On the Scharfetter-Gummel Box-Method

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Abstract

For a linear potential function one-dimensional constant current drift-diffusion equations can be integrated in closed form, yielding the Scharfetter-Gummel (SG) discretization. The box-method generalizes the insistence on exact current conservation to higher dimensions by imposing the exact balancing of Scharfetter-Gummel fluxes through box-faces.

It has long been recognized that the one-dimensional SG discretization defines a finite element method that yields the exact solution by employing closed form solutions as an approximant. Finite element analyses of the box-method tend to employ piecewise linear approximating functions and fail to incorporate the exact integration properties of the SG discretization.

Nevertheless, the current conservation validates for the SG box-method an analytical coupling limitation for the differential drift-diffusion equations.

1. The Scharfetter-Gummel Discretization

In the discretization of the one-dimensional zero generation recombination drift-diffusion equations, the Scharfetter-Gummel technique [9] reproduces exactly the constant current. Let \( u \) denote the electrostatic potential \( u \) in units of the thermal potential \( U_T \equiv (k_B T)/q \), where \( k_B \) is Boltzmann’s constant, \( T \) is the ambient temperature, and \( q \) is the size of the electron charge. Then, under the assumption of Einstein’s relations the one-dimensional zero generation-recombination drift-diffusion equation for the conduction electron density \( n \) is given by

\[
[\mu_n(u_n x - n_x)]_x = 0. \tag{1.1}
\]

The solution \( n(x) \) to equation (1.1) can be expressed in terms of a closed form Green’s function, analogously to the procedure in [7]. To a piecewise linear potential function \( U_i(x) \) with nodal values \( u_j \) at nodes \( x_j \) can be associated a vector \( u \). The Scharfetter-Gummel expression for the one-dimensional electron current \( I_n \) on an interval \( [x_{i-1}, x_i] \) with \( x_i - x_{i-1} = h_i \) is expressed in terms of the Bernoulli function \( B(x) = x/\{\exp(x) - 1\} \) as in

\[
I_{n,j} = -\frac{1}{h_j} \mu_n(u_x) k_B T [B(u_{j+1} - u_j) n_{j+1} - B(u_j - u_{j+1}) n_j]. \tag{1.2}
\]

As observed in [4] and elsewhere, the SG approximation coincides with a finite element
method in which the Slotboom variable \( \nu(x) = \exp[-u(x)]n(x) \) is expanded in terms of nodal, \( u(x) \)-dependent basis-functions

\[
\xi_j(x) = \begin{cases} 
\int_{x_{j-1}}^{x_j} \mu_n \exp[-u(t)] \, dt / \int_{x_{j-1}}^{x_j} \mu_n \exp[-u(t)] \, dt & \text{if } x \in [x_{j-1}, x_j], \\
\int_{x_j}^{x_{j+1}} \mu_n \exp[-u(t)] \, dt / \int_{x_j}^{x_{j+1}} \mu_n \exp[-u(t)] \, dt & \text{if } x \in [x_j, x_{j+1}], \\
0 & \text{elsewhere.}
\end{cases}
\] (1.3)

Let the vector with components \( n_j \) solve the SG discretization of (1.1). Then, the function

\[
n(x) = \sum_j n_j \exp[u(x) - u_j] \xi_j(x)
\] (1.4)
also solves equation (1.1). Hence, solution of the SG discretization of (1.1) for a piecewise linear potential \( U_u(x) \) yields the exact solution to (1.1). In terms of quasi-Fermi levels \( n(x) = \exp[u(x) - \nu(x)] \), \( p(x) = \exp[w(x) - u(x)] \).

2. Box Method Discretization

The prevalence in two and three-dimensional computational codes of the SG box-method, see e.g. [2, 10, 11, 3], is possibly due to the consistent handling of current conservation. Discretization by the box-method of the Slotboom variable equations

\[
- \nabla \cdot [\mu_n \exp(u) \nabla \nu] = 0, \tag{2.1}
\]
\[
- \nabla \cdot [\mu_p \exp(-u) \nabla \omega] = 0, \tag{2.2}
\]
is defined on a mesh of boxes \( B_k \) dual to the vertices \( x_k \) in a mesh of simplexes. Box-faces \( f_{jk} \) are planar. Even though the current is not equal to a constant in higher dimensions, in the Scharfetter-Gummel box-method fluxes through box-faces \( f_{ij} \) are approximated analogously to (1.2), yielding for the electron density vector \( n \)

\[
\sum_{x_j \text{ adjacent } x_i} \frac{f_{ij}}{e_{ij}} \mu_n [B(u_j - u_i)n_j - B(u_i - u_j)n_i] = 0. \tag{2.3}
\]
The nodal values of the Slotboom variable \( \nu \) are then given by \( \nu_j = n_j \exp[-u_j] \).

Both in the box-method, and in Galerkin's equations for a piecewise linear approximation \( V_h \), one component \( \nu_j \) of the solution vector \( \nu \) corresponds to every vertex \( x_j \) of a simplicial mesh. In the sequel, the notation \( V_\nu = \sum_j \nu_j \phi_j(x) \) will be employed for the piecewise linear interpolant of the vector of nodal values \( \nu_j \) at the vertices \( x_j \). With a vector \( v \) will also be associated the nodal piecewise polynomial function \( V_{pp,v} = \sum_j v_j \psi_j(x) \). Finally, define piecewise constant box test-functions \( \psi_{B_k}(x) \) that are equal to 1 in the interior of box \( B_k \) and 0 elsewhere.

The analysis of the box-method is simplified significantly by reducing (2.1) on each element \( S_r \) in the mesh to the Laplacean by replacing the coefficient \( \mu_n \exp(u) \) by a function that assumes elemental average values \( \mu_n \exp(u) \). The boundary conditions are set piecewise linear. In [6] mild conditions are presented under which this simplified BVP approximates the original BVP (2.1) to sufficient accuracy.

Finite element analysis of the box-method commences with the observation (for two dimensions in Bank and Rose in [1], for N dimensions in Lemma 2.3 of [6]) that for box-faces \( f_{jk} \) perpendicular to edges \( e_{jk} \) in the finite element mesh the perpendicular biseector box-method Laplacean Element Matrix (LES) is identical to the Petrov-Galerkin LES for piecewise linear functions with box test-functions \( \psi_{B_k} \).
The components of this perpendicular bisector box-method LES, $E_{B,S_r}$, are defined in terms of box-faces $f_{jk}^{(S_r)}$, normal to edges $e_{jk}$ and delimited by the faces $F_k$ of element $S_r$, by

$$E_{B,S_r,jk} = \langle |f_{jk}^{(S_r)}|/|e_{jk}| \rangle. \quad (2.4)$$

The components of the corresponding global Petrov-Galerkin stress-matrix are defined

$$A_{PG,ij} = \sum_{S_r \text{ adjacent } e_{ij}} \bar{\mu}_n \exp(u)_{S_r} E_{B,S_r,ij}. \quad (2.5)$$

The analysis in [6] relies on piecewise linearity of the approximant in a generalization of the two-dimensional results of Bank and Rose in [1] (see also [5]). By the results in Lemmas 2.1 and 2.2 of [6] the Petrov-Galerkin LES $E_{PG,S_r}$ for a linear approximation and test-functions $\psi_i$ that assume on element faces $F_k$ the average values ($\int_{F_k} \psi_i dx / \int_{F_k} dx = p_{ik}$) can be expressed in terms of the piecewise linear $E_{pl,S_r}$ and the differences $q_{ik} = p_{ik} - (1/N)$ of the face-averages $p_{ik}$ of the test-functions $\psi_i$ from the piecewise linear averages $(\phi_i)_{F_k} = (1/N)$ as in

$$E_{PG,S_r} = [I - N Q_{S_r}] E_{pl,S_r}. \quad (2.6)$$

Here the matrix $Q_{S_r}$ is defined by $Q_{S_r,ii} = q_{ii}$, the matrix of the deviations from the mean of the face-averages $p_{ii}$. The equivalence $E_{B,S_r} = E_{PG,\bar{v}_{B,S_r}}$ and equation (2.6) imply immediately (see Corollary 2.4 of [6]) that if boxes $B_i$ partition equally all faces $F_k$ of an $N$ dimensional simplex $S_r$, then $E_{B,S_r} = E_{pl,S_r}$. This observation combined with equation (2.6) implies that in three dimensions $E_{B,S_r} = E_{pl,S_r}$ and $Q_{S_r} \equiv 0$ if and only if $S_r$ is a regular tetrahedron.

The error analysis in [6] admits this difference in stress matrices subject to the following equivalences of energies defined by the piecewise linear Galerkin LES $E_{pl,S_r} = a_s.(\phi_i, \phi_j)$ and the box-method LES $E_{B,S_r}$ defined in (2.4) (here $\int_S \nabla f \cdot \nabla g dx = a_s.(f,g)$ and $\int_S D_s(u) \equiv a_s.(V_{pp,u},V_{pp,u})$).

$$c_s u^t E_{pl,S_r} u - u^t E_{B,S_r} u \leq C_{DS} u^t E_{B,S_r} u. \quad (2.7)$$

Piecewise polynomial test-functions $\psi_{H,j}(x)$ that assume appropriate face averages are substituted for the $\psi_{B,j}$. Inequality (2.8), below, reflects a special case of Theorem 3.1 in [6].

If $c \leq c_s$, and $C_D \geq C_{DS}$, in (2.7) on all elements $S_r$. If $\hat{v}$ solves the simplified version of (2.1), and the vector $v$ solves the approximate box-method (2.5), then $V_v$ realizes a piecewise linear order of accuracy because for all piecewise linear $V_w$ that satisfy identical boundary conditions as $V_v$

$$\sqrt{\int_G \mu_n \exp(u)|\nabla(V_v - \hat{v})|^2 dx} \leq [1 + \sqrt{C_D/c}] \sqrt{\int_G \mu_n \exp(u)|\nabla(V_w - \hat{v})|^2 dx}. \quad (2.8)$$

Approximation results from [6] and inequality (2.8) yield for the function $n_v(x) = \sum_j n_j \exp(u(x) - u_j) \phi_{pl,j}(x)$, defined in terms of a piecewise linear Slotboom variable $\nu_{pl}(x)$ and the vector $n$ solving the box-method (2.3), a bound similar to (2.8).

3. Equation Coupling and The Scharfetter-Gummel Box-method

The exact current conservation can be employed to validate for the SG box-method discretization an analogy of a simplified coupling limitation for the drift-diffusion
equation for electrons from [8]. The mobilities \( \mu_n \) and \( \mu_p \) are assumed to be functions of the location \( x \) only. In terms of quasi-Fermi levels levels the system (2.1–2.2) is written

\[
-\nabla \cdot [\mu_n \exp(u - v)\nabla v] = 0, \\
-\nabla \cdot [\mu_p \exp(w - u)\nabla w] = 0.
\]

For \( i = 1, 2 \), let \( u_i \) be bounded with square-integrable derivative, let \( v_i \) be the solution to (3.1). We introduce the averages \( \bar{u} = \frac{1}{2}(u_1 + u_2), \bar{v} = \frac{1}{2}(v_1 + v_2) \), and the differences \( \Delta u = u_2 - u_1, \Delta v = v_2 - v_1 \). Then for (3.1)

\[
\sqrt{\int_G \mu_n \exp(\bar{u} - \bar{v})|\nabla \Delta v|^2 dx} \leq \sqrt{\int_G \mu_n \exp(\bar{u} - \bar{v})|\nabla \Delta u|^2 dx}
\]

The SG box-method discretization of the drift-diffusion equations balances the sum of one-dimensional constant-current expressions for the fluxes through box-faces. The following inequality is valid for quasi-Fermi levels on edges \( e_{jk} \), corresponding to the optimized expansion of the Slotboom variables (1.3).

For \( i = 1, 2 \), and the vectors \( u_i \), let \( n_i \) solve the SG box-method equations (2.3). On each edge \( e_{ij} \) in the mesh let \( u \) be the linear interpolant of the nodal values \( u_i \) and \( u_j \) at the vertices \( x_i \) and \( x_j \), and let \( v \) be the univariate quasi-Fermi level \( v(t) \) corresponding to the conduction-electron density function (1.4). Then

\[
\sqrt{\sum_{e_{jk}} \int_{e_{jk}} \exp(\bar{u} - \bar{v})|\Delta u_i|^2 dt} \geq \sqrt{\sum_{e_{jk}} \int_{e_{jk}} \exp(\bar{u} - \bar{v})|\Delta v_i|^2 dt}.
\]

References


