Exfidis Numerical Modelling

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ANR Exfidis

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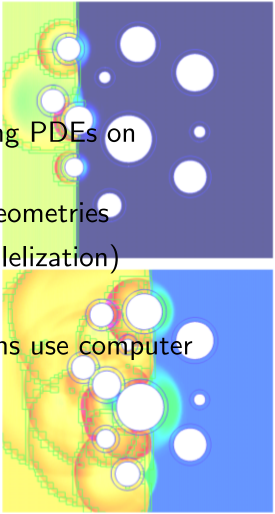
Outline

1. Model Physics And Implementation
2. Code Validation
3. HVND Results
4. To Do

Overture



- Open source C++/Fortran libraries for solving PDEs on overlapping grids
- Efficient mesh generator supports complex geometries
- Efficient array implementation (support parallelization)
- FD/FV operators up to 8th order accuracy
- Structured grids with optimized discretizations use computer time and memory efficiently

Overlapping Grids

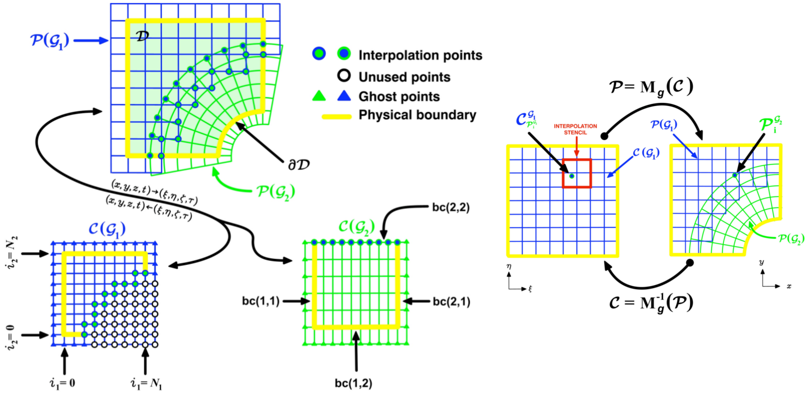
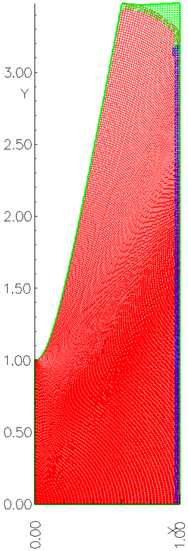
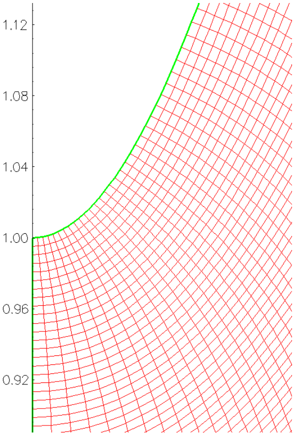


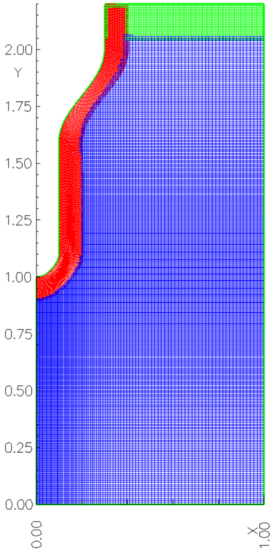
Fig.: Courtesy of Overture team

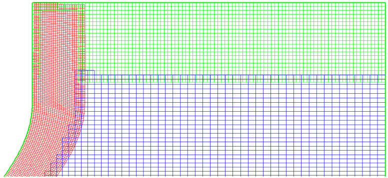
PTP, Hyperboloid-Of-Revolution Anode

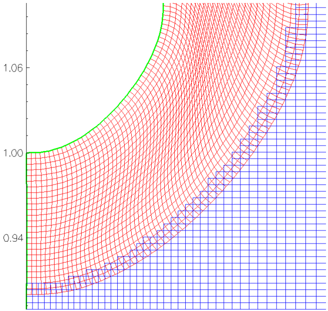




PTP, Exfidis-Like Anode







Chemistry and Transport Parameters

- Plasma chemistry: minimal, nitrogen and air
- Transport parameters (LFA):
  1. Analytical formulas (literature), or
  2. Look-up tables (Bolsig+) with cubic spline interpolation

Electric Field

The electric potential ϕ is governed by

$$\Delta\phi = -\frac{\rho}{\epsilon_0}, \qquad (1)$$

with

$$\Delta \equiv \frac{\partial^2}{\partial x_1^2} + \frac{1}{x_1}\frac{\partial}{\partial x_1} + \frac{\partial^2}{\partial x_2^2},$$

electric field $\mathbf{E} = -\nabla\phi$ and space charge density $\rho = \sum_j q_j n_j$.

Numerical Implementation

- 2nd order FDM on vertex-centered grid
- Banded algebraic system: direct/iterative/PETSC solvers
- Coordinate singularity: L'Hopital's rule
- Dielectrics: surface charge accumul., sub-domain iterations

Semi-Implicit Correction

To remove dielectric relaxation time scale, solve modified Poisson equation

$$\epsilon_0 \nabla \cdot \mathbf{E}^{n+1} \approx \tilde{\rho} = \sum_j q_j \tilde{n}_j, \tag{2}$$

with linearization

$$\tilde{n}_j = n_j + \Delta t \frac{\partial n_j}{\partial t}, \tag{3}$$

and implicit el. field in continuity equation, i.e. $\mathbf{\Gamma}(\mathbf{E}^{n+1}, [\mu, D, n]^n)$. We obtain

$$\left(1 + \frac{\Delta t}{\tau_r}\right) \nabla^2 \phi + \nabla \left(\frac{\Delta t}{\tau_r}\right) \cdot \nabla \phi = -\frac{\rho^D}{\epsilon_0}, \tag{4}$$

where $\tau_r = \epsilon_0 / (e \sum_j \mu_j n_j)$.

Species Densities, Coordinate Transformation

For a smooth grid mapping from a Cartesian to physical space,

$$\mathbf{x} = \mathbf{G}(\mathbf{r}), \quad \mathbf{r} \in [0,1] \times [0,1], \quad \mathbf{x} \in \mathbb{R}^2, \tag{5}$$

we transform to Cartesian space, obtaining

$$\frac{\partial n}{\partial t} + \frac{1}{J}\frac{\partial}{\partial r_1}\hat{f}_1 + \frac{1}{J}\frac{\partial}{\partial r_2}\hat{f}_2 = \hat{R}, \tag{6}$$

where

$$\hat{f}_1 = \frac{\partial x_2}{\partial r_2} f_1 - \frac{\partial x_1}{\partial r_2} f_2, \tag{7}$$

$$\hat{f}_2 = \frac{\partial x_1}{\partial r_1} f_2 - \frac{\partial x_2}{\partial r_1} f_1, \tag{8}$$

$$\hat{R} = R - \frac{f_1}{x_1}, \tag{9}$$

with Jacobian $J = \left|\frac{\partial(x_1,x_2)}{\partial(r_1,r_2)}\right|$ and $\mathbf{\Gamma} = (f_1, f_2)$.

Species Densities, Finite Volume Method

For cell average N over a vertex-centered grid cell $\mathbf{i} = (i, j)$ at time t_n,

$$N_{\mathbf{i}}^n = \frac{1}{\Delta x \Delta y} \int_{y_{j-1/2}}^{y_{j+1/2}} \int_{x_{i-1/2}}^{x_{i+1/2}} n(x, y, t_n)\, dxdy,$$

we apply 1st order operator splitting to flux terms S_F and source terms S_R, so that

$$N_{\mathbf{i}}^{n+1} = S_F(\Delta t) S_R(\Delta t) N_{\mathbf{i}}^n : \; N_{\mathbf{i}}^* = S_F(\Delta t) N_{\mathbf{i}}^n,\; N_{\mathbf{i}}^{n+1} = S_R(\Delta t) N_{\mathbf{i}}^*.$$

S_F represents fully discrete flux-differencing,

$$N_{\mathbf{i}}^* = N_{\mathbf{i}}^n - \frac{\Delta t}{J_{\mathbf{i}}} \left[\frac{\hat{F}_{1,i+1/2,j} - \hat{F}_{1,i-1/2,j}}{\Delta x} + \frac{\hat{F}_{2,i,j+1/2} - \hat{F}_{2,i,j-1/2}}{\Delta y} \right],$$

with flux functions $\hat{F}$ given by an upwind/high-resolution method. S_R is implemented as an explicit Euler.

Photoionization (PI) via Differential Approach

System of $n = 2$ Helmholtz equations gives PI source S_{ph}

$$\left(-\nabla^2 + \lambda_j^2\right) S_{ph,j} = S_i, \qquad S_{ph} = f_q \sum_{j=1}^{n} A_j S_{ph,j} \tag{10}$$

with quenching factor f_q and emission intensity $\propto$ ionization source $S_i = \sum_r^{n_r} \nu_{i,r} n_e$, where $r = 1 \ldots n_r$.

- Equivalent to generalized Eddington approximations of the radiative transfer equation (e.g. Eddington and SP3 models)
- Derived from Zheleznyak integral model by fitting absorption function by n exponential ($\rightarrow \lambda_j$) and interpreting integral photoionization rate as the appropriate Green's function for the corresponding differential model.

Model, Practical Aspects: Computation and Administration

- Model running on our dedicated linux cluster (CentOS), total processing power approx. 114GHz.
- Code maintained through versioning software (Git) allowing for easy collaboration
- All features carefully documented (Latex, Doxygen)
- Results database (MySql) and visualization (Matlab) available through local web interface (LAMP)
- Jobs submitted for computation are handled by a resource manager and scheduler (Torque, Maui)

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Parameters

- Nitrogen at 760 Torr
- Axisymmetric plane-to-plane, 5 mm gap (breakdown at 17.7 kV)
- Analytical transport parameters (LFA)
- Ion diffusion neglected
- External resistor $R = 50\,\Omega$, anode voltage 26 kV
- Gaussian plasma spot at anode for rapid streamer onset
- Background electron density simulates photoionization

Cathode-directed streamer after crossing mid-gap

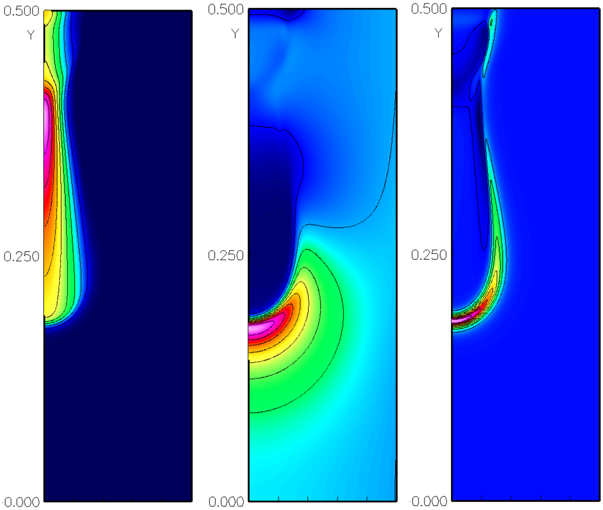

Fig.: Electron density, electric field and space charge density

Cathode-directed streamer, propagation profiles 1/2

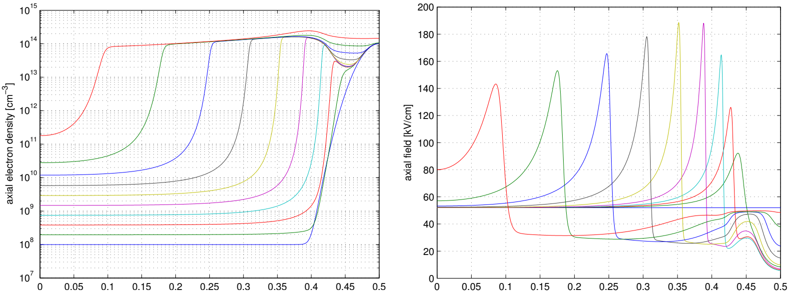

Fig.: Electron density and electric field

Cathode-directed streamer, propagation profiles 2/2

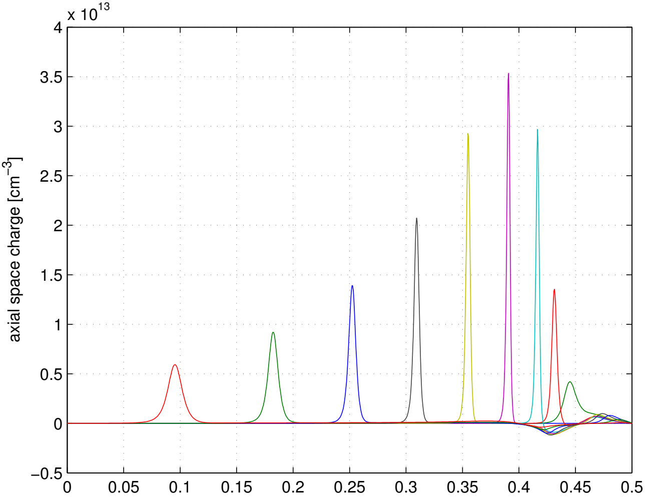

Fig.: Space charge density

Parameters

- Air at atmospheric pressure and room temperature
- Axisymmetric plane-to-plane, 1 cm gap
- Ion mobility and diffusion neglected
- Anode voltage 50 kV
- Photoionization included

Cathode-directed streamer after crossing mid-gap

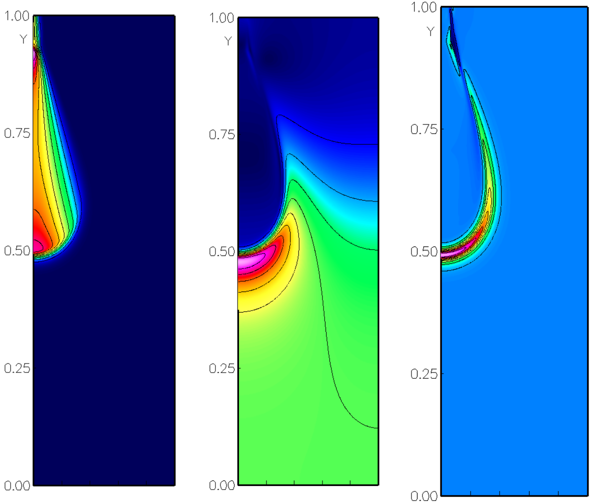

Fig.: Electron density, electric field and space charge density

Propagation profiles 1/2

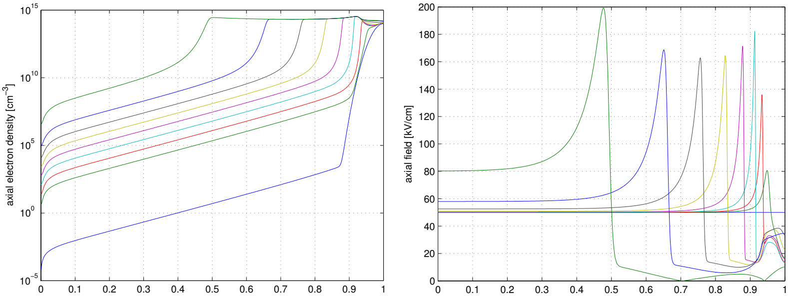

Fig.: Electron density and electric field

Propagation profiles 2/2

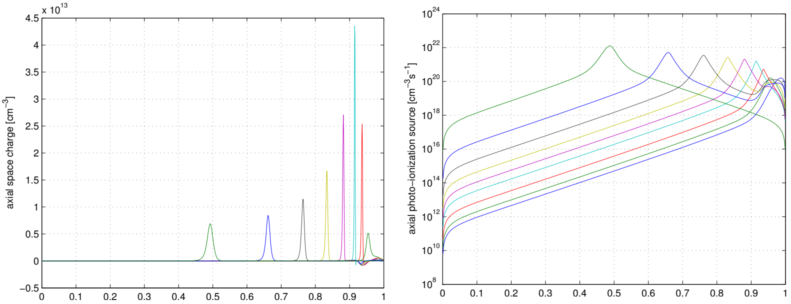

Fig.: Space charge and photoionization source

Parameters

- Air at atmospheric pressure and room temperature
- Axisymmetric point-to-plane, 1 cm gap
- Anode surface: hyperboloid of revolution, tip radius 500 μm
- Ion mobility and diffusion neglected
- Anode voltage 11 kV
- Photoionization included

Cathode-directed streamer near cathode

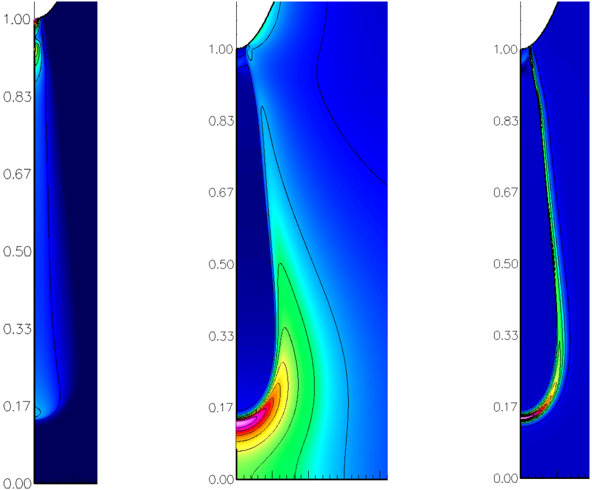

Fig.: Electron density, electric field and space charge density

Propagation profiles 1/2

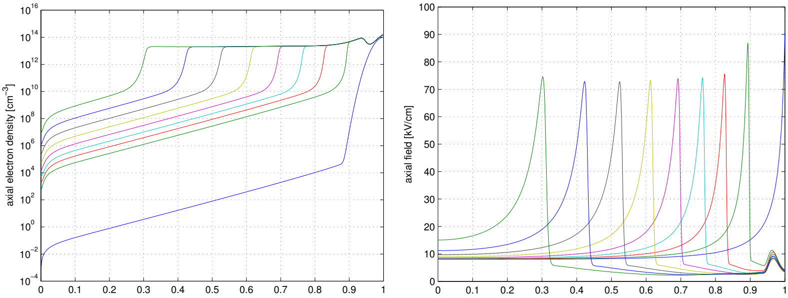

Fig.: Electron density and electric field

Propagation profiles 2/2

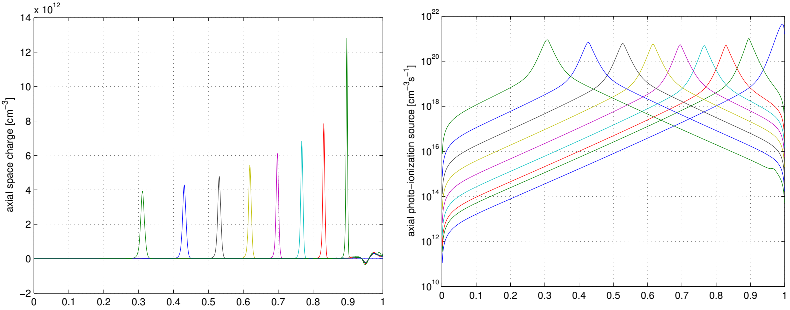

Fig.: Space charge and photoionization source

Streamer parameters 1/2

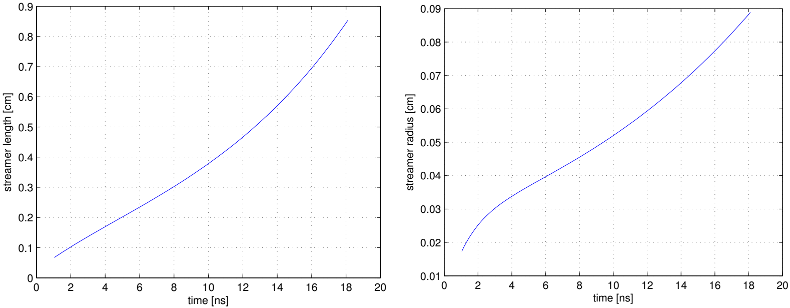

Fig.: Streamer length and radius

Streamer parameters 2/2

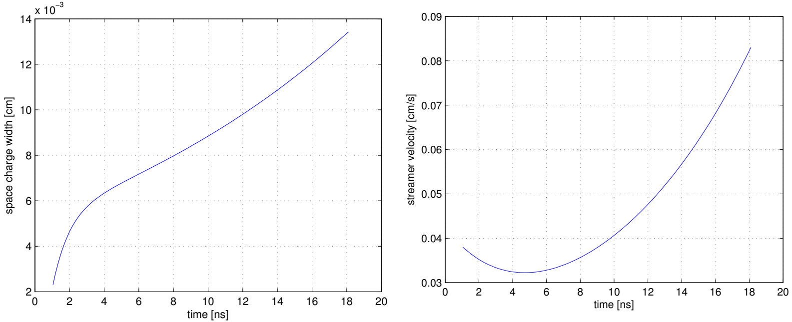

Fig.: Space charge width and streamer velocity (cm/ns)

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4 To Do

Cathode-directed streamer at $t = 1.75$ ns

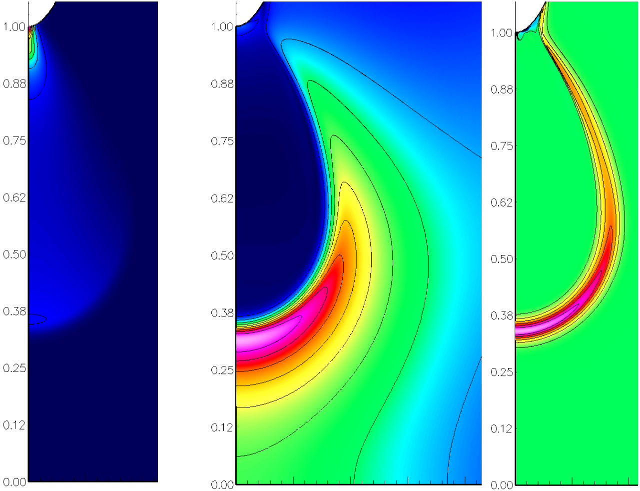

Fig.: Electron density, electric field and space charge density

Cathode-directed streamer, propagation profiles 1/2

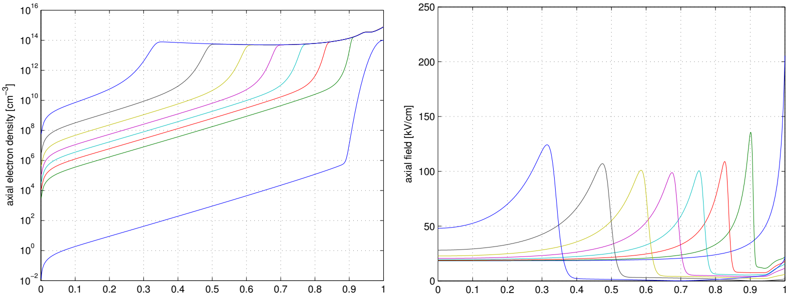

Fig.: Electron density and electric field

Cathode-directed streamer, propagation profiles 2/2

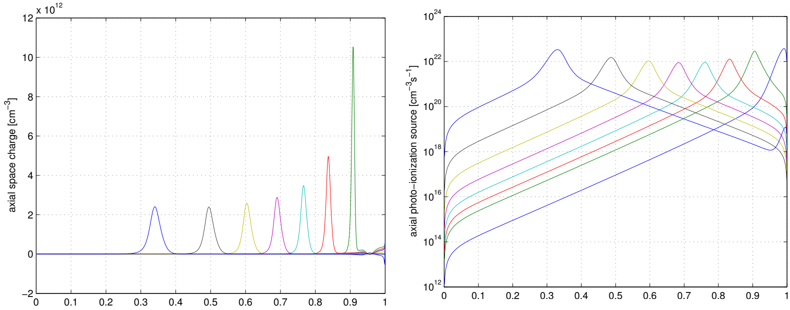

Fig.: Space charge and photoionization source

Cathode-directed streamer at $t = 2.5$ ns

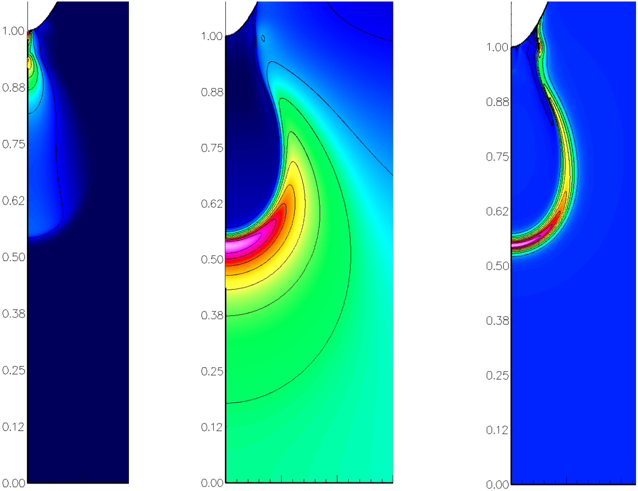

Fig.: Electron density, electric field and space charge density

Cathode-directed streamer, propagation profiles 1/2

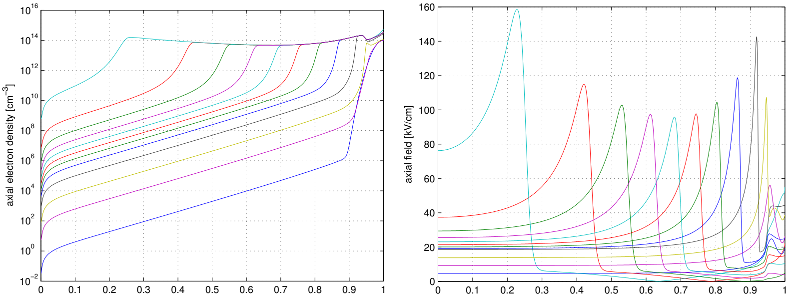

Fig.: Electron density and electric field

Cathode-directed streamer, propagation profiles 2/2

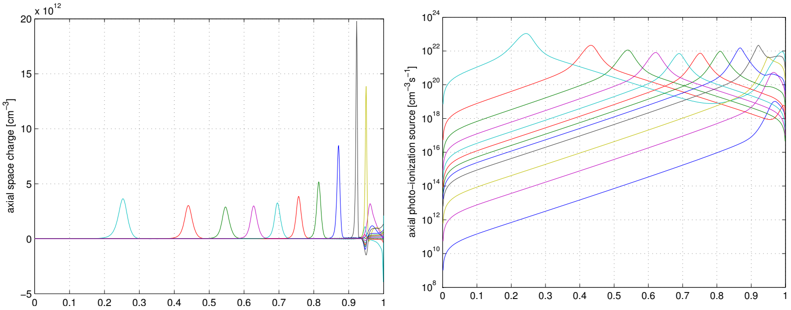

Fig.: Space charge and photoionization source

Supplemental content here.

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Further Plans

- Electron energy equation For energy loss coefficient δ, the energy relaxation length and time, $\Lambda_u \sim l/\sqrt{\delta}$ and $\tau_u = \nu_m^{-1}/\delta$, are on the order of micrometers and nanoseconds $\rightarrow$ LFA is not expected to hold for a pulsed discharge.
- Kinetic (PIC-MCC) model for runaway electrons with forward-backward approximation. Coupling between particle and continuum domains through continuity relations.
- Moving adaptive grid, high-order numerics

Outline

5 50 kV Exfidis Simulations: Physics or Artifact?

Phenomenon Description

- Secondary wave arises at large voltages from anode spot after streamer propagates a certain distance
- Observed for fast streamers (large radius, high conduction current)
- Correlates with electric field reversal ($V_{max} > V_0$)
- Algorithm failure due to high electron density and electric field

Streamer at $t = 0.35$ ns

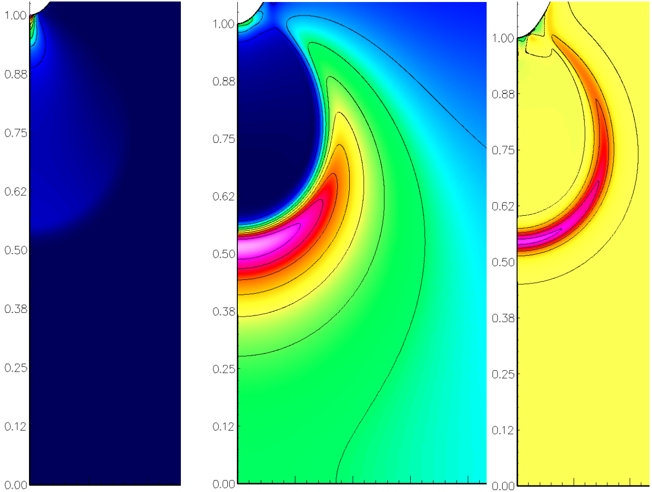

Fig.: Electron density, electric field and space charge density

Streamer at $t = 0.35$ ns, el. field reversal

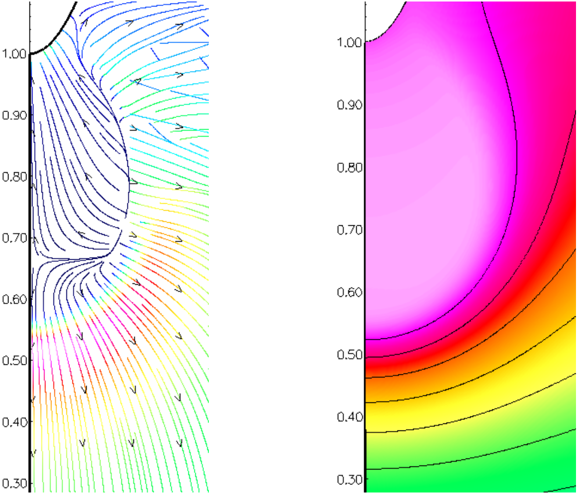

Fig.: Electric field and potential

Time evolution 1/3

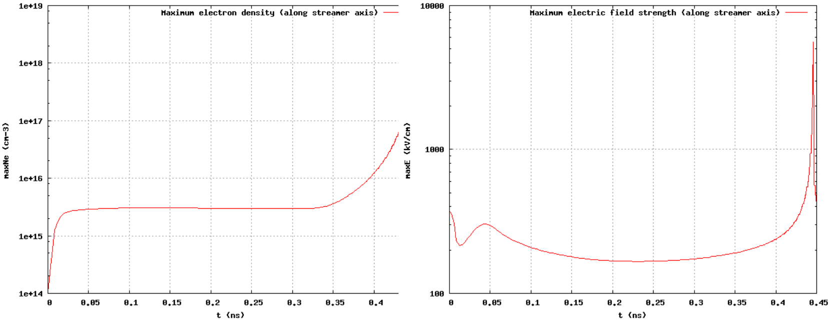

Fig.: Maximum electron density and electric field

Time evolution 2/3

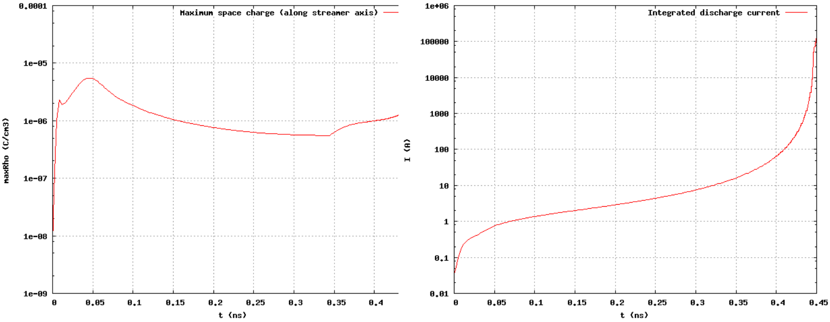

Fig.: Maximum space charge density and conduction current

Time evolution 3/3

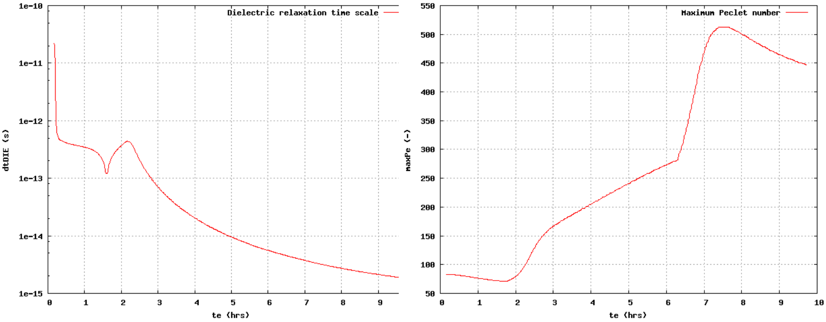

Fig.: Dielectric relaxation time step and max. Peclet number

Propagation profiles 1/2

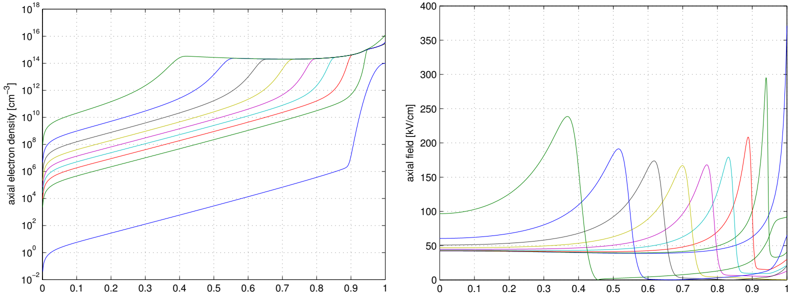

Fig.: Electron density and electric field

Propagation profiles 2/2

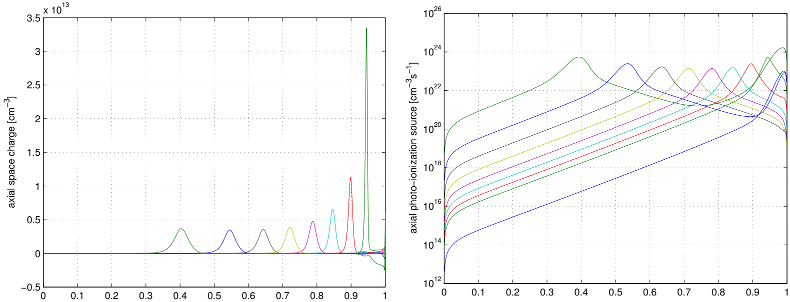

Fig.: Space charge and photoionization source

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