Selected Research Projects

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Outline

1. VSCHT: Control Theory
2. FSU: Stochastic Dynamics
3. LAPLACE: CFD in Plasma

Fuzzy Controll of Traffic Lights

1. Four traffic lights, eight sensors
2. Sugeno-type fuzzy inference model

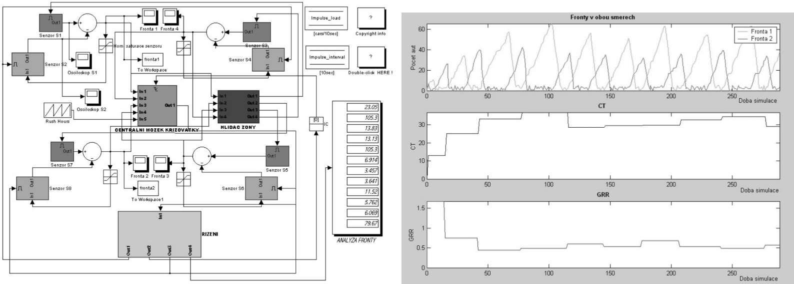

Fig.: *Left: Model in Simulink. Right: Vehicle Count, Cycle Time and Green to Red Ratio under asymmetric load.*

NMR Image Filtering Using M-Estimates

1. Generalized M-Estimates (maximum likelihood): robust
2. New filter design: combine linear descending estimator with inverse hyperbolic functions

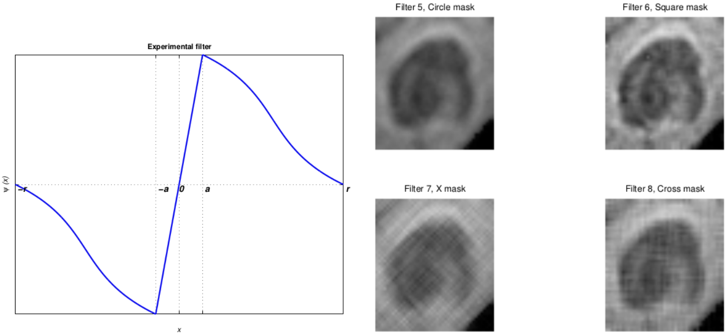

Fig.: *Left: M-Estimator. Right: Sarcoma, Filter Masks.*

3. Superior SNR and MSE compared to median filter

Lyapunov Stabilization of Nonlinear MagLev Systems

1. Nonlinear, open-loop unstable SISO system, 3rd order
2. Exact linearization with Lie algebra: PID regulator synthesis based on Root Locus techniques
3. Stability: Lyapunov function found with Variable Gradient Method

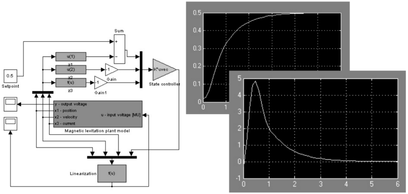

Fig.: *Left: MagLev System. Right: Regulator Synthesis with Root Locus.*

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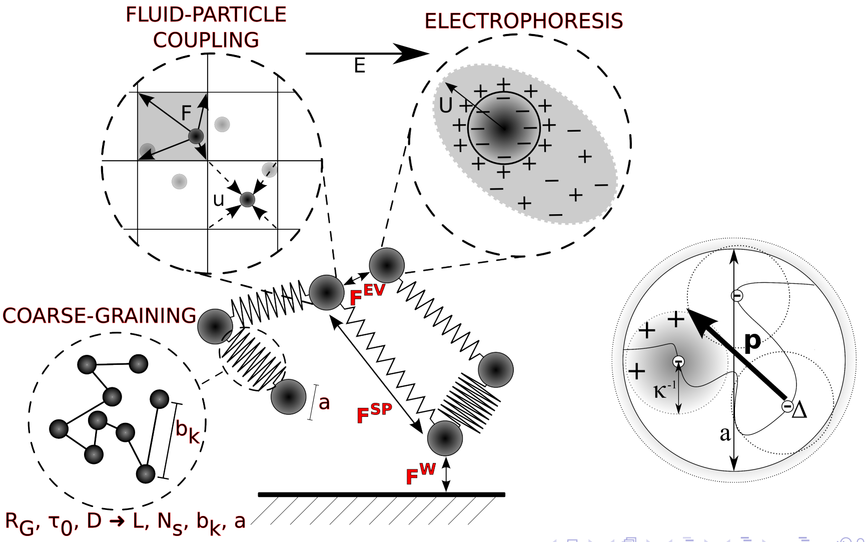
Polymer model



The overall picture

- Elastic dumbells $(\mathbf{r}_c, \mathbf{Q})$ in Newtonian electrolyte
- Continuity + eq. of motion = Fokker-Planck eq.

$$0 = \left\{ -\frac{\partial}{\partial \mathbf{Q}} \cdot \mathbf{D}(\mathbf{Q}) + \frac{\partial}{\partial \mathbf{Q}} \cdot \frac{\partial}{\partial \mathbf{Q}} \boldsymbol{\Delta}(\mathbf{Q}) \right\} \psi$$

- Solve by perturbation series $\rightarrow$ distribution of orientations $\psi(\mathbf{Q}, \mathbf{r}_c)$
- Form averages and let wall-normal COM flux $\mathbf{j}_c$ vanish $\rightarrow$ distribution of positions $n(\mathbf{r}_c)$
- What's new: stiffness (FENE) and wall-mediated HIs due to counter-ion clouds

Fokker-Planck equation for ψ

$$\frac{\partial}{\partial \mathbf{Q}} \cdot (\dot{\mathbf{Q}}\psi) = 0, \frac{\partial}{\partial \mathbf{r}_c} \cdot (\langle \dot{\mathbf{r}}_c \rangle n) = 0, \text{ where } \langle \cdot \rangle = \int \cdot \, \psi d\mathbf{Q}.$$

Balancing Brownian, spring, electric and hydrodynamic forces:

$$\dot{\mathbf{r}}_c = \mathbf{u} + \frac{1}{8}\mathbf{QQ} : \nabla\nabla\mathbf{u} + \frac{1}{2}\bar{\mathbf{\Omega}} \cdot \mathbf{F}^s + \frac{2}{k_b T}\mathbf{D_K} \cdot \mathbf{F}^e - \mathbf{D_K} \cdot \frac{\partial \ln(n\psi)}{\partial \mathbf{r_c}},$$

$$\dot{\mathbf{Q}} = \mathbf{Q} \cdot \nabla\mathbf{u} - 2\mu\mathbf{I} \cdot \mathbf{F}^s - \bar{\bar{\mathbf{\Omega}}} \cdot \mathbf{F}^e - k_b T 2\mu\mathbf{I} \cdot \frac{\partial \ln \psi}{\partial \mathbf{Q}},$$

where $\mathbf{D_K}, \bar{\mathbf{\Omega}}$ and $\bar{\bar{\mathbf{\Omega}}}$ are linearized functions of the HI tensor $\mathbf{\Omega}_{ij}$.

Fokker-Planck equation

$$\frac{2k_b T}{\zeta}\frac{\partial}{\partial \mathbf{Q}} \cdot \frac{\partial}{\partial \mathbf{Q}}\psi - \left(\hat{\boldsymbol{\kappa}} : \frac{\partial \psi}{\partial \mathbf{Q}}\mathbf{Q}\right) + \frac{2a}{\zeta}\mathbf{Q} \cdot \frac{\partial \psi}{\partial \mathbf{Q}} + \frac{2}{\zeta}\left[Q\frac{da}{dQ} + 3a\right]\psi = 0$$

Flow and force in opposition (in electrolyte)

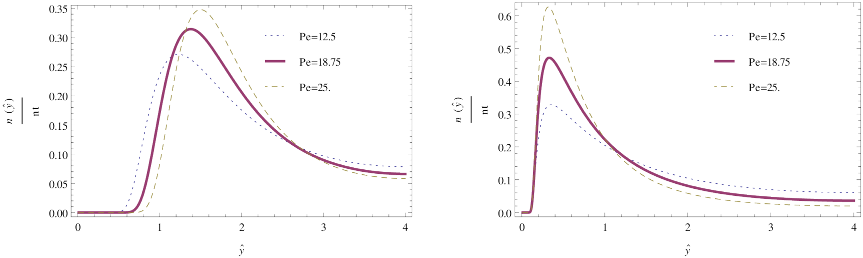


Fig.: *Center-of-mass distribution. Flow and force in opposition,* $Wi = 5/6$. *Left: non-linear spring model, right: linear spring model.*

The overall picture

Objective

Provide a comprehensive treatment of HIs in electric field under confinement within the framework of Brownian Dynamics.

- Use full electrophoretic Stokeslet (short-ranged + long-ranged parts)
- Include the corresponding wall correction

Model equations

$$\dot{\mathbf{r}}_i = \mathbf{u}(\mathbf{r}_i) + \sum_{j=1}^{N} \boldsymbol{\mu}_{ij} \cdot \left(\mathbf{F}_j^b + \mathbf{F}_j^s \right) + \sum_{j=1}^{N} \boldsymbol{\mu}_{ij}^e \cdot \mathbf{F}_j^e$$

- Brownian dynamics:

$$d\mathbf{r} = \left[\mathbf{u} + \frac{1}{k_b T} \mathbf{D} \cdot \mathbf{F} + \frac{\partial}{\partial \mathbf{r}} \cdot \mathbf{D} + \boldsymbol{\mu}^e \cdot \mathbf{F}^e \right] dt + \sqrt{2} \mathbf{B} \cdot d\mathbf{w},$$

$$\mathbf{D} = \mathbf{B} \cdot \mathbf{B}^T.$$

- HI tensor splitting, $\mathbf{u} = \mathbf{u}^{OB} + \mathbf{u}^W$ circumvents the need to resolve Dirac delta function. Price is non-homogeneous BCs.

$$-\nabla p + \eta \Delta \mathbf{u}^W = 0, \;\; \nabla \cdot \mathbf{u}^W = 0,$$

$$\mathbf{u}^W = -\mathbf{u}^{OB} \text{ at walls}$$

Center-of-mass profiles

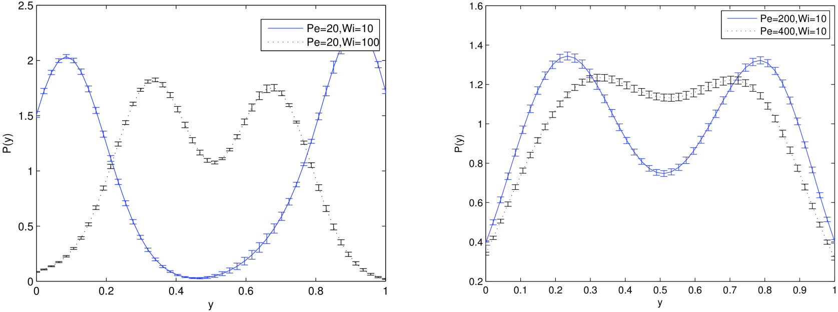


Fig.: *Flow field and electric field in opposition. Debye length* $\lambda_D = 1\,\mu m$

The overall picture

Objective

Derive an analytical form of the Stokeslet in a rectangular channel.

Background

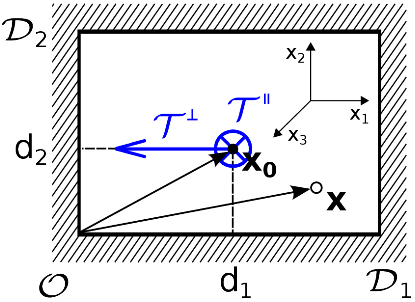


Fig.: *Cross-section of an infinite rectangular channel of dimensions D_1 and D_2. The source point and field point are located at $\mathbf{x}_0 = [d_1, d_2, 0]$ and $\mathbf{x} = [x_1, x_2, x_3]$, respectively. General motion of the source point (T) is decomposed into the translation parallel ($T^{\parallel}$) and perpendicular ($T^{\perp}$) to the walls, $T = T^{\parallel} + T^{\perp}$.*

Problem formulation

$$\eta\nabla^2\mathbf{v} + \delta(\mathbf{x}-\mathbf{x}_0)\mathbf{e}_3 = \nabla p,$$
$$\nabla\cdot\mathbf{v} = 0,$$
$$\mathbf{v} = 0 \qquad \text{at walls.}$$

Papkovich-Neuber formalism:

$$\mathbf{v} = \nabla(\mathbf{x}\cdot\boldsymbol{\phi} + \omega) - 2\boldsymbol{\phi}, \qquad p = 2\eta\nabla\cdot\boldsymbol{\phi},$$

with harmonic functions ω and $\boldsymbol{\phi} = (\phi_1, \phi_2, \phi_3)$ satisfying Laplace equations,

$$\nabla^2\omega = \nabla^2\phi_n = 0, \qquad n = 1, 2, 3.$$

Solution, Final Steps

1. Use FFT (eigenfunction expansions) with the basis functions given by the corresponding Sturm-Liouville problems.
2. Truncate the sums at N terms to de-couple Fourier coefficients to arrive at linear system

$$\mathbf{z} = \mathbf{\Gamma} \cdot \mathbf{z} + \mathbf{p},$$

   where vector $\mathbf{z}$ contains $4N$ elements.
3. Solve for $\mathbf{z}$, compute Fourier coefficients, inverse transform $\hat{\phi}_1$ and $\hat{\phi}_2$ to obtain the desired solutions ϕ_1 and ϕ_2.

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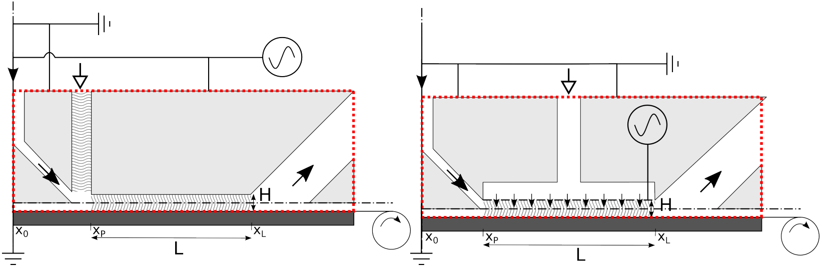
Modeling Objectives Achieved

- Optimize the AP-DBD reactor in terms of selectivity, deposition rate and product yield using a confining stream
- Examine deposition dynamics with modified T-injection and showerhead (limiting case of repeated confinements)
- Propose an injection head design with spatially uniform flow field of discharged gas using a CFD model
- Couple 1D and 2D fluid models of plasma discharge to examine plasma physics

Computational Domain – 2D cross-section



- Plasma source: $V_{RF} = 6$ kV, $f = 5$ kHz, $P = 1$ W/cm^2
- Total gas flow rate $Q(N_2) = 5$ slm
- Precursor concentration $c_{A0} = 50$ ppm
- Confinement strength as a dilution factor $D = 1 - f_Q$, where f_Q is fraction of gas flow rate in precursor inlet
- Electrode length $L/H \in \langle 10..100)$, $H = 1$ mm

Vector Optimization

A composite objective function β, based on a linear scalarization

$$\beta = \sum_{i=1}^{3} w_i f_i(\mathbf{x}), \quad \sum_{i=1}^{3} w_i = 1, \quad \mathbf{x}^* = \max_{\mathbf{x} \in \mathbf{X}} \beta(\mathbf{x}), \tag{1}$$

where $\mathbf{f} = (S, v_N, Y_D)$ are, respectively, the individual objective functions, normalized to $(0, 1)$ range and $\mathbf{w} = (w_S, w_V, w_G)$ is a corresponding weight vector. The solution vectors $\mathbf{x} = (D, L)$ are chosen from a set $\mathbf{X} = \mathbf{x} : \{0 \leq D < 1, 10 \leq L/H \leq 100\}$, with the feasible solution denoted by asterisk.

Vector Optimization

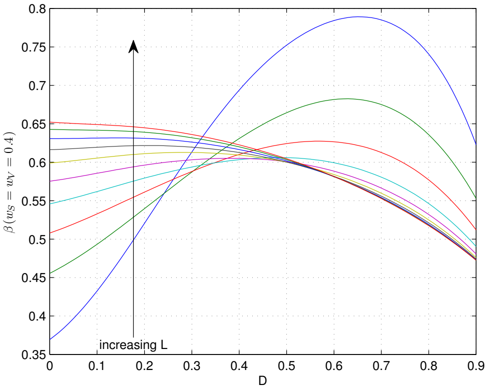


Fig.: *For a specific weighting scheme of* $w_S = w_V = 0.4$, *we obtain* $D^* = 0.65$ *and* $L^*/H = 10$, *based on the objective function* $\beta(D, L)$. *T-injection.*

Optimal Solutions

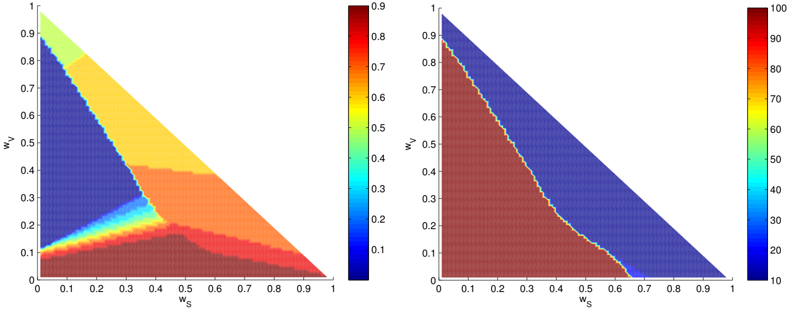


Fig.: *Optimal solutions with selectivity, deposition rate and* **product yield** *as component objective functions. Left: Optimal dilution factor* $D^* = D^*(w_S, w_W)$. *Right: Optimal electrode length* $L^* = L^*(w_S, w_W)$.

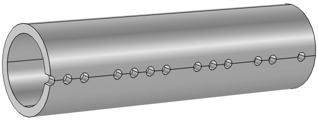
Design Objective

Design Objective

Increase spatial uniformity of gas flow field injected onto the substrate in a AP-PECVD

1. While it is desirable to maintain uniform hole density close to the substrate, it is also beneficial to increase the linear density of holes with the decreasing Peclet number (convective flow strength).
2. Increasing gas residence time and turbulence inside the injector should increase flow field homogenization by increasing eddy diffusivity for momentum transfer.

Injector Geometry



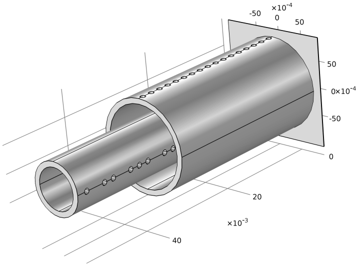
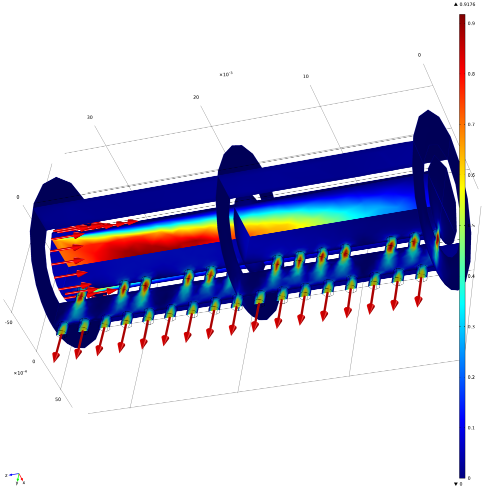


Fig.: *Left: Inner tube with non-uniform hole distribution. Right: Composite injector with inner tube retracted for visualization in the direction of gas inlet. Rotation angle $\phi = \pi/2$, symmetry plane far right.*

Velocity Magnitude with Representative Velocity Vectors

Fig.: *Uniform velocity field along the length of the outer tube.*



Effect of hole alignment and uniformity, cont'd (vorticity)

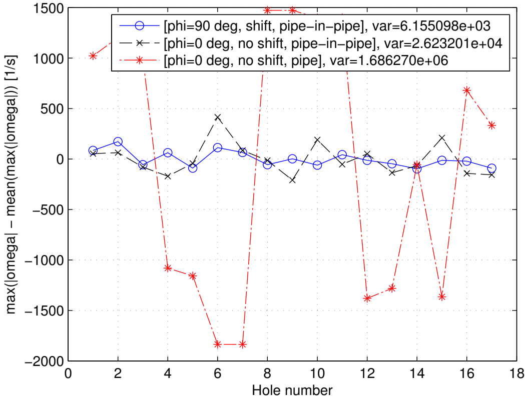


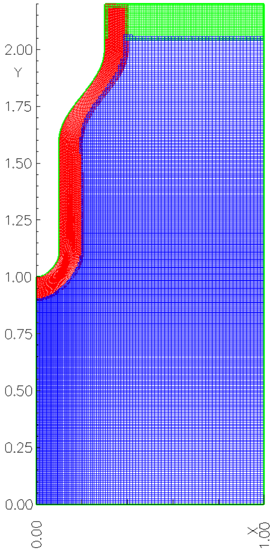
Fig.: *'Shift' denotes mutual misalignment of inner tube and outer tube holes. 'Pipe-in-pipe' denotes injector head with auxiliary inner tube. Reference injector denoted with red asterisks.*

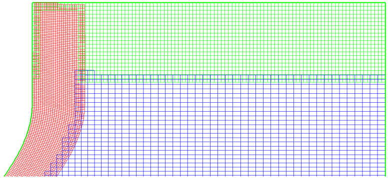
Overture

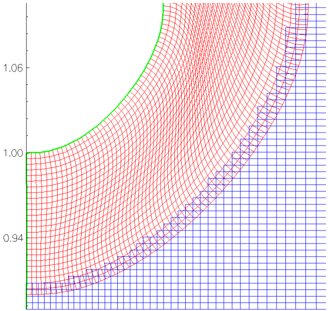
- Open source C++/Fortran libraries for solving PDEs on overlapping grids
- Efficient mesh generator supports complex geometries
- Efficient array implementation (support parallelization)
- FD/FV operators up to 8th order accuracy
- Structured grids with optimized discretizations use computer time and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

Application: Ignition in a combustion engine

PTP, Exfidis-Like Anode







Electric Field

The electric potential ϕ is governed by

$$\Delta\phi = -\frac{\rho}{\epsilon_0}, \tag{2}$$

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

Species Densities, Coordinate Transformation

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

$$\mathbf{x} = \mathbf{G}(\mathbf{r}), \quad \mathbf{r} \in [0,1] \times [0,1], \quad \mathbf{x} \in \mathbb{R}^2, \tag{3}$$

we transform to Cartesian space, obtaining

$$\frac{\partial n}{\partial t} + \frac{1}{J}\frac{\partial}{\partial r_1}\hat{f}_1 + \frac{1}{J}\frac{\partial}{\partial r_2}\hat{f}_2 = \hat{R}, \tag{4}$$

where

$$\hat{f}_1 = \frac{\partial x_2}{\partial r_2} f_1 - \frac{\partial x_1}{\partial r_2} f_2, \tag{5}$$

$$\hat{f}_2 = \frac{\partial x_1}{\partial r_1} f_2 - \frac{\partial x_2}{\partial r_1} f_1, \tag{6}$$

$$\hat{R} = R - \frac{f_1}{x_1}, \tag{7}$$

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

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)

Cathode-directed streamer after crossing mid-gap

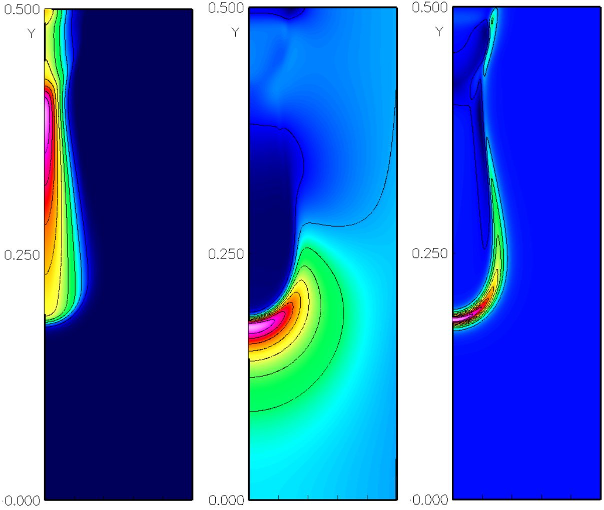


Fig.: *Electron density, electric field and space charge density*

Cathode-directed streamer, propagation profiles 1/2

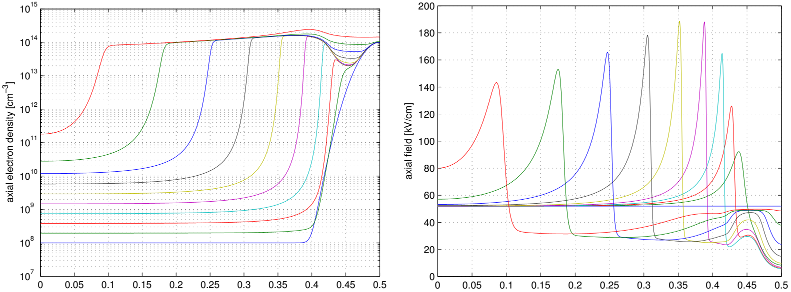


Fig.: *Electron density and electric field*