SAND2017-5062C

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Three-dimensional Wedge Simulation of an Ionization Wave in Nitrogen/Helium Gas

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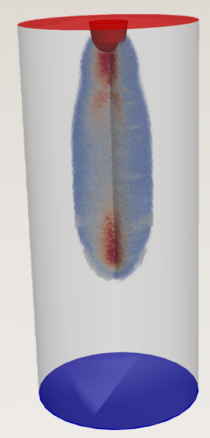
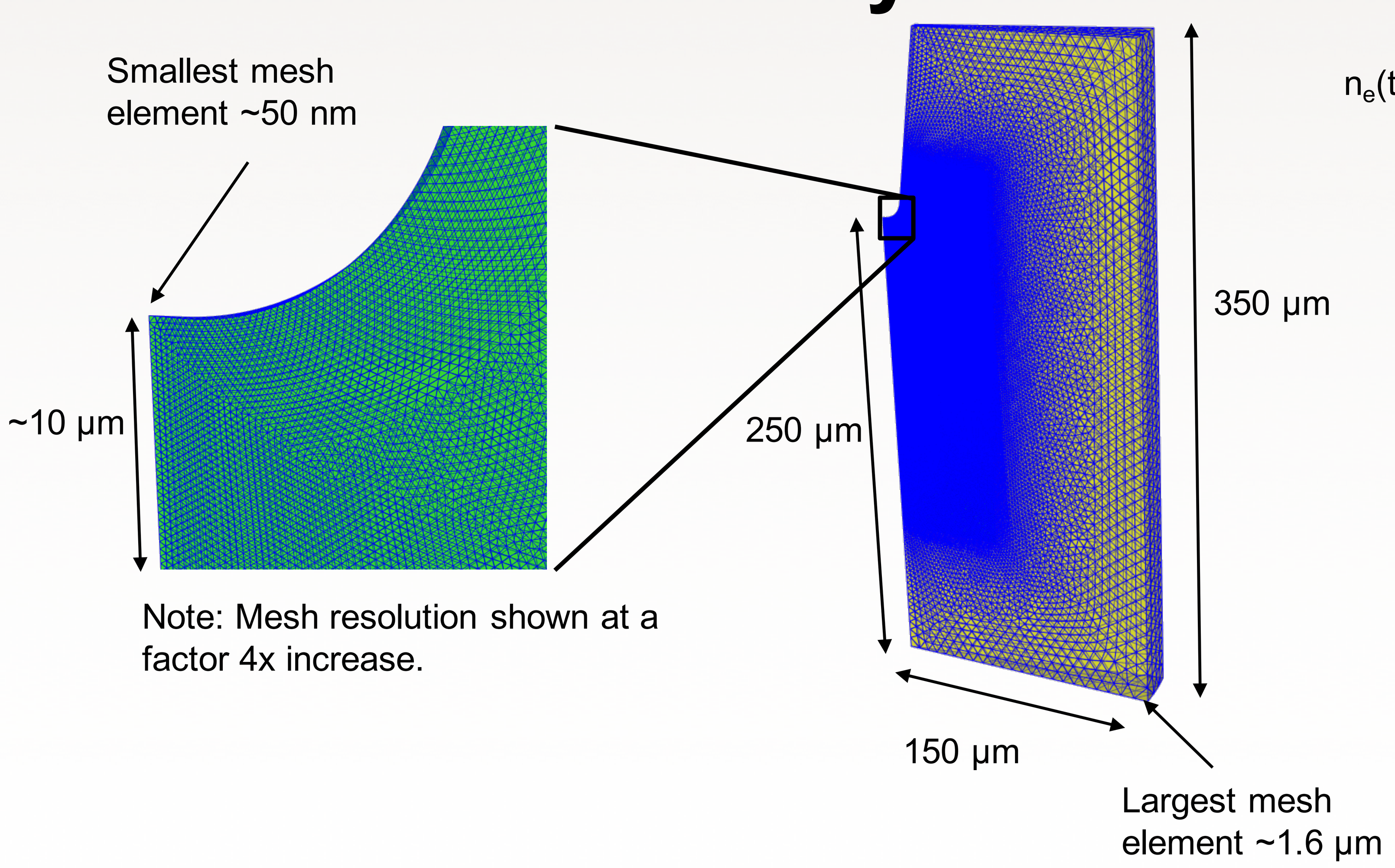
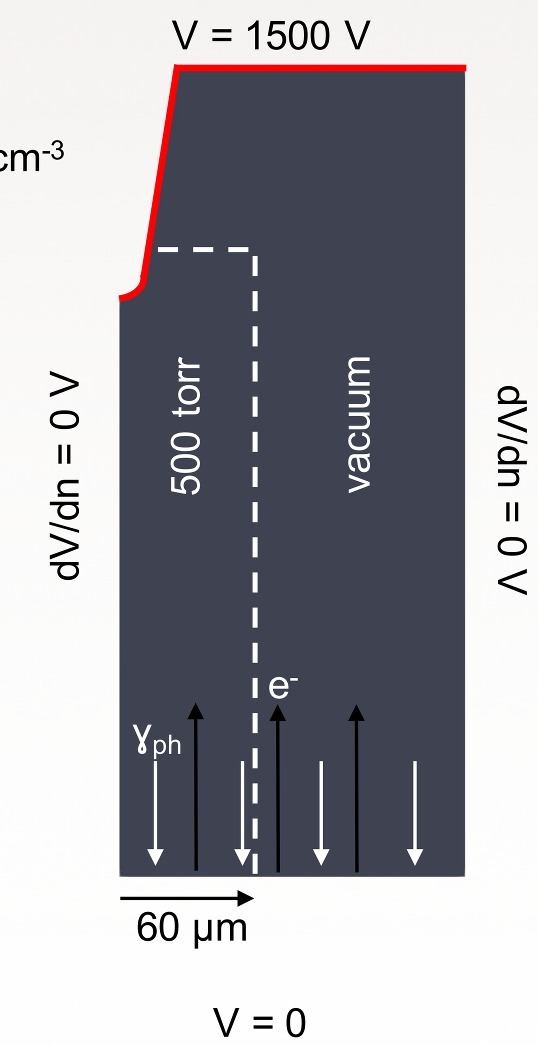
Abstract



Three-dimensional simulations of pulsed plasma formation in non-equilibrium conditions still represents a significant challenge even for modern supercomputers. The high-resolution time and length scales required to accurately simulate near-atmospheric pressure ionization waves or streamers are on the order of femtosecond and tens of nanometers, respectively. To alleviate some of the most demanding computational requirements, only a 10 degree wedge of a needle-plane gap with a 250 micron gap distance is simulated. Regardless, this results in nearly 200 million mesh elements while simultaneously tracking hundreds of millions of computational particles. Simulation time is on the order of many days on 5000 processing cores executed on the Sky Bridge supercomputer at Sandia National Laboratories. Here, a state-of-the-art best effort three-dimensional simulation in nitrogen with a helium gas admixture is presented. Helium gas exhibits strong emission in the extreme ultraviolet (EUV) regime that is capable of direct photoionization of the nitrogen molecule. Recent developments in the advanced particle code, Aleph, have allowed for the discrete tracking of photons that can interact with other particles in the simulation domain [1-3]. As a result, a quantitative study of the role of photoionization in a nitrogen/helium gas discharge is performed by comparing the discharge behavior across varying helium concentrations.

Mesh and Boundary Conditions





Numerical Parameters

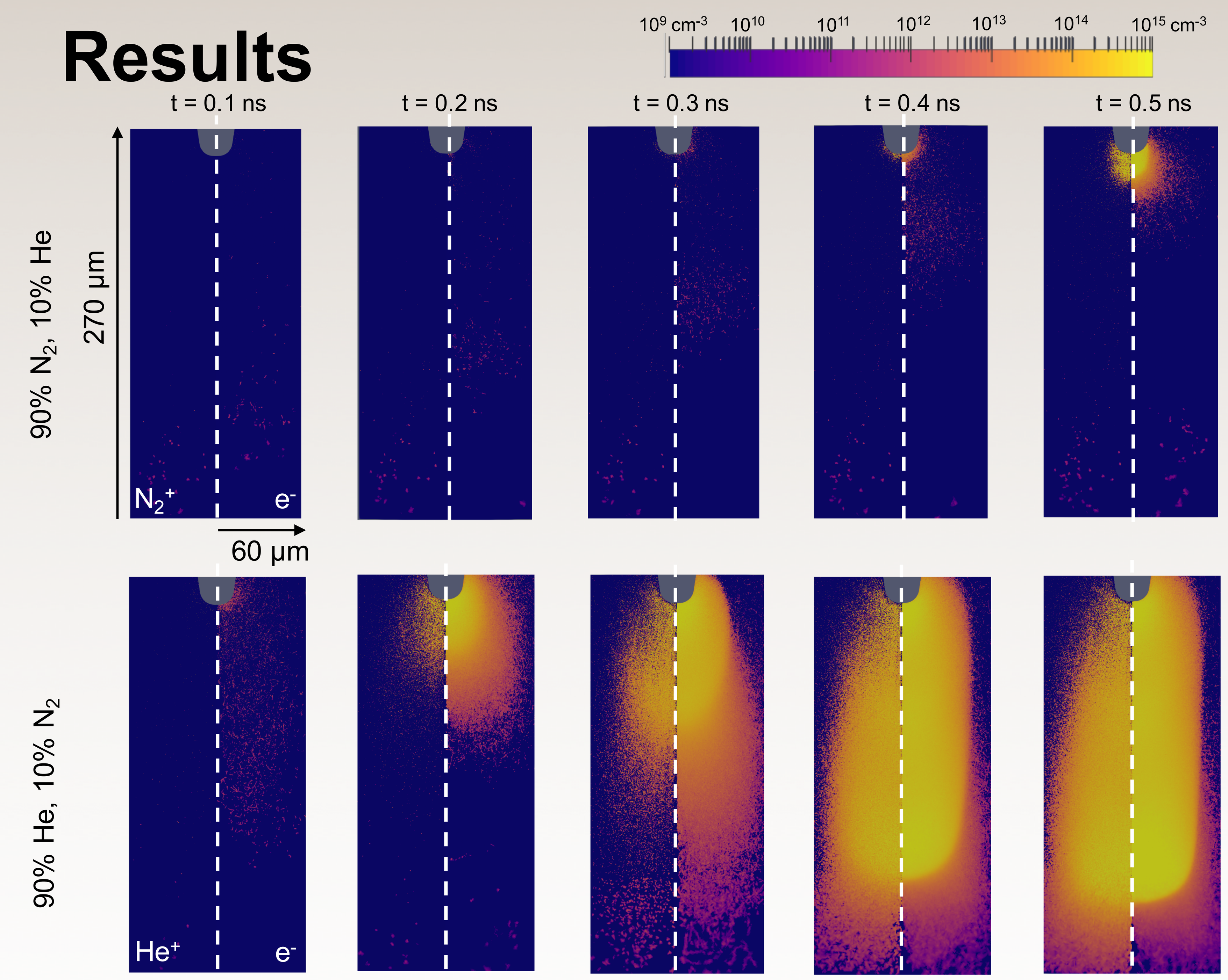
Anticipated electron densities are on the order of 10^{15} cm^{-3} with a temperature of 0.5 eV. The Debye length for electrons and photon CFL condition set the maximum Δx and Δt. Mesh grading is chosen to limit the number of elements in the simulation volume. Choose:

- Δx ~ 50 nm near needle tip and increase smoothly to ~350 nm at a location 70 µm above the cathode.
- Δt = 2 x 10^{-15} s which easily resolves electron dynamics but approaches the limit for photons.

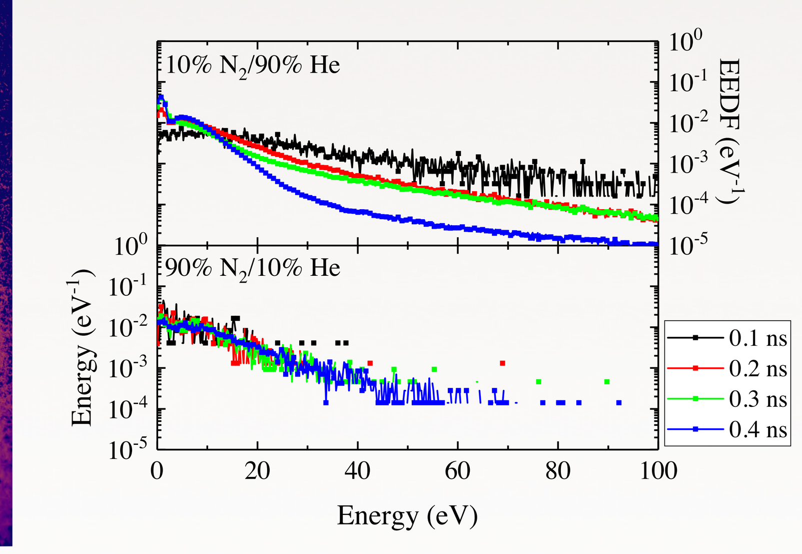
Expected plasma parameters that define the computational requirements.

Parameter	Spatial or Time Scale
Debye Length - λ_D	~150 nm
Electron Mean Free Path - λ_{mfp}	~200 nm
Photon Mean Free Path - γ_{mfp}	~25 µm
Inverse plasma frequency - $(\omega_{pe})^{-1}$	~1 x 10^{-13} s
Inverse collision frequency - $(\nu_c)^{-1}$	~300 x 10^{-12} s
Electron CFL @ 5 x 10^6 m/s	~1 x 10^{-13} s
Photon CFL	1-2 x 10^{-15} s
Charged particles per element (Np/Nx)	50

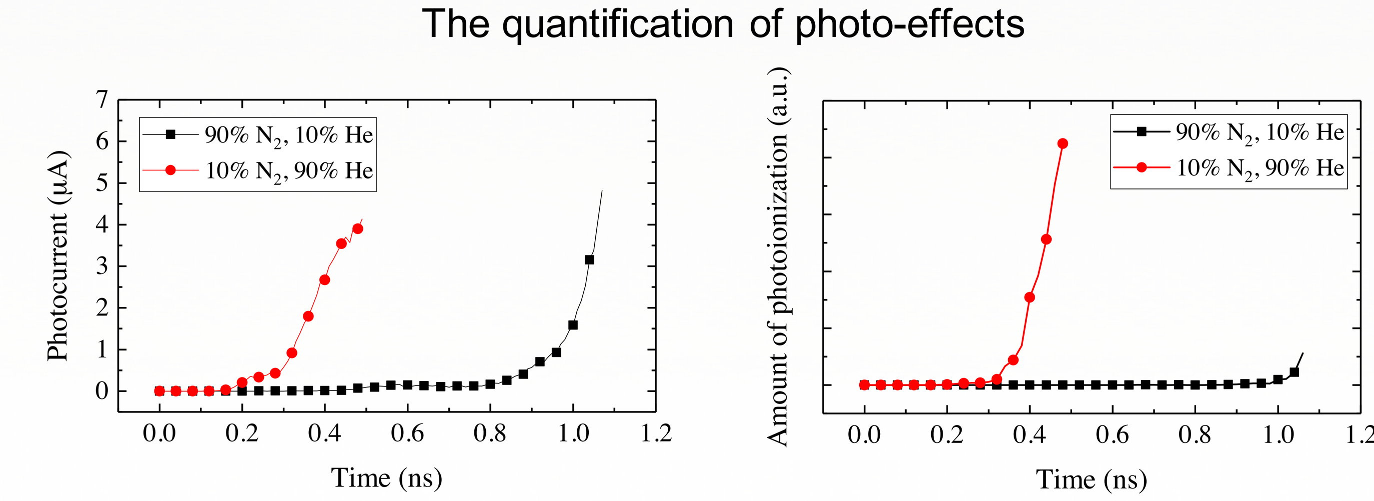
Results



EEDF over entire domain



The quantification of photo-effects



90% N_2, 10% He:

- Plasma formation stalls around 0.6 ns as the initially seeded electrons are swept away towards the needle tip.
- Subsequent photoemission from the cathode allows the ionization wave to progress.

10% N_2, 90% He:

- The decrease in nitrogen density, and thus less energy loss to vibrational or rotational modes, allows for a distribution of electrons with increasing energy.

Conclusions

- Computational requirements were eased by only simulating a small angle wedge of the entire 3D domain, gradual grading of the mesh from the high field region towards the cathode, and limiting the region of space where computational particles exist (far boundaries are used only for electrostatic boundary conditions). Still requires over 5000 processing cores for many days.
- Discharge in mostly nitrogen requires longer time to develop as opposed to a discharge in mostly helium.
- Comparison of photo-effects reveals that there is indeed more photoionization and photoemission occurring in the mostly helium discharge, although it is currently unclear if it is merely due to the higher electron density at these times.

References

[1] C. Moore, H. Hjalmarson, L. Biedermann, K. Williamson, P. Schultz, R. Jorgenson, “Development and Validation of PIC/DSMC Air Breakdown Model in the Presence of Dielectric Particles,” Pulsed Power Conference, May 31 – June 4, Austin, TX, 2015.

[2] A. Fierro, J. Stephens, S. Beeson, J. Dickens, A. Neuber, “Discrete Photon Implementation for Plasma Simulations,” Physics of Plasmas, 23, 013506, 2016.

[3] A. Fierro, C. Moore, B. Scheiner, B. Yee, M. Hopkins, “Radiation Transport in Kinetic Simulations and the Influence of Photo-emission on Electron Current in Self-Sustaining Discharges,” Journal of Physics D: Applied Physics, vol. 50, 065202, 2017.

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