# Comparison of flux discretizations for varying band edge energies

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***Abstract*—Recently, a multiscale framework was developed where drift-diffusion is combined with atomistic tight-binding models [1]. A naive flux discretization was proposed to tackle the problem of heavily fluctuating band edge energies which does not take into account mathematical complications. Here we would like to present several alternatives and compare them.**

## I. Introduction

Random alloy fluctuations significantly affect the electronic, optical, and transport properties of (In,Ga)N-based optoelectronic devices. To bridge the gap between macroscale drift-diffusion simulations and atomistic band-edge fluctuations, recently a multiscale framework was developed to integrate the macroscopic and microscopic worlds [1]. In order to combine atomistic tight-binding theory and continuum-based drift–diffusion solvers, it is necessary to develop flux discretizations for variable band-edge energies. While in [1] a first scheme was formulated, flux discretizations are conceivable which avoid the gradient of the fluctuating band-edge energies. We present and discuss these numerical fluxes here.

## II. The van Roosbroeck system

We consider a version of the stationary van Roosbroeck system for charge transport in semiconductors using the potential $\psi$ and the quasi-Fermi potentials $\varphi_n$ and $\varphi_p$ as unknowns:

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

$$\nabla\cdot\mathbf{j}_n = qR, \qquad \mathbf{j}_n = -q\mu_n n\nabla\varphi_n, \tag{1b}$$

$$\nabla\cdot\mathbf{j}_p = -qR, \qquad \mathbf{j}_p = -q\mu_p p\nabla\varphi_p \tag{1c}$$

where the electron and hole densities are defined by

$$n = N_c\mathcal{F}(\eta_n), \qquad \eta_n = \frac{q(\psi-\varphi_n)-E_c}{k_BT}, \tag{2a}$$

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

Here $\mu_n, \mu_p$ are the mobilities, $N_c, N_v$ the effective density of states, $k_B$ is the Boltzmann constant and $T$ the temperature. The difference to the standard van Roosbroeck system is that the conduction $E_c = E_c(\mathbf{x})$ and valence band-edge energies $E_v = E_v(\mathbf{x})$ are heavily spatially fluctuating. From a mathematically point of view, defining the fluxes in (1b) and (1c) becomes problematic because we have to take the gradient of a *nonsmooth* function since the quasi Fermi potentials depend on the band-edge energies via (2). In order to avoid the gradient, we can introduce a Slotboom-type variable transformation for the Boltzmann case ($\mathcal{F} = \exp$) by setting

$$u_i = \frac{c_i}{N_i\exp\left(\frac{z_i}{qU_T}E_i\right)}, \quad i\in\{n,p\} \text{ with } c_n = n, c_p = p, \tag{3}$$

where we let $U_T = \frac{k_BT}{q}$. Formal computations lead to the following flux for the transformed variable $u_i$:

$$\mathbf{j}_i^u = -q\mu_i\frac{U_T}{z_i}N_i\exp\left(\frac{z_i}{qU_T}E_i\right)\left(\nabla u_i + z_iu_i\nabla\frac{\psi}{U_T}\right). \tag{4}$$

This flux avoids the gradient of the band-edge energy $E_i$ and can therefore be used as a foundation to define a modified system of equations which has a clear meaning, irregardless of the regularity of $E_i$.

Here, we propose to adapt this strategy to general statistics $\mathcal{F}$. To do so, similar to (3), we set

$$u_i = \exp\left(\eta_i - \frac{z_i}{qU_T}E_i\right), \tag{5}$$

and formally compute the flux associated to this new variable:

$$\mathbf{j}_i^u = -q\mu_i\frac{U_T}{z_i}N_i\frac{\mathcal{F}\left(\log(u_i)+\frac{z_i}{qU_T}E_i\right)}{u_i}\left(\nabla u_i + z_iu_i\nabla\frac{\psi}{U_T}\right). \tag{6}$$

As for the flux (4), one can notice that this new expression avoids the gradient of the band-edge energies, and could therefore be used as a base to define numerical fluxes. Notice that (5) coincide with (3) when $\mathcal{F} = \exp$, which means that the variable transformation (5) is a natural generalisation of the Slotboom one.

## III. Flux discretizations

We use a finite volume method to discretize model (1), see [2] for details. We focus here on the flux discretizations.

### A. Discrete thermodynamic consistency

In order to ensure a reliable approximation of the van Roosbroeck system, we require the numerical flux approximation to satisfy a discrete thermodynamic consistency property. Such a property can be expressed from a local point of view: vanishing currents shall lead to 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

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[2] for more details), we want to have the following: If the numerical flux vanishes, i.e.

$$j_i = j_i(\eta_{i,L}, \eta_{i,K}, \psi_L, \psi_K, E_{i,L}, E_{i,K}) = 0$$

then the associated discrete quasi-Fermi potentials has to be constant, in the sense that $\delta\eta_i = \frac{z_i}{U_T}\left(\frac{1}{q}\delta E_i - \delta\psi\right)$, where

$$\delta\eta_i = \eta_{i,L} - \eta_{i,K},\ \delta\psi = \psi_L - \psi_K,\ \text{and}\ \delta\psi = \psi_L - \psi_K. \quad (7)$$

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

### B. Classical thermodynamically consistent approaches

In [1], in the Boltzmann regime the following flux approximation was used:

$$j_i = -q\mu_i \frac{U_T}{z_i} N_i \frac{1}{h}\left\{ B\left( -z_i \frac{\delta\psi - \delta E_i/q}{U_T}\right)\exp(\eta_{i,L}) - B\left(z_i \frac{\delta\psi - \delta E_i/q}{U_T}\right)\exp(\eta_{i,K})\right\}, \quad (8)$$

where $h = \|\mathbf{x}_L - \mathbf{x}_K\|$ and $B(x) = \frac{x}{e^x - 1}$. The question of generalising this numerical flux to other statistics arises naturally, and can be tackled via generalized Scharfetter-Gummel fluxes. The fluxes in the classical framework, that is $E_c = 0$ [2], are good approximations and preserve the thermodynamic consistency. Hence, using for example the SEDAN flux [3], we obtain

$$j_i = -q\mu_i \frac{U_T}{z_i} N_i \frac{1}{h}\left\{ B\left(\delta M(\eta_i) - z_i \frac{\delta\psi - \delta E_i/q}{U_T}\right)\mathcal{F}(\eta_{n,L}) - B\left( -\delta M(\eta_i) + z_i \frac{\delta\psi - \delta E_i/q}{U_T}\right)\mathcal{F}(\eta_{i,K})\right\}, \quad (9)$$

where $\delta M(\eta_i) = \delta\eta_i - \delta\log(\mathcal{F}(\eta_i))$ is a difference in excess chemical potentials. Note that (9) coincides with (8) in the Boltzmann regime where $\mathcal{F} = \exp$.

However, as pointed out in Section II both numerical fluxes (8) and (9) rely on the continuous expression of the flux (1b) and (1c) where the gradient of the band-edge energy $\nabla E_i$ needs to be computed which is problematic from a mathematical point of view. In fact, we expect the numerical fluxes (9) to be a good approximation of the continuous flux when $\delta E_i \to 0$, which is not necessarily the case when we consider very irregular band-edge energy profiles.

### C. Exponentially-fitted approaches

Because of the previous observation, we introduce a new discretisation of the flux, based on the Slotboom trick presented in (5)-(6). From a numerical point of view, such a technique is inspired by the exponential-fitting scheme [4], introduced in the framework of the finite element method. Here, we propose a generalization of this strategy to handle the irregularity of the band-edge energies as well as general statistics $\mathcal{F}$. Following the idea introduced in [5] to design the "inverse activity based scheme", we define an exponentially-fitted numerical flux which discetize (6):

$$j_i = -q\mu_i \frac{U_T}{z_i} N_i \frac{1}{h} m(\beta_i(u_{i,K}), \beta_i(u_{i,L})) \left\{ B\left(\frac{-z_i}{U_T}\delta\psi\right)u_{i,L} - B\left(\frac{z_i}{U_T}\delta\psi\right)u_{i,K}\right\}, \quad (10)$$

where $m(x,y)$ is a mean function and

$$\beta_i(u_{i,K}) = \frac{\mathcal{F}\left(\log(u_{i,K}) + \frac{z_i}{qU_T}E_{i,K}\right)}{u_{i,K}}. \quad (11)$$

From a numerical point of view, the choice of $m$ proved to be challenging, since it has to handle the strong spatial heterogeneity of $E_i$. The relevant choices seem to be the arithmetic, geometric and harmonic averages, namely

$$m(x,y) = \frac{x+y}{2},\ m(x,y) = \sqrt{xy}\ \text{and}\ m(x,y) = \frac{2xy}{x+y}.$$

The numerical flux (10) is devised to handle generic band-edge energy profiles $E_i$, irregardless of their regularity.

## IV. Summary

Although the numerical fluxes (8) and (9) are natural discretizations, they rely on an ambiguous continuous expression if the $E_i$ are irregular. Hence, we introduce a change of variable which leads to the new numerical flux (10). We expect that the underlying scheme is asymptotic preserving with respect the regularity of $E_i$.

| | Flux (8)-(9) | Flux (10) |
|---|---|---|
| Definition of the continuous terms | ✘ | ✔ |
| Hope to show convergence result | ✘ | ✔ |
| Preserve the positivity | ✔ | ✔ |
| Thermodynamic consistency | ✔ | ✔ |
| Manage strong heterogeneities in diffusion & choice of averaging procedure | ✔ | ✘ |
| Unified formulation for irregular and smooth $E_i$ | ✘ | ✔ |

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