Inverse Problems For PNP Systems

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Semiconductor Devices

Considering semiconductor devices the Poisson-Nernst-Planck (PNP) equations on a bounded domain Ω are given by

$$\begin{aligned}
\lambda^2 \Delta V &= n - p - C \\
\partial_t n &= \operatorname{div} J_n - R \\
\partial_t p &= -\operatorname{div} J_p - R \\
J_n &= \mu_n \left(\nabla n - n \nabla V \right) \\
J_p &= \mu_p \left(-\nabla p - p \nabla V \right).
\end{aligned}$$

Boundary conditions

$$n = n_D(x), \quad p = p_D(x), \quad V = U(x,t) + U_T \log\left(\frac{n_D}{2\sigma^2}\right) \qquad \text{on } \Gamma_D$$

$$\frac{\partial V}{\partial \nu} = 0, \quad J_n \cdot \nu = J_p \cdot \nu = 0 \qquad \text{on } \Gamma_N$$

Initial Conditions

$$n(x,0) = n_I(x) \quad p(x,0) = p_I(x)$$

Indirect Measurements

Measurements used in practice on a contact $\Gamma_1 \subset \partial\Omega_D$:

- Current measurements

$$\mathrm{I}_{\Gamma_1} = \int_{\Gamma_1} (J_n + J_p)\, d\nu$$

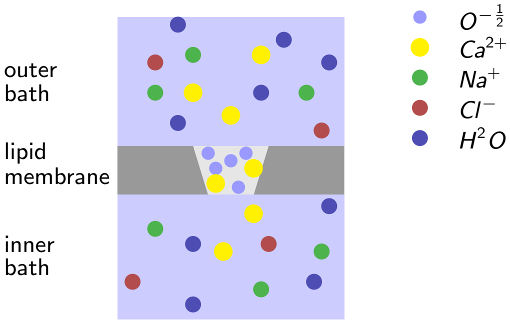
- Capacitance measurements

$$Cap_{\Gamma_1} = \frac{d}{dU}\left(\int_{\Gamma_1} \nabla V d\nu\right)$$

Geometry of an Ion Channel

Ion channels are

- proteins with a hole, which allow ions to move through the impermeable cell membrane.
- selective - they conduct ions of one type much better than others.



Ion Channels

A simplified model of an ion channel is given by the PNP equations

$$\lambda^2 \; \Delta V = \sum_k z_k \rho_k$$
$$-\nabla \cdot (m_j \; \rho_j \nabla \mu_j) = 0 \qquad j = 1, \ldots M.$$

- $V \ldots$ electric potential
- $\rho_k \ldots$ density of ionic species
- $M \ldots$ number of ionic species, $M \geq 4$
- $z_k \ldots$ relative charge
- $\mu_j \ldots$ potential

Ion Channels

The potentials μ_j are calculated as the variation of the energy functional

$$\mu_k = \frac{\partial}{\partial \rho_k} E\left[\rho_1, \ldots, \rho_M; V\right]$$

which is given by

$$E\left[\rho_1, \ldots, \rho_M; V\right] = \int_\Omega \left(-\lambda^2 |\nabla V|^2 + z_k V \rho_k + c_k \rho_k \log \rho_k + \mu_0^k \rho_k\right) dx + \\ + E^{ex}\left[\rho_1, \ldots, \rho_M\right].$$

- $\mu_0^k \ldots$ external force via potential
- $E^{ex} \ldots$ direct and chemical interactions

Ion Channels

Boundary conditions are

$$
\begin{aligned}
V = U, \quad \rho_j = \eta_j \qquad & \text{on } \Gamma_D,\ j = 1, \ldots, M-1 \\
\frac{\partial \mu_M}{\partial \nu} = 0 \qquad & \text{on } \Gamma_D \\
\frac{\partial V}{\partial \nu} = 0, \quad \frac{\partial \mu_j}{\partial \nu} = 0 \qquad & \text{on } \Gamma_N,\ j = 1, \ldots, M.
\end{aligned}
$$

The total number of confined particles N_M, which is needed to specify ρ_M is given by

$$\int_\Omega \rho_M \, dx = N_M.$$

Ion Channels

An output measurement of a channel is the current flowing out at one side

$$I = \sum_{k=1}^{M-1} \int_{\Gamma_0} z_k \; J_k \cdot d\nu.$$

Here J_k denotes the flux of species k given by

$$J_k = -\rho_k \nabla \mu_k = -c_k \nabla \rho_k - z_k \rho_k \nabla V - \rho_k \left(\nabla \mu_k^0 + \nabla \mu_k^{ex} \right)$$

Given the measured current flow the following inverse problems arise:

- Identification of the confining external potential μ_M^0.
- "Design" of the confining external potential μ_M^0 to obtain special selectivities.

Semiconductors versus Ion Channels

Semiconductors	**Ion Channels**
two species (electrons and holes)	more than 4 different species
same type of boundary conditions for all species	different types of boundary conditions for each species
	additional excess electrochemical potentials
capacitance and current measurements	current measurements
variation of applied voltage at the Dirichlet boundaries	variation of concentration at the Dirichlet boundaries

$\Rightarrow$ *M. Burger, R.S. Eisenberg, H.W. Engl, "Inverse problems related to ion channel selectivity", submitted*

Linearization

Unipolar transient PNP equations

$$\lambda^2 \Delta V - n = -C$$
$$n_t = \operatorname{div}\left(\mu_n \left(\nabla n - n \,\nabla V\right)\right).$$

We introduce the variables μ and J given by

$$\mu = \log n - V \approx \log \tilde{n} + \frac{n}{\tilde{n}} - 1 - V$$
$$J = n \,\nabla \mu \approx \tilde{n}\, \tau \,\nabla \mu$$

and replace the time derivative by finite differences. This gives

$$\lambda^2 \Delta V - n = -C$$
$$-V + \frac{n}{\tilde{n}} - \mu = -\log \tilde{n} + 1$$
$$-n + \tau \operatorname{div} J = -\tilde{n}$$
$$-\tau \nabla \mu + \frac{J}{\bar{\mu}_n \tilde{n}} = 0.$$

Linearization

Discretizing the linearized system in time, with time steps τ, we obtain

$$
\begin{aligned}
\lambda^2 \Delta \left(\mathsf{V}^{k+1}\right) - \mathsf{n}^{k+1} &= -C \\
-\mathsf{V}^{k+1} + \frac{\mathsf{n}^{k+1}}{\mathsf{n}^{k}} - \mu_{\mathsf{n}}^{k+1} &= -\log \mathsf{n}^{k} + 1 \\
-\mathsf{n}^{k+1} + \tau \operatorname{div} \mathsf{J}_{\mathsf{n}}^{k+1} &= -\mathsf{n}^{k} \\
\frac{\mathsf{J}_{\mathsf{n}}^{k+1}}{\bar{\mu}_n \, \mathsf{n}^{k}} - \tau \nabla \mu_{\mathsf{n}}^{k+1} &= 0
\end{aligned}
$$

Dirichlet boundary conditions

$$
\begin{aligned}
\mathsf{n}^{k+1}(x,t) &= \frac{1}{2}\left(C(x) + \sqrt{C(x)^2 + 4\sigma^4}\right) \\
\mathsf{V}^{k+1}(x,t) &= U(x,t) + \ln\left(\frac{1}{2\sigma^2}\left(C(x) + \sqrt{C(x)^2 + 4\sigma^4}\right)\right) \\
\mu^{k+1}(x,t) &= \log \mathsf{n}^{k+1}(x,t) - \mathsf{V}^{k+1}(x,t)
\end{aligned}
$$

Existence and Uniqueness

Mixed Formulation

Let $f \in V',\ g \in Q'$ be given, find $u \in V$ and $p \in Q$ solutions of

$$\begin{aligned} a(u,v) + b(v,p) &= \langle f, v\rangle \quad \forall\ v \in V \\ b(u,q) - c(p,q) &= \langle g, q\rangle \quad \forall\ q \in Q. \end{aligned}$$

Here a, b and c are continuous bilinear forms on $V \times V$, $V \times Q$ and $Q \times Q$ respectively.

Existence and Uniqueness

Under the assumptions that

- a is bounded and coercive, i.e.

$$
\begin{aligned}
|a(u,v)| &\le \|a\|\|u\|_V\|v\|_V && \forall\ u,v\in V\\
\exists\ \alpha>0 \quad a(v,v) &\ge \alpha\|v\|_V^2 && \forall\ v\in V
\end{aligned}
$$

- b is bounded, i.e. $|b(v,q)| \le \|b\|\|v\|_V\|q\|_Q$
- b satisfies the inf-sup condition, i.e.

$$\exists\ \beta>0 \quad \sup_{v\in V}\frac{b(v,\mu)}{\|v\|_V} \ge \beta\|\mu\|_Q$$

- c is bounded and coercive, i.e.

$$
\begin{aligned}
|c(\mu,v)| &\le \|c\|\|\mu\|_Q\|v\|_Q && \forall \mu,q\in Q\\
\exists\ \gamma>0 \quad c(q,q) &\ge \gamma\|q\|_Q^2 && \forall q\in Q
\end{aligned}
$$

the system has a unique solution.

Existence and Uniqueness

The linearized PNP equations can be rewritten as

$$\begin{aligned}\tilde{a}\left(\left(\mu_n, J_n\right), \left(\psi_2, \varphi_2\right)\right) + \tilde{b}\left(\left(\psi_2, \varphi_2\right), \left(V, n\right)\right) &= F_1 \\ \tilde{b}\left(\left(\mu_n, J_n\right), \left(\varphi_1, \psi_1\right)\right) - \tilde{c}\left(\left(V, n\right), \left(\varphi_1, \psi_1\right)\right) &= F_2.\end{aligned}$$

We can verify these conditions for

$$\begin{array}{ll} n \in L^2\left(\Omega\right) & V \in H^1\left(\Omega\right) \\ \mu \in L^2\left(\Omega\right) & J \in H\left(\mathrm{div}, \Omega\right) \end{array}$$

$\Rightarrow$ existence and uniqueness of a solution.

Identification Problems

Consider identification of the doping profile $C = C(x)$ from transient current measurements.

Abstract Formulation

$$F(C) = Y^\delta$$

with

$$\begin{aligned} F \colon \mathcal{D} &\to \mathcal{Y} \\ C &\mapsto \mathrm{I}_{\Gamma_1}(U) \end{aligned}$$

Applying Tikhonov regularization to the abstract problem gives

$$Q(C) = \sum_k \left\| F(C) - Y_k^\delta \right\|^2 + \alpha \left\| C - C^* \right\|^2 \to \min_C$$

where the index k denotes the time steps.

Adjoint Equations

The adjoint equations (calculated via the corresponding Lagrange functional) are given by

$$
\begin{aligned}
\lambda^2 \Delta\, \theta^{\mathrm{k+1}} - \gamma^{\mathrm{k+1}} &= 0 \\
-\,\theta^{\mathrm{k+1}} + \frac{1}{\mathrm{n^k}}\, \gamma^{\mathrm{k+1}} - \rho^{\mathrm{k+1}} &= \frac{n^{k+2} - \mathrm{n^{k+1}}}{(\mathrm{n^{k+1}})^2}\ \gamma^{k+2} - \rho^{k+2} + \frac{J^{k+2}}{\bar{\mu}_n\, (\mathrm{n^{k+1}})^2}\ \omega^{k+2} \\
-\,\gamma^{\mathrm{k+1}} + \tau\, \mathrm{div}\, \omega^{\mathrm{k+1}} &= 0 \\
-\tau \nabla\, \rho^{\mathrm{k+1}} + \frac{1}{\bar{\mu}_n\, \mathrm{n^k}}\, \omega^{\mathrm{k+1}} &= 0.
\end{aligned}
$$

with the Dirichlet boundary conditions

$$
\begin{aligned}
\rho^{\mathrm{k+1}}(\Gamma_1) = \mathrm{J_n^{k+1}} - f^{\,k+1} \quad \rho^{\mathrm{k+1}}(\Gamma_2) &= 0 \\
\theta^{\mathrm{k+1}}\,(\Gamma_1) = \theta^{\mathrm{k+1}}\,(\Gamma_2) &= 0 \\
\omega^{\mathrm{k+1}}\,(\Gamma_1) = \omega^{\mathrm{k+1}}\,(\Gamma_2) &= 0
\end{aligned}
$$

and homogenous Neumann boundary conditions on the rest of the boundary.

Discretization for one-dimensional Problems

For the discretization in space we use

- piecewise linear basis functions for V and J and
- piecewise constant ones for n and μ.

The weak formulation of the linearized PNP system is given by

$$\begin{pmatrix} -\lambda^2 K & -M_1 & 0 & 0 \\ -M_1^T & A_n & -M_2 & 0 \\ 0 & -M_2^T & 0 & \tau D \\ 0 & 0 & \tau D^T & B_n \end{pmatrix} \begin{pmatrix} V \\ n \\ \mu \\ J \end{pmatrix} = \begin{pmatrix} f_1 \\ f_2 \\ f_3 \\ f_4 \end{pmatrix}.$$

K	stiffness matrix
$M_1, \ M_2$	mass matrices (depending on the basis functions)
$A_n, \ B_n$	matrices which depend on the solution of the last time step
D	"differentiation" matrix

Problem Setup: Unipolar Diode

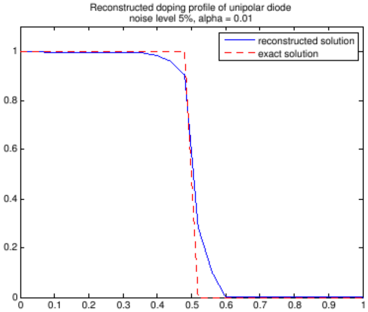
Predefined doping profile

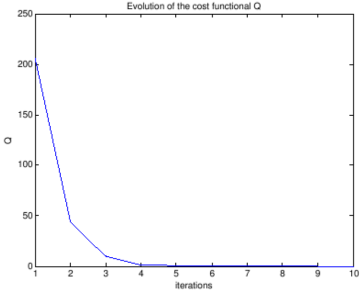
$$C(x) = \begin{cases} C_{max} \cdot 1.0 \ \mathrm{cm}^{-3} & x \leq 0.5 \\ 0 \quad \mathrm{cm}^{-3} & x > 0.5 \end{cases}$$

Length	$L = 10^{-4}\mathrm{cm}$
Time steps	$\tau = 0.5$
Number of time steps	$t_k = 200$
Applied voltage	$U(t) = 10^{-2}(t + \sin(t))$
Discretization parameter	$h \approx \lambda$
Stabilization parameter	$\varepsilon \approx \lambda$
Software package	Matlab

Reconstructed Doping Profile with 5 % noise

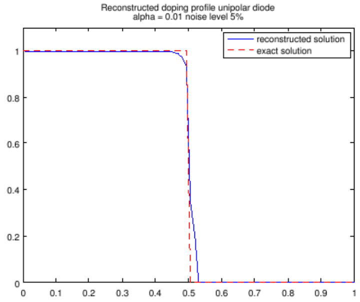
$C_{max} = 10^{16}$, Noise 5 % and $C(x) \geq 0$

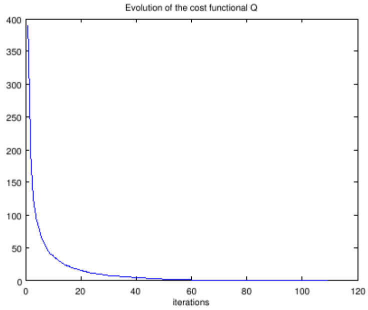




Reconstructed Doping Profile with 5 % noise

$C_{max} = 10^{17}$, Noise 5 % and $C(x) \geq 0$





Identification Problems for Bipolar Semiconductor Devices

Linearized PNP Equations for bipolar device

$$
\begin{aligned}
\lambda^2 \Delta \mathsf{V}^{k+1} - \mathsf{n}^{k+1} + \mathsf{p}^{k+1} &= -\mathsf{C} \\
-\mathsf{V}^{k+1} + \frac{\mathsf{n}^{k+1}}{\mathsf{n}^{k}} - \mu_{\mathsf{n}}^{k+1} &= -\log \mathsf{n}^{k} + 1 \\
\mathsf{V}^{k+1} + \frac{\mathsf{p}^{k+1}}{\mathsf{p}^{k}} - \mu_{\mathsf{p}}^{k+1} &= -\log \mathsf{p}^{k} + 1 \\
-\mathsf{n}^{k+1} + \tau \operatorname{div} \mathsf{J}_{\mathsf{n}}^{k+1} &= -\mathsf{n}^{k} + \tau \frac{\mathsf{n}^{k} \mathsf{p}^{k} - \sigma^4}{\tau_n (\mathsf{p}^{k} + \sigma^2) + \tau_p (\mathsf{n}^{k} + \sigma^2)} \\
-\mathsf{p}^{k+1} + \tau \operatorname{div} \mathsf{J}_{\mathsf{p}}^{k+1} &= -\mathsf{p}^{k} + \tau \frac{\mathsf{n}^{k} \mathsf{p}^{k} - \sigma^4}{\tau_n (\mathsf{p}^{k} + \sigma^2) + \tau_p (\mathsf{n}^{k} + \sigma^2)} \\
\frac{1}{\bar{\mu}_n \mathsf{n}^{k}} \mathsf{J}_{\mathsf{n}}^{k+1} - \tau \nabla \mu_{\mathsf{n}}^{k+1} &= 0 \\
\frac{1}{\bar{\mu}_p \mathsf{p}^{k}} \mathsf{J}_{\mathsf{p}}^{k+1} - \tau \nabla \mu_{\mathsf{p}}^{k+1} &= 0.
\end{aligned}
$$

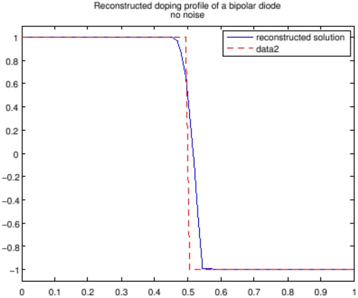
Problem Setup: Bipolar Diode

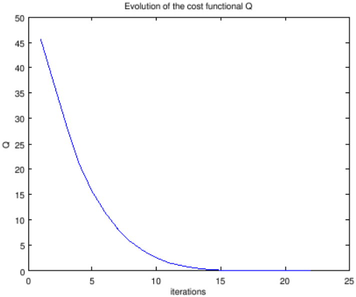
Predefined doping profile

$$C(x) = \begin{cases} 10^{16} \quad \mathrm{cm}^{-3} & x \leq 0.5 \\ -10^{16} \ \mathrm{cm}^{-3} & x > 0.5 \end{cases}$$

Length	$L = 10^{-3}\mathrm{cm}$
Time steps	$\tau = 10$
Number of time steps	$t_k = 100$
Applied voltage	$U(t) = 10^{-3}(t + \sin(t))$
Discretization parameter	$h \approx \lambda$
Stabilization parameter	$\varepsilon \approx \lambda^2$
Software package	Matlab

Reconstructed Doping Profile





Discretization of the two dimensional problem

The solution of the linearized PNP equations is in the following Sobolev spaces

$$V \in H^1(\Omega) \quad n \in L^2(\Omega),$$
$$\mu_n \in L^2(\Omega) \quad J_n \in H(div; \Omega).$$

Discretization

- $n,\ \mu_n \ldots$ piecewise constant basis functions
- $V \ldots$ piecewise linear basis function
- $J_n \ldots$ low order Raviart-Thomas elements

Approximation of $H\,(\mathrm{div}; K)$

Some notations:

- Let $\Omega = \bigcup_{r=1}^{m} K_r$, where K_r denote triangles
- n : dimension of space
- $P_k\,(K)$: space of polynomial of degree $\leq k$

Raviart-Thomas Elements
The Raviart-Thomas space is given by

$$RT_k = (P_k\,(K))^n + \underline{x}\; P_k\,(K)\,.$$

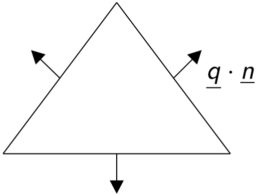
For any $\underline{q} \in RT_k\,(K)$ we have

$$\begin{aligned} \mathrm{div}\,\underline{q} &\in P_k\,(K)\,, \\ \underline{q}\cdot\underline{n}\,|_{\partial K} &\in R_k\,(\partial K)\,. \end{aligned}$$

Low Order Raviart-Thomas Elements

The space RT_0 is given by

$$q_1(x, y) = a + cx,$$
$$q_2(x, y) = b + cy.$$



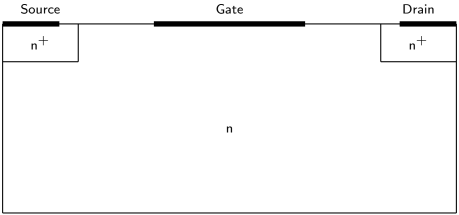
Used in

- electromagnetics
- fluid dynamics

Forward Solver for a MESFET

MESFET - Metal-Semiconductor Field Effect Transistor

- made of n-type III-V compound semiconductors, such as gallium arsenide (GaAs) or silicon carbide (SiC)
- used for high frequency applications (radar) or microwave integrated circuits



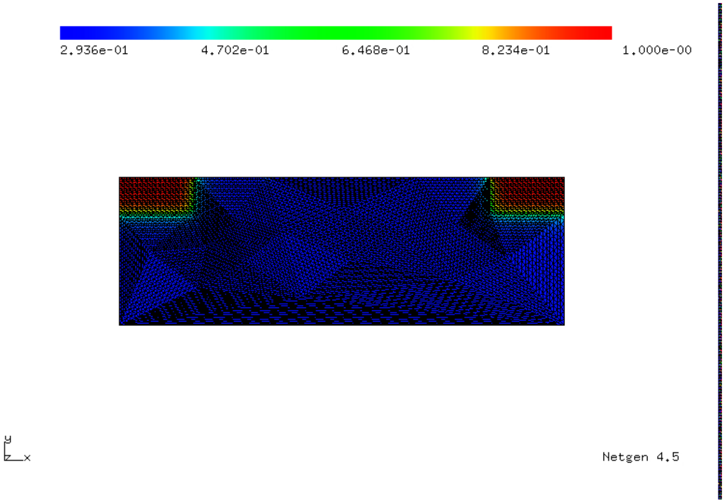
Problem Setup: GaAs MESFET

Predefined doping profile

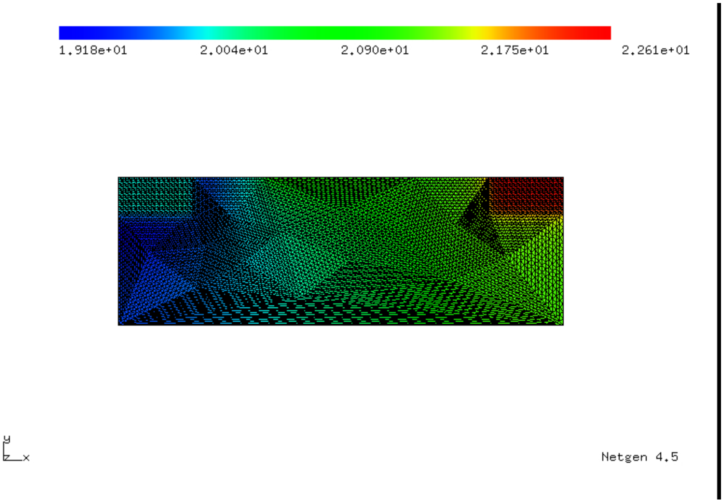
$$C(x) = \begin{cases} 10^{16} & \mathrm{cm}^{-3} & x \in \text{n}^{+}\text{region} \\ 0.3 \cdot 10^{16} & \mathrm{cm}^{-3} & x \in \text{n region} \end{cases}$$

Length	$L = 10^{-4}\mathrm{cm}$
Time steps	$\tau = 0.01$
Number of time steps	$t_k = 100$
Applied voltage	$U_{Source} = 0.4$
	$U_{Gate} = 0$
	$U_{Drain} = -1.1$
Number of triangles	$n_K = 9728$
Computation time	196 s
Software package	NGSolve V4.5

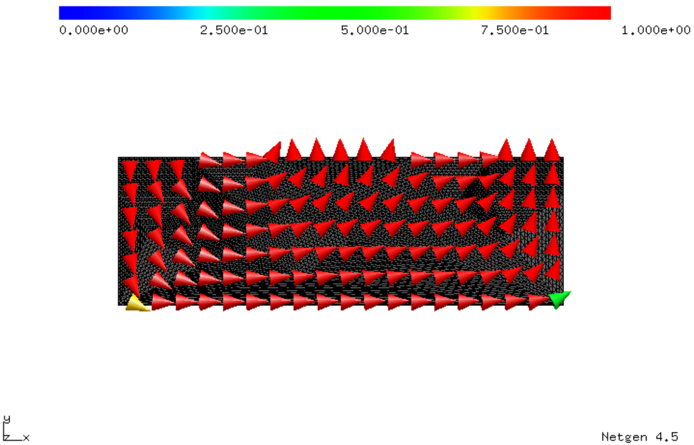
Numerical Simulation of a MESFET



Numerical Simulation of a MESFET



Numerical Simulation of a MESFET



Further Work

What's still left to do (or what we are just working on)

- Backward Solver for two dimensional problems using NGSolve
- Development of efficient numerical methods for two-dimensional identification problems using NGSolve
- Two dimensional solver for ion channels