SAND2010-0619C

Arc simulations using *Aleph*, a DSMC/PIC code

Presented at the "Workshop on Unipolar Arcs,"
Argonne National Laboratories

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Presentation Outline

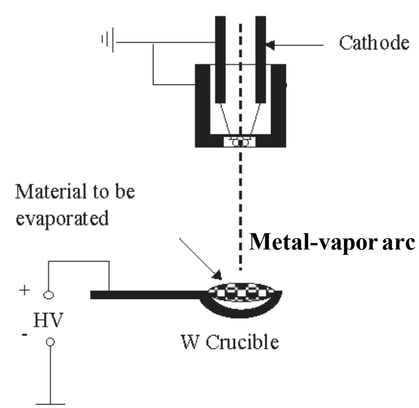
I. Motivation
II. Our goal
III. Overview of the *Aleph* code
IV. Critical infrastructure pieces
V. Description of our arc simulations
VI. Criticisms of our model
VII. Attempt to copy CERN's simple arc model
VIII. Conclusions
IX. Questions/comments/suggestions

I. Motivation

- "Arcs" are high-current density, low voltage discharges in partially-ionized gases

- Of interest for
  - gas switches
  - ion sources
  - vacuum coatings (Thermionic Vacuum Arc: TVA)

- In TVA, evaporating anode generates arc plasma



II. Our goal

Perform PIC/DSMC simulation of vacuum arc formation

- Start with vacuum gap between two electrodes
- Can be 1-D, or quasi-1D
- Simulate emission of electrons, ions, and/or neutrals from electrodes
- Include important ionization processes
- Exponential growth of gap current
- Current avalanche --- breakdown
- Simple circuit in series with arc
- Simulate beyond breakdown

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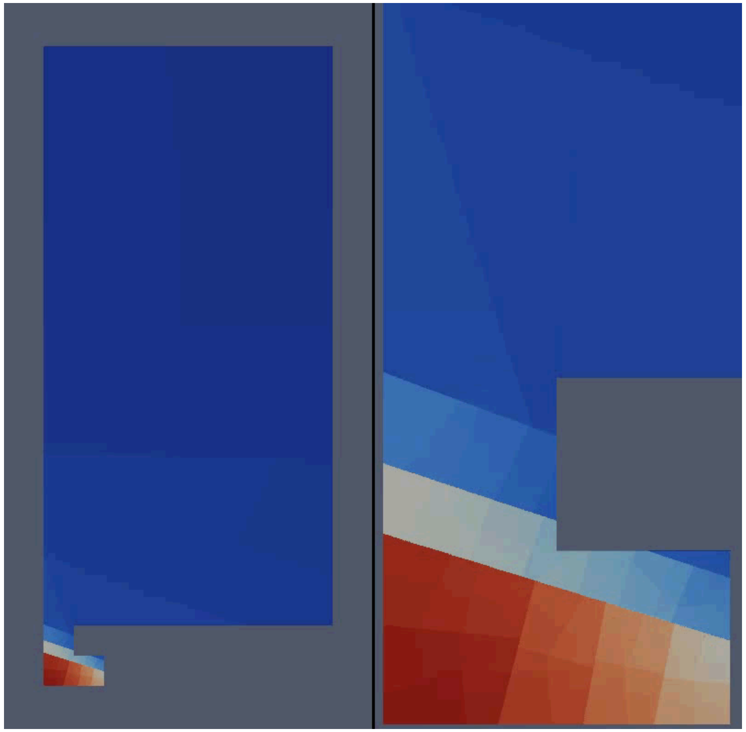
III. Overview of the *Aleph* code

- Hybrid PIC + DSMC
- Electrostatics
- Fixed B field
- Conduction
- Ambipolar approximation
- Dual mesh (Particle and Electrostatics/Output)
- Advanced surface (electrode) physics models
- Collisions, charge exchange, chemistry, ionization
- Advanced particle weighting methods
- Unstructured FEM (compatible with CAD)
- Massively parallel
- Dynamic load balancing (tricky)
- Restart (with all particles)
- Agile software infrastructure for easily extending BCs, post-processed quantities, etc.
- Uses elements of SIERRA, Trilinos and other ASC investments
- Currently utilizing up to 8192 processors (>30M elements, >1B particles)



128 core particle load balancing example

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The Basic *Aleph* Simulation Steps

Basic algorithm for one time step of length Δt:

1. Given known electrostatic field $\mathbf{E}^n$, move each particle for $\frac{\Delta t}{2}$ via:

$$v_i^{n+1/2} = v_i^n + \frac{\Delta t}{2}\left(\frac{q_i}{m_i}\mathbf{E}^n\right)$$

$$x_i^{n+1} = x_i^n + \Delta t v_i^{n+1/2}$$

2. Compute intersections (non-trivial in parallel).
3. Solve for $\mathbf{E}^{n+1}$

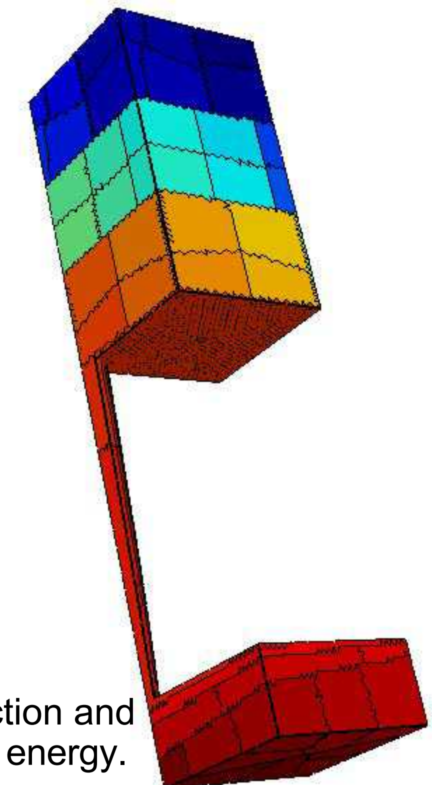
$$\nabla \cdot \left(\epsilon \nabla V^{n+1}\right) = -\rho(\mathbf{x}^{n+1})$$

$$\mathbf{E}^{n+1} = -\nabla V^{n+1}$$

4. Update each particle for another $\frac{\Delta t}{2}$ via:

$$v_i^{n+1} = v_i^{n+1/2} + \frac{\Delta t}{2}\left(\frac{q_i}{m_i}\mathbf{E}^{n+1}\right)$$

5. Perform particle re-weighting.
6. Perform DSMC collisions: sample pairs in element, determine cross section and probability of collision. Roll a digital die, and if they collide, re-distribute energy.
7. Perform chemistry: for each reaction, determine expected number of reactions. Sample particles of those types, perform reaction (particle creation/deletion).
8. Reweight particles. Sometimes.
9. Compute post-processing and other quantities.
10. Output.
11. Rebalance particle mesh if appropriate (variety of determination methods).



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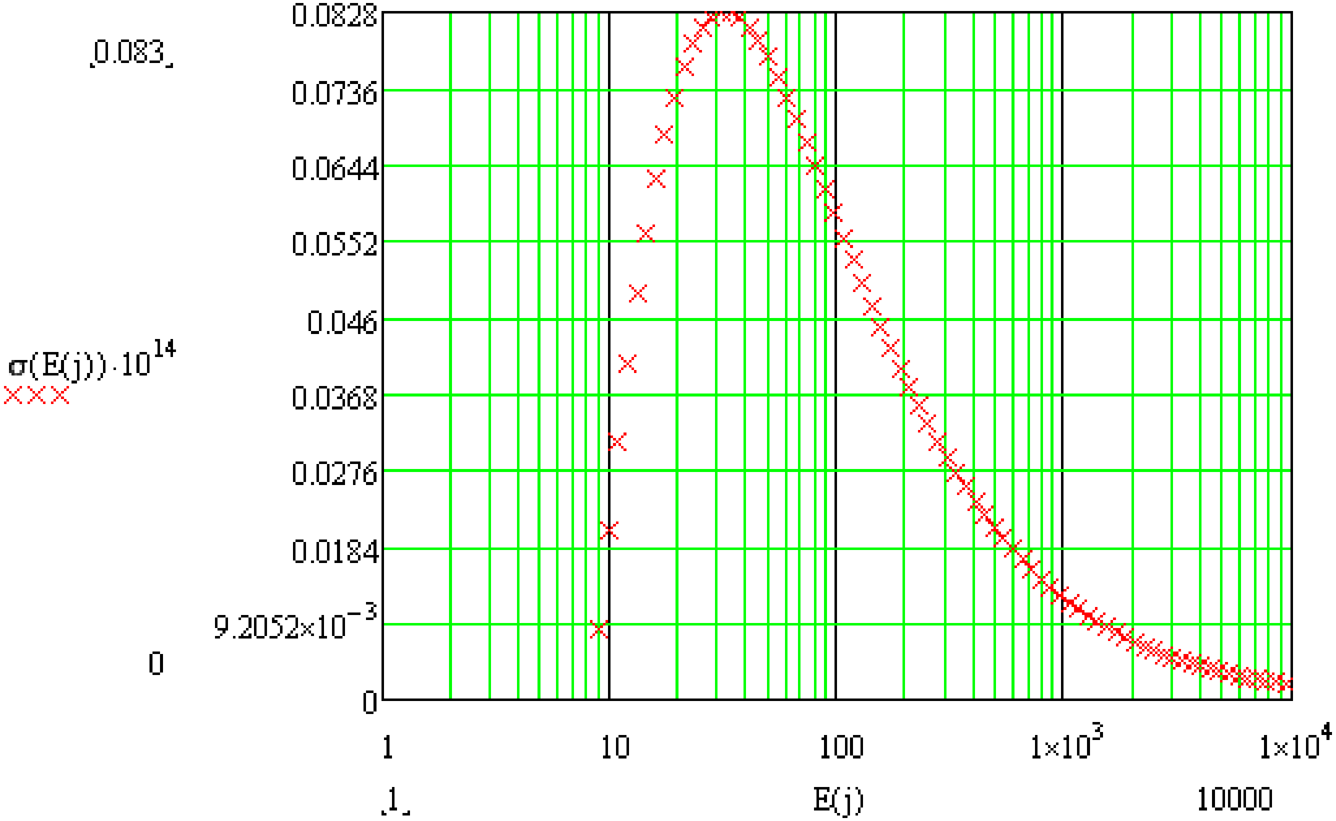
IV. Critical infrastructure pieces

- Computation of cross sections
  - Need ionization cross sections in order to simulate breakdown
  - Use the cross-section summation approach, or treat the individual collisions/reactions independently
  - Our model for ionization cross-section computation
- Dynamic particle reweighting
  - Vast density changes in space and time
  - For best computational efficiency, need a way to adjust particles’ weighting

Ionization cross-section model

Ionization cross-section (10^{-14} cm^2)



collision energy (eV)

Data from: "Electron-Impact Ionization Cross-Sections and Ionization Rate Coefficients …," Wolfgang Lotz, "Z. Physik 220, 466 - 472 (1969).

V. Description of our arc simulations

Stage 0: geometry, initial conditions, and setup of our model system
Stage 1: bulk plasma stability, sheaths formed
Stage 2: heating of the anode
Stage 3: emission from the anode
Stage 4: ionization
Stage 5: growth in plasma density
Stage 6: breakdown, or explosive growth in current to the anode
Stage 7: circuit model kicks in

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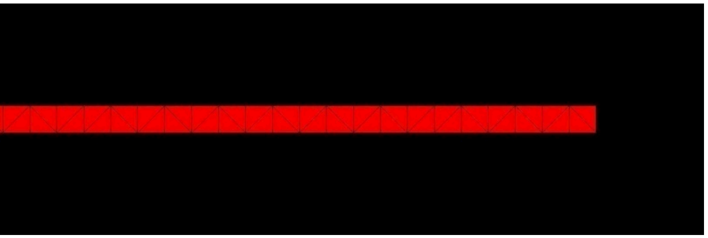
Stage 0: geometry, initial conditions, and setup of our model system



```
create vertex 0 0 0
create vertex 6e-3 0 0
create vertex 6e-3 6e-6 0
create vertex 0 6e-6 0
create surface vertex 1 2 3 4
delete vertex 1 2 3 4
surface 1 size 6e-6
surface 1 scheme trimesh
mesh surface 1
block 1 surface 1
block 1 element type tri
sideset 1 curve 4
sideset 2 curve 3
sideset 3 curve 2
sideset 4 curve 1
nodeset 1 curve 4
nodeset 2 curve 3
nodeset 3 curve 2
nodeset 4 curve 1
export mesh "arc.g" dimension 2 overwrite
```

- Quasi-1D, simple geometry, tri mesh
- Aspect ratio: 1000:1
- 2000 triangular elements
- 6 mm arc gap, 6 μm in the other direction
- Simple plasma cathode model
- Lay in of plasma at 1e20 density
- Start the anode already hot to save time and avoid lengthy heating stage
- Neutral metal atoms emitted from hot anode according to Antoine equation and Hertz-Knudsen vaporization equation
- 1D heat equation solved on anode, including cooling effects due to conduction, radiation, and evaporation
- 1e8 weighting on all particles
- Dynamic particle reweighting on neutrals
- 1800 V drop between the anode and the cathode

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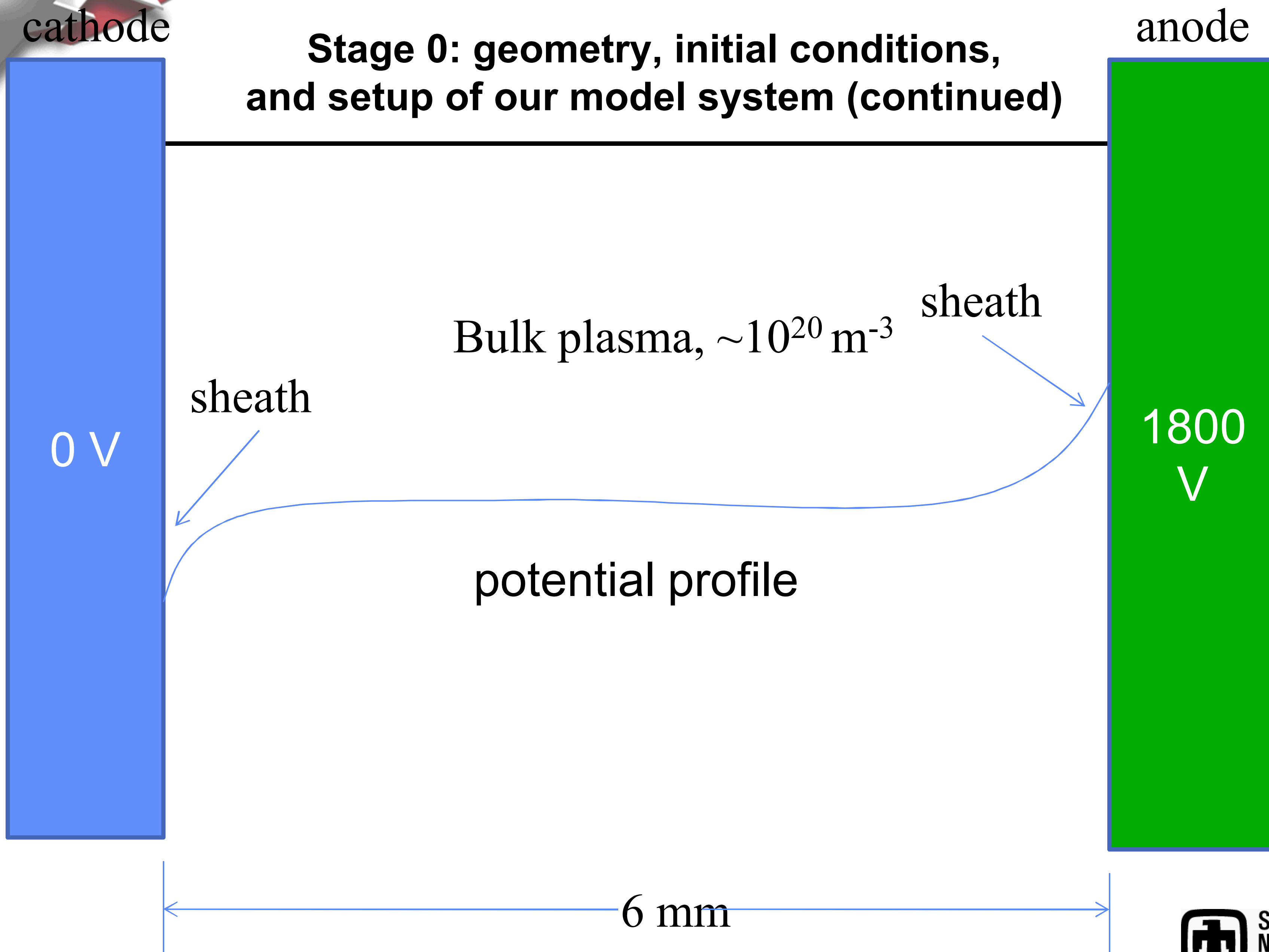
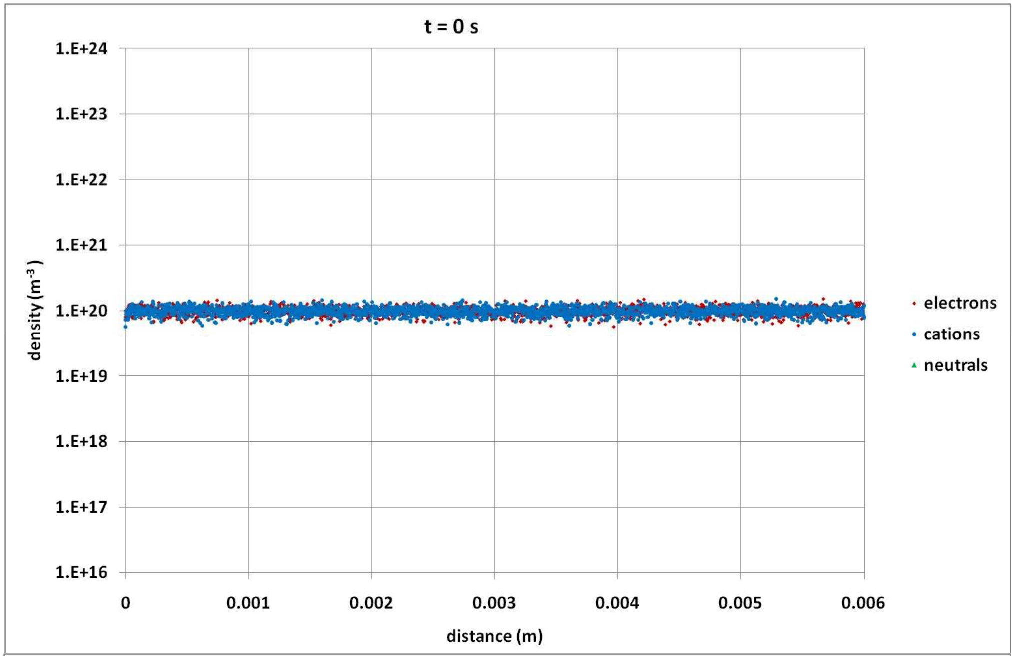
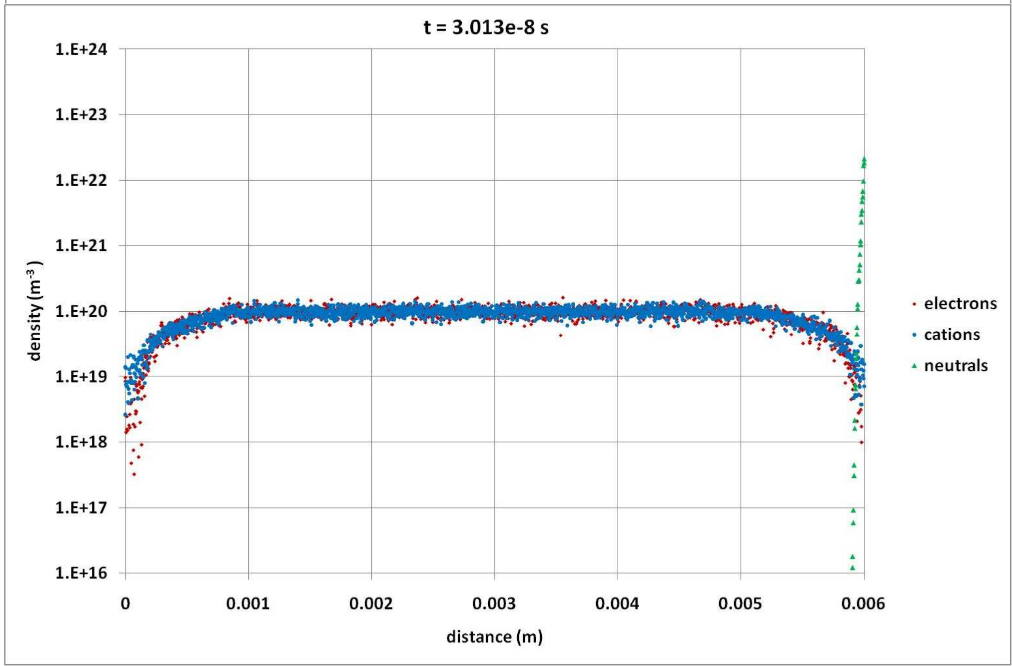
Stage 0: geometry, initial conditions, and setup of our model system (continued)



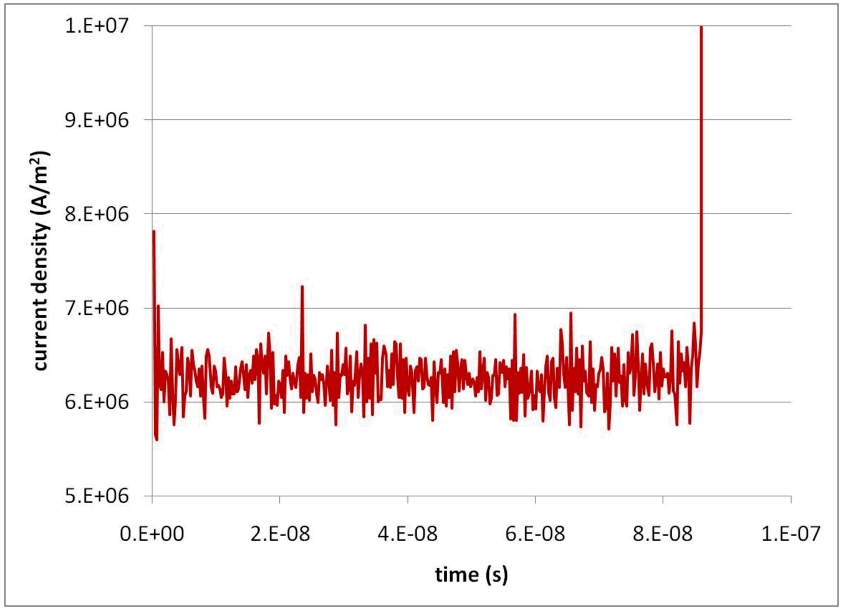
Stage 1: bulk plasma stable, sheaths formed

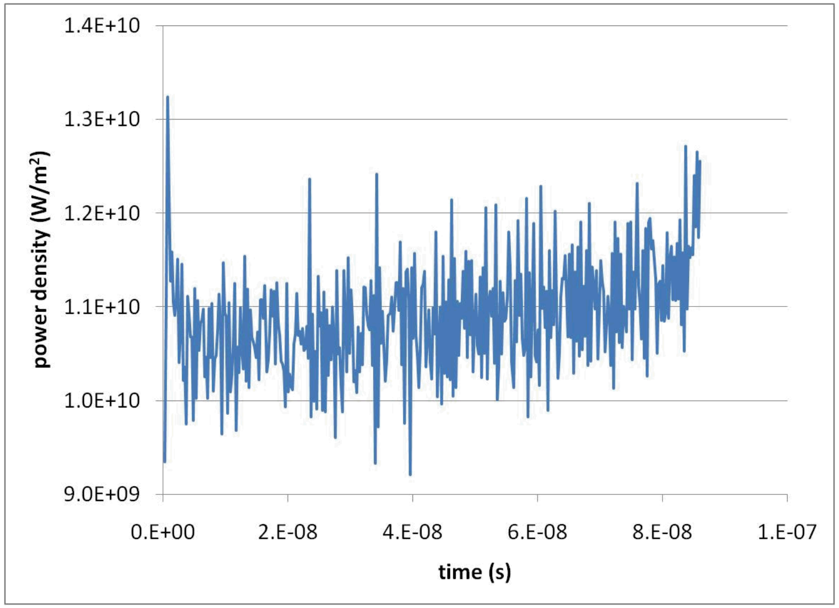
- **Simple cathode plasma model working**
- **Sheath formation at both the anode and the inert cathode.**





Stage 2: heating of the anode





- **P = IV = 6 MA/m^2 * 1800 V = 10.8 GW/m^2**
- **Extremely high heating rate → lower CPU cost**
- **Heat loss via radiation and evaporation negligible**

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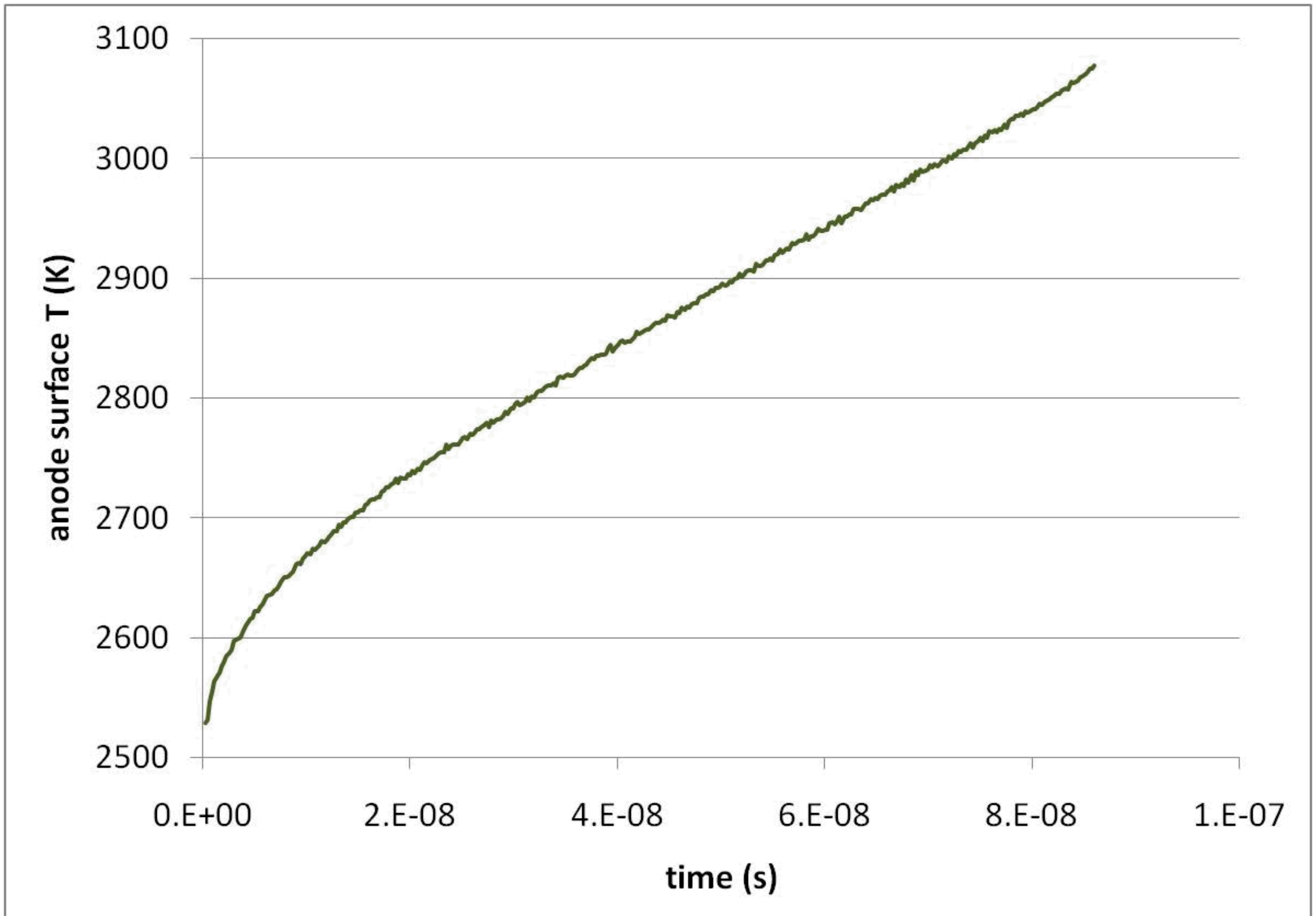
Stage 2: heating of the anode (continued)



Stage 3: emission from the anode

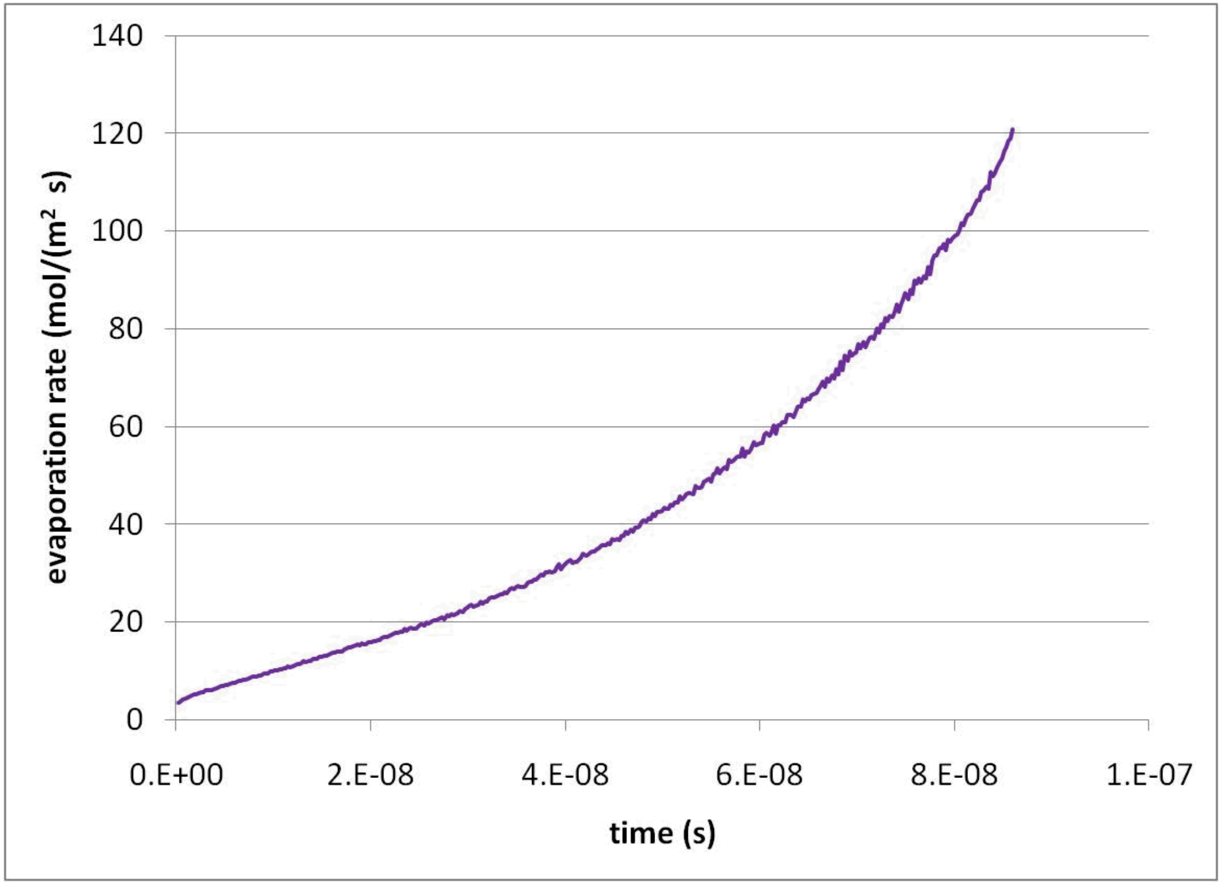
- **Antoine equation is used to compute vapor pressure on surface as a function of anode surface temperature.**

$$\log_{10}(p) = A + BT^{-1} + C\log_{10}(T) + DT^{-3}$$

- **Hertz-Knudsen equation is used to convert vapor pressure into flux.**

$$flux = \frac{P}{\sqrt{2\pi mkT}}$$

- **Anode emission model is working**



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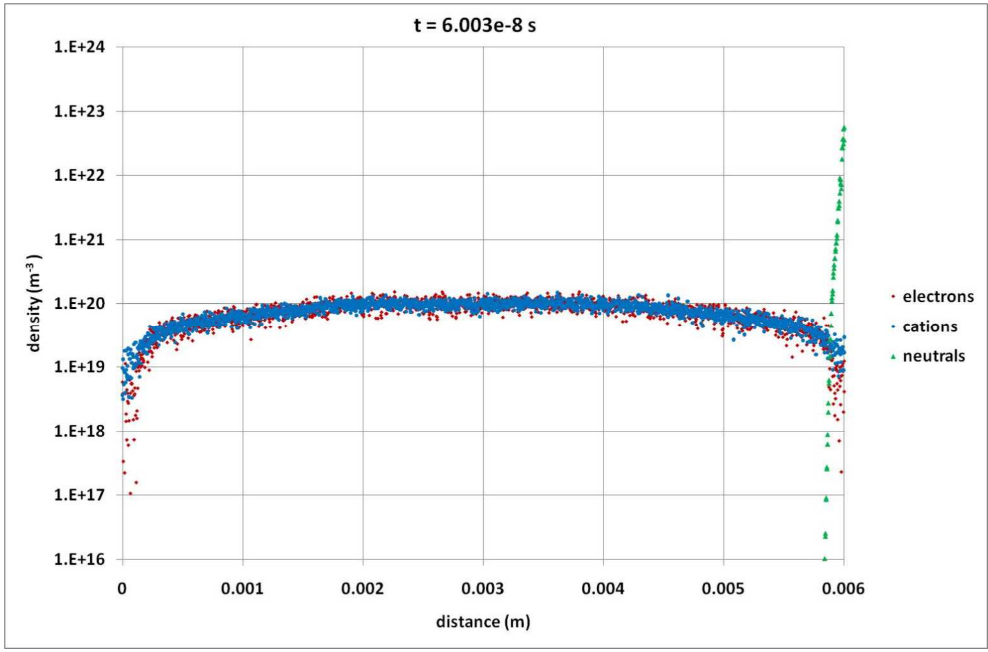
Stage 3: emission from the anode (continued)

- **Densities of electrons, cations, and neutrals given as a function of position.**
- **Neutrals constrained to 20 particles per cell by dynamic reweighting algorithm, but "real" density varies by orders of magnitude --- dynamic particle reweighting working**



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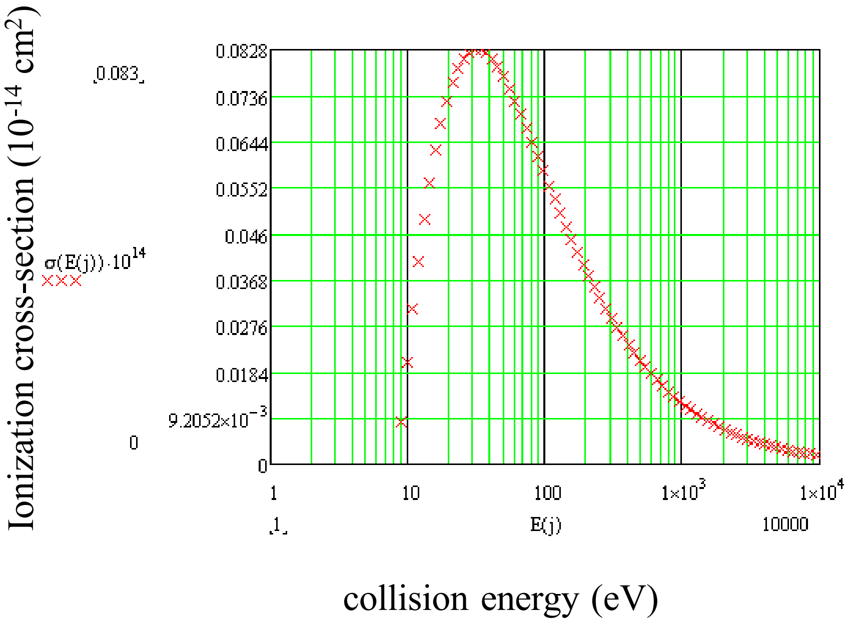
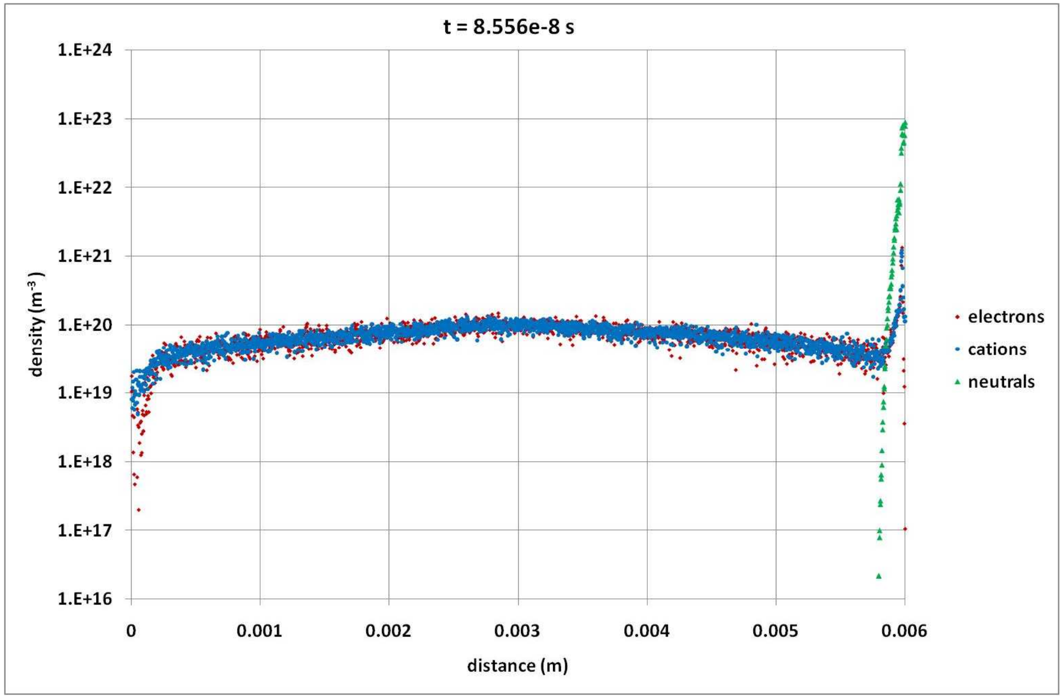
Stage 4: ionization

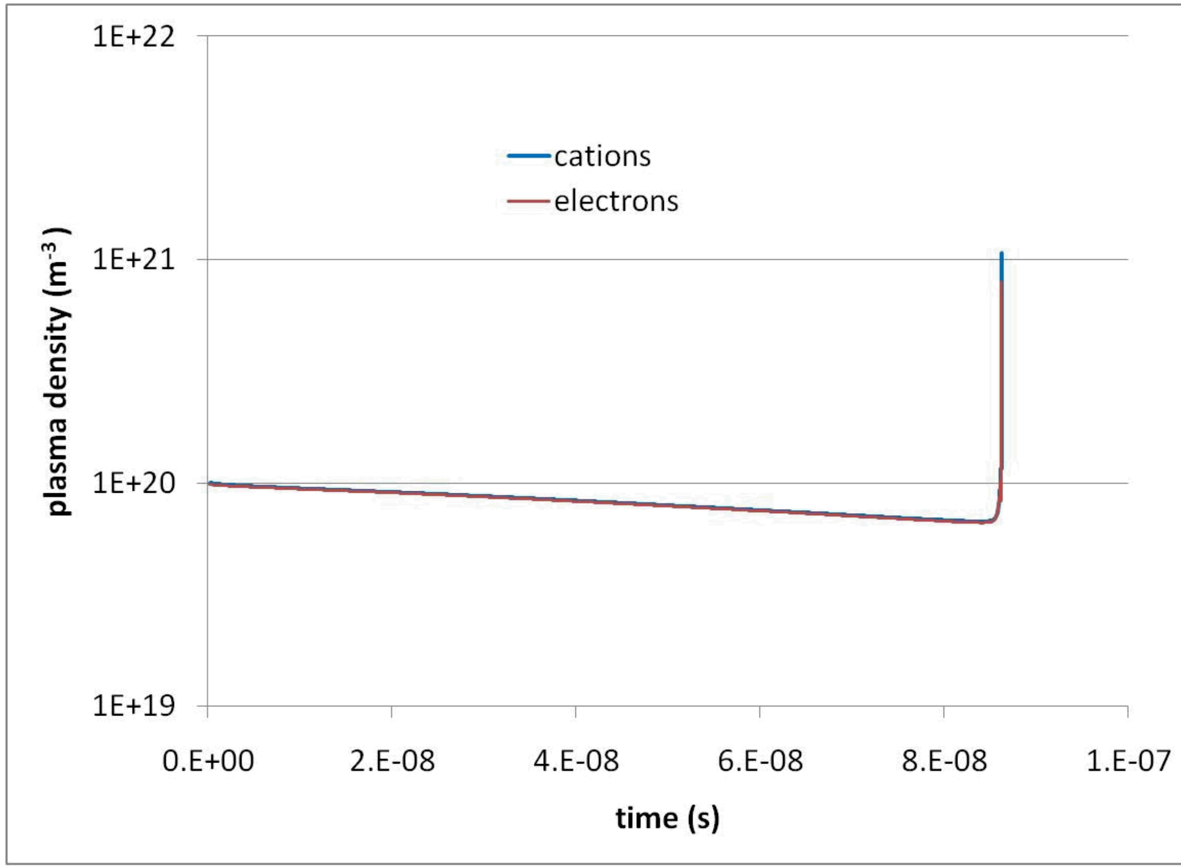




Rapid ionization is occurring where there is a high density of neutrals.

Stage 5: growth in plasma density

- During most of the simulation, the average bulk plasma density gradually drops as it is eaten away at the electrodes.
- Then, in the final ps of the simulation, ionization of neutrals produces huge quantities of plasma, boosting the overall density.
- Ionization is occurring as expected



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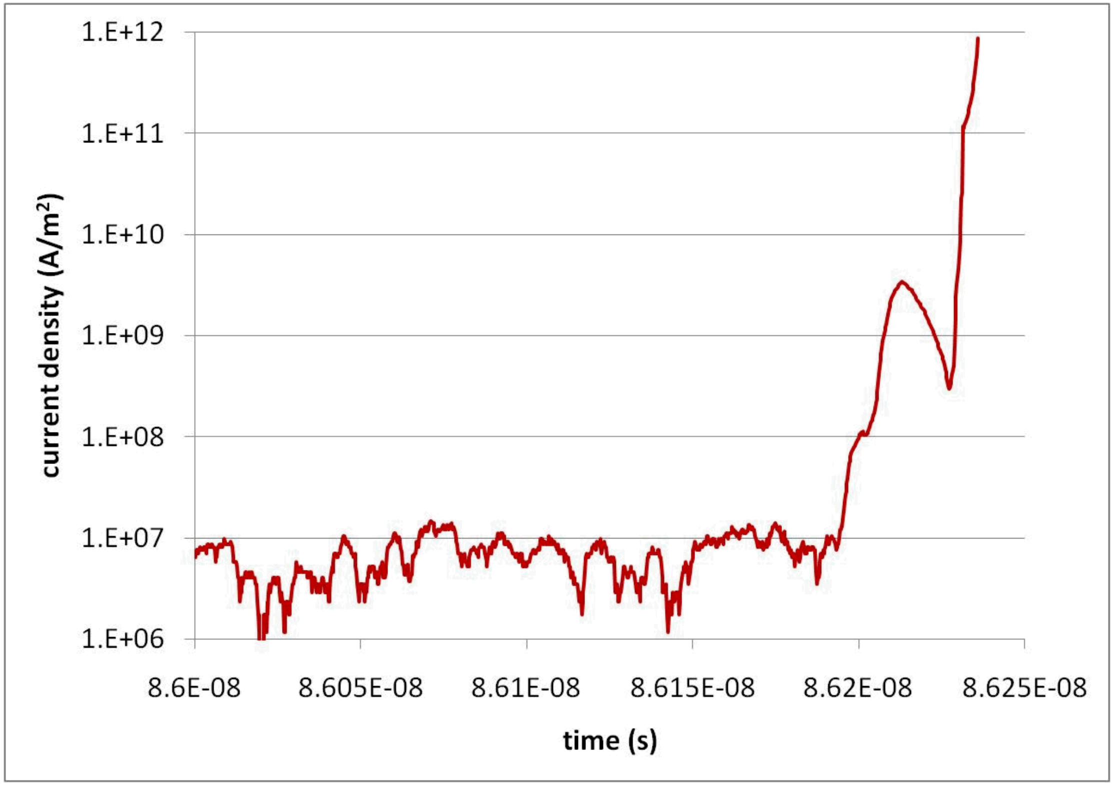
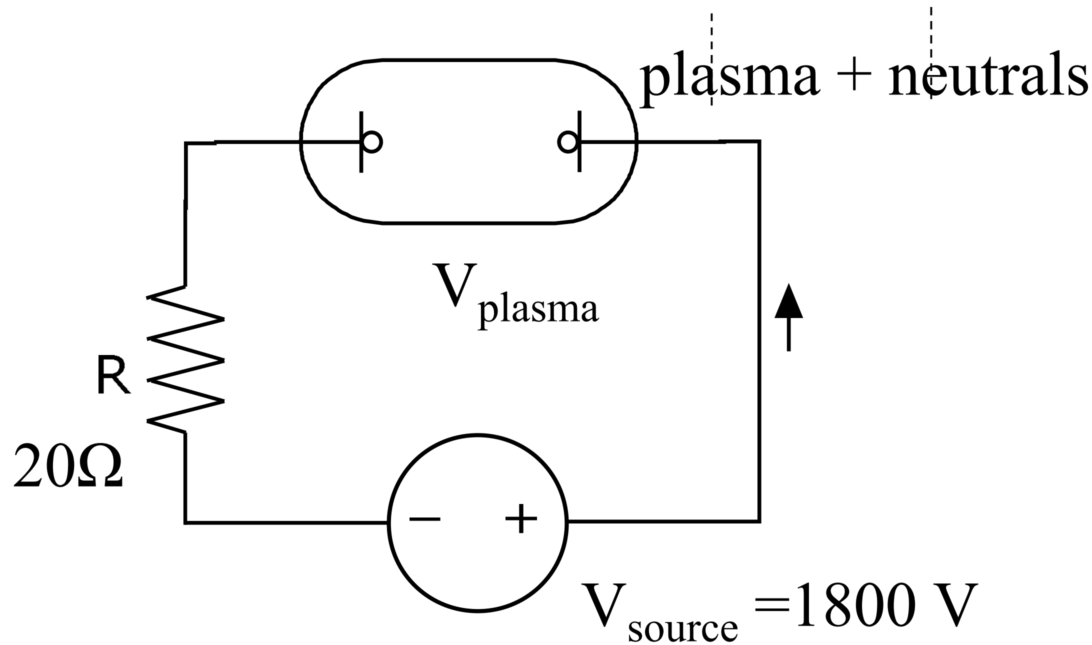
Stage 6: breakdown:
explosive growth in current to the anode

- **The final 50 ps of the simulation shows explosive growth in the current to the anode.**
- **Note that this is a semi-log plot. Current grows by orders of magnitude.**
- **Breakdown!**



Stage 7: circuit model



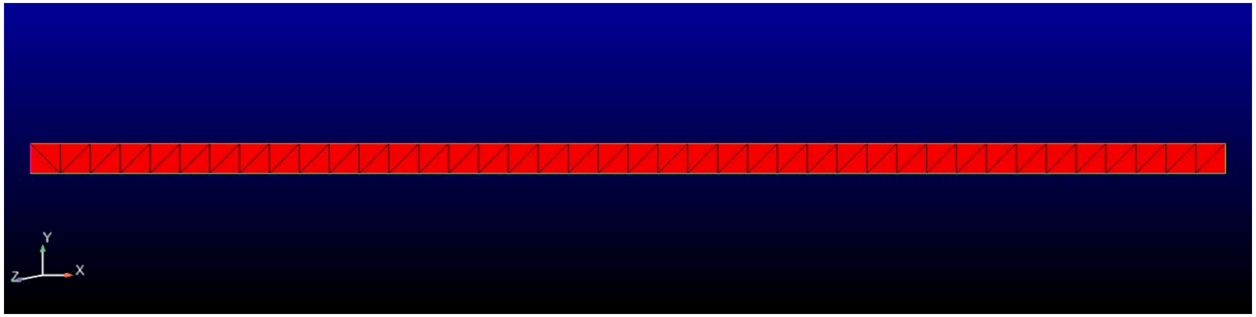
VI. Criticisms of our model

- Our present dynamic particle reweighting doesn't do so well at modeling sheaths. So we turned it off for ions and electrons and only used it for neutrals. Would be nice to use it for all species.
- Not a "real" cathode model --- will remedy this in the future.
- Our models for particle emission at the electrodes appear to be lacking.
- Would be better to start the anode at room T.
- Would be better to do a full 3D thermal solve of the anode.

VII. Attempt to reproduce CERN's simple arc model

- **Early CERN effort available on the internet: http://www.ipp.mpg.de/~knm/CERN/spark.html**

- **Simulation domain used in my effort to reproduce their simulation results:**



Surface 1 (left hand side) is the cathode, surface 3 (right hand side) is the anode. Surface 2 (top) and surface 4 (bottom) reflect particles. The spatial domain is 20 microns from cathode-to-anode, and 0.5 microns high, and is divided into 80 triangular elements with 0.5 micron length sides.

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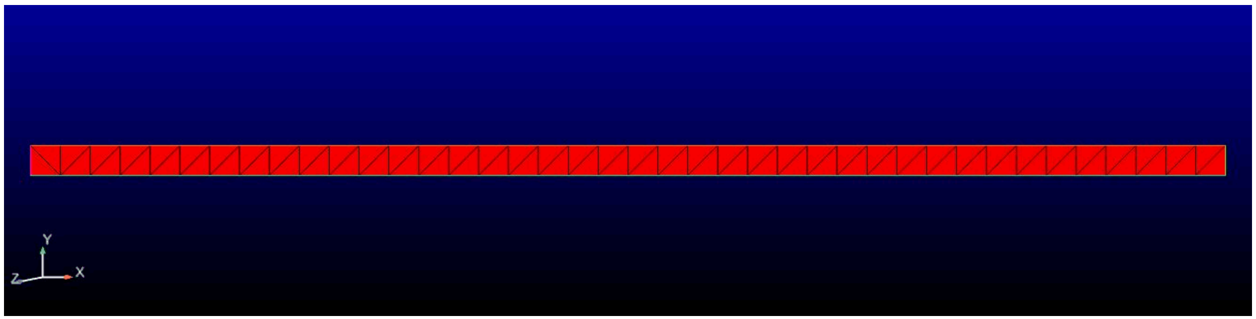
VII. Attempt to reproduce CERN's simple arc model



Surface 1 (left hand side) is the cathode, surface 3 (right hand side) is the anode. Surface 2 (top) and surface 4 (bottom) reflect particles. The spatial domain is 20 microns from cathode-to-anode, and 0.5 microns high, and is divided into 80 triangular elements with 0.5 micron length sides.

Boundary conditions:

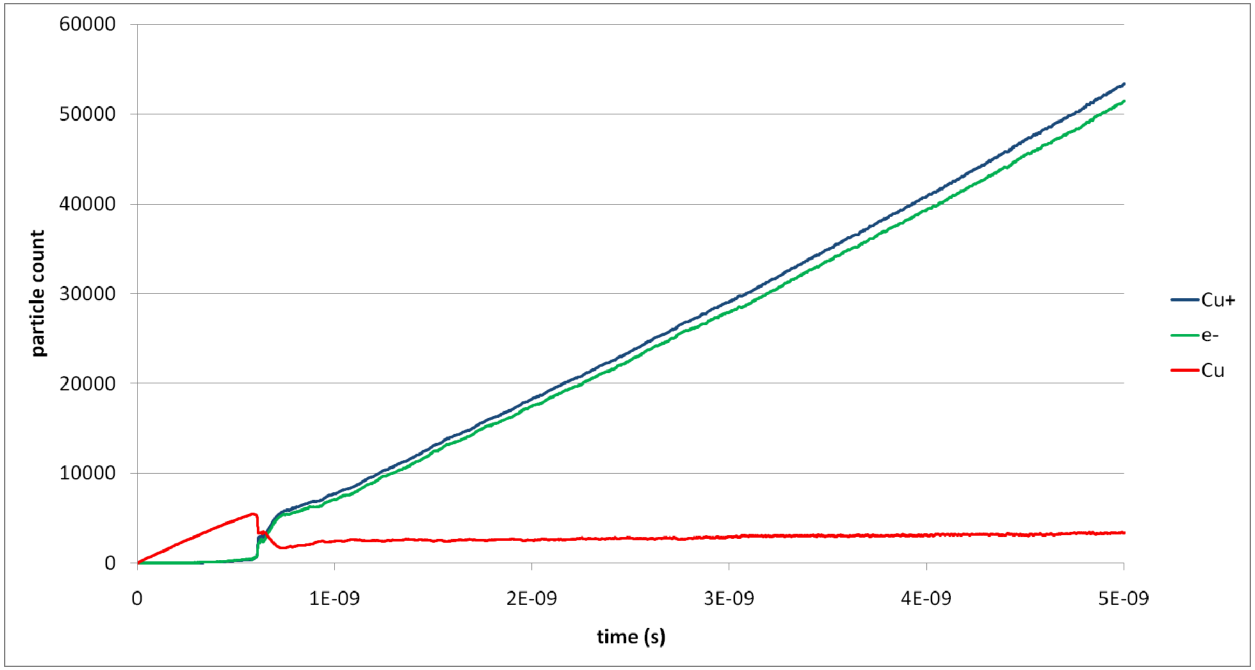
1. Dirichlet V = 0 V on surface 1.
2. Dirichlet V = 10000 V on surface 2.
3. Influx of e- on surface 1 is 10^{30} m^{-2} s^{-1} at T = 2500 K.
4. Influx of Cu on surface 1 is 10^{28} m^{-2} s^{-1} at T = 2500 K.
5. Electrons or ions that hit surface 1 or 3 disappear. Impacting electrons cause emission of a Cu atom with 1% probability, at T = 2500 K, and x-velocity of 100,000 m/s. Impacting Cu+ cause emission of a Cu atom with 100% probability, at T = 2500 K, and x-velocity of 100,000 m/s.
6. Cu atoms that hit surface 1 or 3 bounce.
7. Particles that hit surface 2 or 4 bounce.

VII. Attempt to reproduce CERN's simple arc model

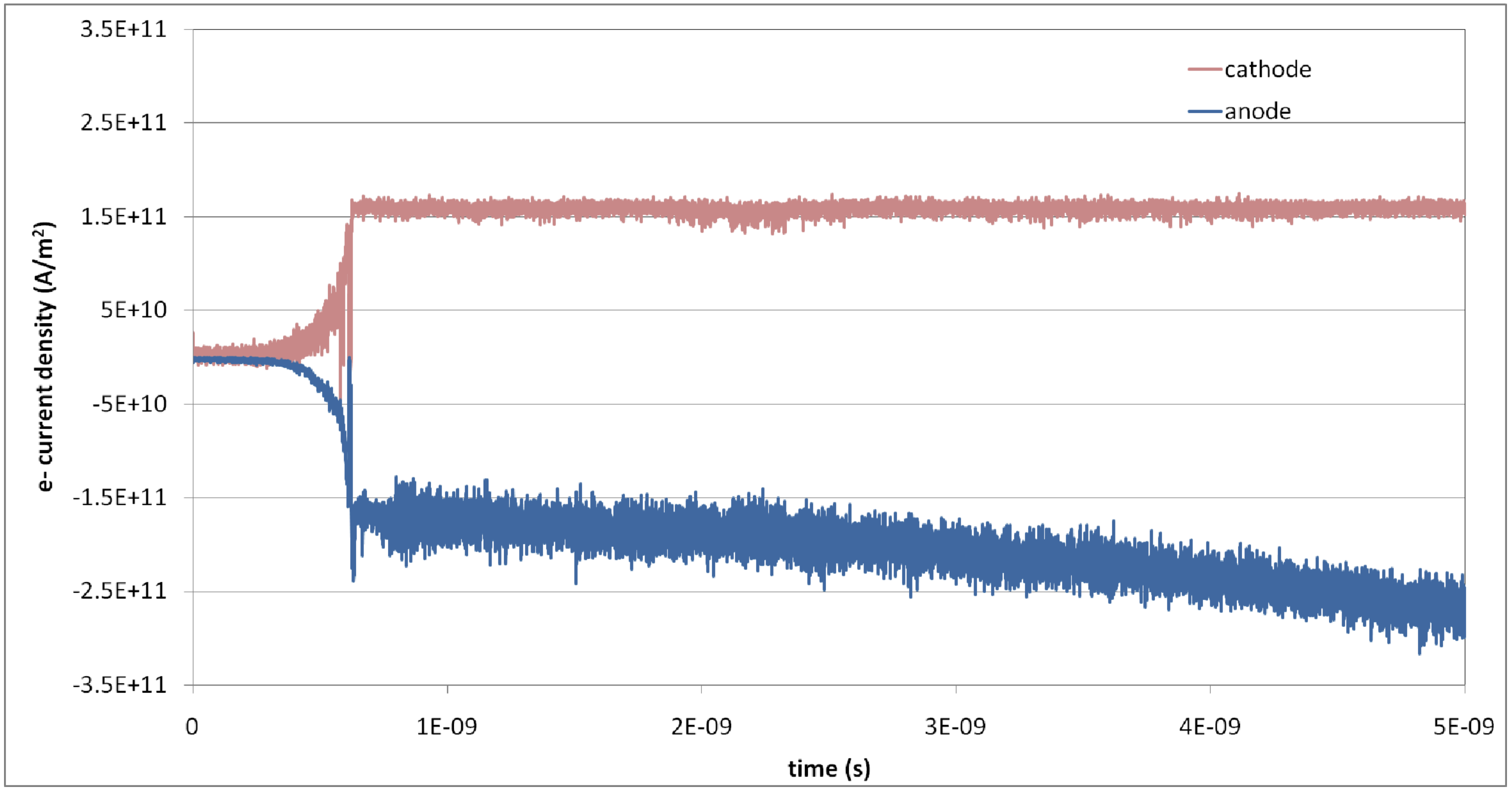
Additional input parameters:

1. Time-step size is 3.5e-15 s.
2. Ran for 1,430,000 time-steps for a total of 5 ns of simulated time.
3. Ignoring all collisions except the impact ionization: e- + Cu -> e- + Cu+ + e-
4. Using particle weighting of 10^9.

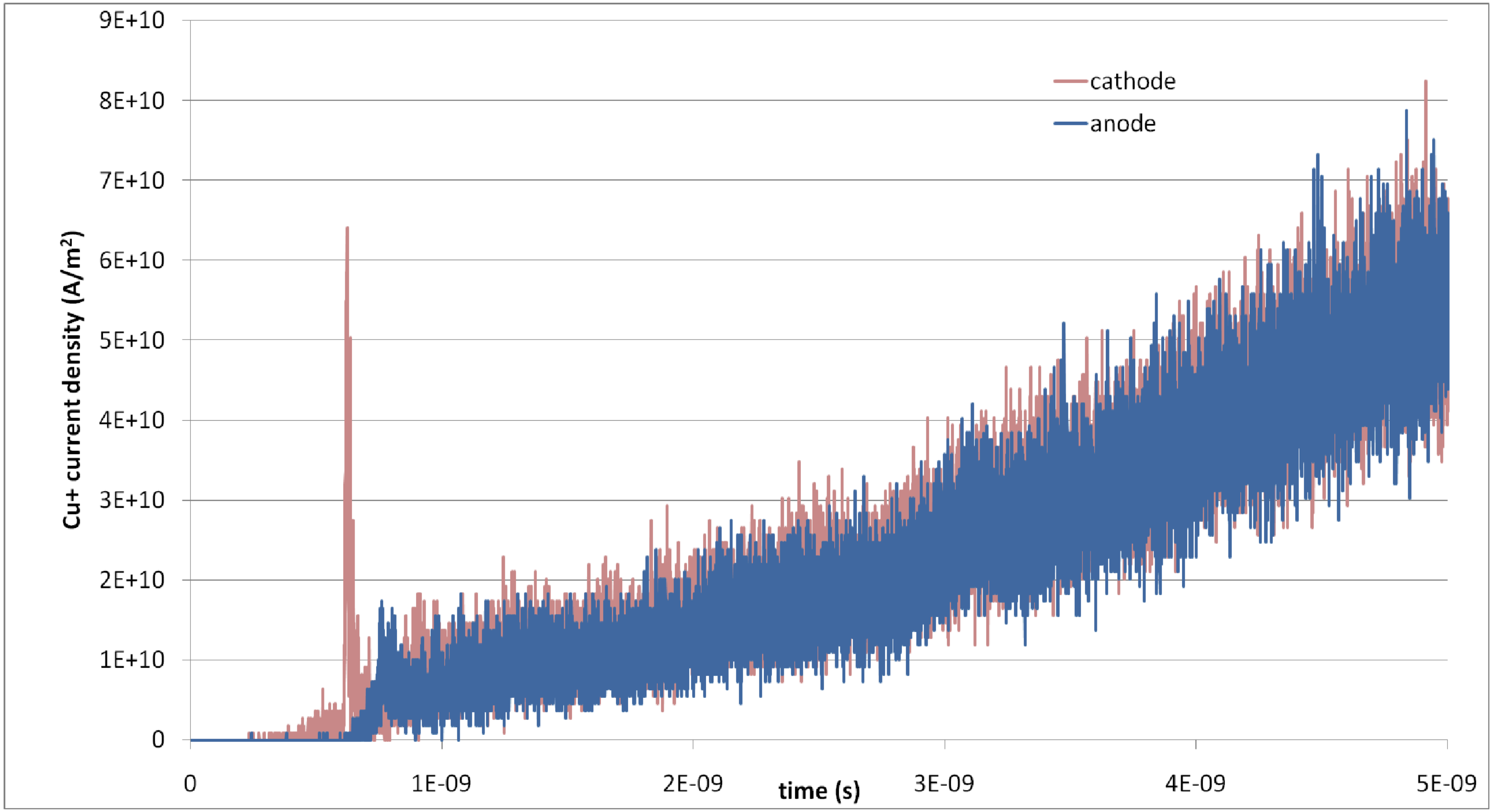
Simulation results:



VII. Attempt to reproduce CERN's simple arc model



VII. Attempt to reproduce CERN's simple arc model



VII. Attempt to reproduce CERN's simple arc model

(Play simulation movies here:
ftp://dropzone.sandia.gov/pscrozi/density.avi
ftp://dropzone.sandia.gov/pscrozi/potential.avi)

VII. Attempt to reproduce CERN's simple arc model

Observations:

1. This is clearly a lumped-physics, "surfaces-for-dummies" approach to modeling electrode emission.
2. Able to start from vacuum and establish a stable bulk plasma.
3. A really good reweighting scheme would be immensely useful. Probably doesn't need to be bullet-proof.
4. We've initiated a collaborative effort with the CERN folks: code-to-code comparisons, sharing of information, possible joint publication of results.

VIII. Conclusions

1. We need to better understand and model the following:
   - electron emission from the electrodes
   - neutral or ion emission from the electrodes

2. We should continue to take a lumped physics, “surfaces-for-dummies” approach to modeling emission from the electrodes rather than try to model minute surface asperities.

3. We need a better particle reweighting method to deal with the huge variations in particle density vs time, space, and species.

4. We need to push “sputtering” simulations out to longer times:
   - Can we achieve a steady-state anode-to-cathode current by putting a current-limiting circuit in series?
   - What happens to the particle densities and electrode temperatures at long times?

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VIII. Questions/comments/suggestions