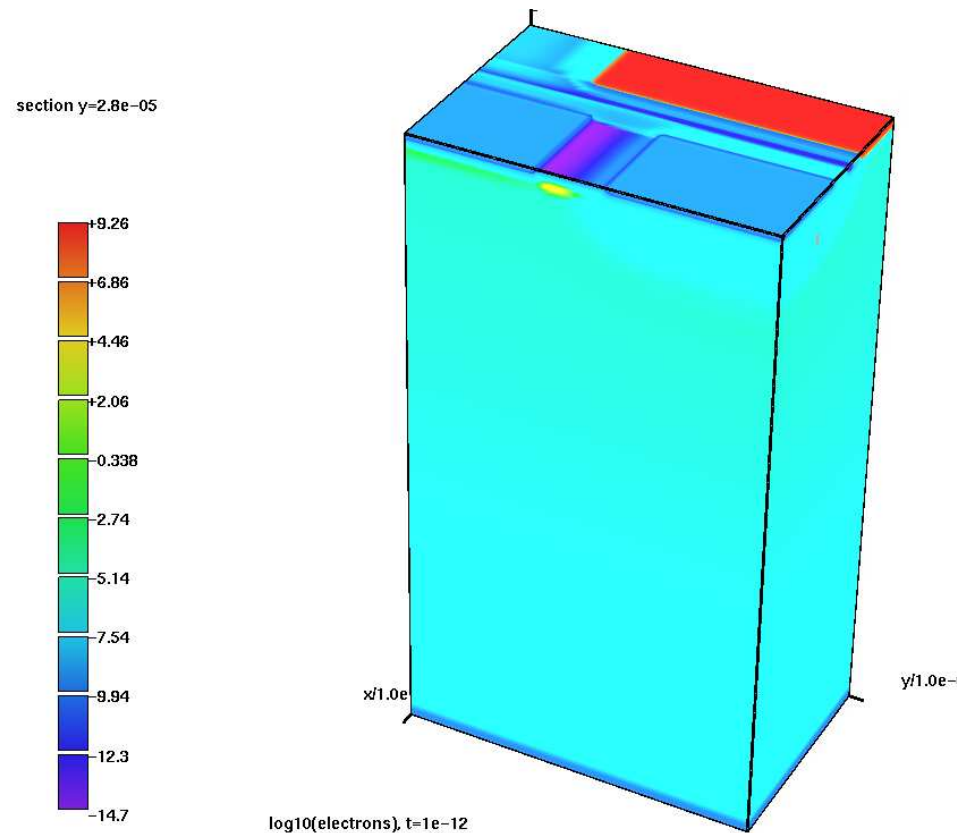


K. Gärtner

3d simulations of DEPFET based sensors: algorithms and results

DEPFET design: R. Richter,
HLL of the MPG in Munich



Outline

- Part A:

 - Van Roosbroeck's Equations

 - Finite volumes schemes and Delaunay grids

 - Useful properties of the Scharfetter-Gummel discretization

 - Sketch of the algorithms

- Part B:

 - DEFFET sensors

 - Simulation results

Warm up: Van Roosbroeck's Equations

$$\begin{aligned} & -\nabla \cdot \epsilon \nabla \psi = f - n + p, \\ (1) \quad & \frac{\partial n}{\partial t} + \nabla \cdot \mu_n n \nabla \phi_n = R, \\ (2) \quad & \frac{\partial p}{\partial t} - \nabla \cdot \mu_p p \nabla \phi_p = R, \end{aligned}$$

in $S \times \Omega$, $S = (0, T)$,

$\Omega \subset \mathbb{R}^N$, $2 \leq N \leq 3$, a bounded Lipschitzian domain,

$\partial\Omega = \Gamma_D \cup \Gamma$, Γ_D closed, positive surface measure.

Boundary conditions:

hom. Neumann on insulating parts,

Dirichlet on Ohmic contacts,

and gates: hom./inhom. Neumann ϕ/ψ

$(\partial\psi/\partial\vec{n} + \alpha(\psi - \psi_\Gamma) = 0$, $\vec{n}$ outer normal vector).

Van Roosbroeck's Equations

The physical meaning of the quantities is :

- $\phi_n = \psi - \log n$ - quasi-Fermi potential n ,
- $\phi_p = \psi + \log p$ - quasi-Fermi potential p ,
- $n = e^{\psi - \phi_n}$ - electron density,
- $p = e^{\phi_p - \psi}$ - hole density,
- ψ - electrostatic potential,
- ϵ - dielectric permittivity,
- f - density of impurities,
- R - recombination / generation rate $R = r(x, n, p)(1 - np)$,
- $\mu_{n,p}$ - carrier mobilities $\mu_{n,p} > 0$, Einstein relation.

Scaling of the potentials: U_T , 'temperature voltage', $1V \approx 40U_T$.

Van Roosbroeck's Equations

Rewriting yields:

$$(3) \quad \frac{\partial n}{\partial t} - \nabla \cdot \mu_n (\nabla n - n \nabla \psi) = R,$$

$$(4) \quad \frac{\partial p}{\partial t} - \nabla \cdot \mu_p (\nabla p + p \nabla \psi) = R,$$

or

$$(5) \quad \frac{\partial n}{\partial t} - \nabla \cdot \mu_n e^{\psi} \nabla e^{-\phi_n} = R,$$

$$(6) \quad \frac{\partial p}{\partial t} - \nabla \cdot \mu_p e^{-\psi} \nabla e^{\phi_p} = R,$$

$(e^{-\phi_n}, e^{\phi_p}$ Slotboom variables).

Free energy, dissipation rate

Let $\psi^* \in H^1$ be the (unique weak) solution of the boundary value problem

$$-\nabla \cdot \epsilon \nabla \psi^* = f + e^{-\psi^*} - e^{\psi^*} \text{ in } \Omega,$$

$$\psi^* = \psi_D^* \text{ on } \Gamma_D, \quad \vec{n} \cdot \nabla \psi^* + \alpha(\psi^* - \psi_\Gamma) = 0 \text{ on } \Gamma_{gate}, \quad n^* = e^{\psi^*}, \quad p^* = e^{-\psi^*}.$$

Definition 1 *The triple (ψ^*, n^*, p^*) is called thermal equilibrium solution; the functionals*

$$F(\psi, n, p) = \int [n(\log \frac{n}{n^*} - 1) + n^* + p(\log \frac{p}{p^*} - 1) + p^*] d\Omega + \frac{1}{2} \|\psi - \psi^*\|^2,$$

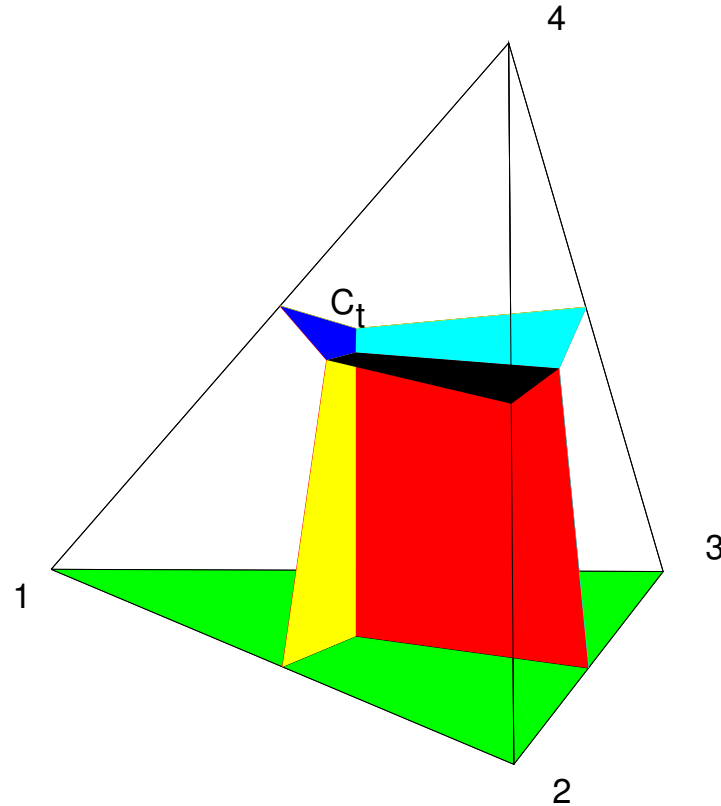
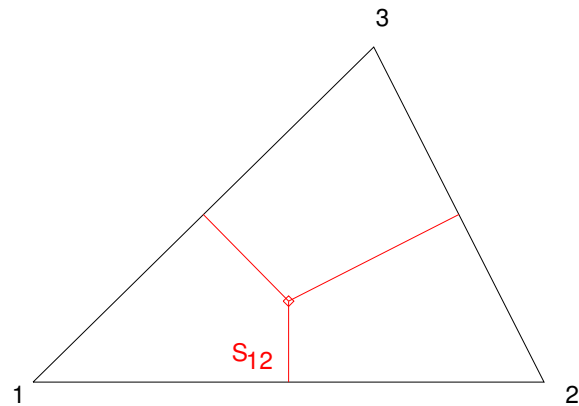
with $\|h\|^2 = \int \epsilon |\nabla h|^2 d\Omega + \int \alpha h^2 d\Gamma$, and

$$d(\psi, n, p) = \int [n\mu_n |\nabla \phi_n|^2 + p\mu_p |\nabla \phi_p|^2 + r(x, n, p)(np - 1) \log(np)] d\Omega \geq 0$$

are the free energy and the dissipation rate, respectively.

Delaunay grids

Example:



A triangle $\mathbb{E}^2$ and a tetrahedron $\mathbb{E}^3$ and the related Voronoi faces.

Delaunay grids, notations

N -dimensional simplices $\mathbf{E}_l^N$ such that

$$\Omega = \cup_l \mathbf{E}_l^N$$

l simplex index, with positive volume in a right-handed coordinate system.

The $N \times (N+1)$ matrix of the vertex coordinates represents the simplex:

$$P = \begin{pmatrix} x_{1,1} & \cdot & \cdot & \cdot & x_{1,N+1} \\ x_{2,1} & \cdot & \cdot & \cdot & x_{2,N+1} \\ \cdot & \cdot & \cdot & \cdot & \cdot \\ x_{N,1} & \cdot & \cdot & \cdot & x_{N,N+1} \end{pmatrix}, \quad \hat{P} = \begin{pmatrix} x_{1,1} - x_{1,N+1} & \cdot & \cdot & \cdot & x_{1,N} - x_{1,N+1} \\ x_{2,1} - x_{2,N+1} & \cdot & \cdot & \cdot & x_{2,N} - x_{2,N+1} \\ \cdot & \cdot & \cdot & \cdot & \cdot \\ x_{N,1} - x_{N,N+1} & \cdot & \cdot & \cdot & x_{N,N} - x_{N,N+1} \end{pmatrix}.$$

$\mathbf{x}_i^T = (x_{1,i}, x_{2,i}, \dots, x_{N,i})$ is the vector of the space coordinates of the vertex i of the simplex.

Edges (simplices with $N = 1$) are denoted by $\mathbf{e}_{ij} = \mathbf{x}_j - \mathbf{x}_i$. The simplex $\mathbf{E}_i^{N-1}$ is the 'surface' opposite to vertex i of the simplex $\mathbf{E}^N$.

Delaunay grids, definitions

Definition 2 A discretization by simplices $\mathbf{E}_i^N$ is called a Delaunay grid

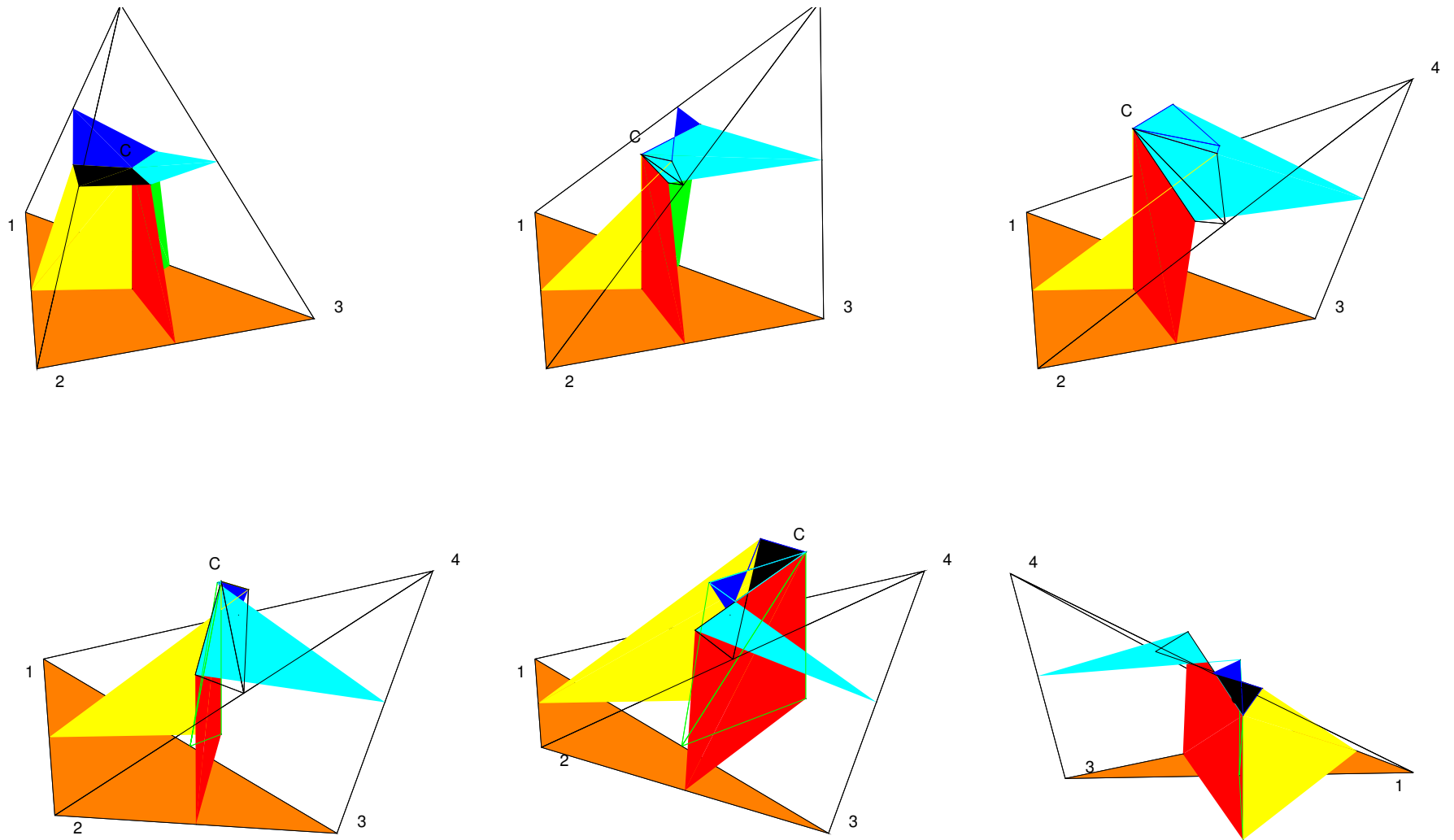
if the balls defined by the $N+1$ vertices of $\mathbf{E}_i^N \forall i$ do not contain any vertex $\mathbf{x}_k$, $\mathbf{x}_k \in \mathbf{E}_j^N$, $\mathbf{x}_k \notin \mathbf{E}_i^N$.

Definition 3 Let $V_i = \{\mathbf{x} \in \mathbb{R}^N : \|\mathbf{x} - \mathbf{x}_i\| < \|\mathbf{x} - \mathbf{x}_j\|, \forall \text{ vertices } \mathbf{x}_j \in \Omega\}$

and $\partial V_i = \bar{V}_i \setminus V_i$. V_i is the Voronoi volume of vertex i and ∂V_i is the corresponding Voronoi surface.

The Voronoi volume element V_{ij} of the vertex i with respect to the simplex $\mathbf{E}_j^N$ is the intersection of the simplex $\mathbf{E}_j^N$ and the Voronoi volume V_i of vertex i .

Delaunay grids, Voronoi surfaces



Finite volume schemes

Functions u defined at $\mathbf{E}^N$ are replaced by discrete vectors $\mathbf{u} = (u(\mathbf{x}_1), \dots, u(\mathbf{x}_{N+1}))^T$.

Volume integral of a function:

$$\int f d\Omega \approx \sum_m f_m |V_m|, \quad \sum_m |V_m| = |\Omega|,$$

With respect to the differential operators Gauss's theorem is supposed to hold

$$-\nabla \epsilon \nabla u = 0, \quad \epsilon = \text{const on } E_l^N, \forall l.$$

on each V_{ij} , this yields

$$\int_{V_{ij}} -\nabla \cdot \epsilon \nabla u dV = -\epsilon_j \sum_k \int_{S_k} \nabla u \cdot d\mathbf{S}_k \approx [\gamma_{k(i)}] \tilde{G}_i \mathbf{u}|_E + \text{boundary integrals},$$

$$\gamma_{k(i)} = \frac{\partial V_{i,k(i)}}{|\mathbf{e}_{i,k(i)}|} \geq 0 \quad (\text{compensation over neighbors possible}).$$

Finite volume schemes

What is $\sum_{i, V_i \in \mathbf{E}_j^N} \int_{V_{ij}} -\nabla \cdot \epsilon \nabla u dV$?

$$\sum_{i, V_i \in \mathbf{E}_j^N} \int_{V_{ij}} -\nabla \cdot \epsilon \nabla u dV = \epsilon \tilde{G}^T[\gamma] \tilde{G} \mathbf{u}|_E + \text{boundary integrals}$$

where

$$\tilde{G}_2 = \begin{pmatrix} 0 & 1 & -1 \\ -1 & 0 & 1 \\ 1 & -1 & 0 \end{pmatrix}, \quad \tilde{G}_3 = \begin{pmatrix} 1 & -1 & 0 & 0 \\ 0 & 1 & -1 & 0 \\ -1 & 0 & 1 & 0 \\ -1 & 0 & 0 & 1 \\ 0 & -1 & 0 & 1 \\ 0 & 0 & -1 & 1 \end{pmatrix}, \quad \dots,$$

the difference matrix along all edges, hence a mapping from nodes to edges.

$$\tilde{G}^T[\gamma] \tilde{G} = \begin{pmatrix} 0 & -1 & 1 \\ 1 & 0 & -1 \\ -1 & 1 & 0 \end{pmatrix} \begin{pmatrix} 0 & \gamma_1 & -\gamma_1 \\ -\gamma_2 & 0 & \gamma_2 \\ \gamma_3 & -\gamma_3 & 0 \end{pmatrix} = \begin{pmatrix} \gamma_2 + \gamma_3 & -\gamma_3 & -\gamma_2 \\ -\gamma_3 & \gamma_1 + \gamma_3 & -\gamma_1 \\ -\gamma_2 & -\gamma_1 & \gamma_1 + \gamma_2 \end{pmatrix}.$$

Finite volume schemes

Testing the expression $\tilde{G}^T[\gamma]\tilde{G}\mathbf{u}|_E$ on the simplex E_j with a unit vector

$e_i^T = (0, \dots, 0, 1, 0, \dots, 0)$ specified on the simplex vertices, yields

$$e_i^T \tilde{G}^T[\gamma]\tilde{G}\mathbf{u}|_E = \sum_{\mathbf{e}_{k(i)}} \pm 1[\gamma_{k(i)}]\tilde{G}\mathbf{u}|_E = \sum_{\mathbf{e}_{k(i)}} -\mathbf{j}_{k(i)}\partial V_{i,k(i)},$$

hence the surface integral of a current

$$\mathbf{J}_i = \int_{\Gamma_{D_i}} \mathbf{j} d\mathbf{S} = \int_{\Gamma_{D_i}} h_i(x) \mathbf{j} d\mathbf{S}$$

$$h_i(x) = \begin{cases} 1 & \text{on } \Gamma_{D_i} \\ 0 & \text{on } \Gamma_{D_j}, j \neq i. \end{cases}$$

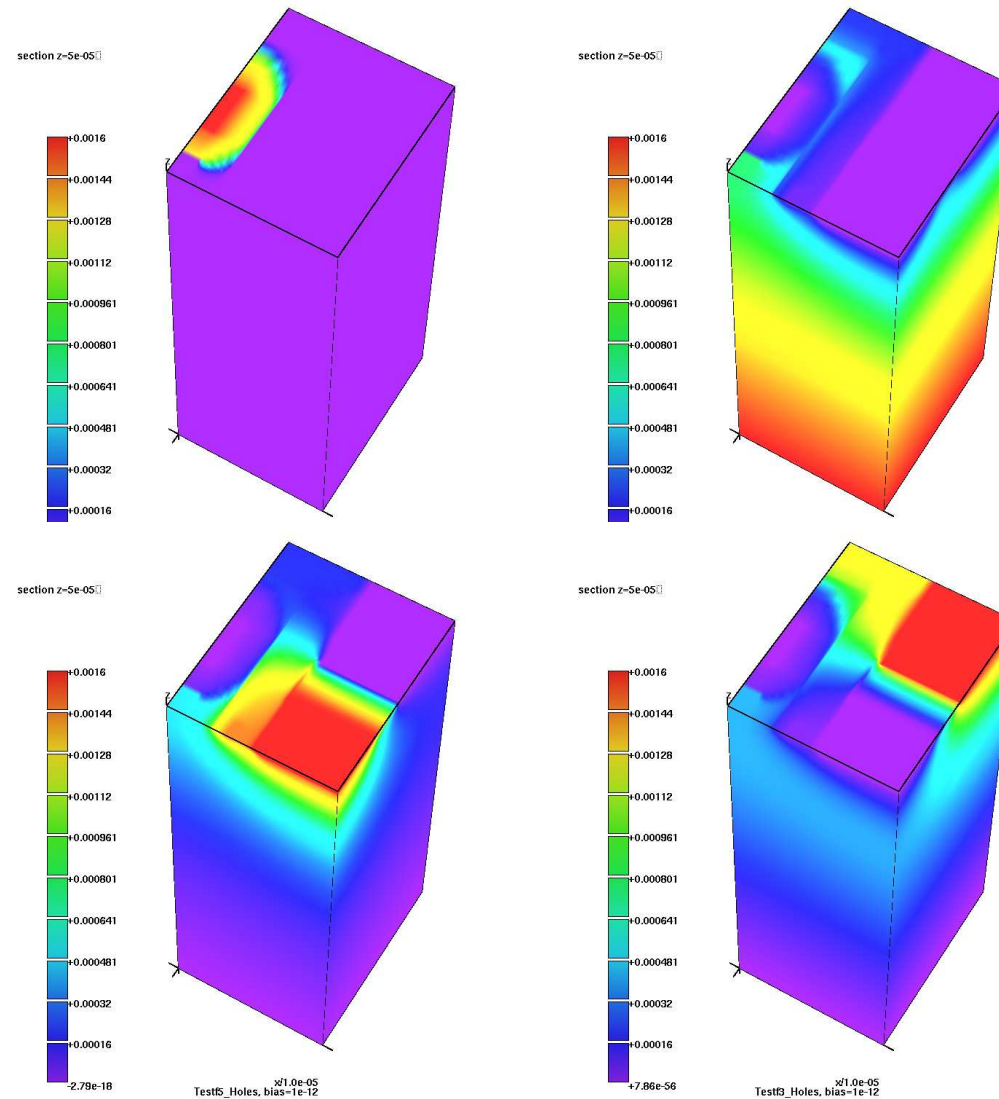
can be expressed in complete analogy to integration by parts

$$\mathbf{J}_i = -\mathbf{h}_i^T \tilde{G}^T[\gamma]\tilde{G}\mathbf{u}.$$

What is the optimal h_i for contact current evaluation?

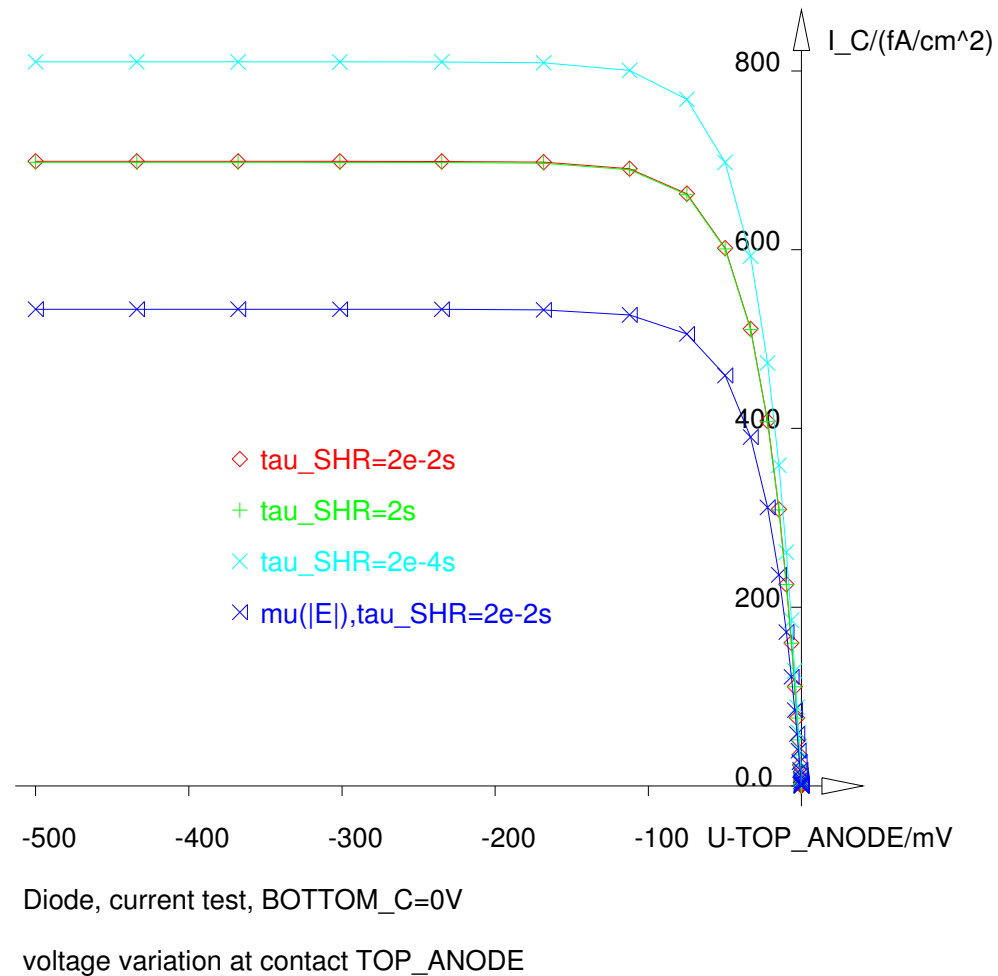
Weak finite volume formulation and contact currents

Approximations of the adjoint problem (contacts, holes):



Weak finite volume formulation and contact currents

Numerical noise
contact currents,
a '3d' diode:



Useful properties of the Scharfetter-Gummel scheme

The Scharfetter-Gummel scheme yields for any step size h :

- discrete maximum principle for $\phi_{n,p}$,
- is dissipative together with the Euler backward scheme.

To discretize $-\nabla \mu e^\psi \nabla e^{-\phi_n}$ on a simplex one has to approximate $e^\psi|_{\partial V_{i,k(i)}}$.

Scharfetter-Gummel (69) (Allen, Southwell (55); Il'in (69); ...): solution of a two point boundary value problem $j' = 0$, hence $j = \text{const.}$

(For more general convection diffusion equations see Eymard, Fuhrmann, Gärtner (05).)

Scharfetter-Gummel scheme

The solution along the edge e_{ij} of $-\mu e^\psi (e^{-\phi_n})' = \text{const}$ yields

$$\langle e^\psi \rangle_{ij} := e^{(\psi_i + \psi_j)/2} / \text{sh}((\psi_i - \psi_j)/2), \quad \text{sh}(s) = \text{sh}(-s) = \frac{\sinh(s)}{s},$$

$$-\nabla \mu e^\psi \nabla e^{-\phi_n} \approx \mu_n \tilde{G}^T[\gamma] [\langle e^\psi \rangle_{i,k(i)}] \tilde{G} e^{-\phi_n} := A_{\text{Slotb}}(\psi) \mathbf{e}^{-\phi_n}.$$

Proposition 1 $A_{\text{Slotb}}(\psi)$ is a *S-matrix* on $E_l^N \forall \psi$.

PROOF: $\mathbf{1}^T A_{\text{Slotb}} = \mathbf{0}^T$, $a_{ii} > 0$, $a_{ij} \leq 0$, $i \neq j$.

Hence for $\mathbf{e}^{-\phi_n}$ holds a discrete maximum principle.

Scharfetter-Gummel scheme

Changing variables ($\mathbf{n} := [e^\psi] \mathbf{e}^{-\phi_n}$) yields the classical Scharfetter-Gummel scheme:

$$\begin{aligned} A_{Slotb}[e^{-\psi}] \mathbf{n} &= \mu_n \tilde{G}^T[\gamma] [\langle e^\psi \rangle |_{i,k(i)}] \hat{G}\{e^{-\psi_i}, -e^{-\psi_{k(i)}}\} \mathbf{n}, \\ &= \mu_n \tilde{G}^T[\gamma] \hat{G}\{e^{(\psi_{k(i)} - \psi_i)/2} / \text{sh}((\psi_i - \psi_{k(i)})/2), \\ &\quad -e^{(\psi_i - \psi_{k(i)})/2} / \text{sh}((\psi_i - \psi_{k(i)})/2)\} \mathbf{n}, \\ &= \mu_n \tilde{G}^T[\gamma] \hat{G}\{b(\psi_i - \psi_{k(i)}), -b(\psi_{k(i)} - \psi_i)\} \mathbf{n}, \\ &= A_{SG}(\psi) \mathbf{n}. \end{aligned}$$

$\frac{e^{-s}}{\text{sh}(s)} = b(2s)$ is the Bernoulli function $b(s) = \frac{s}{e^s - 1}$, $b'(s) \leq 0$.

For the classical Scharfetter-Gummel scheme and ϕ_n holds a discrete maximum principle due to the diagonal transformation and the monotonicity of $e^{-\phi_n}$.

Scharfetter-Gummel scheme

Proposition 2 *The Scharfetter-Gummel scheme is dissipative.*

PROOF: The recombination term yields

$$d_{rec} := \sum_m |V_m| r (np - 1) \log(np)(\mathbf{x}_m) \geq 0.$$

One gradient term is

$$d_n = \int n \mu_n |\nabla \phi_n|^2 dV.$$

Testing the discrete expression with ϕ_n^T on E_l^N is:

$$d_n^E = \phi_n^T \tilde{G}^T[\gamma][\langle e^\psi \rangle_{i,k(i)}] \tilde{G} \mathbf{e}^{-\phi_n} \geq 0,$$

because e^s is monotone - explicit in vertex notation:

$$d_n^E = \mu_n \sum_{edges} e^{(\psi_i + \psi_k(i))/2} / \text{sh}((\psi_i - \psi_k(i))/2) (\phi_i - \phi_k(i)) e^{\phi_i - \phi_k(i)} \geq 0.$$

Scharfetter-Gummel scheme

Proposition 3 $-\partial A_{SG}(\psi)\mathbf{n}/\partial\psi_i$, $i \in E_l^N$ is a S -matrix on $E_l^N \forall \psi$ and $n > 0$.

PROOF:

$$\partial A_{SG}(\psi)\mathbf{n}/\partial\psi_i = \mu_n \tilde{G}^T[\gamma] \left(\frac{\partial}{\partial\psi_i} \hat{G}\{b(\psi_i - \psi_{k(i)}), -b(\psi_{k(i)} - \psi_i)\} \right) \mathbf{n}$$

$$\frac{\partial}{\partial\psi_i, \psi_{k(i)}} \hat{G}\{b(-\delta), -b(\delta)\} \mathbf{n} = \hat{G}\left\{-b'(-\delta) \frac{\partial\delta}{\partial\psi_i, \psi_{k(i)}}, -b'(\delta) \frac{\partial\delta}{\partial\psi_i, \psi_{k(i)}}\right\} \mathbf{n}$$

$$\frac{\partial}{\partial\psi_i, \psi_{k(i)}} \hat{G}\{b(-\delta), -b(\delta)\} \mathbf{n} = -[b'(-\delta)n_i + b'(\delta)n_{k(i)}](-\tilde{G})$$

Hence $\partial A_{SG}(\psi)\mathbf{n}/\partial\psi_i$ is of the type $\tilde{G}^T[D]\tilde{G}$, but $d_{ii} \leq 0$.

Sketch of the algorithms

- implicit Euler (predictor corrector scheme):
time integration or embedding (any parameter);
- Newton's method:
singular perturbation theory based decoupling,
only scalar equations must be factorized (pardiso),
the linearized equations are solved using cgs,
guaranteed positivity (n, p) for specific Delaunay grids;
- precise contact currents;
- doping extension using 2d $DIOS_{ISE}$ profiles,
- SMP parallel.

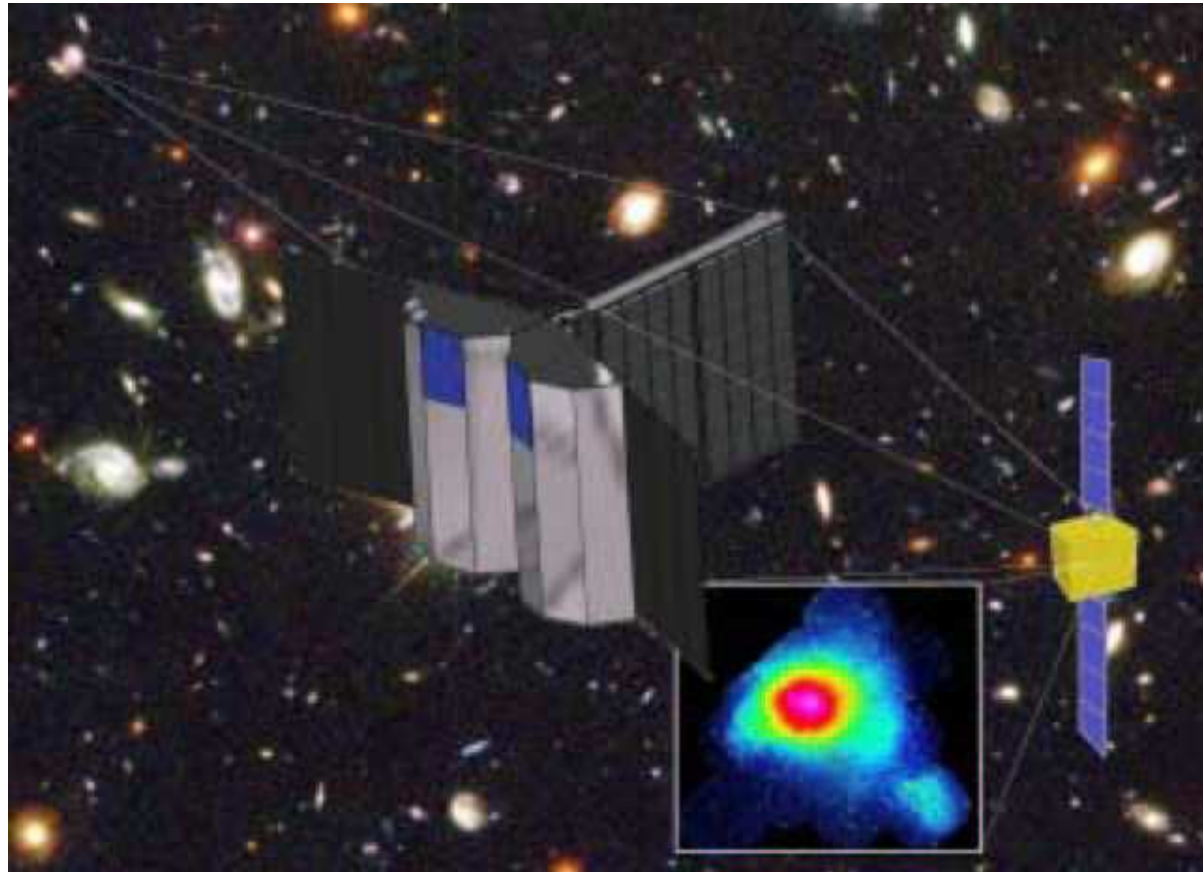
DEPFET sensors

X-ray astronomy sensors:

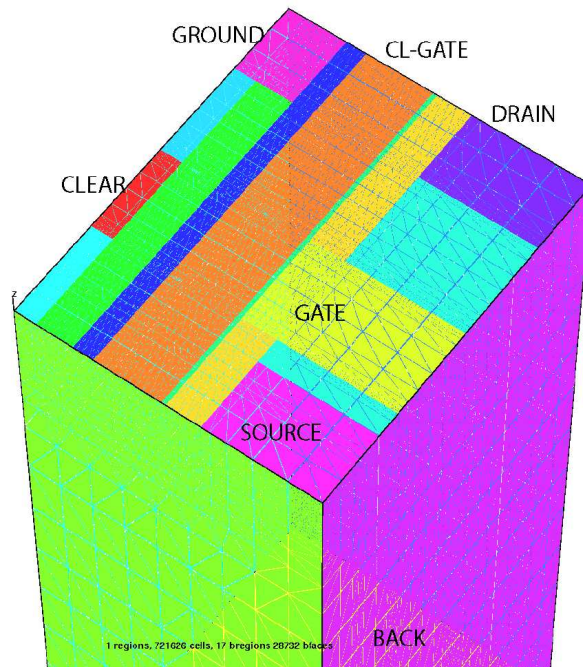
low noise
(1600 ± 2 electrons),
low power,
large amplification,
reasonable readout
frequency.

ILC sensors:

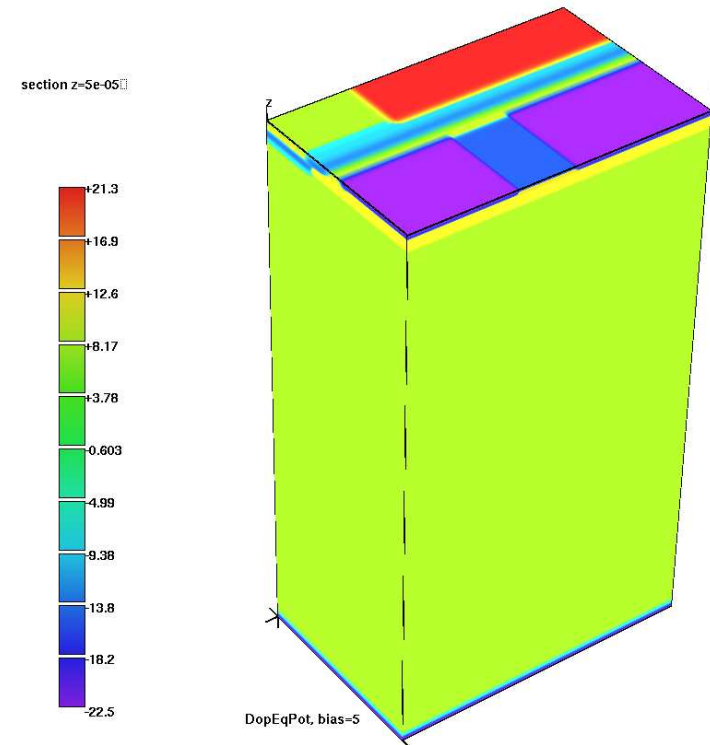
smaller pixels,
fast readout,
a bit relaxed
noise requirements.
2000 x 1000 pixel
per chip, many m^2
detector size.



DEPFET sensors

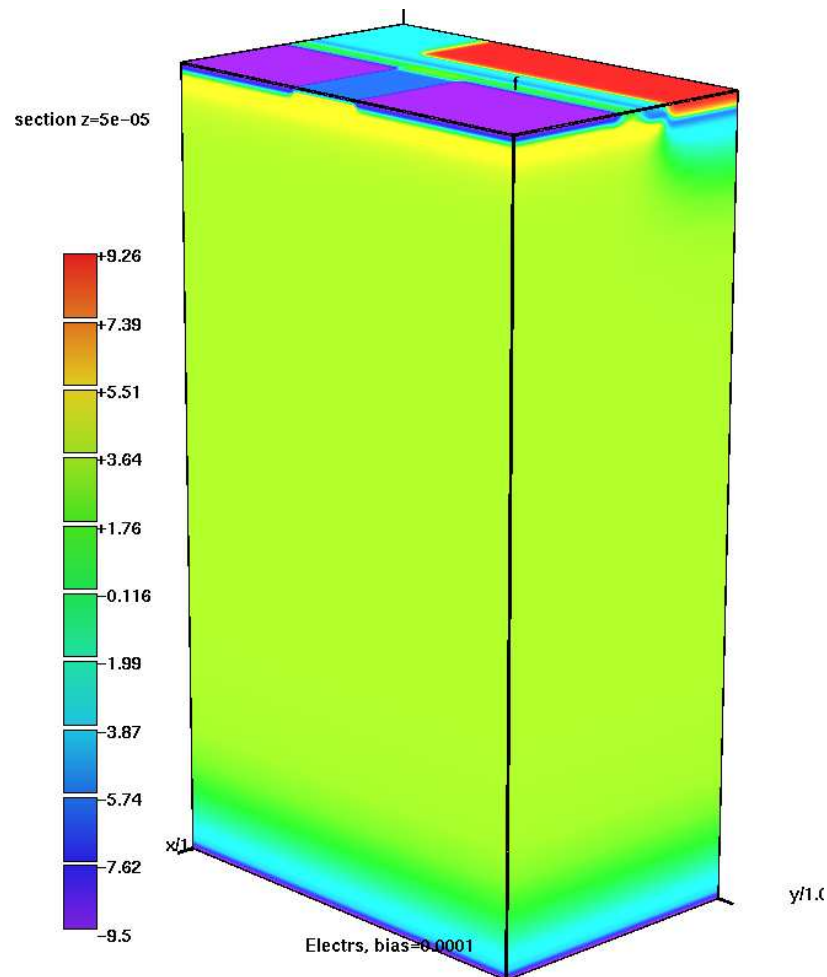


Simulation domain (half pixel)
 $18 \times 22 \times 50 \mu m^3$

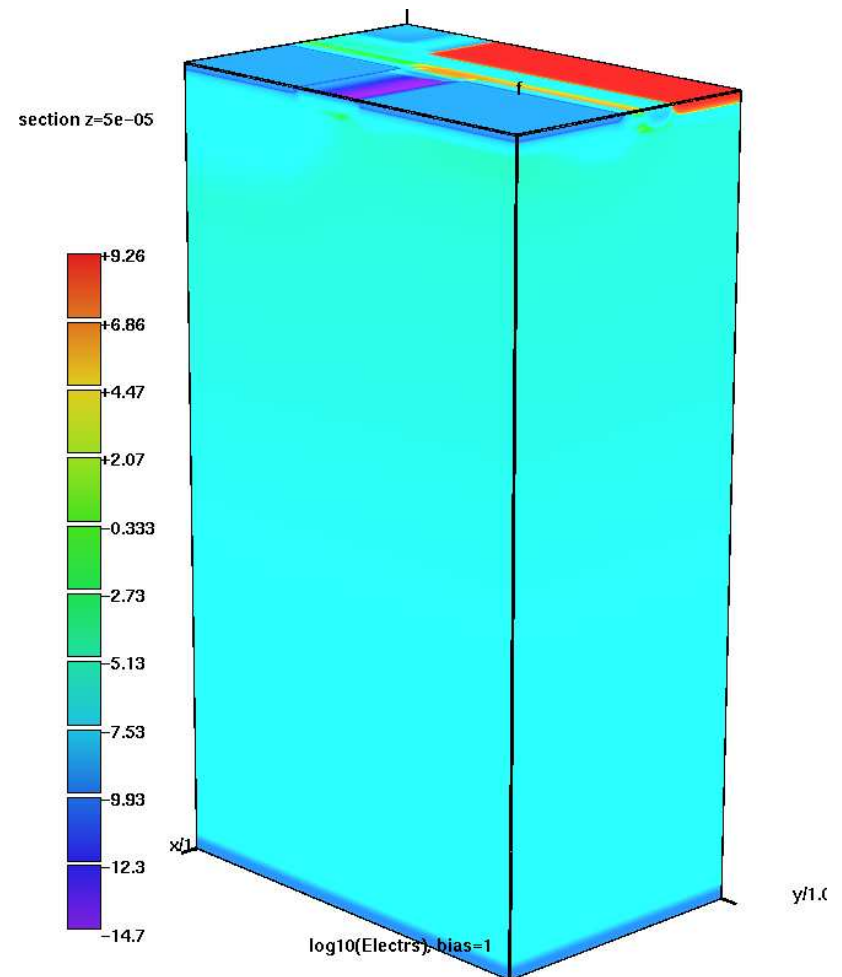


typical doping (equil. pot, $U_T \approx 1/40V$)

DEPFET simulation results

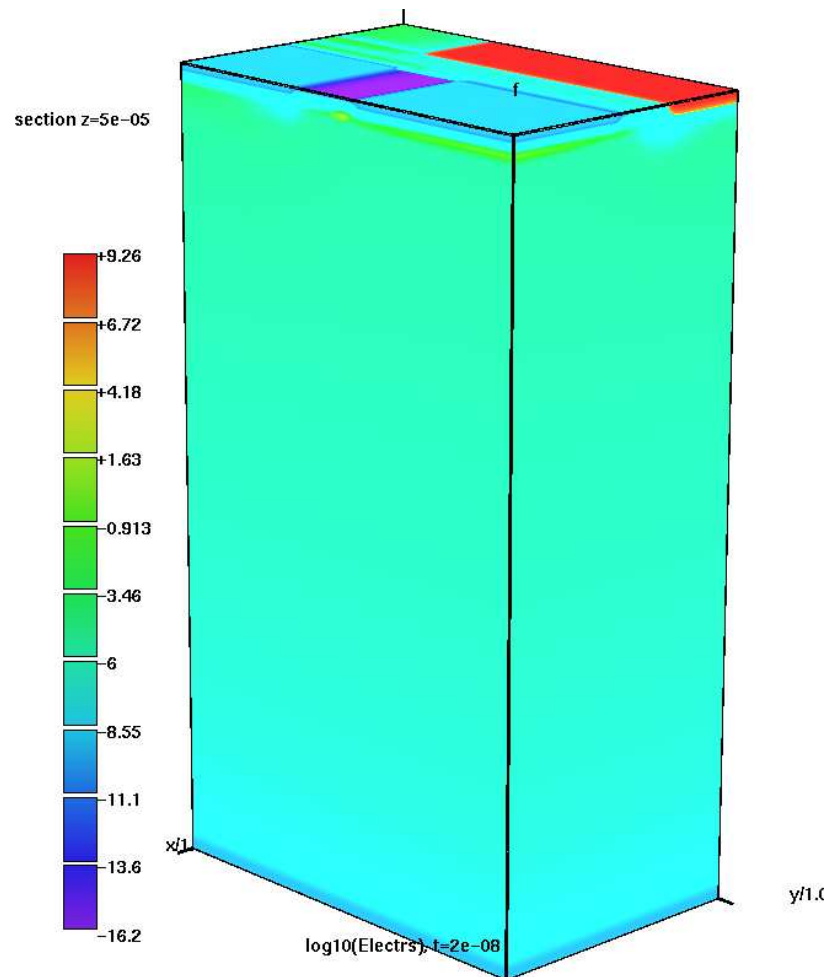


$\log_{10}(n)$, 0.003V 'distance' to equilibrium.

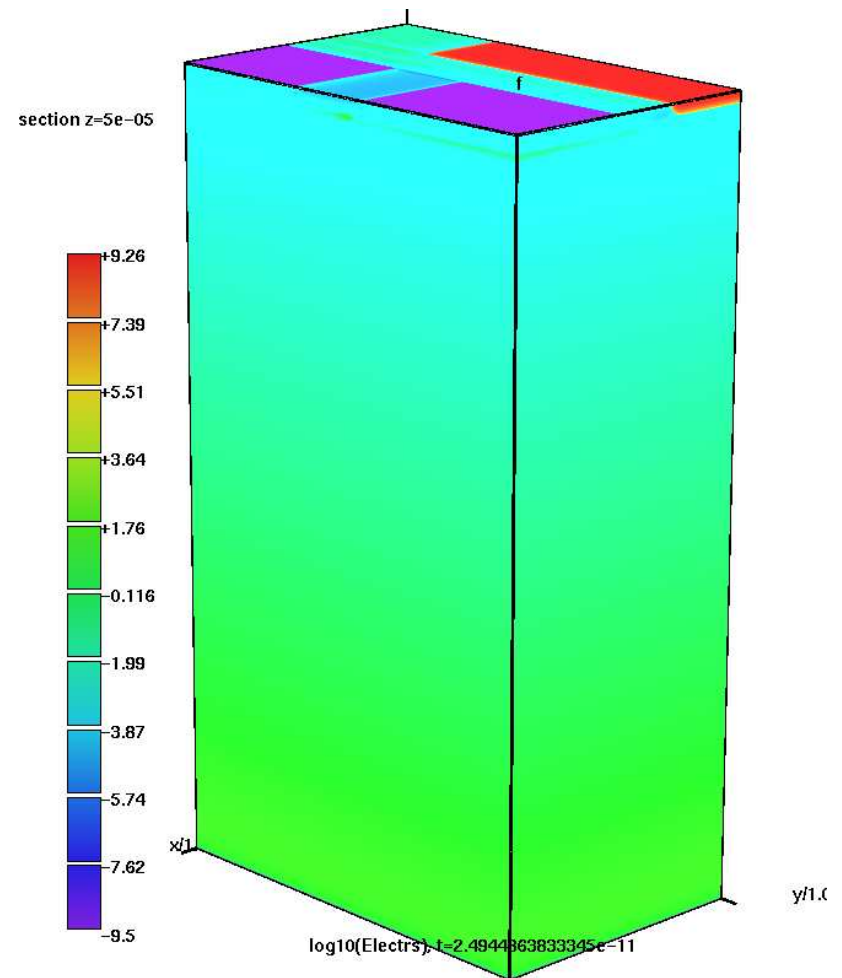


$\log_{10}(n)$, BACK -30V, DRAIN -5V, CL-GATE 10V, CLEAR 15V

DEPFET simulation results

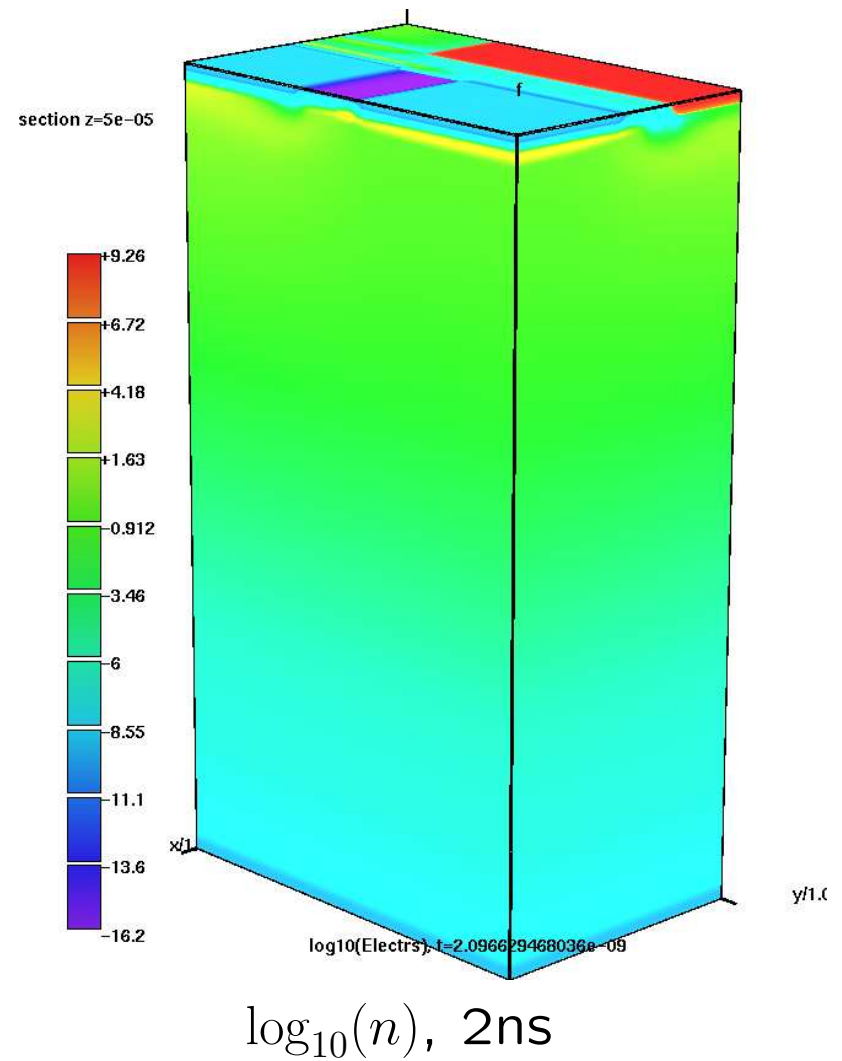
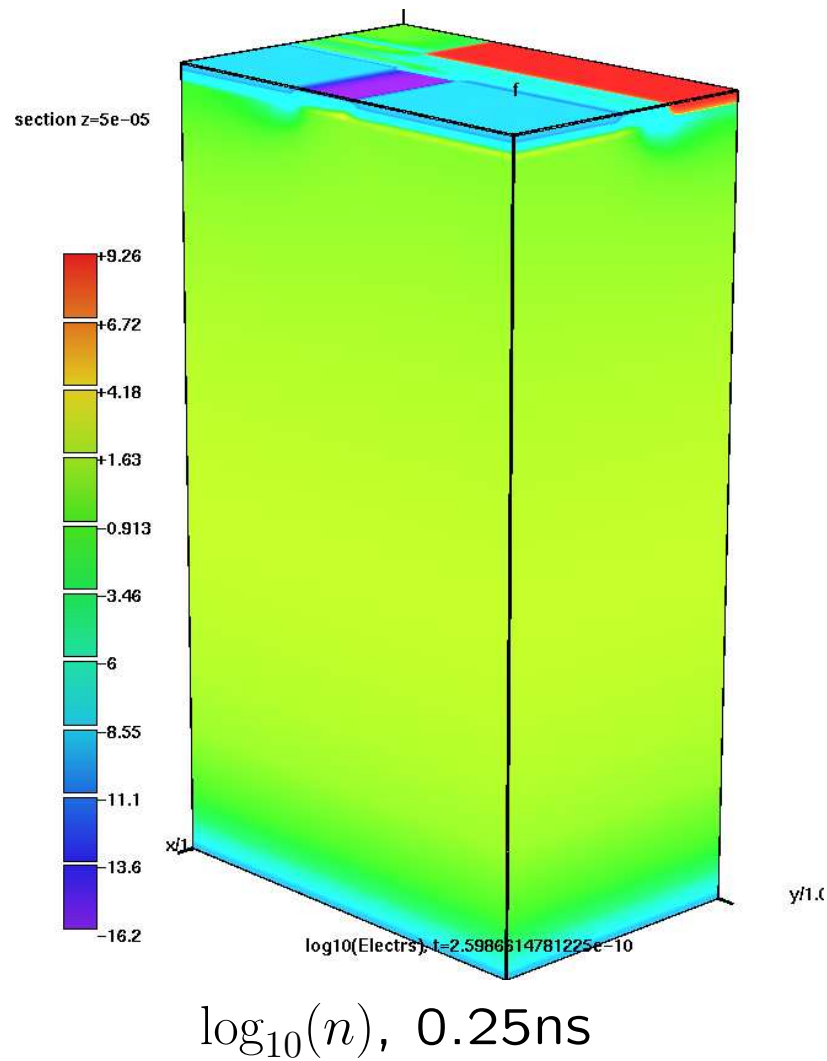


$\log_{10}(n)$, BACK -30V, DRAIN -5V,
CL-GATE 0V, CLEAR 2V

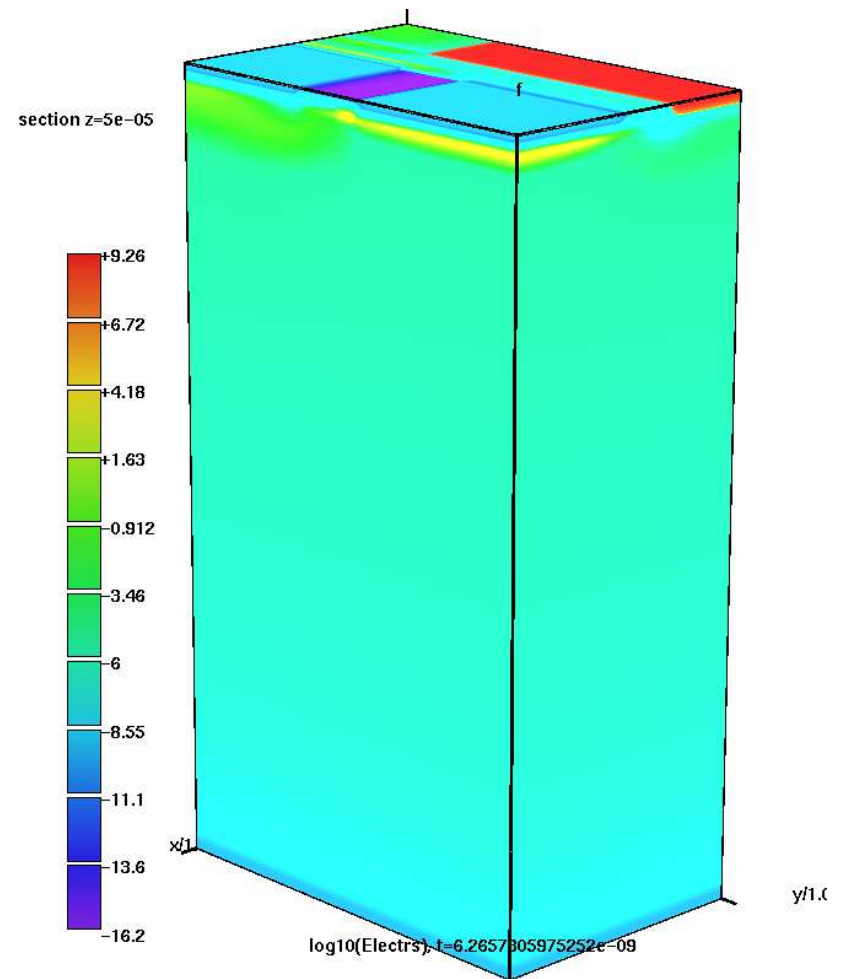
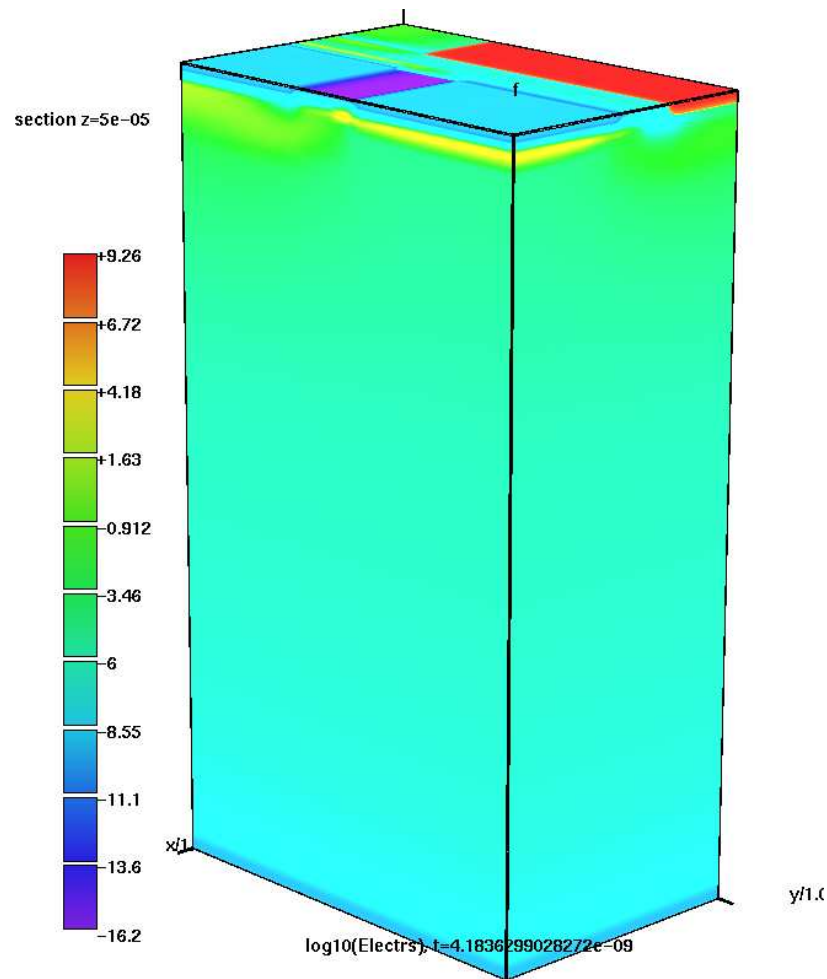


$\log_{10}(n)$, max. source dens., 25ps

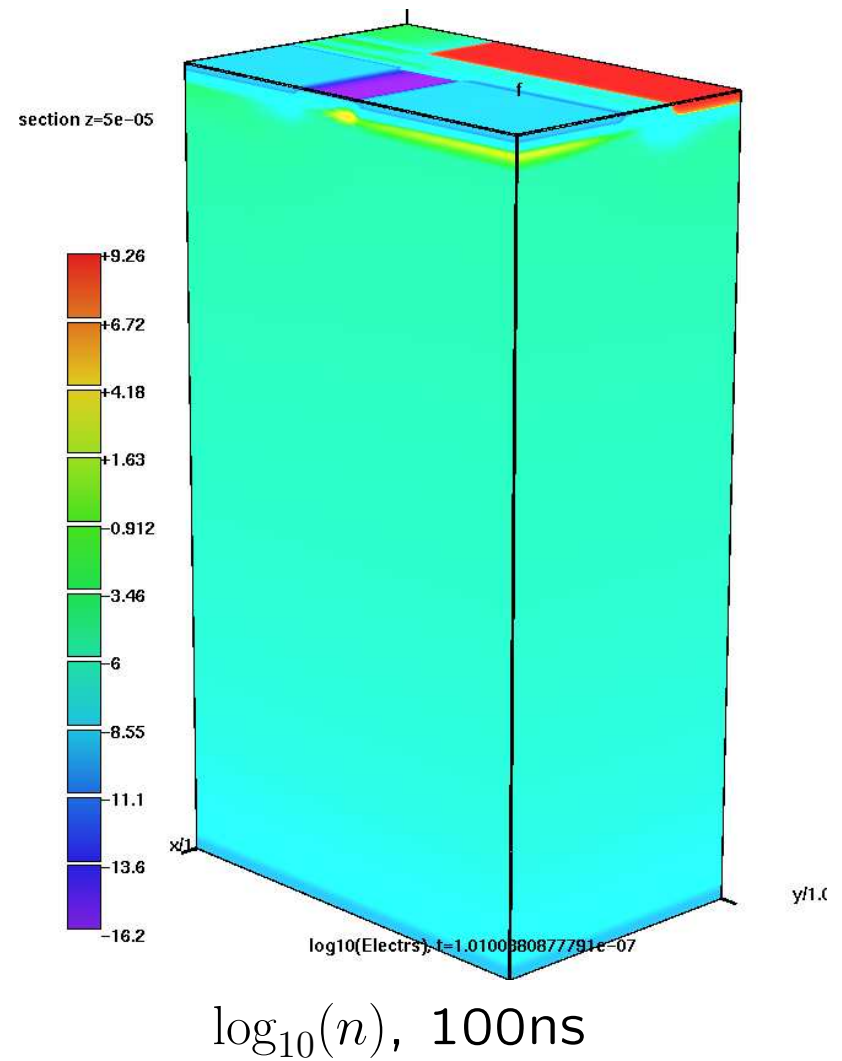
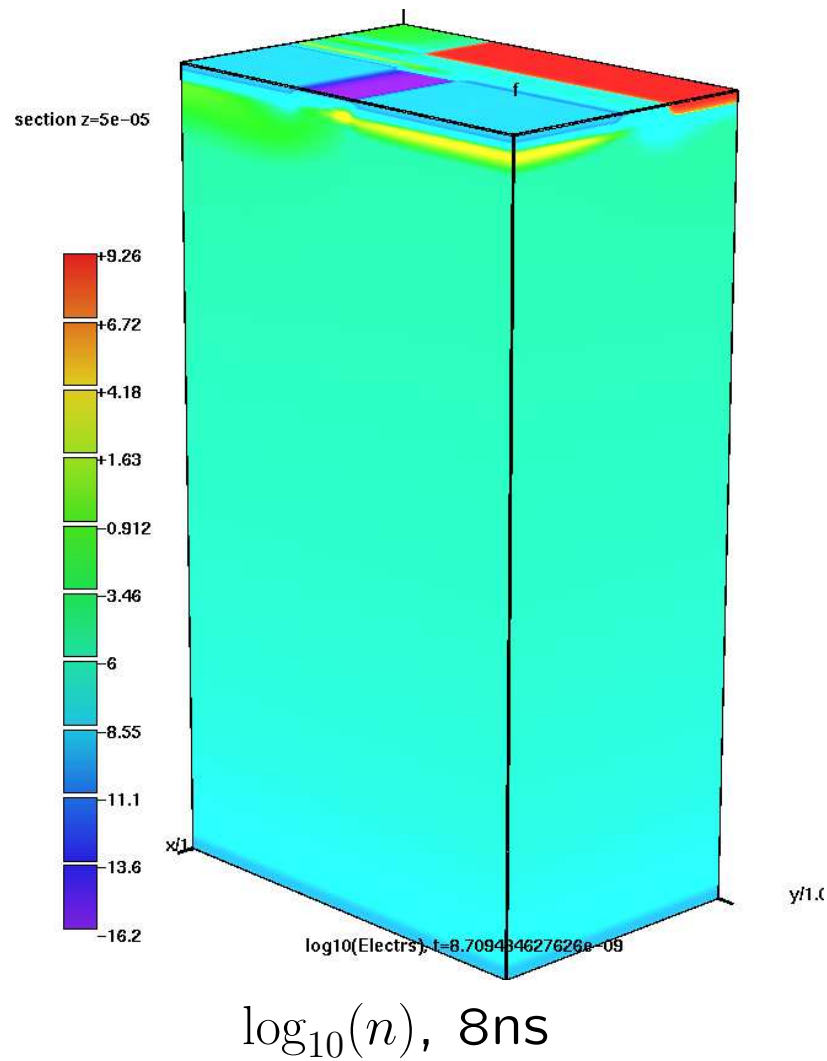
DEPFET simulation results



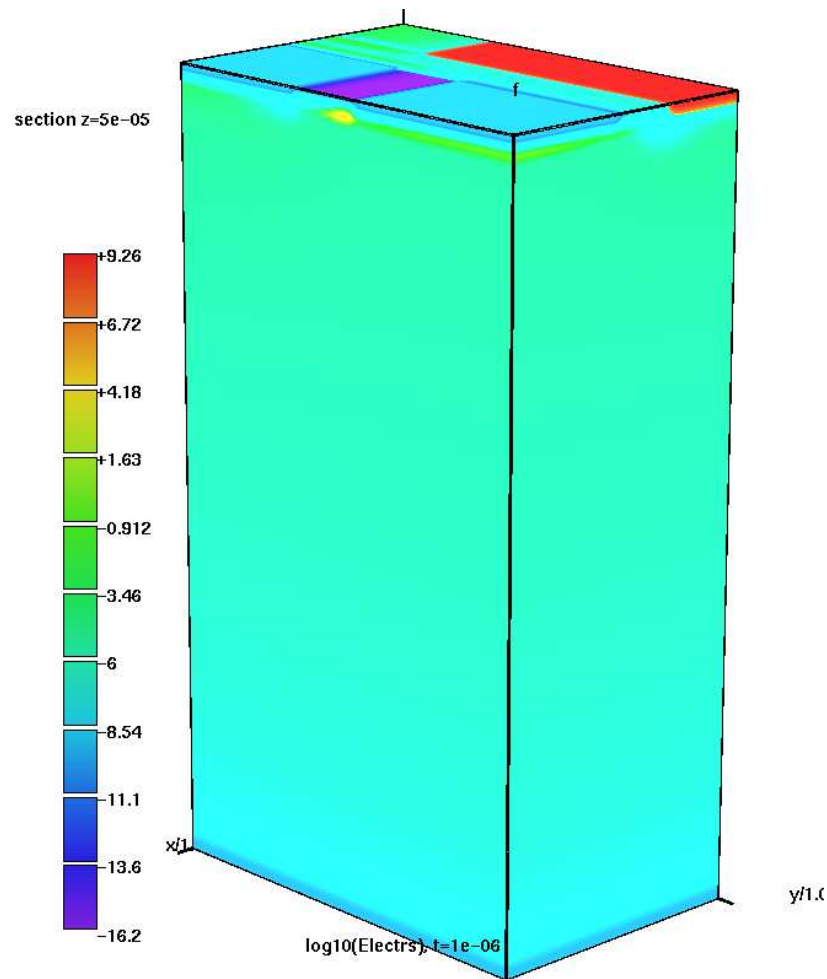
DEPFET simulation results



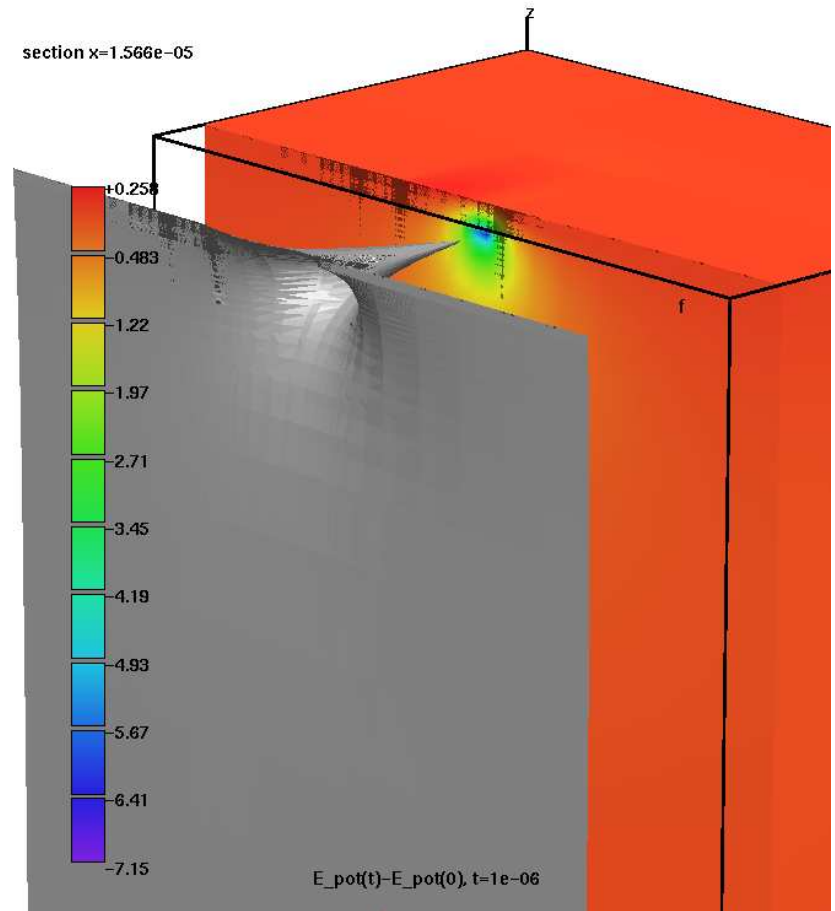
DEPFET simulation results



DEPFET simulation results

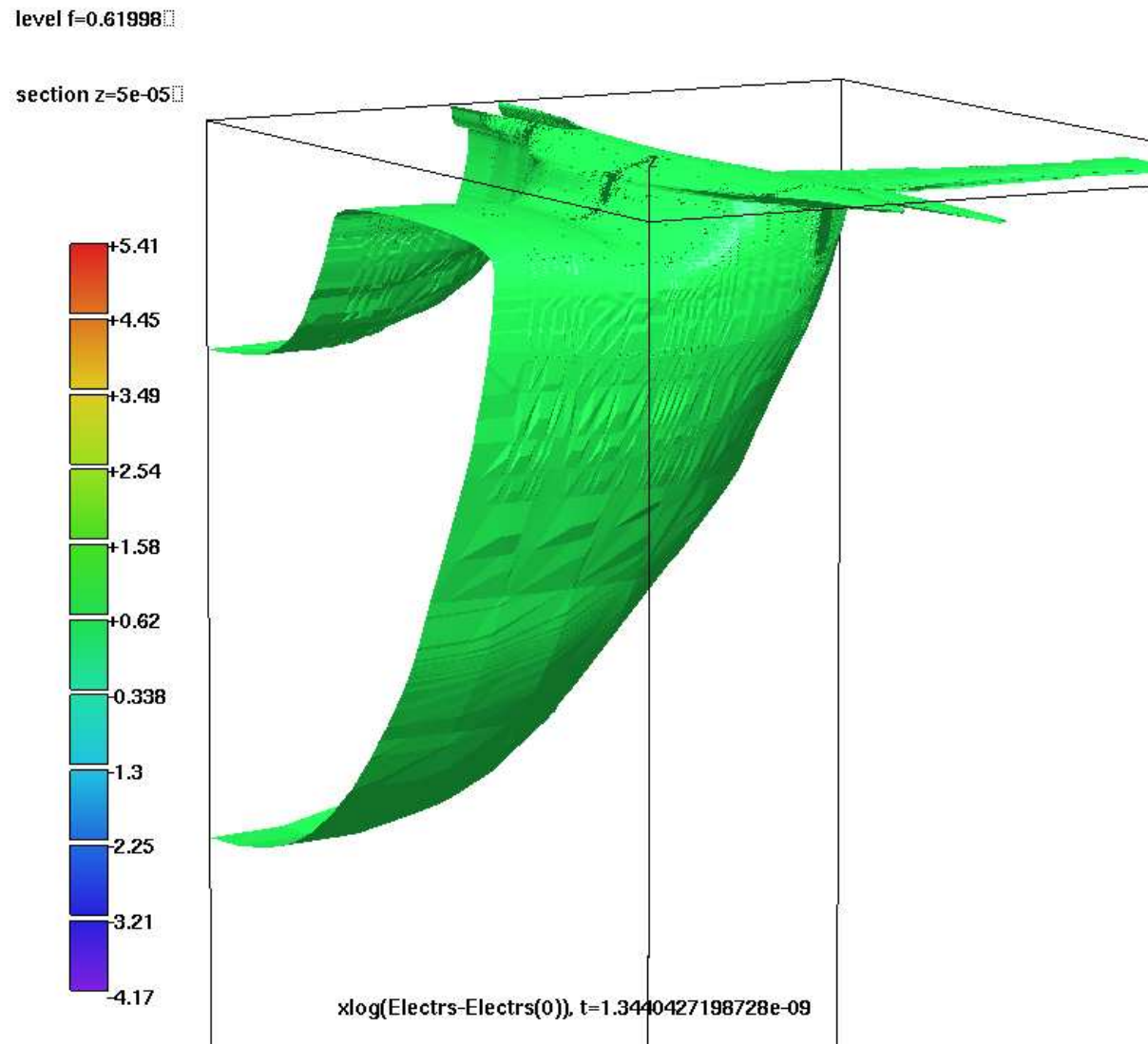


$\log_{10}(n)$, 1000ns



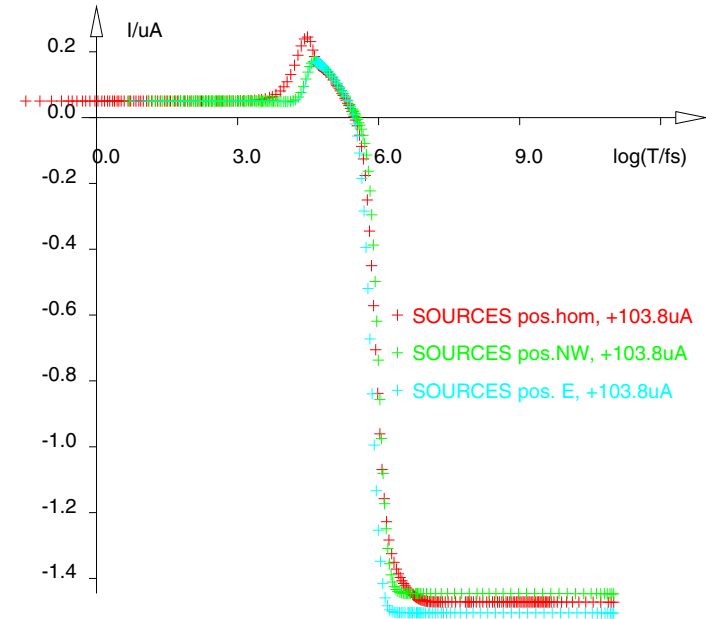
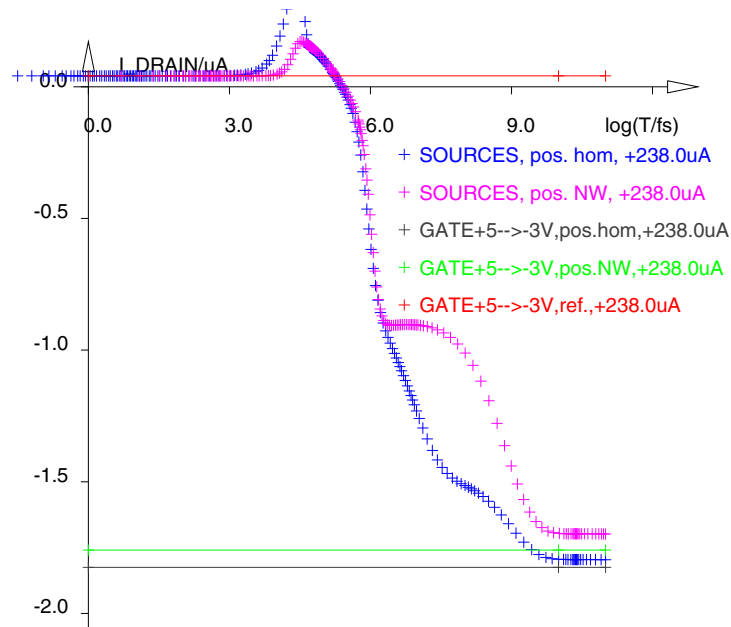
$\psi(1000ns) - \psi(0)$

DEPFET simulation results



$n \approx 10n_i$ isosurface touches the top: losses to CLEAR!

Main result (designer point of view): contact currents



DRAIN current, slow device

DRAIN current, fast device

Computation of some 20 designs:

volume reduction to 70%, sensitivity increase: factor 2,

device speed not critical any more, much better understanding and a pretty stable code.

Final iterations:

```
591 1||d|| 2.8987E-01 5.1989E-02-1.4185E-01-9.6031E-02 time sol 1.7998E+02
591 2||d|| 1.1608E-02-1.9205E-03-5.0442E-03 4.6433E-03 time sol 6.6590E+01
591 3||d|| 4.2353E-05 1.3926E-05 1.4493E-05 1.3934E-05 time sol 1.6270E+02
      Appl. Voltage/V  E_pot      Electrs      Holes      Tot.Cur
CLEAR      1.000000E+00 -1.553598E-13 -3.986510E-11  6.427555E-20 -4.002046E-11
CL-GATE     1.550000E+00  9.197693E-12  0.000000E+00  0.000000E+00  9.197693E-12
DRAIN      -5.000000E+00 -1.241165E-13 -4.641787E-19 -1.288812E-04 -1.288812E-04
BACK       -3.000000E+01 -1.609675E-13 -6.139834E-18  5.088995E-13  3.479259E-13
SOURCE      0.000000E+00 -3.525308E-13 -5.073933E-19  1.288812E-04  1.288812E-04
GATE       -3.000000E+00  6.628627E-13  0.000000E+00  0.000000E+00  6.628627E-13
GROUND      0.000000E+00  8.864205E-15  0.000000E+00  0.000000E+00  8.864205E-15
Time        1.000000E-04 Tot.Cur.Balance -6.122E-19A Rel.Bal.Error -2.375E-15
```

Summary:

-Time integr./embedding:

```
tot. # time steps (i_t_step)      591
tot. # rejected steps              21
```

-Newton it:

```
tot. # factor. (nfactorizations)    2847 , per variable:      949
max. # cgs it. (nmax_cgs)          120
tot. # cgs it. (sum_cgs_iter)      21741
# cgs failures (sum_cgs_fails)      0
tot. # Newton it. (nnewton_tot)     1686
```

Future work

- true 3d doping profiles;
- minor model extensions;
- general anisotropic 3d Delaunay simplex grids (TetGenFuture);
- faster, special algorithms for solving the linear systems;
- 'export' of improvements to WIAS-tesca.

play