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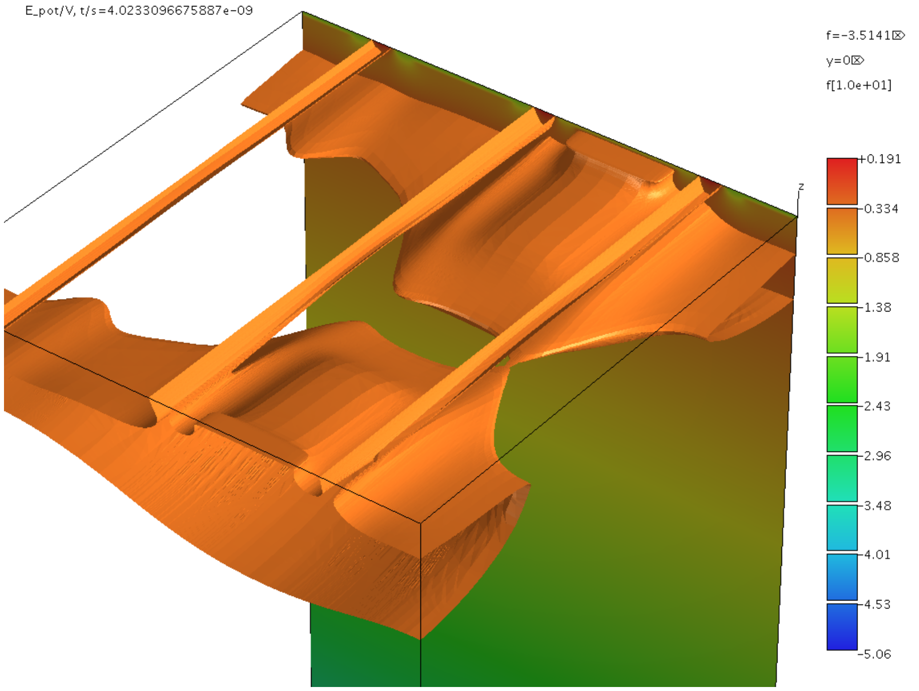
# Existence of bounded discrete steady state solutions of the van Roosbroeck system on boundary conforming Delaunay grids




Mohrenstr 39 10117 Berlin NUSOD, Newark, Sept. 26, 2007

# Aims, Outline

Aim: establish the essential qualitative properties of the analytic problem for a discrete version for some classes of grids independent of $h$ and $\tau$, hence unconditionally stable schemes for arbitrary parameter dependencies.

- uniqueness of the equilibrium
- dissipativity
- bounds for steady state solutions

Outline

- Introduction
- Delaunay grids, discretization
- Bounds by weak discrete maximum principle
- Example X-ray-CCD (candidate LCLS-detector)

# Warm up: Van Roosbroeck's Equations

$$-\nabla \cdot \epsilon \nabla w = C - n + p, \tag{1}$$

$$\frac{\partial n}{\partial t} + \nabla \cdot \mu_n n \nabla \phi_n = R, \tag{2}$$

$$\frac{\partial p}{\partial t} - \nabla \cdot \mu_p p \nabla \phi_p = R, \tag{3}$$

in $S \times \Omega$, $S = (0, T)$,
$\Omega \subset \mathbb{R}^N$, $2 \leq N \leq 3$, a bounded polyhedral domain,
$\partial\Omega = \Gamma_D \cup \Gamma_N$, $\Gamma_D$ closed, positive surface measure.
Boundary conditions:
hom. Neumann on insulating parts,
Dirichlet on Ohmic contacts,
and gates: hom./inhom. Neumann $\phi/w$
($\partial w/\partial\vec{\nu} + \alpha(w - w_\Gamma) = 0$, $\vec{\nu}$ outer normal vector).

# Van Roosbroeck's Equations

The physical meaning of the quantities is :

- $\phi_n = w - \log n$ - quasi-Fermi potential $n$,
- $\phi_p = w + \log p$ - quasi-Fermi potential $p$,
- $n = e^{w-\phi_n}$ - electron density,
- $p = e^{\phi_p - w}$ - hole density,
- $w$ - electrostatic potential,
- $\epsilon$ - dielectric permittivity,
- $C$ - 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:

$$\frac{\partial n}{\partial t} - \nabla \cdot \mu_n(\nabla n - n\nabla w) = R, \qquad (4)$$

$$\frac{\partial p}{\partial t} - \nabla \cdot \mu_p(\nabla p + p\nabla w) = R, \qquad (5)$$

or

$$\frac{\partial n}{\partial t} - \nabla \cdot \mu_n e^{w} \nabla e^{-\phi_n} = R, \qquad (6)$$

$$\frac{\partial p}{\partial t} - \nabla \cdot \mu_p e^{-w} \nabla e^{\phi_p} = R, \qquad (7)$$

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

# Delaunay grids, notations

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

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

$l$ simplex index, with positive volume in a right–handed coordinate system.
The $N \times N$ matrix of the vertex coordinates represents the simplex in a local per simplex coordinate system:

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

$\mathbf{x}_i^T = (x_{1,i}, x_{2,i}, \ldots, x_{N,i})$ 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

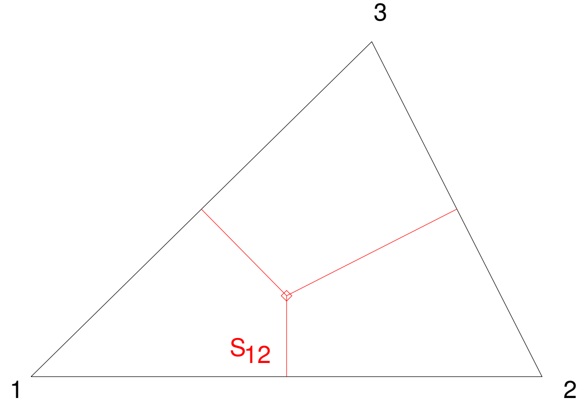
A discretization by simplices $\mathbf{E}_i^N$ is called a Delaunay grid if the balls defined by the $N+1$ vertices of $\mathbf{E}_i^N\ \forall\ i$ do not contain any vertex $\mathbf{x}_k$, $\mathbf{x}_k \in \mathbf{E}_j^N$, $\mathbf{x}_k \notin \mathbf{E}_i^N$.

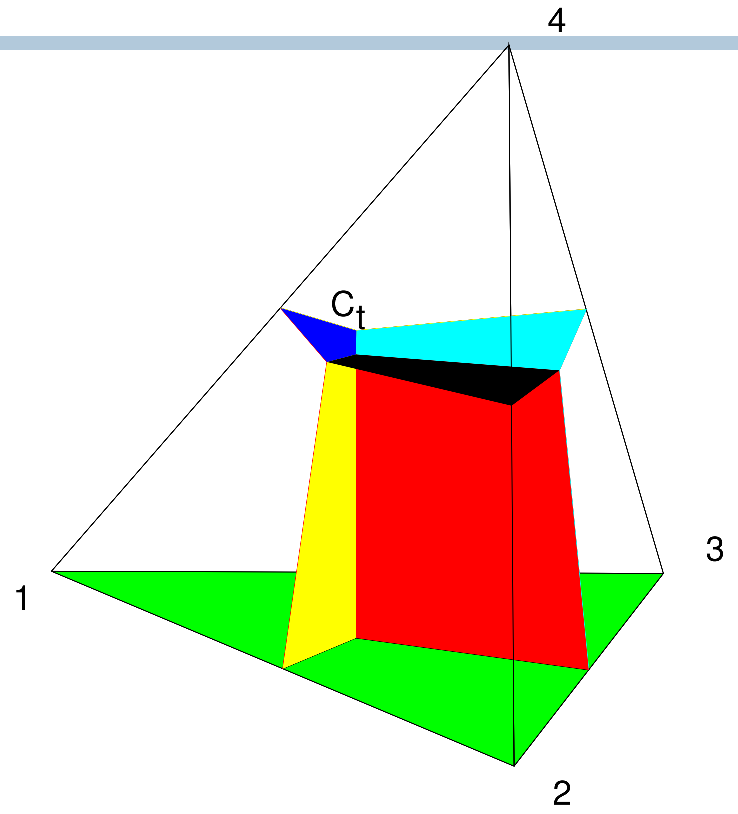
Boundary conforming Delaunay grid:
the circum center of any $\mathbf{E}_l^N \in \mathbf{\Omega}_i$ is in $\bar{\mathbf{\Omega}}_i$.

Let $V_i = \{\mathbf{x} \in I\!R^N : \|\mathbf{x}-\mathbf{x}_i\| < \|\mathbf{x}-\mathbf{x}_j\|, \forall \text{ vertices } \mathbf{x}_j \in \mathbf{\Omega}\}$ and $\partial V_i = \bar{V}_i \setminus V_i$. $V_i$ is the Voronoi volume of vertex $i$ and $\partial V_i$ 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

Example:




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

$$\xi_1 u + \xi_2 \partial u/\partial \nu + \xi_3 = 0$$

# Finite volume scheme

$$-\nabla \cdot \epsilon \nabla u = f,$$

$$\epsilon(x) = \epsilon_l, x \in \Omega_l, \quad \nabla u|_{\partial V_{i,k(i)}} \approx (\mathbf{u}_{k(i)} - \mathbf{u}_i)/|\mathbf{e}_{ik(i)}|$$

$$\begin{aligned} \int_{V_{ij}} -\nabla \cdot \epsilon_l \nabla u \, dV &= -\epsilon_l \sum_{k(i)} \int_{\partial V_{i,k(i)}} \nabla u \cdot d\mathbf{S}_k \\ &\approx -\epsilon_l \sum_k \frac{\partial V_{i,k(i)}}{|\mathbf{e}_{i,k(i)}|}(u_k - u_i) + \mathrm{BI} \\ &= \epsilon_l [\gamma_{k(i)}] \tilde{G}_N(1,-1)\mathbf{u}|_{E_j^N} + \mathrm{BI}. \end{aligned} \quad (8)$$

Summation over all nodes in the simplex $j$:

$$\sum_{V_{ij} \in \mathbf{E}_j^N} \int_{V_{ij}} -\nabla \cdot \epsilon \nabla u dV \approx \epsilon \tilde{G}^T [\gamma] \tilde{G} \mathbf{u}|_{E_j^N} + \mathrm{BI}. \quad (9)$$

$$\mathrm{BI} := \int_{E_j^{N-1} \cap V_i} -\epsilon \nabla u \cdot d\mathbf{S} \approx |E_j^{N-1} \cap V_i| \frac{\epsilon}{\xi_{2_j}} (\xi_{1_j} u_i + \xi_{3_j}).$$

# Finite volume scheme

$$\int_{V_{ij}} f dV \approx V_{ij} f(x_i), \quad [V]_i = \sum_j V_{ij},$$

where $[\cdot]$ denotes a diagonal matrix and

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

the difference matrix along all edges, hence a mapping form 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 scheme

$$(\tilde{G}^T\tilde{G})_{ii} > 0, \quad (\tilde{G}^T\tilde{G})_{i>j} < 0, \text{ and } \mathbf{1}^T\tilde{G}^T = \mathbf{0}^T. \tag{10}$$

If the grid is connected,

$$A(\epsilon) := \sum_{E_l \in \Omega} \epsilon_l G^T[\gamma_l]G$$

is irreducible, weakly diagonally dominant, hence a bounded inverse exists with $0 \leq A^{-1} < \infty$, because

$$\gamma_{k(i)} = \frac{\partial V_{i,k(i)}}{|\mathbf{e}_{i,k(i)}|},$$

$$\sum_{E_j^N \ni \mathbf{e}_{ik}, E_j^N \in \Omega_i} \partial V_{ik} \geq 0. \tag{11}$$

due to the requirement 'boundary conforming Delaunay grid'. Similar to integration by parts test functions can be introduced and a 'weak discrete maximum principle' holds.

# Finite volume scheme

Price to pay:

$$\mathbf{u}^T|_{E_j^N} G^T G \mathbf{u}|_{E_j^N}$$

does not introduce a discrete gradient seminorm on one simplex only. A way out for parameter evaluation is

$$||\nabla u||^2|_{E_j^N} := |E_j^N| \mathbf{u}^T|_{E_j^N} P_j^{-T} P_j^{-1} \mathbf{u}|_{E_j^N},$$

the finite element gradient seminorm.
For any average one requires

$$\bar{\epsilon}_{e_{ik}} = \sum_{E_j^N \ni \mathbf{e}_{ik}, E_j^N \in \Omega_i} \chi(\epsilon(x, u, |\nabla u|)),$$

$$\sum_{E_j^N \ni \mathbf{e}_{ik}, E_j^N \in \Omega_i} \bar{\epsilon}_{e_{ik}} \partial V_{ik} \geq 0.$$

# Scharfetter-Gummel-scheme

The discrete problem reads:

$$G^T \epsilon G \mathbf{w} = [V]\mathbf{g}(\mathbf{C}, \mathbf{n}, \mathbf{p}), \;\; \mathbf{g} = \mathbf{C} - \mathbf{n} + \mathbf{p}, \;\; \mathbf{n} = [e^{w}]\mathbf{u}, \;\; \mathbf{p} = [e^{-w}]\mathbf{v}, \quad (12)$$

$$A_{S_n}(\mu_n, \mathbf{w})\mathbf{e}^{-\phi_n} = G^T[\bar{\mu}_n e^{\bar{w}}/\mathrm{sh}(\tilde{G}\mathbf{w}/2)]G\mathbf{u} = [V][r(\mathbf{x}, \mathbf{n}, \mathbf{p})](\mathbf{1} - [v]\mathbf{u}), \quad (13)$$

$$A_{S_p}(\mu_p, -\mathbf{w})\mathbf{e}^{\phi_p} = G^T[\bar{\mu}_p e^{-\bar{w}}/\mathrm{sh}(\tilde{G}\mathbf{w}/2)]G\mathbf{v} = [V][r(\mathbf{x}, \mathbf{n}, \mathbf{p})](\mathbf{1} - [u]\mathbf{v}). \quad (14)$$

Slotboom variables $u := e^{-\phi_n}$, $v := e^{\phi_p}$,
$\bar{\mu}e^{w}(e^{-\phi_n})' = const$ with
$\bar{w} := (w_i + w_{k(i)})/2$, $\mathrm{sh}(s) := \sinh(s)/s$, $\mathrm{sh}(s) = \mathrm{sh}(-s) \geq 1$,
$b(2s) = e^{-s}/\mathrm{sh}(s) = 2s/(e^{-2s} - 1)$.
Further details and dissipativity see Gajewski,Gä, ZAMM 1996.

# Boundary conditions

On insulating boundary parts the normal derivatives of the quasi-Fermi-potentials vanish $\partial\phi_k/\partial\nu = 0$ ($k = n, p$, $\nu$ outer normal).
The boundary conditions at Ohmic contacts are (due to charge neutrality, infinite recombination velocity, and infinite conductivity of a metallic contact)

$$w|_{\Gamma_{D_k}} = w_k + w_{b,k}, \;\; - e^{w_{b,k}} + e^{-w_{b,k}} = -C|_{\Gamma_{D_k}}, u|_{\Gamma_{D_k}} = e^{-\phi_{n,k}}, \;\; v|_{\Gamma_{D_k}} = e^{\phi_{p,k}}, \tag{15}$$

where $w_k = \phi_{n,k} = \phi_{p,k}$ is the 'applied potential', while $w_{b,k}$ is the 'built-in voltage'.

# Bounds $\mathbf{w}$

Assume

$$\check{u} \leq u_i^0 \leq \hat{u}, \;\; \check{v} \leq v_i^0 \leq \hat{v} \;\forall\; x_i \in \bar{\Omega}. \tag{16}$$

The right hand side of the discrete Poisson equation $g_i(C_i, n_i, p_i)$ is with respect to $w_i$ a monotone mapping of $\mathbb{R}$ onto $\mathbb{R}$ $\forall i$. Let $\check{C} = \min(C(x))$ and $\hat{C} = \max(C(x))$ denote the minimum and maximum of the doping concentration. Hence the solution $\breve{w}_i$ of $\mathbf{g}(\breve{w}_i) = 0$ at any vertex $x_i \in \Omega$ fulfills the bounds

$$e^{\check{w}} := \frac{\check{C}}{2\hat{u}} + \sqrt{\frac{\check{C}^2}{4\hat{u}^2} + \frac{\check{v}}{\hat{u}}} \leq e^{\breve{w}_i} \leq \frac{\hat{C}}{2\check{u}} + \sqrt{\frac{\hat{C}^2}{4\check{u}^2} + \frac{\hat{v}}{\check{u}}} =: e^{\hat{w}}.$$

# Bounds $\mathbf{w}$

**Proposition 1** *The discrete electrostatic potential $\mathbf{w}^0$ unique solution of (12), with $\mathbf{w}$ replaced by $\mathbf{w}^0$, $\mathbf{u}$, $\mathbf{v}$ by $\mathbf{u}^0$, $\mathbf{v}^0$, and fulfilled (16) can be estimated by*

$$\grave{w} := \min(w|_{\Gamma_D}, \check{w}) \leq w_i^0 \leq \max(w|_{\Gamma_D}, \hat{w}) =: \acute{w}. \qquad (17)$$

PROOF: Suppose $w_j^0 > \acute{w}$. Testing (12) with the positive part $(\mathbf{w}^0 - \acute{w})^+$ yields

$$(\mathbf{w}^0 - \acute{w})^{+T} G^T \epsilon G \mathbf{w}^0 - (\mathbf{w}^0 - \acute{w})^{+T} [V] \mathbf{g}(\mathbf{C}, \mathbf{w}^0, \mathbf{u}^0, \mathbf{v}^0) = 0.$$

$\text{sign} G(\mathbf{w}^0 - \acute{w})^+ = \text{sign} G\mathbf{w}^0$ if $G(\mathbf{w}^0 - \acute{w})^+ \neq 0$, $g(\hat{C}, \hat{w}, \check{u}, \hat{v}) = 0$, hence $(\mathbf{w}^0 - \acute{w})^{+T} G^T \epsilon G \mathbf{w}^0 > 0$ and $(\mathbf{w}^0 - \acute{w})^{+T} [V] \mathbf{g}(\mathbf{C}, \mathbf{w}^0, \mathbf{u}^0, \mathbf{v}^0) \leq 0$ holds, this is a contradiction.

# Bounds $\mathbf{w}$

The mapping with respect $\mathbf{w}^0$ is continuous, differentiable, and bounded and maps the convex domain $\grave{w} \le w_i^0 \le \acute{w}$ onto itself. The linear problem with $\mathbf{g} = \mathbf{0}$ has a unique solution ($G^T \epsilon G$ is weakly diagonally dominant) and embedding with respect to $\mathbf{g}$ does not change the degree, uniqueness follows directly from maximum principle: let $\mathbf{w}_1^0$, $\mathbf{w}_2^0$ to be solutions of (12), assume $(\mathbf{w}_1^0 - \mathbf{w}_2^0)^+ > 0$ for at least one $x_i \in \Omega$, testing

$$(\mathbf{w}_1^0 - \mathbf{w}_2^0)^{+T} G^T \epsilon G (\mathbf{w}_1^0 - \mathbf{w}_2^0) - (\mathbf{w}_1^0 - \mathbf{w}_2^0)^{+T} [V] (\mathbf{g}(\mathbf{w}_1^0) - \mathbf{g}(\mathbf{w}_2^0)) = 0,$$

and using the monotonicity of $g$ with respect to $w_i$ yields a contradiction. $\square$

# Bounds $\mathbf{u}$, $\mathbf{v}$

**Proposition 2** *Let* $\mathbf{w}^1$ *be a solution of*

$$G^T \epsilon G \mathbf{w}^1 = [V]\mathbf{g}(\mathbf{C}, \mathbf{w}^1, \mathbf{u}^0, \mathbf{v}^0), \tag{18}$$

*where* $\mathbf{u}^0$*,* $\mathbf{v}^0$ *respect the bounds (16) and suppose* $\mathbf{u}^1$*,* $\mathbf{v}^1$ *to be solutions of the decoupled continuity equations*

$$A_S(\mu_n, \mathbf{w}^1)\mathbf{u}^1 = [V]r(\mathbf{x}, e^{\mathbf{w}^1}\mathbf{u}^0, e^{-\mathbf{w}^1}\mathbf{v}^0)(\mathbf{1} - [v^0]\mathbf{u}^1), \tag{19}$$

$$A_S(\mu_p, -\mathbf{w}^1)\mathbf{v}^1 = [V]r(\mathbf{x}, e^{\mathbf{w}^1}\mathbf{u}^0, e^{-\mathbf{w}^1}\mathbf{v}^0)(\mathbf{1} - [u^0]\mathbf{v}^1). \tag{20}$$

*Assume for some sufficiently large* $w^+$*,*
$\max(w|_{\Gamma_D}) - \min(w|_{\Gamma_D}) \leq w^+ < \infty$*, that*

$$e^{-w^+} \leq \mathbf{u}, \;\; \mathbf{v} \leq e^{w^+},$$

$\forall i$ *is true. Then* $e^{w^-}$*,* $e^{w^+}$ *is an lower, upper solution for equations (13, 14).*

# Bounds $\mathbf{u}$, $\mathbf{v}$

PROOF: Assuming $\mathbf{u}^1 > e^{w^+}$ for at least one $x_i \in \Omega$ and testing (19) with $(\mathbf{u}^1 - e^{w^+})^{+T}$ yields $(\mathbf{u}^1 - e^{w^+})^{+T} A_S(\mu_n, \mathbf{w}^1)\mathbf{u}^1 > 0$ independently of $\mu_n$, $\mathbf{w}^1$. On the other hand $(\mathbf{1} - [v^0]\mathbf{e}^{w^+}) \leq \mathbf{0}$, and $[r(\mathbf{x}, e^{\mathbf{w}^1}\mathbf{u}^0, e^{-\mathbf{w}^1}\mathbf{v}^0)] > 0$ holds, hence $\mathbf{u} \leq e^{w^+}$ follows, and so do the other bounds. $\square$

# Bounds u, v

**Remark 1** *Choosing in (16)* $\check{u}$, $\hat{u}$, $\check{v}$, $\hat{v}$ *accordingly* $\underline{u} = \underline{v} = e^{-w^+}$, $\overline{u} = \overline{v} = e^{w^+}$ *yields*

$$\underline{u} \leq \mathbf{u} \leq \overline{u}, \tag{21}$$

$$\underline{v} \leq \mathbf{v} \leq \overline{v}, \tag{22}$$

*and with (17)*

$$\begin{aligned} \underline{w} &= \min(w|_{\Gamma_D}, \ln((\check{C} + \sqrt{\check{C}^2 + 4})/2) - w^+) \leq w \\ w &\leq \max(w|_{\Gamma_D}, \ln((\hat{C} + \sqrt{\hat{C}^2 + 4})/2) + w^+) = \overline{w}. \end{aligned} \tag{23}$$

*These are the final bounds because Proposition 2 is true with (21,22,23), too.*
*The bounds are identical with the analytic ones.*

# Uniqueness if $|w^+|$ small

Linearization ...

further results and details see WIAS-Preprint

# Summary

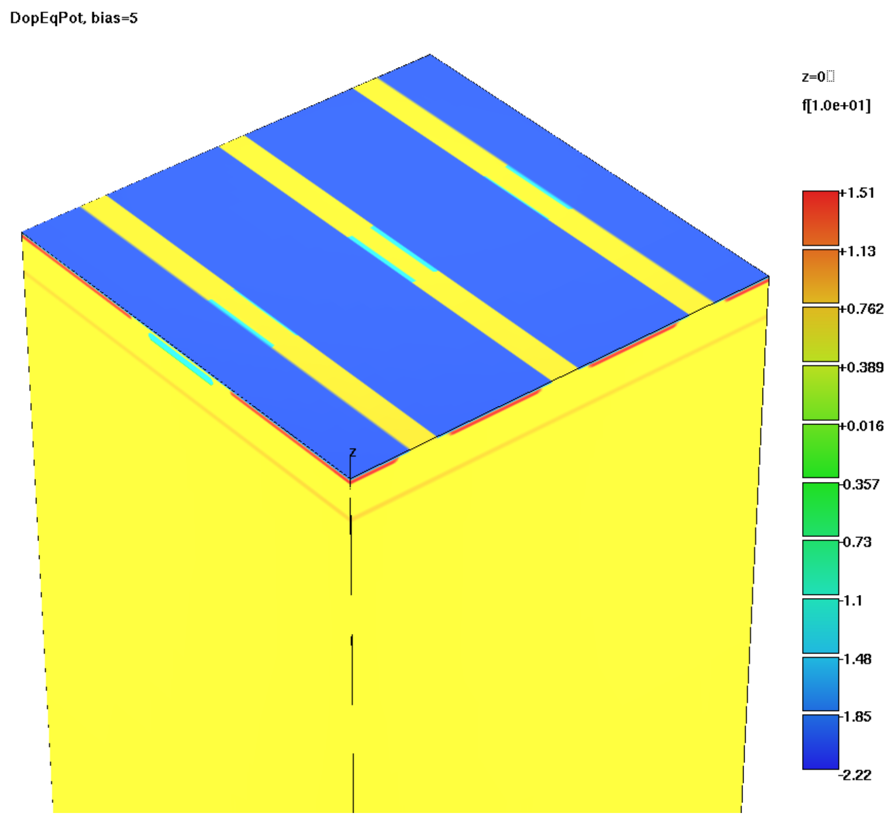
The summary of the results is:

**Theorem 1** *On any connected, boundary conforming Delaunay grid with $n$ vertices, the problem (12,13,14) with positive Dirichlet boundary measure has at least one solution fulfilling the bounds (21, 22, 23).*

PROOF: The established bounds form a convex set in $I\!R^{3n}$ and the two step mapping (proposition 1, 19, 20) is continuous, differentiable, and maps the convex set onto itself, hence Brouwer's fixed point theorem guarantees the existence of at least one fixed point. □

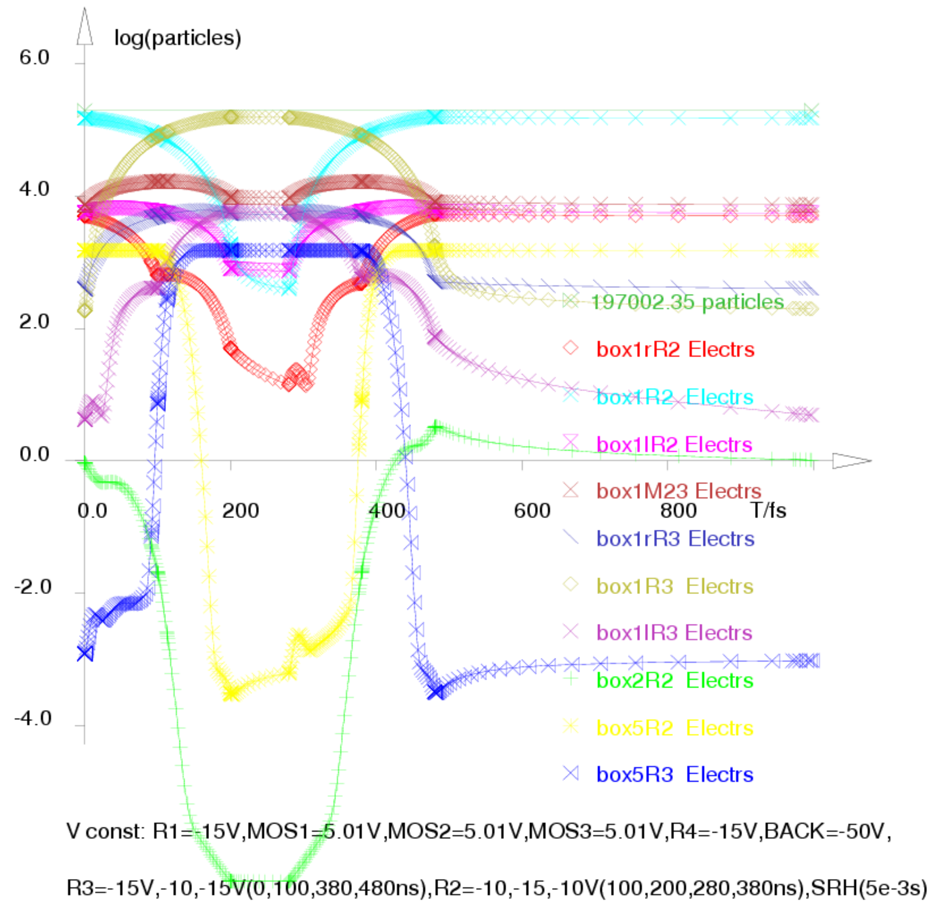
# Example

X-ray CCD (a possible detector for the Stanford LCLS (Linac Coherent Light Source)):



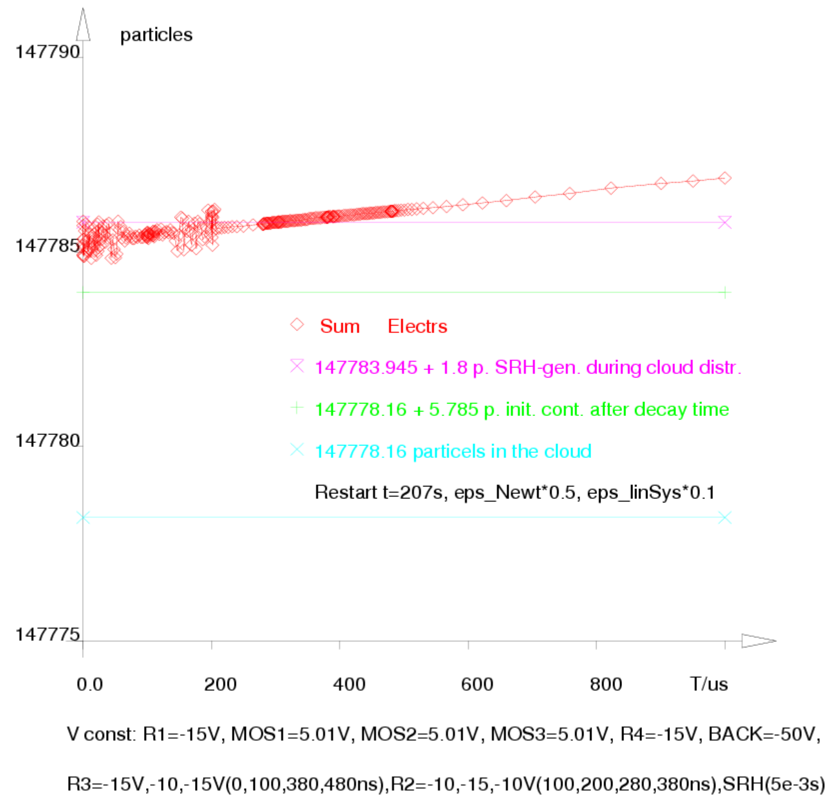

Doping ('equilibrium potential')

# Example




Time dependent paricle numbers in different regions (shifting $R_2 \rightarrow R_3$, $80ns$ wait, $R_3 \rightarrow R_2$, $620ns$ wait, 197002.35 electrons)

# Example




Particle balance over the stages: end of depletion + multiplication of the electron density by $3 \cdot 10^{-7}$ (5.785 electrons in the volume), creation of the electron hole cloud, SRH generation over $1\mu s$,
and restart after the 'Monday-morning-crash'.

# Example

Thank you for your attention

and thanks to the HLL-Munich for the collaboration (R. Richter, G. Lutz, L. Strüder and many others - at WIAS, too)