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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 ϕ 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

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

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 $U_{\mathbf{u}}(x)$ with nodal values u_j at nodes x_j can be associated a vector $\mathbf{u}$. 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 Bernouilli 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

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

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

$$n(x) = \sum_j n_j \exp[u(x) - u_j]\xi_j(x) \quad (1.4)$$

also solves equation (1.1). Hence, solution of the SG discretization of (1.1) for a piecewise linear potential $U_{\mathbf{u}}(x)$ yields the exact solution to (1.1). In terms of quasi-Fermi levels $n(x) = \exp[u(x) - v(x)]$, $p(x) = \exp[w(x) - u(x)]$.

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

$$-\nabla\cdot[\mu_n \exp(u)\nabla\nu] = 0, \quad (2.1)$$
$$-\nabla\cdot[\mu_p \exp(-u)\nabla\omega] = 0, \quad (2.2)$$

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 $\mathbf{n}$

$$\sum_{x_j \text{ adjacent } x_i} \frac{|f_{ij}|}{|e_{ij}|}\mu_n[B(u_j - u_i)n_j - B(u_i - u_j)n_i] = 0. \quad (2.3)$$

The nodal values of the Slotboom variable ν 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 ν_j of the solution vector ν 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 ν_j at the vertices x_j. With a vector $\mathbf{v}$ will also be associated the nodal piecewise polynomial function $V_{pp,\mathbf{v}} = \sum_j v_j\psi_j(x)$. 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 $\overline{\mu_n \exp(u)}$. 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 bisector box-method Laplacean Element Matrix (LES) is identical to the Petrov-Galerkin LES for piecewise linear functions with box test-functions ψ_{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

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

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

$$A_{PG,ij} \equiv \sum_{S_r\ adjacent\ e_{ij}} \overline{\mu_n \exp(u)}_{S_r} E_{B,S_r,ij}. \tag{2.5}$$

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 ψ_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 ψ_i from the piecewise linear averages $\langle \phi_i \rangle_{F_k} = (1/N)$ as in

$$E_{PG,S_r} = [I - NQ_{S_r}]E_{pl,S_r}. \tag{2.6}$$

Here the matrix Q_{S_r} is defined by $Q_{S_r,il} = q_{il}$, the matrix of the deviations from the mean of the face-averages p_{il}. The equivalence $E_{B,S_r} = E_{PG,\psi_B,S_r}$ and equation (2.6) imply immediately (see Corollary 2.4 of [6]) that if boxes B_j 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 $E_{pl,S_r} = a_{S_r}(\phi_i, \phi_j)$ and the box-method LES E_{B,S_r} defined in (2.4) (here $\int_{S_r} \nabla f \cdot \nabla g dx = a_{S_r}(f,g)$ and $\mathbf{u}^t D_{S_r} \mathbf{u} \equiv a_{S_r}(V_{pp,\mathbf{u}}, V_{pp,\mathbf{u}})$.)

$$c_{S_r} \mathbf{u}^t E_{pl,S_r} \mathbf{u} \le \mathbf{u}^t E_{B,S_r} \mathbf{u}, \quad \mathbf{u}^t D_{S_r} \mathbf{u} \le C_{D,S_r} \mathbf{u}^t E_{B,S_r} \mathbf{u}. \tag{2.7}$$

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 $c \le c_{S_r}$, and $C_D \ge C_{D,S_r}$ in (2.7) on all elements S_r. If $\tilde{\nu}$ solves the simplified version of (2.1), and the vector $\mathbf{v}$ solves the approximate box-method (2.5), then $V_\mathbf{v}$ realizes a piecewise linear order of accuracy because for all piecewise linear $V_\mathbf{w}$ that satisfy identical boundary conditions as V_ν

$$\sqrt{\int_G \overline{\mu_n \exp(u)} |\nabla(V_\mathbf{v} - \tilde{\nu})|^2 dx} \le [1 + \sqrt{\frac{C_D}{c}}] \sqrt{\int_G \overline{\mu_n \exp(u)} |\nabla(V_\mathbf{w} - \tilde{\nu})|^2 dx}. \tag{2.8}$$

Approximation results from [6] and inequality (2.8) yield for the function $n_\nu(x) = \sum_j n_j \exp[u(x) - u_j]\phi_{pl,j}(x)$, defined in terms of a piecewise linear Slotboom variable $\nu_{pl}(x)$ and the vector $\mathbf{n}$ 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 μ_n and μ_p are assumed to be functions of the location x only. In terms of quasi-Fermi levels the system (2.1–2.2) is written

$$-\nabla\cdot[\mu_n \exp(u-v)\nabla v] = 0, \quad (3.1)$$
$$-\nabla\cdot[\mu_p \exp(w-u)\nabla w] = 0. \quad (3.2)$$

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 $\tilde{u}=\frac{1}{2}(u_1+u_2)$, $\tilde{v}=\frac{1}{2}(v_1+v_2)$, and the differences $\Delta u = u_2-u_1$, $\Delta v = v_2 - v_1$. Then for (3.1)

$$\sqrt{\int_G \mu_n \exp(\tilde{u}-\tilde{v})|\nabla\Delta v|^2 dx} \leq \sqrt{\int_G \mu_n \exp(\tilde{u}-\tilde{v})|\nabla\Delta u|^2 dx} \quad (3.3)$$

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 $\mathbf{u}_i$, let $\mathbf{n}_i$ 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

$$\sqrt{\sum_{e_{jk}} \int_{e_{jk}} \exp[\tilde{u}-\tilde{v}]|\Delta u_t|^2 dt} \geq \sqrt{\sum_{e_{jk}} \int_{e_{jk}} \exp[\tilde{u}-\tilde{v}]|\Delta v_t|^2 dt}. \quad (3.4)$$

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