Highly Accurate Discretizations for non-Boltzmann Charge Transport in Semiconductors

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***Abstract*—We present and analyze a family of highly accurate quadrature-based Scharfetter-Gummel fluxes for charge carrier transport in semiconductors which are particularly useful for non-Boltzmann statistics.**

I. Introduction

Different numerical methods have been proposed to discretize the van Roosbroeck system describing charge carrier transport. The Scharfetter-Gummel (SG) scheme provides a thermodynamically consistent discrete carrier flux approximation for non-degenerate semiconductors in the Voronoï finite volume method [1]–[3]. For a detailed overview see [4].

Degeneracy effects become relevant at cryogenic temperatures [5], for high doping concentrations or in organic materials [6], [7] so that non-Boltzmann (e.g. Fermi-Dirac and Gauss-Fermi) statistics $\mathcal{F}$ are required. Then a carrier flux can be defined implicitly as the solution of an integral equation which one often cannot find analytically. Circumventing this difficulty, modified SG fluxes [2], [8], [9] have become popular. Here, we present a novel way to numerically solve the integral equation via quadratures and Newton's method [3], [10] and demonstrate the high accuracy of the resulting fluxes.

We consider the stationary van Roosbroeck system for charge transport in semiconductors using the potential ψ and the quasi-Fermi potentials φ_n and φ_p as unknown variables:

$$-\nabla\cdot(\varepsilon_0\varepsilon_r\nabla\psi) = q\,(p-n+C)\,, \tag{1a}$$
$$\nabla\cdot\mathbf{j}_n = qR, \qquad \mathbf{j}_n = -q\mu_n n\nabla\varphi_n, \tag{1b}$$
$$\nabla\cdot\mathbf{j}_p = -qR, \qquad \mathbf{j}_p = -q\mu_p p\nabla\varphi_p \tag{1c}$$

where the electron and hole densities are defined by

$$n = N_c\mathcal{F}(\eta_n), \qquad \eta_n = \frac{q(\psi-\varphi_n)-E_c}{k_BT}, \tag{2a}$$
$$p = N_v\mathcal{F}(\eta_p), \qquad \eta_p = \frac{q(\varphi_p-\psi)+E_v}{k_BT}. \tag{2b}$$

For simplicity, we restrict our considerations to the continuity equation for the electrons, partially omitting the index n.

II. Discrete thermodynamic consistency

We require the numerical flux approximation to (at least approximately) satisfy the thermodynamic consistency property expressed as: vanishing currents for constant quasi Fermi potentials. Thus, for two adjacent discretization nodes $\mathbf{x}_K$ and $\mathbf{x}_L$, corresponding to neighboring Voronoï cells K and L (see [2] for more details), numerical fluxes shall also (at least approximately) vanish,

$$j = j(\eta_L,\eta_K,\psi_L,\psi_K) = 0$$

which implies $\delta\eta_{KL} = \delta\psi_{KL}$, where

$$\frac{\psi_L-\psi_K}{U_T} =: \delta\psi_{KL}, \quad \delta\eta_{KL} := \eta_L-\eta_K. \tag{3}$$

Thermodynamic consistency becomes relevant if the van Roosbroeck system has to be coupled to more complex models and avoids unphysical steady state dissipation [9].

III. Generalized SG Schemes

Assuming a constant flux j and a linear variation of the electrostatic potential ψ between two neighboring cells, a numerical flux can be obtained by solving a two-point boundary value problem for the drift-diffusion flux projected onto the line connecting the discretization nodes $\mathbf{x}_K$ and $\mathbf{x}_L$. For Boltzmann statistics, this problem can be solved analytically [1]. In the general case, this leads to an integral equation for the flux [11], [12],

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

with $\eta_K = \eta_n(\psi_K,\varphi_K)$ and $\eta_L = \eta_n(\psi_L,\varphi_L)$.

IV. Quadrature based SG Schemes

Denoting the integrand in (4) with $G(\eta;\delta\psi_{KL},j_{gsg})$, we can approximate (4) for $j_{gsg} = j_n/j_0$ by

$$H(j_{gsg}) := \sum_{i=1}^{N} w_i G(\eta_i;\delta\psi_{KL},j_{gsg}) - 1 = 0, \tag{5}$$

where w_i are some integration weights, η_i the quadrature nodes and N the number of quadrature nodes. The resulting

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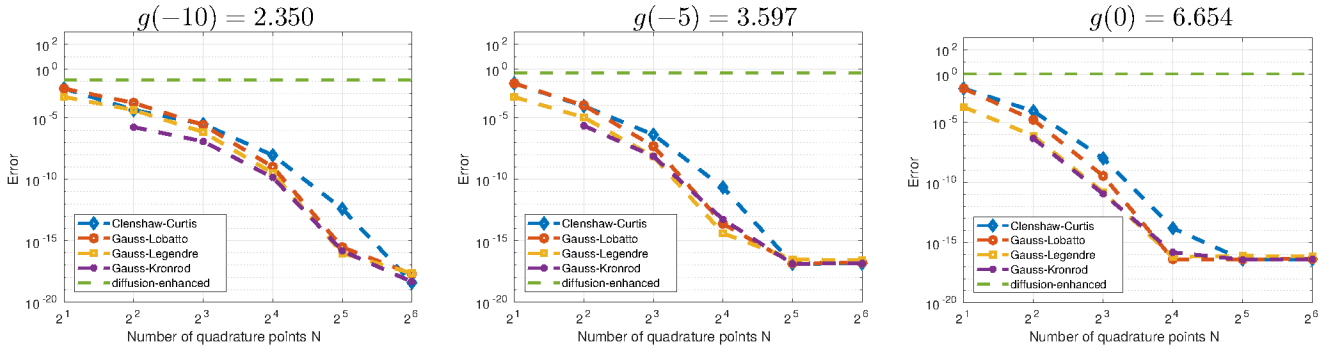

Fig. 1. Logarithmic absolute ℓ_2 errors depending on the number of quadrature points N for Gauss-Fermi distribution functions with different fixed values of $\bar{\eta}_{KL}$ and several quadrature rules. From left to right, errors for $\bar{\eta}_{KL} = -10, -5, 0$. In all figures the errors from the quadrature-based schemes are compared to the corresponding error between the flux obtained via the diffusion enhanced scheme [9] and j_{gsg}^{128} for Gauss-Fermi distribution functions.

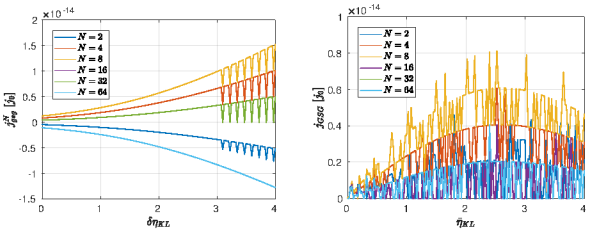

Fig. 2. Numerical verification of validity of the thermodynamic consistency for $\eta \in [\eta_K, \eta_L]$ via Gauss-Legendre quadrature, varying the number of quadrature points N. Left: $\delta\eta_{KL} = \psi_{KL} = 4$ and $\bar{\eta}_{KL} \in [0, 4]$ with step equal to 0.025. Right: $\bar{\eta}_{KL} = 2$ and $\delta\eta_{KL} \in [0, 4]$ with step 0.025.

nonlinear equation for j_{gsg} is solved via Newton's method. As starting guess the diffusion-enhanced flux [8], [9] is used. A detailed explanation of this approach is reported in [10].

V. Discussion

In Figure 1, we present a flux accuracy study in terms of the ℓ_2 norm (similar for the ℓ_∞ norm, [10]) for four different quadratures using the Gauss-Fermi distribution function. We fix $\bar{\eta}_{KL} = \frac{\eta_L + \eta_K}{2} = -10, -5, 0$ and impose $\delta\psi \in [-6, 6]$ with step 0.1, $\delta\eta \in [-4, 4]$ with step 0.1 and an energetic disorder $\sigma = 5$. The error was computed by

$$err(N) := \left| j_{gsg}^{N} - j_{gsg}^{128} \right|. \tag{6}$$

The figure shows the high accuracy of the proposed scheme when compared to a state-of-the-art diffusion-enhanced SG flux [8], [9] (green). All four quadrature rules (Gauss-Legendre, Gauss-Lobatto, Gauss-Kronrod and Clenshaw-Curtis) lead already with just two quadrature nodes to numerical fluxes which are more accurate than the reference flux. For the more challenging case of high diffusion enhancement the accuracy improves further. In addition, in thermodynamic equilibrium our scheme produces numerical flux values on the order of the machine precision (see Figure 2). Thus for all practical purposes it is thermodynamically consistent.

VI. Outlook

We intend to use this approach in the fully coupled nonlinear van Roosbroeck system in order to assess its merits in the simulation of a realistic semiconductor device. Furthermore, we plan comparisons to other numerical schemes such as the finite element method, following ideas from [13].

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