SAND2009-4930P

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

Presented at "A Working Meeting on Computational and Numerical Methods for Modeling Breakdown," hosted by Tech-X Corporation, Boulder, CO

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Presentation Outline

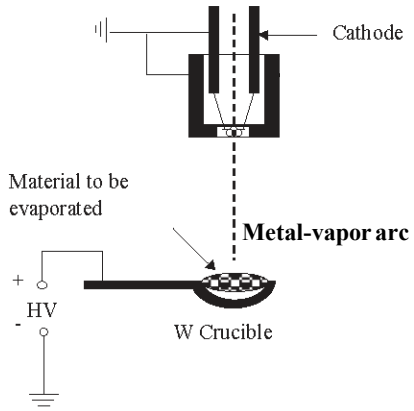
I. Motivation
II. Our goal
III. Overview of the *Aleph* code
IV. Critical infrastructure pieces
V. Description of our arc simulations
VI. Criticisms of our model
VII. Conclusion
VIII. Questions/comments/suggestions

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



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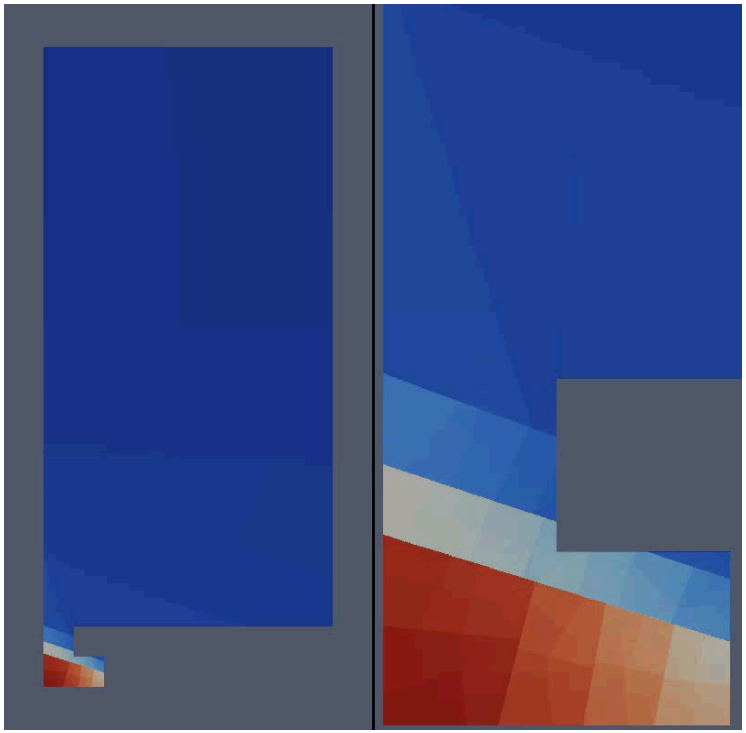
II. Our goal

Perform numerical simulation of breakdown using *Aleph*. Our metrics for success today:

- ❑ **Simple cathode plasma**
- ❑ **Anode emission of neutral metal atoms**
- ❑ **Dynamic particle reweighting**
- ❑ **Ionization of neutrals**
- ❑ **Current avalanche --- breakdown**
- ❑ **Simple circuit is series with arc**

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 $\mathbf{E}^{n+1}$

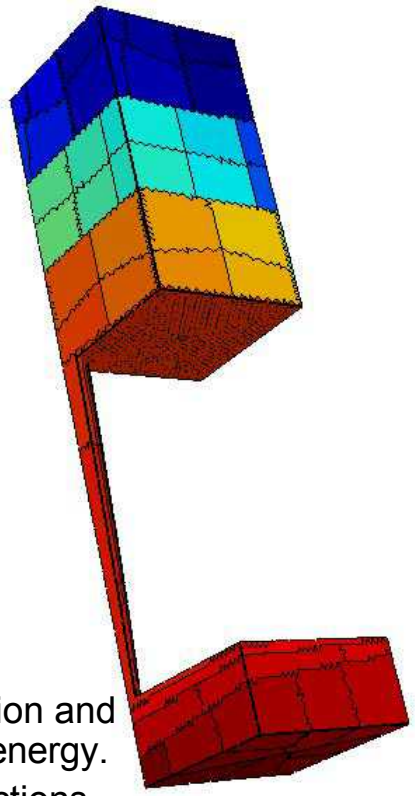
$$\nabla \cdot \left(\epsilon \nabla V^{n+1}\right) = -\rho(\mathbf{x}^{n+1})$$

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

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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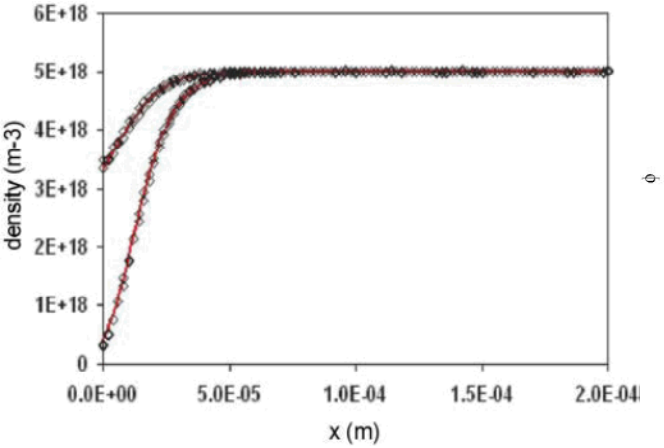
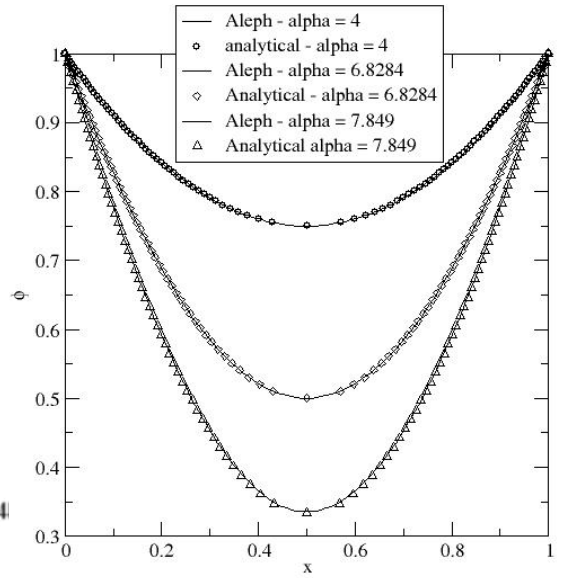
All Interesting Plasma Behavior is Nonlinear and Coupled – Verification is not Enough



Sheaths



Classic diode

Ambipolar fields

We rely very heavily on validation!

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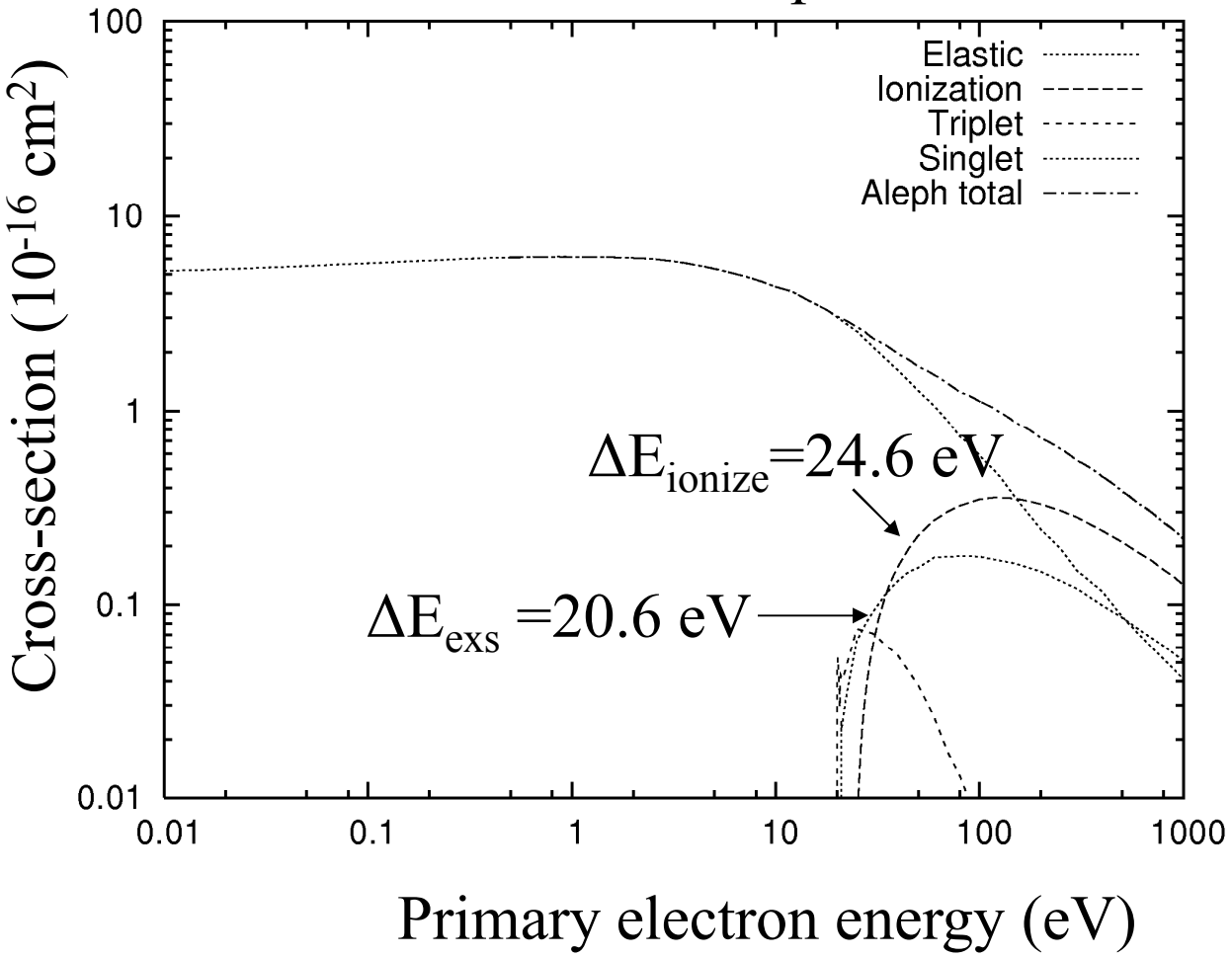
IV. Critical infrastructure pieces

- 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

Aleph gas breakdown algorithm uses Monte Carlo Method:

1. Push swarm of electrons (e) in neutral gas (N)
2. Calculate collision probability based on cross-sections
3. Modify colliding e-N pair, depending on process

He elastic and inelastic processes modeled:



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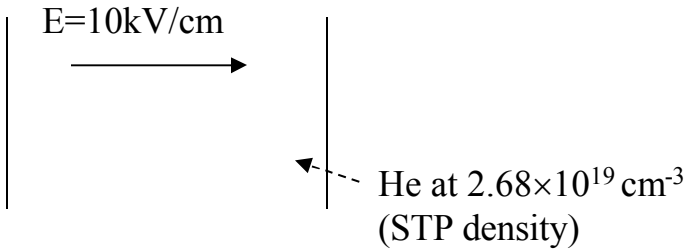
Statistical test: move 2×10^6 electrons for 1 step in Helium at STP

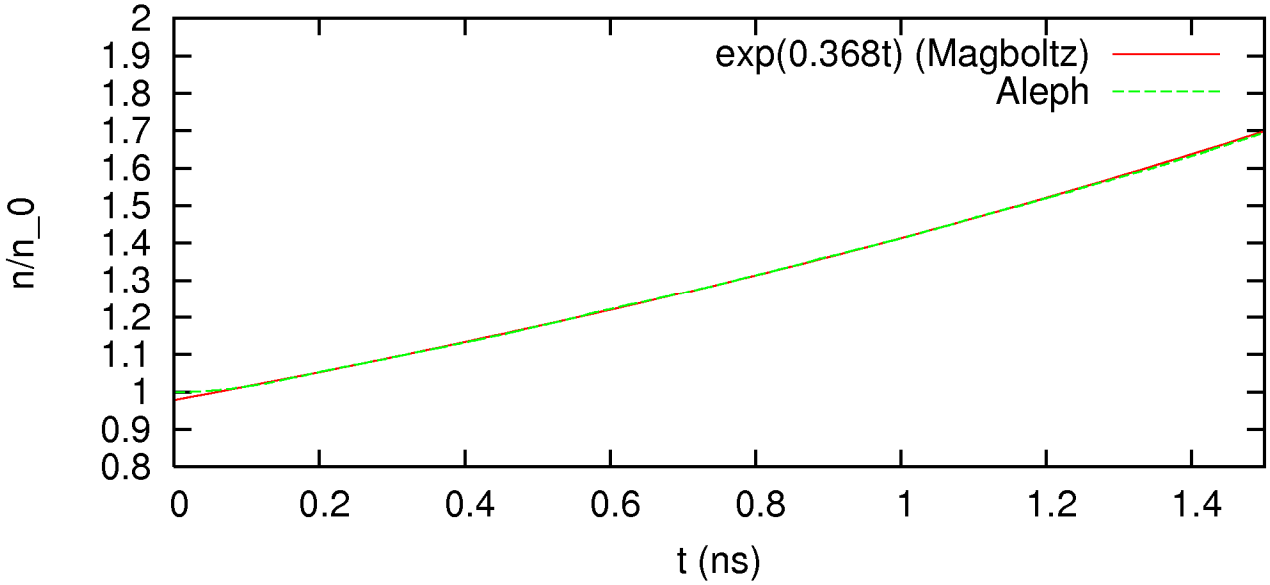
Compare # collisions with predicted number:

	Cross-sections (m^2)			
	Elastic	Ionization	Singlet	Triplet
99.05 eV	5.96×10^{-21}	3.47×10^{-21}	7.68×10^{-23}	1.77×10^{-21}
Actual number of collisions:	94459	54589	1249	27945
Expected:	94285	54901	1216	28035
Difference	0.18%	-0.57%	2.73%	-0.32%
1/sqrt(N)	0.33%	0.43%	2.87%	0.60%

Exponential electron/ion growth agrees with Magboltz code*

Test case:





Have cross-section data for several gases, metal vapors, etc.

(*Magboltz is a 0-D gas-ionization code used to design particle detectors at CERN)

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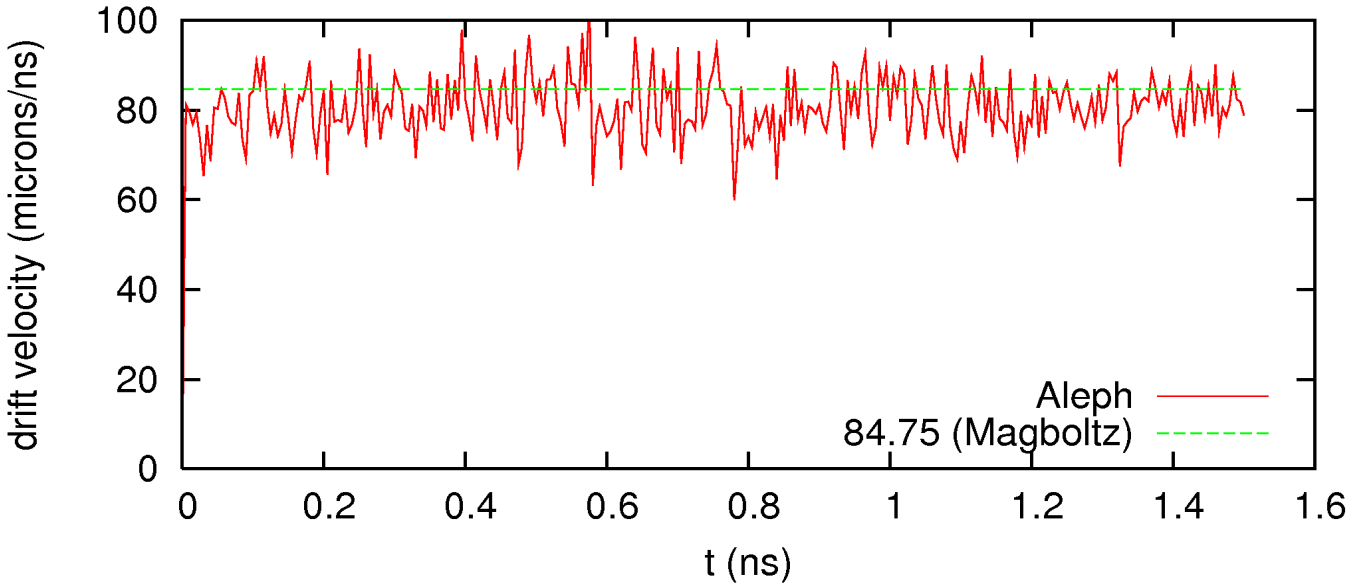
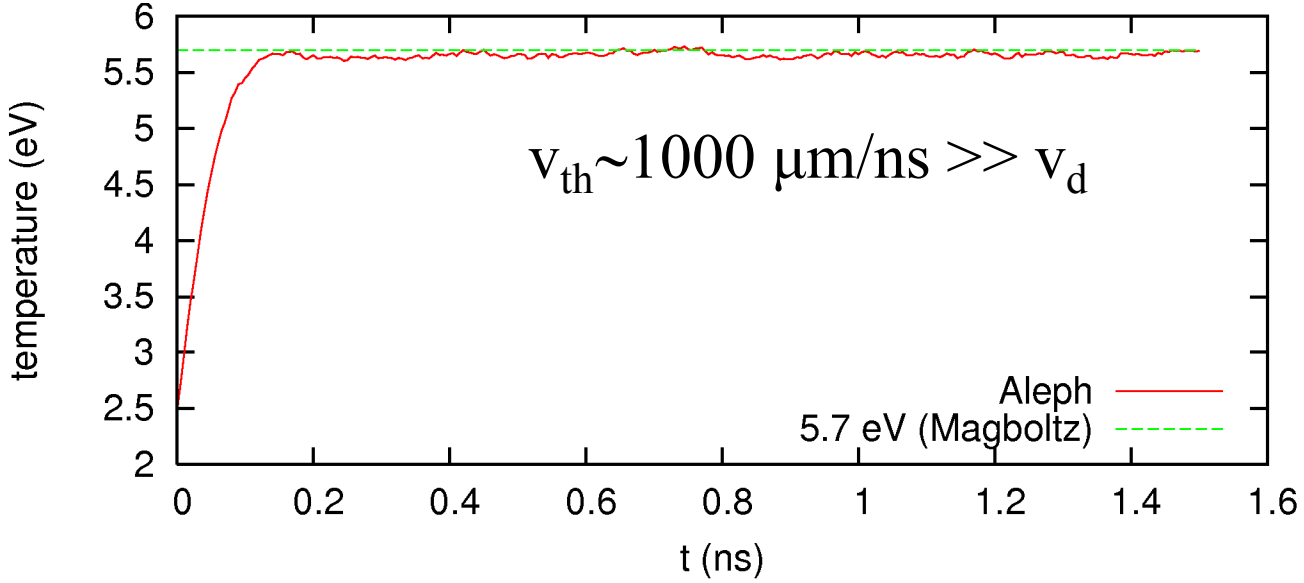
Free electron drift velocity and temperature





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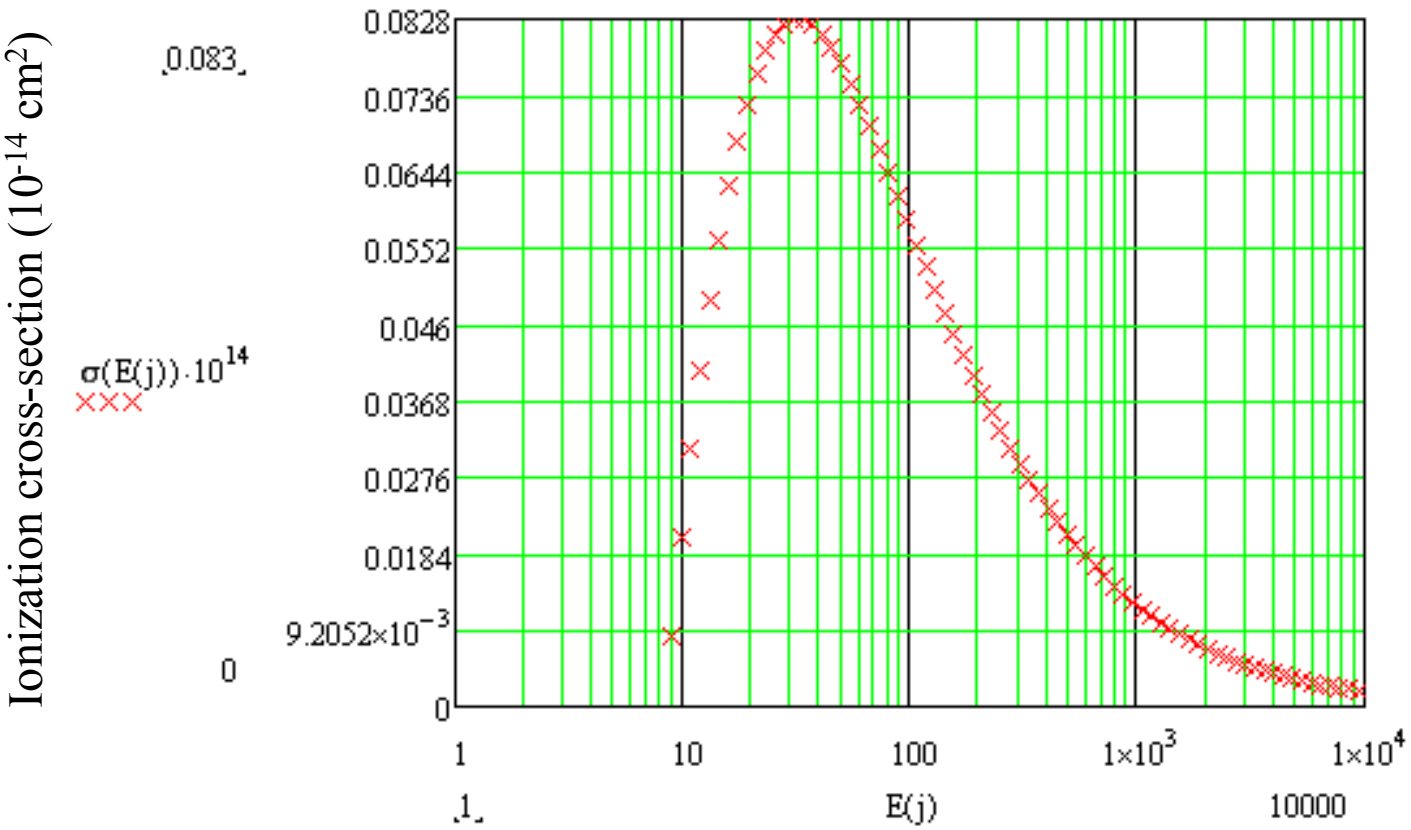
Ionization cross-section model



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

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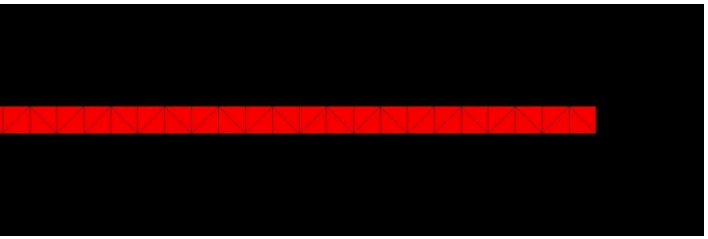
V. Description of our arc simulations

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

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



- Quasi-1D, simple geometry, tri mesh
- Aspect ratio: 1000:1
- 2000 triangular elements
- 6 mm arc gap, 6 um 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

```
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
```

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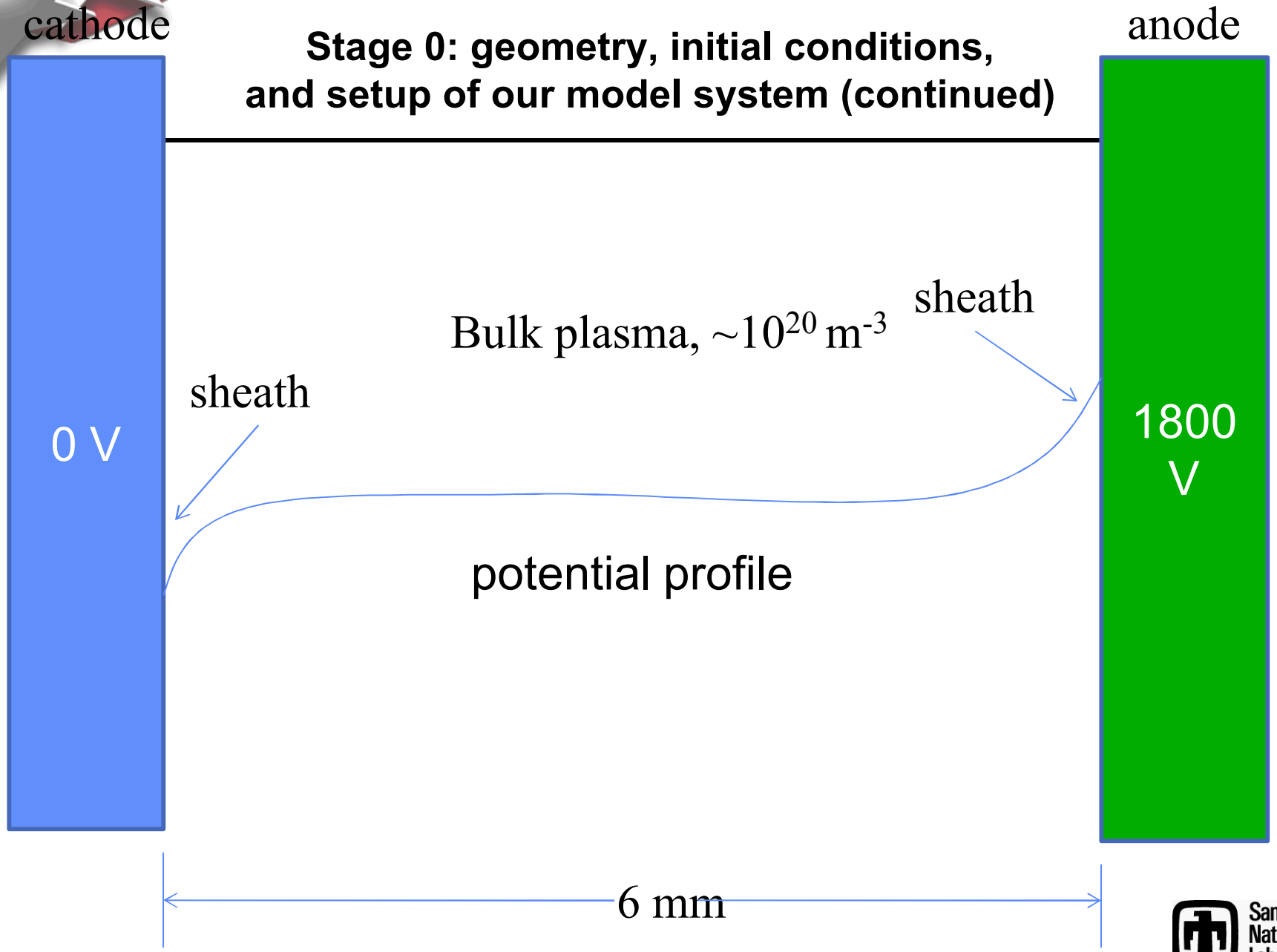
Stage 0: geometry, initial conditions, and setup of our model system (continued)



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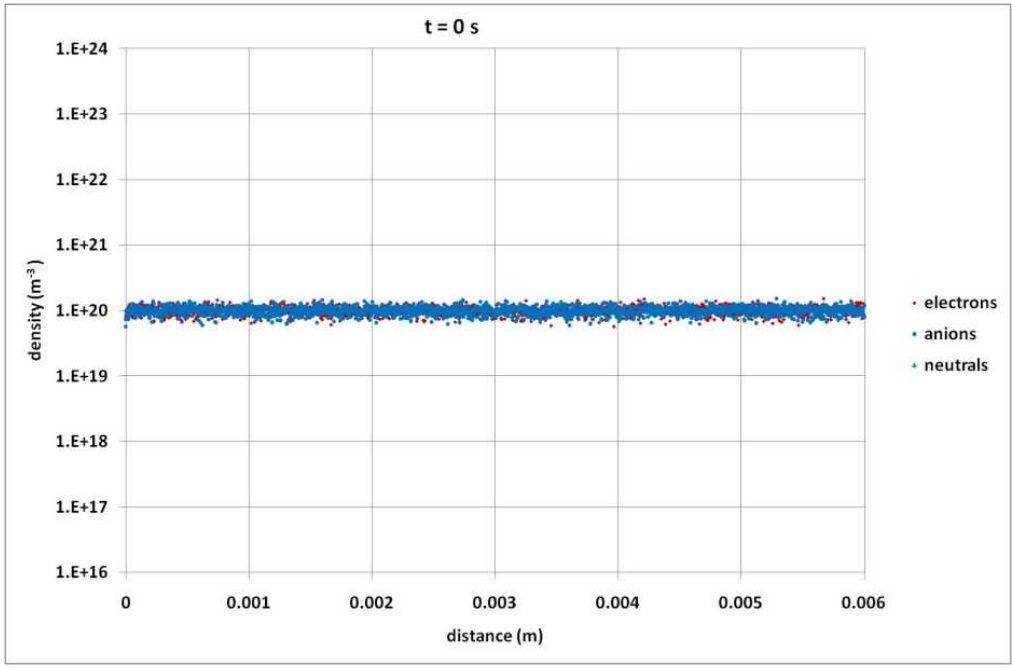
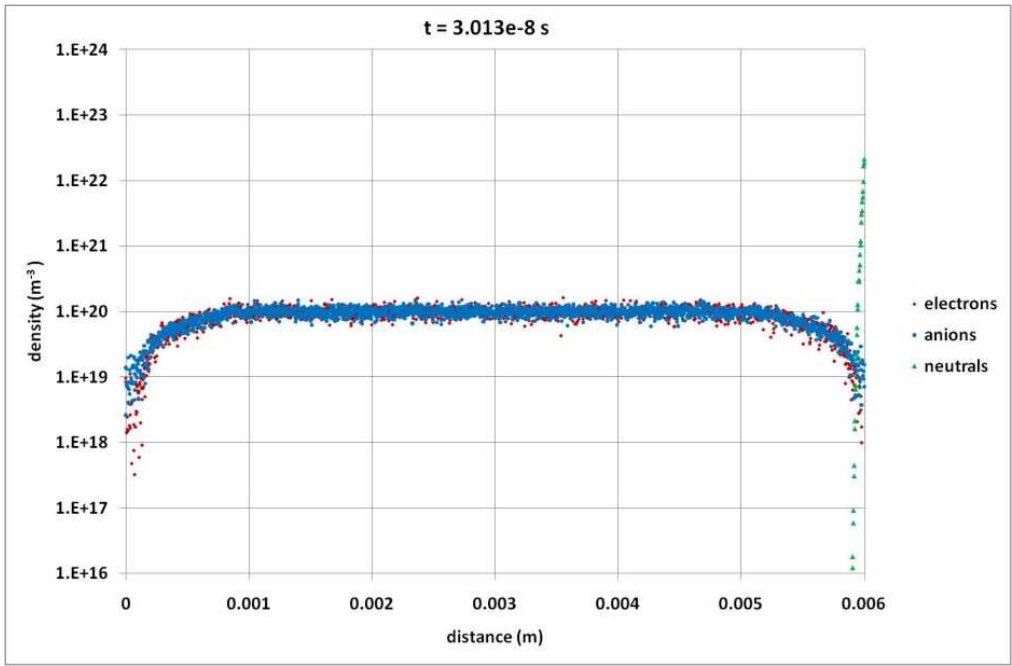
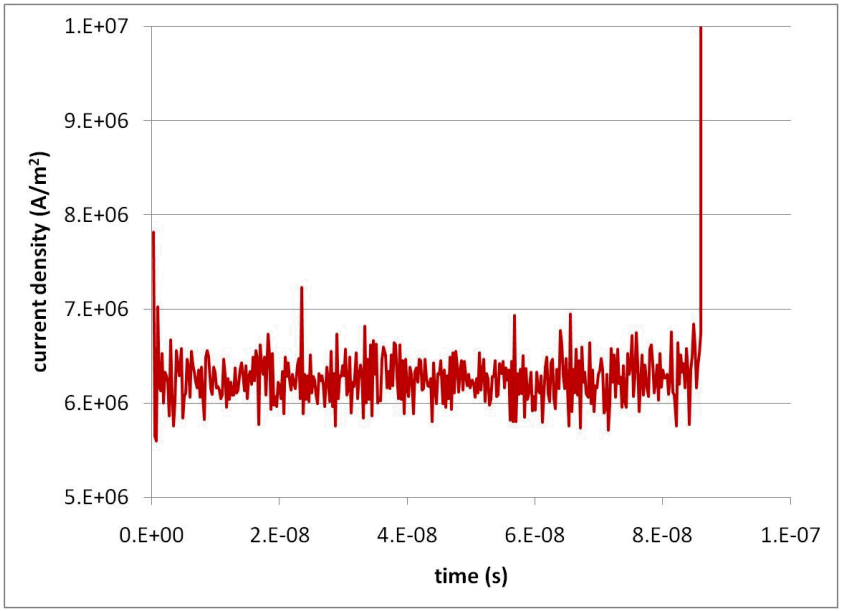
Stage 1: bulk plasma stable, sheaths formed

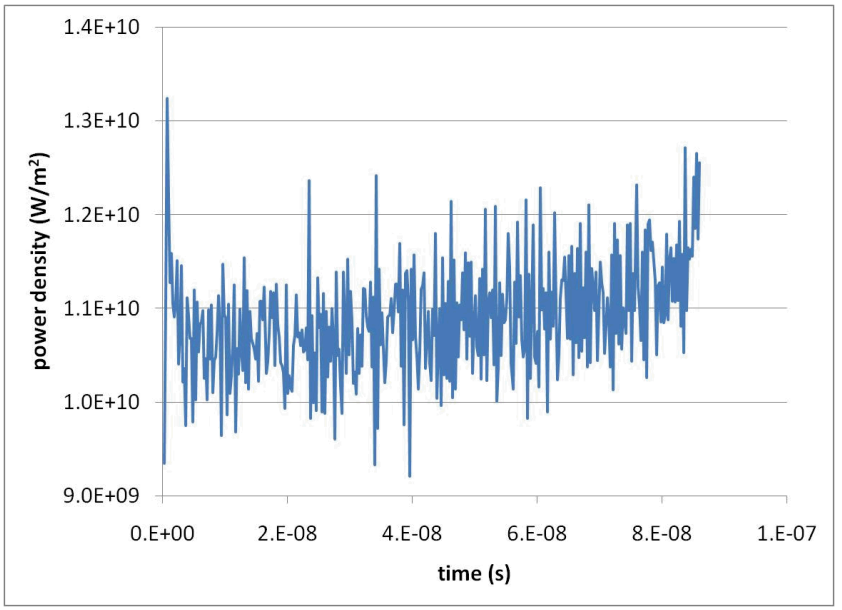
- **Simple cathode plasma model working, CHECK 1!**
- **Sheath formation at both the anode and the inert cathode.**





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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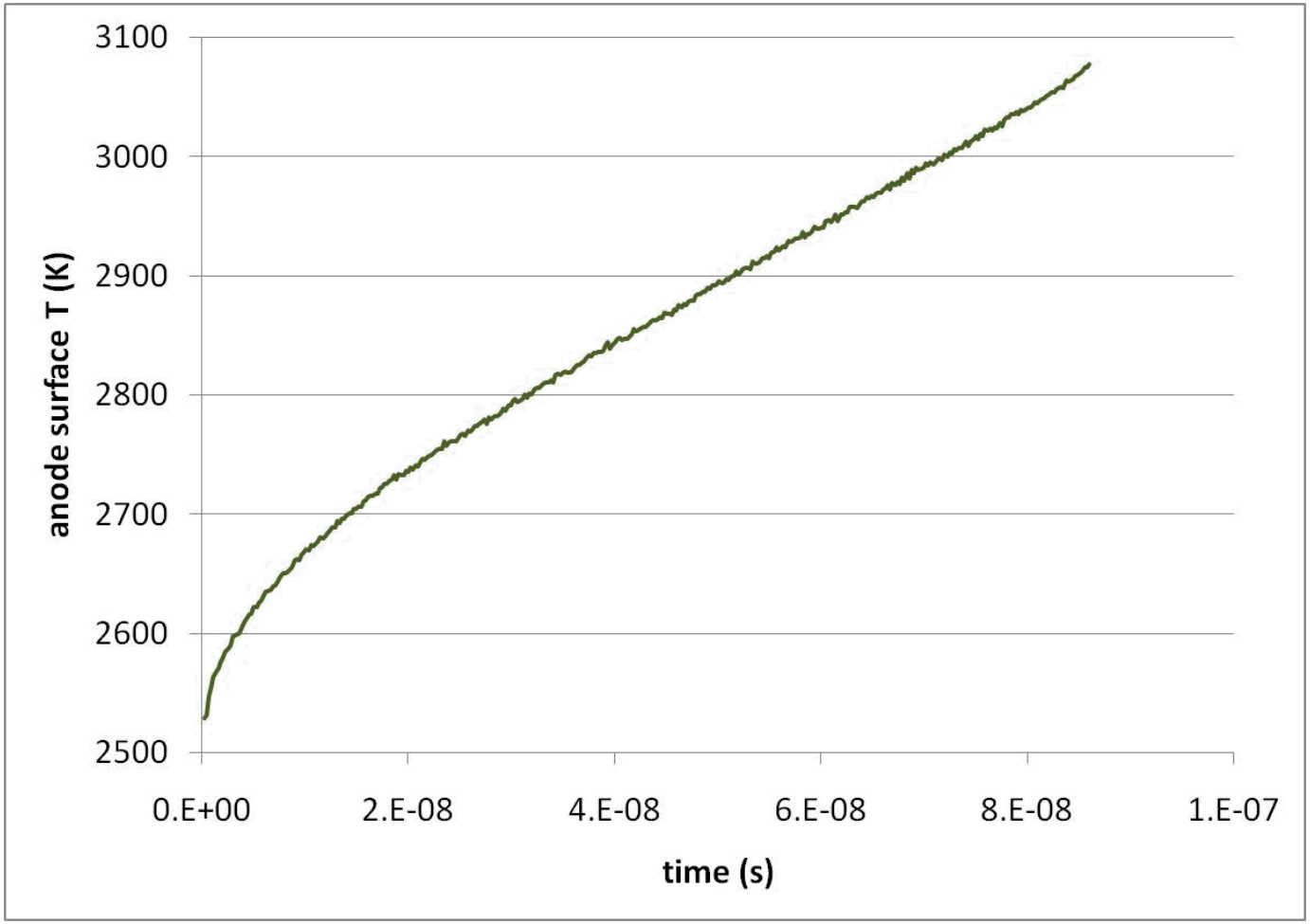
Stage 2: heating of the anode (continued)



Stage 3: emission from the anode

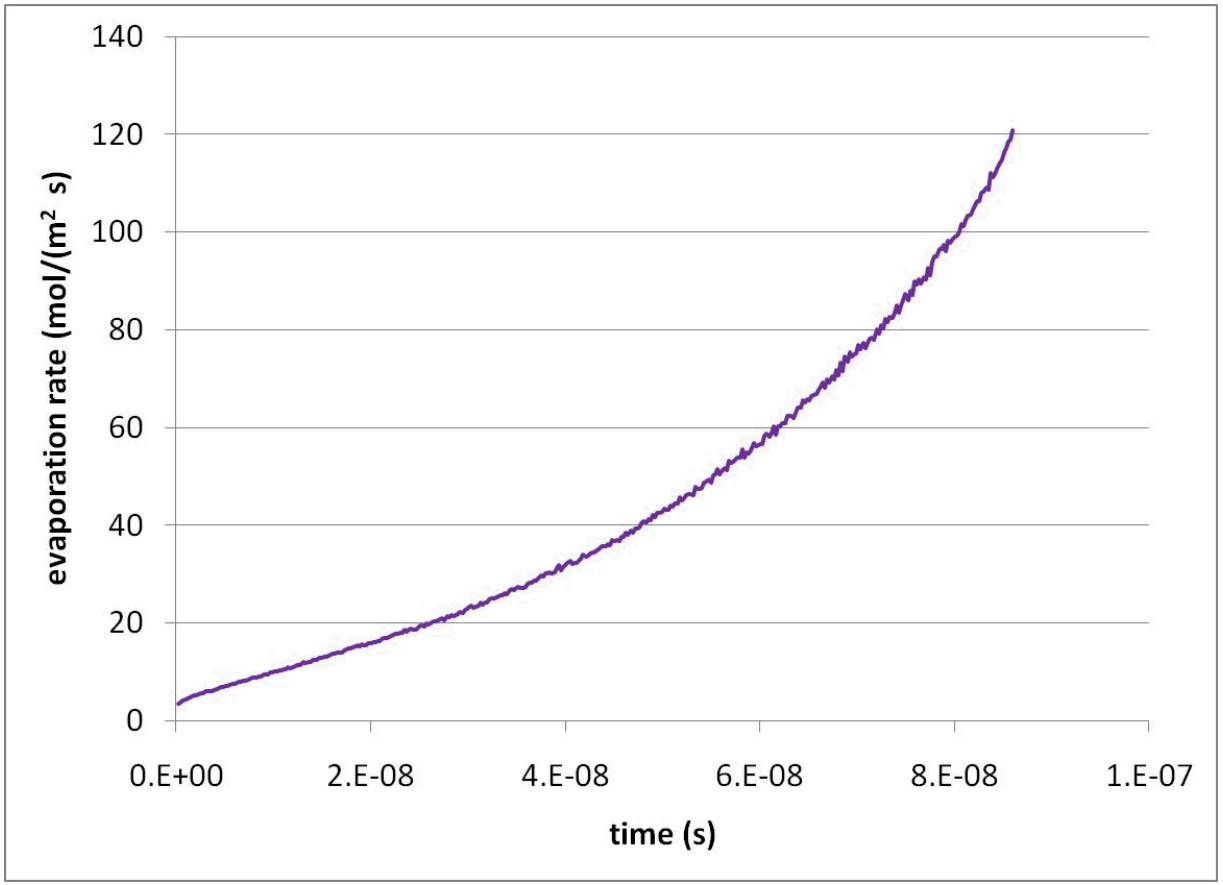
- **Antoine equation is used to compute vapor pressure on surface as a function of anode surface temperature.**

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

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

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

- **Anode emission model is working, CHECK 2!**



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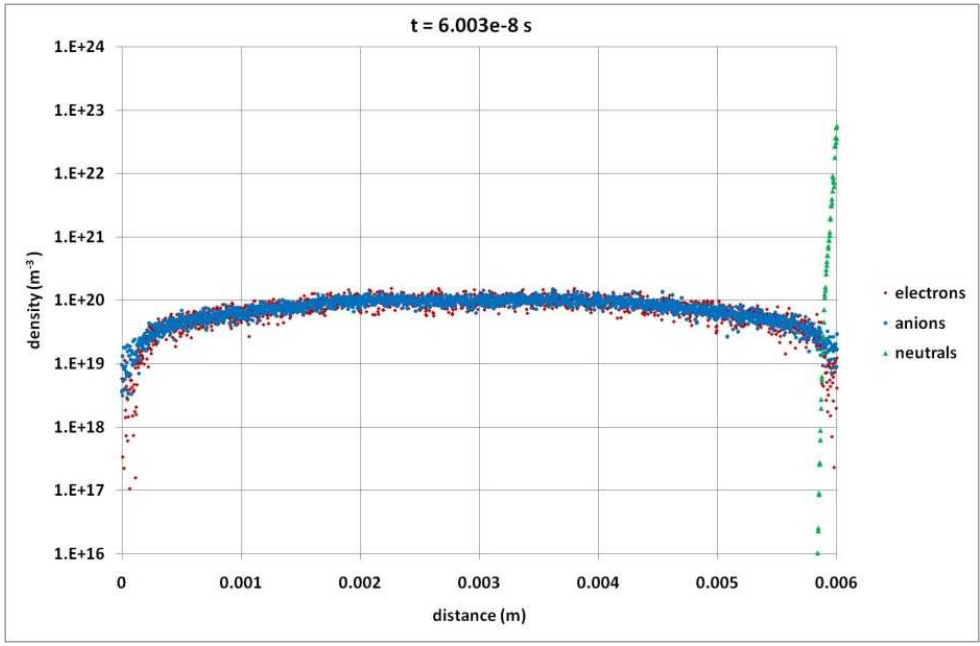
Stage 3: emission from the anode (continued)

- Densities of electrons, anions, 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, CHECK 3!



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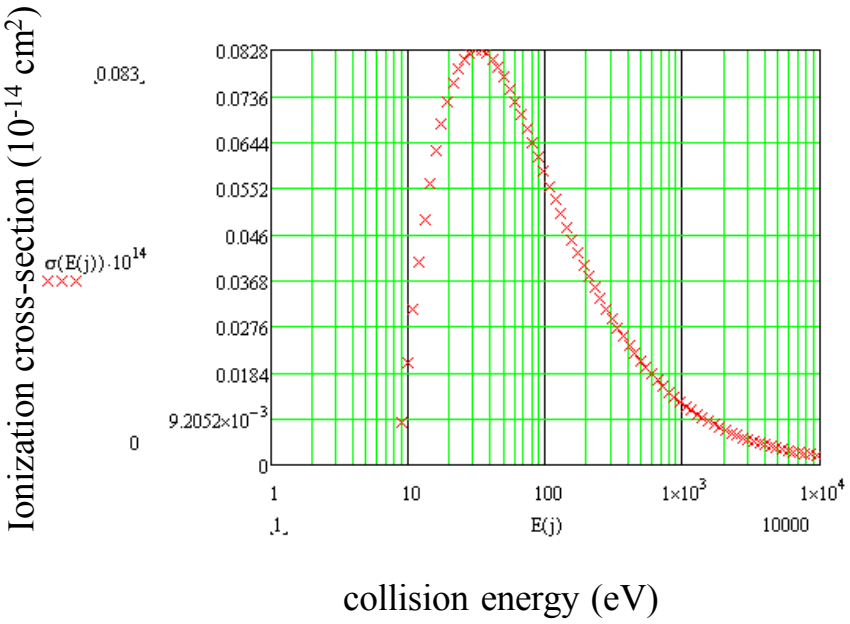
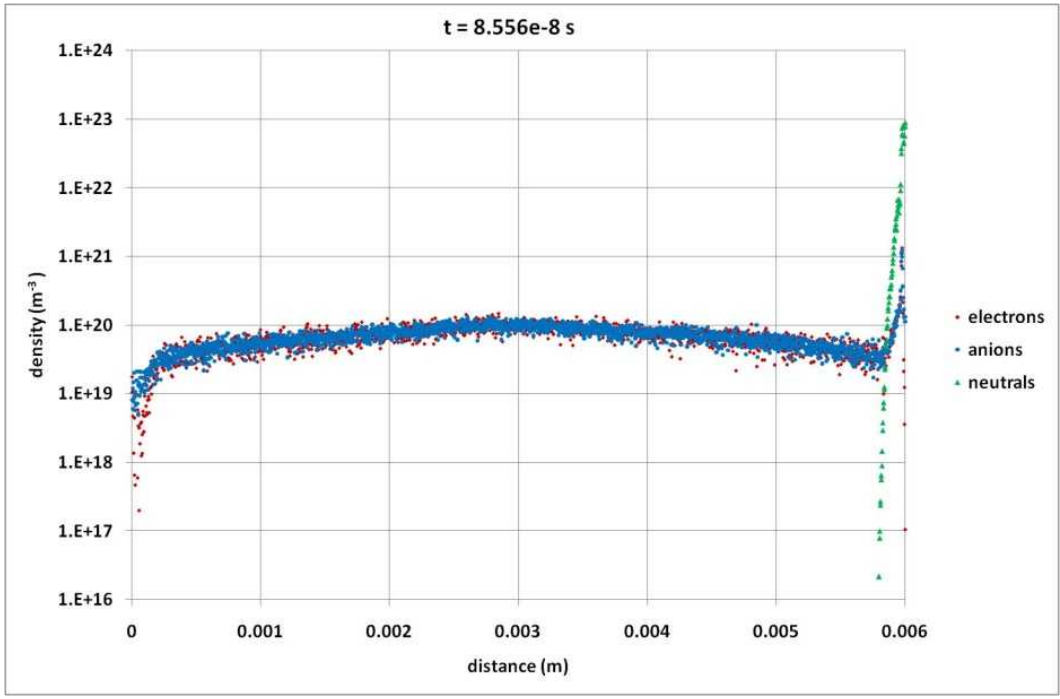
Stage 4: ionization





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

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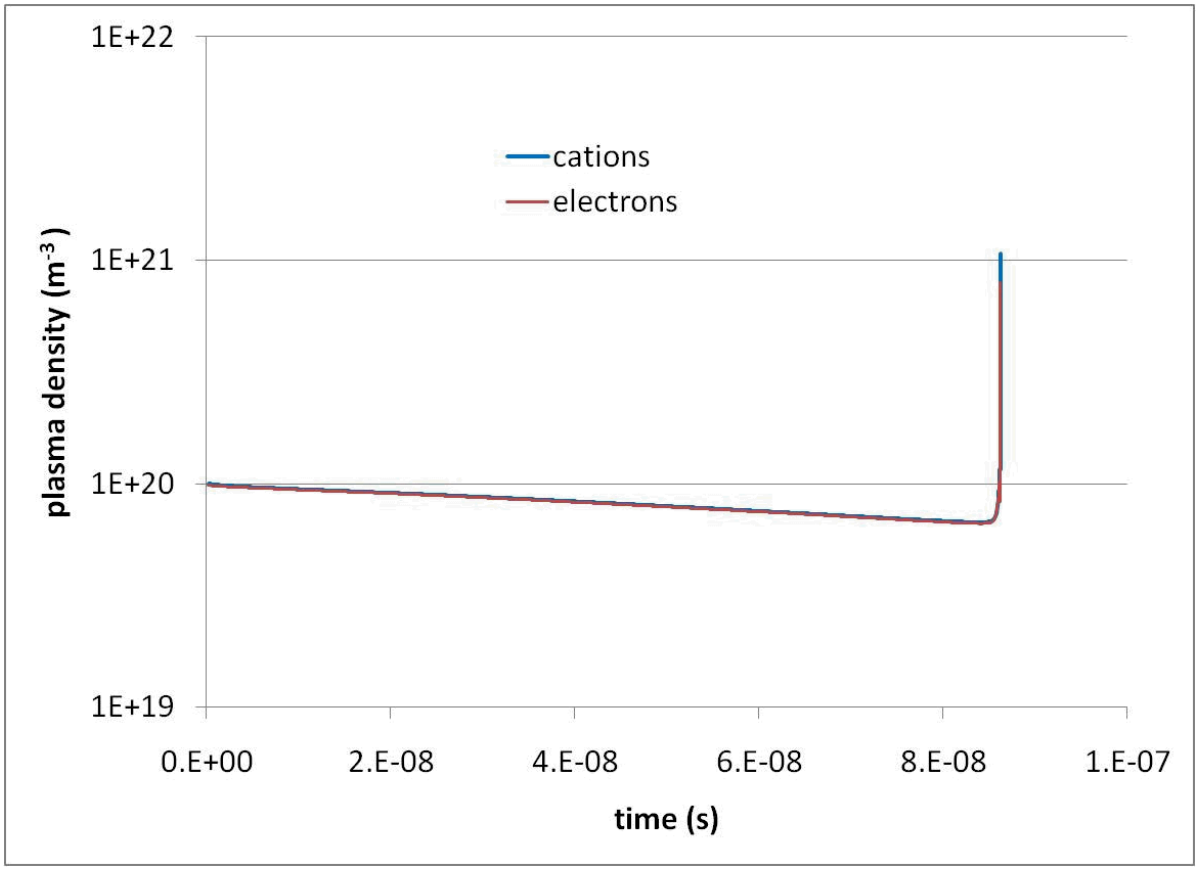
Stage 5: growth in plasma density

- 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 --- CHECK 4!



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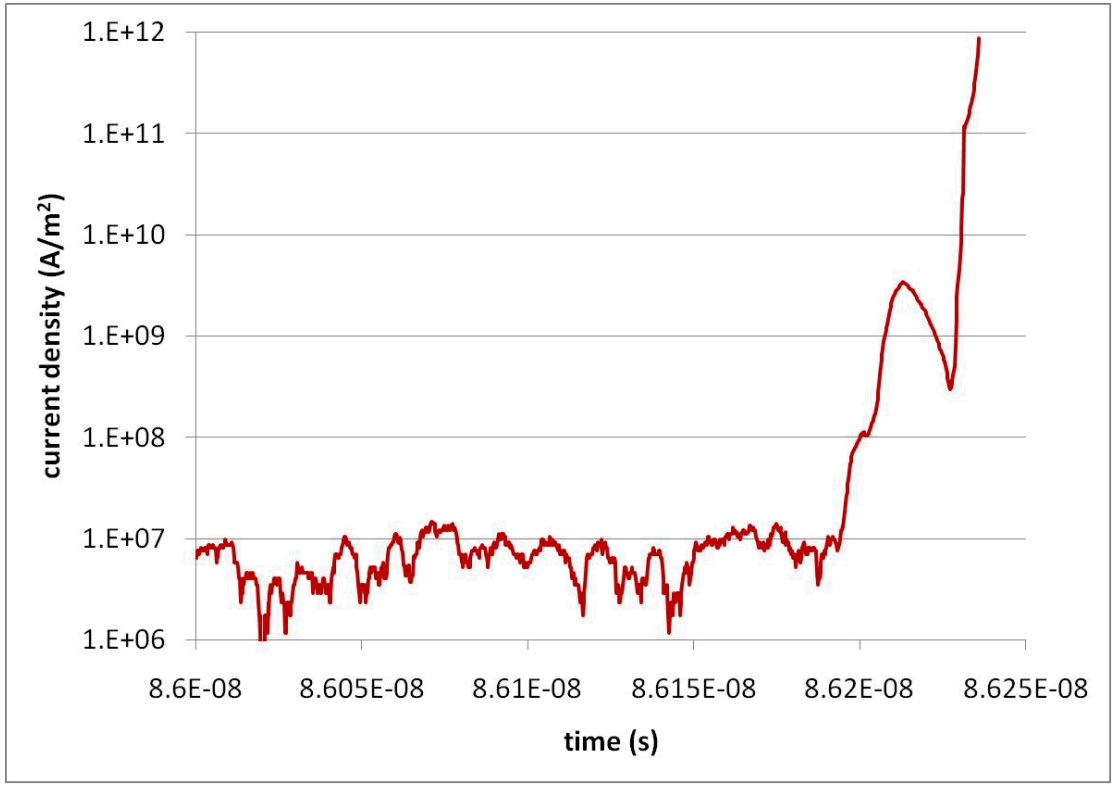
Stage 6: breakdown:
explosive growth in current to the anode

- 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! CHECK 5!



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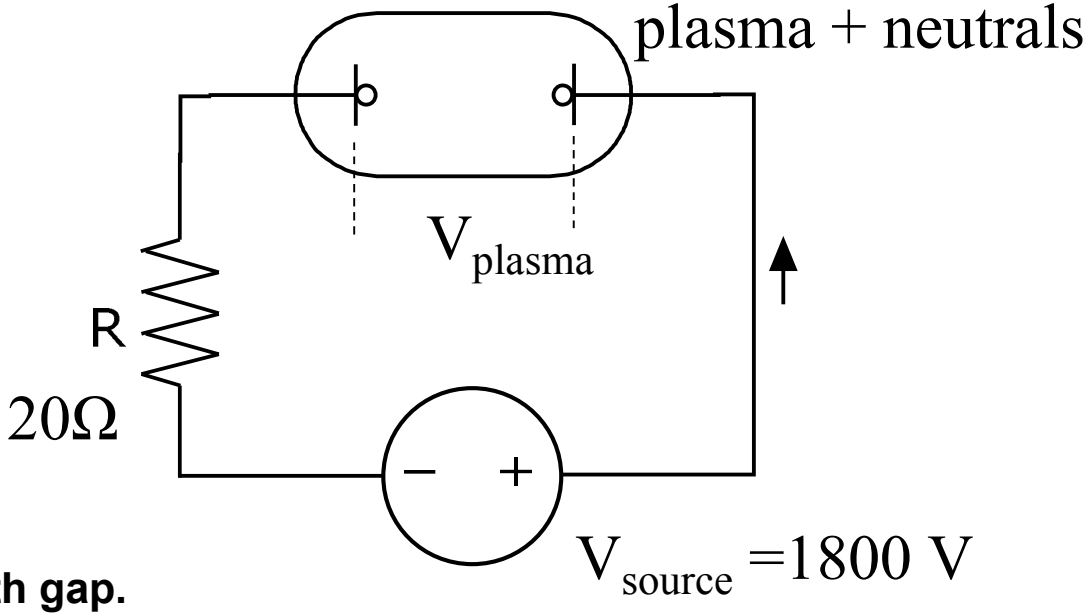
Stage 7: circuit model



- **20 ohm resistor in series with gap.**
- **Did not turn on the circuit model for this simulation --- need to redo with circuit model on.**

VI. Criticisms of our model

- Current growth not arrested due to lack of resistor in series. Will remedy this in subsequent simulations.
- 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.
- Would be better to start the anode at room T.
- Would be better to do a full 3D thermal solve of the anode.

VII. Conclusion

We've nearly achieved our goal, but still have a long way to go in our arc modeling endeavor.

- ✓ **Simple cathode plasma**
- ✓ **Anode emission of neutral metal atoms**
- ✓ **Dynamic particle reweighting**
- ✓ **Ionization of neutrals**
- ✓ **Current avalanche --- breakdown**
- ❑ **Simple circuit is series with arc**

VIII. Questions/comments/suggestions

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Additional material

- More about dynamic particle reweighting
- More about cross section calculations

Dynamic Particle Reweighting Methods for PIC

- Need for particle reweighting
- Special considerations for PIC
- Particle approaches
  - Cloning and merging
  - Position, Velocity, Time
- Element approaches
  - Dynamic reweighting
  - Velocity distribution and moments
  - Finite element reweighting
- Conclusion: Problem dependent

Need for Particle Reweighting

- Flows of practical interest often evolve in time, have strong gradients, trace species, or wide ranges of density and collisionality.
- DSMC and PIC are used to simulate complicated real flows using representative macroparticles.
- Both methods place requirements on cell size and particle count for overall accuracy, and to constrain statistical scatter in instantaneous properties.
- Large simulations require many particles, stressing even massive parallel capabilities.
- Uniform particle weight wastes effort in high density region to maintain resolution in low density region.

What Reweighting Should Do

- Particle reweighting adjusts the local particle weight to maintain a desired number of particles per cell.
- Cloning or merging of particles should conserve mass, momentum, energy, and important features of the velocity distribution functions.
- Reweighting should be isolated from other processes (chemistry, collisions, particle moves).
- Reweighting should not change the final solution.
  - Different problems may require different methods

Reweighting Considerations for PIC

- PIC is used to simulate charged particles in self-consistent electric and magnetic fields.
- Reweighting should conserve charge and current, analogous to mass and momentum.
- Reweighting should also preserve fields, corresponding to conservation of potential energy. (Gauss' Law and Ampere's Law couple the fields to charge distribution and currents.)

- Potential energy also relevant for reweighting in DSMC with body forces such as gravity.

Particle Based Reweighting

- Simple reweighting based on conserving properties at the particle level.
- Clone and merge operate pair-wise on particles.
- Conserves total mass, momentum, and energy on an elemental basis.
- Generally does not conserve properties on the grid except for low order elements. May be better suited to DSMC than PIC.

Cloning and Merging

- **Particle positions, velocities, or “times” are modified when cloning or merging particles.**
- **Ideally the clone and merge process conserves all desired quantities on pair by pair basis: center of mass conservation?**
- **Taking one property as independent, three general schemes are possible.**

Position “Δx” Method

- **Cloned particles are placed at new random position in cell, merged particles are assigned one initial position or mass-average position.**
- **Diffuses particles in space**
  - **Particle beams artificially diffuse across cells**
  - **Total energy conservation constrains velocities, for example in electrostatic sheath**

Velocity “Δv” Method

- **Cloned particles are assigned new velocities, merged particles are assigned one initial velocity or mass-average velocity.**
- **Diffuses particles in velocity space**
  - **Adds “thermal” distortion of velocity distribution**
  - **Diffuses particle pulse in all directions**

Time “Δt” Method

- **Cloned particles are separated by time increment, or a buffer.**
- **Diffuses particles along trajectory.**
  - **Diffuses arrival time for particle pulse**
  - **Preserves discrete combinations of position and velocity**

Element Based Reweighting

- More complicated reweighting to preserve grid properties, suitable for both PIC and DSMC.
- Clone and merge operate on all particles in an element as a group.
- Conserves mass, momentum, and energy on grid points, may be extended to higher elements.

Dynamic Reweighting

- Original number of particles are cloned or merged into target number of particles, with total weight redistributed uniformly.
- “Roulette” deletion instead of merging, exact copy instead of cloning.
- Restore lost momentum or kinetic energy to all particles, expected to be small changes.
  - Great flexibility for target particle count
  - Streamers possible until collisions separate copies
  - Generally does not preserve grid quantities

Distribution Reweighting

- Clones selected from velocity distribution calculated from moments or from a time history record of particle velocities.
  - History introduces lag, undesirable for transient flow
  - Moments imply properties of distribution that are not necessarily valid
  - Fields can distort distributions into non-analytic forms
  - Some distributions may be poorly represented by limited moments, such as crossed beams

Finite Element Reweighting

- Fixed points within the cell for new particles, selected depending on basis functions.
- Matrix equation to determine weights and velocities of particles at fixed points.
  - Designed to preserve grid properties, should maintain fields well
  - Calculated velocities not guaranteed to be consistent with inlet conditions and local potential

Reweighting conclusions

- Reweighting methods should be chosen with the application in mind.
- Particle based reweighting methods are suited to preserving different aspects of particle trajectories. Particles diffuse in space or velocity.
- Element based reweighting methods are suited to preserving element and grid quantities. Particle trajectories may not be reliable.

Uses Okhrimovskyy formulation for anisotropic electron scattering

PHYSICAL REVIEW E, VOLUME 65, 037402

Electron anisotropic scattering in gases: A formula for Monte Carlo simulations

A. Okhrimovskyy, A. Bogaerts, and R. Gijbels
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for anisotropic scattering of electrons, which is generally valid in atomic and nonpolar molecular gases. The general formula will then be applied to a number of atomic and nonpolar molecular gases, to derive formulas that are easy to implement in Monte Carlo algorithms.

II. DIFFERENTIAL CROSS SECTION FOR LOOK-ALIKE SCREENED-COULOMB SCATTERING

In an atomic gas with atomic number Z the electron-neutral interaction potential can be approximated by the screened Coulomb potential

$$U(r) = ZE_0 \frac{r_0}{r} \exp\left(-\frac{r}{r_0}\right). \tag{2}$$

Finally, to find the scattering angle, a random number R uniformly distributed in the interval [0,1] is compared with the probability of scattering; and the reverse function should be found,

$$\cos\chi = 1 - \frac{2R}{1 + 8\varepsilon(1-R)}. \tag{5}$$

Equation (5) is very convenient for Monte Carlo modeling purposes of the electron behavior in atomic gases. We will now derive a similar expression for electron scattering with nonpolar molecules (CH_4, N_2, O_2, etc.), assuming the same functional form of differential cross section as for the idealized atom. Equation (3) can be rewritten in the more general form using one fitting parameter [9],

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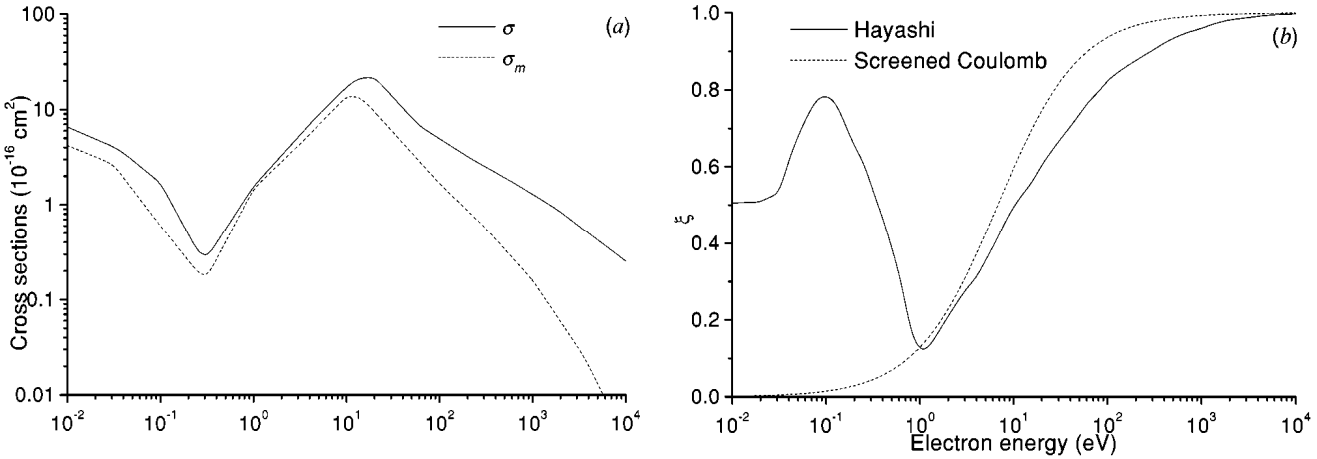

FIG. 1. (a) Integrated elastic σ (solid) and momentum transfer σ_m (dashed) cross sections for Ar from Hayashi [17]; (b) derived ξ based on the data of Hayashi (solid) and for the screened-Coulomb potential (dashed) as a function of electron energy.

$$I(\varepsilon,\chi)=\frac{1}{4\pi}\frac{1-\xi^2(\varepsilon)}{[1-\xi(\varepsilon)\cos\chi]^2}, \tag{6}$$

similar to the procedure described by Phelps [14]. It should be mentioned that we used the notation $\xi(\varepsilon)$, which is equivalent to "$1-2*\beta(n)$" in Phelps notation [14]. This expression reduces to conventional screened-Coulomb scattering if $\xi=4\varepsilon/(1+4\varepsilon)$. In general, ξ is a function of energy (see below), which varies in the interval $(-1,1)$. Depending on the kind of interaction potential, ξ is a different function of energy. Hence, this yields a different scattering formula.

Equally, the probability of electron scattering with an angle χ can be calculated. And again, the scattering angle can be found by comparing a random number R uniformly distributed in the interval $[0,1]$ with the probability of scattering; and reversing the function,

$$\cos\chi=1-\frac{2R(1-\xi)}{1+\xi(1-2R)}. \tag{7}$$

$$\frac{\sigma_m}{\sigma}=\frac{1-\xi}{2\xi^2}\left((1+\xi)\ln\frac{1+\xi}{1-\xi}-2\xi\right). \tag{8}$$

This expression is generally valid for all kinds of interactions between electrons and atoms or nonpolar molecules. In the literature, some experimental data are available for both integrated and momentum transfer cross sections as a function of electron energy, for electron elastic collisions with atoms or molecules [8,15–18]. Hence, the function $\xi(\varepsilon)$ for a specific interaction can be obtained from the ratio of experimental cross sections $\sigma_m(\varepsilon)/\sigma(\varepsilon)$. Finally, when $\xi(\varepsilon)$ is known, the formula for the scattering angle can be obtained with Eq. (7).

The main idea of the procedure to construct differential cross sections based on the screened-Coulomb functional dependence from the data of the integrated and momentum transfer cross sections was first published by Belenguer and Pitchford [9]. In the case of the resonance atom-atom scattering Phelps *et al.* [19] proposed a three fitting parameter

Single-event tests

Elastic

		Before collision			After collision		
		x	**y**	**z**	**x**	**y**	**z**
9.11E-31	Electron:	6502000	0	0	5446091.17	2990301	1915861
6.65E-27	Neutral	-519.93676	29.19455	-800.0567	-375.215667	-380.651	-1062.641
	momentum	2.47E-24	1.94E-25	-5.32E-24	2.47E-24	1.94E-25	-5.32E-24
	loss	0.00E+00	4.36E-40	-5.14E-38			
	energy	1.93E-17			1.92541E-17		
		3.03E-21			4.70201E-21		
		1.93E-17			1.92588E-17		
	loss:	**0.00E+00**					
		1.60E-19					
	eV	**0.0000E+00**					

Excitation

		x	**y**	**z**	**x**	**y**	**z**
9.11E-31	Electron:	6502000	0	0	5195636.417	2672270	944808
6.65E-27	Neutral	-935.31561	159.5363	44.33152	-756.2676154	-206.7205	-85.16228
	momentum	-2.94E-25	1.06E-24	2.95E-25	-2.94E-25	1.06E-24	2.95E-25
	loss:	4.41E-39	0.00E+00	-1.06E-39			
	energy	1.93E-17			1.59546E-17		
		3.00E-21			2.06681E-21		
		1.93E-17			1.59567E-17		
	loss:	3.30E-18					
		1.60E-19					
	eV	**2.0610E+01**					

Ionization

		x	**y**	**z**			**x**	**y**	**z**
9.11E-31	Electron:	6502000	0	0		9.11E-31	5539422.234	-1024479	-1376343
6.65E-27	Neutral	-589.11883	37.77392	-439.5909	Ion	6.65E-27	-457.1895355	178.1873	-250.9516
					Secondary	9.11E-31	-457.1895355	178.1873	-250.9516
	momentum	2.01E-24	2.51E-25	-2.92E-24			2.01E-24	2.51E-25	-2.92E-24
	loss:	-5.29E-37	2.09E-37	-2.98E-37					
	energy	1.93E-17					1.53173E-17		
		1.80E-21					1.00929E-21		
	sum	1.93E-17					1.38351E-25		
	loss:	3.94E-18				sum:	1.53183E-17		
		1.60E-19							
	eV	**2.4587E+01**							

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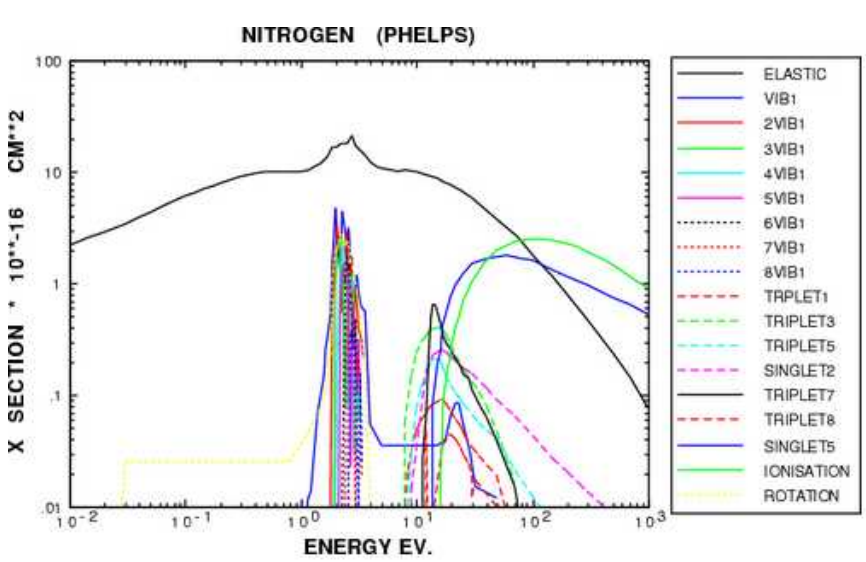
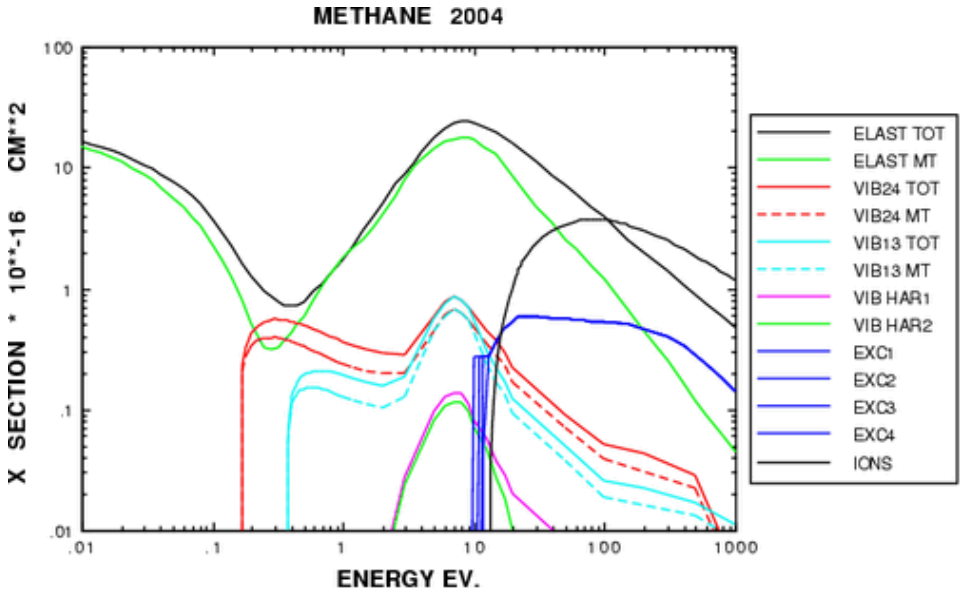
Representative publicly-available cross-section data





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