Numerical simulation of electrostatic spray painting

Matthias Maischak

I fAM

Institute for Applied Mathematics

Hannover University, Germany

BMBF-Projekt 03STM1HV

"3D Adaptive Multilevel FEM-BEM Kopplung für ein Elektrostatisches Teilproblem der Nasslackierung mit Aussenraumaufladung"

Head: Prof. Stephan (Hannover)

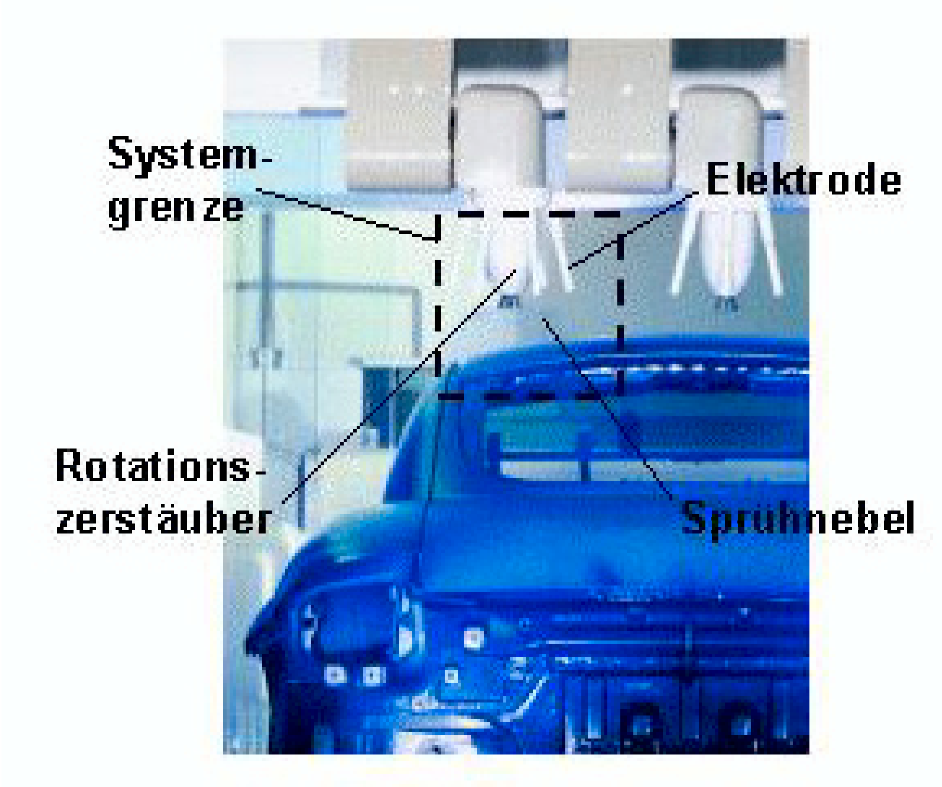
Partners: Prof. Peukert, Dr. Schmid, Hr. Horn (Erlangen)

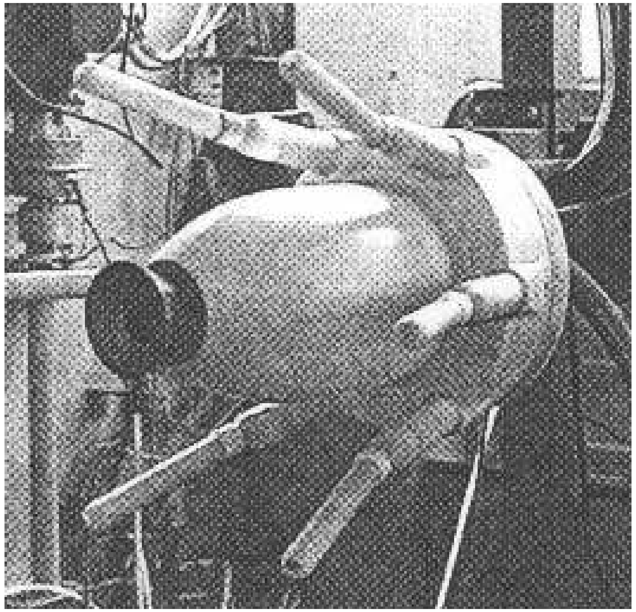
Hr. Sonnenschein, Hr. Poppner (DaimlerChrysler)

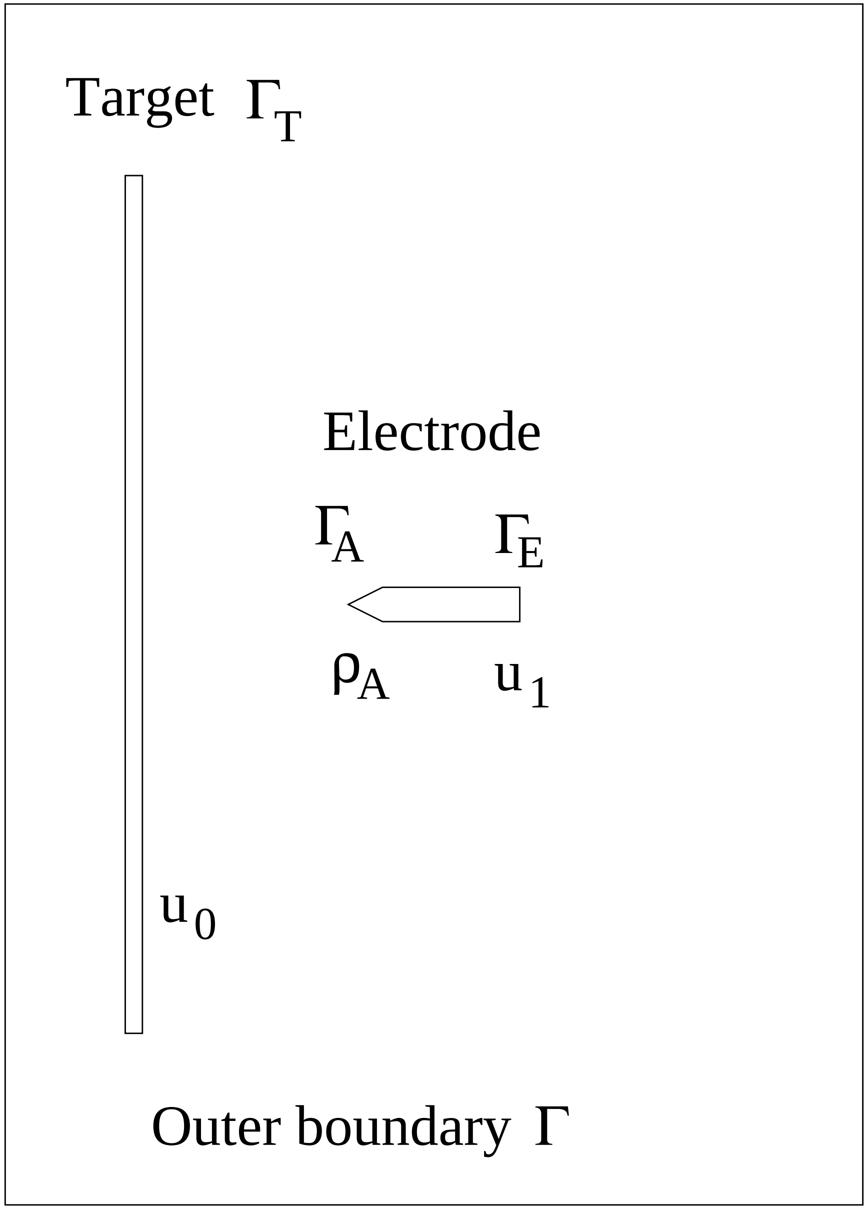
Overview

- Physical/Engineering problem
- Model problem
- Variational Formulation
- Method of Characteristics
- Least-Squares formulation
- Numerical examples

Electrostatic spray painting






Target Γ_T
Electrode
Γ_A
Γ_E
ρ_A
u_1
u_0
Outer boundary Γ

Electric corona discharge configuration

- Applied Voltage between Target and Electrode(s)
- Electrical field (Poisson equation)
- Ion transport (Convection), Space charge density ϱ
- Fluid (Moving Air, CFD) v_{Air}
- Particle tracking, Particle charge ϱ_P
- Corona discharge

Corona discharge: Locally high electric field strength leads to ionization of air, ions are transported along field lines. Cloud of space charge near electrode has influence on local field strength.

Distribution of scalar potential u

$$-\varepsilon_0 \Delta u = \varrho + \varrho_P$$

Electric field

$$E = -\nabla u$$

Density of ionic current

$$j_{\mathrm{Ion}} = \varrho b E + \varrho v_{\mathrm{Air}}$$

Charge conservation law

$$\frac{\partial \varrho}{\partial t} + \mathrm{div}(j_{\mathrm{Ion}}) = S_\varrho$$

Source term S_ϱ due to to charge transfer between ϱ and ϱ_P.

ε_0:	$8.8542 \cdot 10^{-12}$
Electron mobility:	$2 \cdot 10^{-4}\ \frac{\mathrm{m}^2}{V s}$

Electrostatic Model problem

Poisson equation

$$-\Delta u = \frac{\varrho}{\varepsilon_0} \text{ in } \Omega \tag{1}$$

Electrical field

$$E = -\nabla u \tag{2}$$

Boundary conditions (applied voltage)

$$\begin{aligned} u &= u_0 \text{ on } \Gamma_T \text{ (Target)} && (3) \\ u &= u_1 \text{ on } \Gamma_E \text{ (Electrode)} && (4) \end{aligned}$$

Artifical boundary conditions on Γ

$$\frac{\partial u}{\partial n}|_\Gamma = \begin{cases} 0 & \text{(Outflow b.c.)} \\ -Su & \text{(infinite domain)} \end{cases} \tag{5}$$

or

$$u|_\Gamma = 0 \text{ (Faraday)} \tag{6}$$

Using the Poincaré-Steklov operator
$S := -\frac{1}{2}(W + (I - K')V^{-1}(I - K))$ we can describe a charge free exterior domain as a boundary condition for the interior domain.
The symmetric fem-bem coupling formulation approximates the Poincaré-Steklov operator by the Schur-complement of Galerkin matrices.

Linear transport equation Neglecting the air flow and the particle charge we can describe the unipolar ion transport by the linear transport equation

$$\operatorname{div}(E\varrho) = 0 \text{ in } \Omega \tag{7}$$

$$\varrho = \varrho_A \text{ on } \Gamma_E \text{ (Inflow-b.c.)} \tag{8}$$

Non-linear transport equation Inserting the Poisson equation in the linear transport equation we eliminate $\operatorname{div} E$ and we obtain

$$E \cdot \nabla\varrho + \frac{\varrho^2}{\varepsilon_0} = 0 \text{ in } \Omega \tag{9}$$

$$\varrho = \varrho_A \text{ on } \Gamma_E \text{ (Inflow-b.c.)} \tag{10}$$

Kaptzov's assumption

Let E_{onset} be the field strength where corona emission starts. With Kaptzov's assumption we obtain on Γ_E the boundary condition:

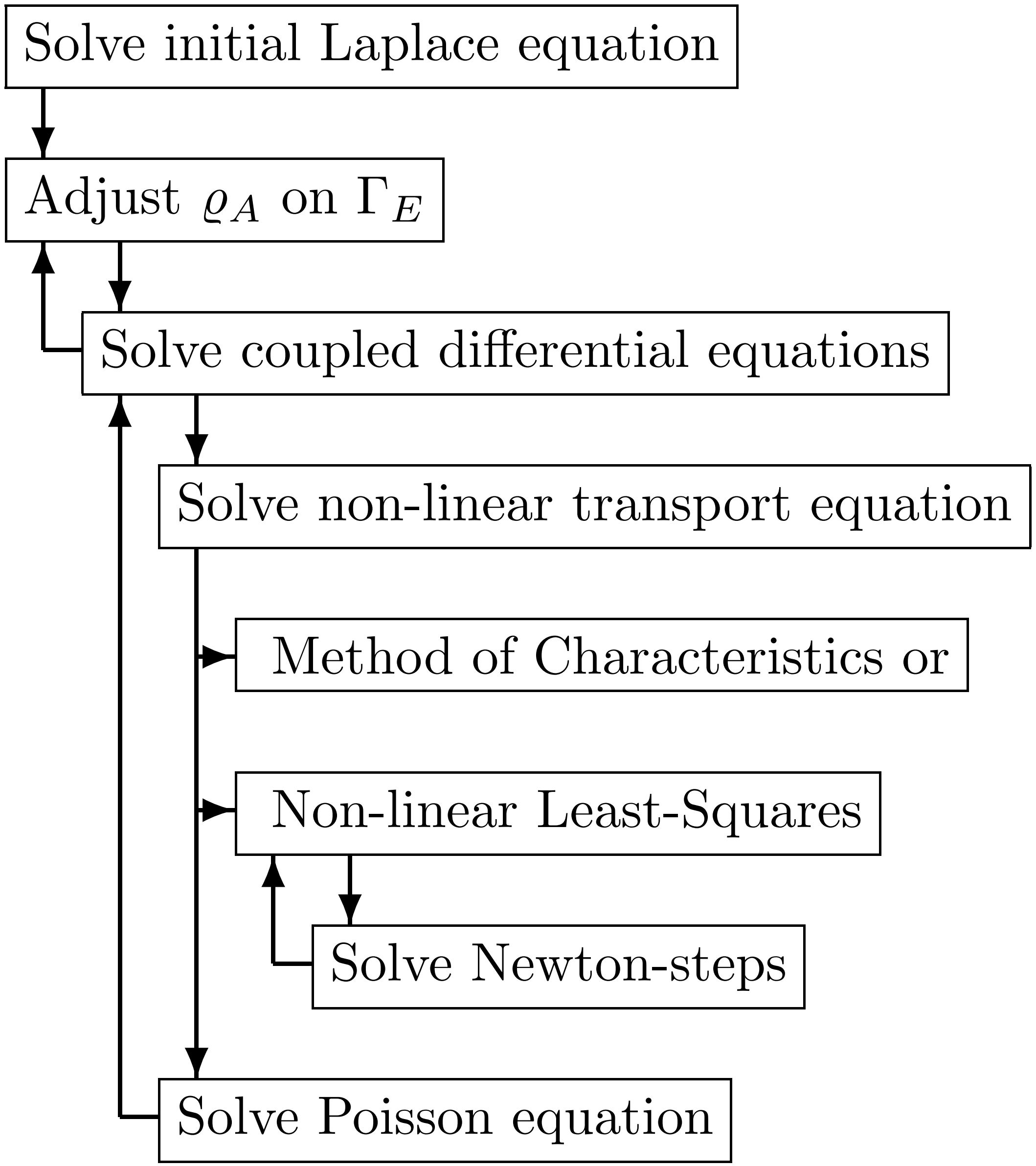
$$\varrho_A \geq 0, \quad -E \cdot n \leq E_{\text{onset}} \tag{11}$$

$$\varrho_A(E \cdot n + E_{\text{onset}}) = 0 \tag{12}$$

Peek-field strength E_{onset} (argument r in cm, result in V/m)

$$E_{\text{onset}} = 3.1 \cdot 10^6 (1 + \frac{0.308}{\sqrt{r}}) \quad \text{(Cylinder)} \tag{13}$$

$$E_{\text{onset}} = 3.1 \cdot 10^6 (1 + \frac{0.308}{\sqrt{r/2}}) \quad \text{(Spherical)} \tag{14}$$


Solve initial Laplace equation
Adjust ϱ_A on Γ_E
Solve coupled differential equations
Solve non-linear transport equation
Method of Characteristics or
Non-linear Least-Squares
Solve Newton-steps
Solve Poisson equation

Poisson equation

Find $u \in H^1_D := \{v \in H^1(\Omega) \,:\, u|_{\Gamma_T} = u_0, \quad u|_{\Gamma_E} = u_1\}$, such that:

$$(\nabla u, \nabla v)_0 = \frac{1}{\varepsilon_0}(\varrho, v)_0 \qquad \forall v \in H^1_{D,0} \tag{15}$$

Solver: diagonal preconditioned Conjugate Gradient

Overlaping domain decomposition as preconditioner for CG

Mixed formulation

Find $(p, u) \in H(\mathrm{div}; \Omega) \times L^2(\Omega)$ such that

$$\begin{aligned} (q, p)_0 + (u, \mathrm{div}\, q)_0 &= \langle u_0, q \cdot n\rangle_{\Gamma_T} + \langle u_1, q \cdot n\rangle_{\Gamma_E} \quad \forall q \in H(\mathrm{div}; \Omega) \\ (v, \mathrm{div}\, p)_0 &= -\frac{1}{\varepsilon_0}(\varrho, v)_0 \quad \forall v \in L^2(\Omega) \end{aligned} \tag{16}$$

Solver: unpreconditioned GMRES

Overlapping domain decomposition as preconditioner for GMRES

Symmetric FEM-BEM-coupling

Find $(u, \sigma) \in H^1_D(\Omega) \times \tilde{H}^{-1/2}(\Gamma)$, such that:

$$\begin{aligned} -\Delta u &= \frac{\varrho}{\varepsilon_0} \quad \text{in } \Omega \\ \sigma &= \frac{\partial u}{\partial n} \quad \text{on } \Gamma \\ 2\sigma &= -Wu + (I - K')\sigma \quad \text{on } \Gamma \\ 0 &= (I - K)u + V\sigma \quad \text{on } \Gamma \end{aligned}$$

Variational formulation:

Find $(u, \sigma) \in H^1_D(\Omega) \times \tilde{H}^{-1/2}(\Gamma)$, such that:

$$\begin{aligned} 2(\nabla u, \nabla v)_0 + \langle Wu, v\rangle + \langle (K' - I)\sigma, v\rangle &= 2\int_\Omega \frac{\varrho}{\varepsilon_0} v\, dx \quad \forall v \in H^1_{D,0}(\Omega) \\ \langle (K - I)u, \psi\rangle - \langle V\sigma, \psi\rangle &= 0 \quad \forall \psi \in \tilde{H}^{-1/2}(\Gamma) \end{aligned}$$

$$V\psi(x) := \frac{1}{2\pi}\int_\Gamma \frac{1}{|x-y|}\psi(y)\,ds_y$$ single layer potential

$$K\psi(x) := \frac{1}{2\pi}\int_\Gamma \frac{\partial}{\partial n_y}\frac{1}{|x-y|}\psi(y)\,ds_y$$ double layer potential

$$K'\psi(x) := \frac{1}{2\pi}\int_\Gamma \frac{\partial}{\partial n_x}\frac{1}{|x-y|}\psi(y)\,ds_y$$ adjoint double layer potential

$$W\psi(x) := -\frac{1}{2\pi}\frac{\partial}{\partial n_x}\int_\Gamma \frac{\partial}{\partial n_y}\frac{1}{|x-y|}\psi(y)\,ds_y$$ hypersingular operator

Smoothing of electrical field

Let $E_\nabla = -\nabla u_h$

Clement-Interpolation: Let $x \in \Omega$ be a node of the mesh $\mathcal{T}_h$.
Then we define

$$U(x) = \bigcup_{T \in \mathcal{T}_h, x \in T} T$$

i.e. $U(x)$ is the union of all elements connected to the node x.
Then the value of E_h in the node x is given by

$$E_h(x) := \frac{\int_{U(x)} E_\nabla(x)\, dy}{\int_{U(x)} 1\, dy}$$

L^2-Projection: The L^2-Projection E_h of E_∇ is given by:

Find $E_h \in V_h^E := \{E_h \in [H^1(\Omega)]^3 \,:\, E_h|_T \text{ ist linear }, T \in \mathcal{T}_h\}$, such that:

$$(E_h, v_h)_{L^2(\Omega)} = (E_\nabla, v_h)_{L^2(\Omega)} \forall v_h \in V_h^E. \tag{17}$$

Method of Characteristics

We compute $\varrho(x)$ along a field line, i.e., along a characteristic line. We write $\varrho(s) = \varrho(x(s))$. $x(s)$ is determined by $b \cdot E(x(s)) = \frac{dx(s)}{ds}$ and $x(0) = x_0$. Then there holds

$$0 = bE \cdot \nabla \varrho + b\frac{\varrho^2}{\varepsilon_0} = \varrho'(s) + b\frac{\varrho^2(s)}{\varepsilon_0} \tag{18}$$

For $\varrho_0 = \varrho(x(0))$ the solution reads

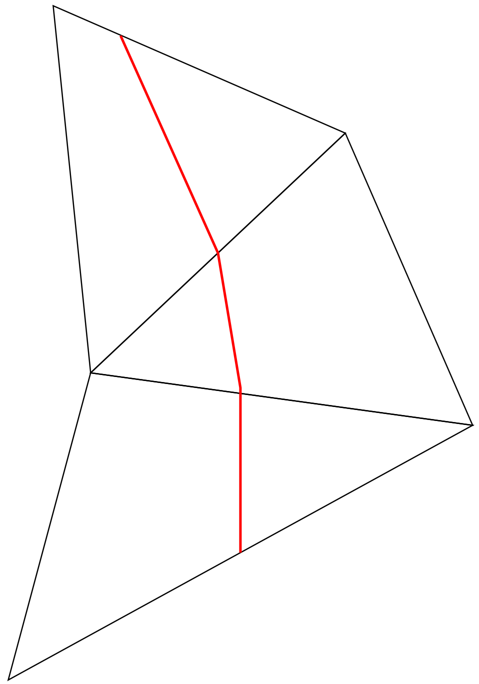
$$\frac{1}{\varrho} = \frac{1}{\varrho_0} + \frac{bs}{\varepsilon_0} \tag{19}$$

resp.

$$\varrho(s) = \varrho_0 \frac{\varepsilon_0}{\varepsilon_0 + b\varrho_0 s} \tag{20}$$

The remaining problem is the determination of the characteristic field line:
Find $x(s)$, such that $bE(x(s)) = \frac{dx(s)}{ds}$, i.e.

$$x(s) = x(0) + \int_0^s bE(x(t))\,dt$$



On the finite element mesh follow the direction of the electrical field. Efficient computation of boundary crossing points is essential.

Computated values of space charge density are averaged on each element. Resulting average density is smoothed using Clement interpolation.

Least-Squares Formulation

Find the minimum of the non-linear least squares functional

$$J(\varrho; f, \varrho_D, \varrho_N) = \| E \cdot \nabla \varrho + \frac{\varrho^2}{\varepsilon_0} - S_\varrho \|^2_{L^2(\Omega} \tag{21}$$

for functions $\varrho \in V^{\varrho_A}$ with

$$V^{\varrho_A} = \{ v \in H^1(\Omega) \, : \, v = \varrho_A \text{ on } \Gamma_E \} \tag{22}$$

The first and second Frechet-derivative of (21) read:

$$\begin{aligned} J'(\varrho; \sigma) =& 2 \int_\Omega (E \cdot \nabla \varrho + \frac{\varrho^2}{\varepsilon_0} - S_\varrho)(E \cdot \nabla \sigma + \frac{2\varrho\sigma}{\varepsilon_0}) \, dx \\ J''(\varrho; \sigma, \xi) =& 2 \int_\Omega (E \cdot \nabla \xi + \frac{2\varrho\xi}{\varepsilon_0})(E \cdot \nabla \sigma + \frac{2\varrho\sigma}{\varepsilon_0}) \, dx \\ &+ 2 \int_\Omega (E \cdot \nabla \varrho + \frac{\varrho^2}{\varepsilon_0} - S_\varrho) \frac{2\xi\sigma}{\varepsilon_0} \, dx \end{aligned}$$

The Newton algorithm applied to (21) reads:

Find $\varrho_{k+1} \in V^{\varrho_A}$, such that

$$0 = J'(\varrho_k; \sigma) + J''(\varrho_k; \sigma, \varrho_{k+1} - \varrho_k) \quad \forall \sigma \in V^0 \tag{23}$$

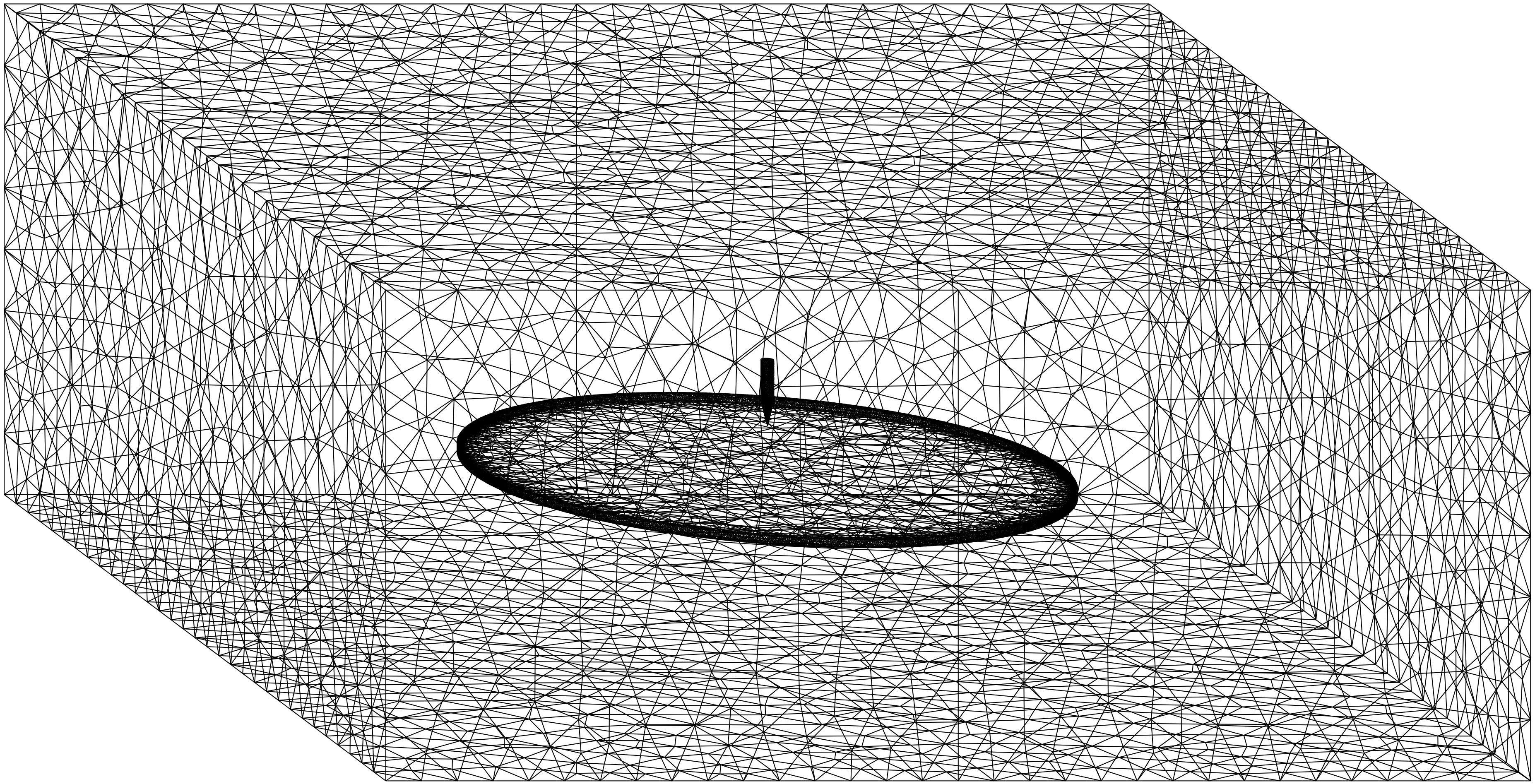
Numerical Examples

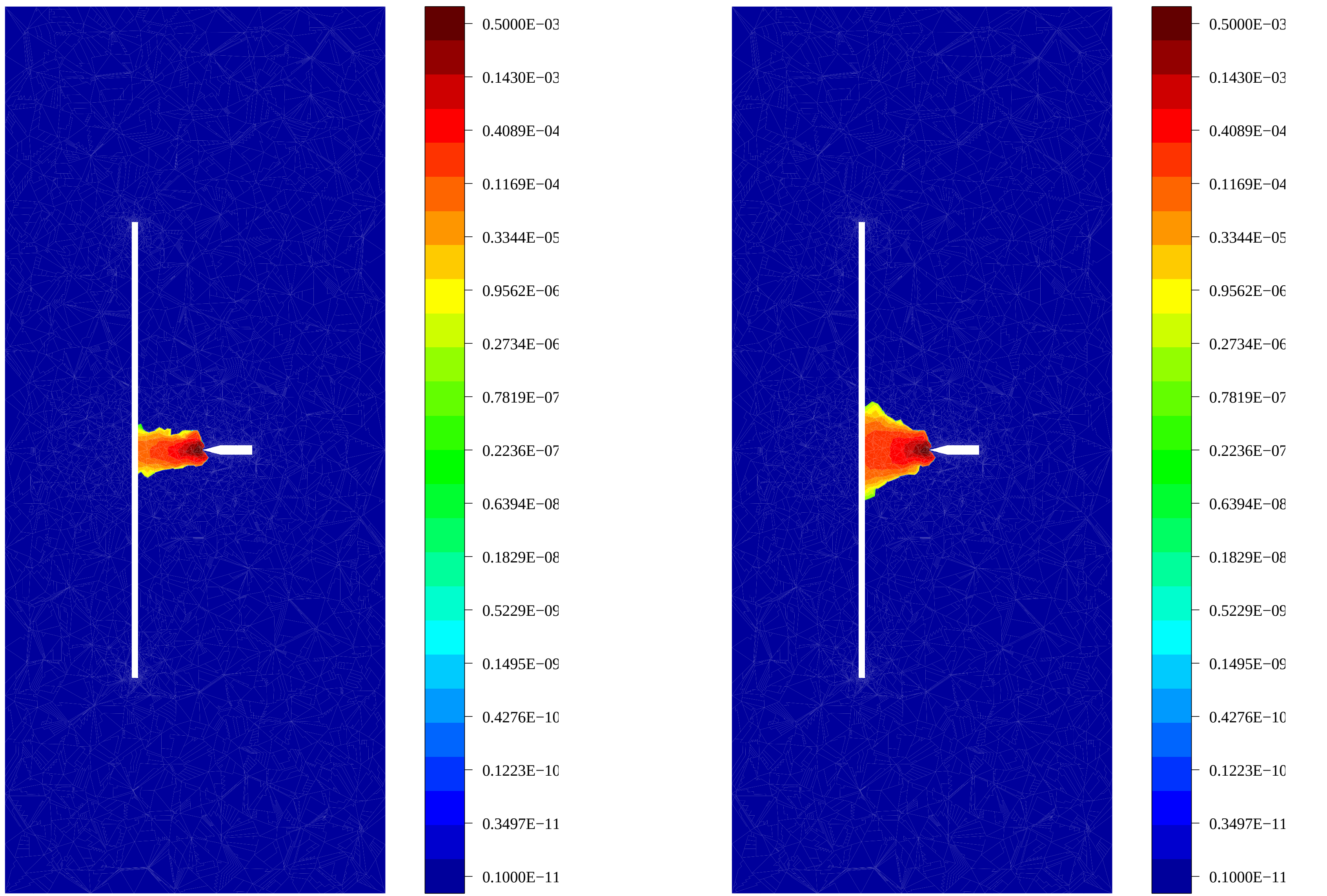
Mesh	Elements	Nodes
Single electrode (tetrahedral,Horn)	347193	68647
Single electrode (tetrahedral,Sonnenschein)	1650233	281829
Six electrodes (tetrahedral,Sonnenschein)	3030803	545429

Using single electrode mesh created by Erlangen-group (Horn)

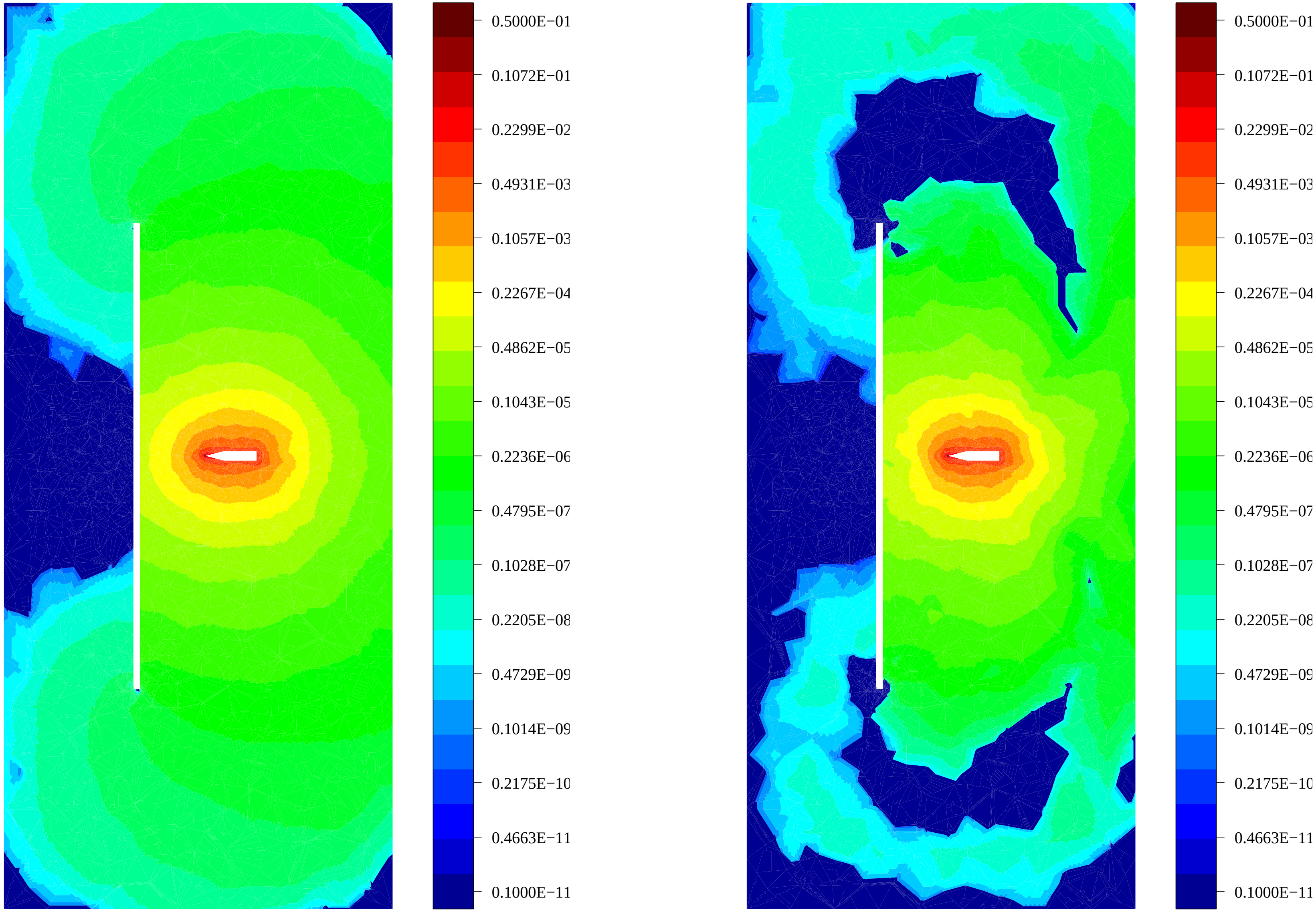
Applied Voltage:	26300 V
Electrode radius:	0.0075 cm
Distance Electrode-Target:	0.32 m
Measured Ion flow density (central target):	$1.4\mathrm{mA/m}^2$
Computed E_{onset}:	$1.4 \cdot 10^7 \frac{\mathrm{V}}{\mathrm{m}}$ (Cylinder),
	$1.86 \cdot 10^7 \frac{\mathrm{V}}{\mathrm{m}}$ (Spherical)

Charge injection law: $\varrho|_{\Gamma_A} = \varrho_0 \max(0, (E \cdot n - E_{\mathrm{onset}})/(E_{\max} - E_{\mathrm{onset}}))$

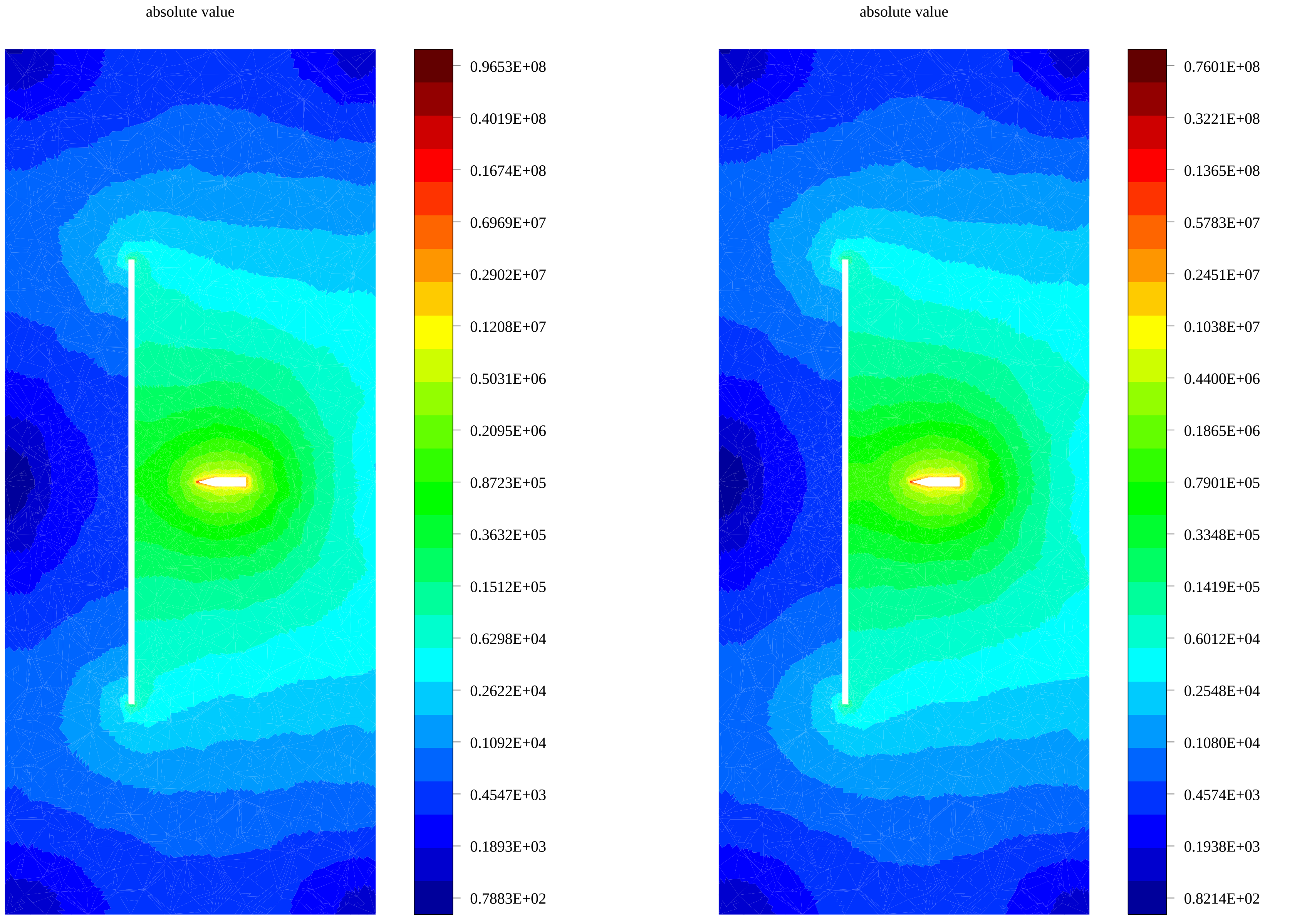




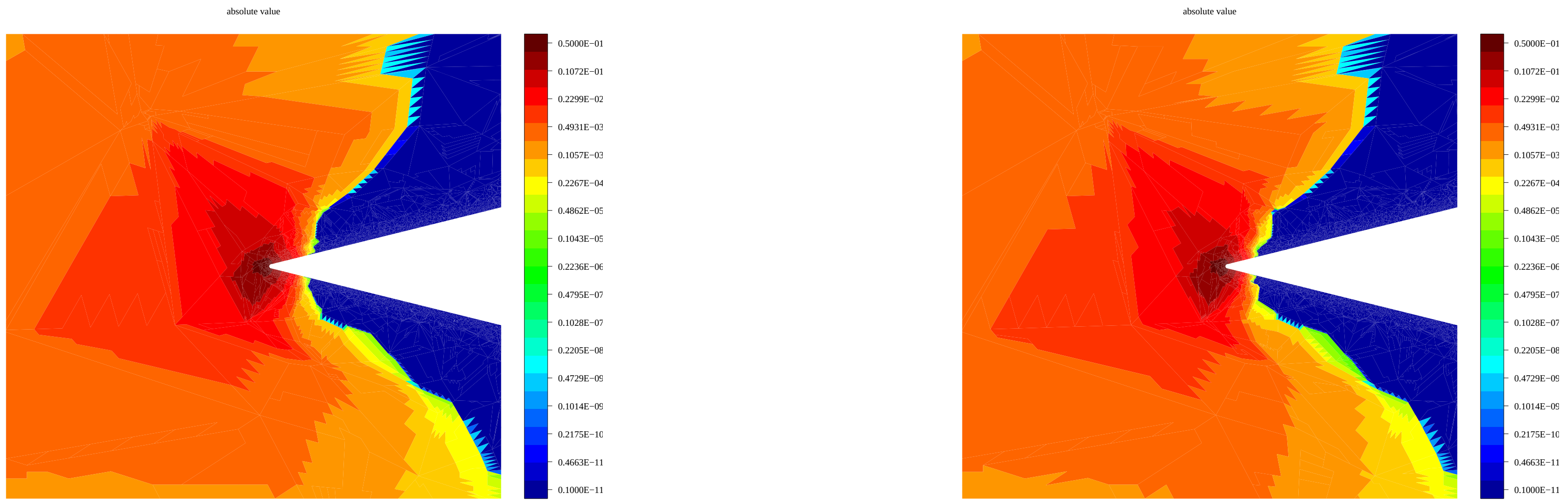
Space charge density (MOC), first and 7th iteration



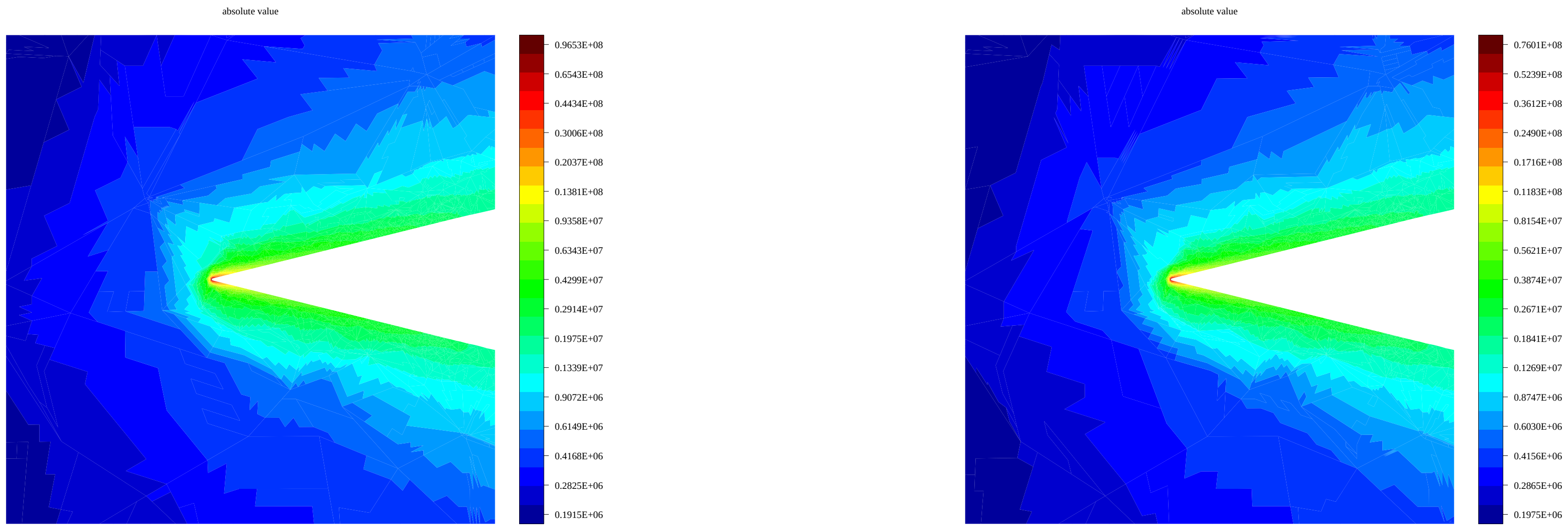
Space charge density (MOC), full injection law ($E_{\text{onset}} = 0$)
Piecewise linear E-Field (left), piecewise constant $-\nabla u$ (right)



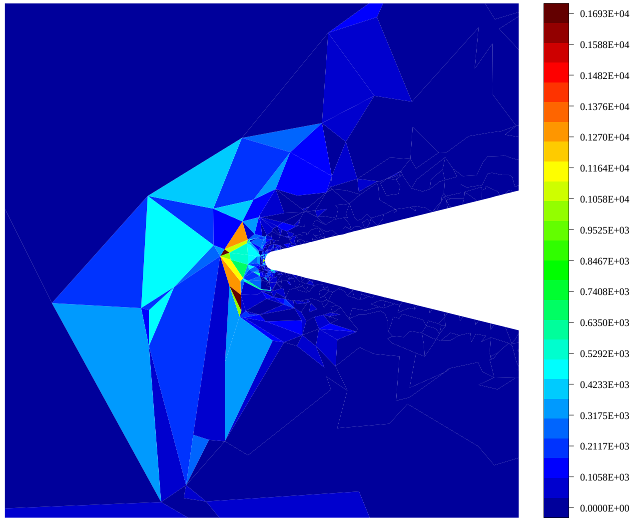
Electric field strength (MOC), first and 7th iteration

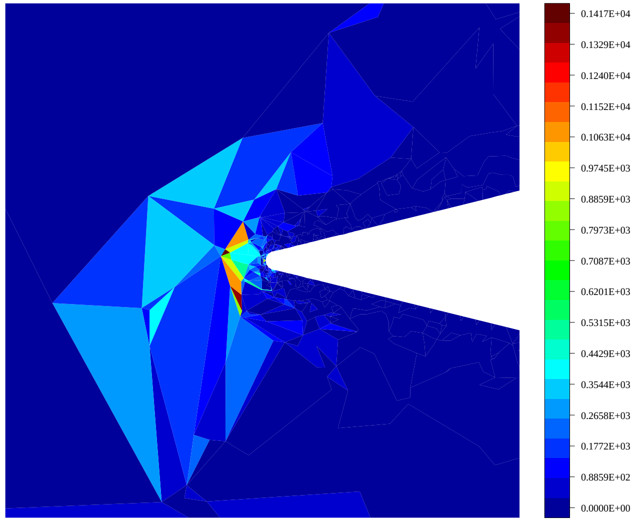


Space charge density near tip (MOC), first and 7th iteration



Electric field strength near tip, first and 7th iteration





n	$\lVert E\cdot\nabla\varrho\rVert_{L^2(\Omega)}$	$\lVert\varrho^2/\varepsilon_0\rVert_{L^2(\Omega)}$	$\lVert E\cdot\nabla\varrho+\varrho^2/\varepsilon_0\rVert_{L^2(\Omega)}$	$E_{\max}$
1	1.2160E+04	1.2068E+03	1.1657E+04	1.0297E+08
2	1.0299E+04	1.1297E+03	9.8192E+03	8.2916E+07
3	1.0067E+04	1.1132E+03	9.5929E+03	8.0682E+07
4	1.0117E+04	1.1163E+03	9.6416E+03	8.1190E+07
5	1.0095E+04	1.1141E+03	9.6202E+03	8.0963E+07

Conclusion/ to do

- Method of Characteristics gives space charge distribution
- Need better E-field (with mixed formulation?)
- Initial mesh should be better adjusted to field lines
- Use Least squares functional of transport problem for adaptive scheme