

# The Role of Metastables in Discharge Evolution



## PRESENTED BY

Matthew M. Hopkins, Andrew S. Fierro,  
George Nail, Edward Barnat  
Sandia National Laboratories



Sandia National Laboratories is a multimission laboratory managed and operated by National Technology & Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.

# Introduction

---

The initiation of a repetitively pulsed discharge system is heavily influenced by the presence of gas constituents, different from an often assumed “clean” background gas of pure ground state atoms, including the presence of contamination species and populations of excited states.

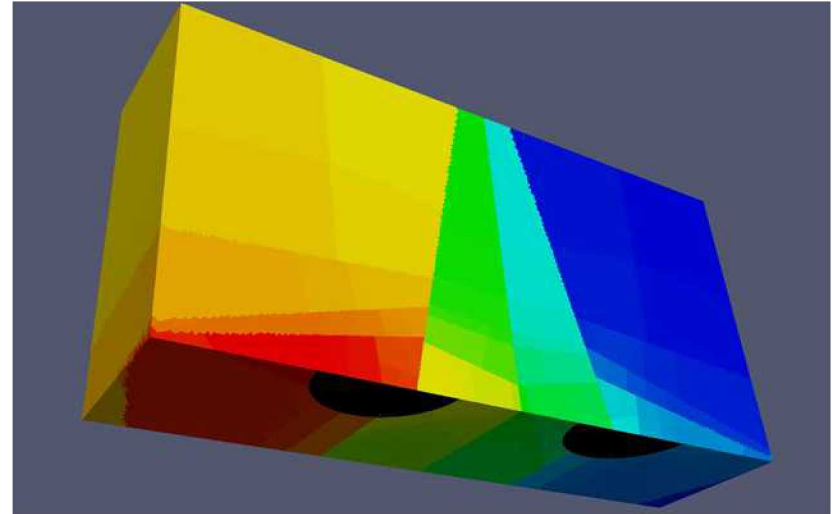
In this work we investigate the role of a background population of metastable excited state helium on discharge and ionization rates.

Here, the physical mechanism for generating this metastable background density is through repetitively pulsed DC discharges building up a background of metastables through multiple shots, whether they result in full discharges or not. After many shots the initial condition for one cycle of the discharge has converged to a persistent metastable density.

We provide and evaluate an effective ionization rate  $\alpha_{\text{eff}}$  as a function of initial background metastable density.

# Aleph: PIC-DSMC Simulation Capability

- 0, 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)



# 0D Model Description

Initial simulations were performed in 0D with a simplified model system:

$e^- + \text{He}$  (elastic)

$e^- + \text{He} \rightarrow e^- + \text{He}^+ + e^-$  (ionization)

$e^- + \text{He} \rightarrow e^- + \text{He}(2^3\text{S})$  (excitation)

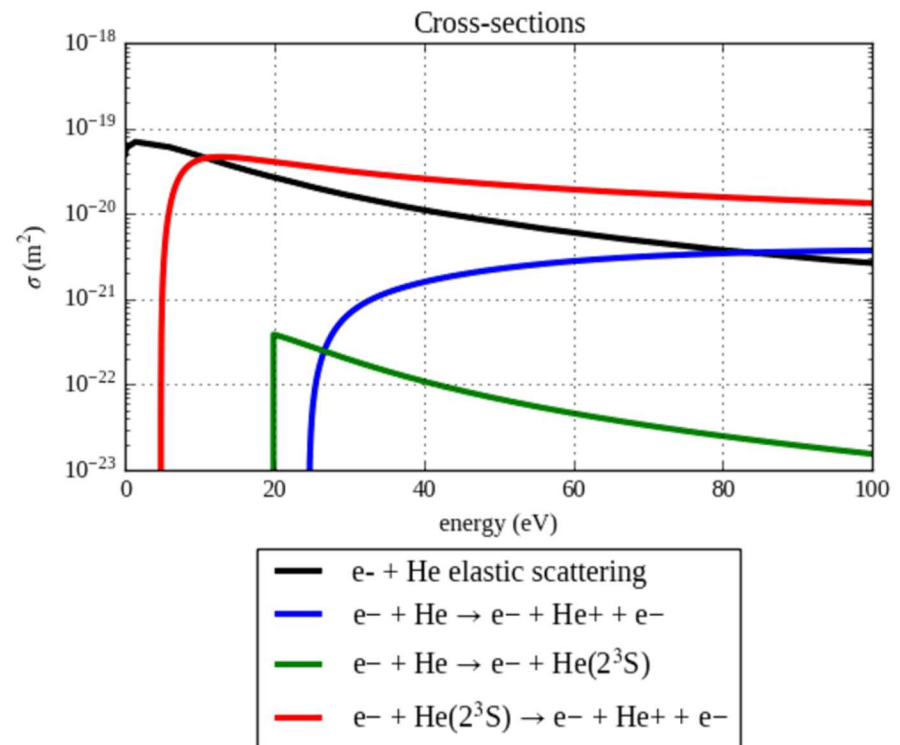
$e^- + \text{He}(2^3\text{S}) \rightarrow e^- + \text{He}^+ + e^-$  (ionization)

Initial  $\text{He}(2^3\text{S})$  ratios are  $10^{-6}$  to  $10^{-1}$ .

Applied  $E/n$  ranges from  $T_d = 20$  to 2000.

Pressure of mixed initial gas is 76 torr.

We employ dynamic load balancing and target computational # of ( $e^-$ ,  $\text{He}^+$ ,  $\text{He}(2^3\text{s})$ ,  $\text{He}$ ) to be approximately (1000, 16, 16, 10)



# Effective ionization rate, $\alpha_{\text{eff}}$

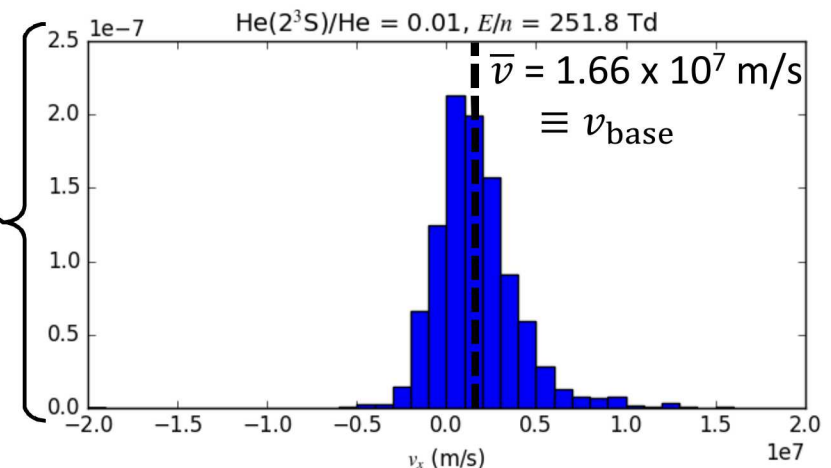
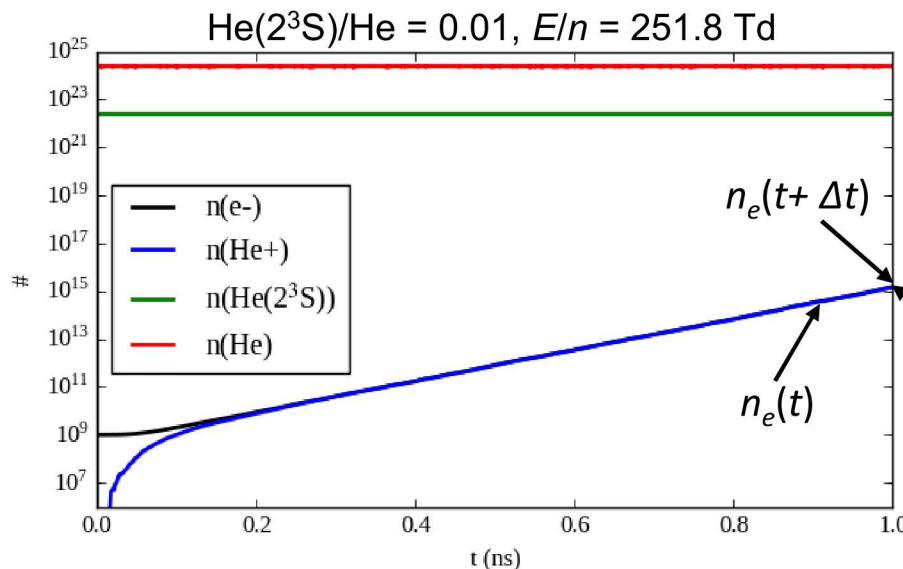
As with Townsend discharge descriptions, the ionization rate  $\alpha$  is defined as:

$$e^{\alpha d} = \frac{I(d)}{I(0)}$$

Where  $I(d)$  is the current at  $x = d$ , and  $I(0)$  is the initial current at  $x = 0$ .

For our 0D model we exchange length for time in the simulation using the mean velocity of the EVDF at long times when the electron growth is in the exponential regime, and total number of electrons for current,

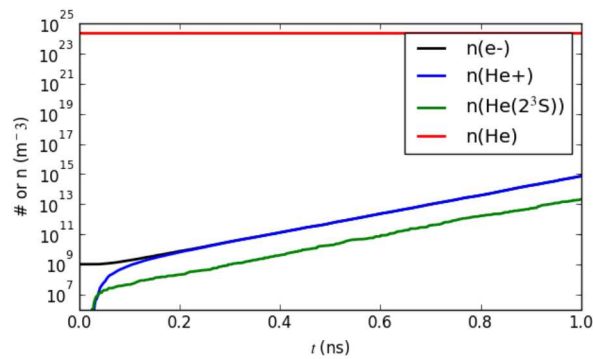
$$e^{\alpha_{\text{eff}}(\bar{v}\Delta t)} = \frac{n_e(t + \Delta t)}{n_e(t)}, \Delta t = 0.1 \text{ ns}$$



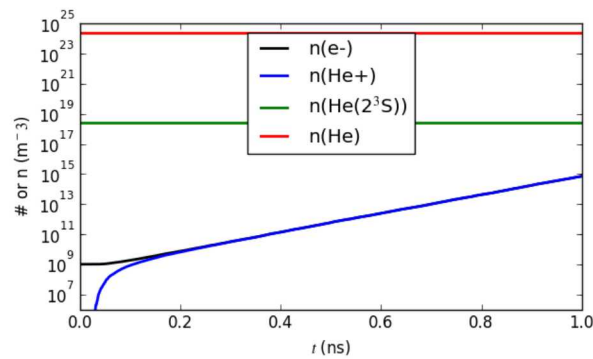
# Effect of Initial Background Metastable Density

In all cases,  $E/n = 251.8$  Td.

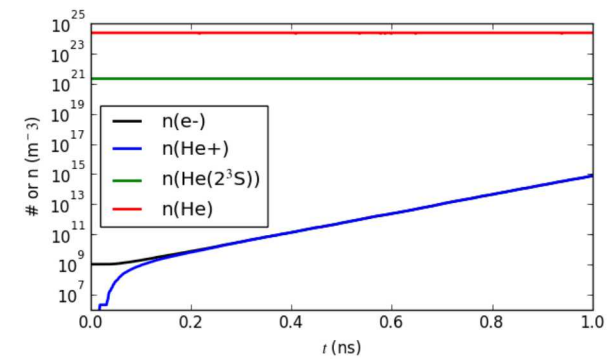
He( $2^3S$ )/He = 0



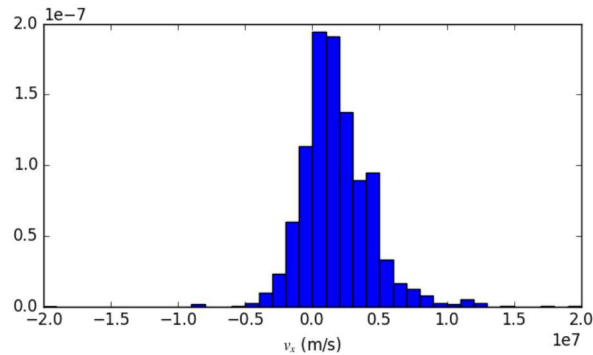
He( $2^3S$ )/He =  $10^{-6}$



He( $2^3S$ )/He =  $10^{-3}$

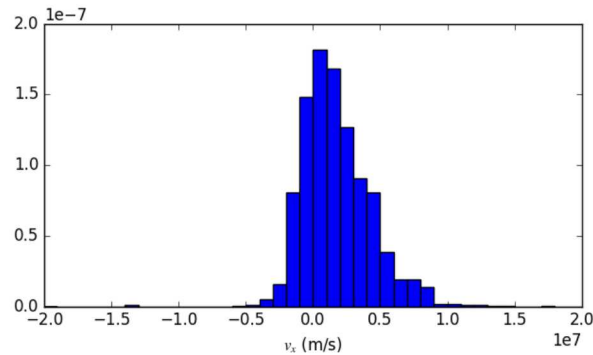


EVDFs at  $t = 1$  ns



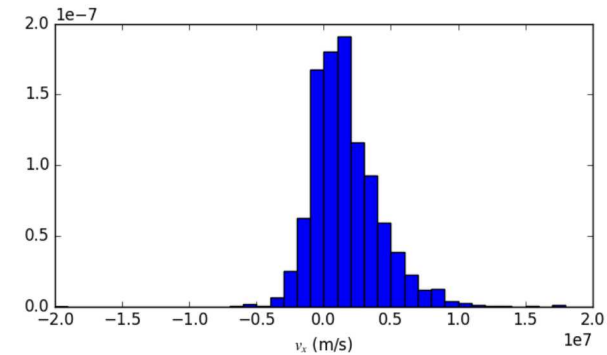
$$\bar{v} = 1.80 \times 10^6 \text{ m/s} = 1.08 \times v_{\text{base}}$$

$$\alpha_{\text{eff}} = 7801 \text{ m}^{-1}$$



$$\bar{v} = 1.75 \times 10^6 \text{ m/s} = 1.05 \times v_{\text{base}}$$

$$\alpha_{\text{eff}} = 7932 \text{ m}^{-1}$$



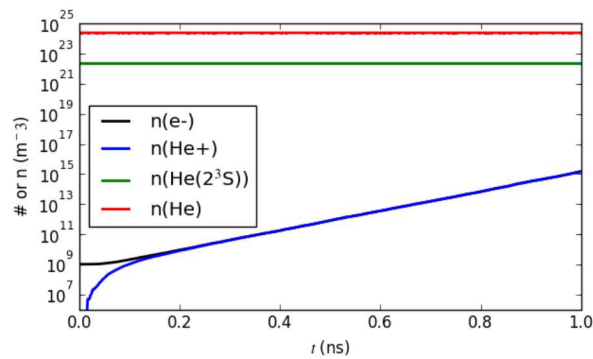
$$\bar{v} = 1.67 \times 10^6 \text{ m/s} = 1.01 \times v_{\text{base}}$$

$$\alpha_{\text{eff}} = 8463 \text{ m}^{-1}$$

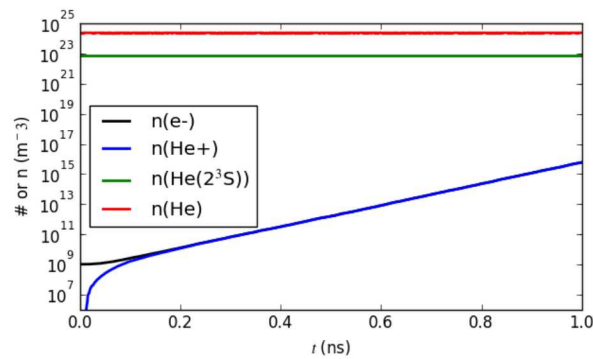
# Effect of Initial Background Metastable Density

In all cases,  $E/n = 251.8$  Td.

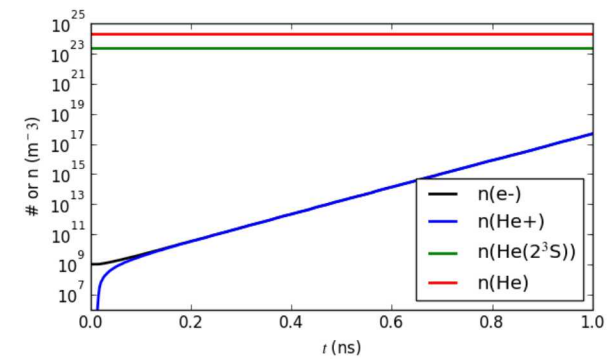
He( $2^3S$ )/He = 0.01



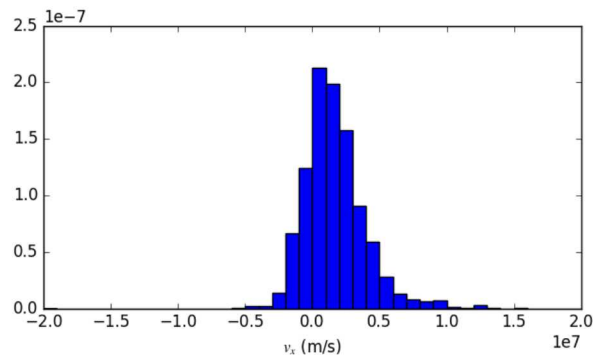
He( $2^3S$ )/He = 0.032



He( $2^3S$ )/He = 0.1

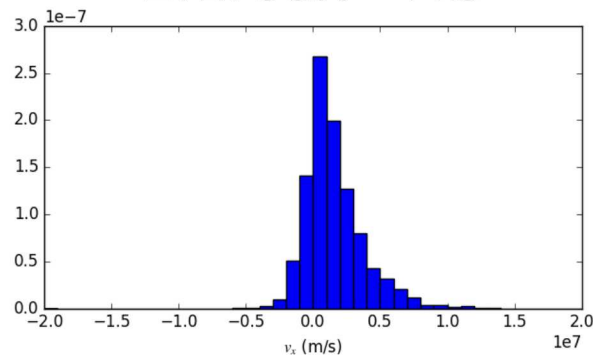


EVDFs at  $t = 1$  ns



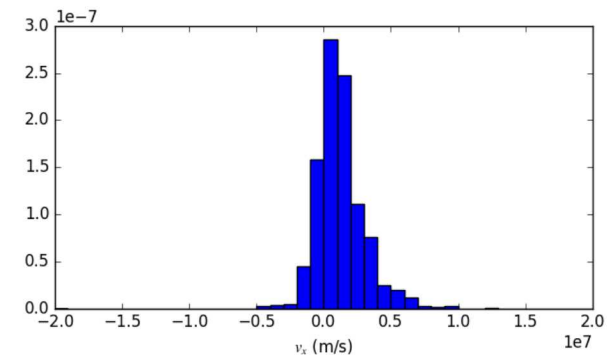
$$\bar{v} = 1.66 \times 10^6 \text{ m/s} \equiv v_{\text{base}}$$

$$\alpha_{\text{eff}} = 8944 \text{ m}^{-1}$$



$$\bar{v} = 1.57 \times 10^6 \text{ m/s} = 0.946 \times v_{\text{base}}$$

$$\alpha_{\text{eff}} = 10420 \text{ m}^{-1}$$



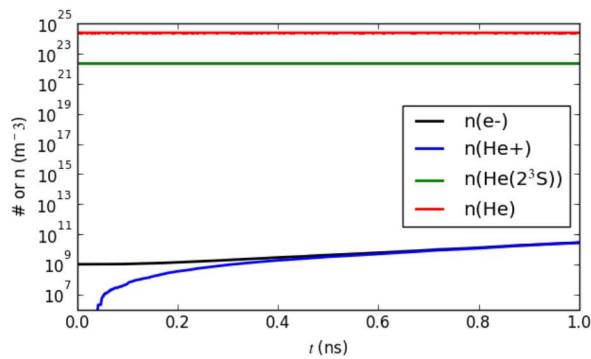
$$\bar{v} = 1.23 \times 10^6 \text{ m/s} = 0.741 \times v_{\text{base}}$$

$$\alpha_{\text{eff}} = 17050 \text{ m}^{-1}$$

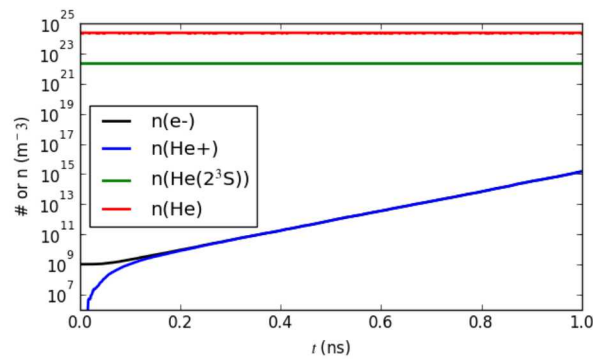
# Effect of Reduced Field

In all cases,  $\text{He}(2^3\text{S})/\text{He} = 0.01$

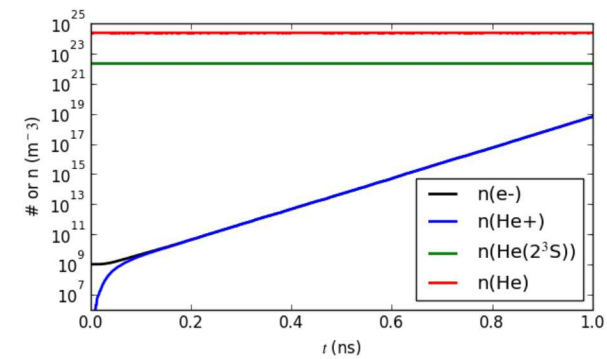
$E/n = 100.2 \text{ Td}$



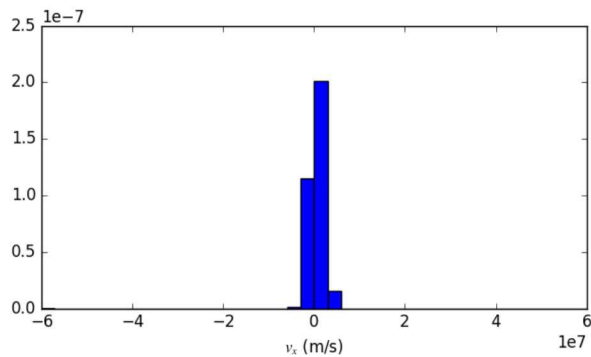
$E/n = 251.8 \text{ Td}$



$E/n = 399.1 \text{ Td}$

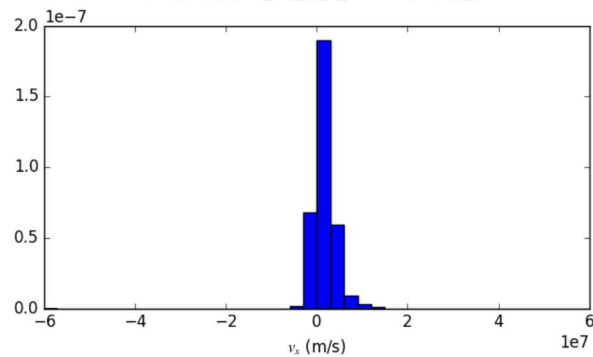


EVDFs at  $t = 1 \text{ ns}$



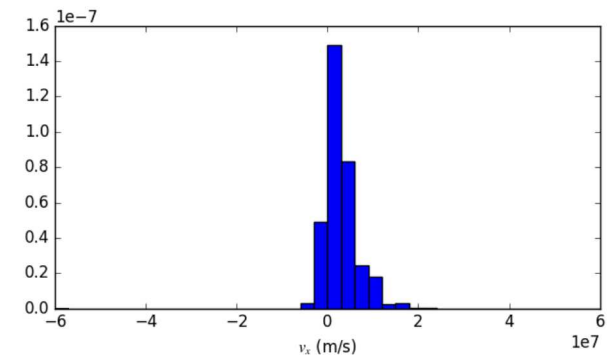
$$\bar{v} = 0.483 \times 10^6 \text{ m/s} = 0.291 \times v_{\text{base}}$$

$$\alpha_{\text{eff}} = 7599 \text{ m}^{-1}$$



$$\bar{v} = 1.66 \times 10^6 \text{ m/s} \equiv v_{\text{base}}$$

$$\alpha_{\text{eff}} = 8944 \text{ m}^{-1}$$



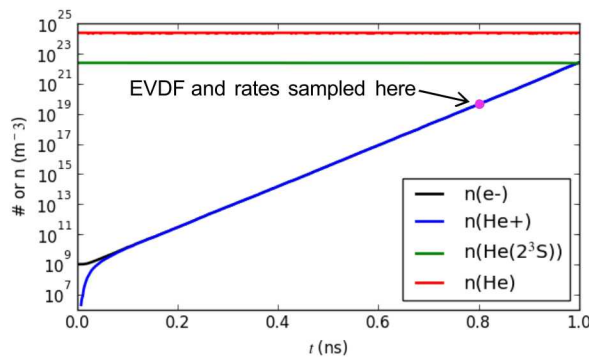
$$\bar{v} = 2.97 \times 10^6 \text{ m/s} = 1.79 \times v_{\text{base}}$$

$$\alpha_{\text{eff}} = 7954 \text{ m}^{-1}$$

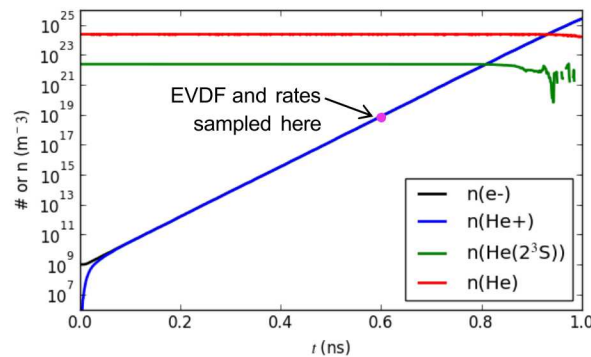
# Effect of Reduced Field

In all cases,  $\text{He}(2^3\text{S})/\text{He} = 0.01$

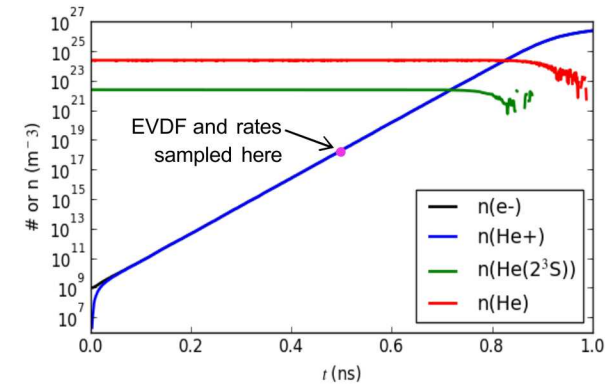
$E/n = 632.5 \text{ Td}$



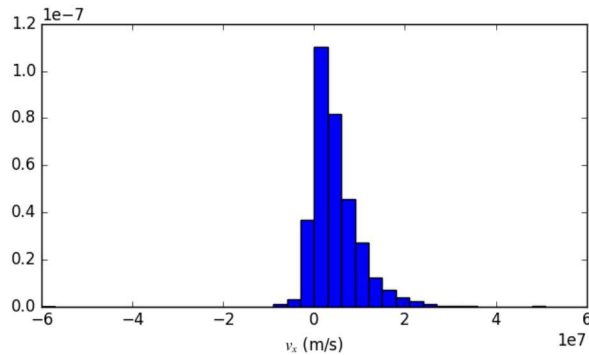
$E/n = 1002 \text{ Td}$



$E/n = 2000 \text{ Td}$

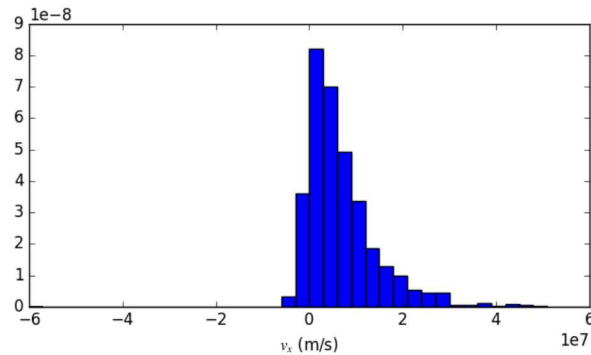


EVDFs at  $t = 0.5 - 0.8 \text{ ns}$



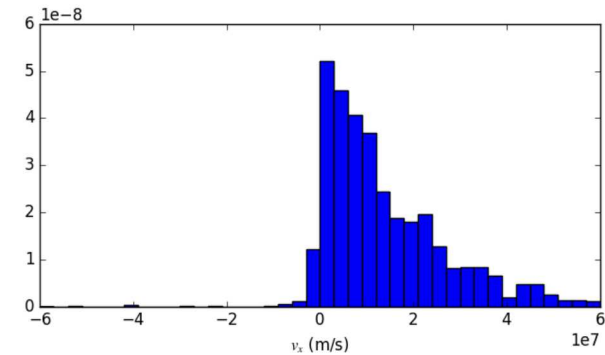
$$\bar{v} = 4.57 \times 10^6 \text{ m/s} = 2.75 \times v_{\text{base}}$$

$$\alpha_{\text{eff}} = 6868 \text{ m}^{-1}$$



$$\bar{v} = 6.81 \times 10^6 \text{ m/s} = 4.10 \times v_{\text{base}}$$

$$\alpha_{\text{eff}} = 5652 \text{ m}^{-1}$$

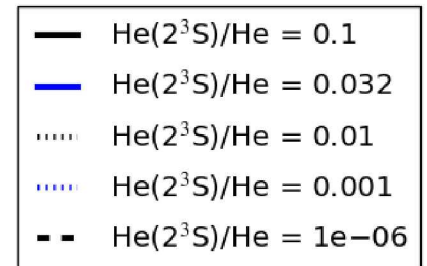
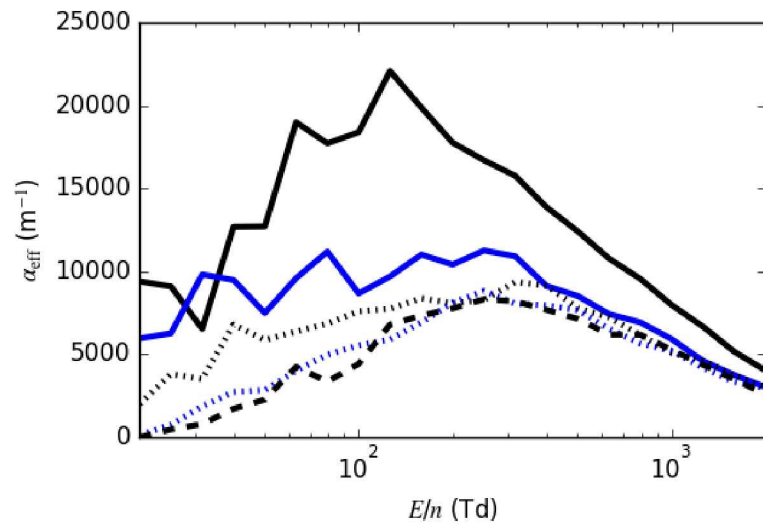
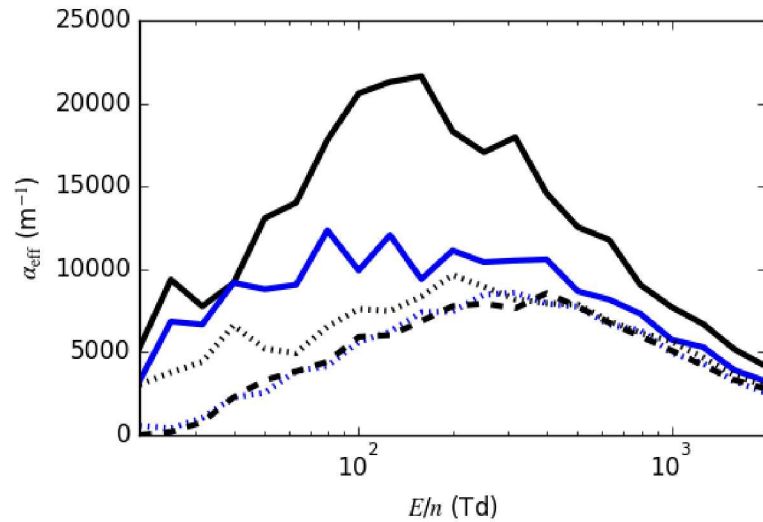


$$\bar{v} = 14.7 \times 10^6 \text{ m/s} = 8.86 \times v_{\text{base}}$$

$$\alpha_{\text{eff}} = 2950 \text{ m}^{-1}$$

# Full Variation of $\alpha_{\text{eff}}$

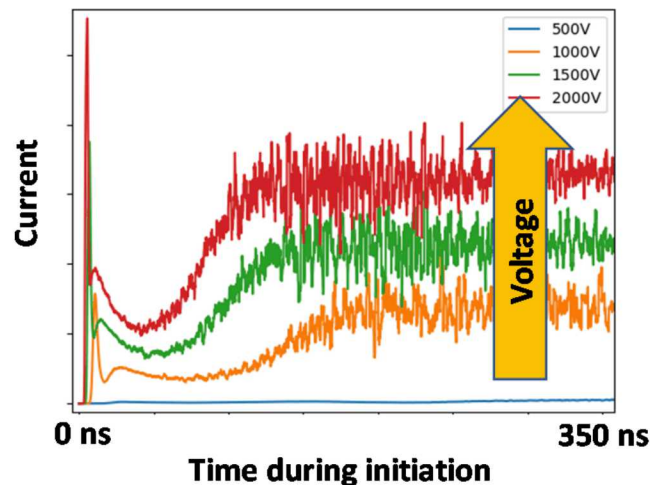
(2 different random  
number seeds)



# Initial 1D Simulations

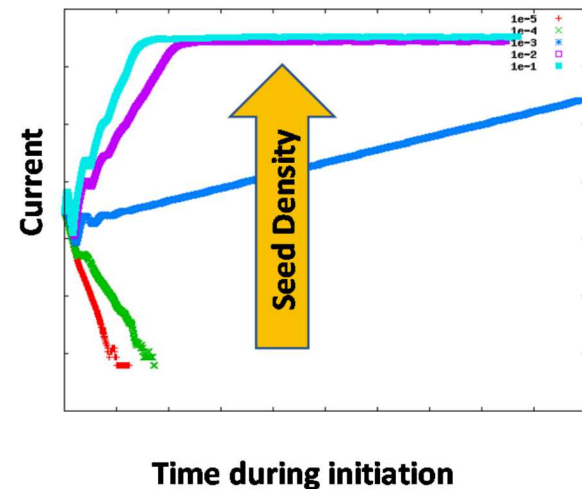
We are further investigating the timing, breakdown thresholds, and ionization rates in experiments, leading up to 3D (potentially axisymmetric) systems.

## “Injection seeded Breakdown”



As reduced fields increase the time to breakdown decreases.

## “Memory effect”



As initial He(23S)/He increases,  $\alpha_{\text{eff}}$  can reach a level where breakdown can now occur because of the presence of He(23S) – breakdown in He alone would not occur.

# Summary

---

- Demonstrated the reduction in  $\alpha_{\text{eff}}$  as  $E/n$  increases past a critical point, explained by the increase in  $\bar{\nu}$ .
- Demonstrated the quicker time to reach the exponential growth phase with increase in initial metastable population.
- He( $2^3\text{S}$ )/He must be O(0.01) or higher to influence initial ionization rate.

## Future Work

---

- Further develop 1D (and eventually 3D) models to show how spatially (and temporally) varying  $E/n$  influences discharge evolution
- Further develop 1D (and eventually 3D) models to show how spatially varying initially He( $2^3\text{S}$ ) distributions influence discharge evolution.

## Acknowledgement

---

This work was supported by the Office of Fusion Energy Science at the U.S. Department of Energy under contract DE-AC04-94SL85000.