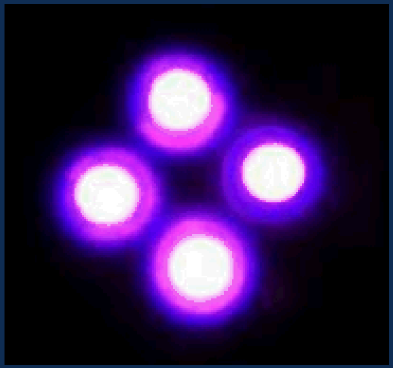

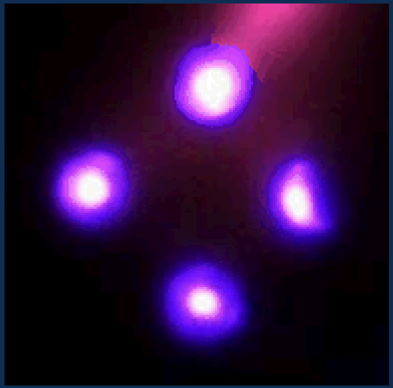

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SAND2015-8679C

Fully Kinetic Simulation of Atmospheric Pressure Microcavity Discharge Device

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Sandia National Laboratories

International Conference on Plasma Science (ICOPS), May 24-28, 2015, Belek, Turkey

U.S. DEPARTMENT OF ENERGY

NNSA National Nuclear Security Administration

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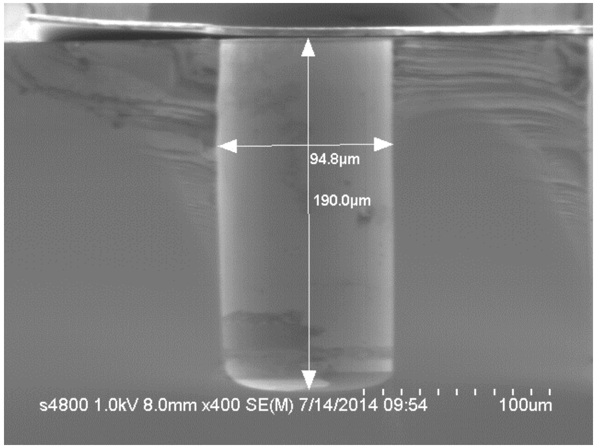
Introduction

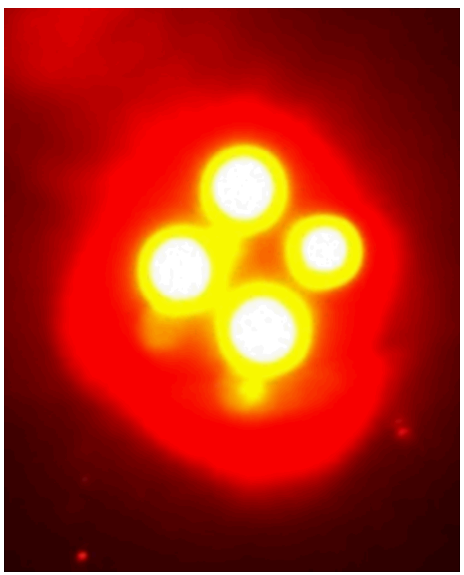
This work addresses the completely kinetic description of a microscale discharge device operating at atmospheric pressure. Such devices are often used in arrays for a variety of light generation purposes.

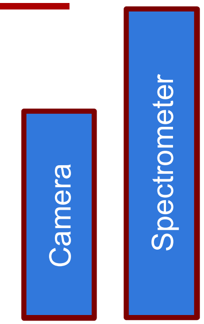
The separation and control of specific excited states is the goal of the overall work. Developing a computational model will allow us to better design and assess operating efficiencies, trade-offs, etc.

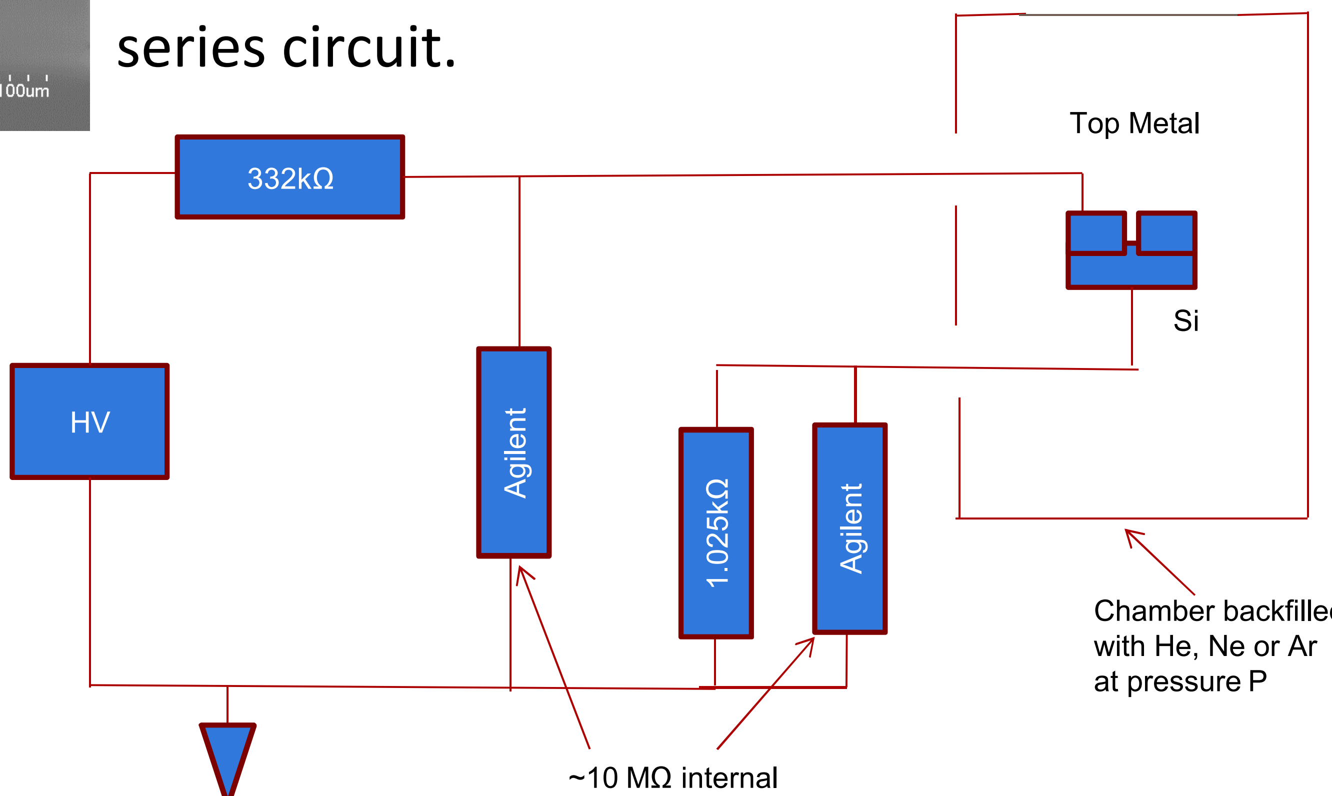
Experiments



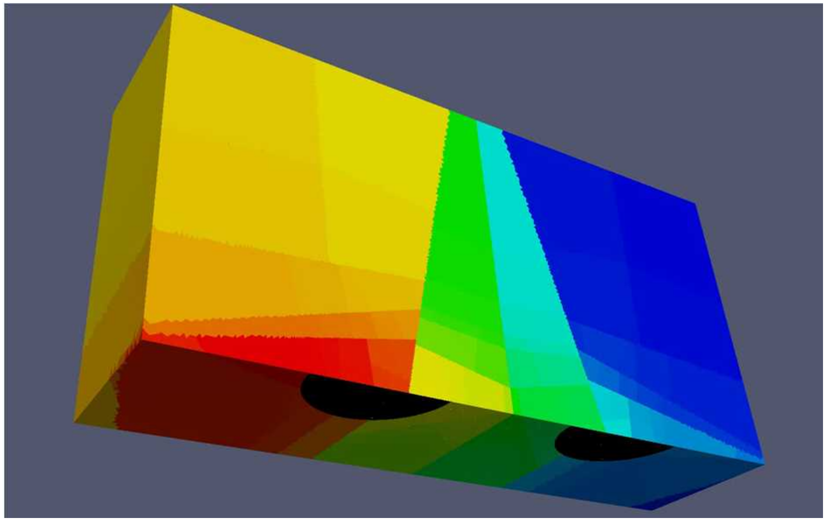
Experiment uses 4 cylindrical 50 μm radius cavities (up to 200 μm deep) all connected to the same ballast resistor-in-series circuit.





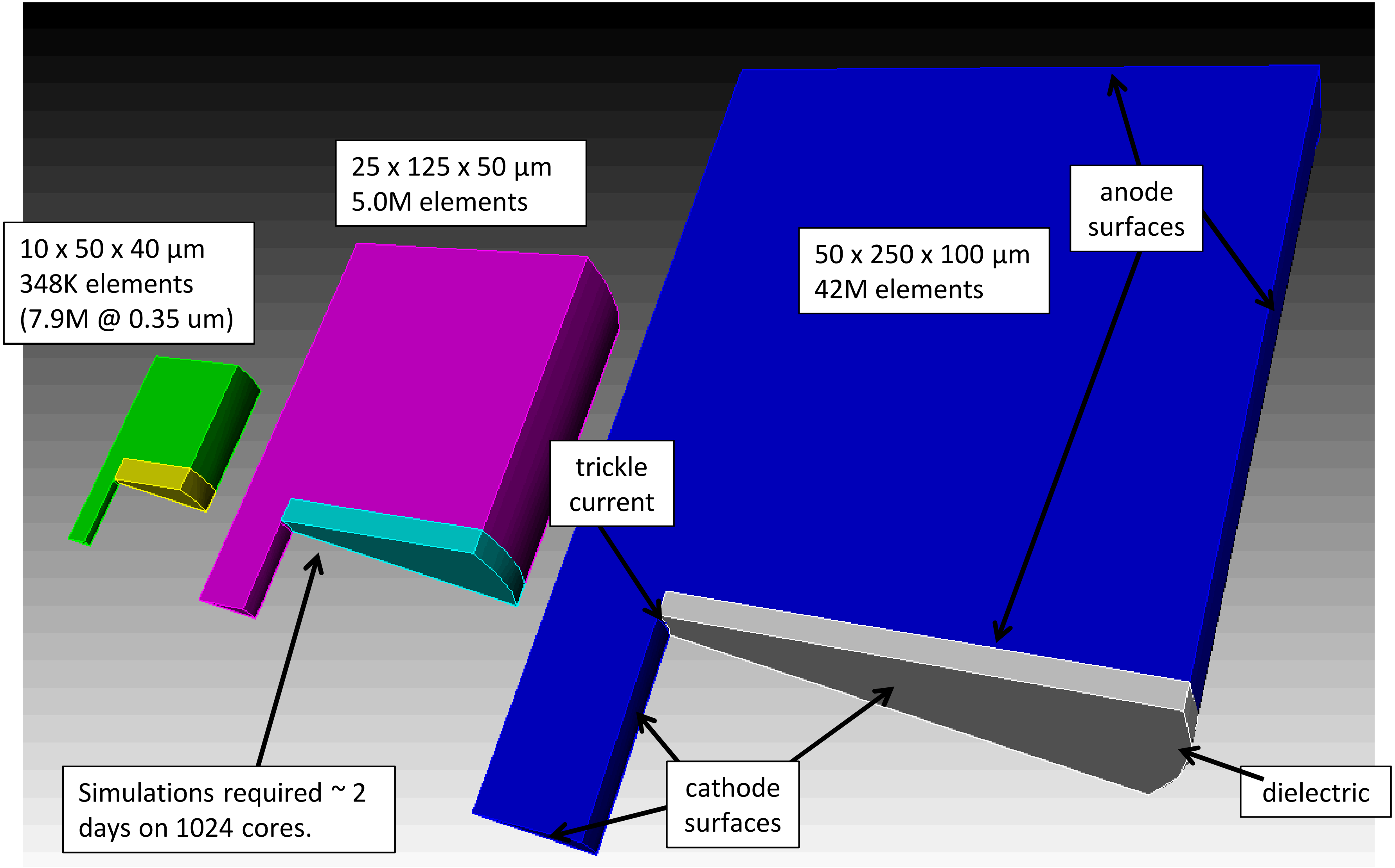


Description of *Aleph*



- 1, 2, or 3D Cartesian
- Unstructured FEM (compatible with CAD)
- Massively parallel
- Hybrid PIC + DSMC (PIC-MCC)
- Electrostatics
- Fixed B field
- Solid conduction
- Advanced surface (electrode) models
- e- approximations (quasi-neutral ambipolar, Boltzmann)
- Collisions, charge exchange, chemistry, excited states, ionization
- Photon transport, photoemission, photoionization
- Advanced particle weighting methods
- Dual mesh (Particle and Electrostatics/Output)
- Dynamic load balancing (tricky)
- Restart (with all particles)
- Agile software infrastructure for extending BCs, post-processed quantities, etc.
- Currently utilizing up to 64K processors (>1B elements, >1B particles)

Model Description



Model Description

Experiment

655 Torr 300 K Ne

332 kΩ resistor-in-series w/circuit elements

50 μm radius, 200 μm depth, 10 μm spacer

4 full microcavities

Full chemistry

ε = 3 10 μm polyimide dielectric

Model

655 Torr 300 K Ne (n_{Ne} = 2.1 x 10^{25}/m^3)

$V_A = V_{PS} - IR$, R = 332 kΩ, I averaged ~ 10 ps

25 μm radius, 40 μm depth, 10 μm spacer

Single 3D 30 degree sector

Ionization, excitation, elastic (7 tracked species), from LXCat, www.lxcat.net

ε = 3 10 μm polyimide dielectric w/ surface charging

SEE γ = 0.15 for Ne+ and Ne++

Computational Parameters

Targeting $n_{e-} < 10^{20}$/m^3, T_e = 4 eV,

λ_D > 1.1 μm → Δx < 1.1 um, [Debye length]

λ_{mfp} > 1.6 μm → Δx < 1.6 um, [Collision mean free path]

Use Δx = 1.0 μm.

Targeting ΔV < 200 V, v_{max} = maximum e- speed (~ 9.4 x 10^6 m/s including thermal],

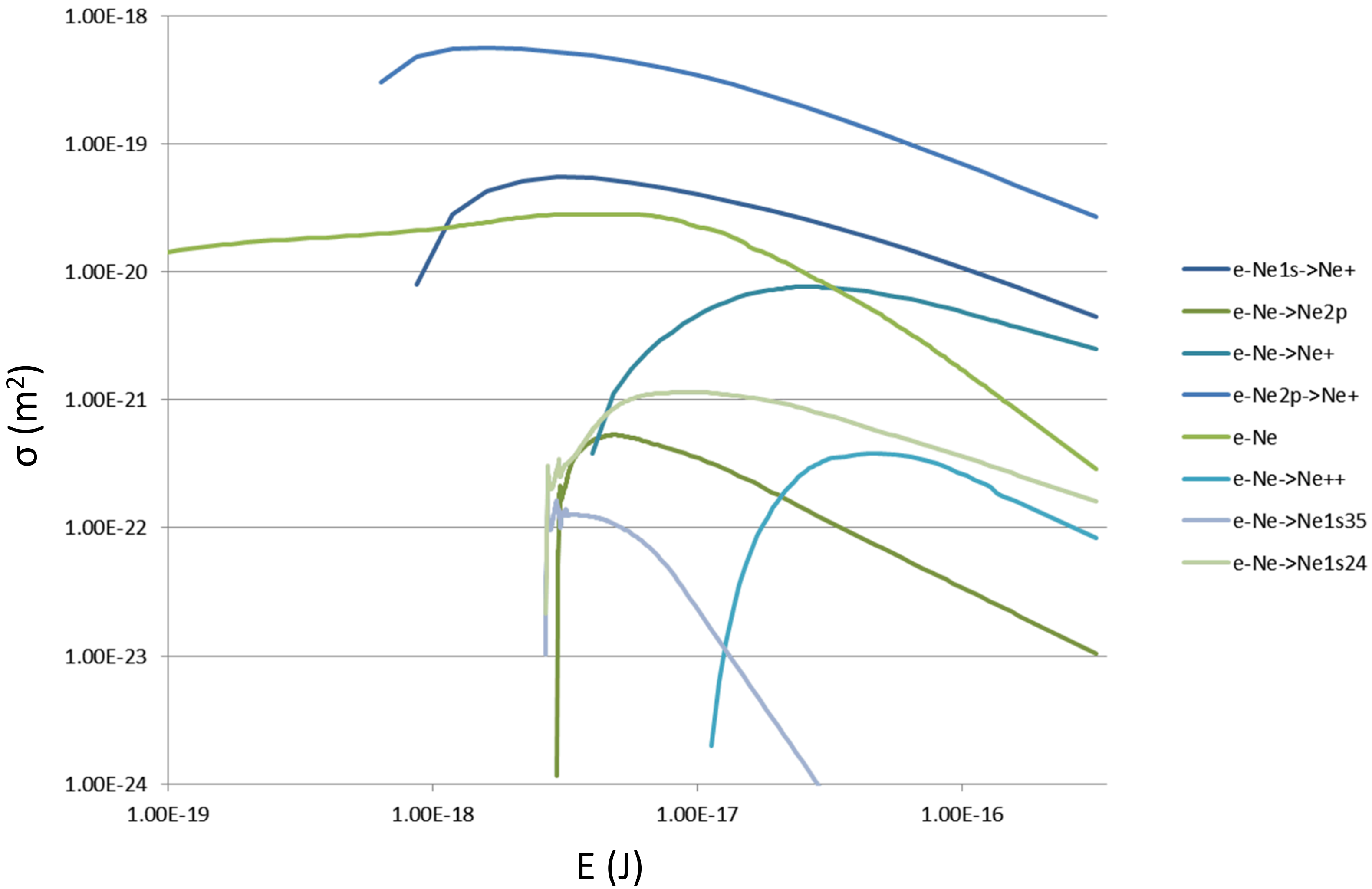
$\omega_p < 5.6 \times 10^{11}$/s → Δt < 3.5 ps, [Plasma e- frequency]

$\Delta t < \Delta x / v_{max}$ → Δt < 100 fs, [CFL]

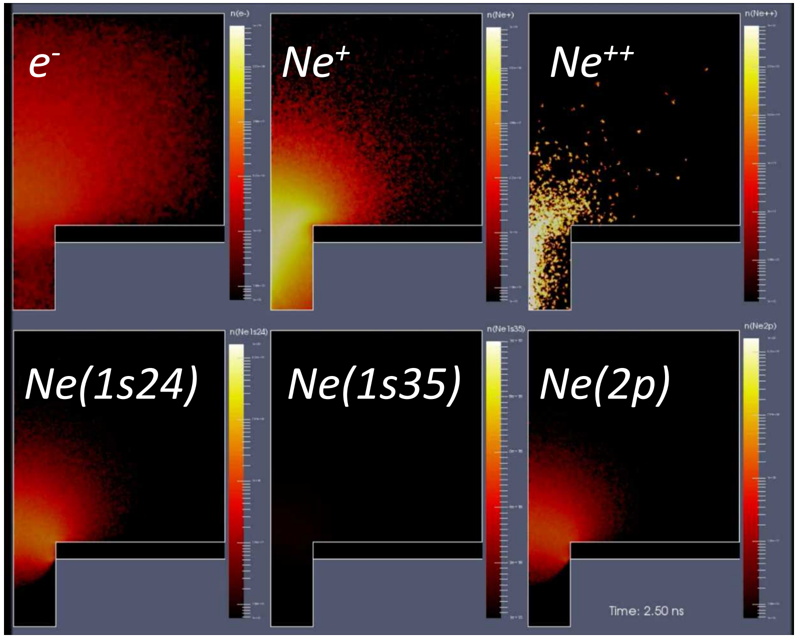
$\Delta t_{collide} < (n_{Ne}\sigma_{max}v_{max})^{-1}$ → Δt < 170 fs, [Collision frequency]

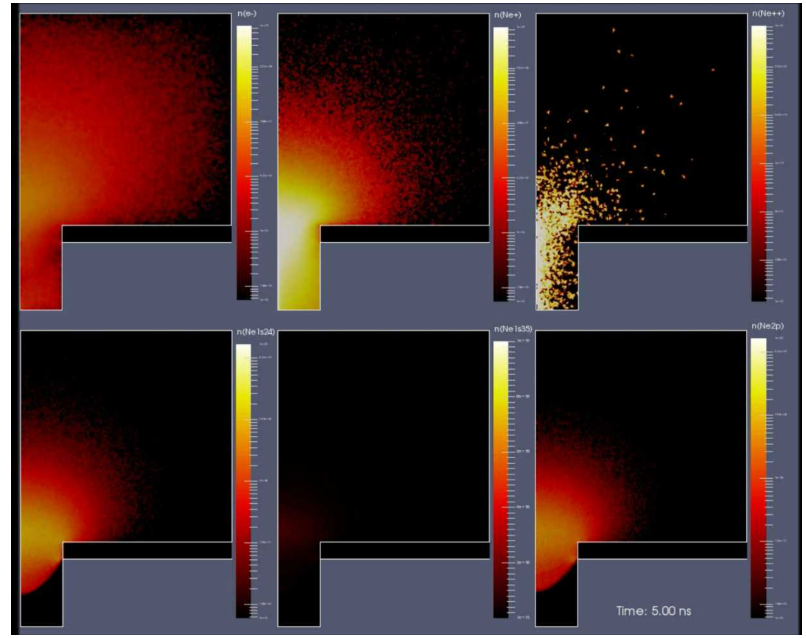
Use Δt = 50 fs.

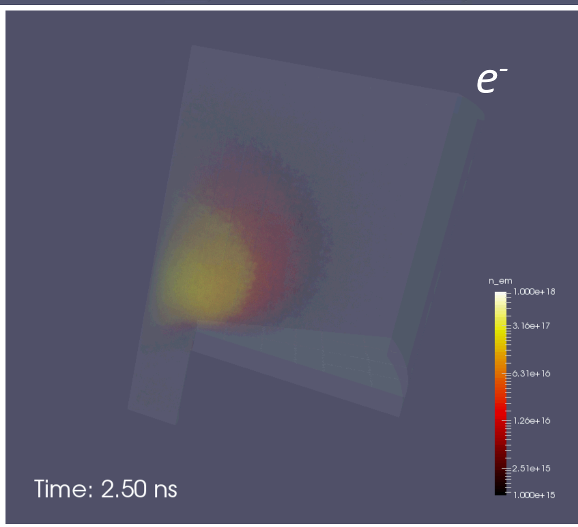
Cross-sections (from LXCat)

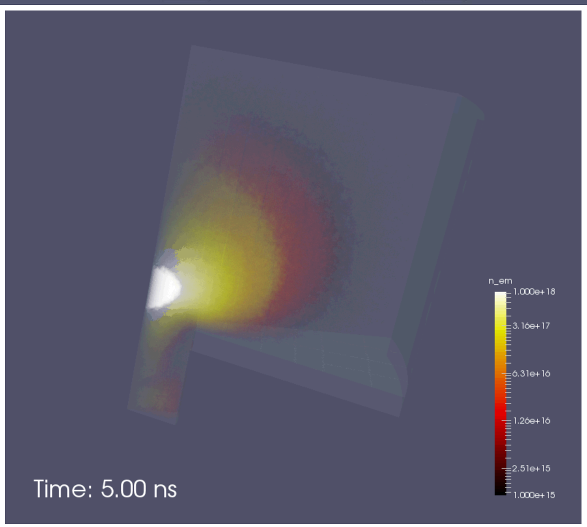


Results (V_{PS} = 200 V): Spatial Evolution

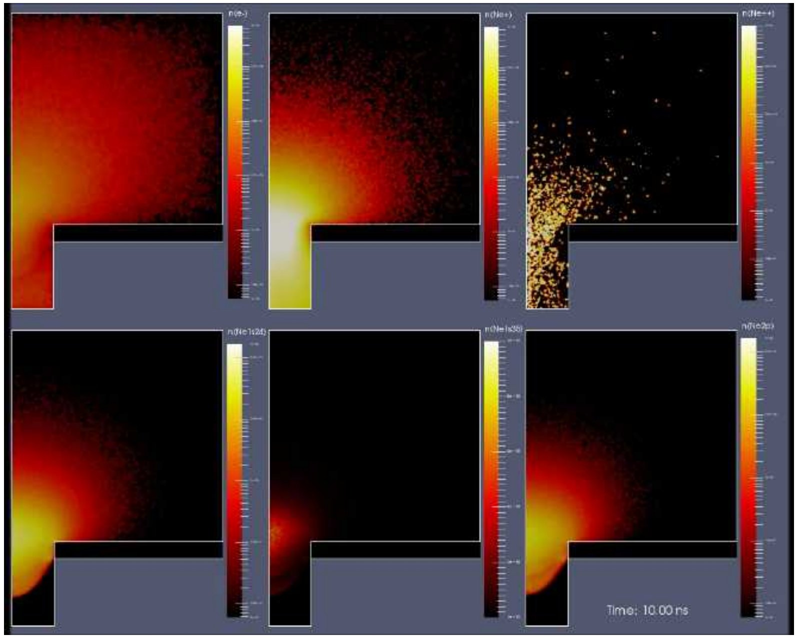


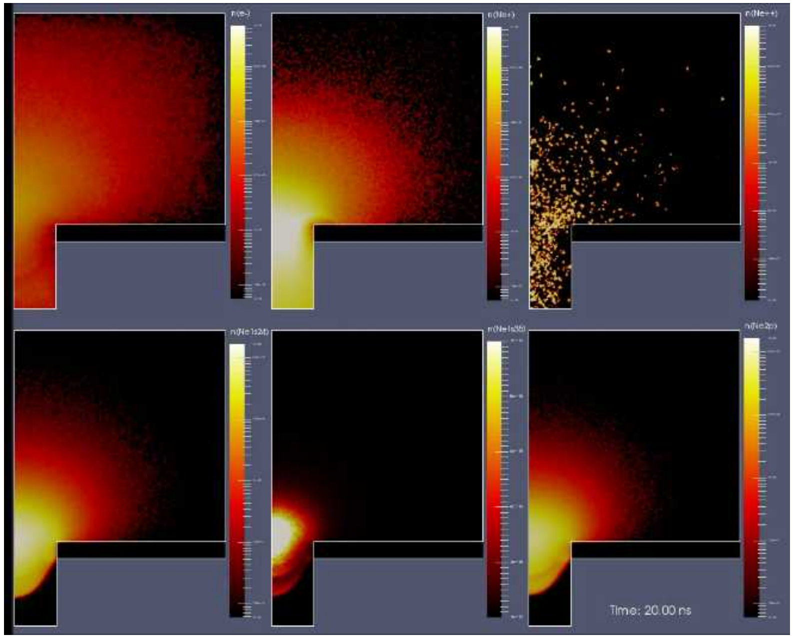


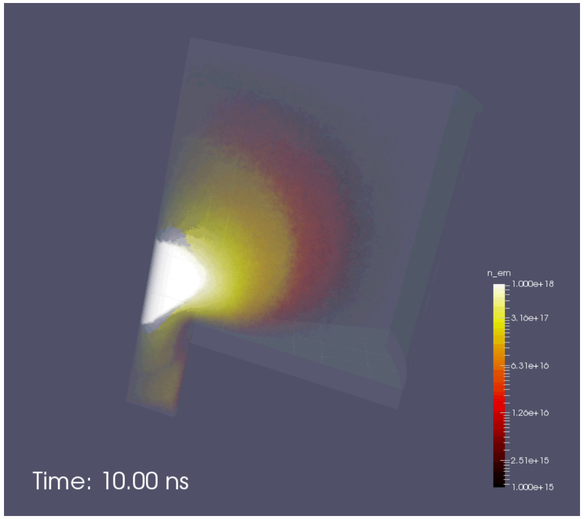


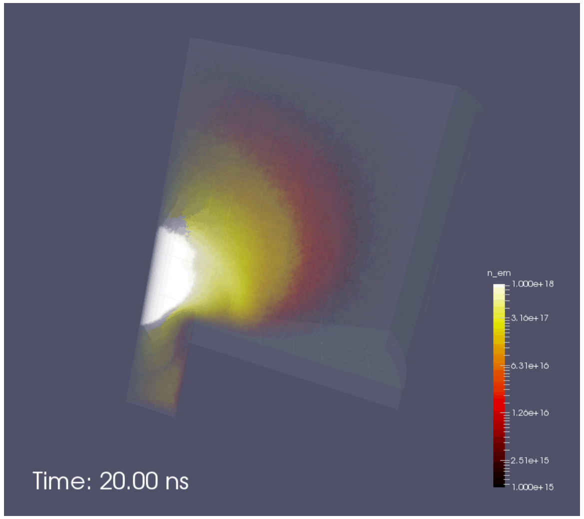


Results (V_{PS} = 200 V): Spatial Evolution

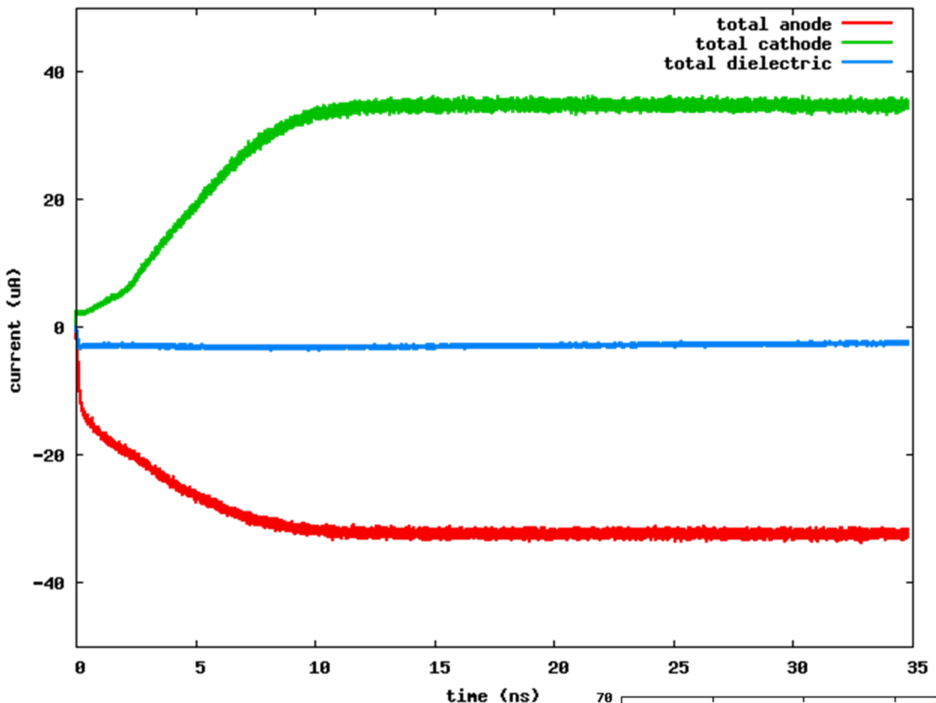


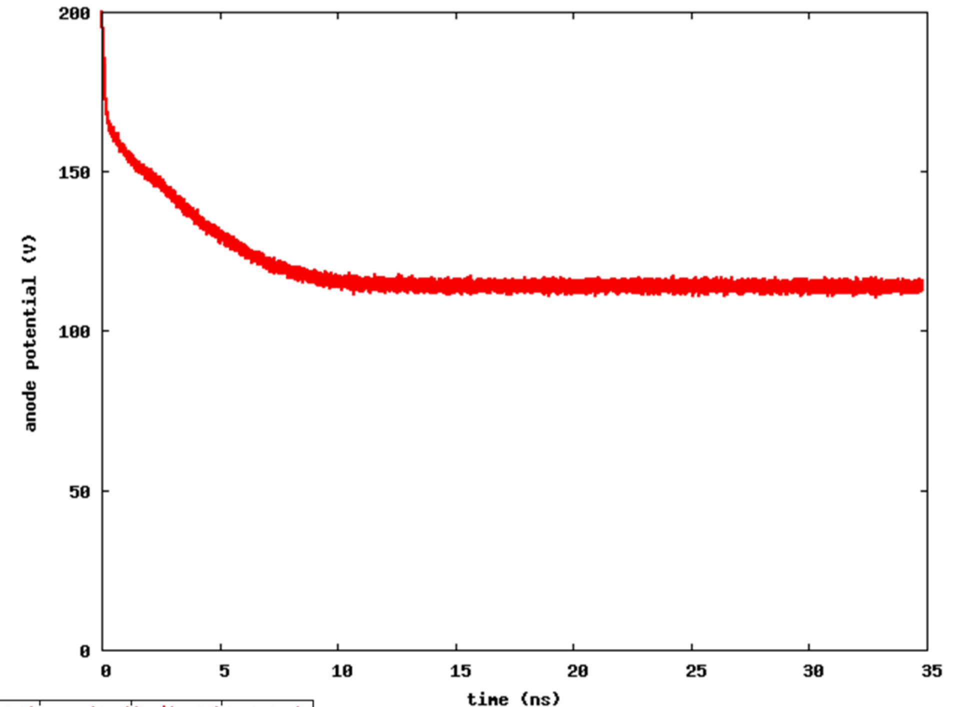




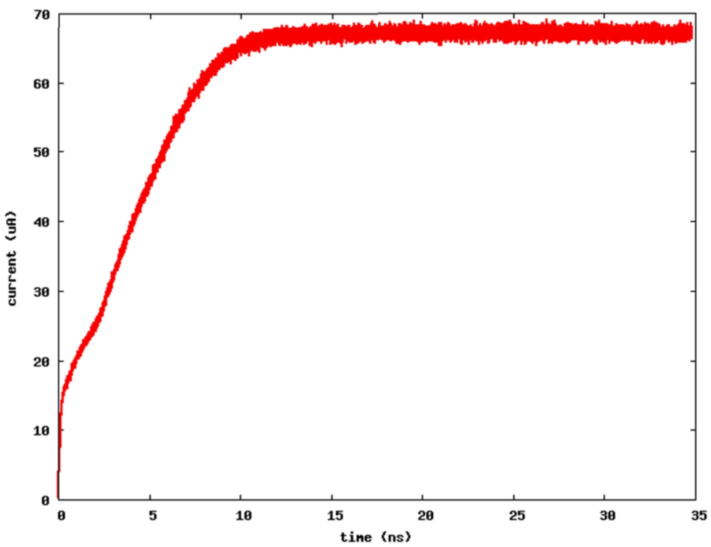


Results (V_{PS} = 200 V): *I* and *V* Evolution





Anode current
– cathode current =



Results (operating *I* vs. *V*)

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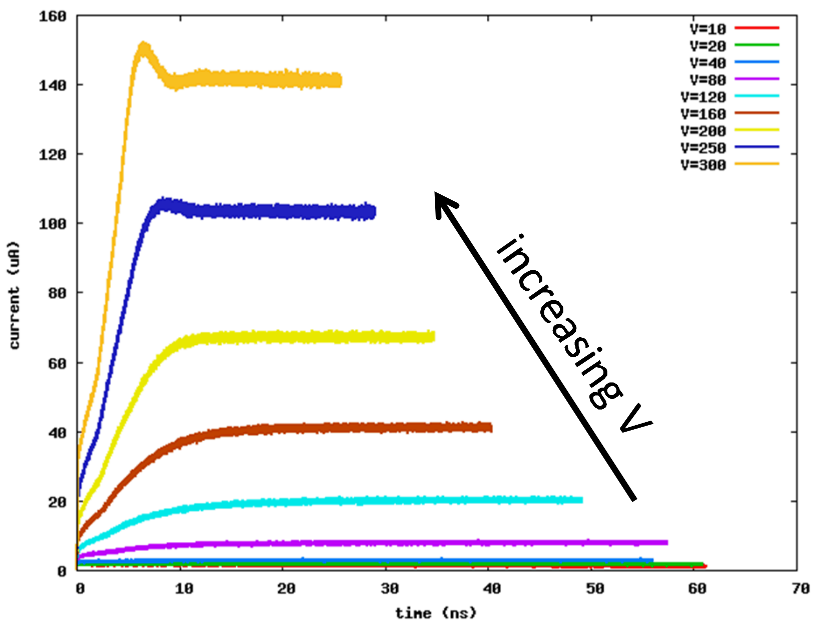
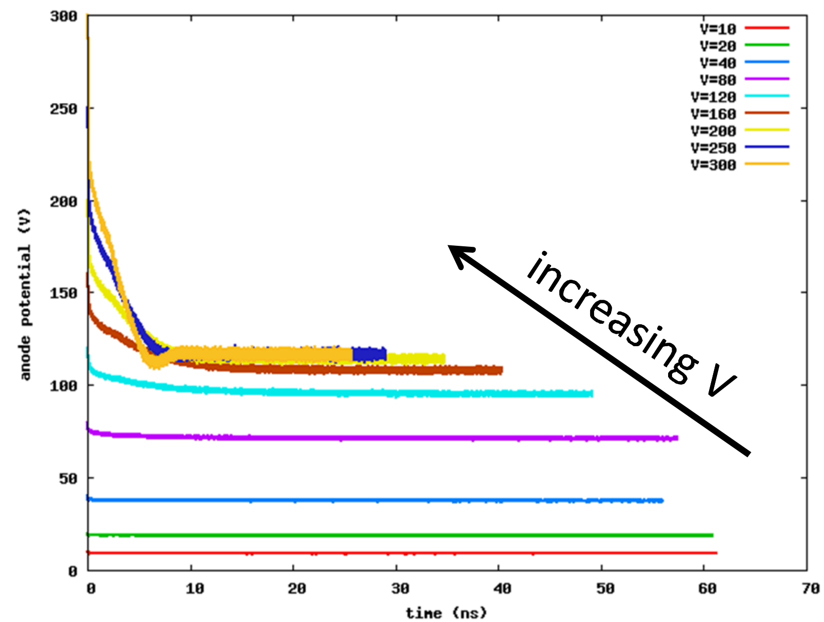
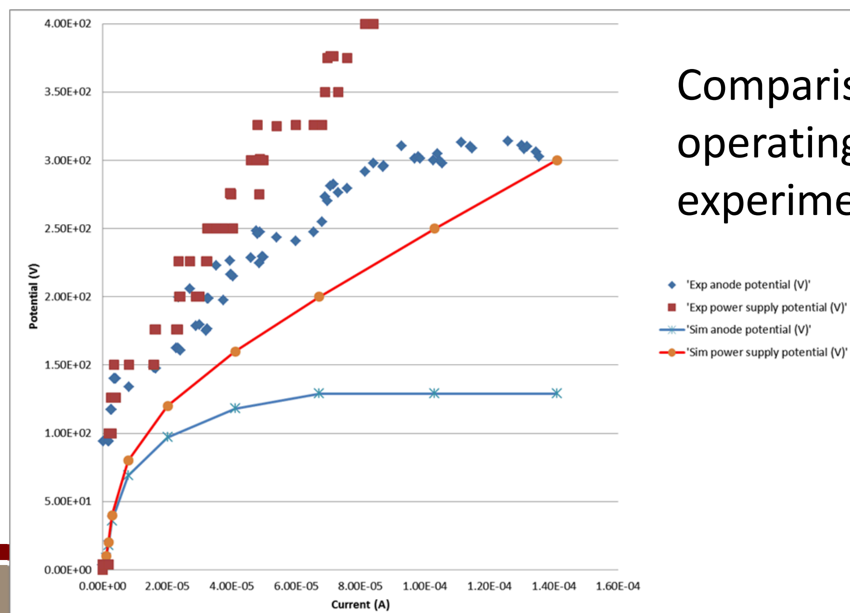
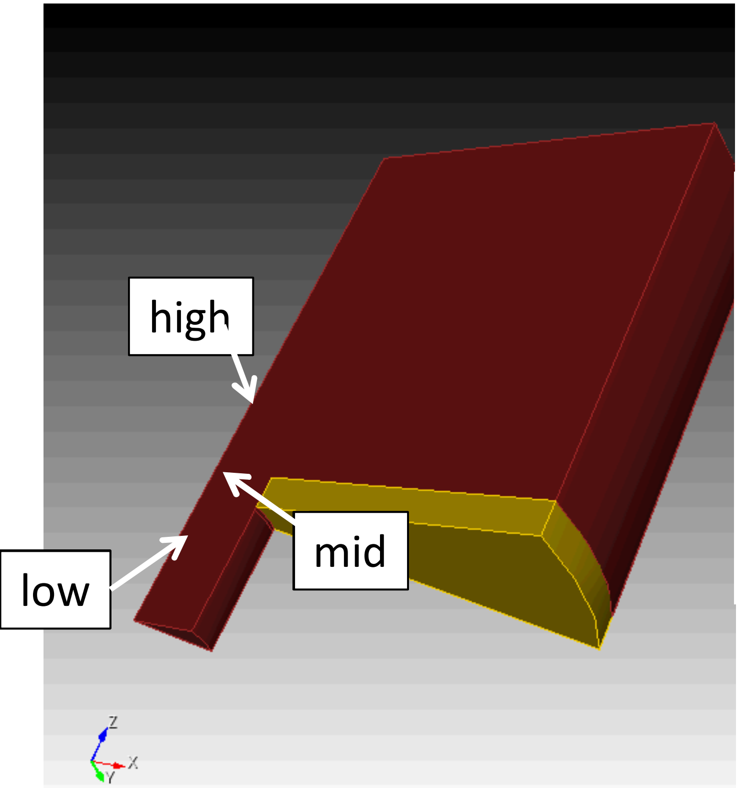


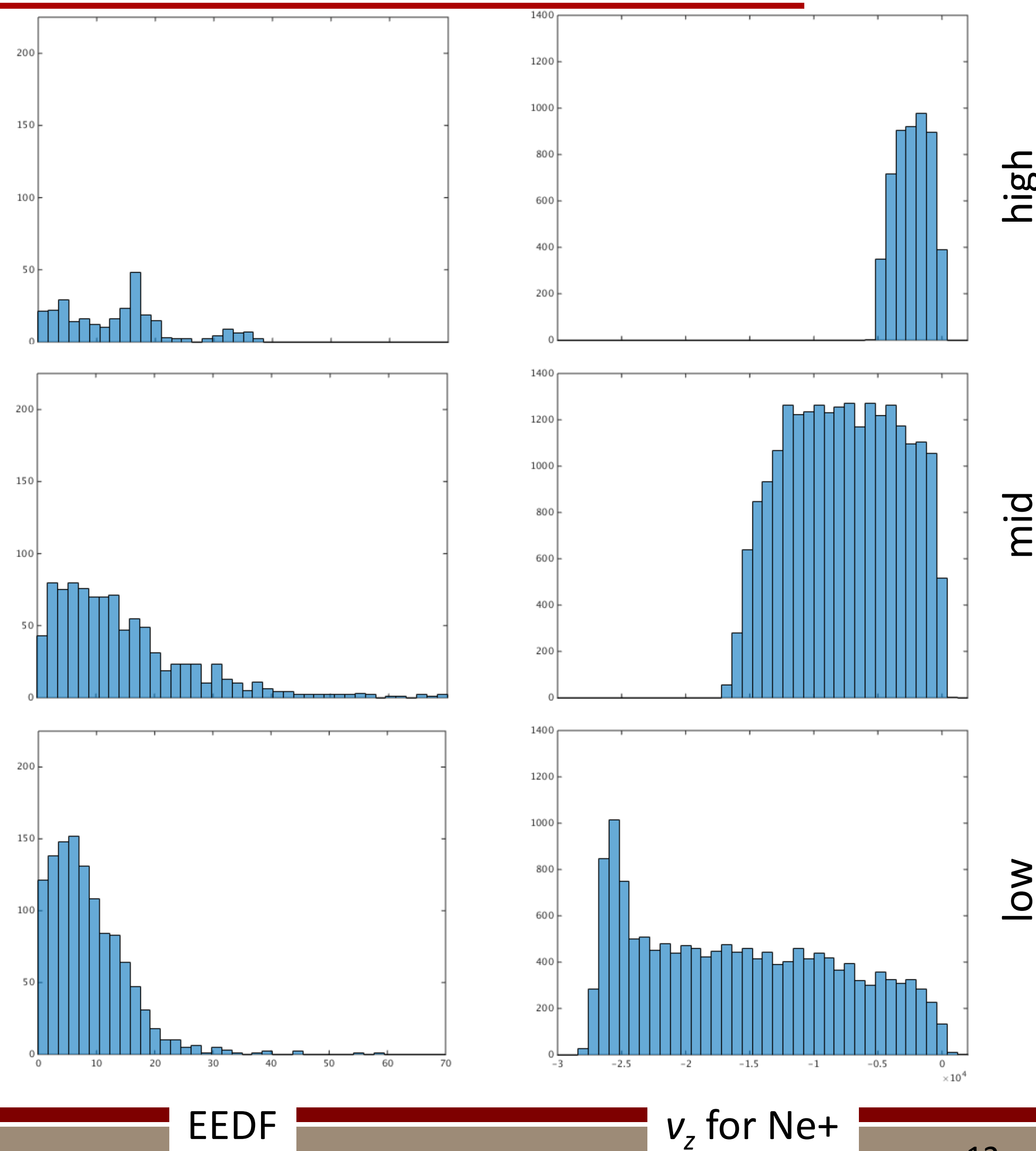




Comparison to operating conditions of experiment

Results: Distribution Functions





The Truth about Particle Weights

In these simulations, the particle weights for all species except Ne is initially 0.01.

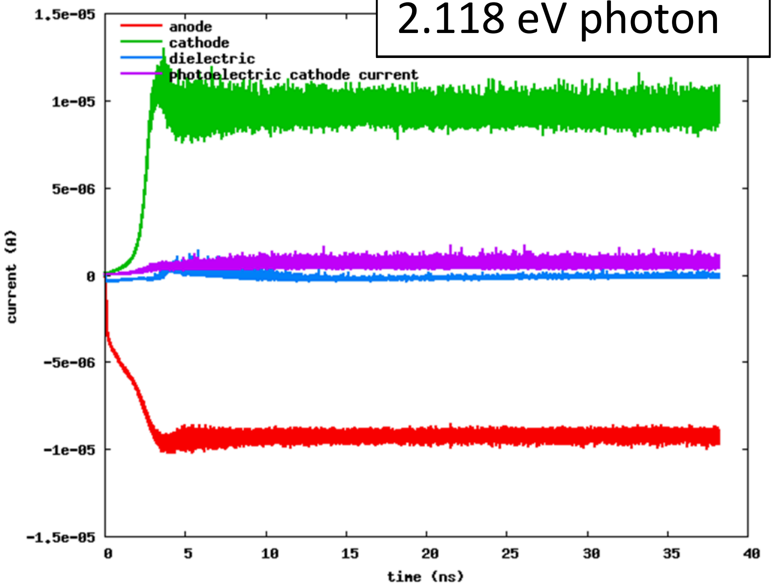
- We are supposedly still a plasma as the plasma number is ~500 (# particles in a Debye sphere).
- One advantage of the tiny particle weight is the exponential multiplicative effect is essentially guaranteed to begin at $t = 0$.
- Circuit noise is also impacted with a lower particle weight.
- Laying in a low density plasma to initiate discharge is non-physical and can lead to premature overshooting.

Conclusion & Future Steps

- Have developed a fully kinetic capability for simulation atmospheric pressure microscale discharges.
- Can track vdf's for all species in space and time.
- Agreement within factor of 2x with experiment (first comparison for us).

- Need more electron chemistry.
- Should add spontaneous emission.
- Looking into photoemission.
- Recombination?
- Question about experimental ground at bottom of silicon vs. model ground at silicon surface.
- Turn off trickle current after some initial time.

Photoelectric current from 2.118 eV photon



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