Comparison of Scharfetter-Gummel Schemes for (Non-)Degenerate Semiconductor Device Simulation

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***Abstract*—We consider Voronoi finite volume schemes for the discretization of the van Roosbroeck system and pay particular attention to the choice of flux approximations. The classical Scharfetter-Gummel scheme yields a thermodynamically consistent numerical flux, but cannot be used for general charge carrier statistics. We compare and analyze aspects of two state-of-the-art *modified* Scharfetter-Gummel schemes to simulate (non-)degenerate semiconductors.**

I. Van Roosbroeck model

The standard drift-diffusion model for the description of semi-classical transport of free electrons and holes due to a self-consistent electric field in a semiconductor device is the van Roosbroeck system. The stationary model is given by

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

$$\nabla \cdot \mathbf{j}_n = qR(n,p), \tag{1b}$$

$$\nabla \cdot \mathbf{j}_p = -qR(n,p), \tag{1c}$$

where q denotes the elementary charge, ε_s the dielectric permittivity, C describes the doping profile and $R(n,p)$ the recombination. The set of unknowns is expressed by the electrostatic potential ψ and the quasi-Fermi potentials for electrons φ_n and holes φ_p. We have the current densities

$$\mathbf{j}_n = -q\mu_n n \nabla \varphi_n, \qquad \mathbf{j}_p = -q\mu_p p \nabla \varphi_p, \tag{2}$$

where the electron and hole densities n and p are defined by

$$n = N_c \mathcal{F}(\eta_n), \qquad \eta_n = \frac{q(\psi - \varphi_n) - E_c}{k_B T}, \tag{3a}$$

$$p = N_v \mathcal{F}(\eta_p), \qquad \eta_p = \frac{q(\varphi_p - \psi) + E_v}{k_B T}. \tag{3b}$$

The valence band density of states are identified by N_c and N_v, the mobilities by μ_n and μ_p and the Boltzmann constant by k_B. The conduction and valence band-edge energies are denoted by E_c and E_v and T refers to the temperature.
Non-degenerate semiconductors can be simulated with the Boltzmann approximation $\mathcal{F}(\eta) = \exp(\eta)$ as choice for the strictly monotonously increasing statistics function $\mathcal{F}$. Here, we focus on degenerate semiconductors. To compare our flux approximations, we choose the Blakemore statistics function $\mathcal{F}(\eta) = \dfrac{1}{\exp(-\eta) + \gamma}$ with $\gamma = 0.27$ for which an expensive but accurate numerical flux is known.
Without loss of generality, we consider only the current density for electrons from now on, thus partially omitting the index n.

II. Scharfetter-Gummel Current Expressions

A. Generalized Scharfetter-Gummel Scheme

Under the assumption that the flux j and the electric field $-\nabla\psi$ are constant along each face of a cell, an integral equation can be derived [2], which shall be satisfied by the unknown flux

$$\int_{\eta_K}^{\eta_L} \left(\frac{j_n/j_0}{\mathcal{F}(\eta)} + \delta\psi_{KL} \right)^{-1} d\eta = 1, \quad j_0 = q\mu_n N_c \frac{U_T}{h_{KL}}, \tag{4}$$

where $\delta\psi_{KL} = (\psi_L - \psi_K)/U_T$ and $U_T = \frac{k_B T}{q}$. The integration limits are given by $\eta_K = \eta_n(\psi_K, \varphi_K)$ and $\eta_L = \eta_n(\psi_L, \varphi_L)$. The existence of a solution to (4) was proven in [4]. We refer to the solution of (4) as *generalized* Scharfetter-Gummel flux. Note that for non-degenerate semiconductor devices the generalized Scharfetter-Gummel scheme reduces to the classical Scharfetter-Gummel scheme [5]

$$j_{sg} = B(\delta\psi_{KL})\, e^{\eta_L} - B(-\delta\psi_{KL})\, e^{\eta_K}, \tag{5}$$

for a non-dimensionalized edge current $j_{sg} = j_n/j_0$ and the Bernoulli function $B(x) := x/(e^x - 1)$. Additionally, it was shown in [3] that for Blakemore statistics the integral equation (4) can be reduced to a fixed point equation, namely

$$j_g = B(\delta\psi_{KL} + \gamma j_g)\, \mathrm{e}^{\eta_L} - B\left(-\left[\delta\psi_{KL} + \gamma j_g\right]\right) \mathrm{e}^{\eta_K}. \tag{6}$$

B. "Sedan" Scheme

Rearranging the drift part in (2) to include the *excess chemical potential*, $\mu^{ex} = \log \mathcal{F}(\eta) - \eta$, allows to derive the following *modified* Scharfetter-Gummel scheme

$$j_s = B(Q_{KL})\, \mathcal{F}(\eta_L) - B(-Q_{KL})\, \mathcal{F}(\eta_K) \tag{7}$$

with

$$Q_{KL} = \delta\psi_{KL} + \mu_L^{ex} - \mu_K^{ex}. \tag{8}$$

This approach to handle degenerate semiconductors appears to be customary in parts of the device simulation community. The earliest reference we could find is the source code of the SEDAN III simulator [7], therefore in the sequel we will call this scheme the *Sedan scheme*.

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C. Diffusion Enhanced Scheme

Recently, in [6] another *modified* Scharfetter-Gummel scheme was introduced. The idea is based on a logarithmic average of the diffusion enhancement $g(\eta) = \mathcal{F}(\eta)/\mathcal{F}'(\eta)$,

$$g_{KL} = \frac{\eta_L - \eta_K}{\log \mathcal{F}(\eta_L) - \log \mathcal{F}(\eta_K)}, \tag{9}$$

resulting in the local flux approximation

$$j_d = g_{KL}\left[B\left(\frac{\delta\psi_{KL}}{g_{KL}}\right)\mathcal{F}(\eta_L) - B\left(-\frac{\delta\psi_{KL}}{g_{KL}}\right)\mathcal{F}(\eta_K)\right]. \tag{10}$$

We stress that, if $\eta_K \approx \eta_L$, regularization strategies need to be developed to handle the removeable singularity.

III. Comparison of Flux Discretizations

Based on the comparison made in [1], the discussion in the aforementioned work is extended by the Sedan flux approximation. We define $\delta\eta_{KL} := \eta_L - \eta_K$ and consider the logarithmic error between modified flux schemes and the generalized scheme for a fixed average $\bar{\eta}_{KL} = \frac{\eta_L+\eta_K}{2}$. The errors for the simulation of a degenerate semiconductor can be seen in Figure 1. The black dashed lines correspond to thermodynamic consistency, i.e. vanishing currents for constant quasi-Fermi potentials, as well as pure drift currents, i.e. $\eta_K = \eta_L$. In both cases, modified schemes agree exactly with the generalized Scharfetter-Gummel scheme. The red dashed line indicates agreement of the Sedan scheme and the exact solution of (4) for a pure diffusion current $\mathbf{j}$, i.e. $\delta\psi_{KL} = 0$. This can be proven analytically, see [8].

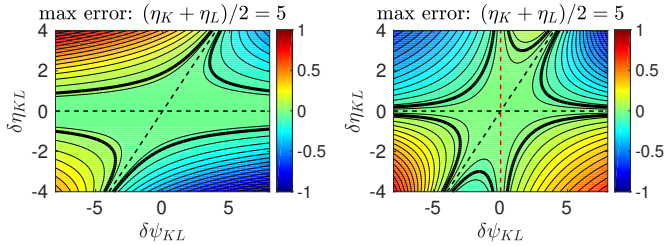

Fig. 1. Logarithmic absolute errors between the generalized Scharfetter-Gummel and the diffusion enhanced scheme (left) and the Sedan scheme (right) for $\bar{\eta}_{KL} = 5$.

When neglecting third-order terms, error bounds between the modified and the generalized flux dependent on the diffusion enhancement can be derived, see [1], [8]

$$|j_s - j| \leq \frac{1}{2}\frac{\mathcal{F}(\bar{\eta}_{KL})}{g(\bar{\eta}_{KL})}\left(|\delta\psi_{KL}\delta\eta_{KL}| + \delta\eta_{KL}^2\right) \tag{11}$$

$$|j_d - j| \leq \frac{1}{2}\frac{\mathcal{F}(\bar{\eta}_{KL})}{g(\bar{\eta}_{KL})}|\delta\psi_{KL}\delta\eta_{KL}|. \tag{12}$$

The error bounds indicate a better performance of the diffusion enhanced scheme for large values of the diffusion enhancement g, i.e. for statistics strongly deviating from the Boltzmann. Both, the error estimates (11), (12) and Figure 1 indicate a larger area, where the diffusion enhanced and the generalized scheme agree well for small values of $\delta\eta_{KL}$ and large values of the potential difference $\delta\psi_{KL}$.

IV. Numerical Example

The impact of the different flux discretization schemes on the simulation of degenerate semiconductor devices was studied for a GaAs p-i-n diode. A Julia-based solver `VoronoiFVM.jl` [9] was used. Noteworthy is the possibility to work with `ForwardDiff.jl` [10], a package based on automatic differentiation, which provides the ability to compute Jacobians analytically without needing any additional information in Julia. Figure 2 shows that the errors in the computed total currents based on the flux schemes converge with order $\mathcal{O}(h^2)$. Furthermore, it suggests that on coarse meshes, which are essential for complex geometries or 3D simulations, the Sedan flux performs more accurate than the diffusion enhanced scheme.

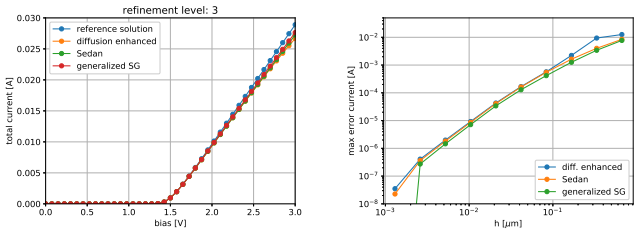

Fig. 2. Left: The I-V curves computed with the different schemes for fixed mesh refinement. The reference solution was computed using the generalized Scharfetter-Gummel scheme on refinement level 10. Right: Convergence studies for the absolute errors of the total currents.

V. Conclusion

A discussion of advantages and issues of the presented schemes was made and in Section IV an impression of their performance in a real device setup was given. For an extensive discussion further applications will be part of future research.

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