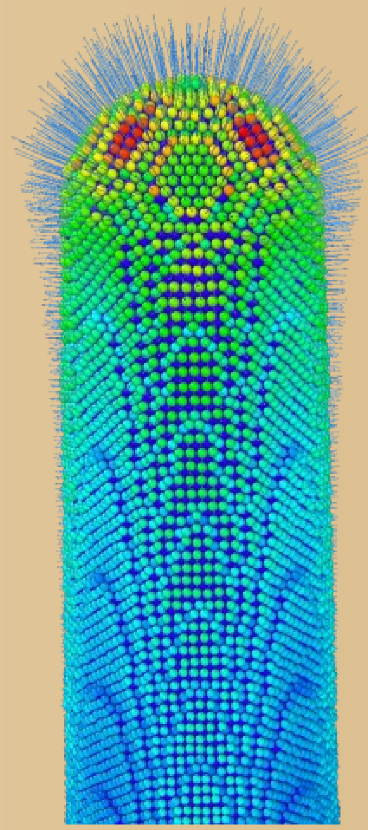
Thermal runaway of metal nano-tips during intense electron emission



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Outline

- Motivation
- Methods:
  - Molecular Dynamics – Electrodynamics
  - Electron emission
  - Heat diffusion
- Results:
  - Thermal runaway in intensively emitting Cu nanotips
  - Evaporation rate – connection to plasma onset simulations
- Open questions - future plans
- Conclusions

Motivation

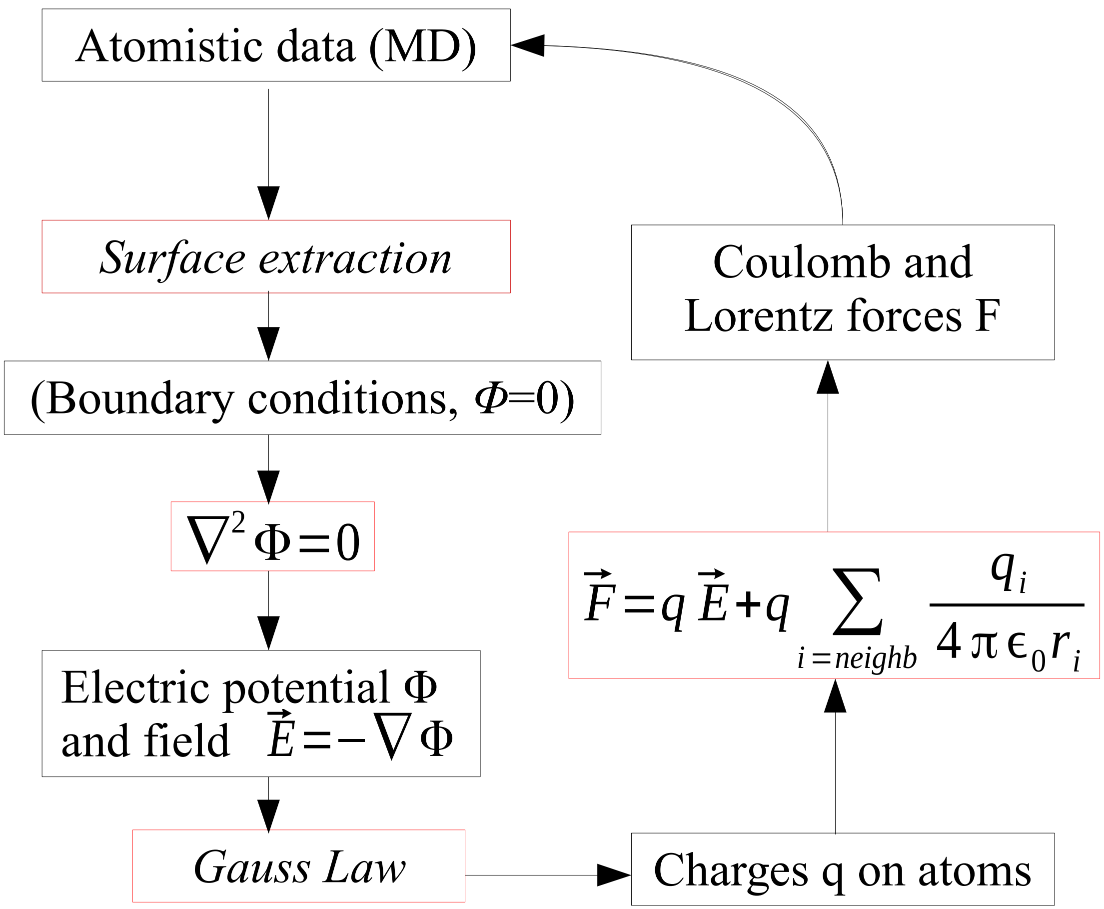
- Electron emission is known to initiate vacuum arcs. However, the exact mechanism is still unclear.
- Reveal and understand the mechanisms leading from **intense electron emission** to **plasma formation**
- Plasma PIC simulations [1]: plasma can ignite from a Cu field emitter assuming:
  - Intense field electron emission up to mA
  - Evaporation of Cu neutral atoms to a rate of 0.015 atoms/emitted e.
- **What is the origin of those neutrals?**
- **What mechanisms lead to their evaporation?**

[1]: H. Timko et. al., Contrib. Plasma. Phys. 4 , p229 (2015)

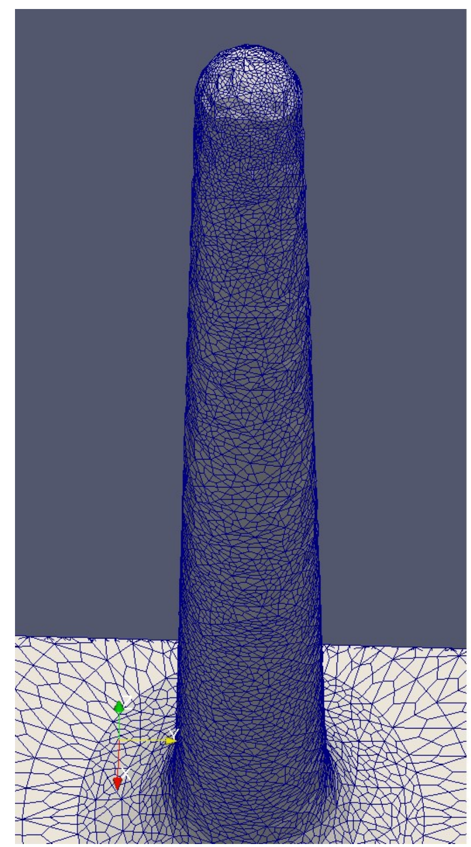
Need for multi-physics simulations

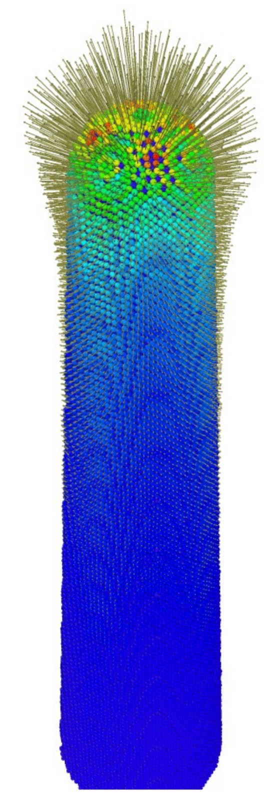
- Existing hypothesis:
  - Intense electron emission → heating → thermal-field-assisted evaporation
  - Is this evaporation enough??
- A simulation of this process must include:
  - Material deformations: *Molecular Dynamics*
  - Electric field effects: *Finite Element Method*
  - Electron emission: *GETELEC*
  - Heat diffusion: *Finite Difference Method*
- All the above processes have to be calculated **concurrently** and **self-consistently**

Concurrent MD-ED

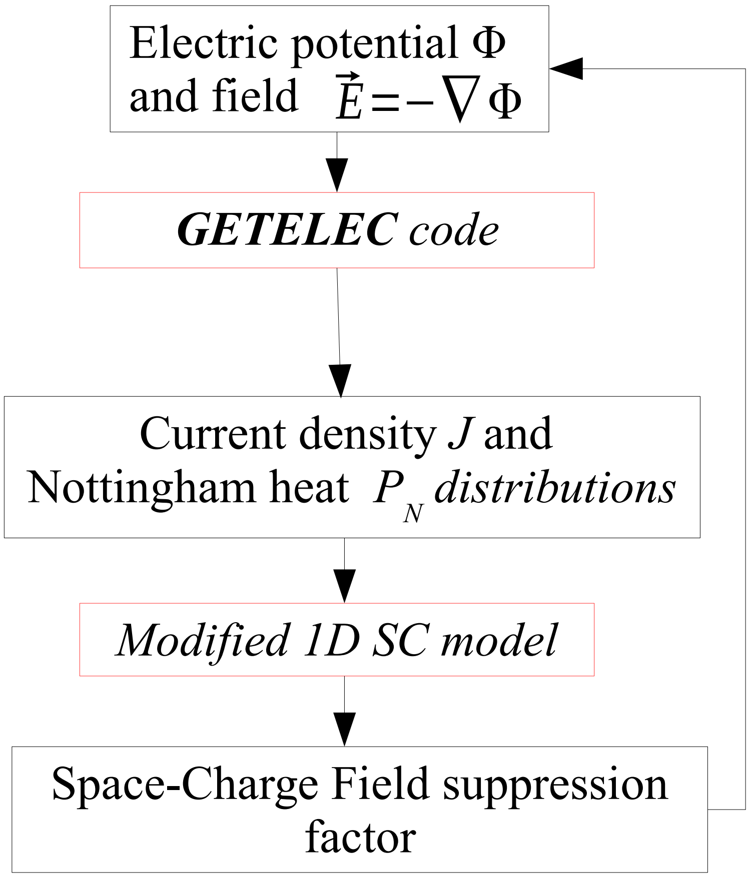


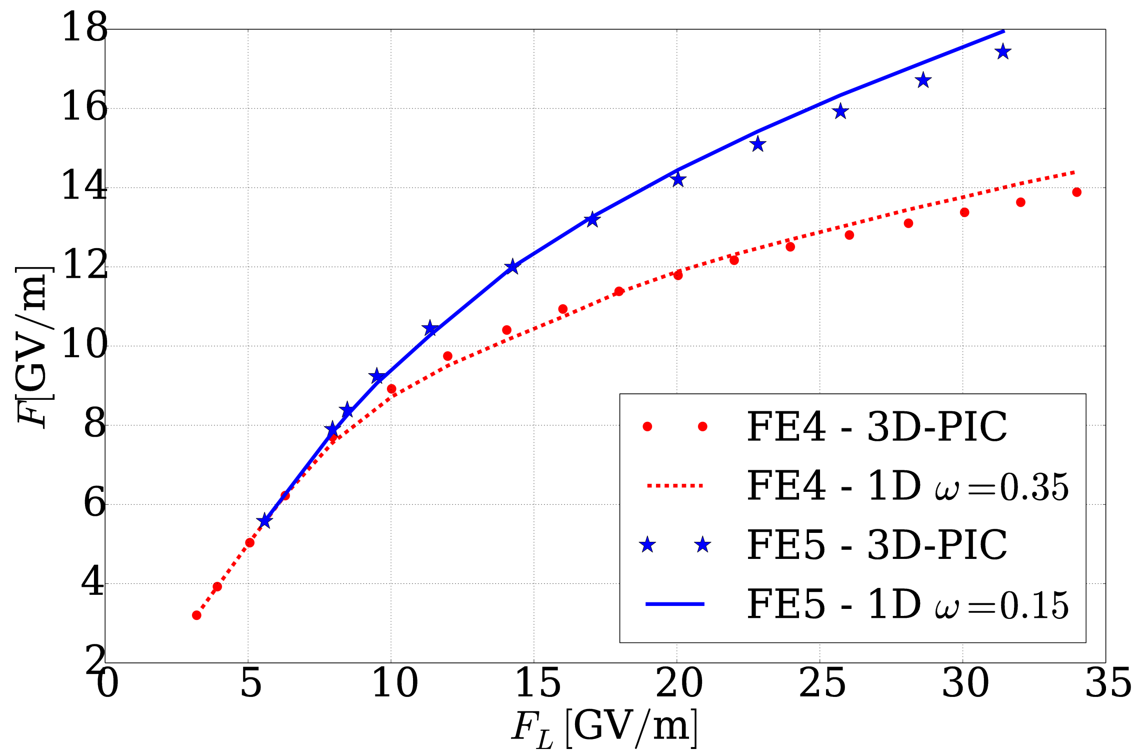
h = 93nm, r=3nm, sa = 3°





Electron emission in the space-charge limited regime

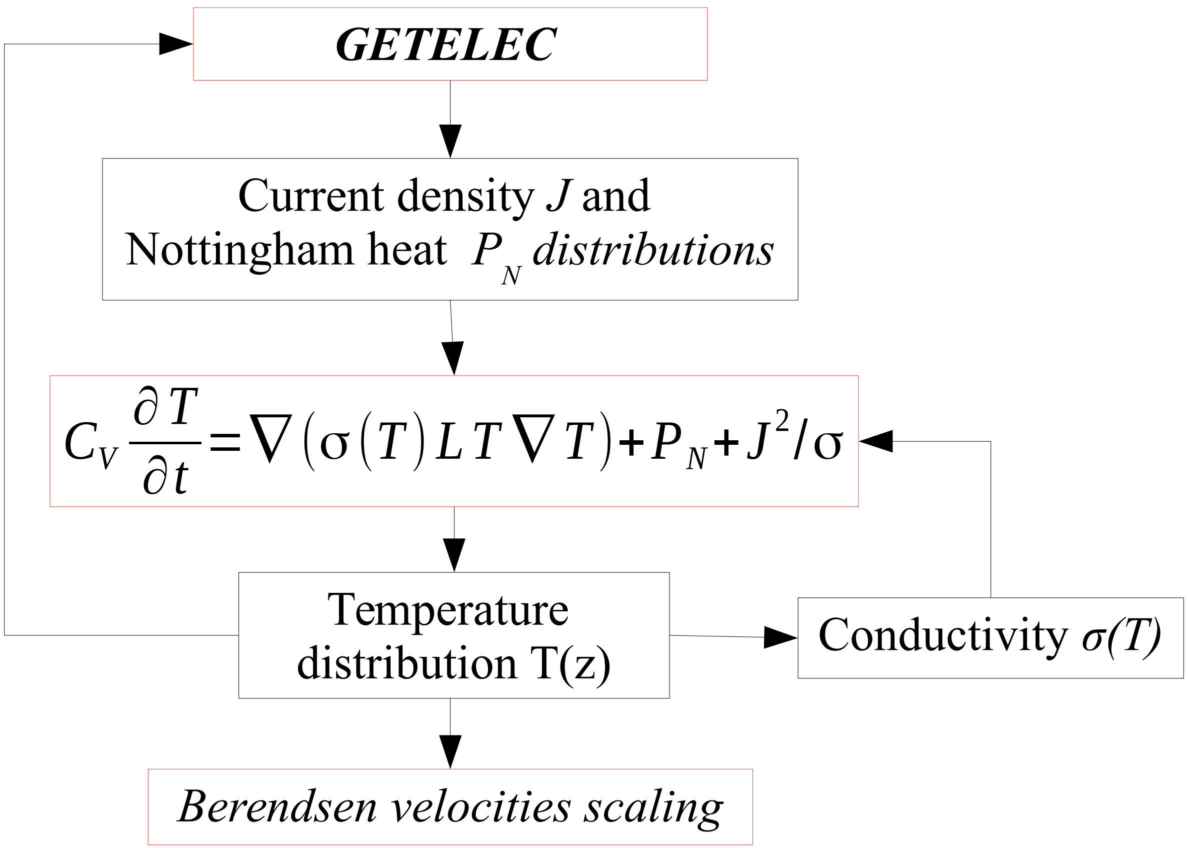


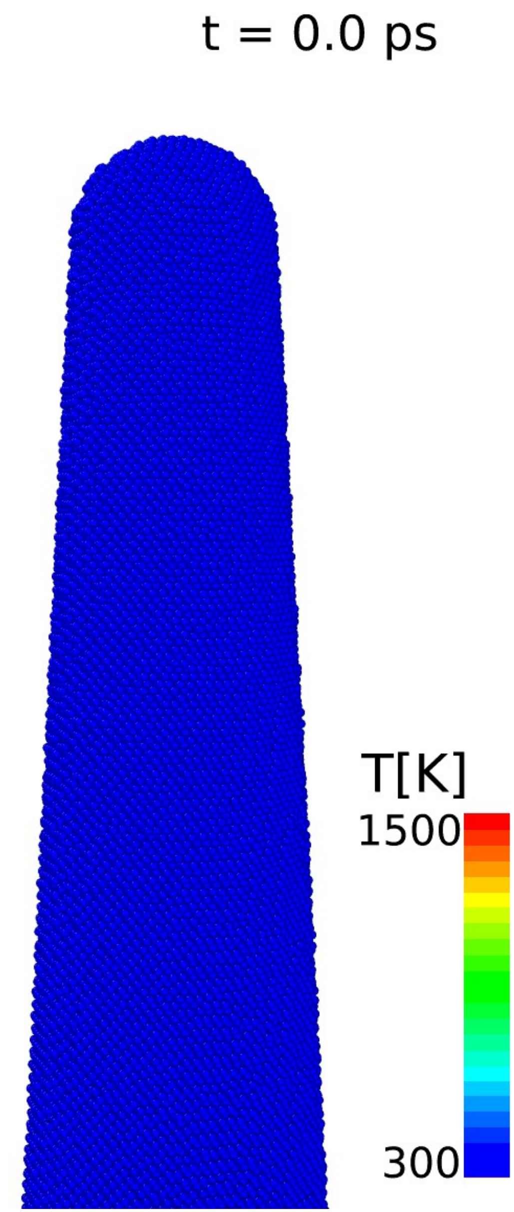


- Modified 1-D model: multiply the total voltage by ω<1, use representative values for ***E, J*** distributions
- Fitting to full 3D simulation data by Uimanov [1]
- Good agreement: The 1D SC model is sufficient

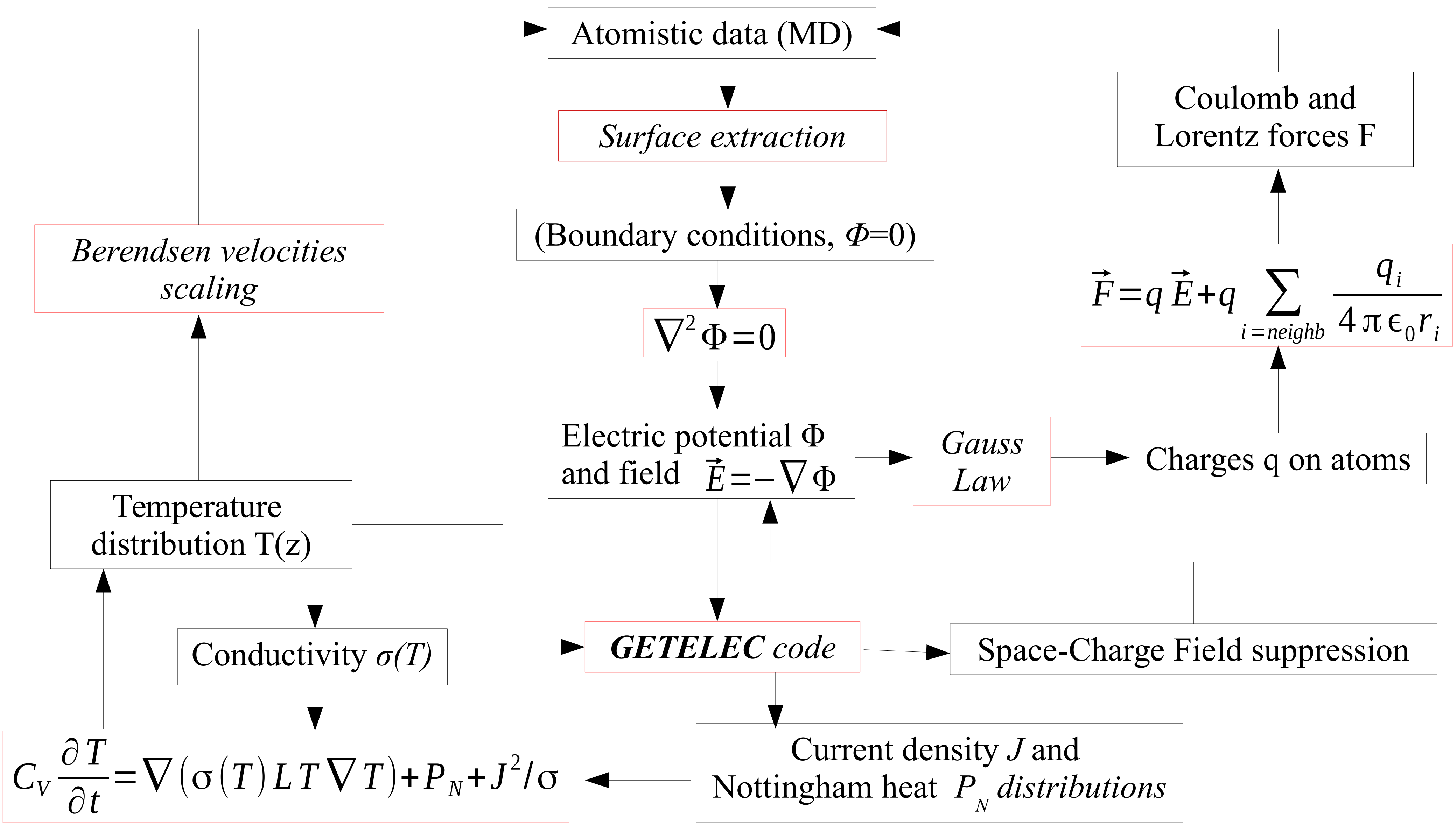
[1] I. Uimanov, IEEE Trans. Dielectr. Electr. Insul. 18, 924 (2011)

Heating: Joule and Nottingham



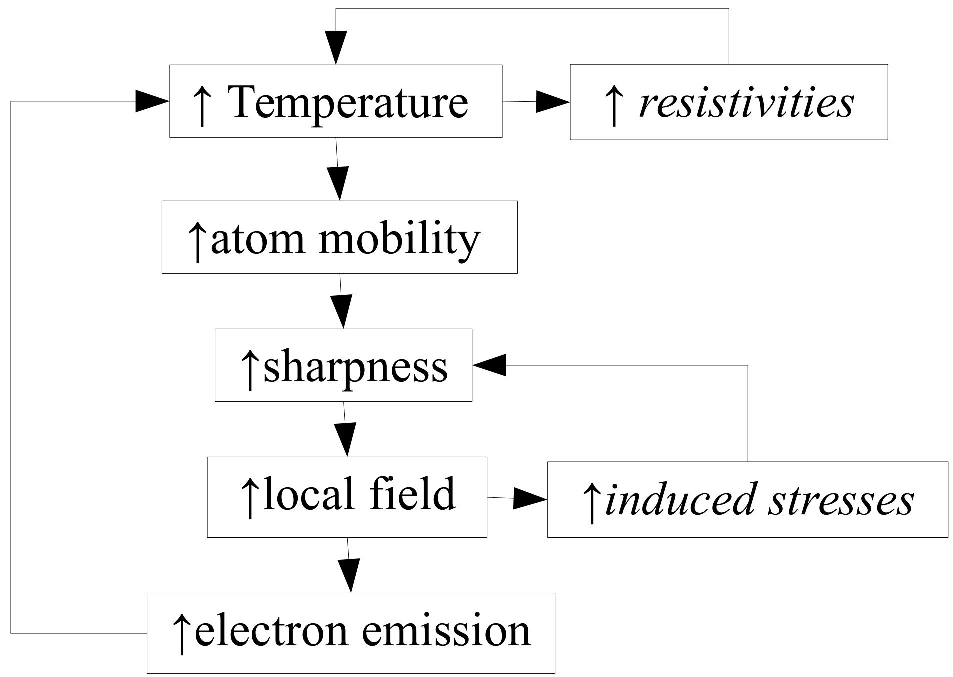


The whole simulation model

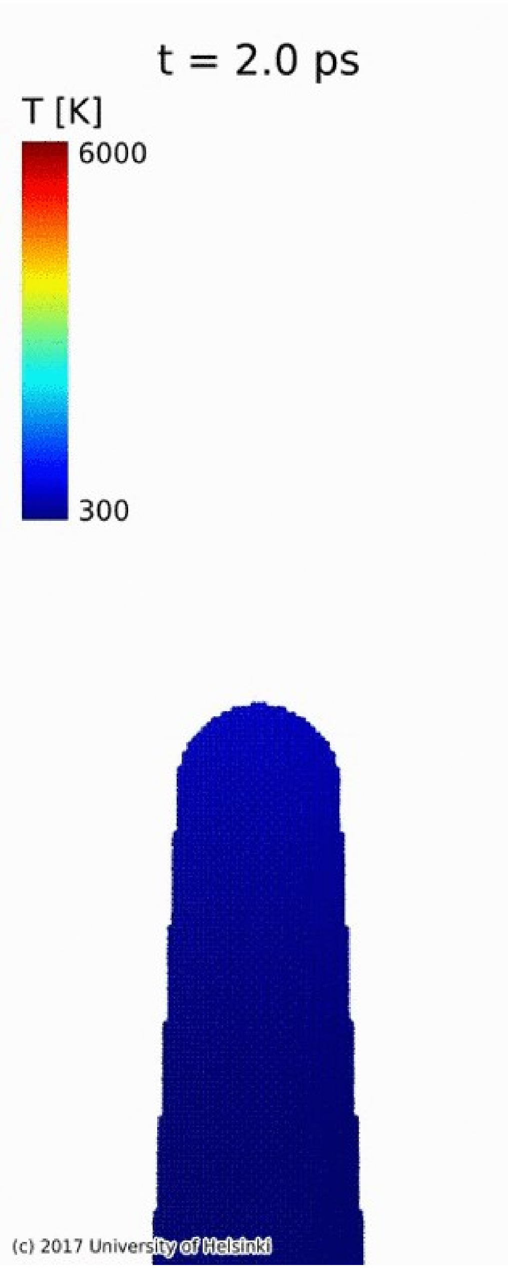


Results: Thermal runaway-evaporation

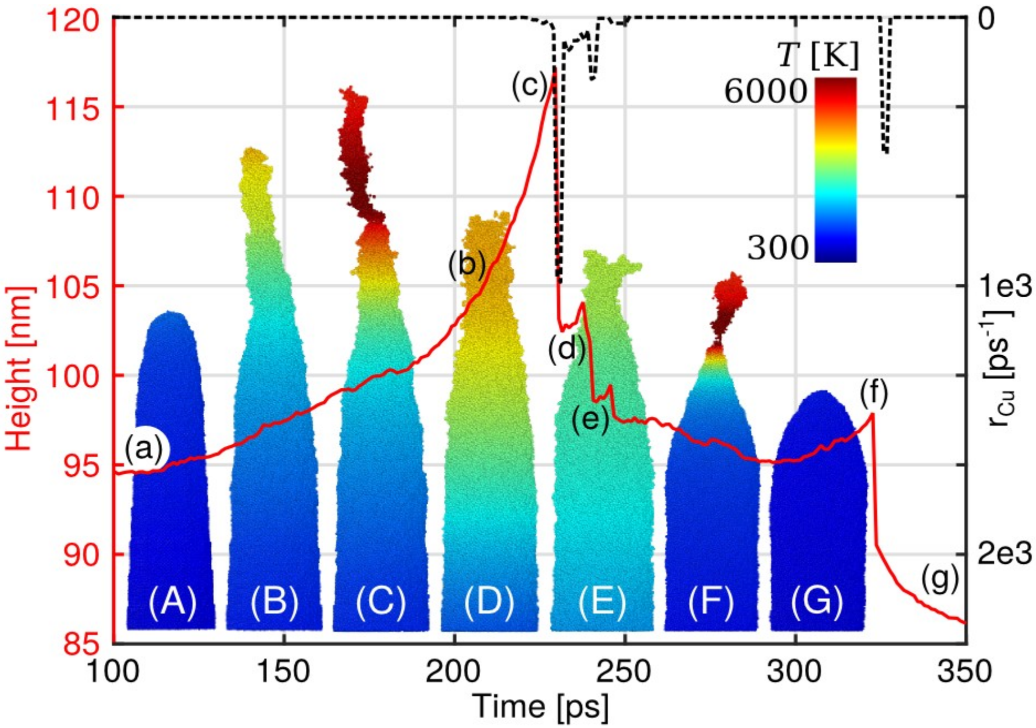
- Simulating for E_{appl}=0.8GV/m, V_{appl}=3kV DC
- **Thermal runaway:**



- **Evaporation** of large parts of the tip in forms of atoms and nanoclusters
- Eventually the tip has not enough length and it cools down gradually.



Evaporation analysis



- Tested for two different Cu inter-atomic potentials
- 7 independent runs for each potential with different seeds
- The same qualitative behaviour for all (the numbers might deviate)

- Mean evaporation rate between first and last evaporation events: R_{Cu} = 75±11 atoms/ps
- Mean current I = 2807±153 e/ps
- $R_{Cu/e}$ = 0.025±0.003 atoms/e
- **Exceeds** the minimum 0.015 found in the ArcPIC simulations!!!

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Conditions to runaway

- Prerequisites for the thermal runaway process to be initiated:
  a) **Heating** enough to cause melting of a significant area at the apex region. T reach ~1400-1500K
  b) **Current densities** that cause this high heating are of the order 10^{12} A/m^2 (agreement with experiments)
  c) **Local field** at the top (after SC lowering) must be more than ~10GV/m to "pull" the tip upwards
- Tips of 20-100nm height must be present to initiate this process

Open questions - Future plans

- **Still open questions:**
  - What happens with the evaporated atoms and clusters?
  - How do they affect the electrostatics?
  - What is the transient effect of the space charge?

- **Further development:**
  - Develop full 3D simulation for the space charge
  - Simulate the impact of the nanoclusters on the anode
  - Include the evaporated atoms in the electrostatic simulation
  - Integrate PIC simulations in the vacuum region and track all evaporated particles until plasma ignition.

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Conclusions

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- The mechanism leading from intense field emission to vacuum arc has still a lot of questions to be answered
- The integrated multi-physics simulations can reveal and give an insight in several processes
- A **thermal runaway** process leads to **evaporation** of large parts of a nanotip in the form of both **atoms** and **nanoclusters**
- The number of evaporated atoms matches well the minimum number required in plasma simulations to initiate plasma
- Further investigation of the behaviour of the vapour is needed to understand the behaviour of mechanisms and fully connect to the plasma calculations.

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Acknowledgements

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Thank you!!!!