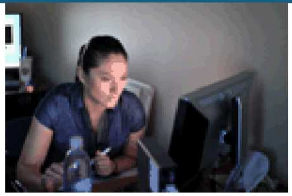
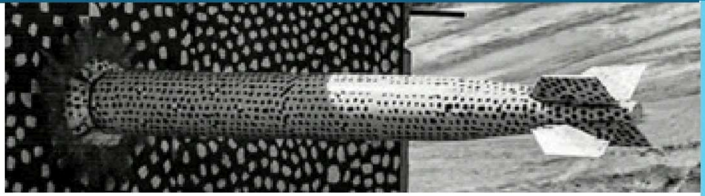
SAND2019-10462C

Initial Comparison to Experiments of EMPIRE Simulations with Diodes Driven by the Photoelectric Effect





PRESENTED BY

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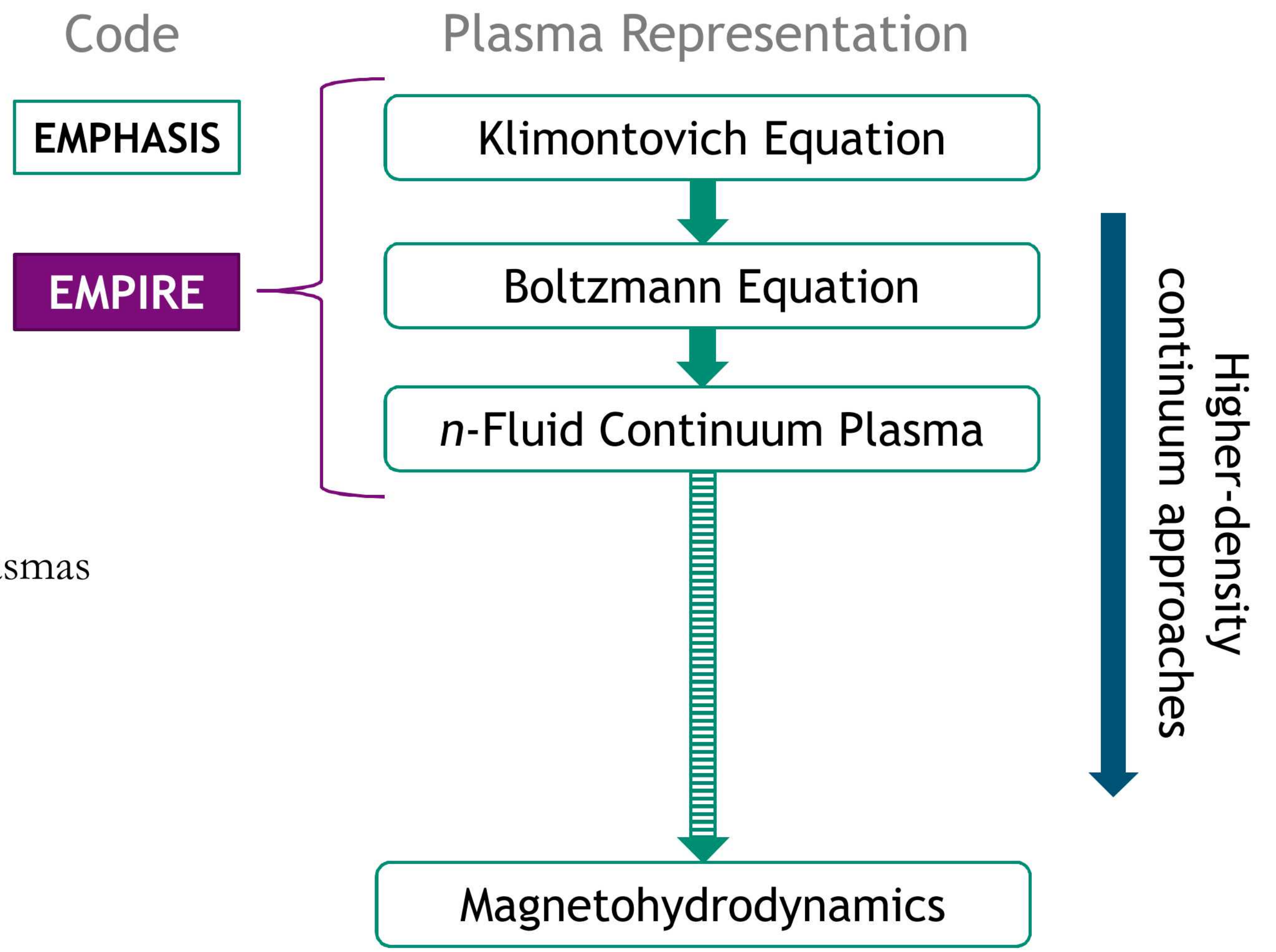
Outline

- What is EMPIRE
  - Research in Algorithms and Computer Science
- Simulations of diodes driven by photoelectric effect on Z and NIF
  - Vacuum
  - Gas filled
  - Surface Heating

EMPIRE’s Grand Vision: Plasma Physics Modeling

EMPHASIS is our current production low density plasma simulation tool



EMPIRE adds new capabilities:

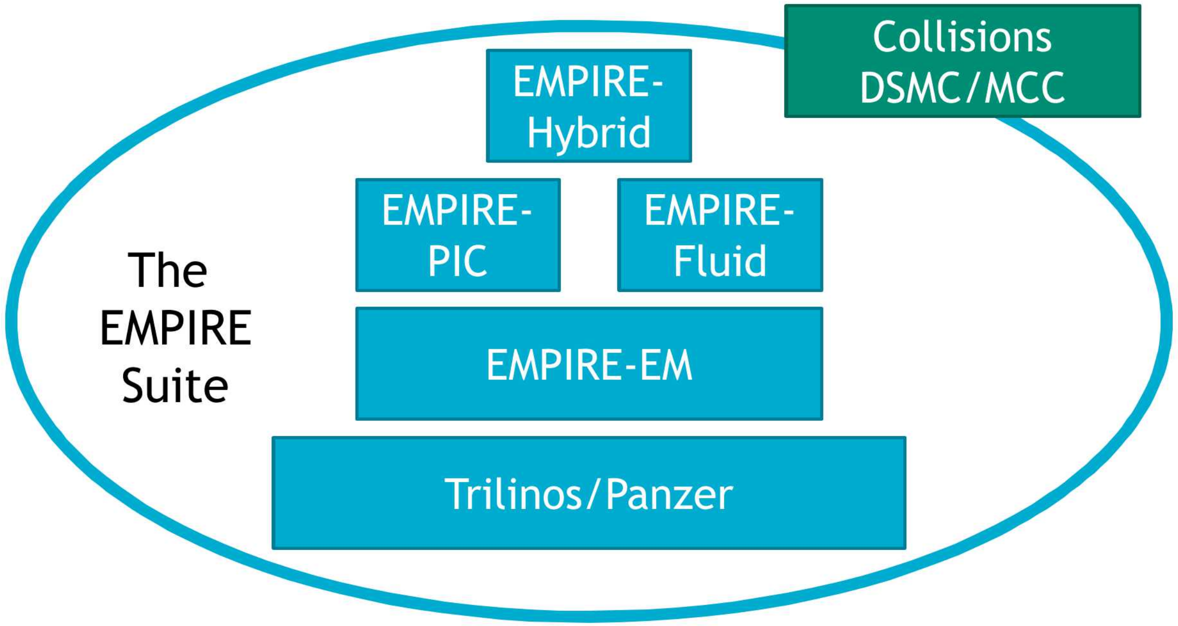
- Written for advanced computing architectures
  - GPGPU, Intel Phi, ARM…
- Expanded particle-based modeling regime
  - DSMC (changing background)/MCC
  - Implicit PIC in term of plasma density and magnetic field
- Full continuum fluid plasma modeling for high-density plasmas
  - Drift-Diffusion approximation
    - Local Mean Energy Approximation (LMEA)
    - Local Field Approximation (LFA)
- Hybrid particle-fluid modeling for intermediate densities

EMPIRE's Grand Vision: Integrated Suite of Capabilities

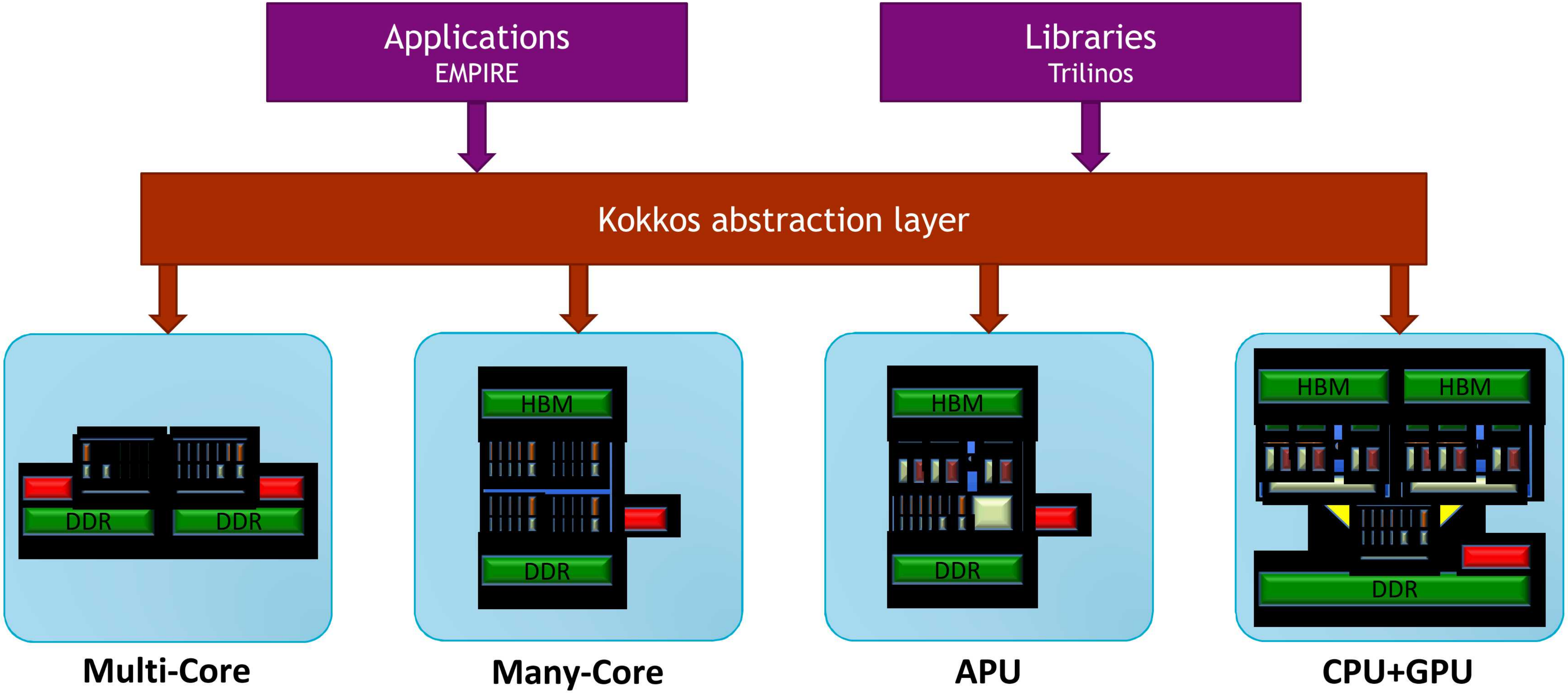
EMPIRE is being designed to be our "next-generation" "low density" plasma modeling tool

EMPIRE builds off various components to achieve performance portable physics representation
- EMPIRE-EM: Core time-domain Maxwell's equations for electromagnetics
- EMPIRE-PIC: Particle-in-Cell plasma modeling
- EMPIRE-Fluid: Multi-species fluid plasma modeling
- EMPIRE-Hybrid: Coupled Fluid/PIC plasma modeling

EMPIRE is built upon Trilinos components:
- Panzer: FEM discretization tools
- Tempus: General time integration package
- Uses the modern Tpetra-based linear solver stack
- Kokkos: Portable threading library



Performance Portability Through Kokkos



Kokkos is the cornerstone for performance portability across next generation HPC architectures at multiple DOE laboratories and other organizations.

Basic Equations

Maxwell's Dynamical Equations:

$$\nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t} \qquad \nabla \times \mathbf{H} = \mathbf{J} + \frac{\partial \mathbf{D}}{\partial t}$$

Subject to the initial value constraints:

$$\nabla \cdot \mathbf{B} = 0$$

$$\nabla \cdot \mathbf{D} = \rho$$

With the definitions for macroscopic media:

$$\mathbf{D} = \varepsilon \mathbf{E} \qquad \mathbf{J} = \sigma \mathbf{E}$$

$$\mathbf{B} = \mu \mathbf{H}$$

Relativistic Lorentz Force Law for relativistic velocity *u=vγ*:

$$\frac{d\mathbf{u}}{dt} = \frac{q}{m}\left[\mathbf{E} + \frac{\mathbf{u}\times\mathbf{B}}{\gamma}\right]$$

The Plasma Models

Relativistic Klimontovich Equation

$$\frac{\partial N_s(\boldsymbol{x},\boldsymbol{u},t)}{\partial t} + \boldsymbol{v}\cdot\nabla_x N_s + \frac{q_s}{m_s}\left(\mathbf{E} + \frac{\boldsymbol{v}}{c}\times\mathbf{B}\right)\cdot\nabla_u N_s = \left.\frac{\partial N_s(\boldsymbol{x},\boldsymbol{u},t)}{\partial t}\right|_c$$

$$\rho(\boldsymbol{x},t) = \sum_{species} q_s \int d\boldsymbol{u} N_s(\boldsymbol{x},\boldsymbol{u},t) \qquad \boldsymbol{J}(\boldsymbol{x},t) = \sum_{species} q_s \int d\boldsymbol{u}\boldsymbol{u} N_s(\boldsymbol{x},\boldsymbol{u},t)$$

Maxwell’s Equations

$$\nabla\cdot\boldsymbol{D}(\boldsymbol{x},t) = \frac{\rho(\boldsymbol{x},t)}{\epsilon_0}$$

$$\nabla\cdot\mathbf{B}(\boldsymbol{x},t) = 0$$

$$\nabla\times\mathbf{E}(\boldsymbol{x},t) = -\frac{\partial\mathbf{B}(\boldsymbol{x},t)}{\partial t}$$

$$\nabla\times\boldsymbol{H}(\boldsymbol{x},t) = \mu_0\boldsymbol{J}(\boldsymbol{x},t) + \mu_0\epsilon_0\frac{\partial\boldsymbol{D}(\boldsymbol{x},t)}{\partial t}$$

The Radiation Transport Models

Relativistic Klimontovich Equation

$$\frac{\partial N_s(\boldsymbol{x},\boldsymbol{u},t)}{\partial t} + \boldsymbol{v}\cdot\nabla_x N_s + \frac{q_s}{m_s}\left(\mathbf{E} + \frac{\boldsymbol{v}}{c}\times\mathbf{B}\right)\cdot\nabla_u N_s = \left.\frac{\partial N_s(\boldsymbol{x},\boldsymbol{u},t)}{\partial t}\right|_c$$

Fixed **E** and **B,** often zero

This contains the uncertainty in the model

Fluid formulation for plasma modeling

A multi-species 5-moment model derived by taking moments of the collisional Boltzmann equation over velocity space:

$$\frac{\partial \rho_\alpha}{\partial t} + \nabla \cdot (\rho_\alpha \mathbf{u}_\alpha) = \sum_{\text{srcs}} m_\alpha \Gamma^{\text{src}} - \sum_{\text{sinks}} m_\alpha \Gamma^{\text{sink}}$$

$$\begin{aligned}\frac{\partial (\rho_\alpha \mathbf{u}_\alpha)}{\partial t} + \nabla \cdot (\rho_\alpha \mathbf{u}_\alpha \otimes \mathbf{u}_\alpha + p_\alpha I + \Pi_\alpha) &= \frac{q_\alpha}{m_\alpha} \rho_\alpha \left(\mathbf{E} + \mathbf{u}_\alpha \times \mathbf{B}\right) \\ &+ \sum_{\text{srcs}} m_\alpha \mathbf{u}_{\text{src}} \Gamma^{\text{src}} - \sum_{\text{sinks}} m_\alpha \mathbf{u}_\alpha \Gamma^{\text{sink}} + \sum_{\beta \neq \alpha} \mathbf{R}^{\alpha,\beta}\end{aligned}$$

$$\begin{aligned}\frac{\partial \mathcal{E}_\alpha}{\partial t} + \nabla \cdot ((\mathcal{E}_\alpha + p_\alpha)\mathbf{u}_\alpha + \mathbf{u}_\alpha \cdot \Pi_\alpha + \mathbf{h}_\alpha) &= \frac{q_\alpha}{m_\alpha} \rho_\alpha \mathbf{E} \cdot \mathbf{u}_\alpha + \sum_{\beta \neq \alpha} \left(\mathbf{u}_\alpha \mathbf{R}^{\alpha,\beta} + Q^{\alpha,\beta}\right) \\ &+ \frac{1}{2} \sum_{\text{srcs}} m_\alpha u_{\text{src}}^2 \Gamma^{\text{src}} - \frac{1}{2} \sum_{\text{sinks}} m_\alpha u_\alpha^2 \Gamma^{\text{sink}}\end{aligned}$$

Much faster than PIC for simulating high-density collisional plasma environments

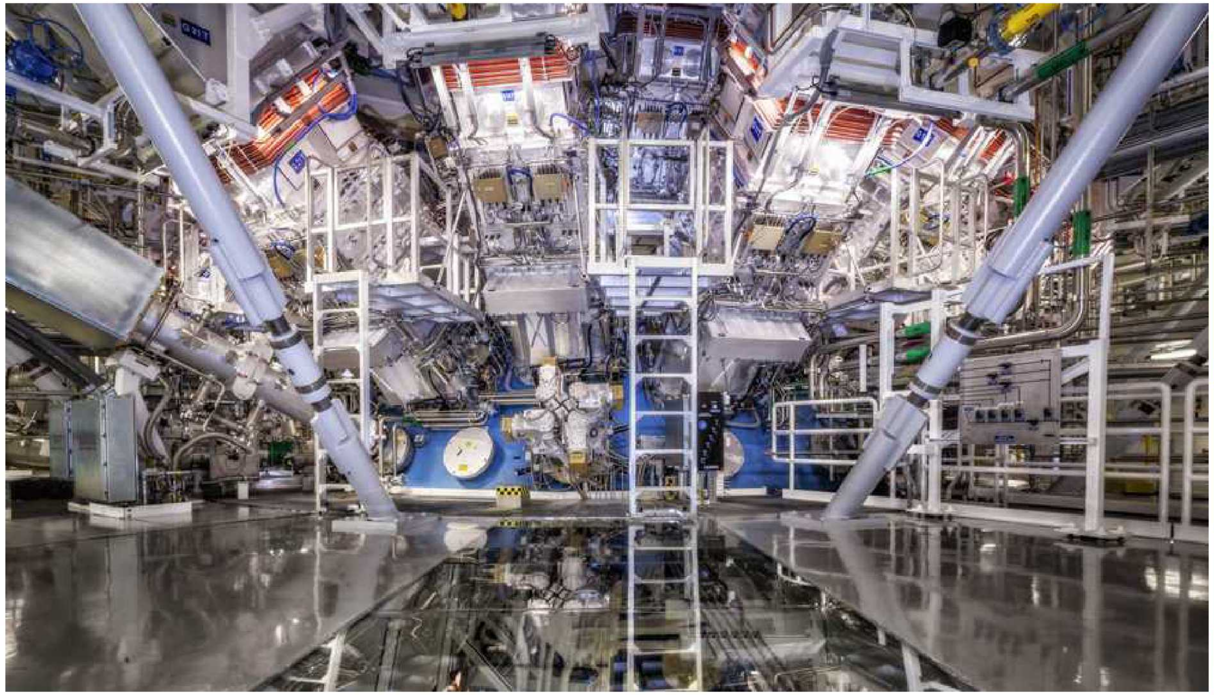
EMPIRE Simulations of Diodes Driven by the Photoelectric Effect

Comparison of EMPIRE Simulations with Diodes Driven by the Photoelectric Effect:

- Benchmark capability and identify missing physics in EMPIRE
- Advance capability in particle emission and collision models

Motivation:

- Drive development of necessary physics (sources, collisions, heating)
- Drive development of software capability (solvers, load balancing, particle merge algorithms)
- Use simple verification and validation problems to build confidence in physics capability
- Build understanding in simulation uncertainties
- Build understanding in experimental measurement uncertainties



Outside NIF Target Chamber

EMPIRE Simulations of Diodes Driven by the Photoelectric Effect

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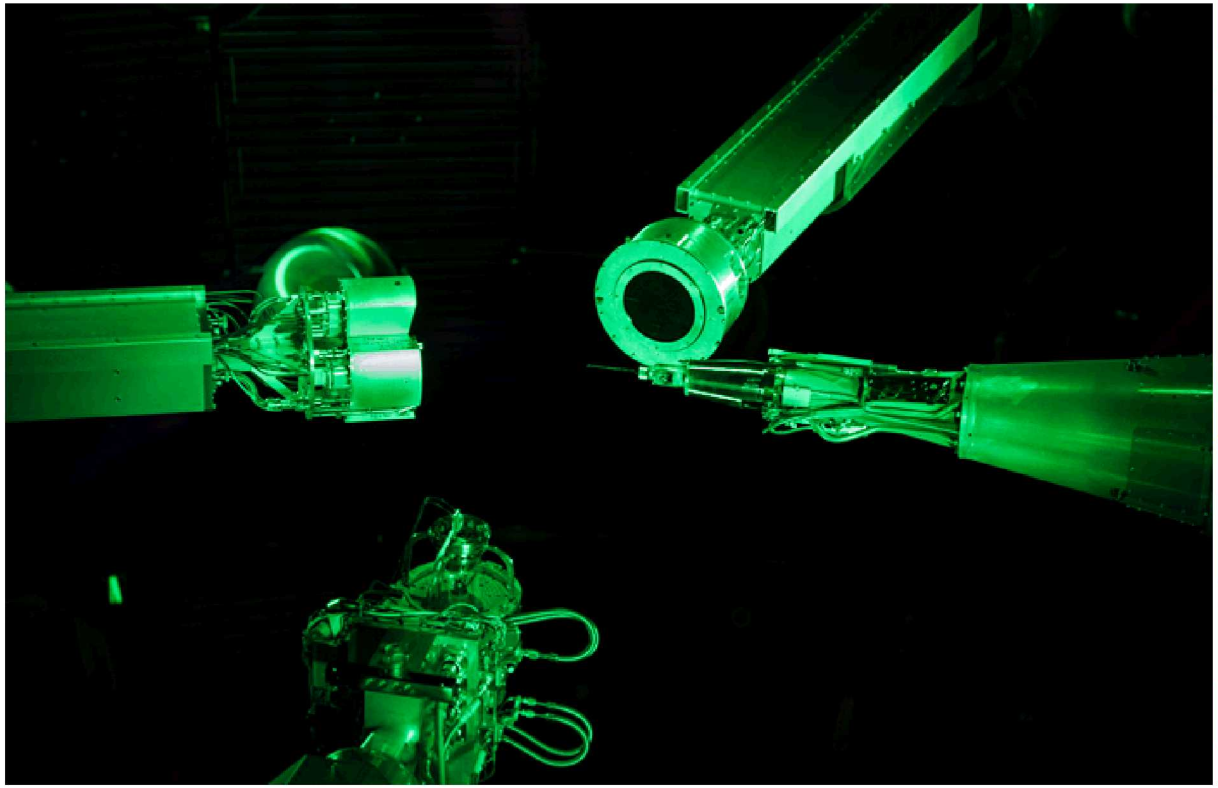

Inside NIF Target Chamber

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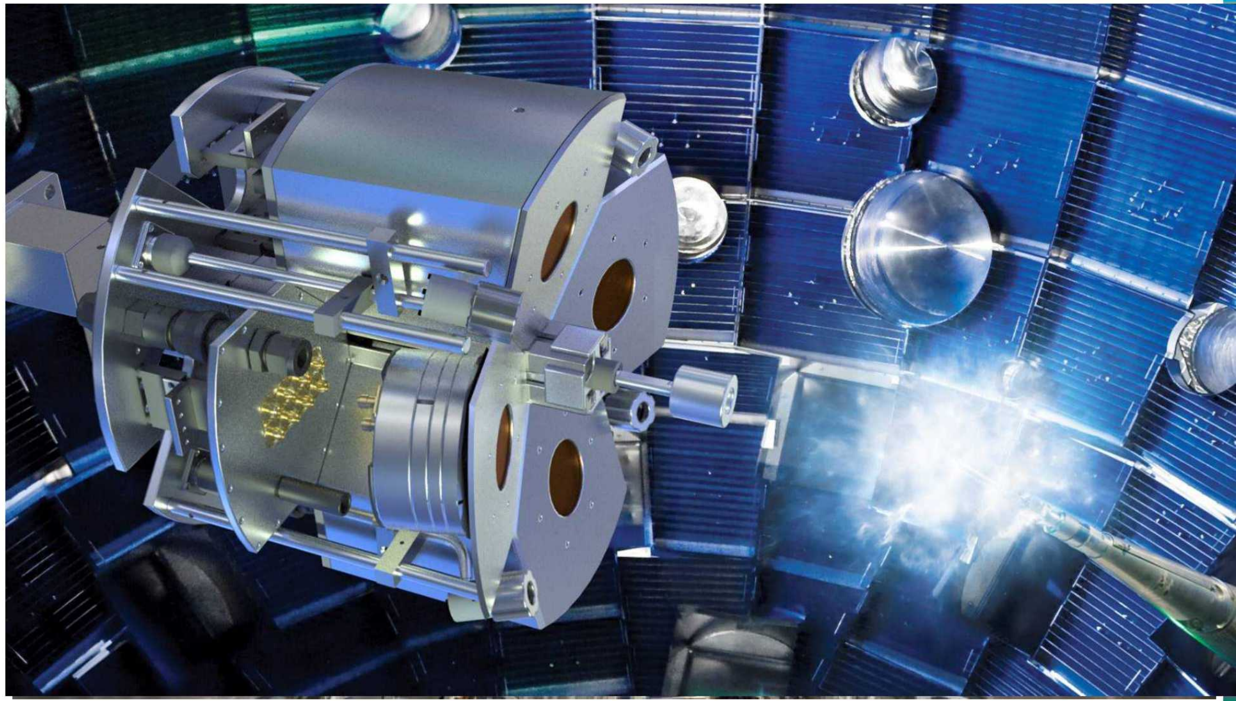

Four cavity experiments on a diagnostic instrument manipulator

EMPIRE Simulations of Diodes Driven by the Photoelectric Effect

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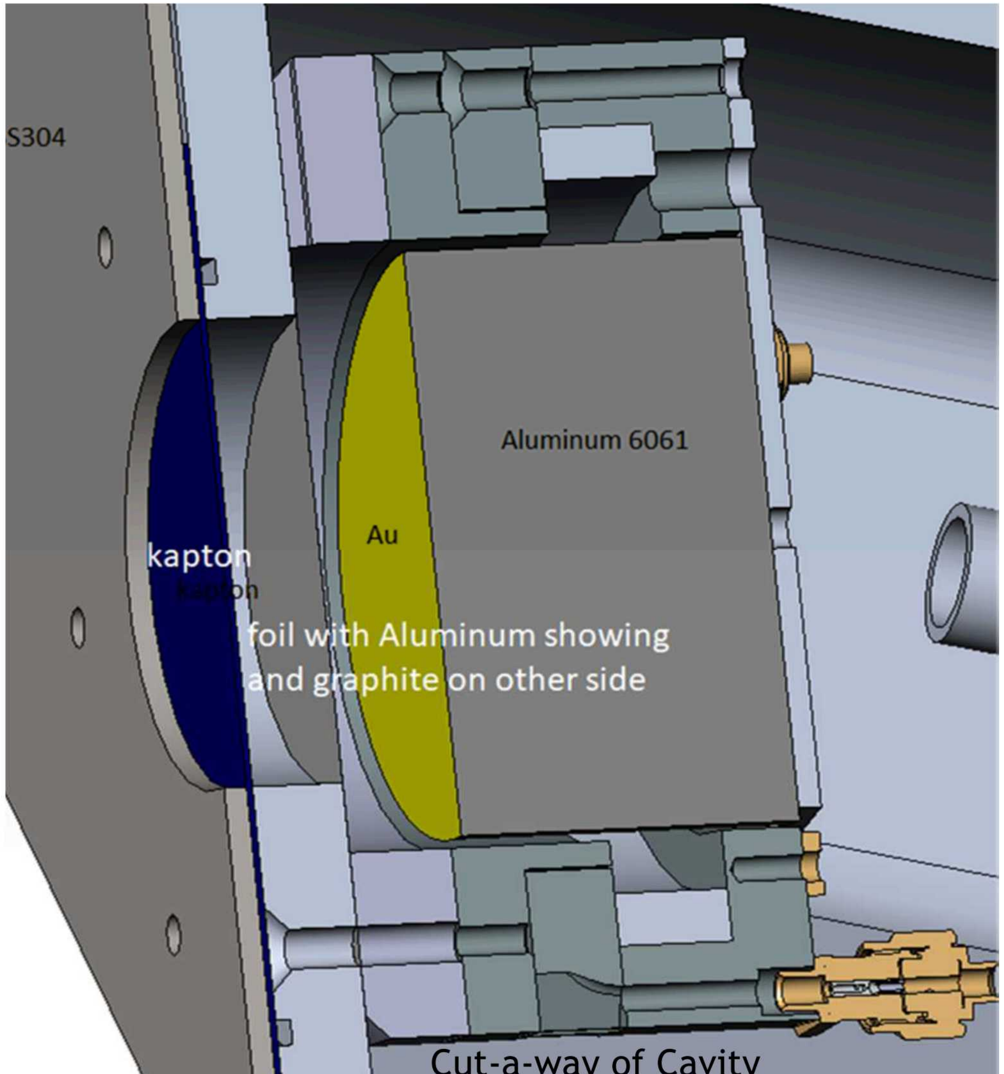
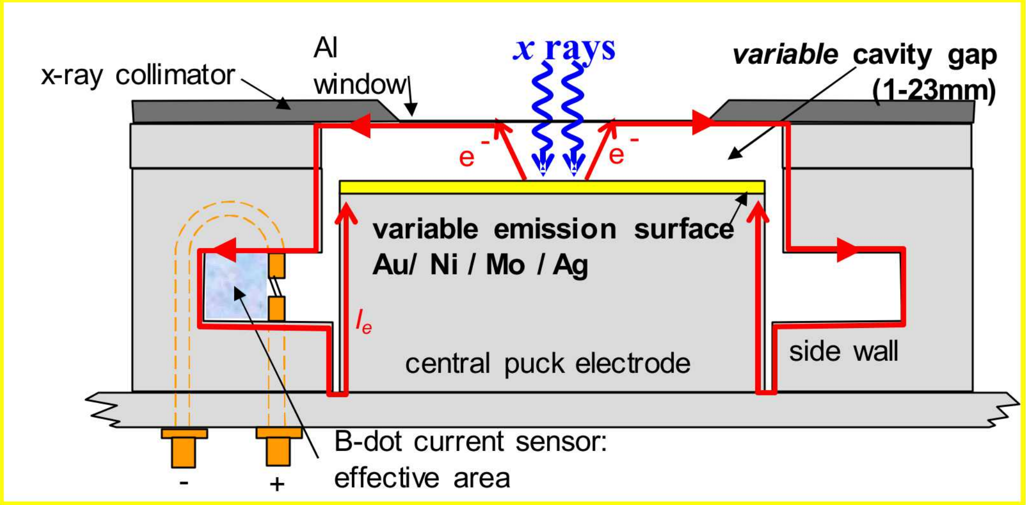


Cut-a-way of Cavity

Parameterized B-Dot Cavity



Problem Parameters:

Cavity height (mm)

Wedge angle (degrees)

Base mesh scale (mm)

Time step (s)

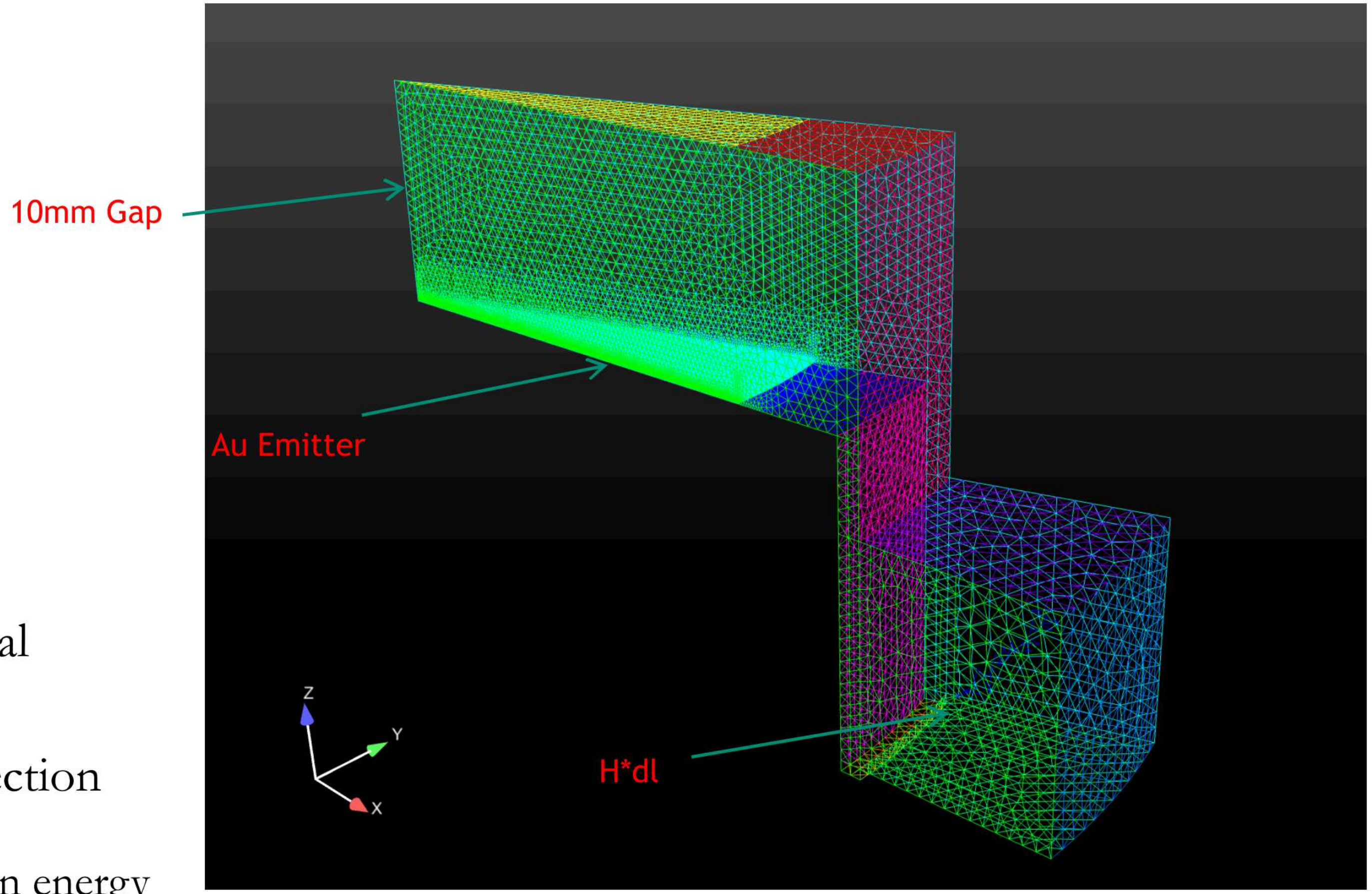
Simulation time (s)

Number of processors

Background neutral pressure

Parameterized injection boundary for:

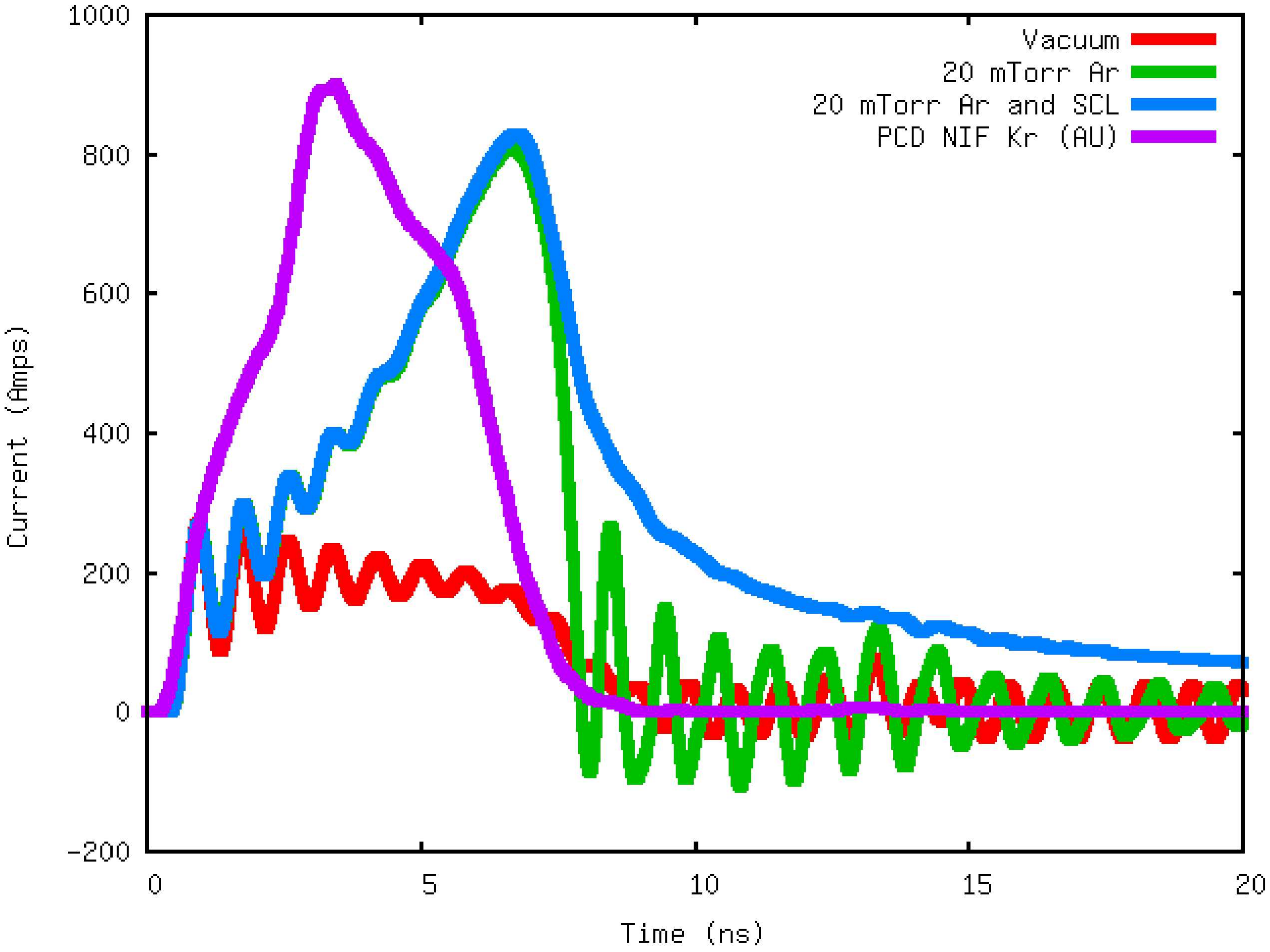
- Thermal emission energy
- ITS source
- SCL
- Neutral particle emission



Prototype Milestone Mesh

B-Dot Nightly Testing: Includes a vacuum B-Dot with two vastly different currents. An argon-filled pressurized B-Dot with e-Ar collisions is under review.

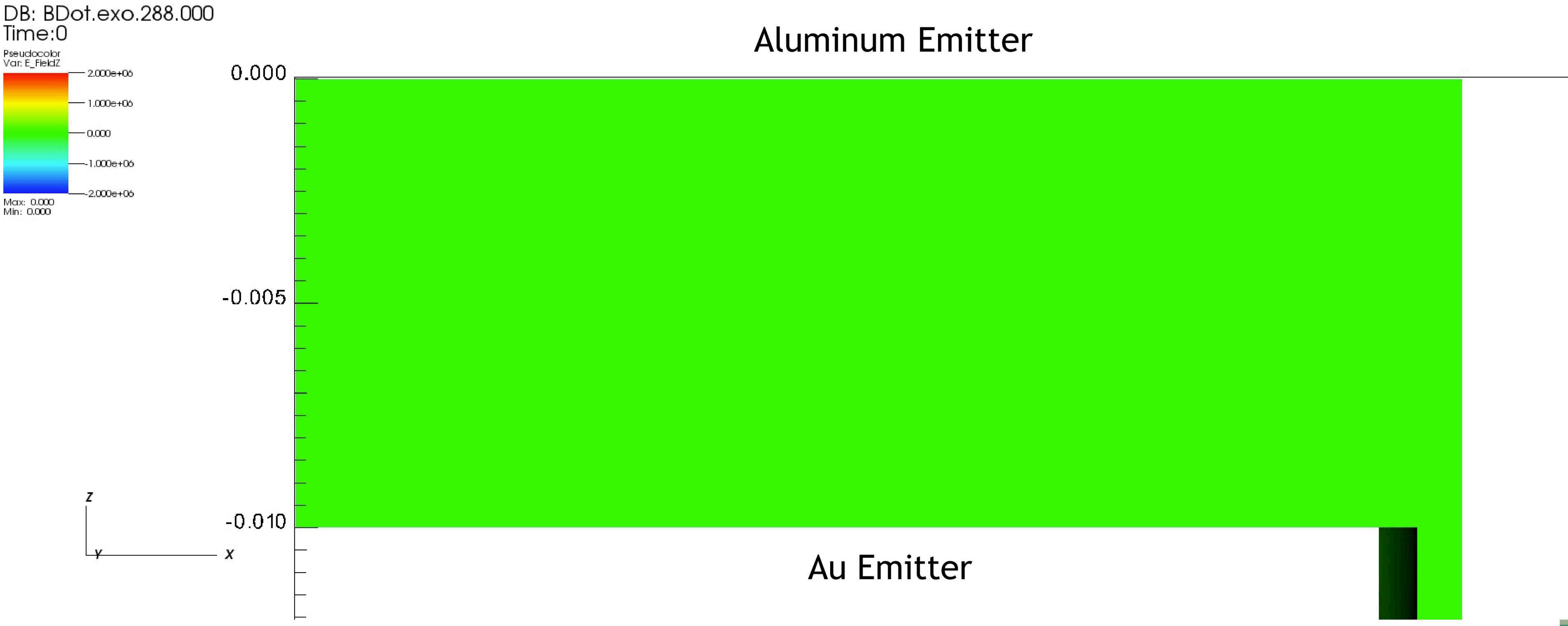
Summary of Vacuum, Gas, and SCL emission



- Adding a background gas neutralizes the space charge barrier
- Adding space charge limited emission increases the tail and smooths the tail
  - Early time response is mostly ionization (collisions)
  - Late time with SCL is the SCL boundary and the inductance of the system and scattering collisions (not ionization)
  - With out SCL ionizations continue through late time

- These effects have been explore in EMPHASIS

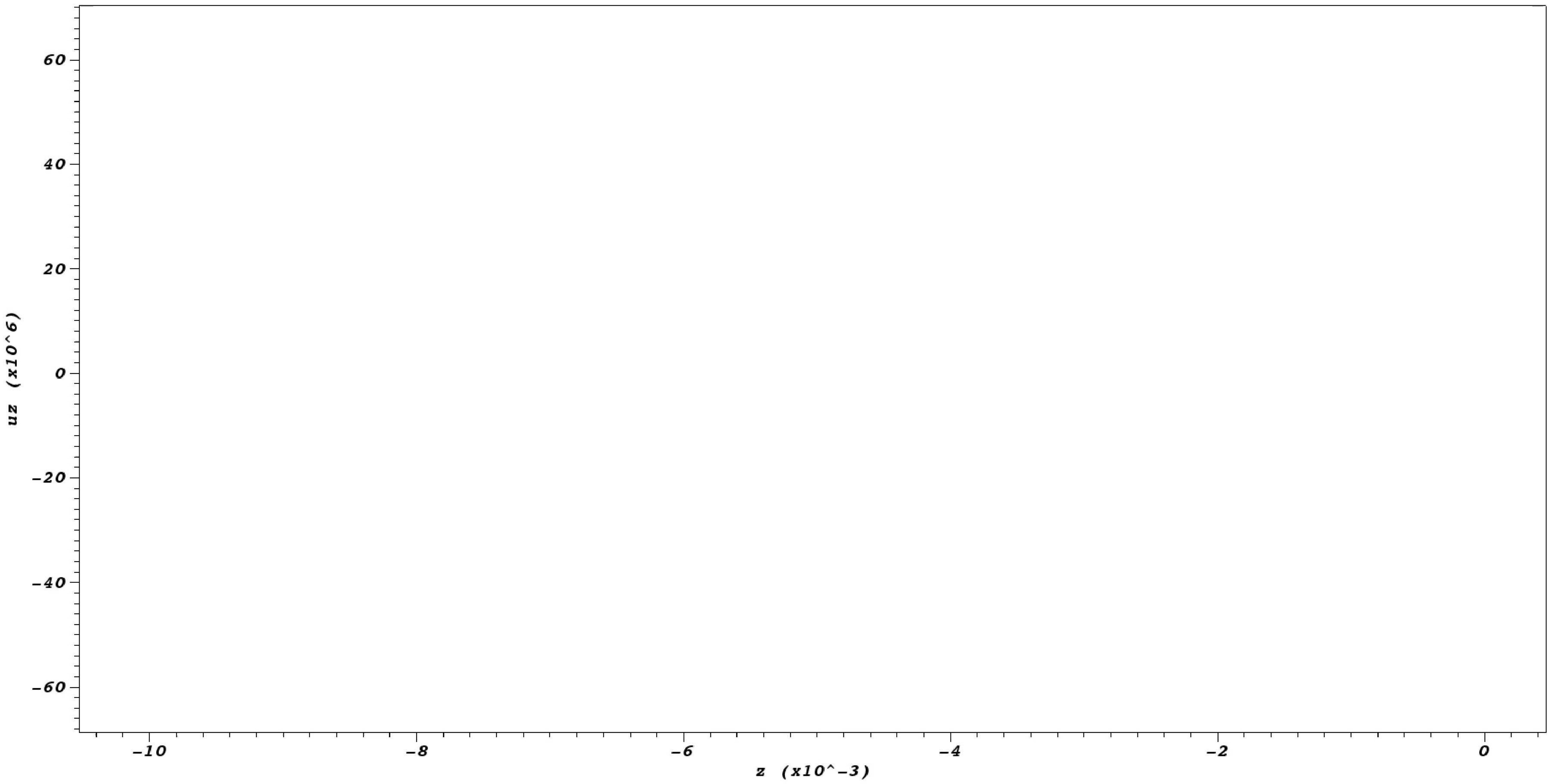
Vacuum B-dot: Electric Field in Z



Vacuum B-dot: Phase Space

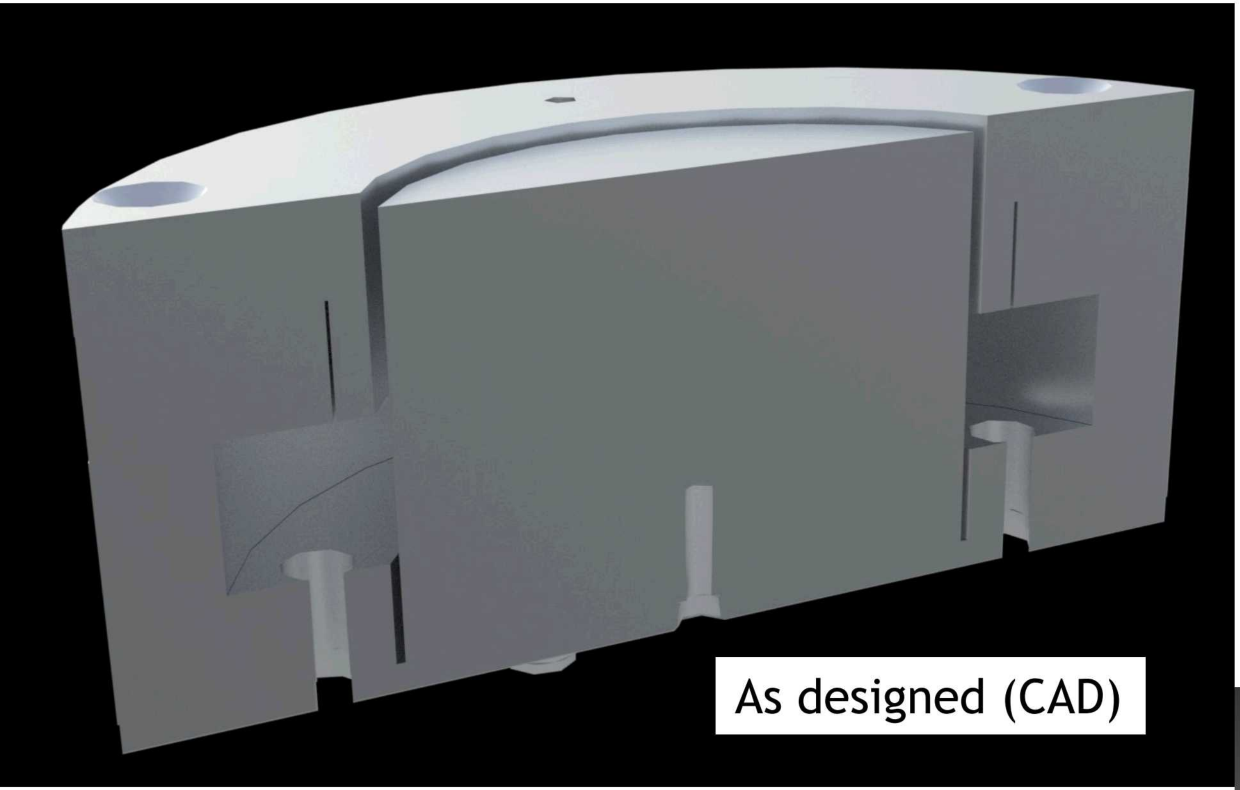
DB: BDot.h5part
Cycle: 3 Time:6.00415e-10

Au Emitter

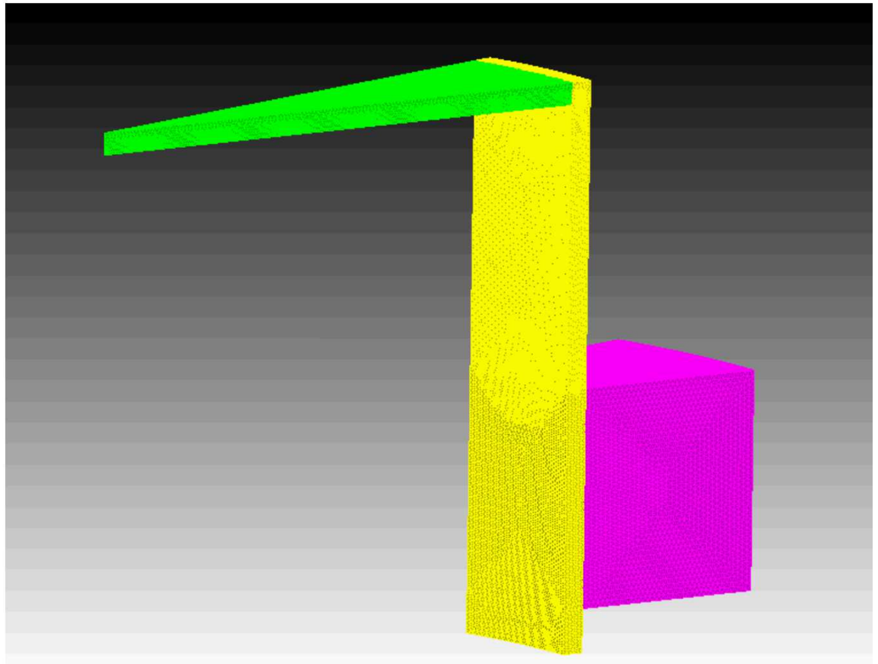


Aluminum Emitter

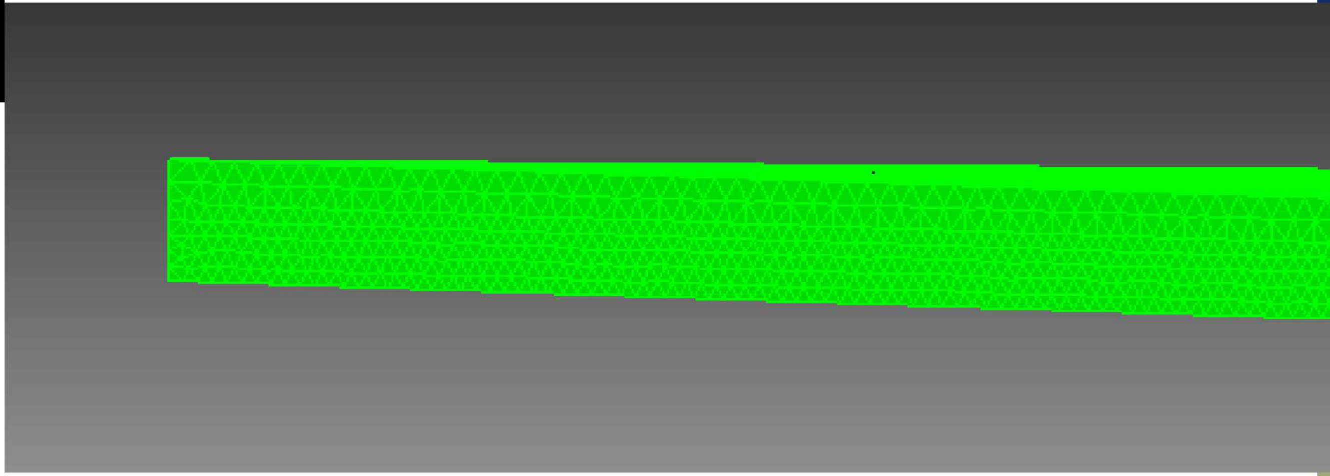
Introduction to 1mm B-Dot



As designed (CAD)



As Meshed



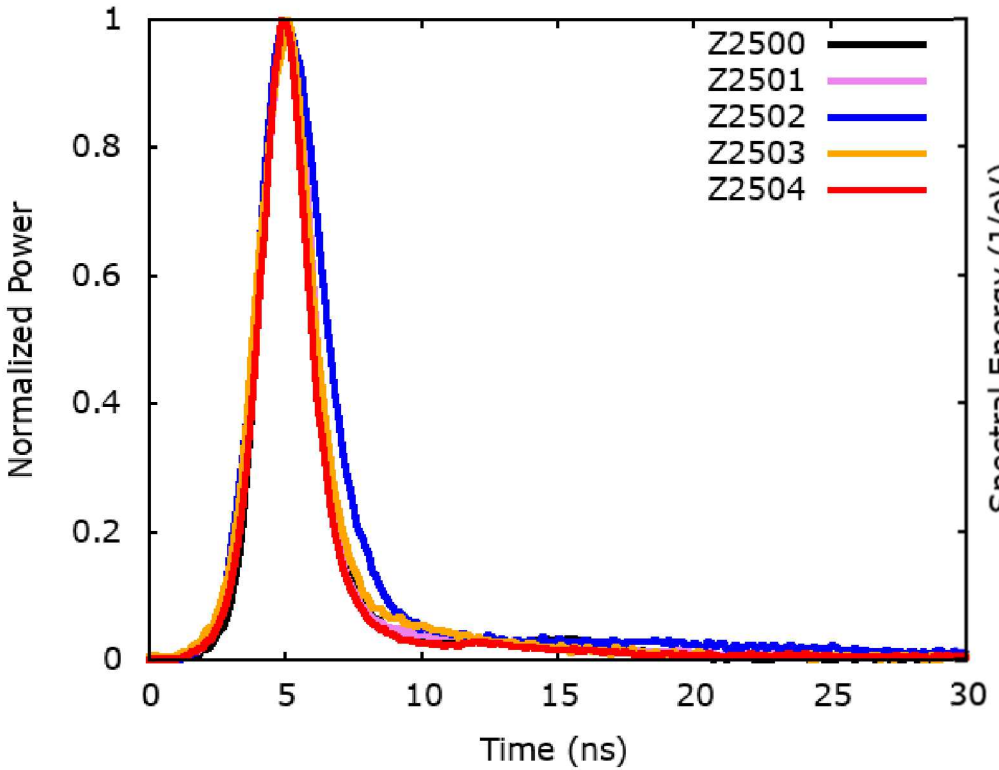
Below the space change limit

- Testing photo electron emission
- Limited out gassing from surfaces

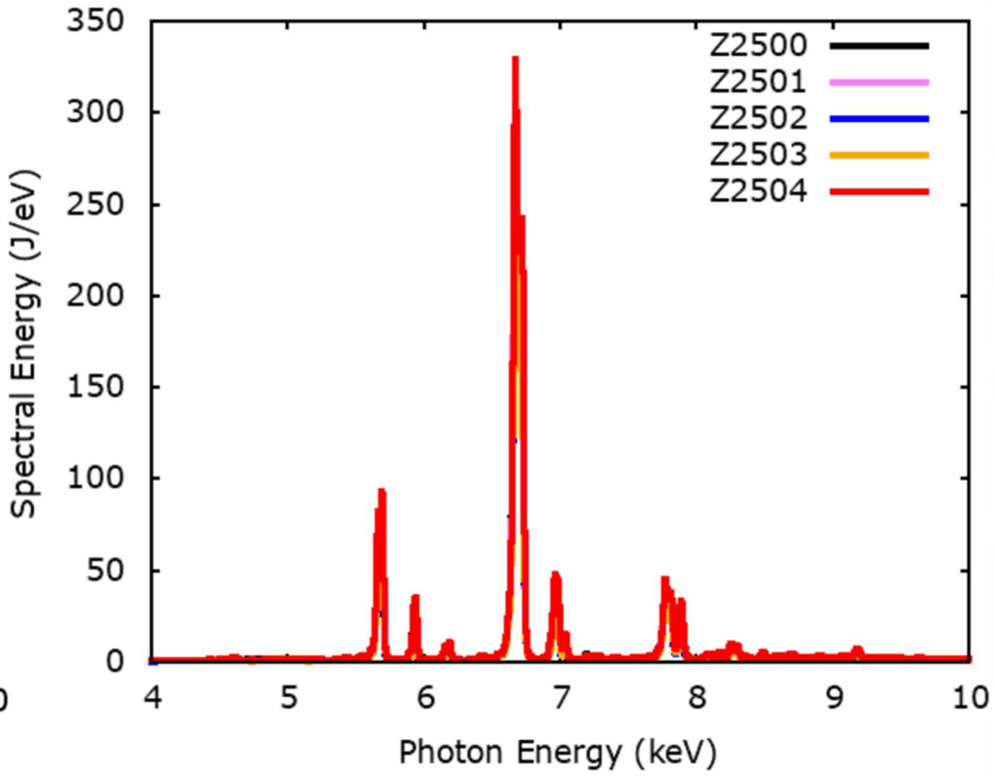
Input into Vacuum B-Dot Simulation

Shot	Yield (kJ)
2500	72 +/- 11
2501	89 +/- 14
2502	62 +/- 9
2503	60 +/- 6
2504	90 +/- 9

Yield is strongest driver



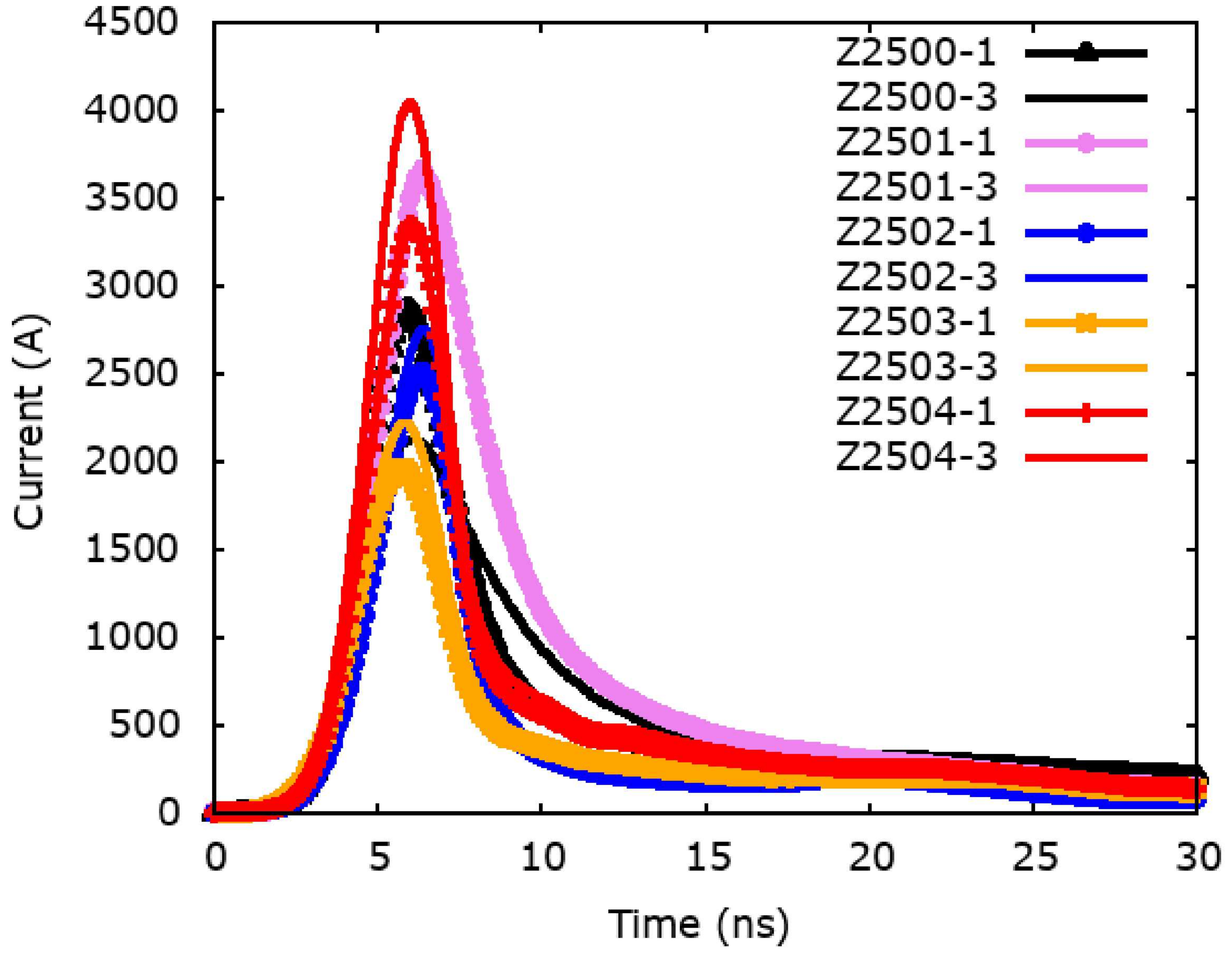
Pulse shape is second strongest driver

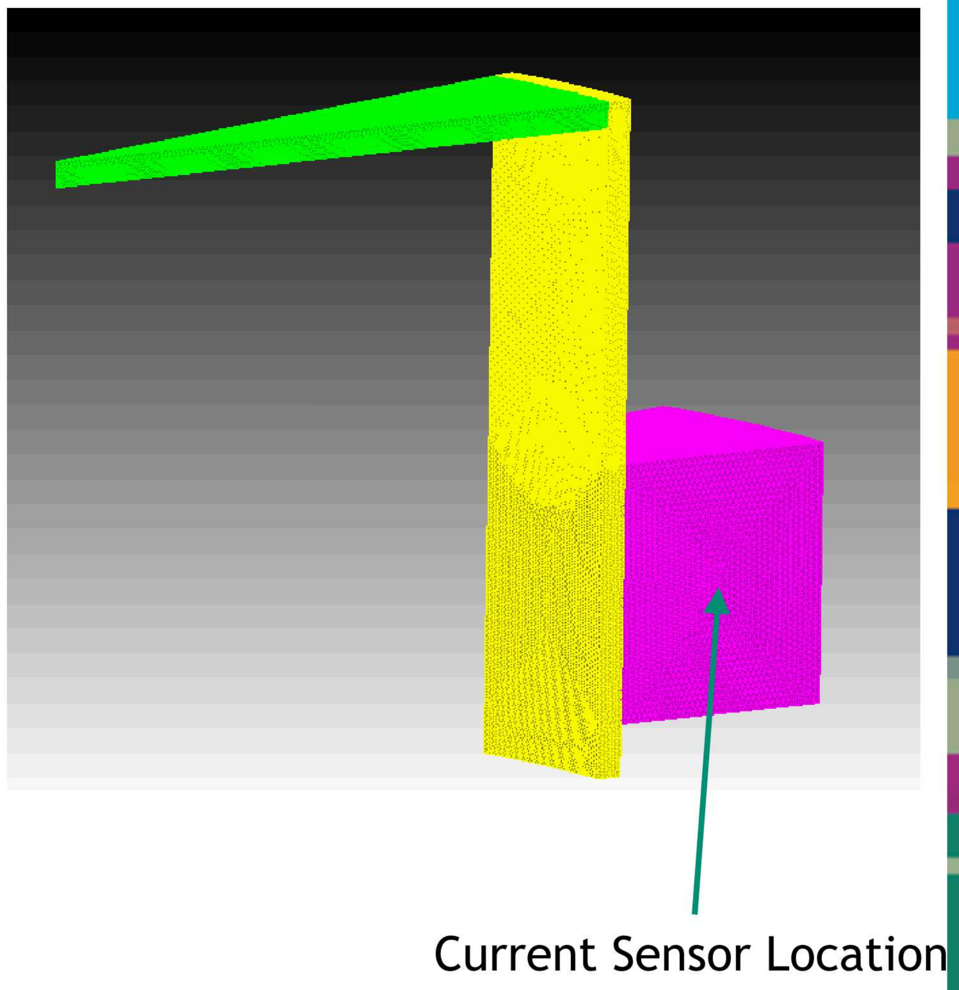


Spectrum is least driver

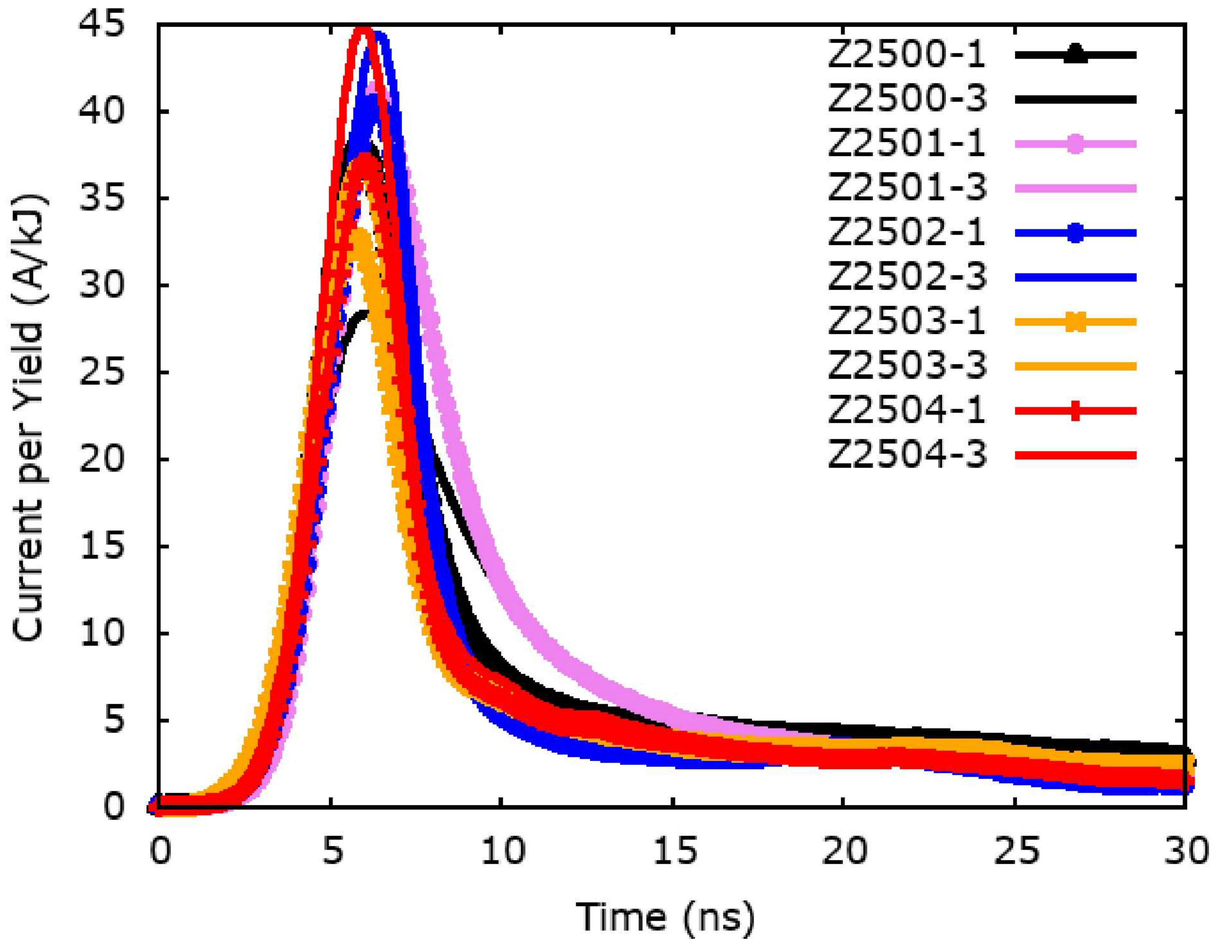
Ranking is driven by experiment variability

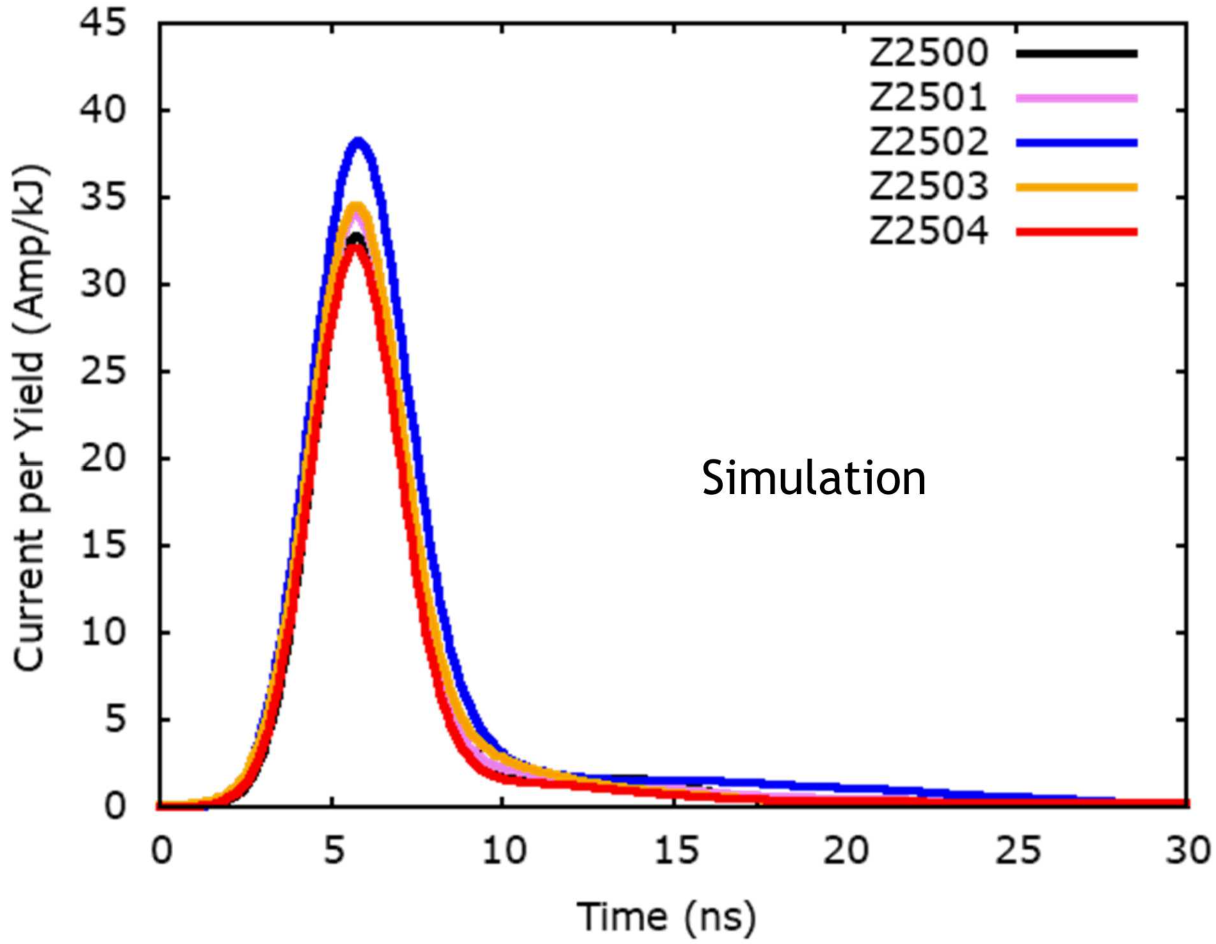
Current from Experimental





Good Experimental Comparison For Low Fluence Vacuum B-Dot





Error Bound on Z Shot 2503: 95% Confidence Interval

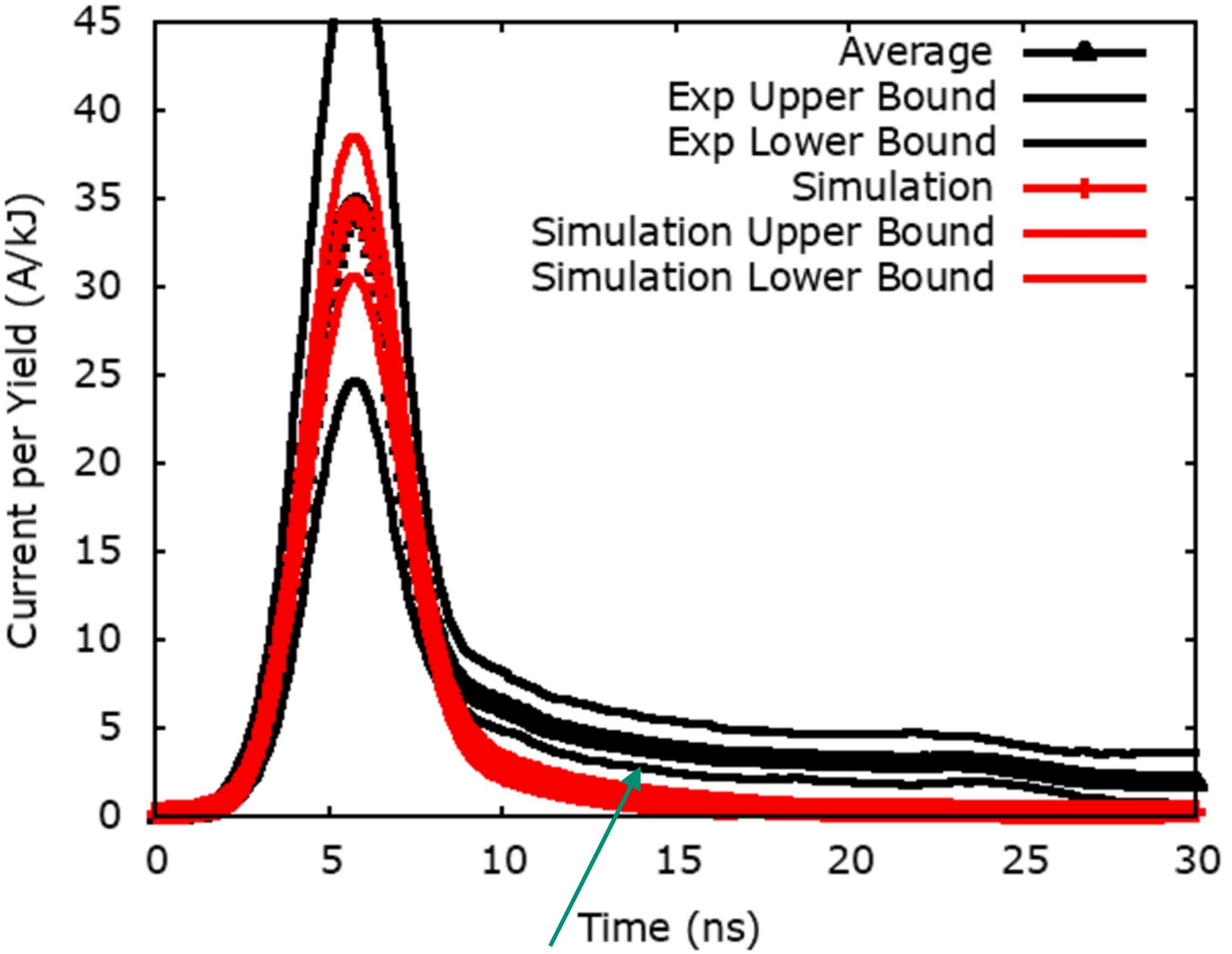
Assume 4 current sensors are independent measurements

- Use Student's *t*-distribution to estimate the bounds
- Yield is 60kJ+/-12kJ (2 sigma)

Over estimation of the error because the environment might not be the same

Simulation error is the confidence interval assuming first order in dx, dt (CFL=6), and number or particles

- dx=~height/8, ~height/16, and ~height/32

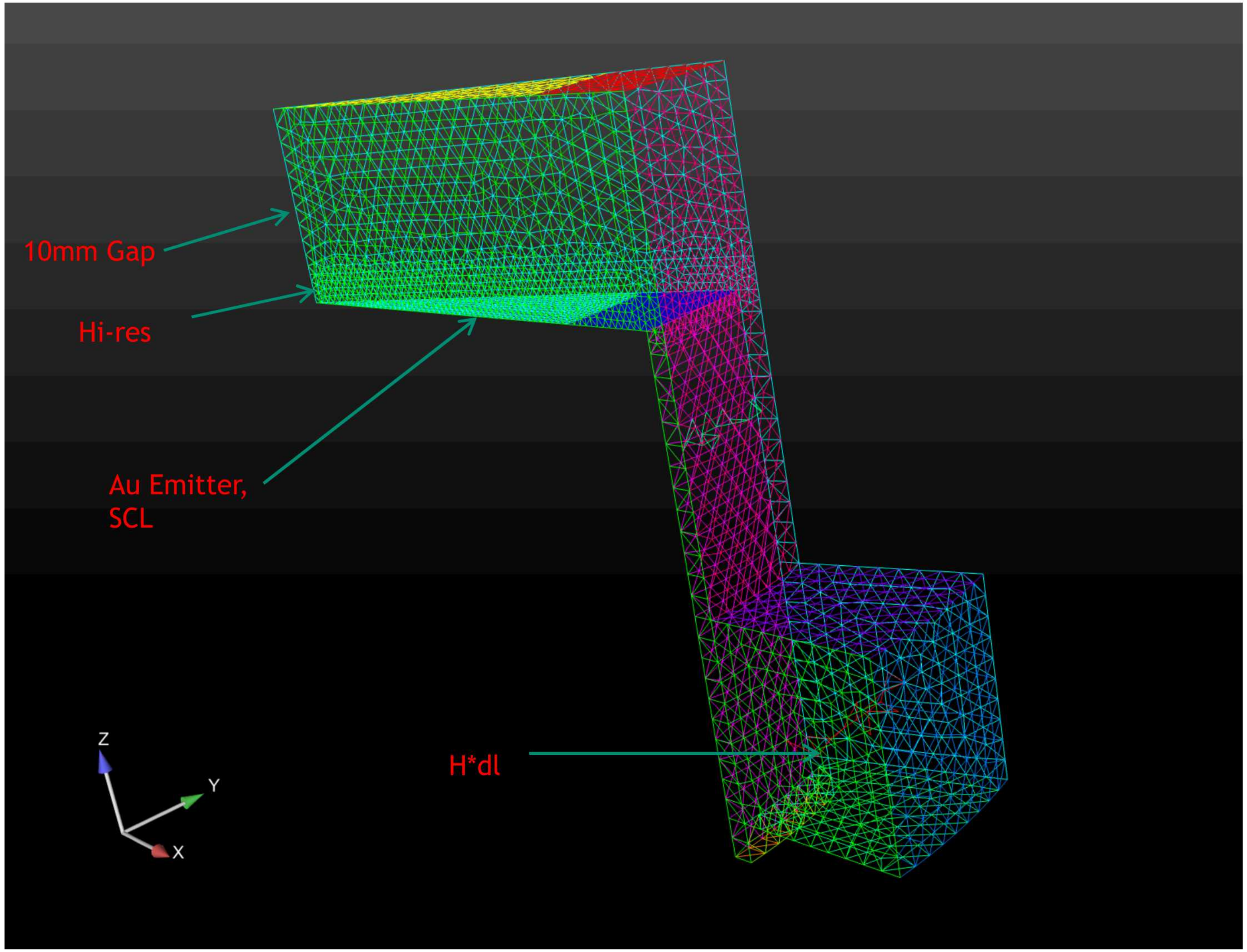


Late time current is larger in experiment could be because of outgassing

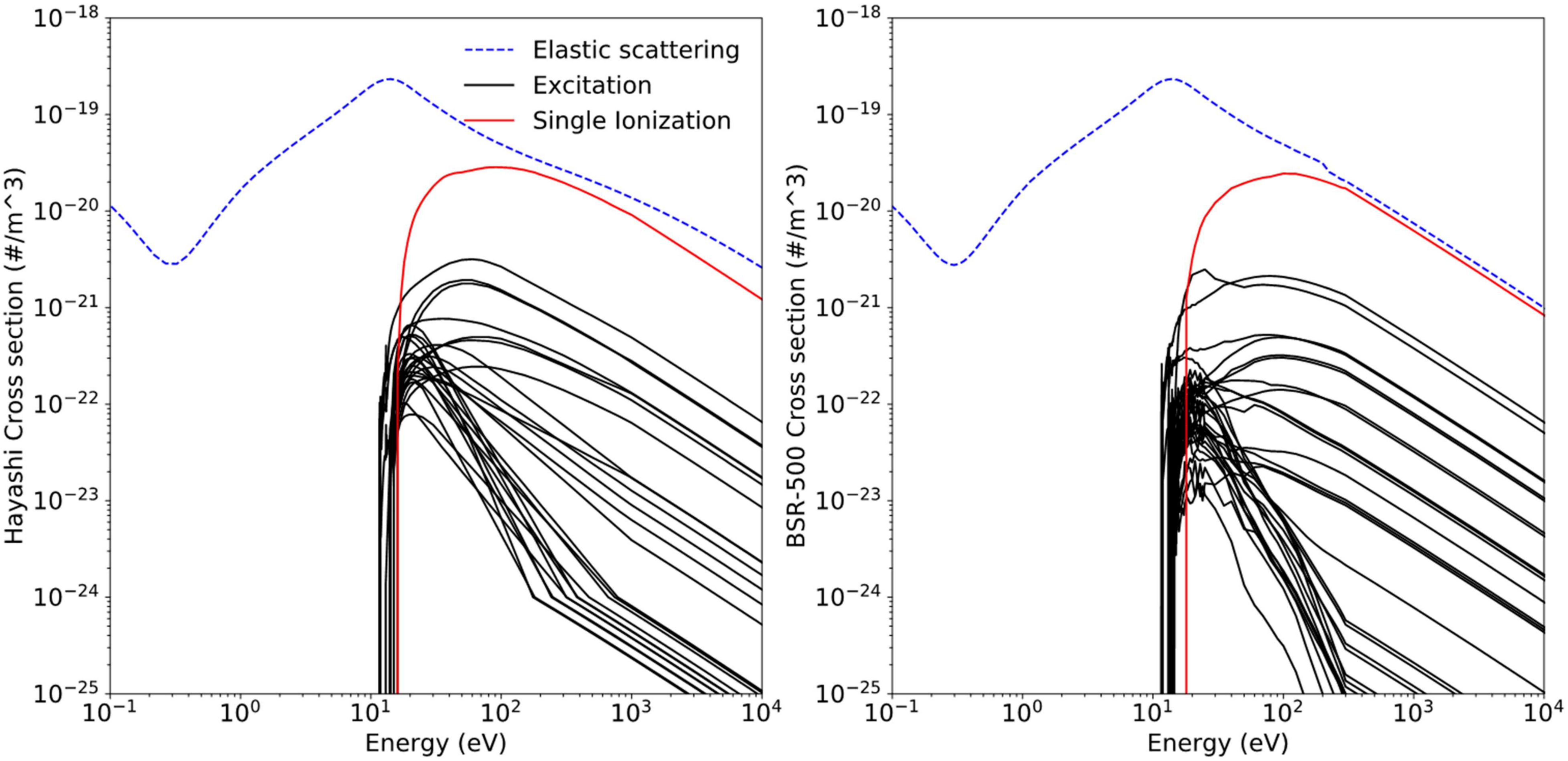
Introduction to 10mm Argon B-Dots

Goal of these experiment was to provide data with a simpler gas than N_2
- Selecting the correct Ar set of reactions and cross-section is ongoing
- Scaling/extrapolation to higher energy

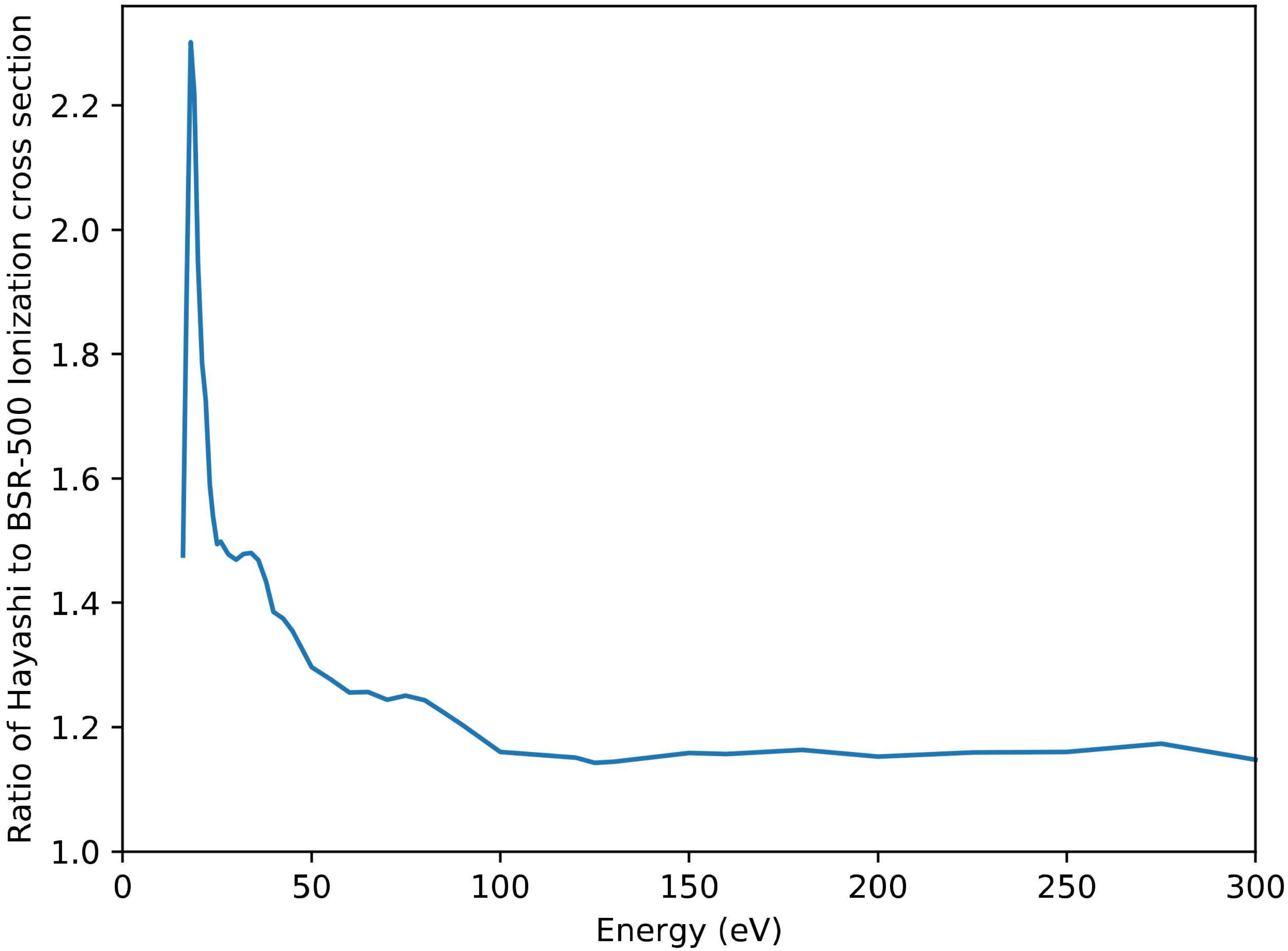
Open issues
- Differential cross-section/Energy Partitioning
- Two-step ionization
- Multiply ionized ions
- Initial ionization
- Particle merge



Argon Cross Section

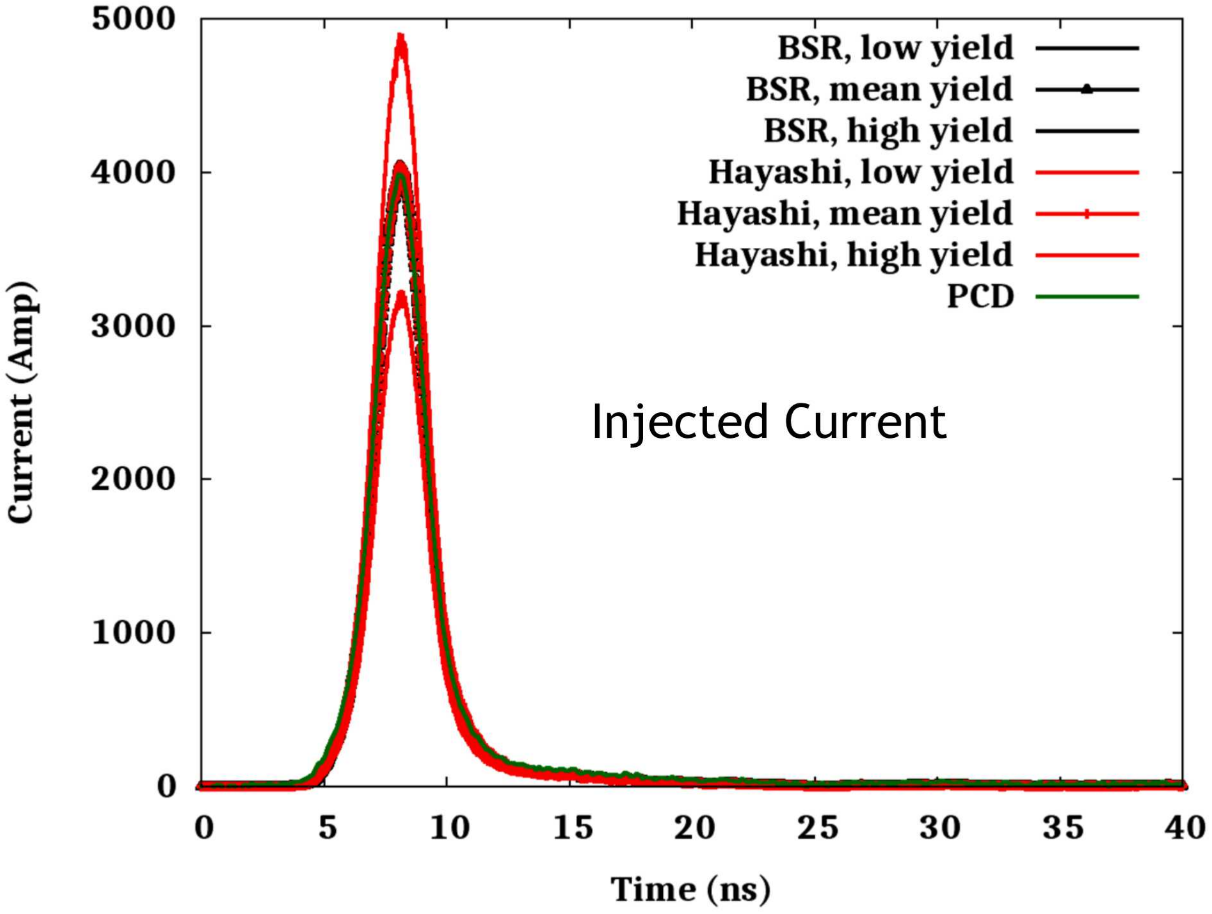


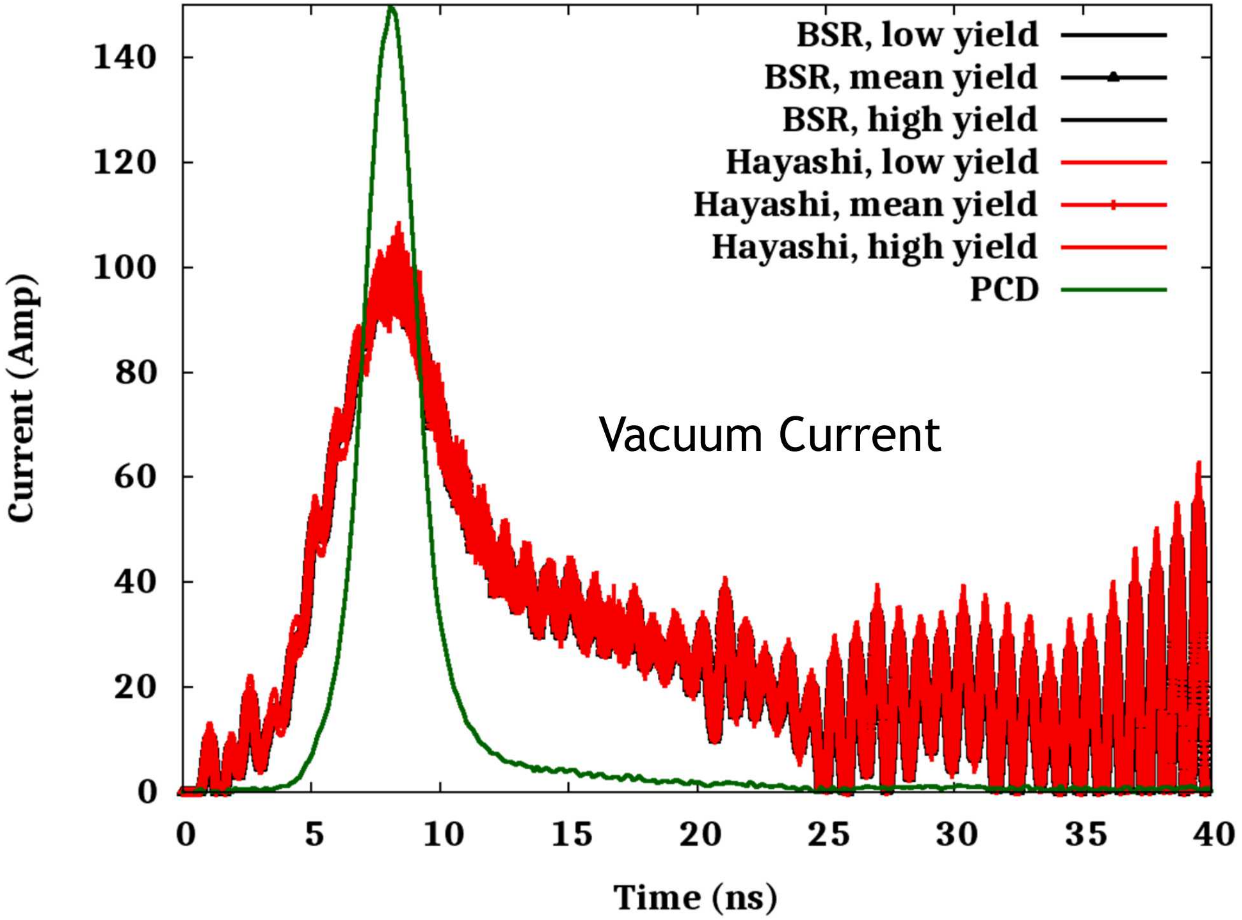
Ratio of Ionization Argon Cross Section



0mTorr Argon 10mm B-Dots

Well over the space charge limit





50mTorr Argon 10mm B-Dots

Both the Haysahi and BSR (B-spline R-matrix with pseudostates) give results lower than experiment

- Differential Cross Section
- Energy Partitioning, questionable at this energy ranges
- Two-step ionization
- Electronic excitation

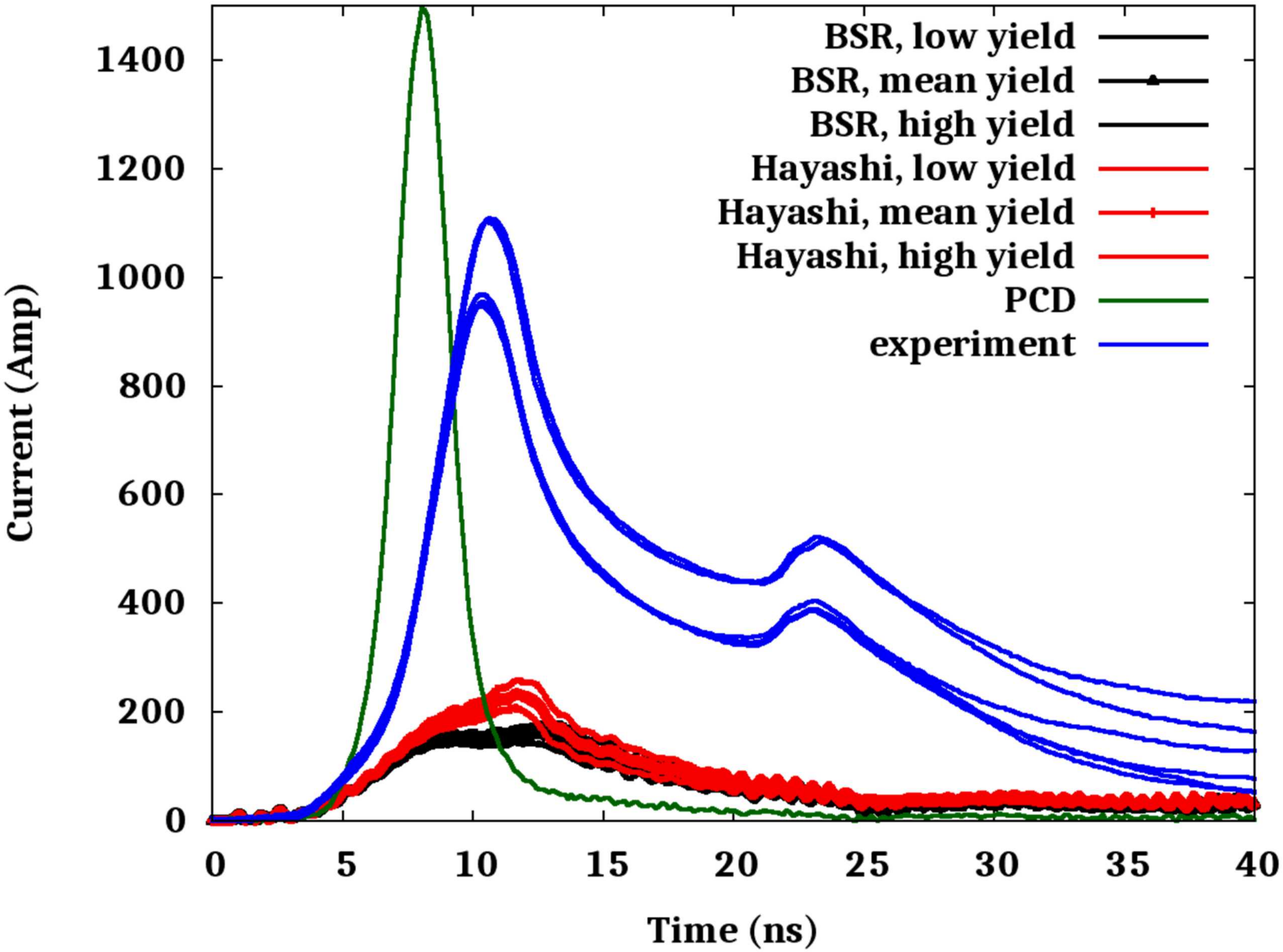
Numerical uncertainty has not been assessed

Uncertainty from yield is shown, but not gas pressure

Shape of the peak in simulations is shifted

Second peak is not seen in simulations

- Could be the PCD doesn't have enough resolution
- Could be increase gas pressure due to outgassing



100mTorr Argon 10mm B-Dots

Both the Haysahi and BSR (B-spline R-matrix with pseudostates) give results lower than experiment

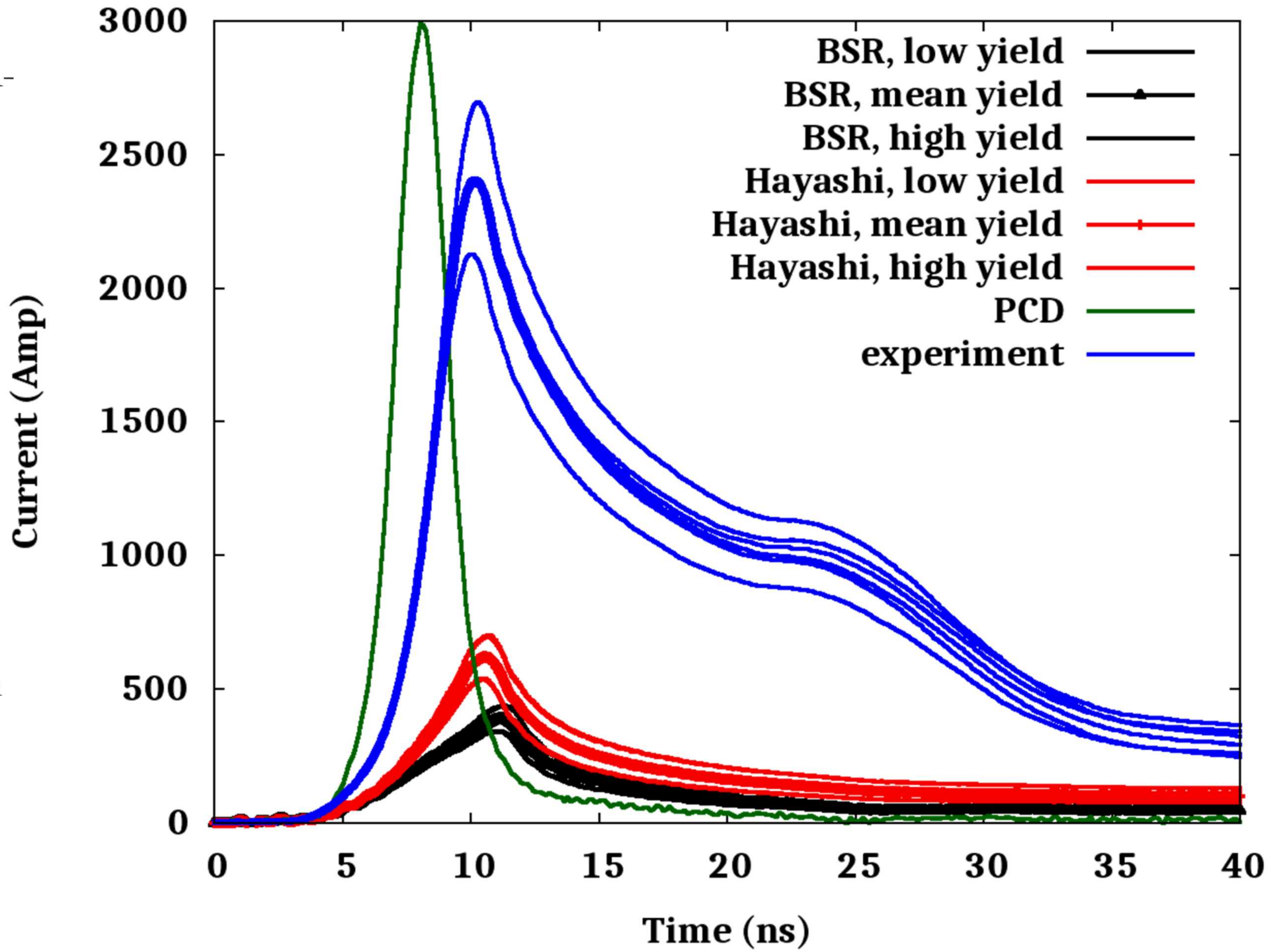
Numerical uncertainty has not been assessed

Uncertainty from yield is shown, but not gas pressure

Shape of the current with the Hayashi cross-section looks closer to experiment

Second peak is not seen in simulations

- Could be the PCD doesn't have enough resolution
- Could be increase gas pressure due to outgassing



200mTorr Argon 10mm B-Dots

Both the Haysahi and BSR (B-spline R-matrix with pseudostates) give results lower than experiment

Numerical uncertainty has not been assessed

- Numerical heating is large at late time

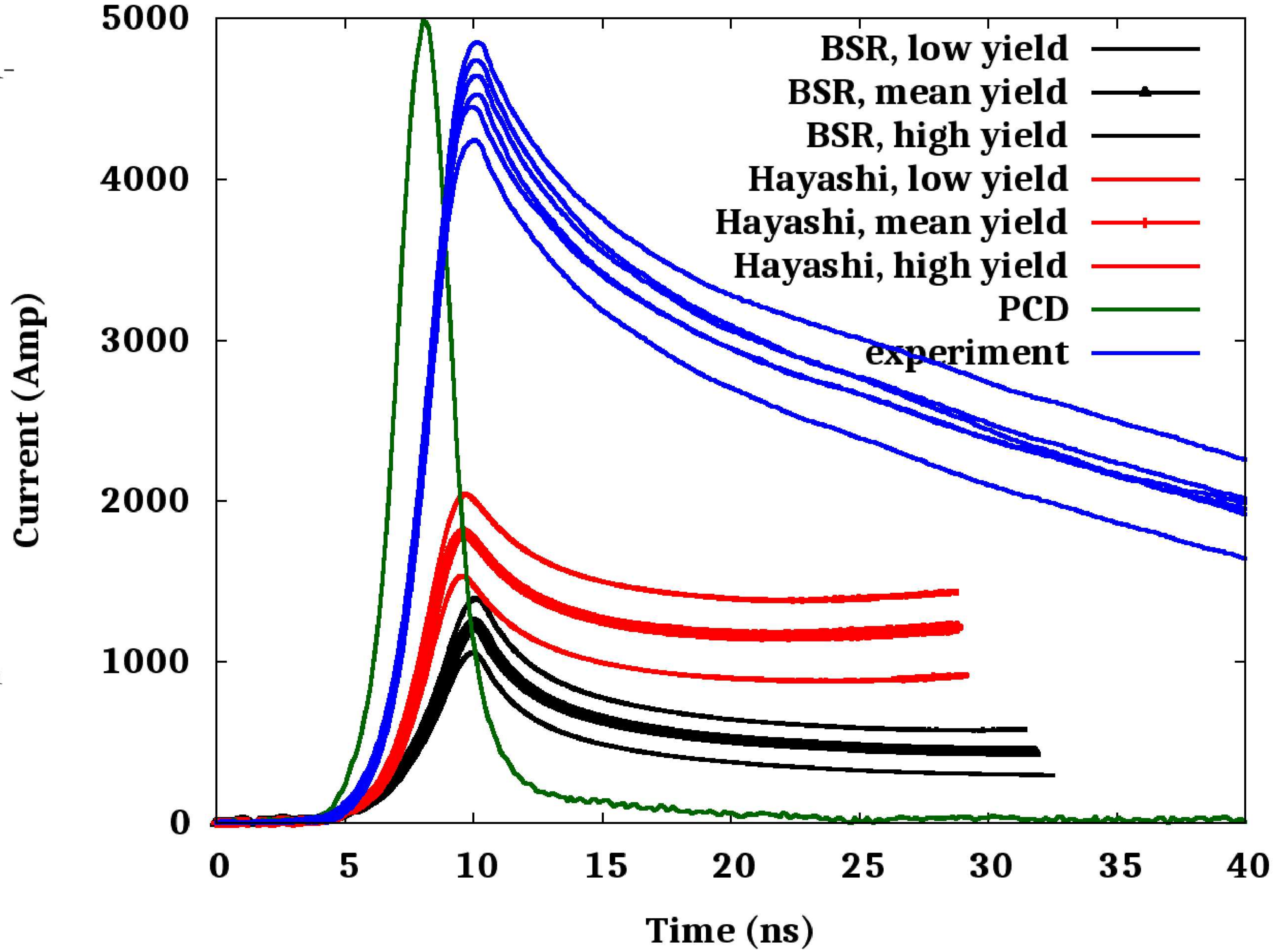
Uncertainty from yield is shown, but not gas pressure, etc.

Shape of the current with the Hayashi cross-section looks closer to experiment

Second peak is not seen in simulations

- Could be the PCD doesn't have enough resolution
- Could be increase gas pressure due to outgassing

70M Ar particles



300mTorr Argon 10mm B-Dots

Both the Haysahi and BSR (B-spline R-matrix with pseudostates) give results lower than experiment

- At 300mTorr the difference between BSR and Hayashi is less

Numerical uncertainty has not been assessed

- Numerical heating is large at late time

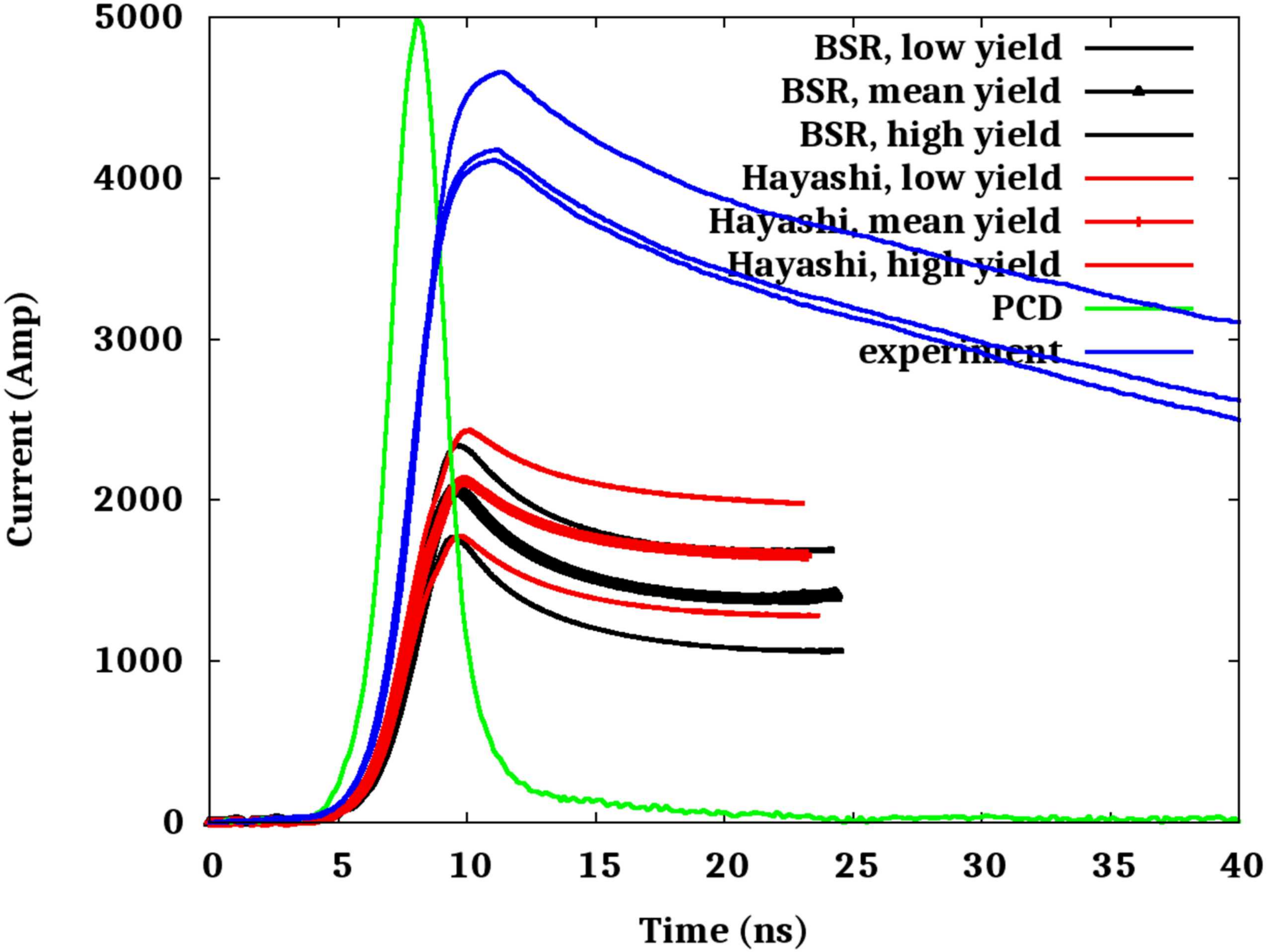
Uncertainty from yield is shown, but not gas pressure, etc.

Shape of the current with the Hayashi cross-section looks closer to experiment

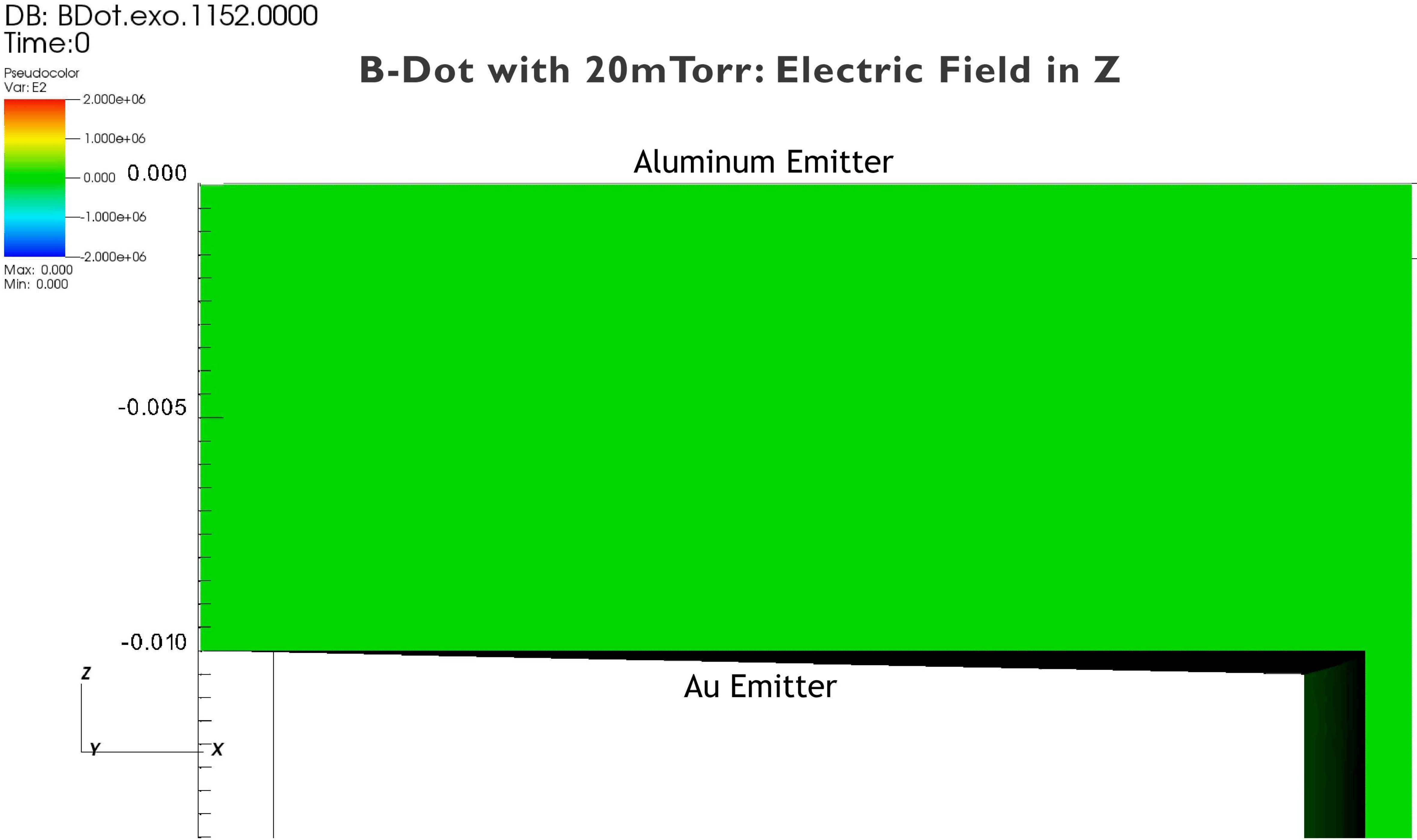
Second peak is not seen in simulations

- Could be the PCD doesn't have enough resolution
- Could be increase gas pressure due to outgassing

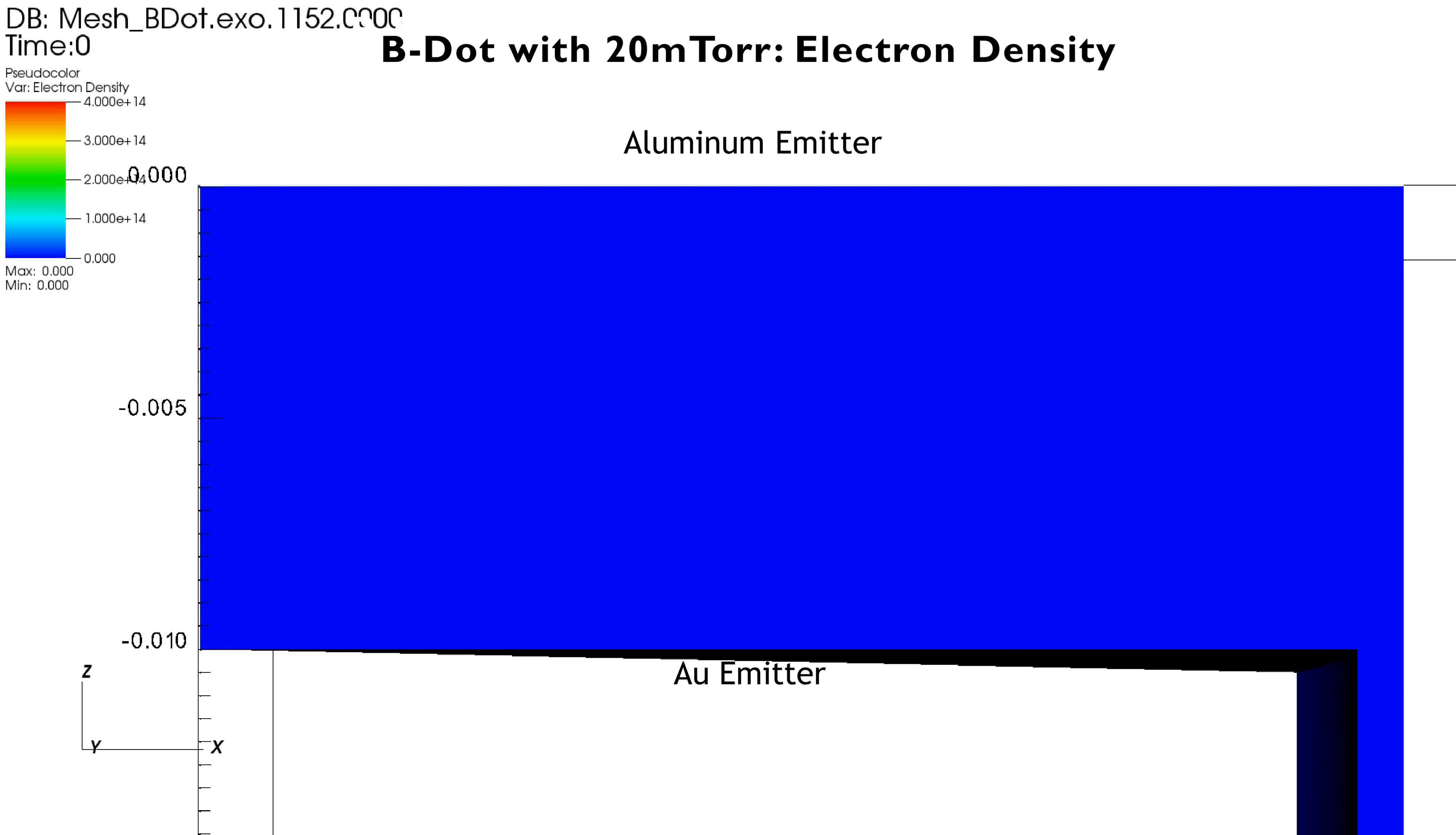
70M Ar particles



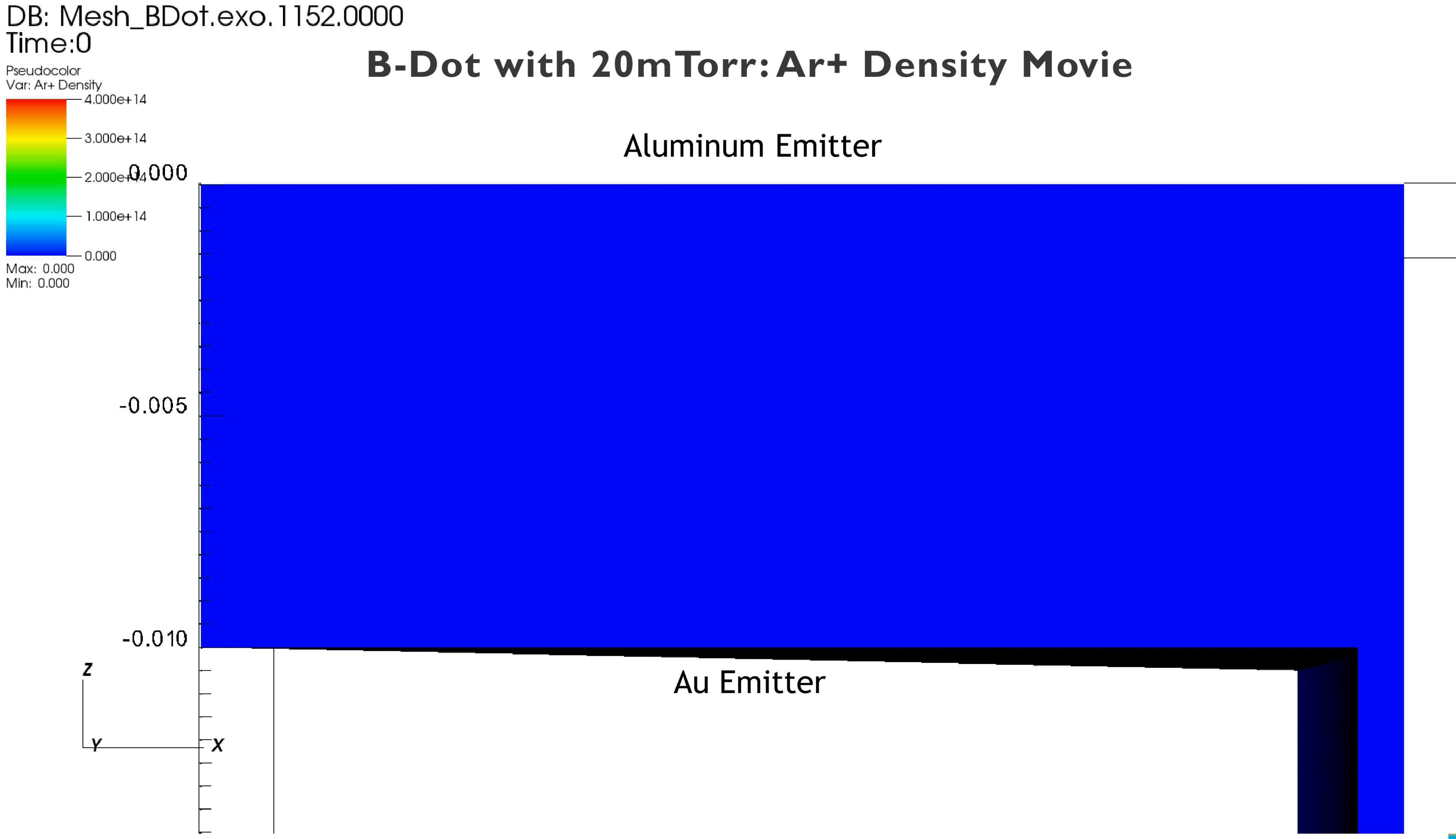
B-Dot with 20mTorr: Electric Field in Z



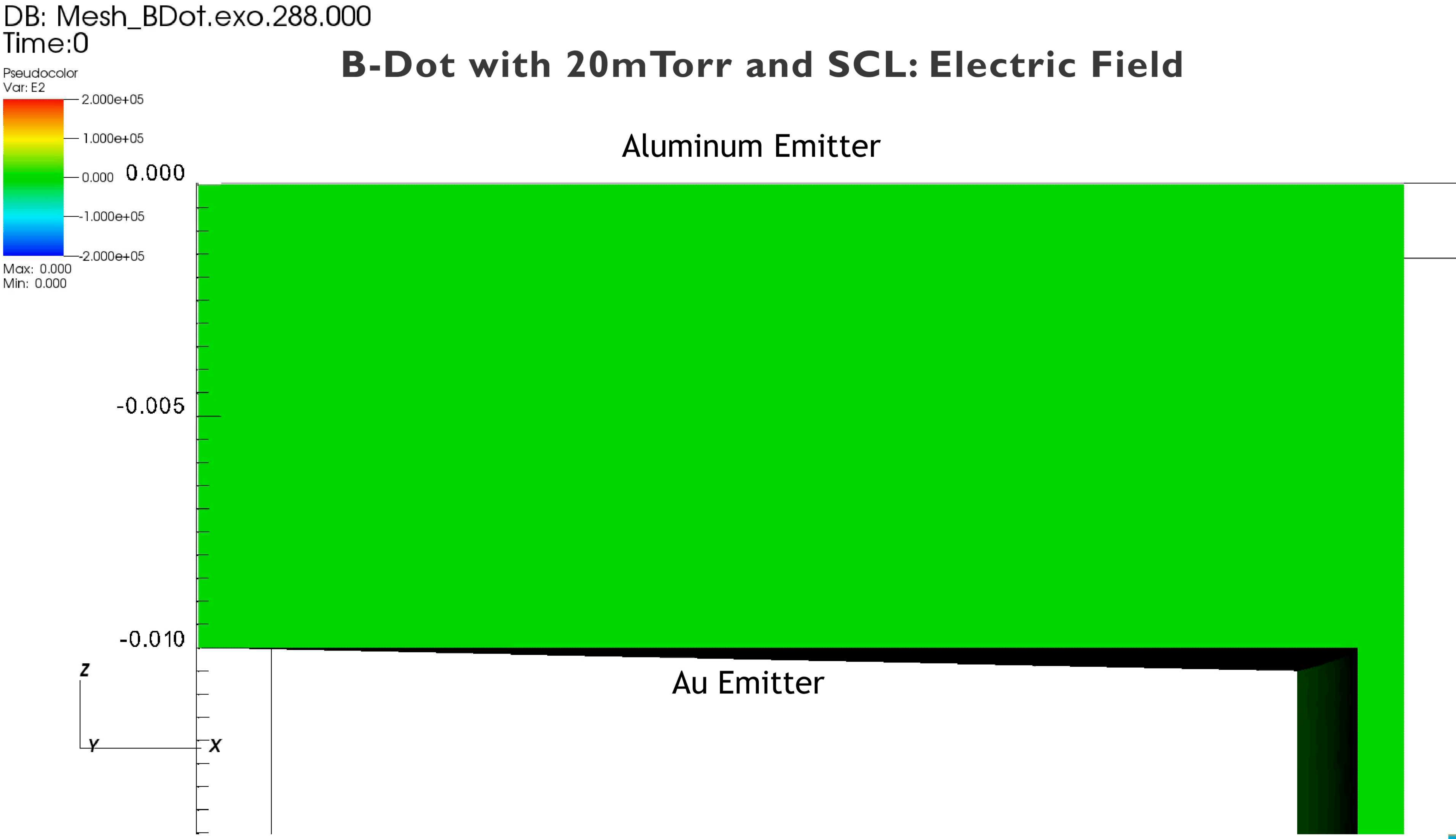
B-Dot with 20mTorr: Electron Density



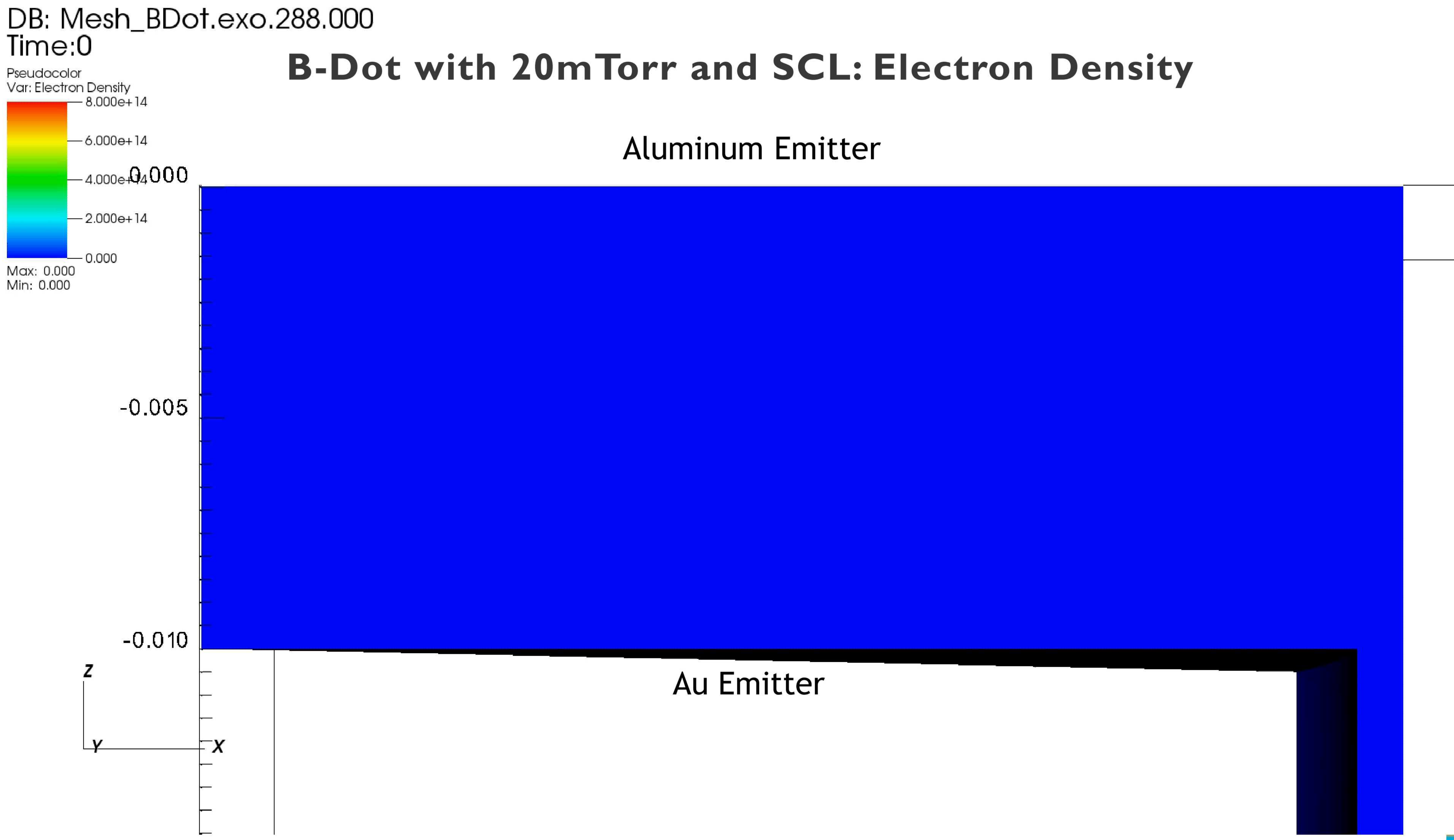
B-Dot with 20mTorr: Ar+ Density Movie



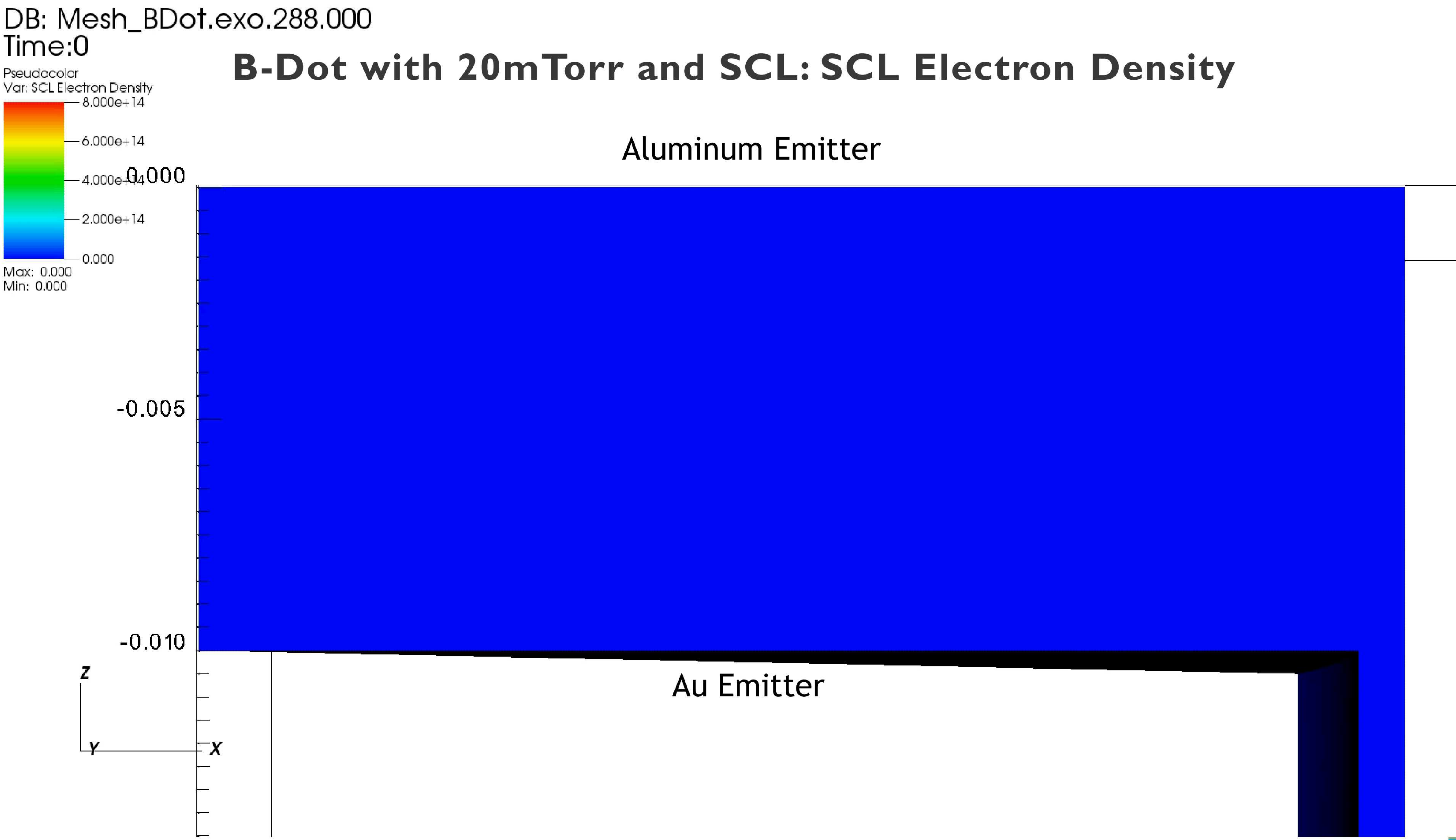
B-Dot with 20mTorr and SCL: Electric Field



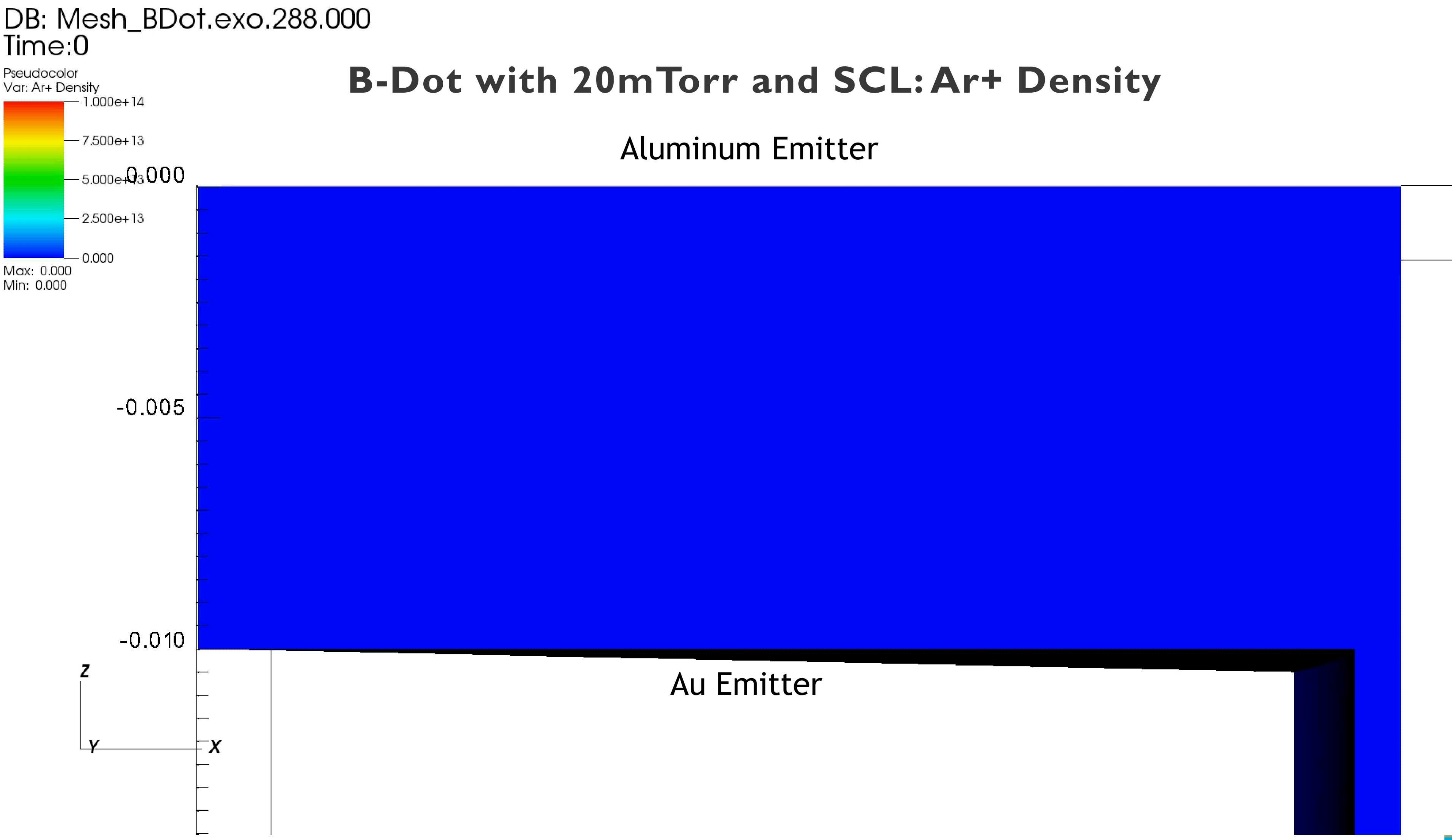
B-Dot with 20mTorr and SCL: Electron Density



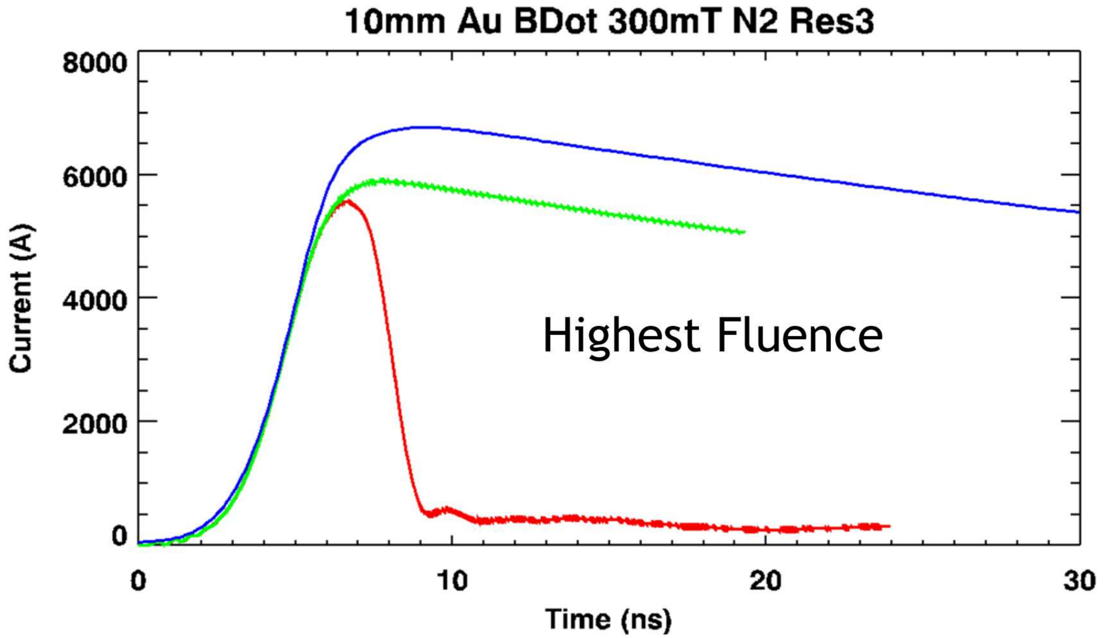
B-Dot with 20mTorr and SCL: SCL Electron Density

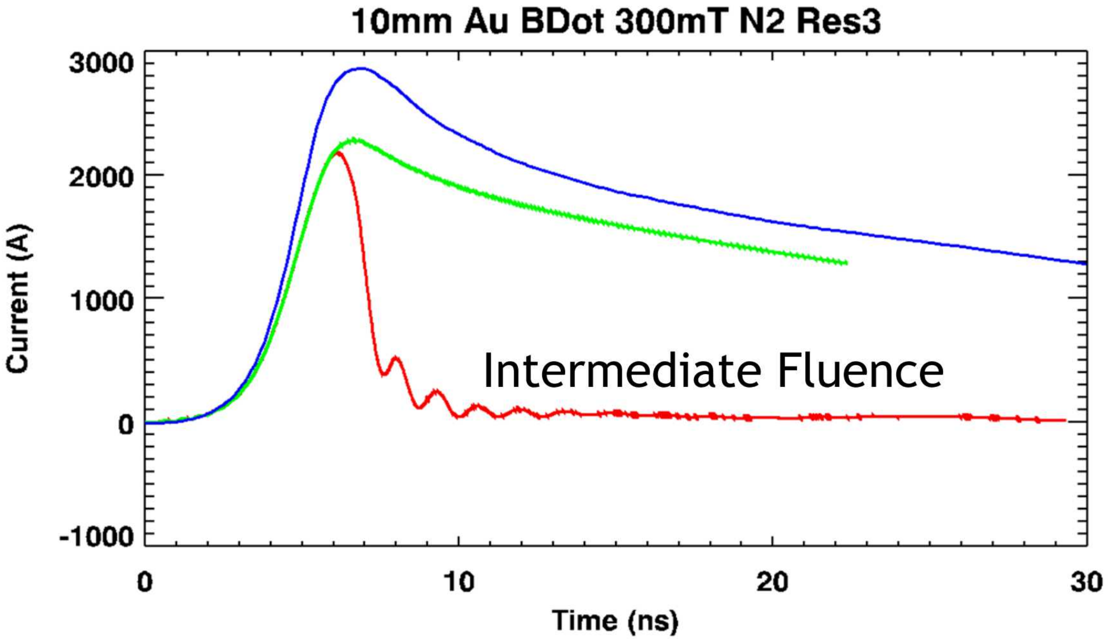


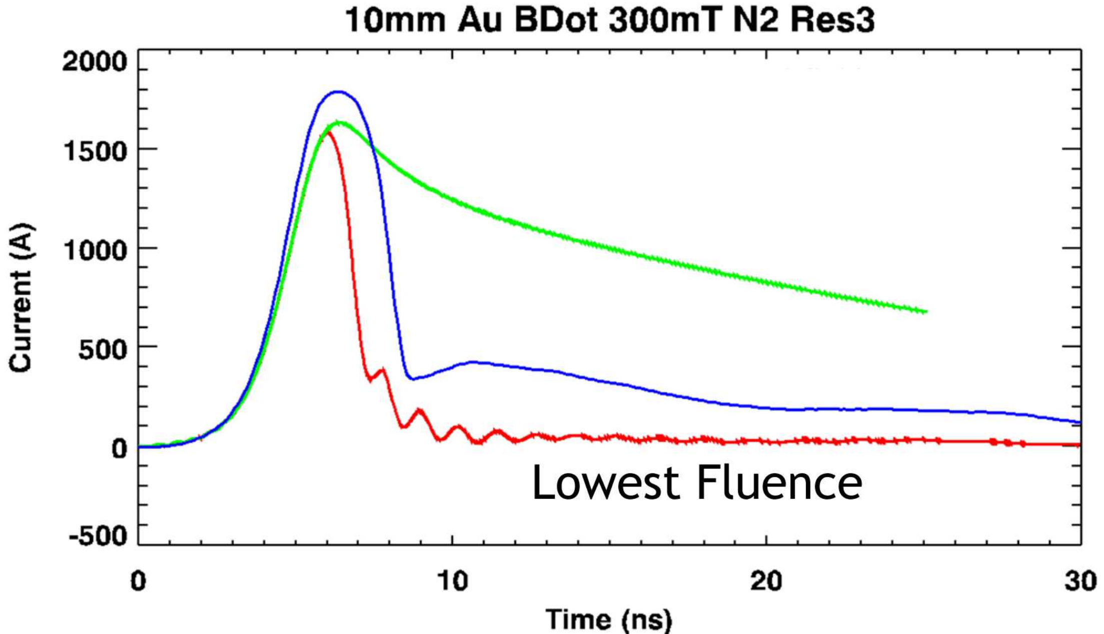
B-Dot with 20mTorr and SCL: Ar+ Density



Focusing on the Uncertainty of the Surface Emission







Red is simulations without SCL
Green is simulation with SCL
Blue is Measurement

10 mm, N2 filled, B-Dot, fluence scan

- N2 Collisions control the current ramp: good collision set
- Surface plasma models control the shape of the tail: not predictive, but captures the phenomenon

Conclusions

There is a lot of physics that need to come together to simulate radiation driven cavities

- Electromagnetics: Finite Element
- Chemistry/Collisions: DSMC
- Plasma Facing Surface: Heating and desorption/emission (See Nick Roberds Poster for more details)