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Developing a kinetic approach to radiation transport and its interaction in He/N_2 ionization waves

Andrew Fierro, Ed Barnat, Chris Moore, Matthew Hopkins
Sandia National Laboratories, Albuquerque NM

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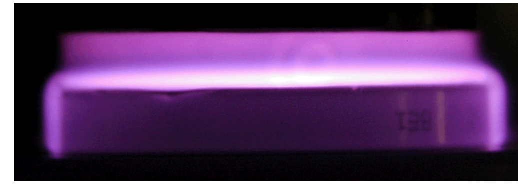
Motivation

- Interested in transient response times of plasma formation as well as steady quantities which may be sensitive to photonic processes.

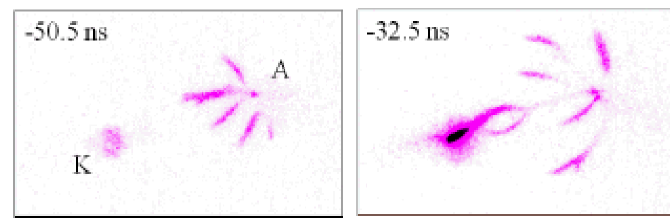
- Light emission is one of the defining characteristics of plasma discharges. Another tool to make comparisons to experiments for validation purposes.

- Would like to begin to quantify the effect of self-produced radiation on plasma development and its secondary effects.

- Develop a method to discretely model photons in a kinetic code that allows for the incorporation of energy dependent photo-processes.



- Pulsed helium discharge operating at 30 torr (A. Fierro, E. Barnat)

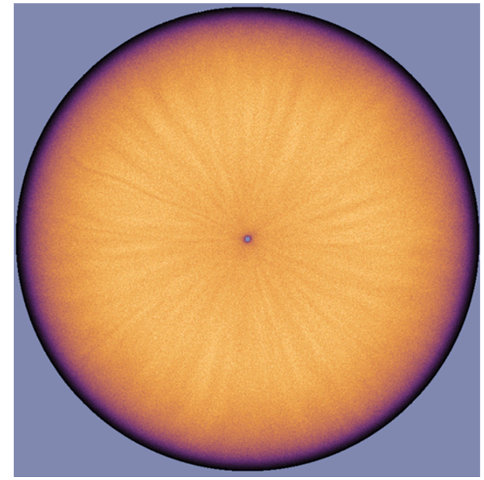


- Fast-gated imaging of streamer propagation.

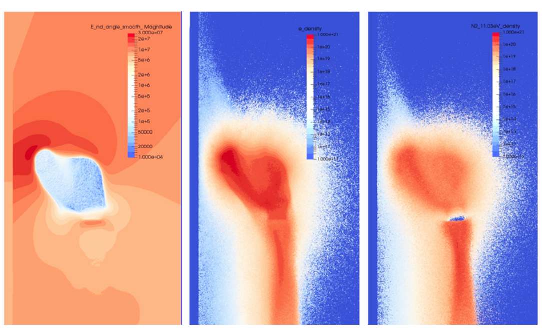
A. Fierro, *et al.*, J. Phys. D: Appl. Phys., 2012.
A. Fierro, *et al.*, Plasma Sources Sci. Technol., 2017, to be submitted.

The Kinetic Code - *Aleph*

- Unstructured FEM (compatible with CAD)
- Massively parallel (scales up to 100k proc.)
- Hybrid PIC + DSMC, also PIC-MCC
- Electrostatics with fixed B Field
- Advanced surface (electrode) models
- Collisions, charge exchange, chemistry, excited states, ionization
- Photon transport, photoemission, photoionization
- Advanced particle weighting methods
- Dynamic load balancing restart (with all particles)



- 2D simulation of a Langmuir probe in the electron saturation regime demonstrating unexpected streaming instabilities (B. Yee).



- Simulation of streamer formation along a dielectric surface (C. Moore).

Radiation Transport Method

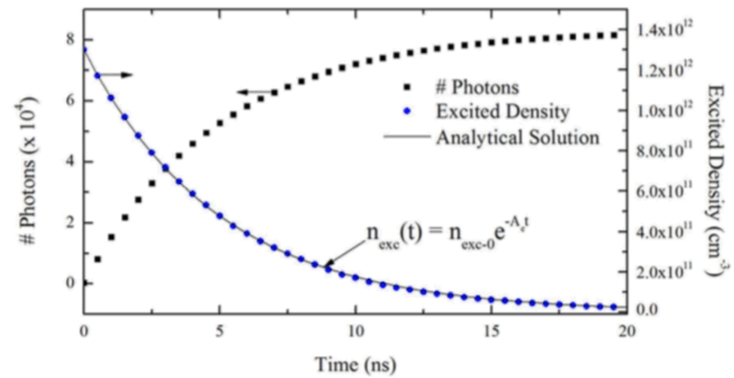
- **$e^- + A \rightarrow A^* + e^-$**
  - **leads to an accumulation of A^***
- **for each A^* evaluate:**
  - **$R < 1 - e^{-t/\tau}$, τ = lifetime of A^***
- **If evaluated to be true**
  - **$A^* \rightarrow A + h\nu$**
  - **$|v_{ph}| = c$, v_{ph} = isotropic**
  - **$\lambda_{ph} = hc / (E(A^*) - E(A))$**
    - **Lorentz shape**

$$\lambda_s = \tan[(R - 0.5)\pi] \cdot \Delta\lambda_r + \lambda_0$$

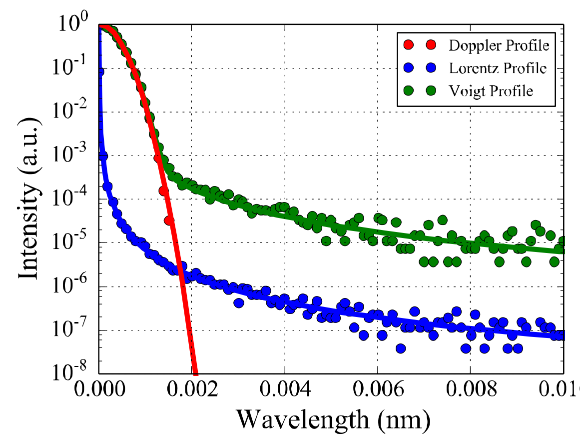
    - **Doppler shape**

$$\lambda_f = \frac{(c + \hat{v}_{ph} \cdot v_p)\lambda_c}{c}$$

- **Each photon is pushed through the computational domain and interactions are handled with traditional DSMC procedures.**



- **Verification of the method.**

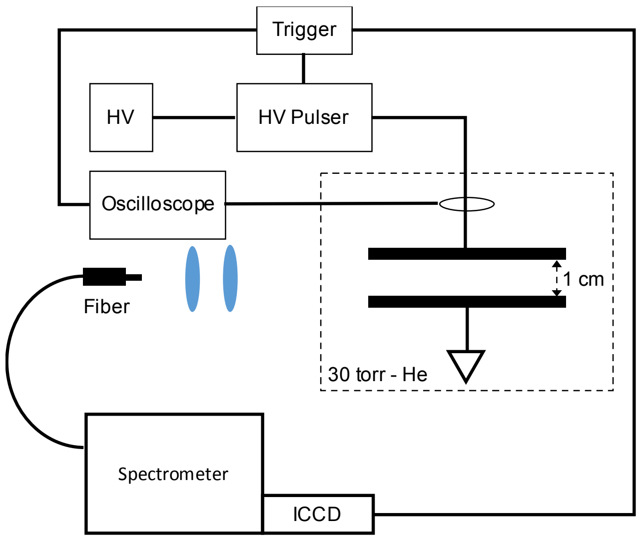


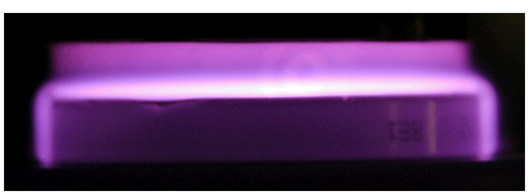
- **Simulated line profiles.**

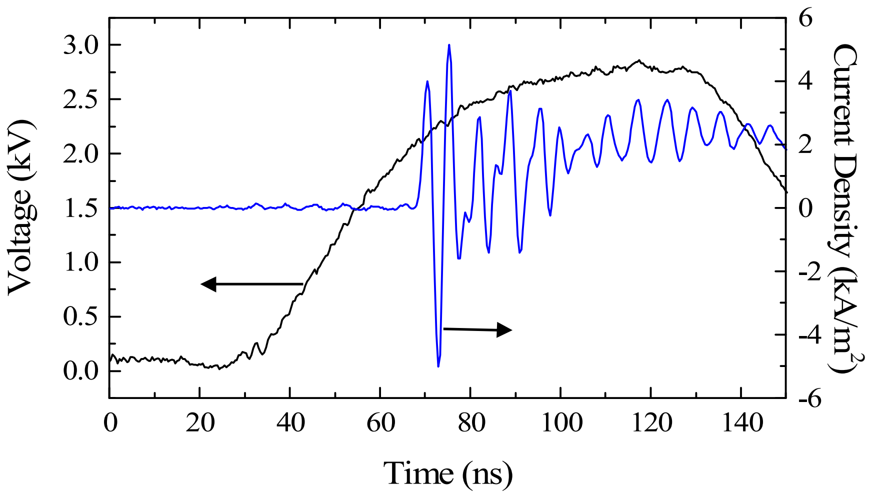
A. Fierro, *et al.*, Phys. Plasmas, 2016.
A. Fierro, *et al.*, Phys. Plasmas, 2014.

Towards Validation

- **With this method, we are able to generate spatially-resolved line emission spectra that does not assume LTE.**
  - **Can we begin to use emission spectra as a viable validation tool?**



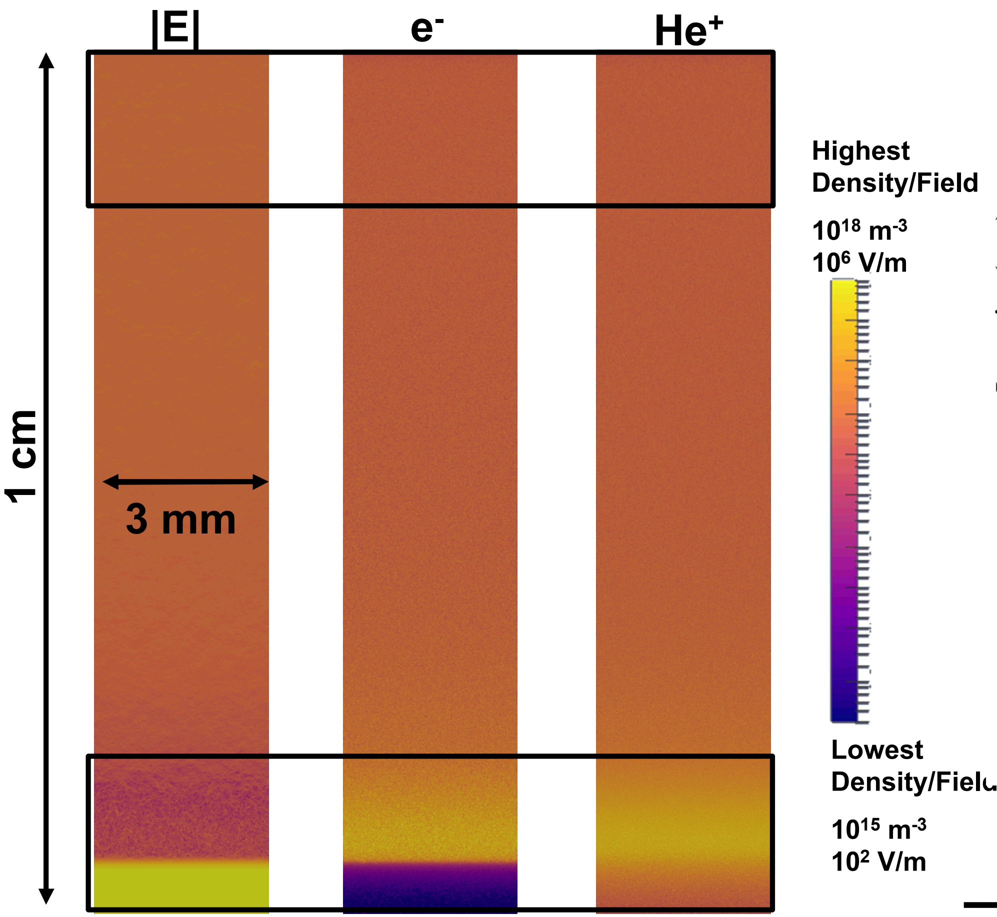


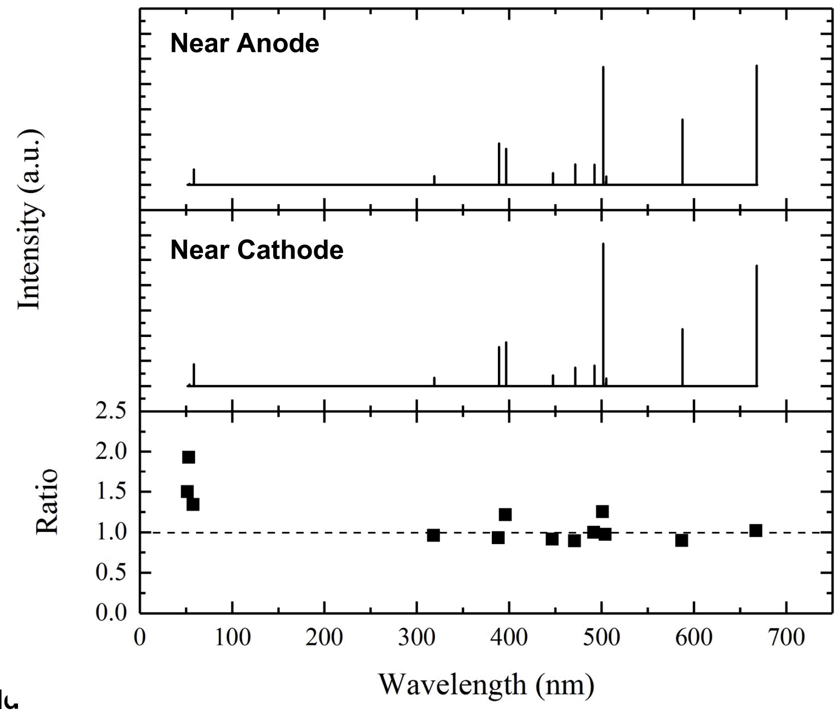


- **Experimental setup focused on capturing time-resolved optical emission spectroscopy in the visible regime.**

Towards Validation

- **With this method, we are able to generate spatially-resolved line emission spectra that does not assume LTE.**

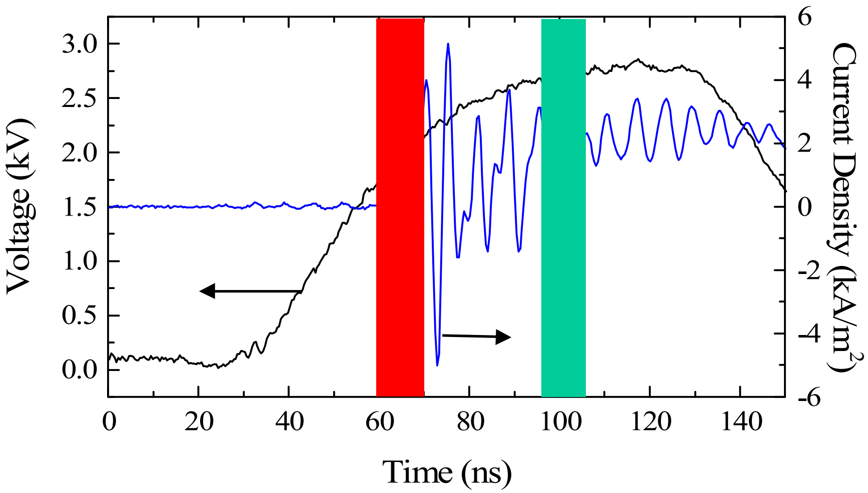


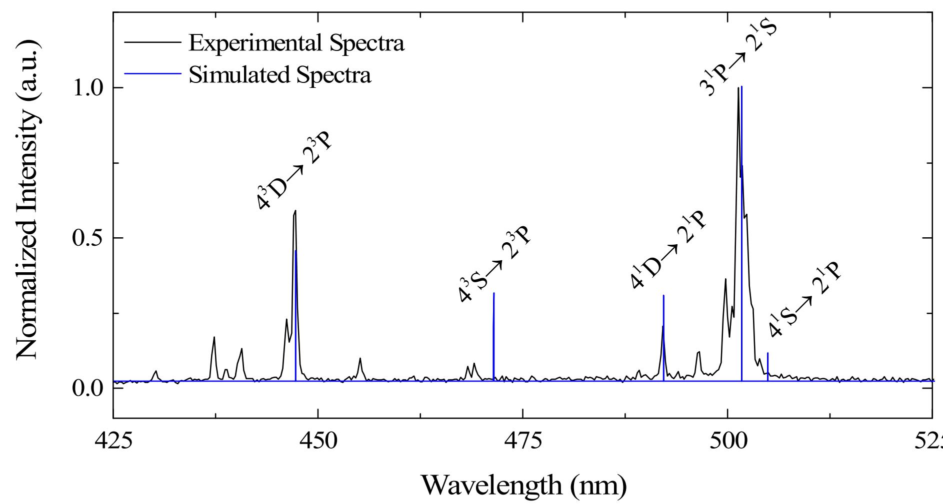


- **Log contour plots from a simulation of pulsed plate-plate discharge, t = 60ns**

Towards Validation

- **Initial comparisons to experimental data**
  - **10 ns camera gate, timing indicated by green window.**
  - **Simulation spectra taken at t = 60 ns**
  - **Working on time correlation between experiment and simulation**





- **The simulation produces realistic line ratios for the He lines shown.**
- **Assume pure He gas, no impurities are included.**

Application to Large Scale Simulations

- **How do photonic mechanisms impact near atmospheric pressure discharges? The goal is to simulate a three-dimensional system of a pulsed, near atmospheric pressure discharge.**
  - **How big of a system is capable of being simulated in *reasonable* time.**
  - **What assumptions can be made to alleviate computational requirements?**
  - **What are the numerical challenges (timestep, space step)?**
  - **What are the computational resource challenges (memory, processors)?**

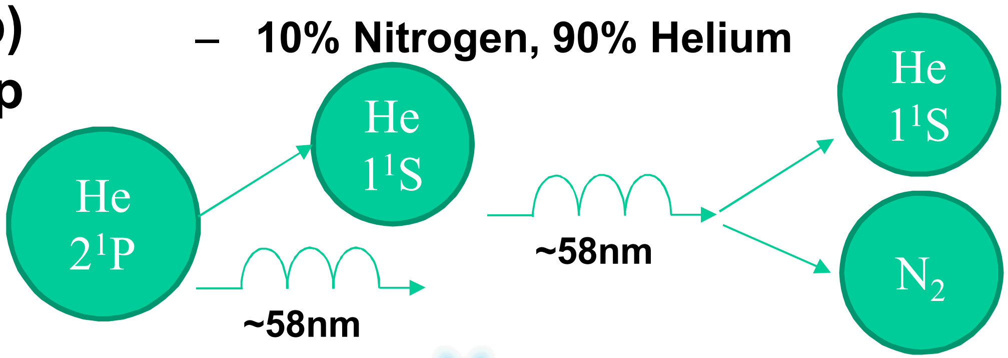
- **Simulations at higher pressures are extremely challenging due to the anticipated large electron densities. This results in a smaller mesh to resolve Debye lengths and avoid numerical heating.**

Ionization Wave Simulation

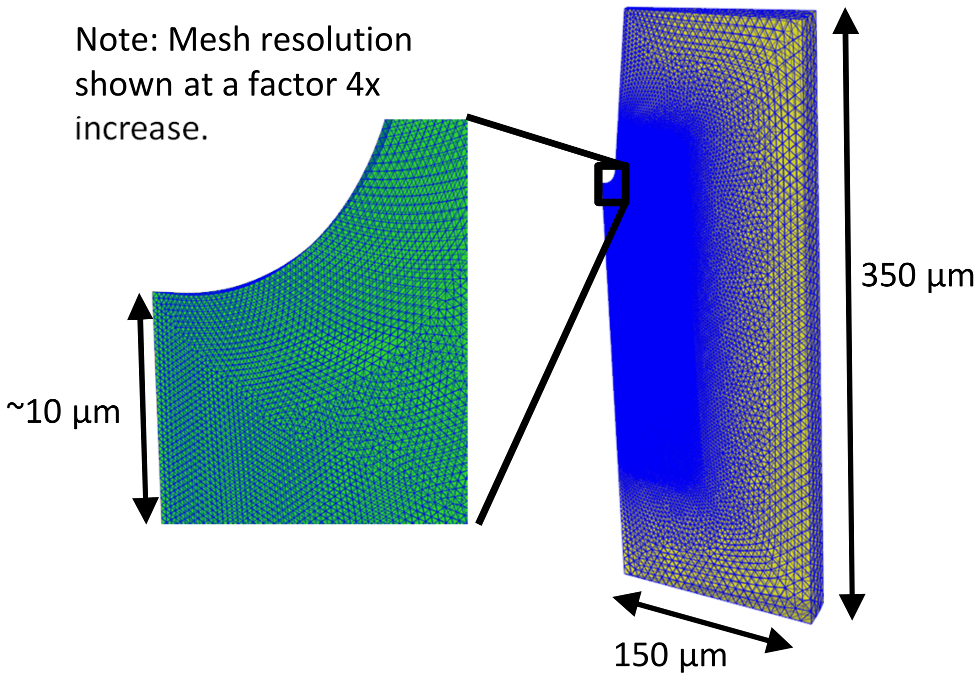
- **Numerical parameters are guided by experiments of similar type discharges**
  - **500 torr background pressure**
  - **10^{15} cm^{-3} electron density**
  - **0.5 eV electron temperature**
- **Debye length and Photon CFL conditions (photon does not cross more than 1 element in a time step) set the minimum time step and spatial step.**
  - **dx = 50 nm**
  - **dt = 2 x 10^{-15} s**

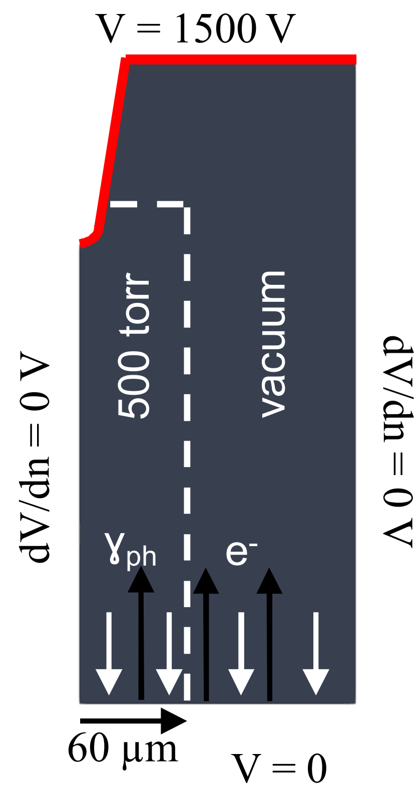
Parameter	Spatial or Time Scale
Debye Length - λ_D	**~150 nm**
Electron Mean Free Path - λ_{mfp}	~200 nm
Photon Mean Free Path - γ_{mfp}	~25 μm
Inverse plasma frequency - $(\omega_{pe})^{-1}$	~1 x 10^{-13} s
Inverse collision frequency - $(\nu_c)^{-1}$	~5 x 10^{-13} s
Electron CFL @ 5 x 10^6 m/s	~1 x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

- **Compare 2 different cases:**
  - **90% Nitrogen, 10% Helium**
  - **10% Nitrogen, 90% Helium**



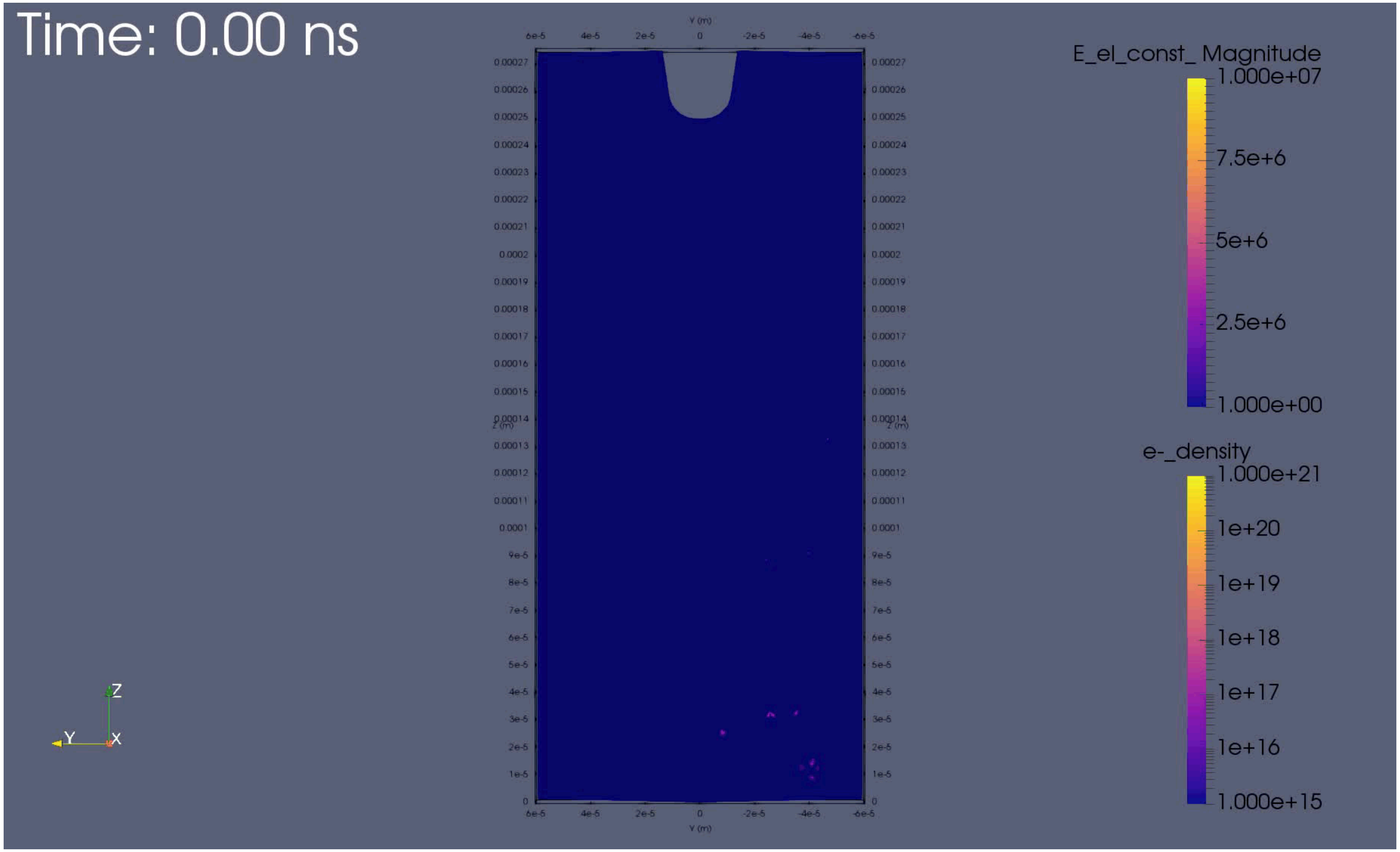
Simulation Setup



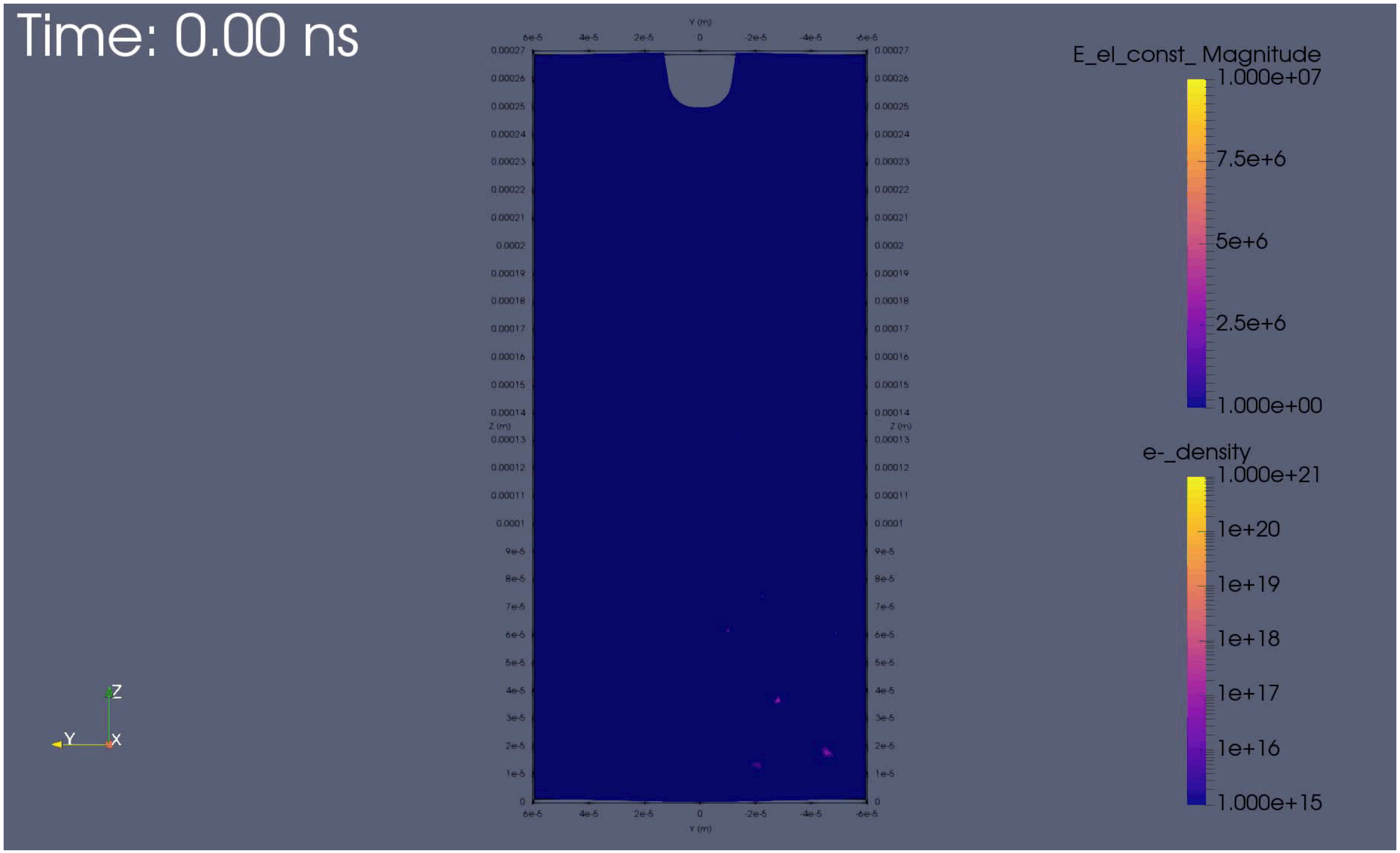


- **~170 million elements for only a 10 degree wedge.**
- **To ease particle requirements, for r > 60 um, we assume vacuum. Executed on 5120 cores on the Skybridge super computer.**
- **In summary, this is a very challenging simulation for even modern computers and numerical techniques.**

90% N_2, 10% He


Time: 0.00 ns
Y (m)
Z (m)
E_el_const_ Magnitude
1.000e+07
7.5e+6
5e+6
2.5e+6
1.000e+00
e-_density
1.000e+21
1e+20
1e+19
1e+18
1e+17
1e+16
1.000e+15

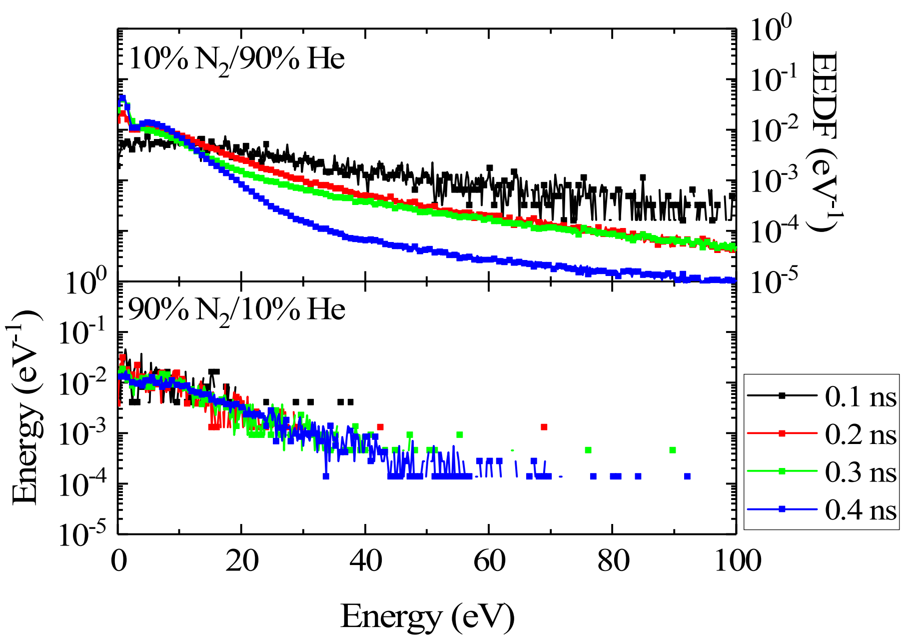
10% N_2, 90% He



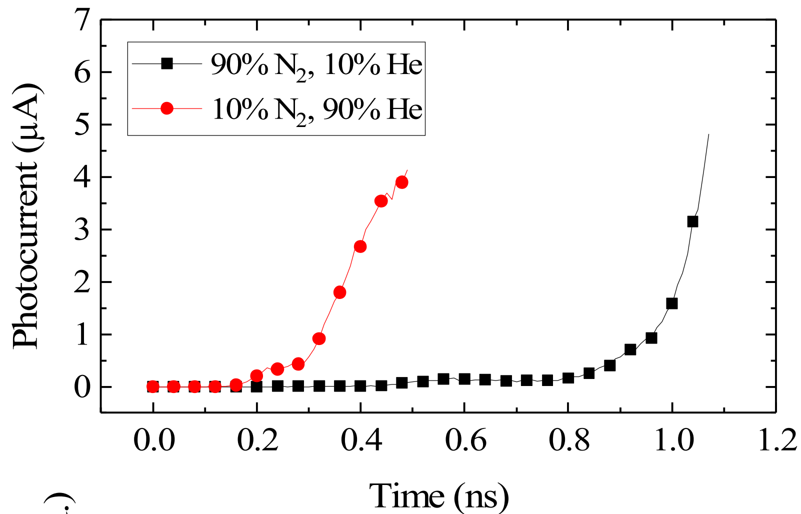
Time: 0.00 ns
Y (m)
Z (m)
E_el_const_ Magnitude
1.000e+07
7.5e+6
5e+6
2.5e+6
1.000e+00
e-_density
1.000e+21
1e+20
1e+19
1e+18
1e+17
1e+16
1.000e+15
Z
Y
X

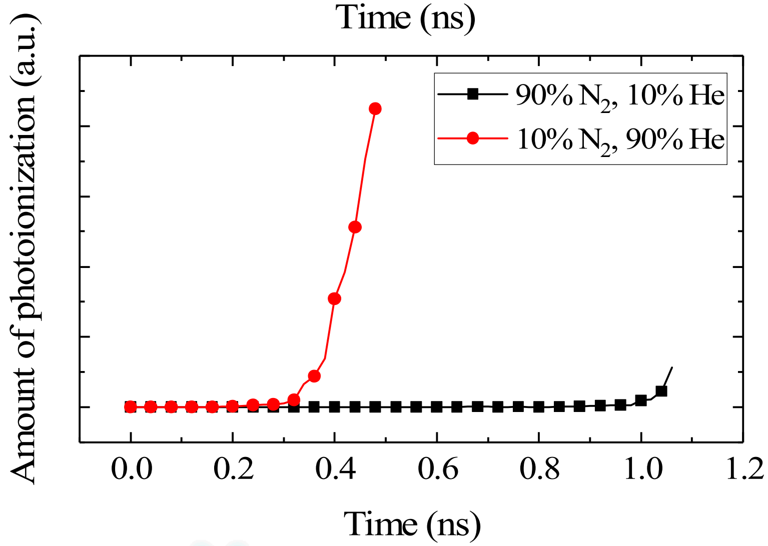
Results

- **Comparing photo-effects from each case**
  - **Both photo-emission and photo-ionization occur earlier for 90% He**



  - **EEDF's are shifted towards higher energies for the 90% He case due to less energy loss to vibrational or rotational energy modes.**

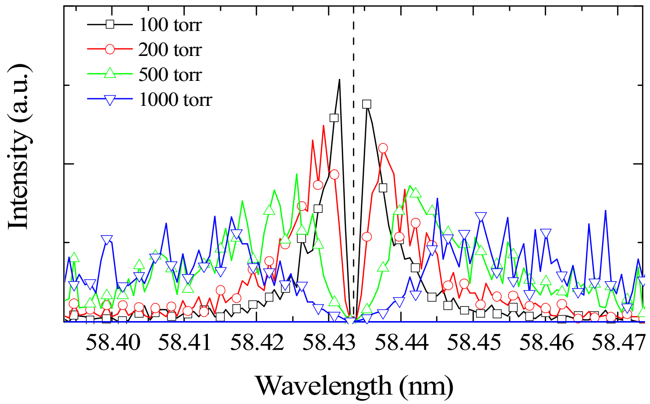




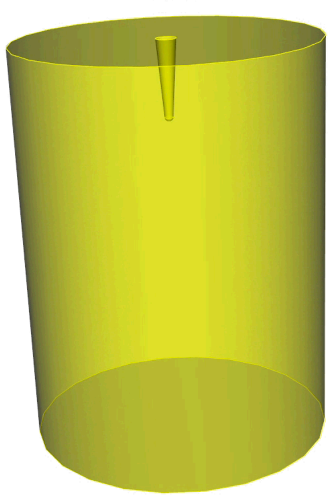
Conclusion and Outlook

- **Have incorporated a method to discretely track photons and include energy-dependent photo-processes.**

- **Can generate non-LTE emission spectra that is both spatially and temporally resolved. On-going work is comparing simulation data versus experiment.**



- **Gain knowledge in simulating large-scale, near atmospheric pressure plasmas.**



- **Even on large super computing systems, modeling larger plasma devices (> 1 mm) at near atmospheric pressures with a kinetic code is still very much a challenging problem, and likely still years away with current algorithms and hardware.**