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Computational and analytical comparison of flux discretizations for the semiconductor device equations beyond Boltzmann statistics

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ABSTRACT

We compare three thermodynamically consistent numerical fluxes known in the literature, appearing in a Voronoï finite volume discretization of the van Roosbroeck system with general charge carrier statistics. Our discussion includes an extension of the Scharfetter–Gummel scheme to non-Boltzmann (e.g. Fermi–Dirac) statistics. It is based on the analytical solution of a two-point boundary value problem obtained by projecting the continuous differential equation onto the interval between neighboring collocation points. Hence, it serves as a reference flux. The exact solution of the boundary value problem can be approximated by computationally cheaper fluxes which modify certain physical quantities. One alternative scheme averages the nonlinear diffusion (caused by the non-Boltzmann nature of the problem), another one modifies the effective density of states. To study the differences between these three schemes, we analyze the Taylor expansions, derive an error estimate, visualize the flux error and show how the schemes perform for a carefully designed p-i-n benchmark simulation. We present strong evidence that the flux discretization based on averaging the nonlinear diffusion has an edge over the scheme based on modifying the effective density of states.

1. Introduction

The van Roosbroeck system [1] (also known as the semiconductor device equations) has become a standard model to describe the flow of electrons and holes in semiconductor devices. Its numerical approximation is very well understood if Boltzmann statistics accurately describes the electron and hole densities. In this case, one refers to the semiconductor as *non-degenerate*. Scharfetter and Gummel [2] presented in the late 1960ies a flux discretization scheme which could deal with the numerical challenges such as stability and preservation of maximum principles posed by these equations, see for example [3–5]. The generalization to non-Boltzmann statistics (in *degenerate* semiconductor materials), however, presents very similar challenges which are not satisfactorily solved yet. Hence, the goal of this paper is to study the influence of three thermodynamically consistent flux approximations used in a Voronoï finite volume discretization of the van Roosbroeck system when assuming more general statistics functions. We will compare these schemes analytically and numerically to assess their quality for semiconductor device simulations.

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A very general and computationally rather expensive finite volume flux approximation was studied in [6]. In order to determine the numerical flux between two control volumes this method needs to solve an integral equation. This integral equation is a reformulation of a nonlinear two-point boundary value problem which one obtains from projecting the continuity equation for the charge carriers onto the interval between two nodes belonging to neighboring cells. For so-called Blakemore statistics [7] the integral equation is known to simplify to a nonlinear algebraic equation which can be solved with a few Newton steps [8]. No corresponding simplification is known for more general statistics. For this reason several ideas were proposed. In [9], piecewise approximations (e.g. Padé interpolants) for the statistics function are discussed. However, this approach may still be rather costly. Hence, *modified* Scharfetter–Gummel schemes which only approximately solve the two-point boundary value problem may yield a good compromise between efficiency and accuracy by averaging certain quantities.

Several such schemes have been suggested to deal with more general statistics [10–12]. Unfortunately, these discretizations are not consistent with the thermodynamic equilibrium, i.e. they do not satisfy an analogous discrete version of the continuous property that the fluxes vanish if the quasi Fermi potentials are constant. Thermodynamic consistency is extremely important to avoid unphysical steady state dissipation. Furthermore, the consistent discretization of dissipative effects is crucial when coupling the semiconductor device equations to heat transport models.

Bessemoulin-Chatard suggested a scheme which averages the diffusion enhancement in such a way that the resulting flux approximation is thermodynamically consistent [13]. The diffusion enhancement can be interpreted as a measure for how far the system is from the Boltzmann regime. It leads to a nonlinear diffusion coefficient whose particular form is induced by the statistical distribution function for the charge carrier densities, e.g., the Fermi–Dirac integral of order one half. Using this flux, Bessemoulin-Chatard proved convergence of a semi-implicit finite volume scheme. This *diffusion enhanced* scheme was translated into the context of semiconductor device models in [14], making the dependency on the diffusion enhancement explicit.

It is also possible to derive another class of schemes by modifying the effective density of states. This so-called *inverse activity* scheme was introduced in [15] for the numerical solution of the generalized Nernst–Planck system which is similar to the van Roosbroeck system. A variant of this scheme for Fermi–Dirac statistics is described in [16,17]. Here the adaption to general statistics is realized via averaging the inverse activity coefficient. Even though any such average will yield a thermodynamically consistent scheme, we will focus on two practical choices: an arithmetic and geometric mean of the inverse activity coefficients at neighboring nodes. However, some of our results apply to any average for the inverse activity coefficient that satisfies very mild additional assumptions.

We continue this paper by introducing the van Roosbroeck system in Section 2 and present its discretization as well as the different flux approximations in Section 3. In order to compare these schemes, we study their Taylor series expansions in Section 4, derive a general error estimate in Section 5, compare the flux error visually in Section 6 and finally analyze the influence of the different numerical fluxes to the coupled van Roosbroeck system by simulating a carefully chosen device setup consisting of a p-doped, intrinsic and n-doped region (p-i-n device) in Section 7.

This publication is supplemented with a Mathematica notebook, Matlab files and simulation data, which can be used to verify the presented results [18].

2. The van Roosbroeck system

The van Roosbroeck system describes the charge carrier flow and the electrostatic potential in a semiconductor device. It consists of three coupled nonlinear partial differential equations: one for the electrostatic potential ψ and two continuity equations, one for the electron and one for the hole density which we denote with n and p. We consider a homogeneous material and some domain $\Omega \subseteq \mathbb{R}^d$ for $d \in \{1, 2, 3\}$.

Then the stationary van Roosbroeck system is given by

$$-\nabla \cdot (\varepsilon_0 \varepsilon_r \nabla \psi) = q\,(p - n + C)\,, \tag{1a}$$

$$\nabla \cdot \mathbf{j}_n = qR, \tag{1b}$$

$$\nabla \cdot \mathbf{j}_p = -qR. \tag{1c}$$

The constants q, ε_0 and ε_r denote the elementary charge, the vacuum dielectric permittivity and the relative permittivity of the semiconductor, respectively. The recombination rate R depends on the electron and hole densities and the doping profile C may vary spatially.

The electron density and the hole density are related to the electrostatic potential ψ as well as the quasi Fermi potentials of electrons and holes φ_n and φ_p via a statistical distribution function $\mathcal{F}$, namely by

$$n = N_c \mathcal{F}\left(\frac{q(\psi - \varphi_n) - E_c}{k_B T}\right) \quad \text{and} \quad p = N_v \mathcal{F}\left(\frac{q(\varphi_p - \psi) + E_v}{k_B T}\right). \tag{2}$$

The effective densities of states for electrons in the conduction band N_c and holes in the valence band N_v as well as the corresponding band-edge energies E_c and E_v are material parameters and assumed to be constant in this paper. However, in applications they can vary with the material (for example due to abrupt or graded heterojunctions). The temperature