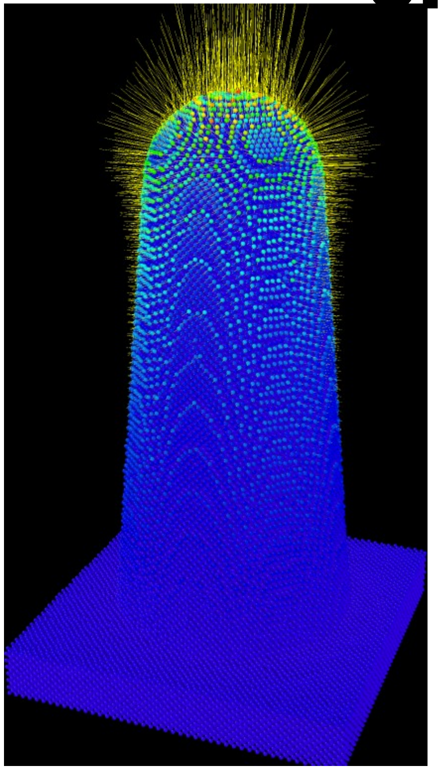
# A generalized method for calculating electron emission and thermal evolution of metallic nanotips



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# Motivation

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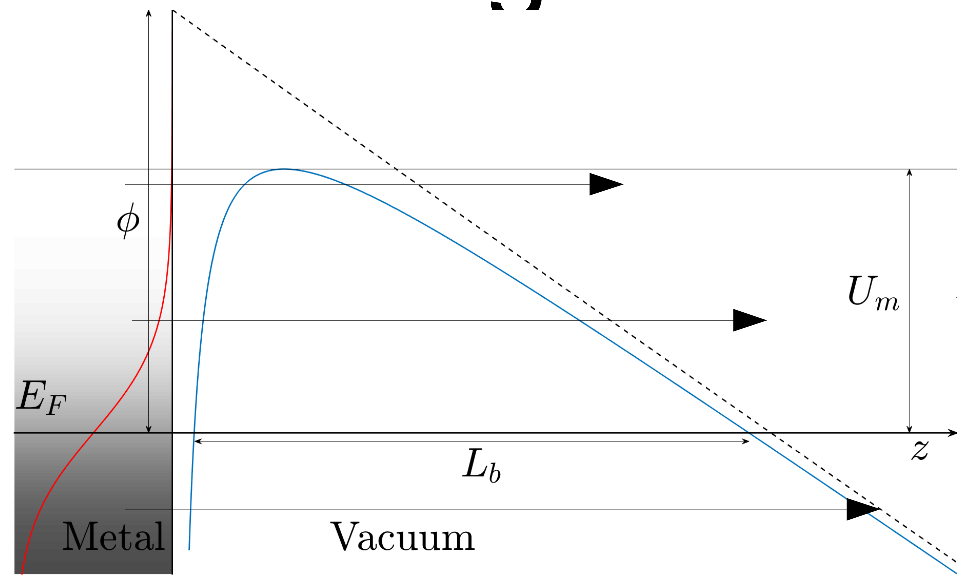
- It is established that electron emission plays an important role in the initiation of vacuum arcs.
- However the exact mechanism that leads from intense emission to plasma initiation is still unclear
- Fundamental questions:
  - How do we go from field emission to plasma?
  - PIC simulations assume supply of neutral atoms. What is their source?
- Need for simulations that take into account more phenomena:
  - Electron emission from sharp tips
  - Joule and Nottingham heating
  - Field-induced stress

# Electron emission: problems and challenges

- Problem I: T-F Emission

Thermionic and Field emission cannot be always separated. General Thermal-Field (GTF) theory is needed (especially in the case of high-temperature melting nanotips.)




- Problem II: Sharp nano-tips

Sharp emitters have curved potential.The classical Shottky-Nordheim (SN) barrier, based on planar geometry and linear potential cannot describe them. The emission might be overestimated by orders of magnitude

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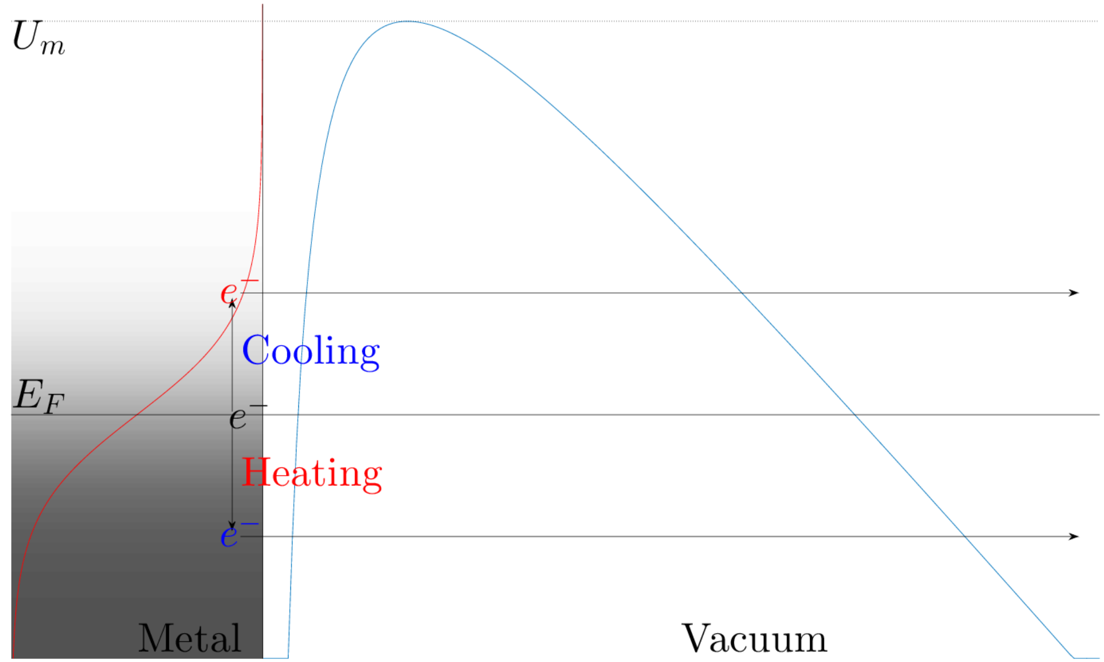
# Heating processes

- Nottingham heating

Electrons leaving from the surface cause either heating or cooling, depending on the conditions




- Joule Heating

Current running through the emitter causes Joule heating. In standard metallic tips conditions, Nottingham heating is dominant. **However** this might change when tips reach **high temperatures beyond melting point**.

# Electron emission computational tool requirements

- Field emission calculations are much more complicated than applying simple equations.
- Need for a general computational tool for electron emission that:
  - Calculates emitted current density and Nottingham heating power
  - Is applicable to all regimes (thermal, field, intermediate)
  - Takes into account the curvature of the emitters
  - Costs affordable computational time
  - Is versatile and generally applicable to various emission calculations
- Development of a new tool named GETELEC.

!!Download it from https://github.com/AndKyr/GETELEC

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# What can GETELEC do?

- Take as input the work function $\varphi$, temperature T and electrostatic data as:
  - Either already calculated electrostatic potential distribution $\Phi(x)$
  - Or the parameters $(F,R,\gamma)$ of a simple electrostatic model
- Find the regime (thermal, field, intermediate, blunt, sharp)
- Calculate the current density J and the Nottingham heating power $P_N$
- Automatically analyse experimental I-V data and extract:
  - Enhancement factor $\beta$
  - Radius of curvature R

# GETELEC Results

- GETELEC calculations for various regimes and comparison to previous theories:

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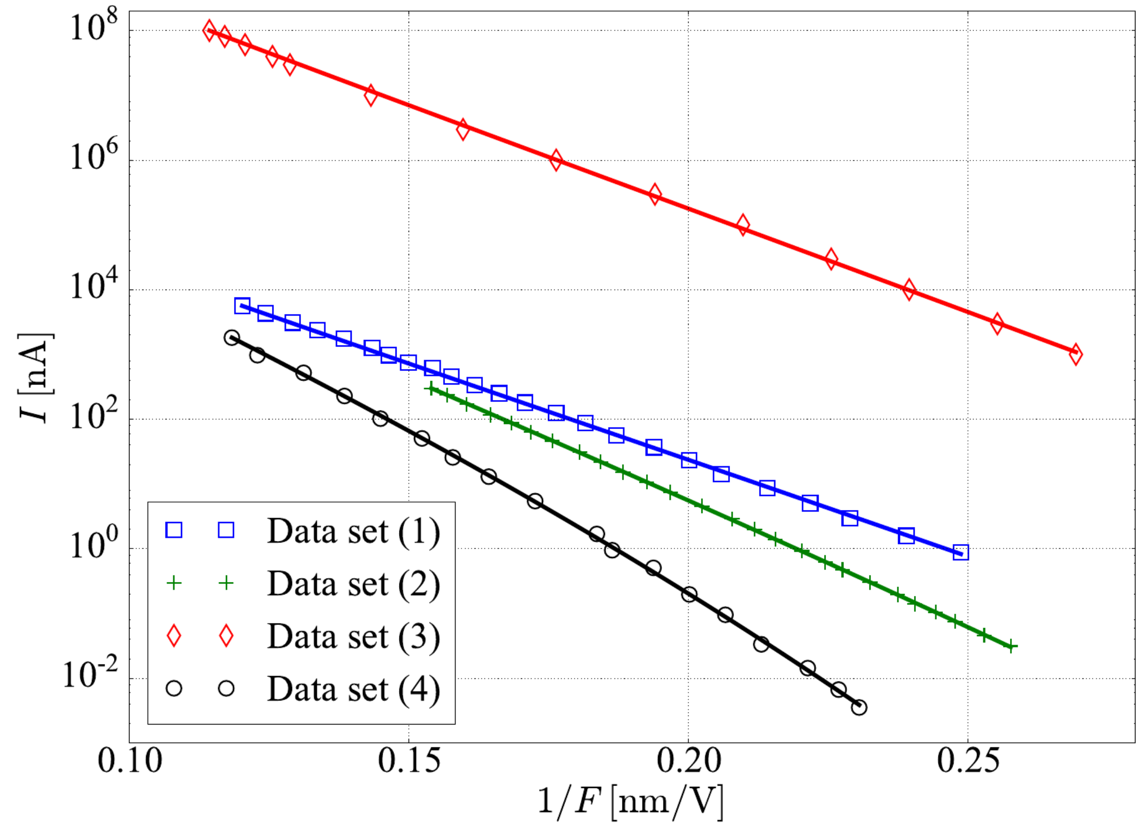
- Current and Nottingham heat are overestimated by several orders of magnitude by the standard GTF or FN theory

# GETELEC Results II: Experimental I-V data

- Fitting data from various experimental groups
- Extracted parameters in good agreement with

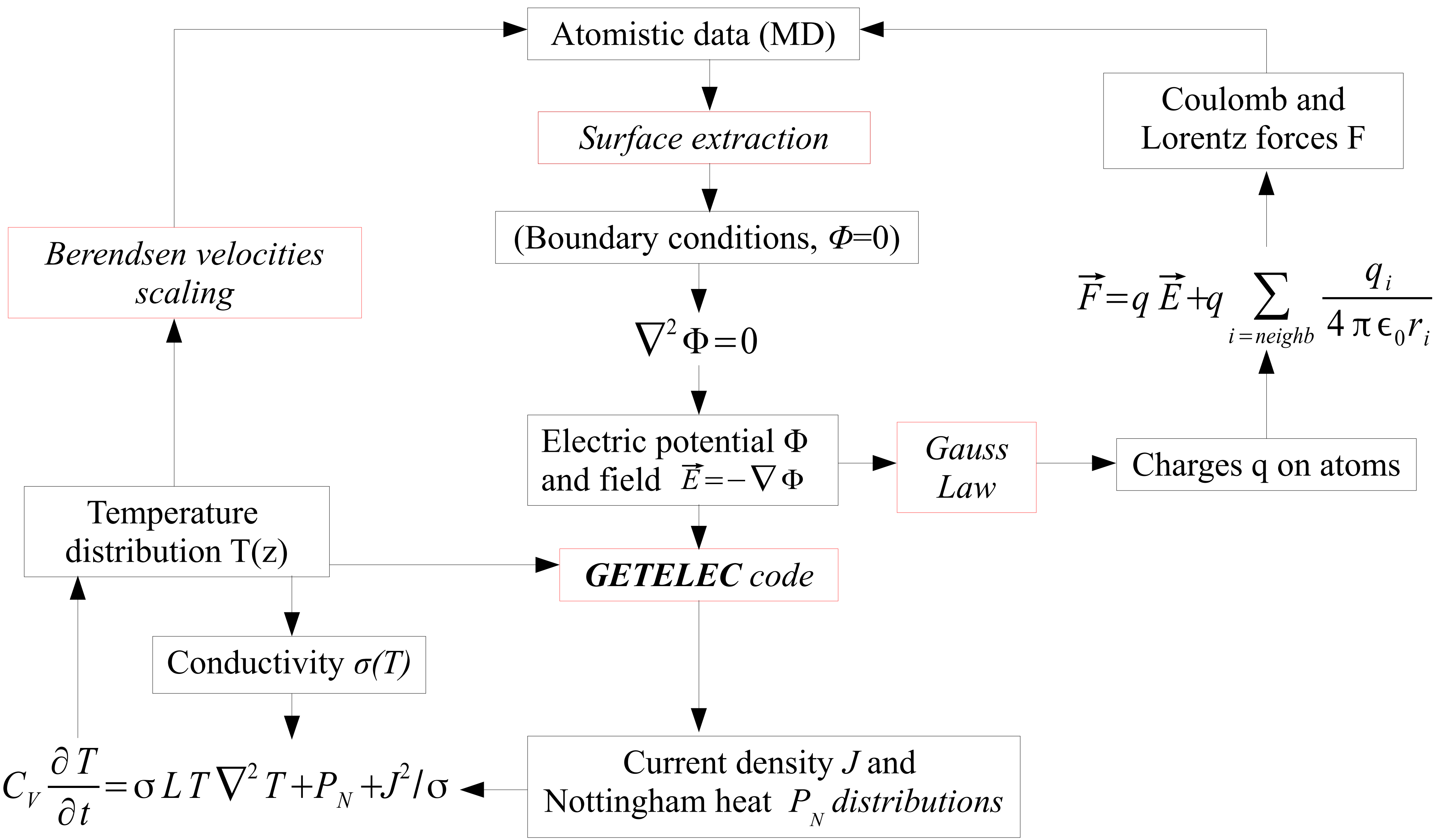
| Set | φ(eV) | β | R(nm) |
|---|---|---|---|
| 1 | 4.05 | 0.017/nm | 10.08 |
| 2 | 4.5 | $1.007\beta_{exp}$ | 6.87 |
| 3 | 4.35 | 0.065/nm | 16.22 |
| 4 | 4.5 | 68.6 | 2.96 |

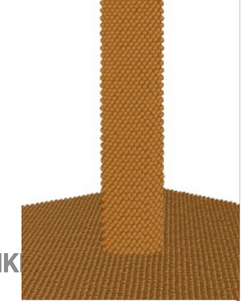


# Integrating GETELEC into multi-physics simulation tools

- The power of GETELEC is that it is general, versatile and computationally efficient
- It can be easily integrated with other simulation tools
- We combined it with our multi-physics codes under development into a complete simulation tool that combines various processes:
  - Molecular Dynamics (MD): Parcas
  - ElectroDynamics (ED): Helmod or Femocs
  - Electron Emission (EE): GETELEC
  - Heat Evolution (HE): Helmod or Femocs

# Integrated Multi-physics simulations





# Results: Temperature

- Test on a simple cylindrical tip with R=1.5nm, h=21nm and applied field = 1.25GV/m
- Two modes for comparison on a :
  - **Mode A:** Full calculation with GETELEC, including both Nottingham and Joule heating components
  - **Mode B:** Simple Classical F-N equation, including only Joule heating

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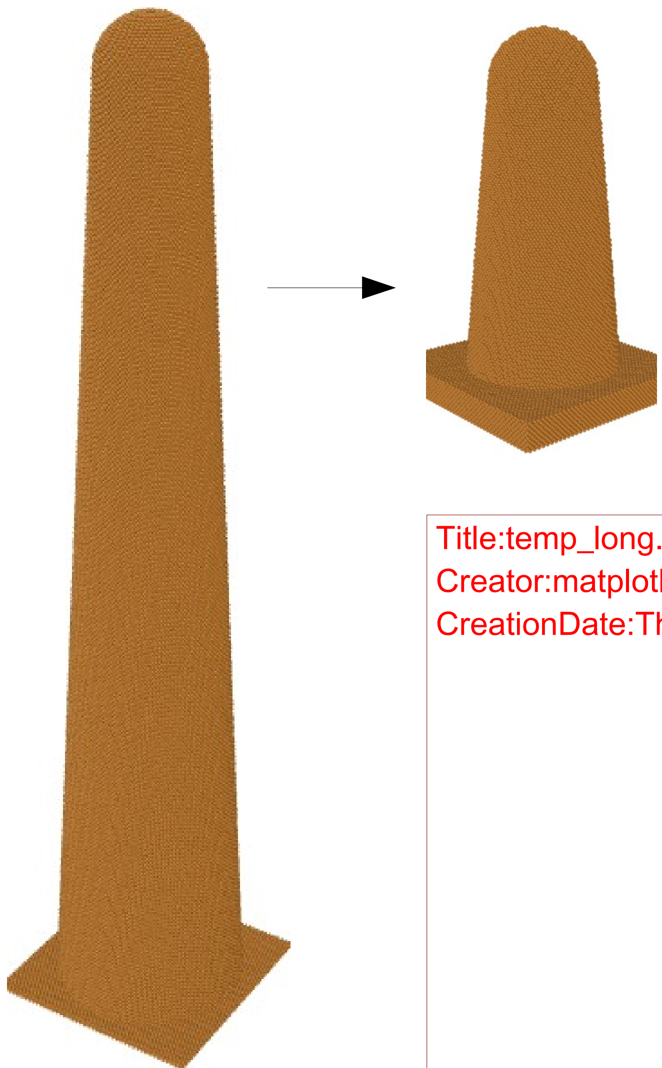
# A bigger tip



- Experiments have shown enhancement factors of the order of β~20-50
- Assuming tips of the size that can produce an enhancement factor of β~20: h=61nm, R=4nm
- Emitters with this enhancement easily reach melting temperature at the top for an applied field of about 0.43GV/m
- To simulate in a plausible computational time, we assume a smaller system, but apply higher field to get the same local, and higher bottom temperature 600K

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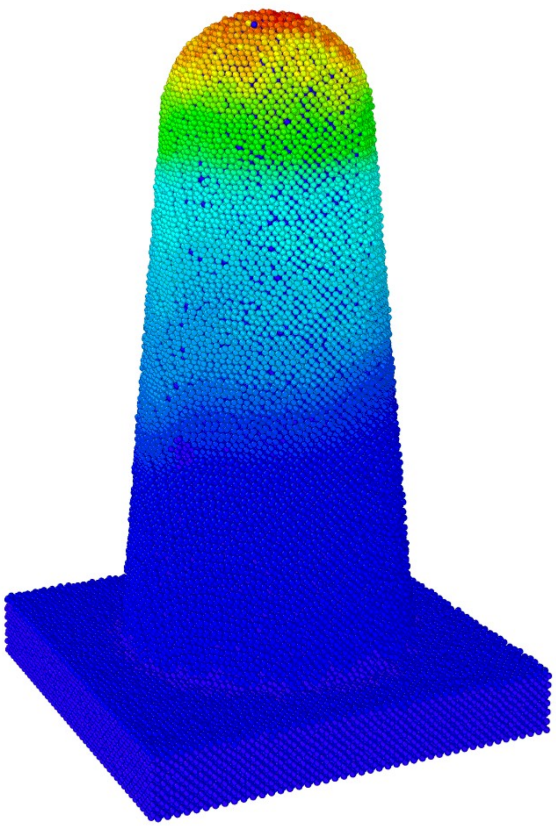
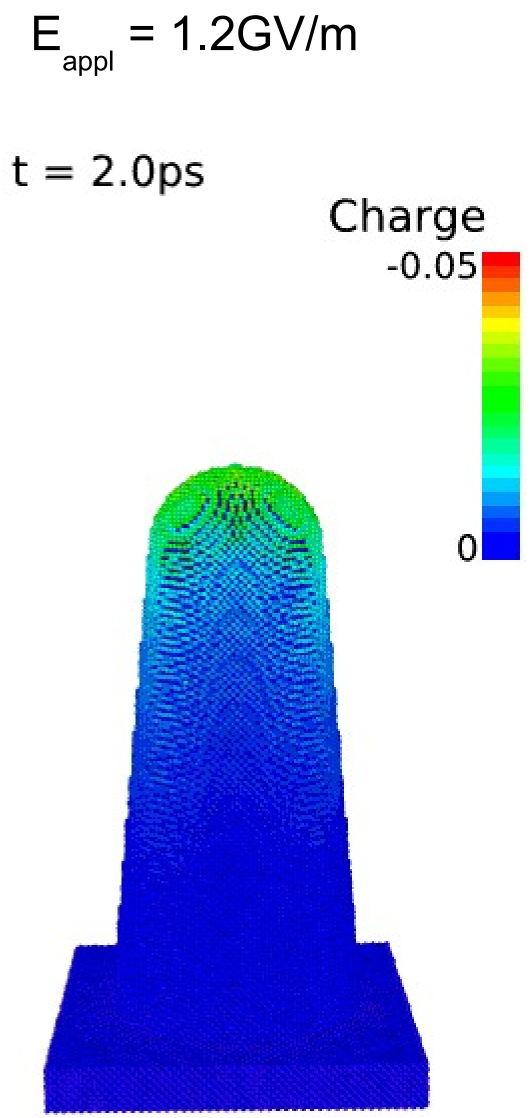
# Positive feedback and evaporation



If the applied field is enough to melt the top, the tip enters in a positive feedback loop:

- The field-induced stress make it pointier and the current increases
- The current increases the temperature
- The temperature increases the thermal and electric resistivity and makes the tip more “flexible”, tending to grow higher and pointier
- Eventually it will reach temperatures as high as 3000K and start evaporating

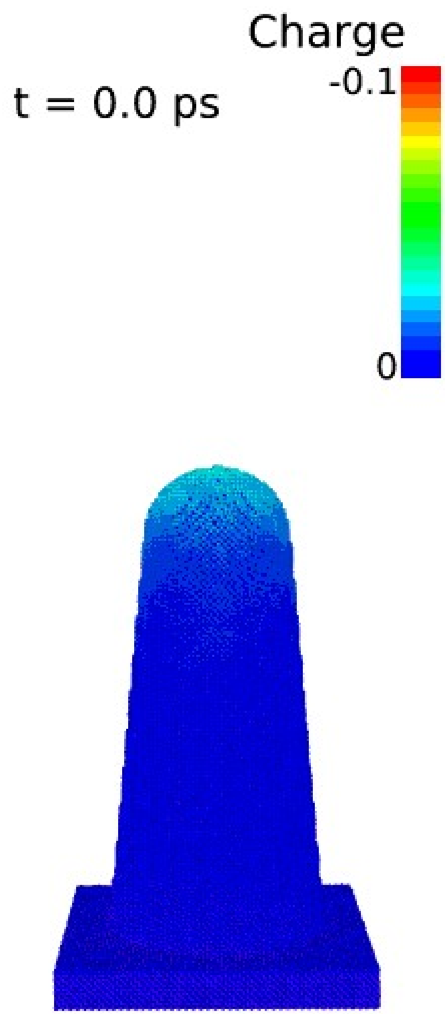
# Including the space charge




- Beyond a point the electron emission enters the space-charge limited regime.
- We took it into account with the simple analytical 1-D approximation.
- The space charge does not let the local field and the emitted current reach too high levels.
- However as the temperature rises, the resistivity of the material rises a lot and the Joule heating leads it to very high temperatures
- The result does not change qualitatively but the whole process becomes slower

# Running at constant temperatures

$E_{appl}$ = 1.2GV/m
$T_{top}$ = 1600K




- We ran at constant temperature distributions, to investigate under what conditions the tips enter this positive feedback loop
- With constant temperature  the shape is kept much smoother as the tip does not reach boiling temperatures
- A large cluster with total charge of ~20e  is evaporating in the end
- We found that a temperature of at least ~1300K is required to see a deformation in MD timescale
- We found that a minimum local field of about ~8GV/m is required to pull the structures upwards and not let them melt down

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# Future plans

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- Run more extensive simulations to see what are the exact conditions that lead to tip "explosion"
- Include space charge effects with better models
- Improve the tools and run various geometries and fields
- Investigate the size and the charge of the evaporated clusters
- Simulate the possibility that the evaporated clusters get more charge due to the electron beam.
- Simulate the bombardment of the anode side with the charged clusters, and the resulting possible sputtering.

# Thank you!!!!