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Towards EM/ES hybrid Fluid-PIC simulations of arc discharge in EMPIRE

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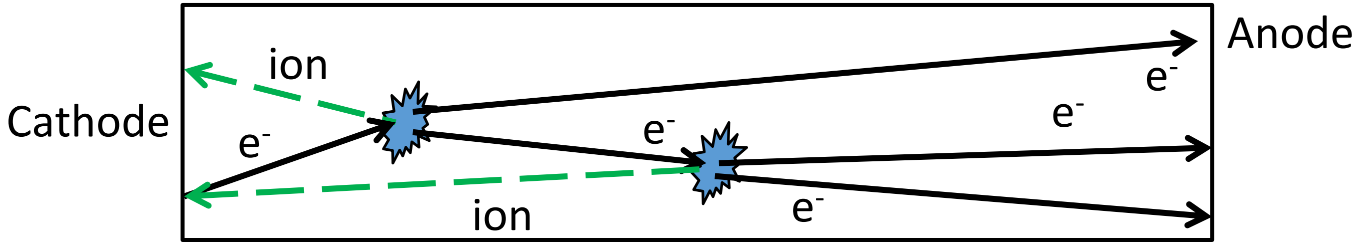
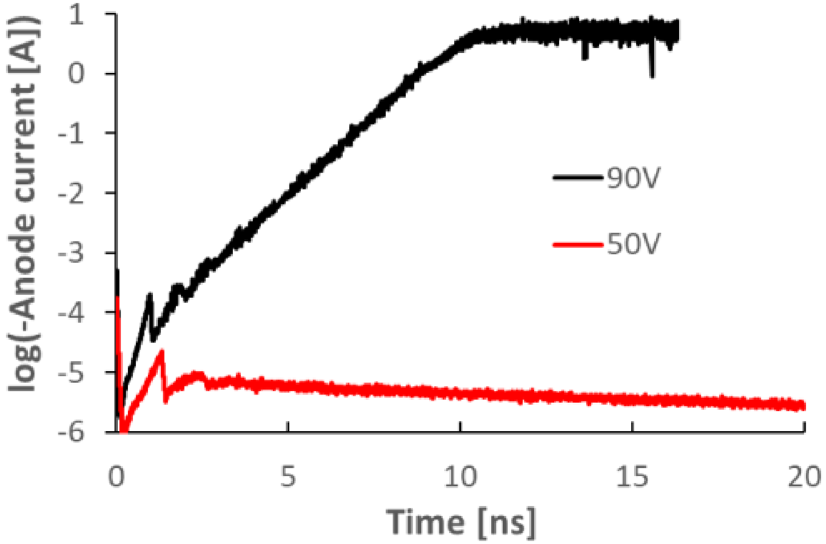
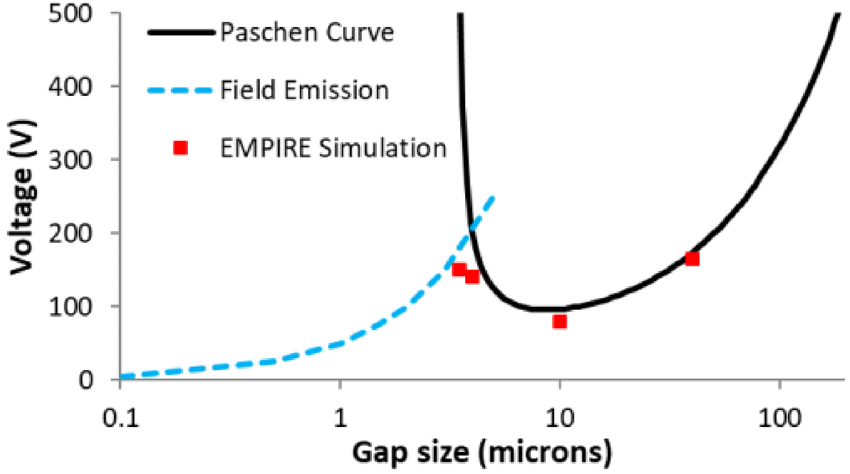
EMPIRE

- EMPIRE is a "new" code with the lofty goal of solving plasma problems across a large range of density ranges on unstructured meshes
  - Goal to have PIC, Fluid, and Hybrid capability
  - Built to be scalable from the start (Bettencourt's talk)
  - Electrostatic and Electromagnetic Maxwell solvers
  - Transmission line model (Edward and Duncan's talk)
  - DSMC and MCC collisional models: e.g. ionization, excitation
  - Surface physics: e.g. thermal desorption (David and Nick's talk), ion-induced SEE
- Paschen curve: Test case for self-sustained discharge physics (ion-induced SEE and collision models)



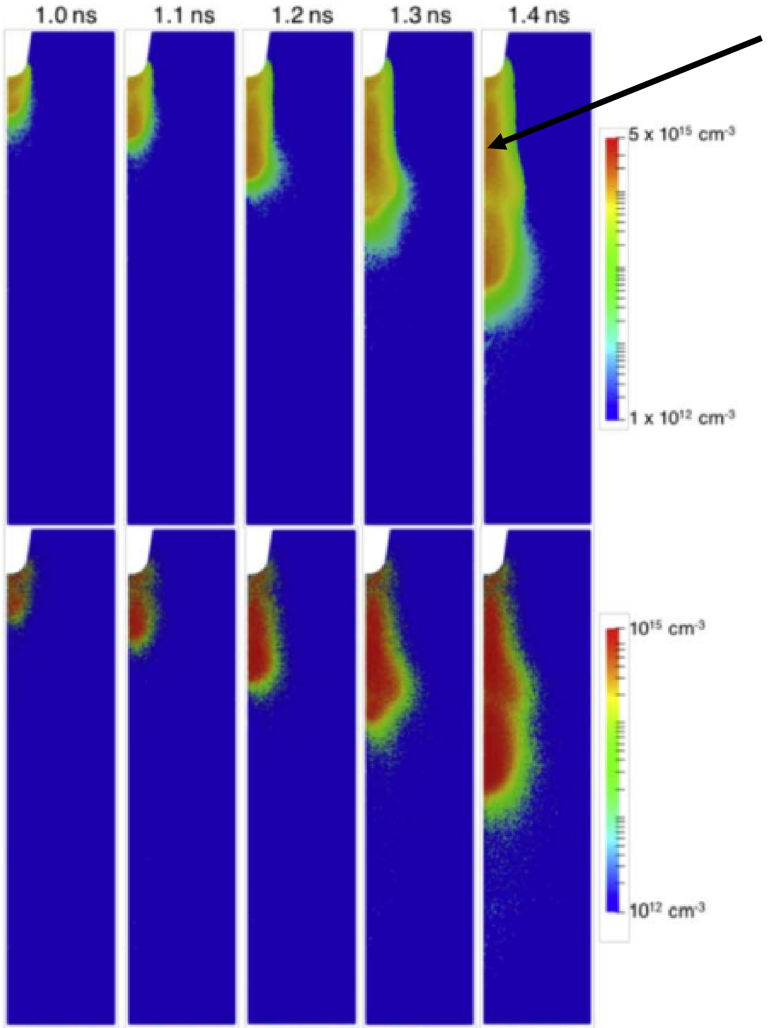


Current vs. time for 10 μm Gap at different voltages. Current decays for $V < V_B$



EMPIRE simulation of Paschen curve (Ar)

Atmospheric Pressure Simulations - motivation

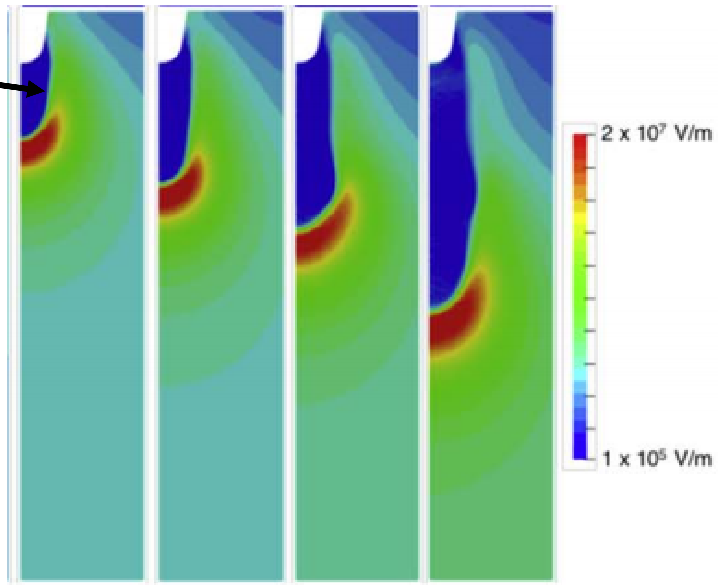


Dense Plasma Core

At atmospheric pressure, the formation of positive ionization waves (Streamers) are possible. Characterized by:

- Propagation due to new electrons ahead of the ionization front – photoionization, field detachment, photo emission
- A dense plasma core where the electric field is screened out.

Small electric field



Fully spatially resolved simulations – num elements = ~180 million, L = ~250 micron

A. Fierro, *et al.*, Plasma Sources Sci. Technol., **27**, 105008, 2018.

The (current) Hybrid Approach

GOAL: Implement this atmospheric pressure ionization wave in a hybrid simulation

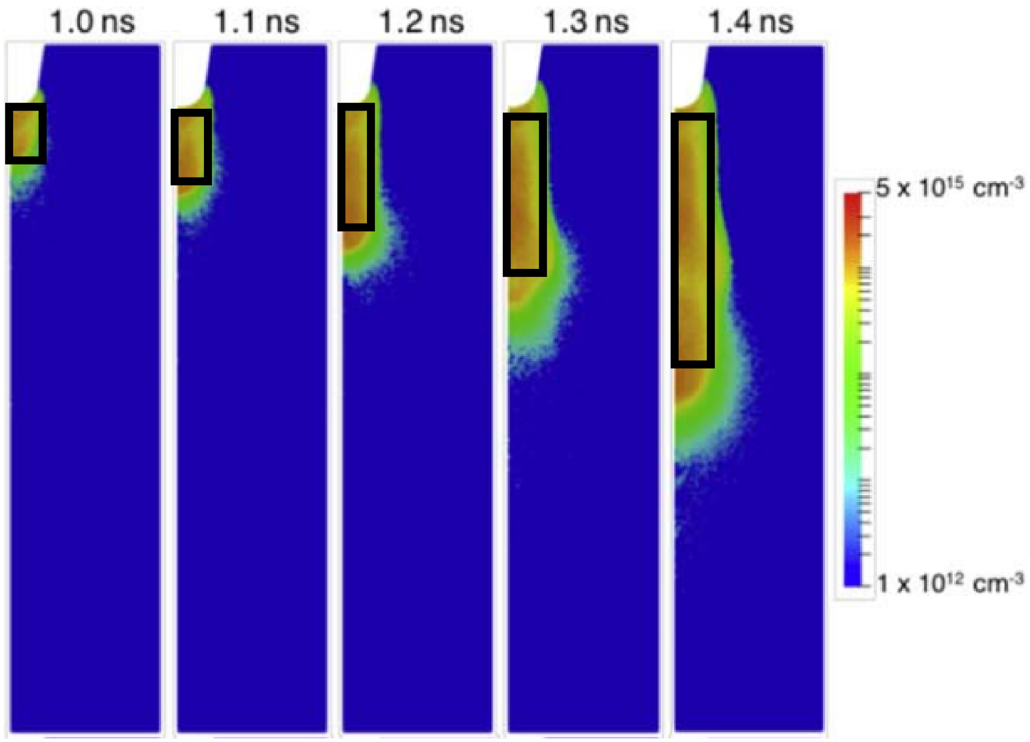
Hybrid in this context refers to in a single simulation, a representation of charged and neutral species by both fluids and particles

- Ideally, some transfer of information between the two representations
  - particle electrons ↔ fluid electrons

Kinetic in this context refers to every species being modeled as particles

Due to the dense and cold plasma core, λ_D very small → small space steps! Can we instead represent this area of a fluid?

- In this work, we are showing the beginning stages of model development and testing and just modeling the neutral states as a fluid as previous results were done with a different code (Aleph)
  - Leads to MCC
  - Testing components in this regime as they become available from developers



▯ Proposed fluid regions

Can lead to two improvements: relaxed mesh sizing and reduced particle counts over full Direct Simulation Monte Carlo (DSMC) approach

A. Fierro, *et al.*, Plasma Sources Sci. Technol., **27**, 105008, 2018.

A simplified gas model

Focused on the propagation of positive streamer at atmospheric pressure. Not necessary to have a real gas environment.

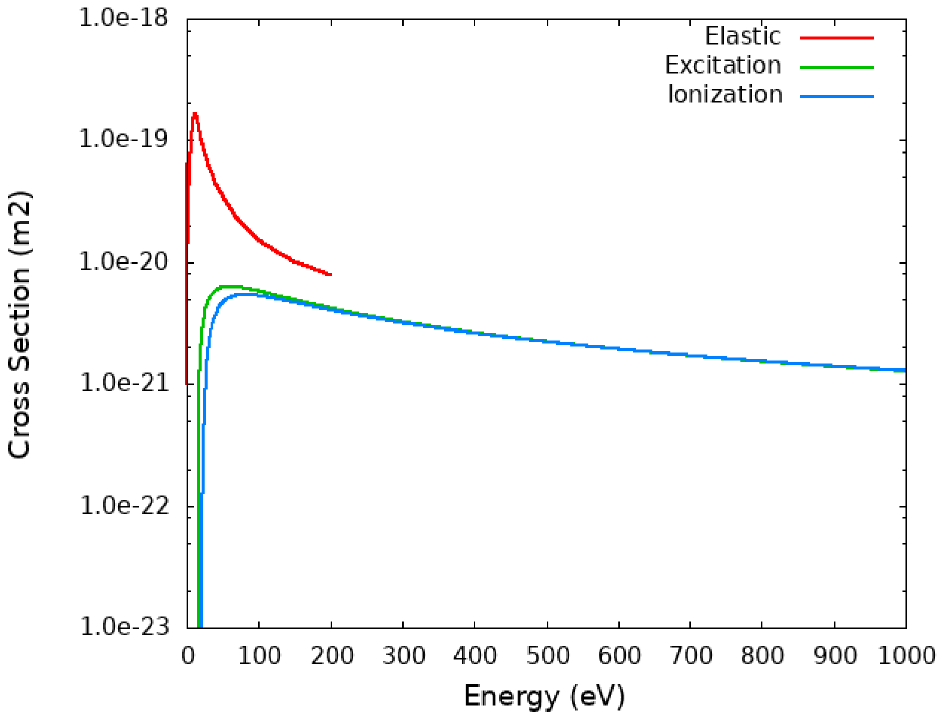
Three included collision mechanics:

- Elastic (taken from helium)
- Excitation (single process)
- Ionization

Excitation and ionization cross section created from the form

$$\sigma(E_s) \cdot E_s = A \ \ln E_s + \frac{[B \ln E_s + C(E_s - 1)]}{E_s + D}$$

COEFFICIENT	EXCITATION	IONIZATION
A	0.75	0.75
B	-5.5	-5.0
C	6.0	4.0
D	3.0	0.5
THRESHOLD ENERGY (E_{th})	15 eV	20 eV



In the future: can study different photonic effects on the propagation of the ionization wave (e.g. photon absorption length)

Y. Kim, J. Res. Natl. Inst. Stand. Technol., 1992.

One-dimensional electron avalanche

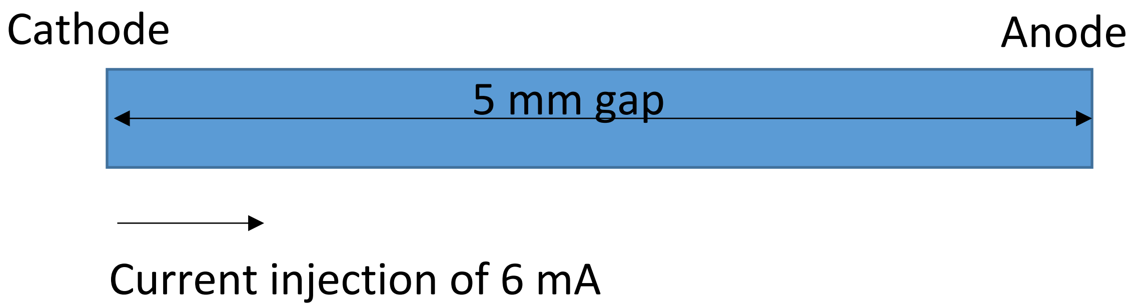
Compare one dimensional electron avalanche for fully kinetic vs. hybrid approach

- Only neutrals modeled as fluid
- Background gas pressure = ~10 Torr

Electrostatic simulations currently not supported with the hybrid model. Three different electrical coupling simulations shown:

- Electrostatic kinetic
- Electromagnetic kinetic
- Electromagnetic hybrid

One-dimensional geometries approximated by 2D simulations with only 4 elements in the y-direction. Periodic boundary conditions used on these surfaces



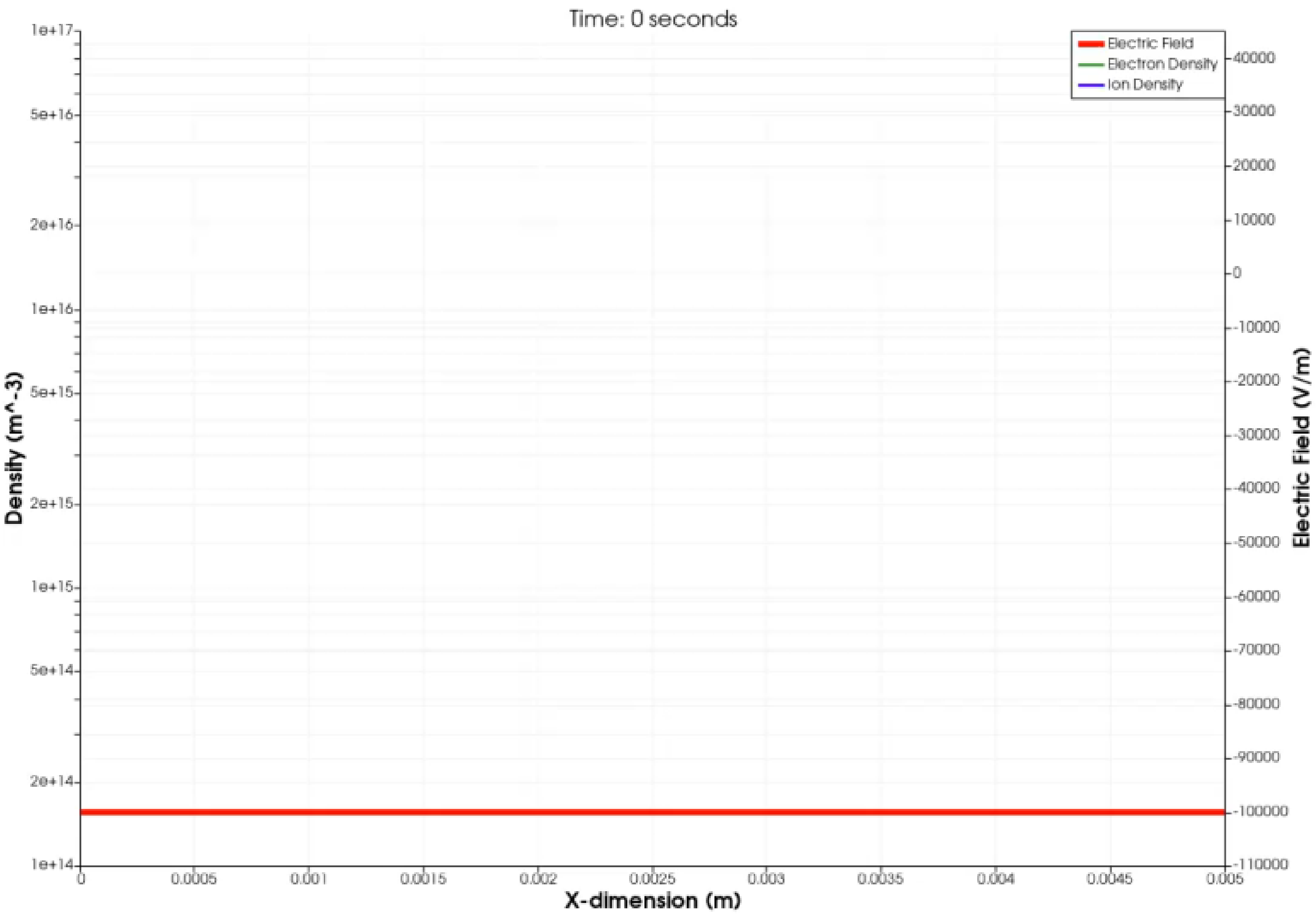
Boundary/Initial Conditions:

Electrostatic: V(cathode) = 0, V(anode) = 500 V

Electromagnetic: $E_x = -10^5$ V/m, $E_y = E_z = 0 = B = 0$

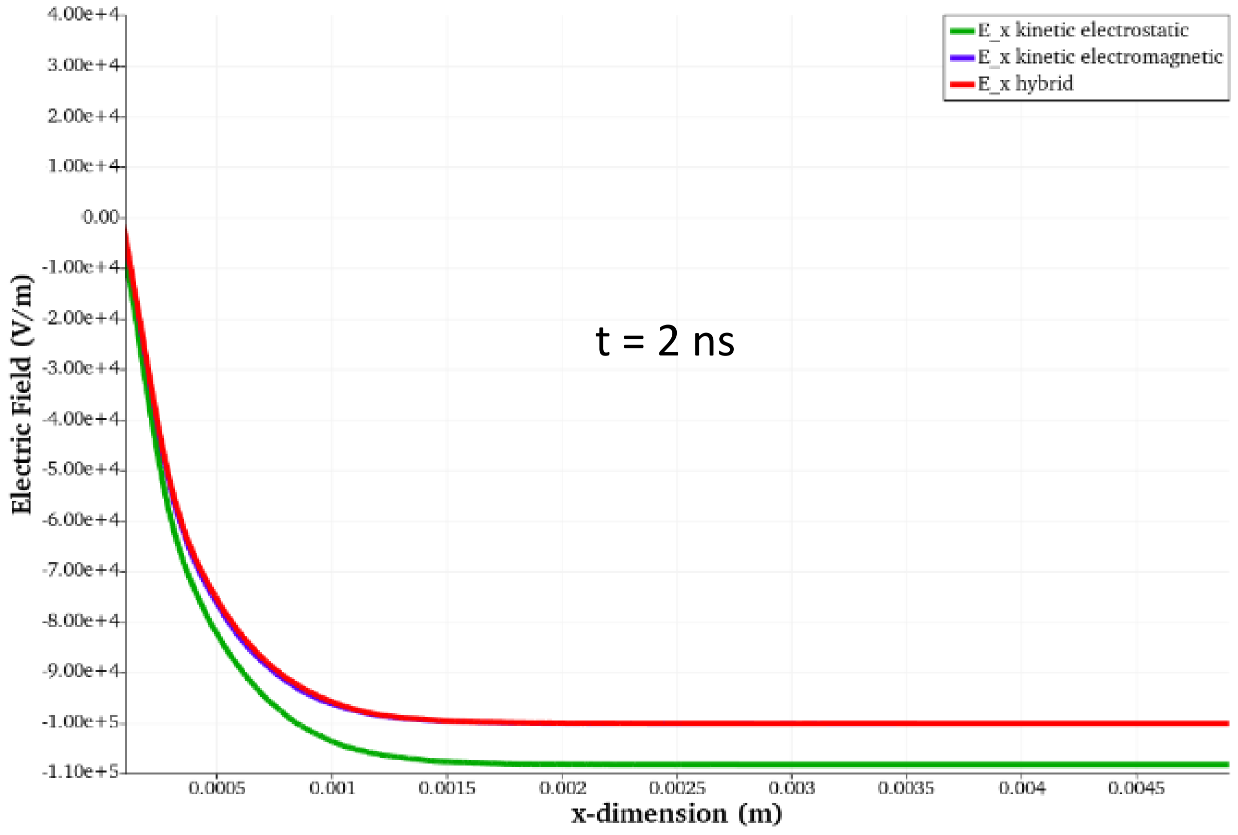
How equivalent are these two conditions?

Characteristic Development



Development of electron avalanche in the gas using the fully kinetic **electromagnetic** solution from t = 0 ns to 10 ns

One-dimensional electron avalanche



Electric field comparisons for

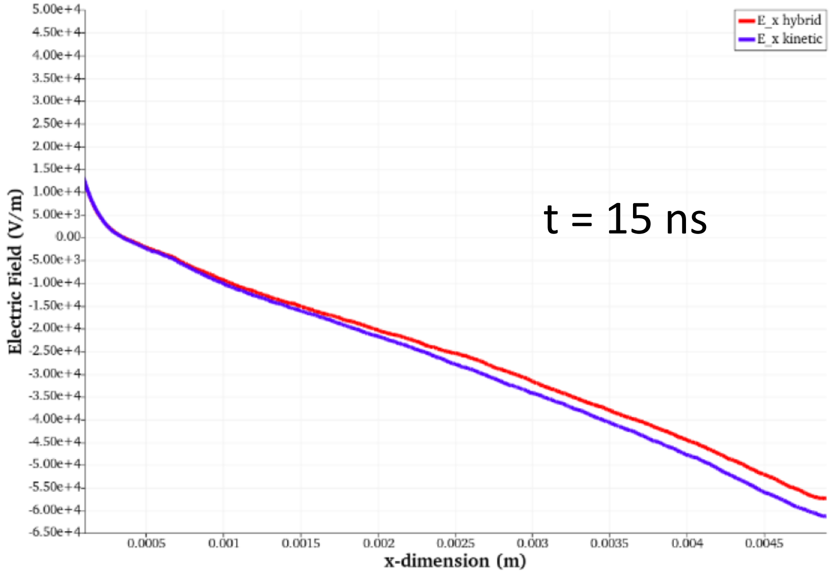
- (green) electrostatic kinetic
- (blue) electromagnetic kinetic
- (red) electromagnetic hybrid

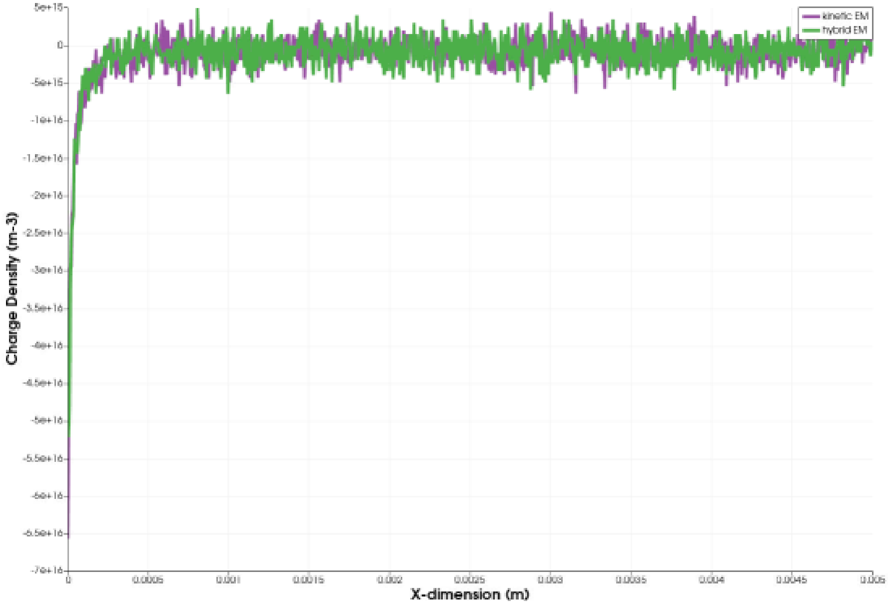
The electromagnetic solutions agree well with each other, differences observed in the electrostatic case (is this to be expected?)

Integration of the electric field shows that

- The integral $\int \boldsymbol{E}\, dx = 500$ is maintained as expected in the electrostatic case.
- In the electromagnetic cases, this is not the case and in general, becomes smaller with simulation progression time.

One-dimensional electron avalanche





Electric field and charge density comparisons for

- electromagnetic kinetic
- electromagnetic hybrid

As simulation progresses, begin to see some differences in electric field calculation between hybrid and kinetic approach

Net charge density “looks” consistent between the two simulation. Is it error accumulation?

Speed benefit over 96 hours of simulation time:

- Kinetic simulation ran to 15 ns
- Hybrid simulation ran to 86 ns

Note: no particle merging – difference likely due to presence of neutral particles

In the future

Observing some differences between the electrostatic vs. electromagnetic and hybrid vs. kinetic simulations

- Determine the differences here and see if they are real
- If so, determine when important (time scales, pressures, etc)

Hybrid charged species

- Including electrons/ions as a fluid and allowing particles to transitions to the fluid representation could save a lot in particle counts

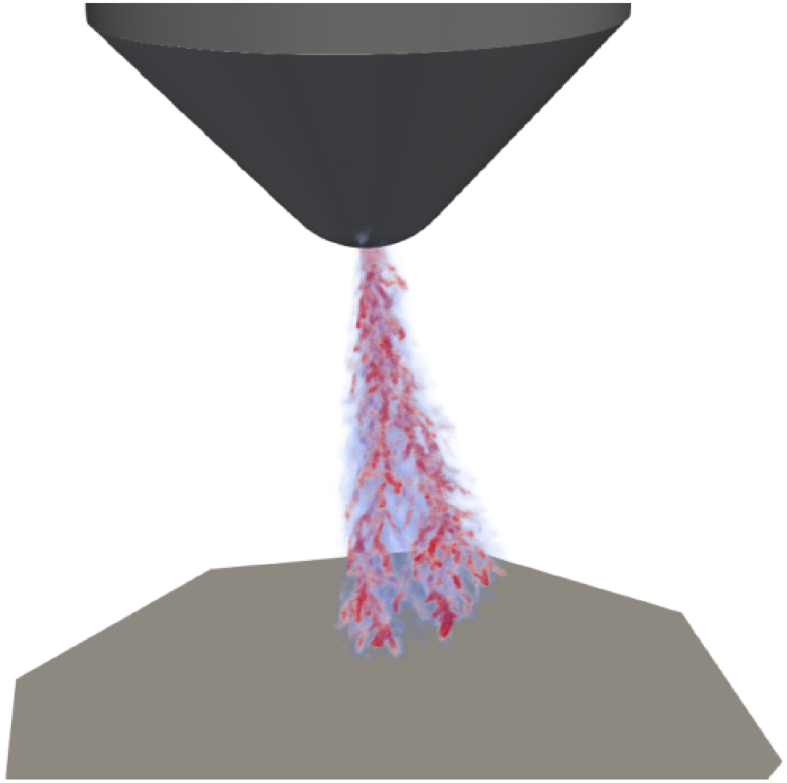
Higher dimensionality simulations (2D → 3D)

- Scaling the size of the simulation can show the benefit of hybrid approach further when applied to really big simulation domains

Basic ionization wave physics

- Role of photons
- Front speeds
- Breakdown voltages (Paschen)

3d simulation run on 6000 cores for 10 days! t = 1.2 ns



A. Fierro, *et al.*, European J. Phys. D., invited, in review, 2020.