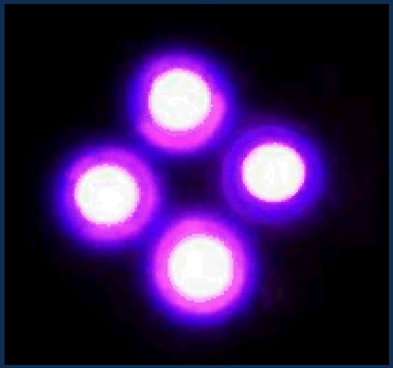

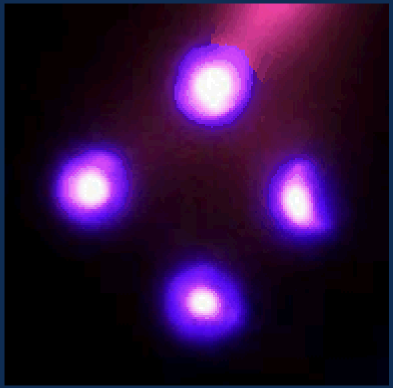

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Experiences with Kinetic Modeling of Atmospheric Pressure Discharge

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Sandia National Laboratories

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University of Maryland, College Park
College Park, MD, USA

U.S. DEPARTMENT OF ENERGY

NNSA National Nuclear Security Administration

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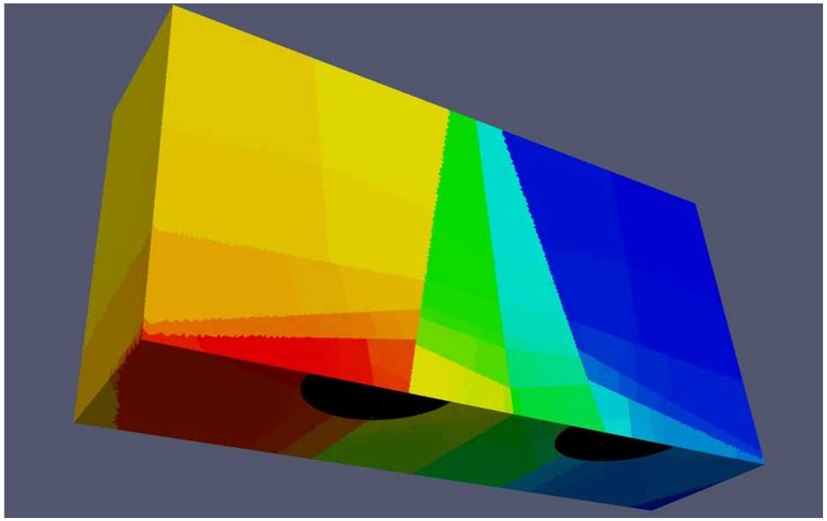
Introduction

We present a number of techniques and challenges in simulating the transient behavior of discharge at atmospheric pressures. All of the following work is performed with the Aleph simulation tool, with newly added capabilities for three-body interactions and photonic process (spontaneous emission, absorption, excitation, and line broadening).

We describe three related systems:

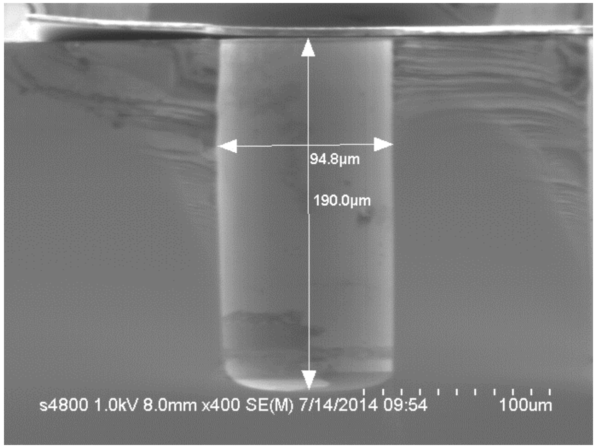
1. Microscale discharge in 1 atm Ne, ~250V across 10 μm.
2. Microscale discharge in ~1 atm He with photonic and three-body processes.
3. Exploration of particle dE/dt constraint.

Description of *Aleph*

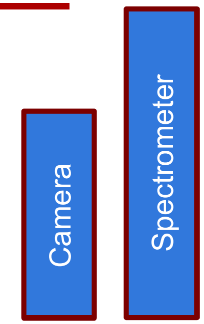


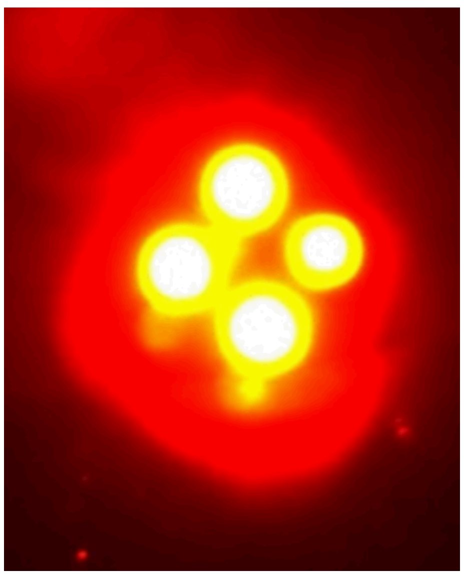
- 1, 2, or 3D Cartesian
- Unstructured FEM (compatible with CAD)
- Massively parallel
- Hybrid PIC + DSMC (+ PIC-MCC)
- Electrostatics
- Fixed B field
- Solid conduction
- Advanced surface (electrode) models
- e- approximations (quasi-neutral ambipolar, Boltzmann)
- Collisions, charge exchange, chemistry, excited states, ionization
- Photon transport, photoemission, photoionization, absorption
- 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)

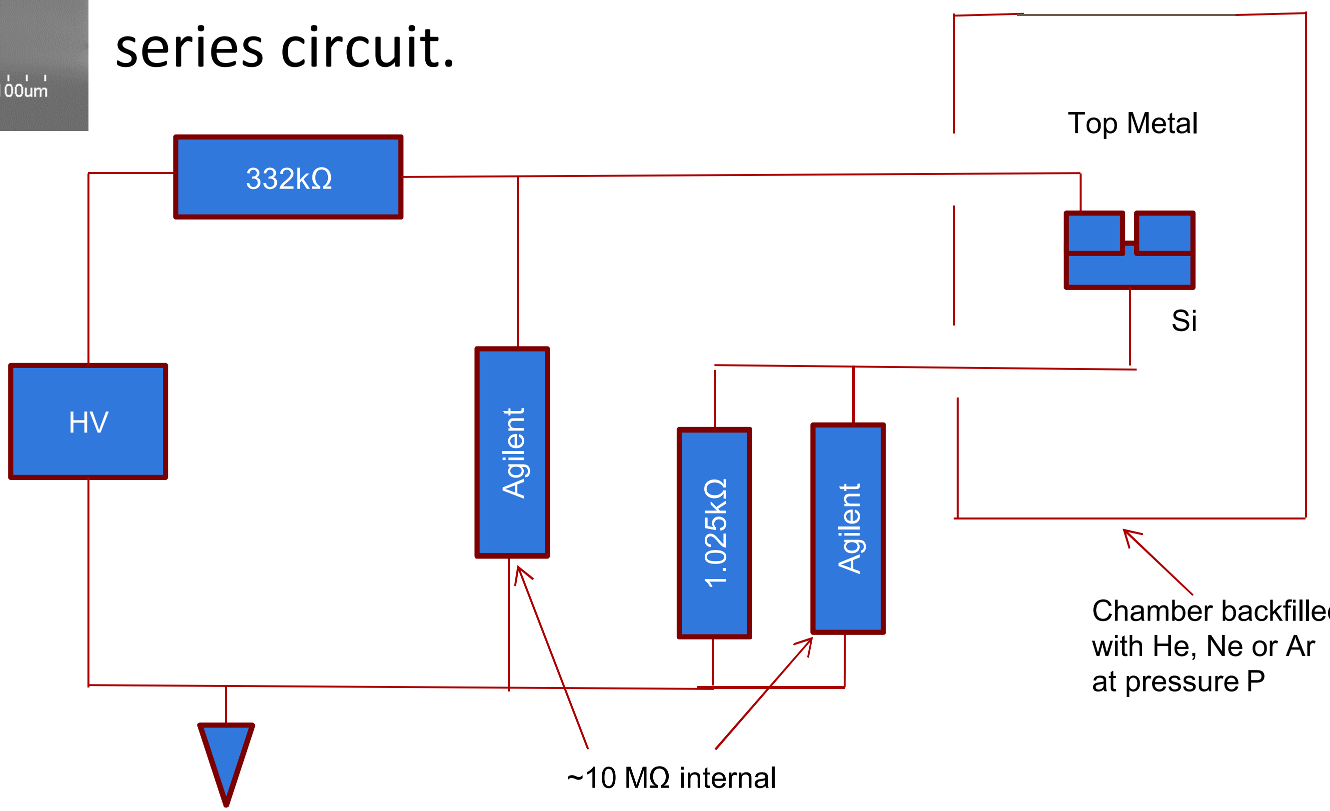
3D Microscale Discharge in 655 Torr Neon



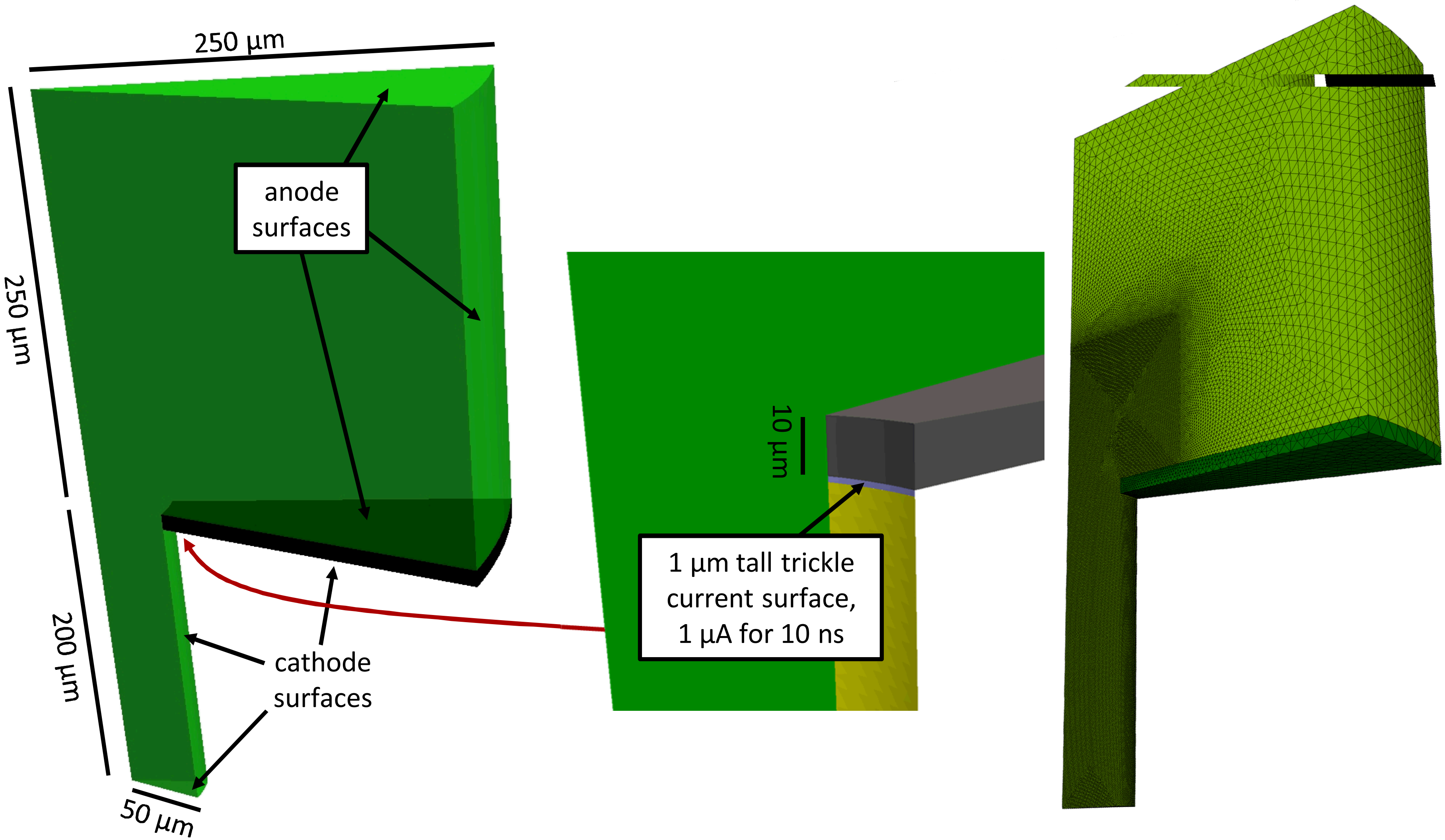
Experiment uses 1-4 cylindrical 50 µm radius cavities (up to 200 µm deep) all connected to the same ballast resistor-in-series circuit.







3D Microscale Discharge in 655 Torr Neon



3D Microscale Discharge in 655 Torr Neon

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Experiment

655 Torr 300 K Ne
332 kΩ resistor-in-series w/circuit elements
50 μm radius, 200 μm depth, 10 μm spacer
1-4 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
50 μm radius, 200 μm depth, 10 μm spacer
Single 3D 20 degree sector
Ionization, excitation, elastic (6 tracked species), from LXCat, www.lxcat.net
ε = 3 10 μm polyimide dielectric w/ surface charging
SEE γ = 0.15 for Ne+

Computational Parameters

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

- $\lambda_D > 1.1$ μm → $\Delta x < 1.1$ um, [Debye length]
- $\lambda_{mfp} > 1.6$ μm → $\Delta x < 1.6$ 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),

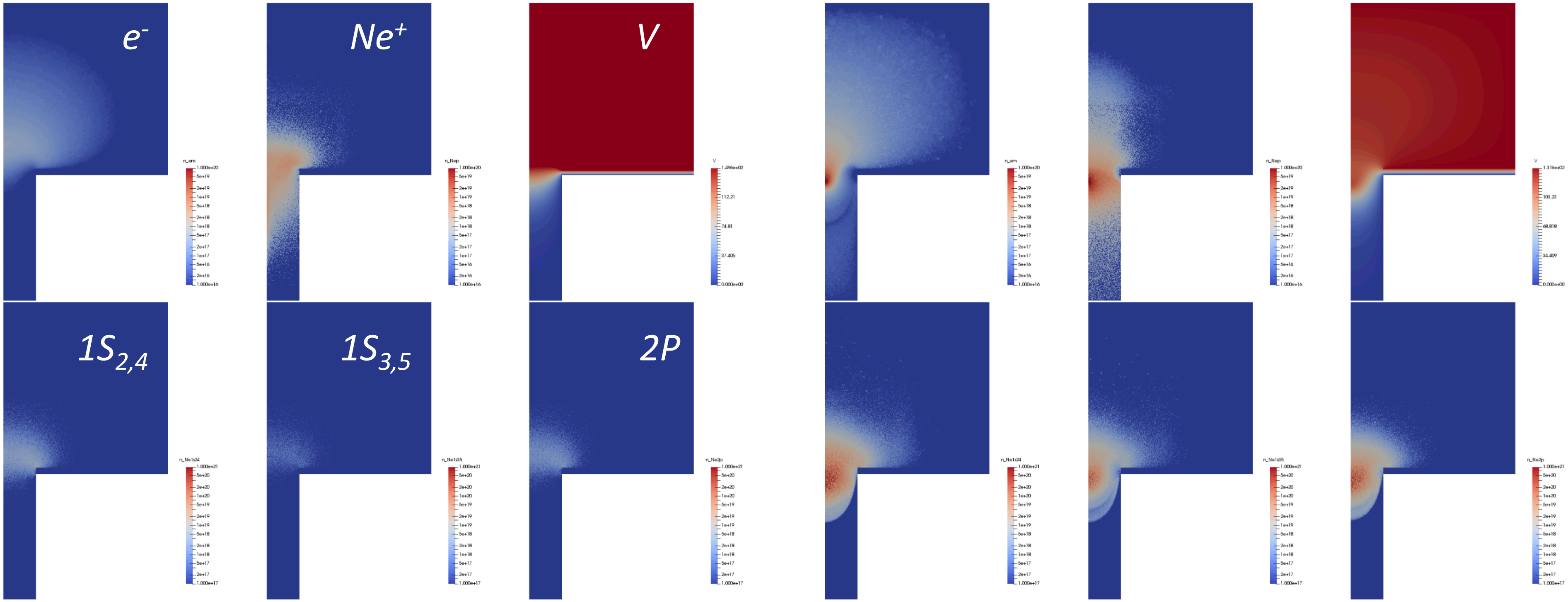
- $\omega_p < 5.6 \times 10^{11}$/s → $\Delta t < 3.5$ ps, [Plasma e- frequency]
- $\Delta t < \Delta x / v_{max}$ → $\Delta t < 100$ fs, [CFL]
- $\Delta t_{collide} < (n_{Ne}\sigma_{max}v_{max})^{-1}$ → $\Delta t < 170$ fs, [Collision frequency]

Use Δt = 50 fs.

3D Microscale Discharge in 655 Torr Neon

Drive voltage = 300 V

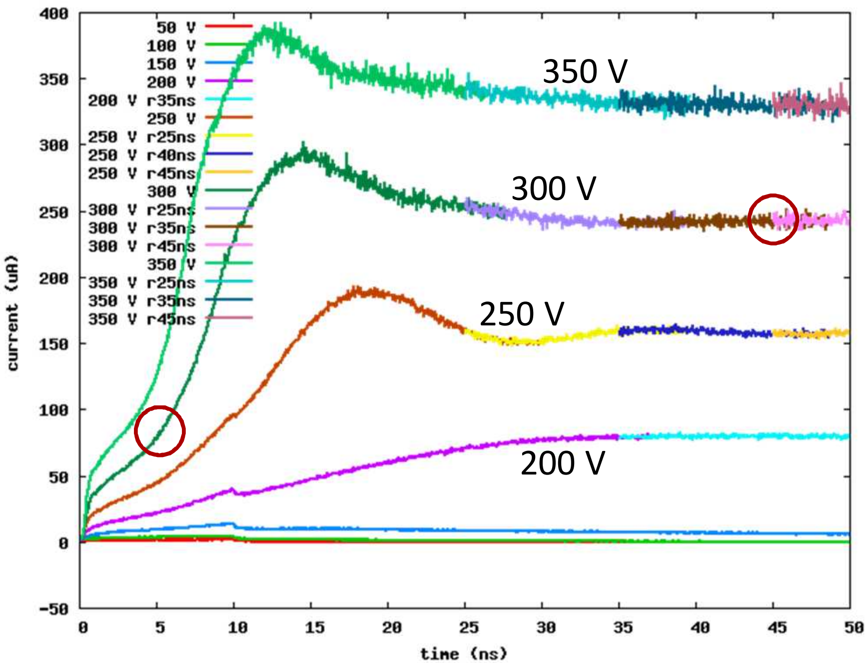
time = 5 ns time = 45 ns

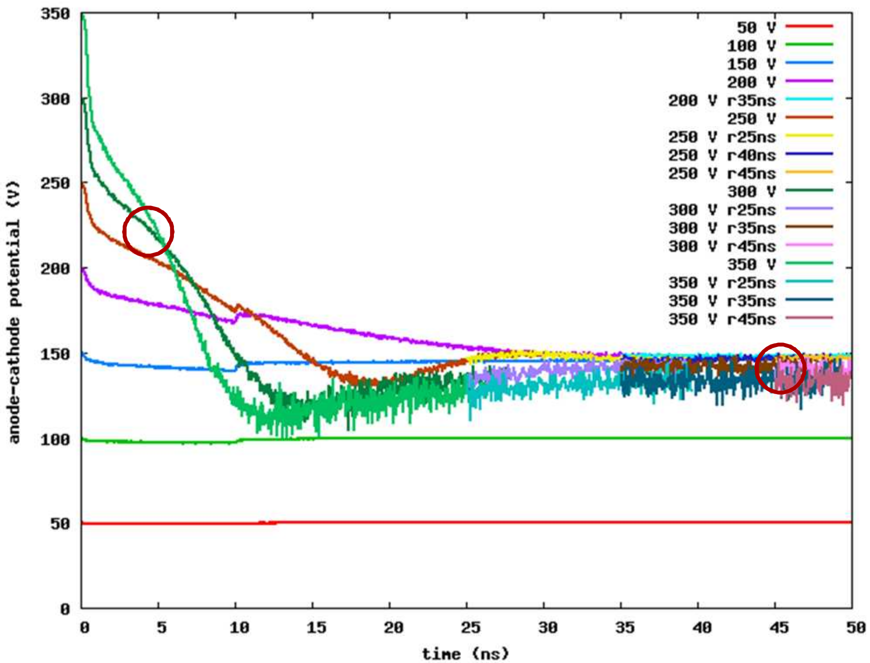


e- and Ne+ scales are $[10^{16}, 10^{18}]/m^3$, excited states are $[10^{17}, 10^{21}]/m^3$, V_{max} ~ 140 V

3D Microscale Discharge in 655 Torr Neon

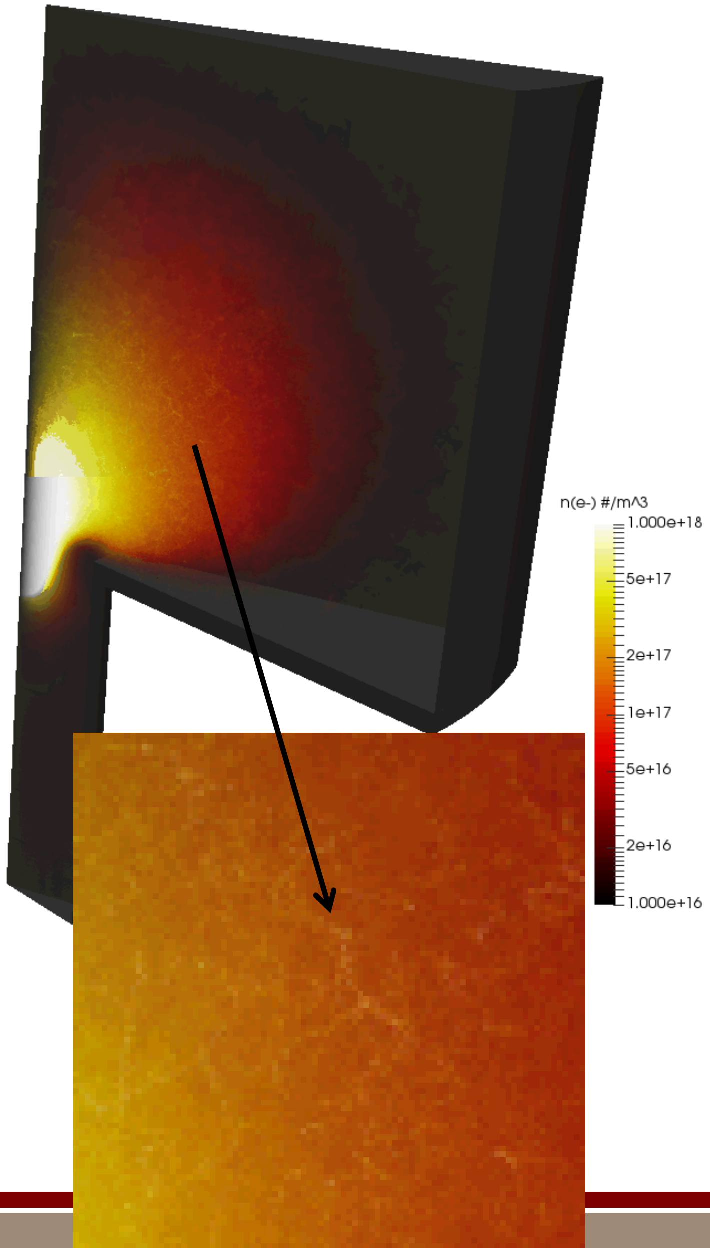
Time-resolved results varying drive voltage over 50-350 V. Breakdown at 200 +/- 50 V. Calibrated Paschen model (*A* = 4.4/Torr/cm, *B* = 111 V/Torr/cm) estimates 210 V.

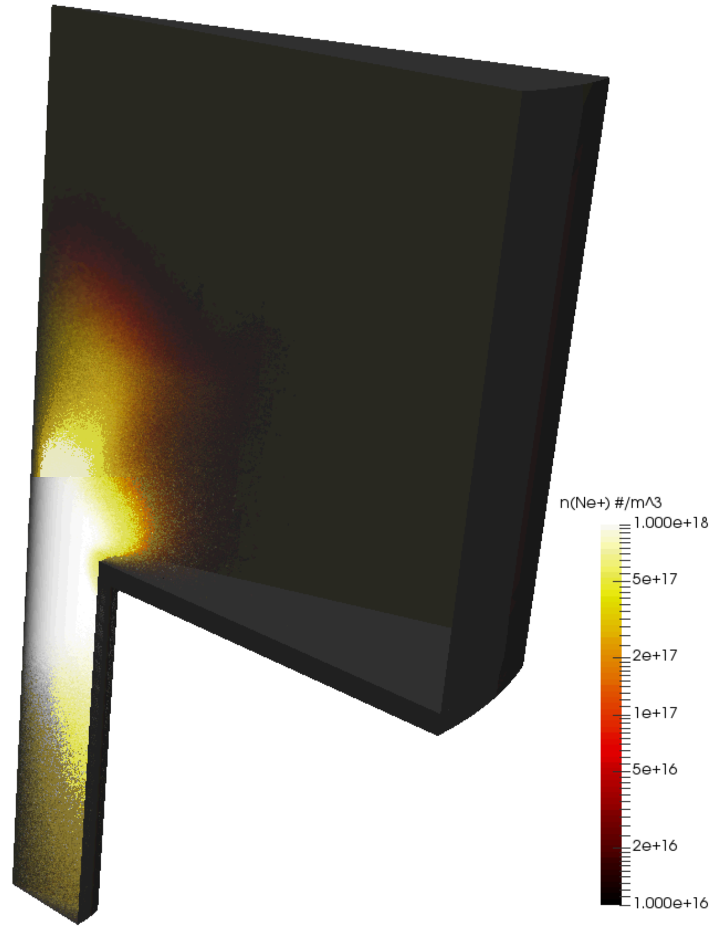




Each simulation is 48 hours on 512 cores. Results required multiple restarts (each different color above is a separate simulation).

3D Microscale Discharge in 655 Torr Neon





3D Microscale Discharge in 655 Torr Neon

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

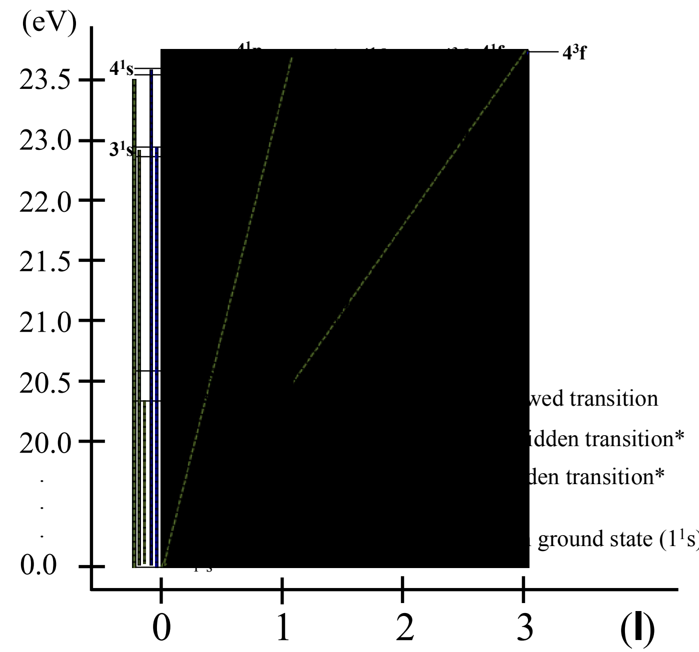
- We are supposedly still a plasma as the plasma number is ~500 (# particles in a Debye sphere).
- One advantage of the tiny particle weight is the exponential multiplicative effect is essentially guaranteed to begin at $t = 0$.
- Circuit noise is also impacted with a lower particle weight.

3D cell volume with Δx = 1 um → volume ~10^{-19} m^3. One particle of weight 1 → $n_e >= 10^{19}/m^3$! Not a problem in < 3D.

1D 1 mm Helium Discharge: Photo-Emission Effect

Model

- 100, 200, 500, 1000 Torr, 300 K He.
- 1 mm gap, variable applied anode voltage.
- Over 50 electron-neutral impact excitation cross sections.
- Tracking of over 25 photon wavelengths including self-absorption mechanisms and photo-emission from the cathode (SEE = 0.1).
- SEE for He+ = 0.01.



Computational Parameters

Dominated by photo-processes

- Spatial Parameters

  $P_{mfp} > 0.4$ µm → $\Delta x < 0.4$ um [Photon absorption MFP]

  Use Δx = ~300 nm

- Time Parameters (**still under investigation**)

  $\Delta t < \Delta x/c$ → $\Delta t < 1$ fs, [CFL]

  $\Delta t_{absorption} < (n_{He}\sigma_{max}c)^{-1}$ → $\Delta t < 0.2$ fs, [Collision frequency]

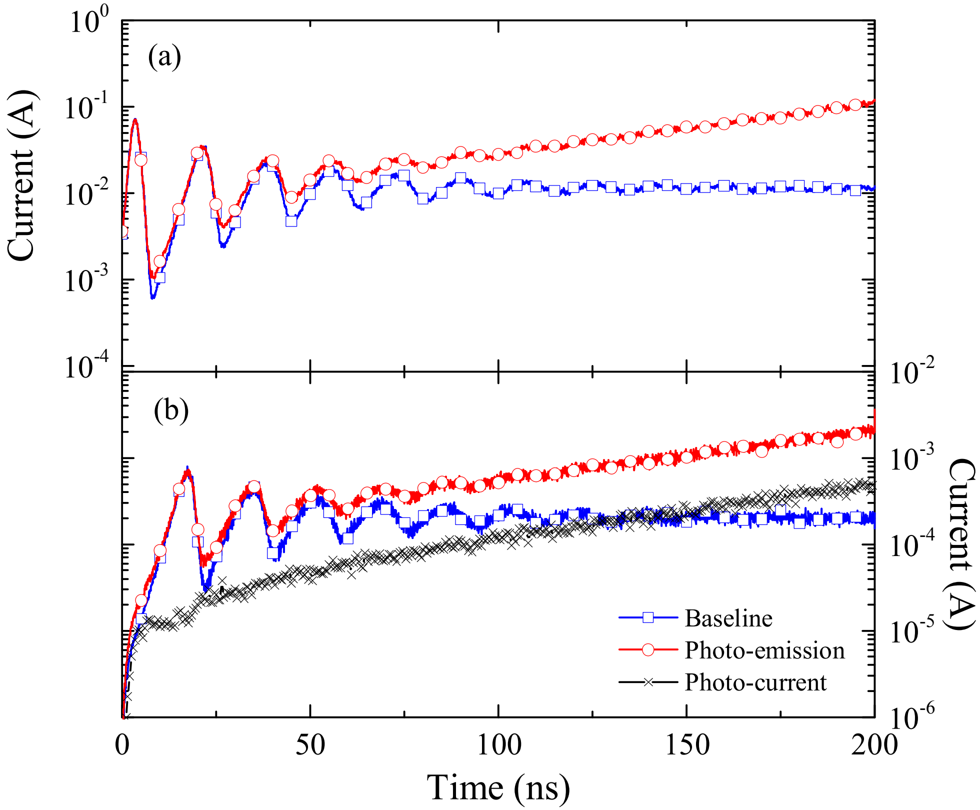
  Currently using Δt = **50 fs**. (how does this affect simulation results)

1D 1 mm Helium Discharge: Photo-Emission Effect

200 Torr comparison with and without photo-emission. *E*/*n* = 55 Td

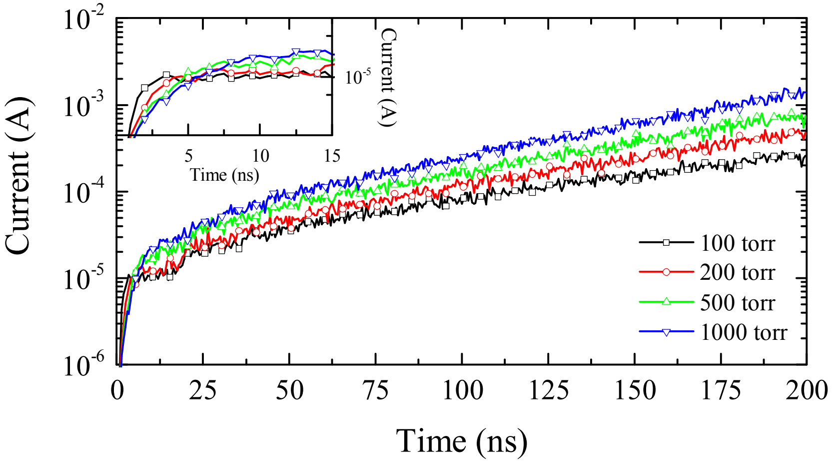
(a) electron current into anode

(b) electron current from cathode



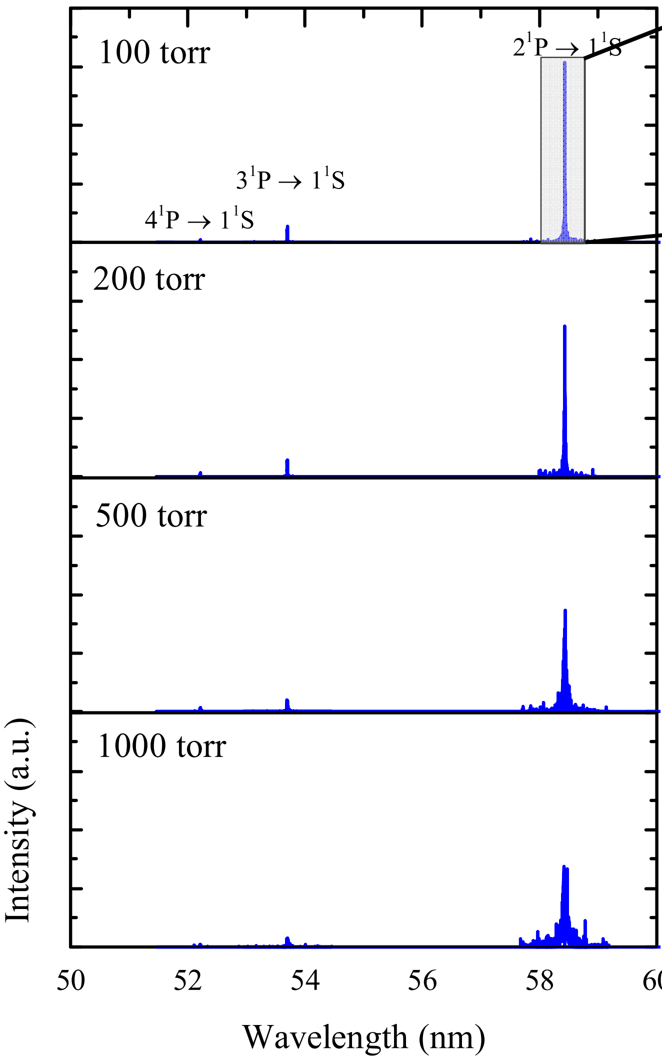
Left: Photo-current accounts for nearly 20% of the total current originating from the cathode as t → 200 ns.

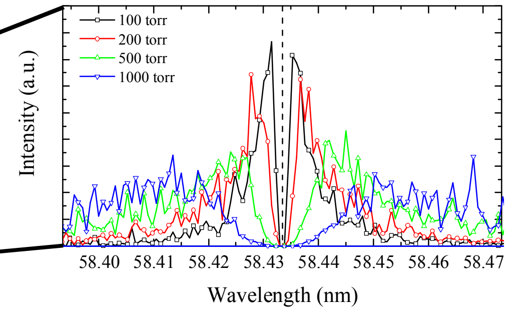
Below: At higher pressures, the magnitude of photo-current increases although still 20% of the cathode electron current.



Observed photo-current at various pressures. *E*/*n* was set to result in steady-state without photo-current.

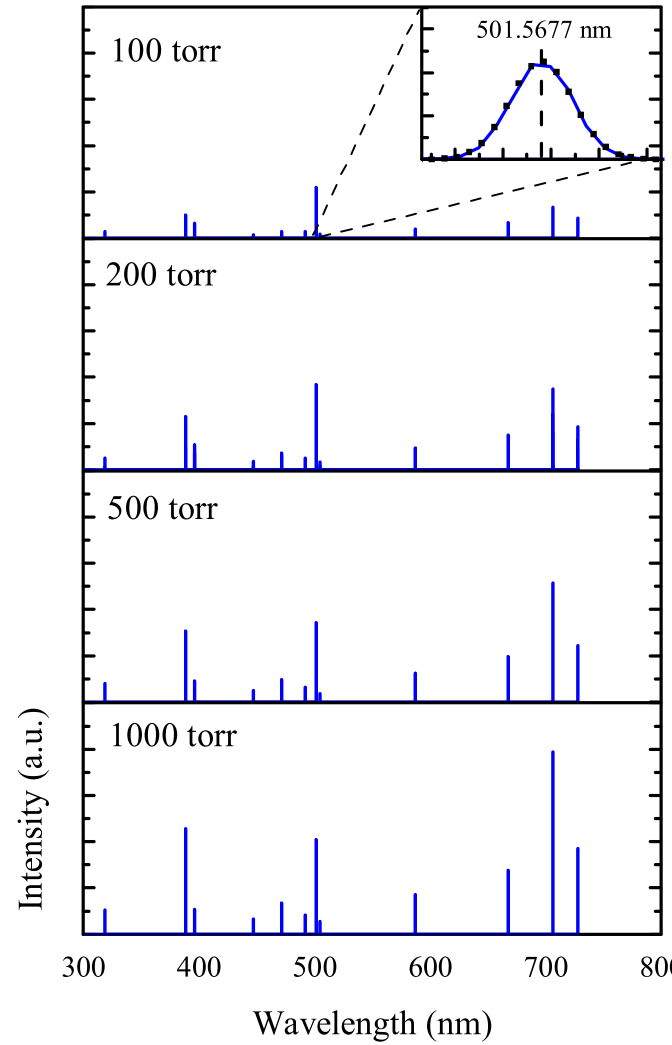
1D 1 mm Helium Discharge: Photo-Emission Effect





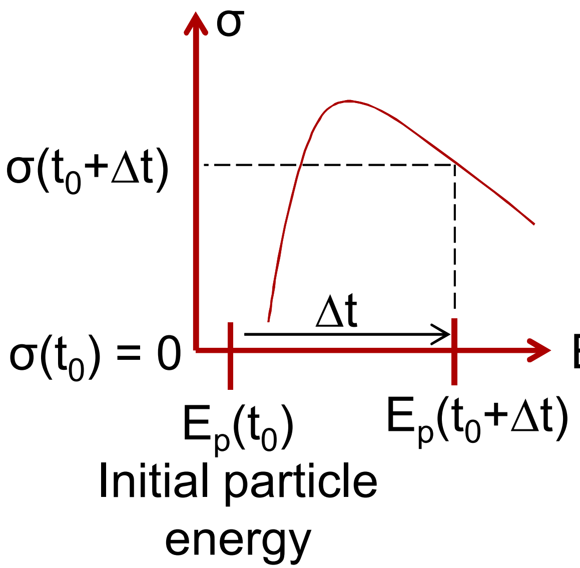
Left and middle: VUV Emission spectra taken at *t* = 50 ns integrated over 10 ns. Zoomed in image shows the strong self-absorption profile of these transitions.

Right: VIS Emission spectra taken at *t* = 50 ns integrated over 10 ns. Inset graph shows theoretical Voigt emission profile.



Cross-section Energy Accuracy

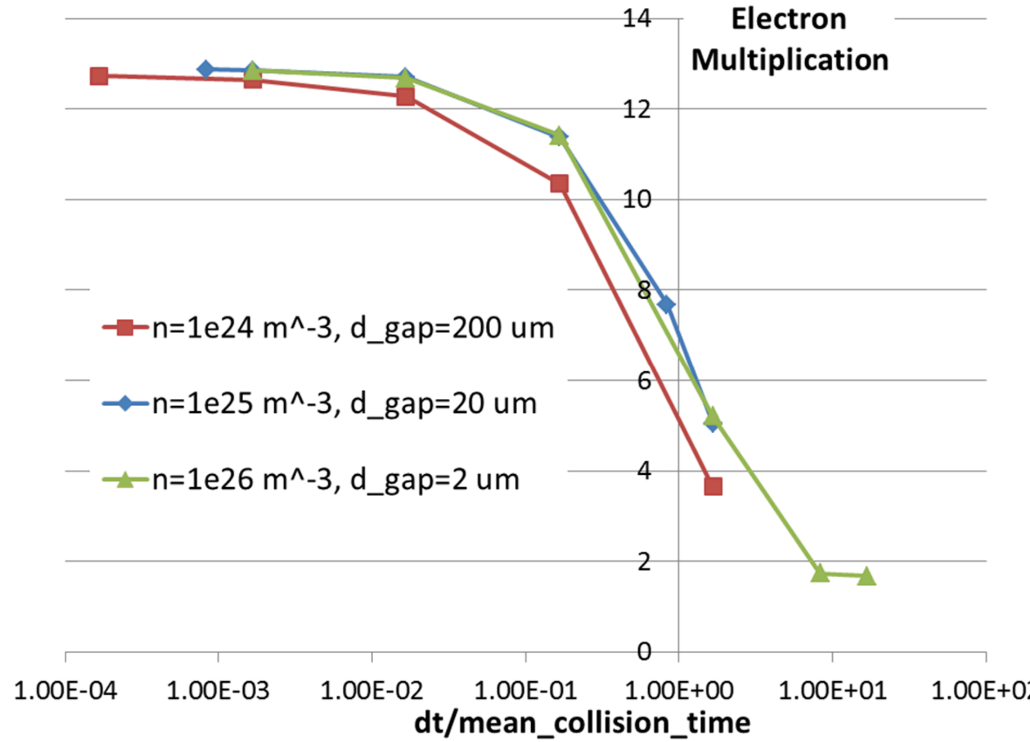
- Charged particles gain/loose energy over the time step.
  - Can have significant cross section changes over *Δt* due to energy change → Local collision rate can change dramatically during *Δt.*



- For an avalanche across a fixed potential drop (e.g. in the cathode fall) the e^- gains energy and finite *Δt* results in error for the effective collision rate across the drop.
  - Accurate simulation requires *Δt* resolve changes in the cross sections.
- Error source due to time step size that is not related to resolving the collision rate (or particle CFL).
  - Still converges with *Δt*. This is just an additional limit on *Δt* for accuracy.

Cross-section Energy Accuracy

- Examine electron multiplication across gap versus time step size.
  - Space charge ignored when solving for E-field → Plasma frequency not meaningful timestep constraint.



- Vary density (collision rate) and hold *E*/*n* fixed.
  - Neutral collisional simulations exhibit convergence at $\Delta t \sim \nu^{-1}$
  - Error in ionization efficiency results in significant error in steady state plasma density if $\Delta t = 0.5 \times \nu^{-1}$ is used.
  - Charged particle electron avalanche exhibits convergence at $\Delta t \sim \frac{\nu^{-1}}{100}$.

6th International Workshop on Mechanisms of Vacuum Arcs