Weierstrass Institute for Applied Analysis and Stochastics

Klaus Gärtner, Annegret Glitzky, Jens A. Griepentrog

Voronoi Finite Volume Methods for Semiconductor Problems

Halbleiterlabor der Max-Planck-Institute für Physik und extraterrestrische Physik

Model Equations

- reversible reactions

$$\alpha_1 X_1 + \dots + \alpha_m X_m \rightleftharpoons \beta_1 X_1 + \dots + \beta_m X_m, \quad (\alpha,\beta) \in \mathscr{R}$$

generation rate of species X_i: $R_i = \sum_{(\alpha,\beta)\in\mathscr{R}} k_{\alpha\beta}(\mathrm{e}^{\zeta\cdot\alpha} - \mathrm{e}^{\zeta\cdot\beta})(\beta_i - \alpha_i)$

- flux density $\quad j_i = -u_i\mu_i\nabla\zeta_i, \quad i = 1,\dots,m,$

Poisson equation and continuity equations

$$-\nabla\cdot(\varepsilon\nabla v_0) = f + \sum_{i=1}^m q_i u_i$$
$$\frac{\partial u_i}{\partial t} + \nabla\cdot j_i = R_i$$
$$u_i(0) = U_i, \quad i = 1,\dots,m$$

v_0	electrostatic potential
q_i	charge number
v_i	chemical potential
$\zeta_i = v_i + q_i v_0$	electrochemical potential
$\bar{u}_i$	reference density
$u_i = \bar{u}_i \mathrm{e}^{v_i}$	density of species X_i

Stationary Spin-Polarized Drift-Diffusion Models

Species: spin-polarized electrons $\mathrm{e}_\downarrow$, $\mathrm{e}_\uparrow$ and holes $\mathrm{h}_\downarrow$, $\mathrm{h}_\uparrow$

spin relaxation reactions: $\mathrm{e}_\downarrow \rightleftharpoons \mathrm{e}_\uparrow, \quad \mathrm{h}_\downarrow \rightleftharpoons \mathrm{h}_\uparrow$

generation/recombination reactions:

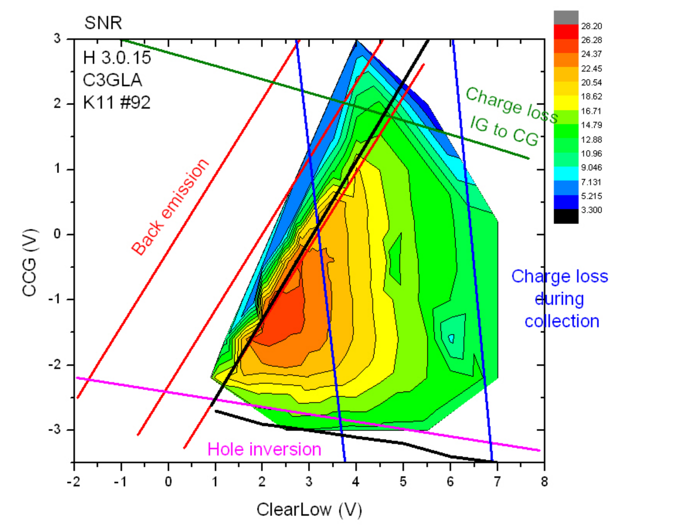
$$\mathrm{e}_\downarrow + \mathrm{h}_\downarrow \rightleftharpoons 0, \quad \mathrm{e}_\downarrow + \mathrm{h}_\uparrow \rightleftharpoons 0, \quad \mathrm{e}_\uparrow + \mathrm{h}_\downarrow \rightleftharpoons 0, \quad \mathrm{e}_\uparrow + \mathrm{h}_\uparrow \rightleftharpoons 0$$

Techniques: Slotboom variables, Scharfetter–Gummel scheme Brouwder's fixed point theorem, implicit function theorem

Results [1]:

- Existence of discrete stationary solutions
- Bounds of the solution coinciding with the corresponding bounds for solutions to the continuous problem
- Uniqueness for small applied voltages

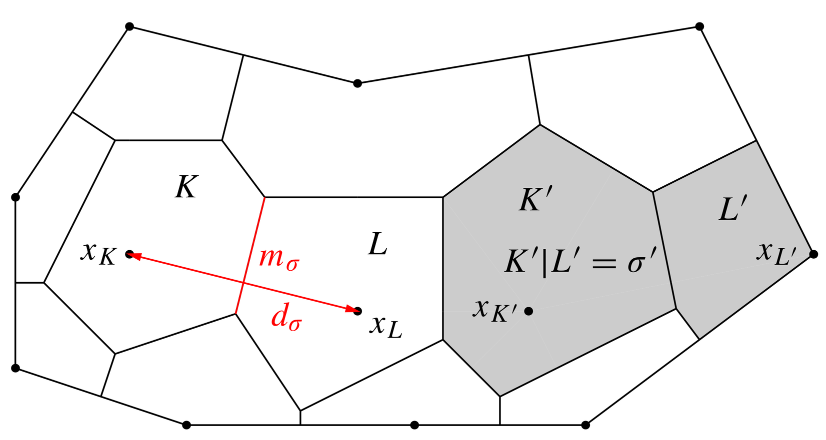
Corresponding results [2] for the van Roosbroeck system are obtained as a special case of the present investigations.



Measured signal to noise ratios for a DEPFET pixel matrix (HLL prototype design for the Belle2 experiment in Japan): the red area is the pretty small operation window. Simulations agree well and indicate the different reasons of the limits and possible improvements. Measurements: J. Ninkovic, HLL.

Voronoi Finite Volume Meshes

Boundary conforming Delaunay grid for a polyhedron $\Omega \subset \mathbb{R}^n$:



meshes $\mathscr{M} = (\mathscr{P},\mathscr{T},\mathscr{E})$:

- family $\mathscr{P}$ of grid points x_K in $\overline{\Omega}$,
- family $\mathscr{T}$ of Voronoi control volumes K,
- family $\mathscr{E} = \mathscr{E}_{int} \cup \mathscr{E}_{ext}$ of interior and exterior Voronoi faces σ,
- set $\mathscr{E}_K$ of Voronoi faces forming the boundary of $K \in \mathscr{T}$,
- Voronoi face $\sigma = K|L$ between $K, L \in \mathscr{T}$ with surface area m_σ, Euclidean distance $d_\sigma = |x_K - x_L|$ between their centers.

Discrete Sobolev–Poincaré Inequality

- Set $X(\mathscr{M})$ of functions $\underline{u}: \Omega \to \mathbb{R}$ being constant on each $K \in \mathscr{T}$, where u^K is the value of $\underline{u}$ in the Voronoi box K,
- Discrete H^1-seminorm for $\underline{u} \in X(\mathscr{M})$:

$$|\underline{u}|^2_{1,\mathscr{M}} = \sum_{\sigma\in\mathscr{E}_{\mathrm{int}}} |D_\sigma \underline{u}|^2 \frac{m_\sigma}{d_\sigma}, \quad \text{where } D_\sigma \underline{u} = |u^K - u^L|.$$

Mesh quality of $\mathscr{M}$:

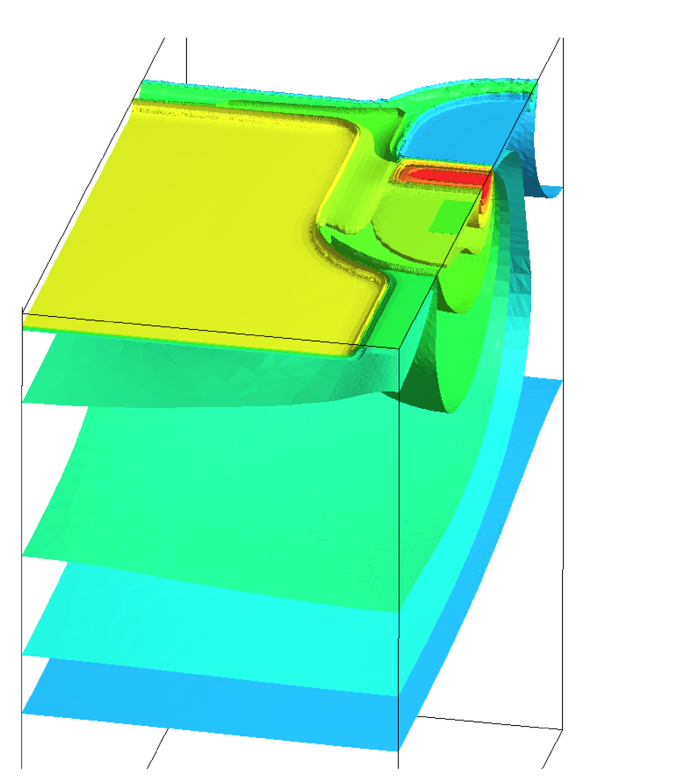
$$\frac{\operatorname{diam}(\sigma)}{d_\sigma} \le \kappa_1 \text{ for all } \sigma \in \mathscr{E}_{int}, \quad \frac{R_{K,out}}{R_{K,inn}} \le \kappa_2 \text{ for all } K \in \mathscr{T} \qquad \text{(Q)}$$

- smallest radius $R_{K,out}$ of balls circumscribing K and centered at x_K, greatest radius $R_{K,inn}$ of balls centered at x_K, fully contained in K.

Discrete Sobolev–Poincaré Inequality [3]: Let $q \in [1,\infty)$ for $n = 2$ and $q \in \left[1, \frac{2n}{n-2}\right)$ for $n \ge 3$. Then there exists a constant $c_q > 0$ depending only on n, q, Ω and the constants κ_1, κ_2 such that

$$\left\| \underline{u} - \tfrac{1}{|\Omega|}\int_\Omega \underline{u}\,\mathrm{d}x \right\|_{L^q(\Omega)} \le c_q |\underline{u}|_{1,\mathscr{M}} \quad \text{for all } \underline{u} \in X(\mathscr{M}).$$

Techniques: Sobolev integral representation, solid angle and weakly singular integral estimates.



The red isosurface of the quasi-Fermi potential includes the floating region of the internal gate of the Belle2-DEPFET. The electrons created in the lower 95% of the half pixel have to be collected in the internal gate within 25ns. The hole current difference of the MOSFET above the internal gate depends linearly of the collected charge.

Voronoi Finite Volume - Implicit Euler - Discretization

discretized Poisson equation

$$-\sum_{\sigma\in\mathscr{E}_K\cap\mathscr{E}_{int}} \varepsilon^\sigma(v_0^L(t_l) - v_0^K(t_l))\frac{m_\sigma}{d_\sigma} + \sum_{\sigma\in\mathscr{E}_K\cap\mathscr{E}_{ext}} (\tau^\sigma v_0^\sigma(t_l) - f^\sigma)m_\sigma = f^K|K| + \sum_{i=1}^m q_i u_i^K(t_l)|K|$$

discretized continuity equations

$$\frac{u_i^K(t_l) - u_i^K(t_{l-1})}{t_l - t_{l-1}}|K| - \sum_{\sigma\in\mathscr{E}_K\cap\mathscr{E}_{int}} Y_i^\sigma Z_i^\sigma(t_l)(\zeta_i^L(t_l) - \zeta_i^K(t_l))\frac{m_\sigma}{d_\sigma} = R_i^K(t_l)|K|$$
$$u_i^K(0) = \frac{1}{|K|}\int_K U_i\,\mathrm{d}x,$$

discretized state equations

$$u_i^K(t_l) = \bar{u}_i^K \mathrm{e}^{v_i^K(t_l)}, \quad n \ge 1$$

where

- $R_i^K(t_l) = \sum_{(\alpha,\beta)\in\mathscr{R}} k_{\alpha\beta}^K(\mathrm{e}^{\alpha\cdot\zeta^K(t_l)} - \mathrm{e}^{\beta\cdot\zeta^K(t_l)})(\beta_i - \alpha_i)$
- $Z_i^\sigma = \frac{1}{2}(\mathrm{e}^{v_i^K} + \mathrm{e}^{v_i^L})$ for $\sigma = K|L$
- Y_i^σ, ε^σ suitable average of $\bar{u}_i\mu_i$, ε corresponding to face σ
- $\bar{u}_i^K$, $k_{\alpha\beta}^K$, f^K average of $\bar{u}_i$, $k_{\alpha\beta}$, f on the box K
- $v_0^\sigma = v_0^K$ for $\sigma \in \mathscr{E}_{ext}\cap\mathscr{E}_K$, f^σ, τ^σ average of boundary data on σ.

Instationary Problems from Device Simulation

Electro-reaction-diffusion systems with homogeneous Neumann boundary conditions for the continuity equations

Results for any fixed Voronoi finite volume mesh $\mathscr{M}$ [4], [5]:

- For all t_n: $\int_\Omega(\underline{u}(t_n) - U)\,\mathrm{d}x$ belongs to the stoichiometric subspace.
- Existence of a unique steady state $(\underline{u}^*, \underline{v}^*)$ respecting the invariants. It is a thermodynamic equilibrium.
- The system is dissipative,

$$D_{\mathscr{M}}(\underline{v}) = \sum_{i=1}^m \sum_{\sigma\in\mathscr{E}_{int}} Y_i^\sigma Z_i^\sigma |D_\sigma \underline{\zeta}_i|^2 \frac{m_\sigma}{d_\sigma} + \int_\Omega \sum_{(\alpha,\beta)\in\mathscr{R}} \underline{k}_{\alpha\beta}\left[\mathrm{e}^{\alpha\cdot\underline{\zeta}} - \mathrm{e}^{\beta\cdot\underline{\zeta}}\right](\alpha - \beta)\cdot\underline{\zeta}\,\mathrm{d}x.$$

- The free energy

$$F_{\mathscr{M}}(\underline{u}) = \int_\Omega \sum_{i=1}^m (\underline{u}_i\underline{v}_i - \underline{u}_i + \bar{\underline{u}}_i)\,\mathrm{d}x + \sum_{\sigma\in\mathscr{E}_{int}} \frac{\varepsilon^\sigma}{2}|D_\sigma \underline{v}_0|^2\frac{m_\sigma}{d_\sigma} + \sum_{\sigma\in\mathscr{E}_{ext}} \frac{\tau^\sigma}{2}|v_0^\sigma|^2 m_\sigma$$

  decays monotonously and exponentially to its equilibrium value.
- Generalizations: anisotropies, more general statistical relations.

Using the discrete Sobolev-Poincaré inequality, for all Voronoi finite volume meshes $\mathscr{M}$ with the property (Q) it results [6]:

- Uniform estimate of the free energy by the dissipation rate.
- Uniform exponential decay of the free energy to its equilibrium value.

Cooperations

R. Richter (Max-Planck-Institut Halbleiterlabor, Otto-Hahn-Ring 6, 81739 München)

R. Eymard (Université de Marne-la-Vallée 5, boulevard Descartes Champs-sur-Marne, 77454 Marne La Vallée Cedex 2, France)

References

[1] A. Glitzky and K. Gärtner, *Existence of bounded steady state solutions to spin-polarized drift-diffusion systems*, SIAM J. Math. Anal. **41** (2010) pp. 2489–2513.

[2] K. Gärtner, *Existence of bounded discrete steady state solutions of the van Roosbroeck system on boundary conforming Delaunay grids*, SIAM J. Sci. Comput. **31** (2009) pp. 1347–1362.

[3] A. Glitzky and J. A. Griepentrog, *Discrete Sobolev-Poincaré inequalities for Voronoi finite volume approximations*, SIAM J. Numer. Anal. **48** (2010) pp. 372–391.

[4] A.Glitzky, *Exponential decay of the free energy for discretized electro-reaction-diffusion systems*, Nonlinearity **21** (2008) pp. 1989–2009.

[5] A. Glitzky and K. Gärtner, *Energy estimates for continuous and discretized electro-reaction-diffusion systems*, Nonlinear Anal. **70** (2009) pp. 788–805.

[6] A.Glitzky, *Uniform exponential decay of the free energy for Voronoi finite volume discretized reaction-diffusion systems*, WIAS-Preprint 1443 (2009).

contact: Annegret Glitzky · WIAS · Mohrenstr. 39, 10117 Berlin · +49 30 20372 568 · glitzky@wias-berlin.de · www.wias-berlin.de