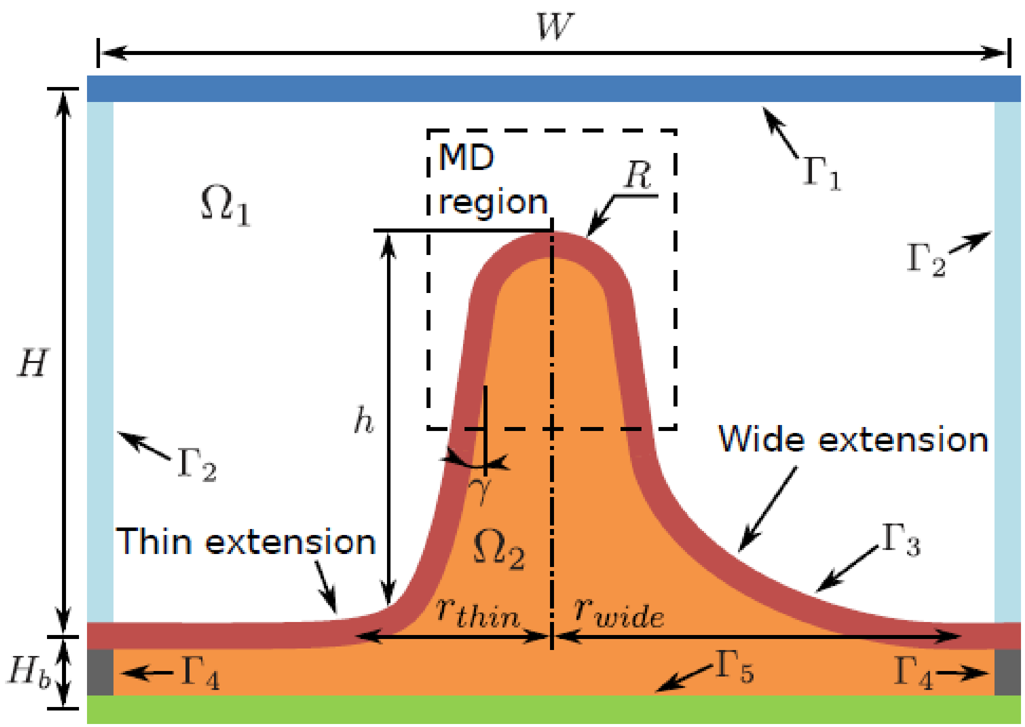


Incorporating PIC in FEMOCS



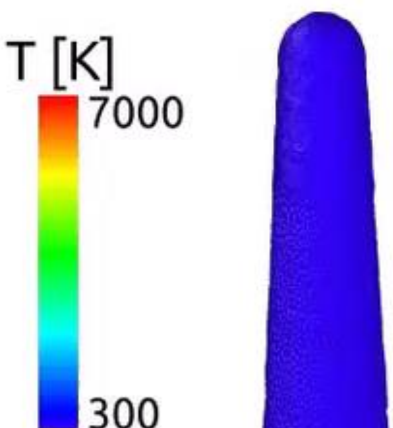
Runaway with full PIC-FEMOCS simulations

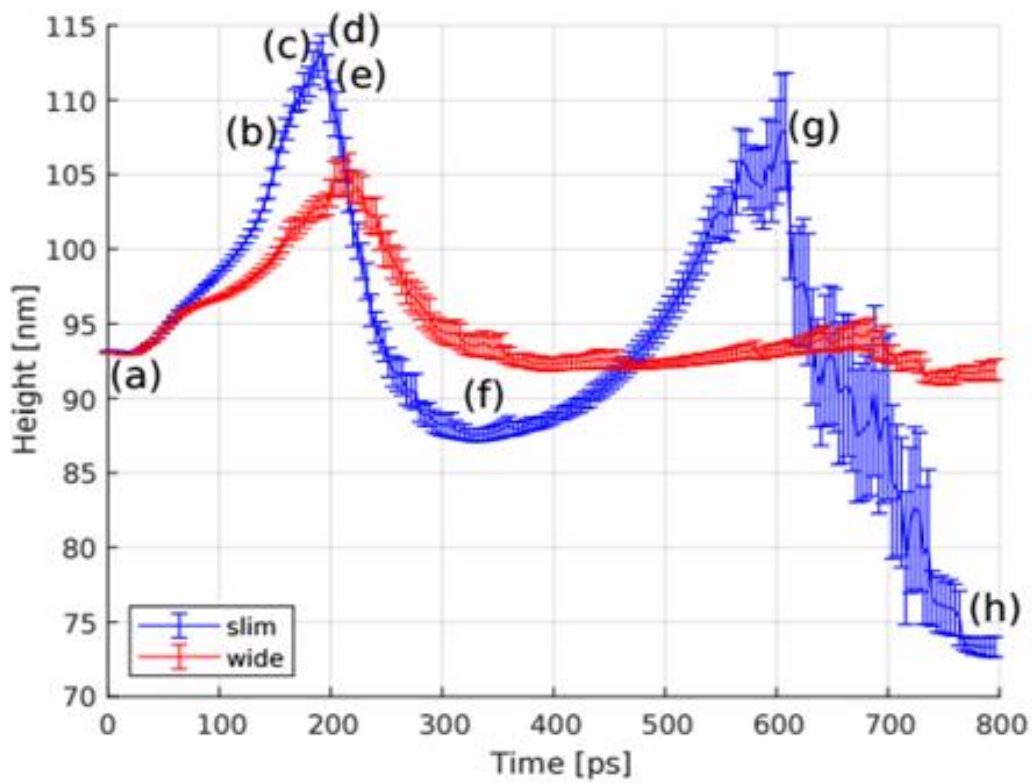
- r_{thin} = 17nm, r_{wide} = 54nm
- E_{appl} = 600MV/m (closer to reality)



Results I

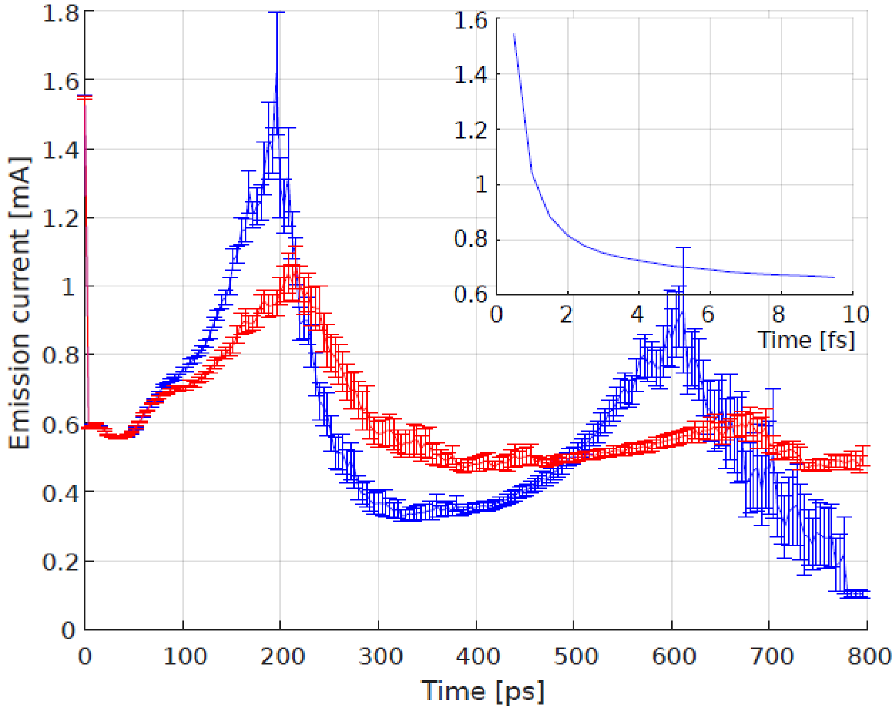
Time = 0.0 ps

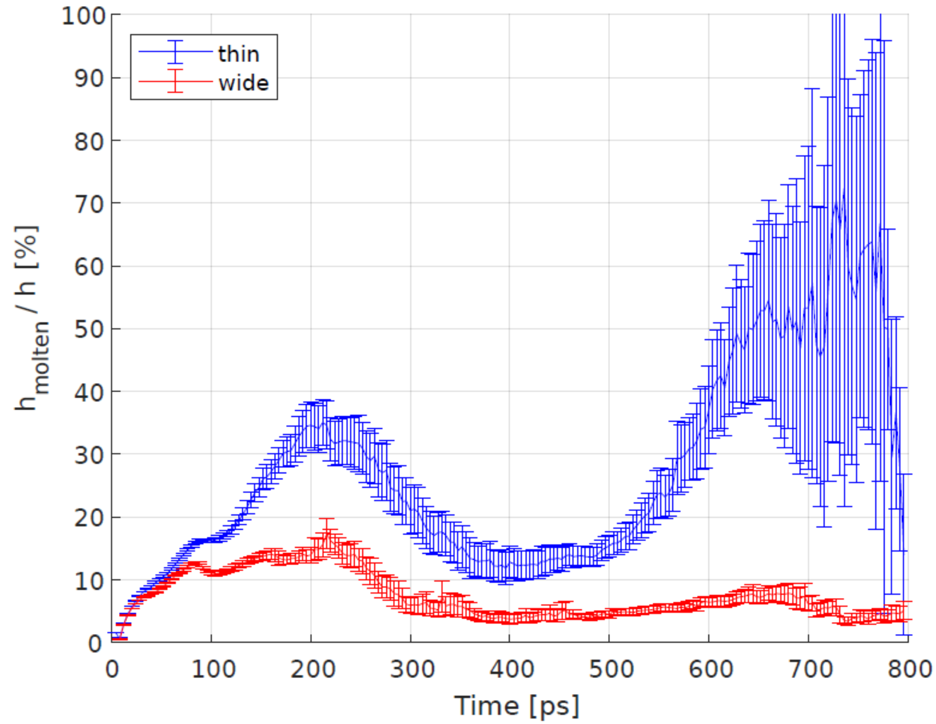




M. Veske, et. al. https://arxiv.org/abs/1906.08125

Results II



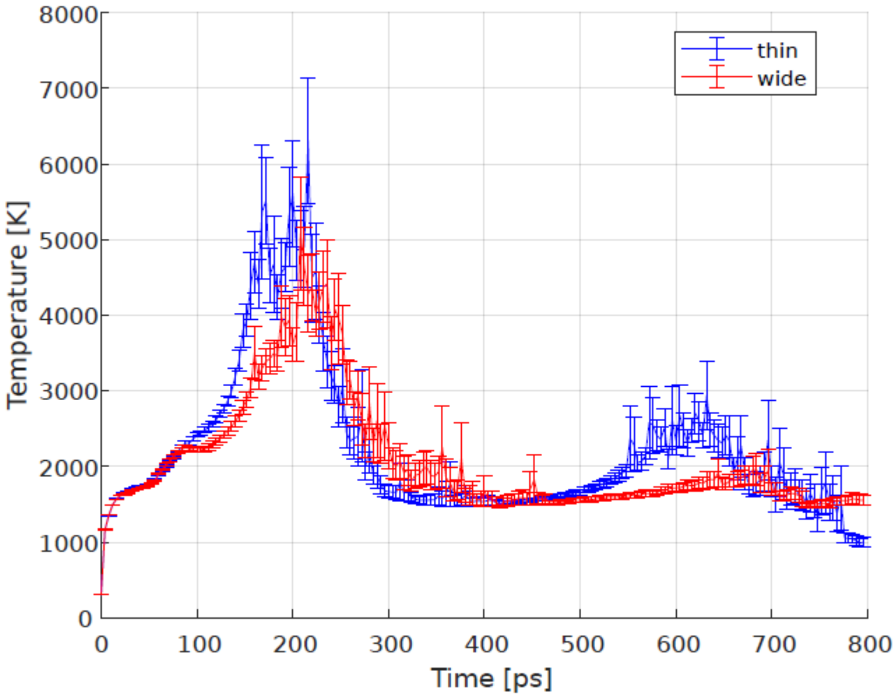


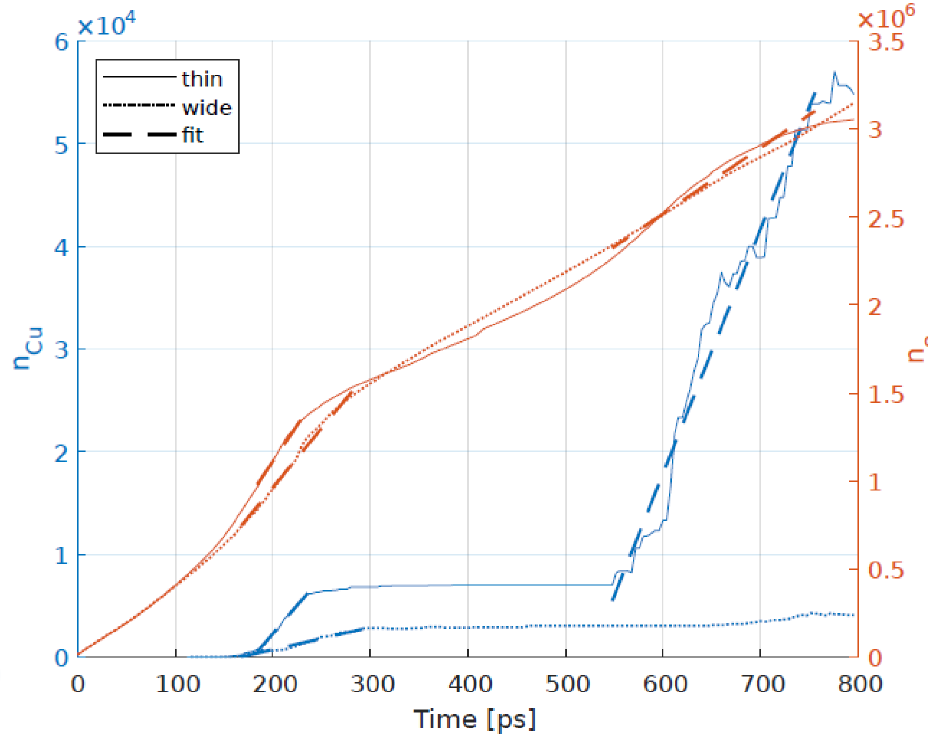
- Power flux density in a cylinder of 10nm radius: 9.5 MW/mm^2
- Similar to SC limit calculations [1]

[1] A. Grudiev et. al. Phys. Rev. accel. beam. 12 102001

Evaporation rates

	wide	thin 1	thin 2	ArcPIC
r_{Cu} [ps^{-1}]	22±2	110±5	238±12	404
r_e [fs^{-1}]	6.7±0.2	8.2±0.6	3.7±0.2	27.1
R_{Cu} [nm^{-2} ns^{-1}]	220±20	1100±50	2380±120	40.4
R_e [nm^{-2} ps^{-1}]	67±2	82±6	37±2	2.7
$r_{Cu/e}$ [$\times 10^{-3}$]	3.2±0.3	13.5±1.6	64±6	15





Outlook for plasma onset simulations

- Ultimate goal: direct connection of stages 2 and 3, simulation of the full BD process
- Including other particle species (Cu, Cu^{+}, Cu^{++} etc)
  - ✓ Managing boundary injection between MD and PIC domains (quite challenging)
  - ✓ Simulating larger systems for longer times to check whether the runaway continues
- Understanding the limitations of the arc ignition progress with respect to:
  - ✓ Power flow and related quantities
  - ✓ Tip size, shape, β, etc

Conclusions

- Getting closer to understanding the transition from intense FE to arc plasma, more complex simulation methods required
- Experiments show that the anode does not play a significant role on BDs. Even the anode flare seems to be caused by cathode material
- Now we know how to properly calculate the biased diffusion parameters, preliminary results indicate a possibility to grow tips by this mechanism
- Surface defects do not affect FE dynamics apart from a slight φ lowering. More evidence that field enhancement is most probably geometric

THANK YOU

CSC

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Magnus Ehrnroothin säätiö