An interpretation of the Scharfetter-Gummel finite difference scheme

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Abstract: We give an interpretation of the Scharfetter-Gummel (SG) scheme in the theory of semiconductor devices. The key fact is that the SG scheme is based on a harmonic relation between the Green function and the Green matrix for a two-point boundary value problem. An a consequence of our interpretation, we obtain error estimates in L^r, $r \in [2, \infty]$, where the coefficient functions may be discontinuous.

Key words: Finite difference method; finite element method; Scharfetter-Gummel scheme; singular perturbation problem.

1. Introduction. The purpose of this short note is to give an interpretation of the Scharfetter-Gummel (SG) scheme, which is widely used as an effective numerical method in the theory of semiconductor devices. The SG scheme is a special finite difference method (FDM) and a few different interpretations are known. Originally, in [6], D. L. Scharfetter and H. K. Gummel applied the box method (the finite volume method) to obtain the SG scheme. In [3], J. W. Jerome derived the SG scheme from a variational principle by taking generalized splines as trial functions. On the other hand, S. Odanaka *et al.* [5] reported that the SG scheme might be regarded as a kind of upwinding. Our approach is completely different from these previous works. The key point is a harmonic relation between the Green function and the Green matrix for a two-point boundary value problem (BVP), which are investigated in detail by T. Yamamoto and his colleagues. As a consequence of our interpretation, we shall give error estimates of the SG scheme in the L^r norm, $r \in [2, \infty]$, where the coefficient functions may be discontinuous.

As a model problem, we consider the following BVP for $u = u(x)$ defined on the interval $I = (0, 1)$:

$$(1) \qquad -\left(e^{-\psi}u'\right)' = f \ (x \in I), \quad u|_{x=0,1} = 0,$$

where $'$ denotes the differentiation in x, and $\psi = \psi(x)$, $f = f(x)$ are given functions. In drift-diffusion system in the theory of semiconductor devices, $ue^{-\psi}$ represents the density of electrons, ψ is the electric potential, and f the recombination and generation of electrons. We are interested in the case where $\psi'(x)$ is very large. However, in that case, (1) becomes a singular perturbation problem. Hence, it is difficult to capture $u(x)$ sharply by using the standard numerical methods on fixed meshes. To overcome this difficulty, D. L. Scharfetter and H. K. Gummel proposed the following special FDM ([6]). Let $\{x_i\}_{i=0}^{N+1}$ be a set of grid points such that $0 = x_0 < x_1 < x_2 < \cdots < x_N < x_{N+1} = 1$ with a positive integer N. We set $h_i = x_i - x_{i-1}$ and $H_i = (h_i + h_{i+1})/2$. Then, find $\{\hat{u}_i\}_{i=1}^{N}$ satisfying

$$(2) \qquad \begin{cases} -\dfrac{1}{H_i}\left(\dfrac{\hat{u}_{i+1} - \hat{u}_i}{b_{i+1}} - \dfrac{\hat{u}_i - \hat{u}_{i-1}}{b_i}\right) = f(x_i) \\ \qquad\qquad\qquad\qquad\qquad\qquad (1 \le i \le N) \\ \hat{u}_0 = \hat{u}_{N+1} = 0. \end{cases}$$

Here, b_i is defined as

$$(3) \qquad b_i = \begin{cases} h_i \dfrac{e^{\psi_i} - e^{\psi_{i-1}}}{\psi_i - \psi_{i-1}} & (\psi_i \ne \psi_{i-1}) \\ h_i e^{\psi_i} & (\psi_i = \psi_{i-1}), \end{cases}$$

where $\psi_i = \psi(x_i)$. We call (2) the SG scheme.

For comparison, we here recall the Shortley-Weller (SW) scheme to (1), which is one of the standard FDM. That is, we find $\{u_i\}_{i=1}^{N}$ satisfying

$$(4) \qquad \begin{cases} -\dfrac{1}{H_i}\left(\dfrac{u_{i+1} - u_i}{h_{i+1}e^{\psi_{i+1/2}}} - \dfrac{u_i - u_{i-1}}{h_i e^{\psi_{i-1/2}}}\right) = f(x_i) \\ \qquad\qquad\qquad\qquad\qquad\qquad (1 \le i \le N) \\ u_0 = u_{N+1} = 0, \end{cases}$$

where $\psi_{i-1/2} = \psi((x_i + x_{i-1})/2)$.

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One may feel that the form of the coefficients (3) is somewhat strange. However, it is really reasonable in a certain sense, especially when ψ is not so regular. Below we shall see this fact.

The organization of this note is as follows: In §2 and §3, we review the standard FEM for a general BVP and its error estimates. In particular, we pay a special attention to the precise error analysis by T. Tsuchiya *et al.* [8]. Then, in §4, we introduce a non-standard FEM (the IG scheme) and state the error estimate. The validity of the IG scheme is also confirmed by some numerical examples. Our interpretation of the SG scheme is described in §5. Finally, we conclude this note by giving some remarks in §6.

In what follows, we use standard function spaces $L^r = L^r(I)$, $W^{s,r} = W^{s,r}(I)$ and $H^s = W^{s,2}$, where $s > 0$ and $r \in [1, \infty]$. As usual, $W_0^{1,r} = \{v \in W^{1,r} |\ v(0) = v(1) = 0\}$ and $H_0^1 = W_0^{1,2}$. Finally, $\mathrm{TD}_N[c_i, d_i, e_i]$ denotes a tridiagonal matrix of the form:

$$\begin{bmatrix} d_1 & e_1 & 0 & & \\ & \ddots & \ddots & & \\ & c_i & d_i & e_i & \\ & & \ddots & \ddots & \\ & & & c_N & d_N \end{bmatrix}.$$

2. Standard FEM. In order to discuss in a general context, we consider a two-point BVP:

$$-(pu')' = f \ (x \in I), \quad u|_{x=0,1} = 0 \tag{5}$$

where $p \in L^\infty$ and $f \in L^2$ are given functions. We assume that there is $p_0 > 0$ such that $p(x) \geq p_0$ a.e. $x \in I$, unless otherwise stated explicitly. By a solution of (5), we mean $u \in H_0^1$ satisfying

$$\int_I pu'v' \ \mathrm{d}x = \int_I fv \ \mathrm{d}x \quad \forall v \in H_0^1. \tag{6}$$

As the discretization parameter, we take $h = \max\{h_1, h_2, \ldots, h_{N+1}\}$. We define V_h by

$$V_h = \left\{ v_h = \sum_{i=1}^N c_i \varphi_i(x) \,\middle|\, \{c_i\}_{i=1}^N \subset \mathbf{R} \right\} \subset H_0^1,$$

where

$$\varphi_i(x) = \begin{cases} h_i^{-1}(x - x_{i-1}) & (x \in I_i), \\ h_{i+1}^{-1}(x_{i+1} - x) & (x \in I_{i+1}), \\ 0 & (\text{otherwise}) \end{cases}$$

with $I_i = (x_{i-1}, x_i)$. Then we consider a FEM for (5): Find $u_h \in V_h$ satisfying

$$\int_I pu_h'v_h' \ \mathrm{d}x = \int_I fv_h \ \mathrm{d}x \quad \forall v_h \in V_h. \tag{7}$$

Setting

$$u_h(x) = \sum_{i=1}^N u_i \varphi_i(x), \quad \{u_i\}_{i=1}^N \subset \mathbf{R},$$

we may rewrite (7) as

$$\begin{cases} -[a_{i+1}(u_{i+1} - u_i) - a_i(u_i - u_{i-1})] = f_i \\ \qquad\qquad\qquad\qquad\qquad\qquad (1 \leq i \leq N) \\ u_0 = u_{N+1} = 0, \end{cases}$$

where

$$a_i = \frac{1}{h_i^2} \int_{x_{i-1}}^{x_i} p \ \mathrm{d}x, \quad f_i = \int_I f\varphi_i \ \mathrm{d}x.$$

The corresponding matrix representation is as follows:

$$\mathsf{A}\mathbf{u} = \mathbf{f},$$

where $\mathbf{f} = [f_i] \in \mathbf{R}^N$, $\mathbf{u} = [u_i] \in \mathbf{R}^N$, and $\mathsf{A} = \mathrm{TD}_N[-a_i,\ a_i + a_{i+1},\ -a_{i+1}]$.

Remark 1. If we let $p(x) = e^{-\psi(x)}$ and evaluate a_i and f_i by the midpoint and trapezoid rules, respectively, we obtain the SW scheme (4).

3. Error analysis for FEM. Error analysis for (7) is well developed. In general, we have $\|u - u_h\|_{H^1} \to 0$ as $h \downarrow 0$. Moreover, if $u \in H^{1+\varepsilon}$ with some $\varepsilon \in (0, 1]$, we have (cf: [2])

$$\|u - u_h\|_{H^1} \leq Ch^\varepsilon \|u\|_{H^{1+\varepsilon}}$$

with a constant $C > 0$. However, if $u \notin H^{1+\varepsilon}$ for any $\varepsilon > 0$, the convergence may be arbitrarily bad. Actually, "negative" examples were pointed out by [1] and [7]; The speed of convergence of finite element approximations could be very slow in that case. On the other hand, a "positive" result was established by T. Tsuchiya *et al.* [8]. To review it, we make the following assumptions:

$$\begin{cases} I \text{ is divided into disjoint} \\ \text{sub-intervals } \{J_k\}_{k=1}^M : \overline{I} = \bigcup_{k=1}^M \overline{J_k}; \end{cases} \tag{8}$$

$$\{\partial J_k\}_{k=1}^M \subset \{x_i\}_{i=0}^{N+1}; \tag{9}$$

$$\exists \alpha, \beta > 0 : \ \alpha \leq |p(x)| \leq \beta \text{ a.e. } I; \tag{10}$$

$$\gamma \equiv \left| \int_I p(s)^{-1} \mathrm{d}s \right| \neq 0; \tag{11}$$

(12) $\exists q \in [1,\infty] :\ p \in W^{2,q}(J_k) \quad (k = 1,\dots,M).$

Moreover, let $f \in L^r$ with some $r \in [2,\infty]$. Under these assumptions, there exists a solution $u \in H_0^1$ of (5). Furthermore, we have $u \in W_0^{1,r}$ and

$$\|u_h - u\|_{L^r} + h\|u_h' - u'\|_{L^r} \le Ch^2\|f\|_{L^r} + C'h^{2-\frac{1}{q}}\|f\|_{L^1}$$

with positive constants C and C'. It should be noticed that *no* regularity assumptions of the form $u \in W^{1+\varepsilon,r}$ with $\varepsilon > 0$ are required and that $p(x)$ may be discontinuous. The proof is based on the decomposition of the error:

$$u(x) - u_h(x) = E_I(x) + E_A(x),$$

where

$$\begin{aligned} E_I(x) &= \int_I [G(x,y) - \Pi_h G(x,y)]\ f(y)\ \mathrm{d}y, \\ E_A(x) &= \sum_{i=1}^N e_i(f)\varphi_i(x), \\ \Pi_h G(x,y) &= \sum_{i,j=1}^N G(x_i,x_j)\varphi_i(x)\varphi_j(y); \\ e_i(f) &= \int_I f(y)\sum_{j=1}^N [G(x_i,x_j) - g_{ij}]\ \mathrm{d}y; \\ \mathsf{G} &= \mathsf{A}^{-1} = [g_{ij}]; \\ G(x,y) &= \begin{cases} \left(\displaystyle\int_I \frac{\mathrm{d}s}{p(s)}\right)^{-1} \int_0^x \frac{\mathrm{d}s}{p(s)} \cdot \int_y^1 \frac{\mathrm{d}s}{p(s)} \\ \qquad\qquad (0 \le x \le y \le 1) \\ \left(\displaystyle\int_I \frac{\mathrm{d}s}{p(s)}\right)^{-1} \int_0^y \frac{\mathrm{d}s}{p(s)} \cdot \int_x^1 \frac{\mathrm{d}s}{p(s)} \\ \qquad\qquad (0 \le y \le x \le 1). \end{cases} \end{aligned}$$

($G(x,y)$ is the Green function associated with (5)). Then, we estimate the *interpolation error* E_I and the *approximation error* E_A separately. It is easy to see that the contribution of E_A to the error is larger than that of E_I.

4. A nonstandard FEM: the IG scheme. From the observation above, we consider the following *nonstandard FEM* instead of (7): Find $\hat{\mathbf{u}} = [\hat{u}_i] \in \mathbf{R}^N$ satisfying

$$(13)\quad \begin{cases} -[\hat{a}_{i+1}(\hat{u}_{i+1} - \hat{u}_i) - \hat{a}_i(\hat{u}_i - \hat{u}_{i-1})] = f_i \\ \qquad\qquad (1 \le i \le N) \\ \hat{u}_0 = \hat{u}_{N+1} = 0, \end{cases}$$

or, equivalently,

$$\hat{\mathsf{A}}\hat{\mathbf{u}} = \mathbf{f},$$

where $\hat{\mathsf{A}} = \mathrm{TD}_N[-\hat{a}_i, \hat{a}_i + \hat{a}_{i+1}, -\hat{a}_{i+1}]$ and

$$\hat{a}_i = \left(\int_{x_{i-1}}^{x_i} \frac{\mathrm{d}x}{p(x)}\right)^{-1}.$$

We shall call (13) the *IG scheme*. Indeed, $\hat{\mathsf{A}}$ is closely related with the *inverse* of the *Green matrix*. Thus, we have

$$(14)\qquad \hat{\mathsf{A}}^{-1} = [G(x_i,x_j)]$$

which is a direct consequence of Yamamoto's inversion formula ([9]). Such a harmonic relation between the Green function and the Green matrix hold true for more general two-point BVPs (cf: [10]). An advantage of (14) is that we have the expression

$$u(x) - \hat{u}_h(x) = E_I(x),$$

where

$$\hat{u}_h(x) = \sum_{i=1}^N \hat{u}_i\varphi_i(x).$$

Thus, the approximation error $\hat{E}_A$ does not appear, and the interpolation error E_I is exactly the same as that of the standard one. Moreover, if we trace [8] carefully, we obtain the following

Theorem 1. *Let $f \in L^r$ with some $r \in [2,\infty]$. Suppose that* (8)–(11) *hold. Moreover, assume that*

$$\exists q \in [1,\infty] :\ p \in W^{1,q}(J_k)\ (j = 1,\dots,M)$$

instead of (12). *Then, for solutions u and $\hat{u}_h$ of* (5) *and of* (13), *we have*

$$\|\hat{u}_h - u\|_{L^r} + h\|\hat{u}_h' - u'\|_{L^r} \le C_1h^2\|f\|_{L^r} + C_2h^{2-\frac{1}{q}}\|f\|_{L^1},$$

where

$$C_1 = \frac{1}{\alpha}, \quad C_2 = \frac{2\gamma}{\alpha^3}\max_{1\le k\le M}\|p'\|_{L^q(J_k)}.$$

From this theorem, we may expect that the IG scheme works well even if p is not so regular. Actually, the efficiency of the IG scheme could be observed by numerical experiments (see Fig. 1 and 2). We use the uniform mesh ($h_i = 1/(N+1)$), and take $f \equiv 1$ and

$$p(x) = \exp(-\psi(x)),$$

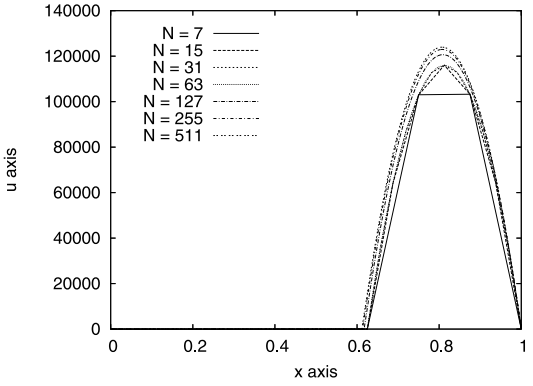

Fig. 1. Solutions $u_h(x)$ of (7).

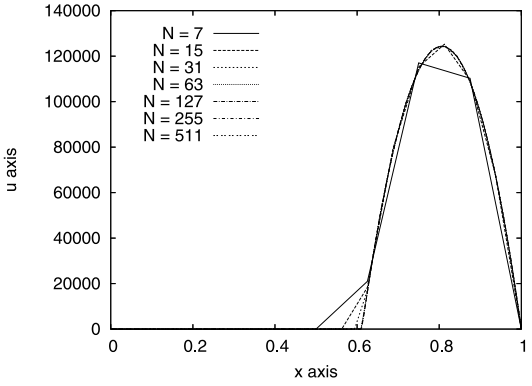

Fig. 2. Solutions $\hat{u}_h(x)$ of (13).

$$\psi(x) = L\left(\tan^{-1}\frac{x-a}{\varepsilon} + \frac{\pi}{2}\right),$$

where $L = 5$, $\varepsilon = 0.0001$, and $a = 0.61$. Numerical quadrature is evaluated by the Clenshaw-Curtis formula. We may observe that the IG scheme can capture $u(x)$ with a small $N \approx h^{-1}$, even if $p'(x)$ is very large.

5. A derivation of the SG scheme. It is divided into two steps.

Step 1 (finite dimensional approximation). Setting $p(x) = e^{-\psi(x)}$, we apply the IG scheme to (1). Then, we have (13) with

$$\hat{a}_i^{-1} = \int_{x_{i-1}}^{x_i} \frac{\mathrm{d}x}{p(x)} = \int_{x_{i-1}}^{x_i} e^{\psi(x)}\mathrm{d}x.$$

Step 2 (numerical quadratures). We take the linear interpolation

$$\psi_h(x) = \sum_{i=1}^{N} \psi_i \varphi_i(x)$$

as an approximation of $\psi(x)$. Then, if $\psi_{i-1} \neq \psi_i$,

$$\begin{aligned}\hat{a}_i^{-1} &\approx \int_{x_{i-1}}^{x_i} e^{\psi_h(x)}\mathrm{d}x \\ &= \frac{h_i}{\psi_i - \psi_{i-1}} \int_{x_{i-1}}^{x_i} \frac{\mathrm{d}}{\mathrm{d}x} e^{\psi_h(x)}\mathrm{d}x = b_i.\end{aligned}$$

Finally, we employ the trapezoid rule to evaluate f_i and obtain $f_i \approx f(x_i)H_i$.

By summarizing these results, we derive the SG scheme (2) as an approximation of (1).

Remark 2. Here, ψ is assumed to be a given function. In the original drift-diffusion problem, however, ψ is also the unknown function to be solved. Thus, we can get the value of ψ only at the nodal points. Hence, the choice $\psi \approx \psi_h$ is natural.

6. Conclusion. As is seen in the previous section, our derivation of the SG shceme (2) consists of two steps:

1. (1) is approximated by the IG scheme (13);
2. The coefficients are evaluted by simple quadrature formulas.

On the other hand, the standard FDMs such as the SW scheme (4) could be interpretated as follows:

1. (1) is approximated by the standard FEM (7) with $p(x) = e^{-\psi(x)}$;
2. The coefficients are evaluted by simple quadrature formulas (see Remark 1).

Moreover, we might say that the FEM and SW scheme are based on the weak formulation (6), whereas the IG and SG schemes are based on the formula

$$u(x) = \int_I G(x,y)f(y)\ \mathrm{d}y.$$

Such a difference between the IG scheme and FEM is of interest in designing numerical methods for a general BVP of elliptic type.

Finally, we present error estimates for the SG scheme. For the sake of simplicity, we consider a modified SG scheme: Find $\{\hat{u}_i\}_{i=1}^N$ satisfying

$$\text{(15)} \qquad \begin{cases} -\left(\dfrac{\hat{u}_{i+1}-\hat{u}_i}{b_{i+1}} - \dfrac{\hat{u}_i - \hat{u}_{i-1}}{b_i}\right) = f_i \\ \qquad\qquad\qquad\qquad (1 \le i \le N) \\ \hat{u}_0 = \hat{u}_{N+1} = 0. \end{cases}$$

Thus, a numerical quadrature of f_i is not taken into account. We have already derived the error estimate of the IG scheme. Therefore, it remains to estimate the error of the numerical quadrature.

Theorem 2. *Let $f \in L^r$ with some $r \in [2, \infty]$. Suppose that* (8) *and* (9) *hold. Moreover, assume that*

$$\exists \alpha, \beta \in (-\infty, \infty) : \ \alpha \le \psi(x) \le \beta \ \text{a.e. } I;$$
$$\exists q \in [1, \infty] : \ \psi \in W^{2,q}(J_k) \quad (k = 1, \dots, M).$$

Then, for solutions u and u_h of (1) *and of* (15), *we have*

$$\|u - \hat{u}_h\|_{L^r} + h\|u' - \hat{u}_h'\|_{L^r} \le K_1 h^2 \|f\|_{L^r} + [K_2 + (1+h)K_3] h^{2-\frac{1}{q}} \|f\|_{L^1},$$

where

$$\hat{u}(x) = \sum_{i=1}^{N} \hat{u}_i \varphi_i(x);$$
$$K_1 = e^{\beta};$$
$$K_2 = 2e^{4\beta^3 - \alpha} \max_{1 \le k \le M} \|\psi'\|_{L^q(J_k)};$$
$$K_3 = e^{2\beta - \alpha}(e^{\beta - \alpha} + 2) \max_{1 \le k \le M} \|\psi''\|_{L^q(J_k)}.$$

This theorem is actually an extension of previous error estimates including [4] where the uniform convergence was proved under some regularity assumptions on u. We again emphasize that no regularity assumptions of the form $u \in W^{1+\varepsilon, r}$, $\varepsilon > 0$, are assumed in Theorem 2. We skip the proof, since it can be done in essentially the same way as the method of [8].

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