On modifications of the Scharfetter-Gummel scheme for drift-diffusion equations with Fermi-like statistical distribution functions

Thomas Koprucki, Markus Kantner, Jürgen Fuhrmann and Klaus Gärtner
Weierstrass Institute for Applied Analysis and Stochastics, Mohrenstr. 39, 10117 Berlin, Germany
Email: thomas.koprucki@wias-berlin.de

***Abstract*—Driven by applications in fields like organic semiconductors there is an increased interest in numerical simulations based on drift-diffusion models with general statistical distribution functions. It is important to keep the well known qualitative properties of the Scharfetter-Gummel finite volume scheme, like positivity of solutions, dissipativity and consistency with thermodynamic equilibrium. A proper generalization to general statistical distribution functions is a topic of current research. The paper presents different state-of-the-art approaches to solve this problem. Their issues and advantages are discussed, and their practical performance is evaluated for real device structures.**

I. Drift-diffusion equations

The dependence of the carrier densities for electrons and holes on the chemical potentials η_n and η_p are described by a statistical distribution function $\mathcal{F}(\eta)$ and the conduction and valence band density of states N_c and N_v with state-equations of the form $n = N_c\mathcal{F}(\eta_n)$ and $p = N_v\mathcal{F}(\eta_p)$. Typical choices of the distribution function are $\mathcal{F}(\eta) = \exp\eta$ (Boltzmann approximation) or $\mathcal{F}(\eta) = F_{1/2}(\eta)$ (Fermi-Dirac integral of order 1/2 describing degenerate semiconductors).

The drift-diffusion equations describe the carrier flow in a semiconductor due to an self-consistent electrical field. They are given by the coupled system consisting of Poisson's equation for the electrostatic potential ψ

$$-\nabla\cdot(\varepsilon\nabla\psi) = q(C + p - n) \tag{1}$$

and continuity equations for the electron and hole densities which in the stationary case are given by

$$-\frac{1}{q}\nabla\cdot\mathbf{j}_n = -R, \quad +\frac{1}{q}\nabla\cdot\mathbf{j}_p = -R, \tag{2}$$

where q denotes the elementary charge, ε the electrical permitivity, C the net doping profile and $R(n,p)$ describes the recombination. The electron and hole currents $\mathbf{j}_n$ and $\mathbf{j}_p$ are defined by

$$\mathbf{j}_n = -q\mu_n N_c\mathcal{F}(\eta_n)\nabla\varphi_n, \quad \mathbf{j}_p = -q\mu_p N_v\mathcal{F}(\eta_p)\nabla\varphi_p, \tag{3}$$

where μ_n and μ_p denote the mobilities, φ_n and φ_p the quasi-Fermi potentials of electrons and holes and η_n and η_p the corresponding (non-dimensionalized) chemical potentials

$$\eta_n = \frac{q(\psi-\varphi_n) + E_{\mathrm{ref}} - E_c}{k_BT}, \; \eta_p = \frac{q(\varphi_p-\psi) - E_{\mathrm{ref}} + E_v}{k_BT}.$$

Here, k_B denotes Boltzmann's constant, T the temperature, E_{ref} a reference energy for the quasi-Fermi potentials and E_c and E_v the conduction and valence band-edge energies.

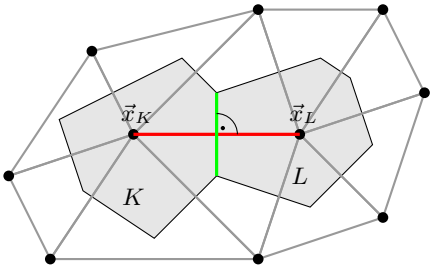

Fig. 1. Collocation points (black), simplices (grey lines) and control volumes (filled) in two space dimensions. Note the right angle between the lines $\overline{\vec{x}_K\vec{x}_L}$ and $\partial K\cap\partial L$, which allows to approximate the normal current through the face boundary $\partial K\cap\partial L$ (green) by a finite difference expression along the edge $\overline{\vec{x}_K\vec{x}_L}$ (red).

II. Finite volume space discretization

The Voronoï box based finite volume method [1], known also as "box method" [2] uses a simplicial grid in the simulation domain $\Omega\subset\mathbb{R}^d$. The boundary conforming Delaunay property [3] of the grid allows to obtain control volumes surrounding each given collocation point $\vec{x}_K$ by joining the circumcenters of the simplices adjacent to it, see Fig. 1.

Let denote by ∂K the boundary of the control volume K, and by $|\xi|$ the measure of a geometrical object ξ. For each control volume K, we integrate the continuity equation (2) and apply the Gauss theorem to the integral of the flux divergence. Without loss of generality, we restrict our considerations to the electron transport equation.

$$\begin{aligned} 0 &= \int_K (-\nabla\cdot\mathbf{j}_n + R)\,d\vec{x} = \int_{\partial K}\mathbf{j}_n\cdot\vec{n} + \int_K R\,d\vec{x} \\ &= \sum_{L\text{ neighbour of }K}\int_{\partial K\cap\partial L}\mathbf{j}_n\cdot\vec{n}_{KL}ds + \int_K R\,d\vec{x} \\ &\approx \sum_{L\text{ neighbour of }K}\frac{|\partial K\cap\partial L|}{|\vec{x}_K-\vec{x}_L|}j_{n;KL} + |K|R(n_K,p_K). \end{aligned} \tag{4}$$

Here, n_K, p_K are the values of n and p at the collocation points $\vec{x}_K$, and $j_{n,KL}$ are approximations of the (scaled by the edge length) normal currents through the interface $\partial K\cap\partial L$ between two neighbouring control volumes, see Fig. 1.

In the same way, one obtains for the Poisson equation

$$\sum_{L\text{ neighbour of }K}\frac{|\partial K\cap\partial L|}{|\vec{x}_K-\vec{x}_L|}E_{KL} = |K|q(C_K + p_K - n_K). \tag{5}$$

978-1-4799-3682-3/14/$31.00 ©2014 IEEE

In a straightforward manner, the scaled electric field projection E_{KL} can be expressed by the finite difference expression

$$E_{KL} = \varepsilon(\Psi_K - \Psi_L). \tag{6}$$

III. Scharfetter-Gummel current expressions

The classical Scharfetter-Gummel scheme [4] approximates the normal current across the interface $j_{n,KL}$ by

$$j = j_0\Big[B(-\delta\psi)n_K - B(\psi)n_L\Big], \tag{7}$$

where $B(x) = \frac{x}{\exp(x)-1}$ is the Bernoulli function, $j_0 = q\mu_n U_T$, $\delta\psi = (\psi_K - \psi_L)/U_T$ and $U_T = \frac{k_B T}{q}$. Assuming the Boltzmann approximation $\mathcal{F}(\eta) = \exp\eta$, the scheme has been derived from solving a two-point boundary value problem resulting from a projection of the continuity equation (neglecting recombination) along the discretization edge $\overline{\vec{x}_K\vec{x}_L}$ assuming constant current $j = \mathbf{j}_n \cdot \vec{n}_{KL}$ and constant electrical field with boundary values $n|_{\vec{x}_K} = n_K, n|_{\vec{x}_L} = n_L$ [4]. It is important that it is consistent with the unique thermodynamic equilibrium ($\mathbf{j}_n = 0$ for $\varphi_n = const.$).

For cases where the Boltzmann approximation is no longer valid (high densities) there exist different ways to extend the Scharfetter-Gummel scheme for the current approximation.

A. Averaging of inverse activity coefficients

Motivated by applications in electrochemical systems, in [5] it has been proposed to reformulate the equations based on the activities e^η. This reformulation results in a Boltzmann-like drift-diffusion expression for the activities scaled by the inverse activity coefficient β:

$$\mathbf{j}_n = -q\mu_n\beta(\eta)N_c e^\eta \nabla\varphi_n, \quad \beta(\eta) = \frac{\mathcal{F}(\eta)}{e^\eta}. \tag{8}$$

This structure can be kept in the discretization:

$$j = j_0\bar{\beta}_{KL}N_c\Big[B(-\delta\psi)e^{\eta_K} - B(\delta\psi)e^{\eta_L}\Big]. \tag{9}$$

Here, η_K and η_L are the chemical potentials corresponding to the densities n_K and n_L. It is consistent with thermodynamic equilibrium for any average $\bar{\beta}_{KL} \in [\beta(\eta_K), \beta(\eta_L)]$.

B. Averaging of diffusion enhancement

Keeping densities as basic variables, the drift-diffusion expression for the current is modified by the diffusion enhancement g:

$$\mathbf{j}_n = -qn\mu_n\big[\nabla\psi - \frac{k_B T}{q}g\big(\frac{n}{N_c}\big)\nabla n\big], \quad g(x) = x(\mathcal{F}^{-1})'(x). \tag{10}$$

As g scales the diffusion coefficient, using an appropriate average $\bar{g}_{KL} = \bar{g}_{KL}(n_K, n_L) \in [g(n_K), g(n_L)]$ leads to the Scharfetter-Gummel like expression

$$j = j_0\bar{g}_{KL}\Big[B\Big(-\frac{\delta\psi}{\bar{g}_{KL}}\Big)n_K - B\Big(\frac{\psi}{\bar{g}_{KL}}\Big)n_L\Big]. \tag{11}$$

However, in this case, consistency with thermodynamic equilibrium can only be achieved for a special choice of the averaging procedure [6].

C. Generalized Schafetter-Gummel scheme

The idea to solve a local two-point boundary value problem in order to derive the current expressions in the finite volume scheme has been generalized to nonlinear drift-diffusion problems in [7]. This idea has been carried out in [8] for the Blakemore approximation $\mathcal{F}(\eta) = \frac{1}{\exp(-\eta)+\gamma}$, which for $\gamma = 0.27$ provides a good approximation of $F_{1/2}$ upto $\eta \leq 1.3$ [9]. This approach leads to a nonlinear equation for j:

$$j = j_0 N_c\Big(B(\delta\psi + \gamma j)e^{\eta_K} - B(-(\delta\psi + \gamma j))e^{\eta_L}\Big). \tag{12}$$

This equation has a unique solution [8], which can be obtained in practice by a Newton method. It is possible to generalize this ansatz to any strictly monotonous distribution functions [10]. The scheme is dissipative and consistent with thermodynamic equilibrium. Based on a proper constant current approximation, the scheme is expected to deliver approximations with high accuracy already on rather coarse grids.

IV. Outlook

The presented schemes have been verified numerically and partially investigated analytically. To our knowledge up to now, no comparative evaluations have been carried out for the fully coupled system. Their application to real device structures is still missing. This contribution attempts to perform a step in this direction.

Acknowledgment

The work of T.K. and M. K. has been supported by the Deutsche Forschungsgemeinschaft (DFG) within the collaborative research center 787 "Semiconductor Nanophotonics" under project B4.

References

[1] R. H. Macneal, "An asymmetrical finite difference network," *Quart. Math. Appl.*, vol. 11, pp. 295–310, 1953.

[2] R. E. Bank and D. J. Rose, "Some error estimates for the box method," *SIAM J. Numer. Anal.*, vol. 24, no. 4, pp. 777–787, 1987.

[3] H. Si, K. Gärtner, and J. Fuhrmann, "Boundary conforming Delaunay mesh generation," *Comput. Math. Math. Phys.*, vol. 50, pp. 38–53, 2010.

[4] D. L. Scharfetter and H. K. Gummel, "Large signal analysis of a silicon Read diode," *IEEE Trans. Electron. Dev.*, vol. 16, pp. 64–77, 1969.

[5] J. Fuhrmann, "Comparison and Numerical Treatment of Generalized Nernst-Planck Models," 2014, WIAS Preprint No. 1940. [Online]. Available: http://www.wias-berlin.de/preprint/1940/wias_preprints_1940.pdf

[6] M. Bessemoulin-Chatard, "A finite volume scheme for convection-diffusion equations with nonlinear diffusion derived from the Scharfetter-Gummel scheme," *Numer. Math.*, vol. 121, pp. 637–670, 2012.

[7] R. Eymard, J. Fuhrmann, and K. Gärtner, "A finite volume scheme for nonlinear parabolic equations derived from one-dimensional local dirichlet problems," *Numer. Math.*, vol. 102, pp. 463–495, 2006.

[8] T. Koprucki and K. Gärtner, "Discretization scheme for drift-diffusion equations with strong diffusion enhancement," *Optical and Quantum Electronics*, vol. 45, no. 7, pp. 791–796, 2013.

[9] J. Blakemore, "The Parameters of Partially Degenerate Semiconductors," *Proc. Phys. Soc. London A*, vol. 65, pp. 460–461, 1952.

[10] T. Koprucki and K. Gärtner, "Generalization of the Scharfetter-Gummel scheme," in *Proceedings of the 13th International Conference on Numerical Simulation of Optoelectronic Devices (NUSOD), 2013*, J. Piprek, L. Chrostowski, eds., IEEE Conference proceedings, 2013, pp. 85–86.