

On the computation of semiconductor device current characteristics by finite difference methods

M. S. MOCK

Courant Institute of Mathematical Sciences, New York University and IBM Systems Product Division, East Fishkill Laboratory, Hopewell Junction, N.Y. 12533, U.S.A.

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SUMMARY

An analysis is presented of the error in numerical approximations to a system of elliptic equations describing the steady-state distribution of mobile carriers in a semiconductor device. Although this system has been extensively studied by finite difference methods, the accuracy of the numerical methods employed has not been previously established. Computation schemes are presented for which suitable error estimates are obtained, without assuming an unreasonably small mesh size. In addition, for the one-dimensional problem, the effect of the inexact solution of the discrete equations is estimated.

1. Introduction

In this paper we are concerned with the accuracy of numerical solutions of a system of non-linear elliptic equations describing steady-state carrier distributions in a semiconductor device. In an open bounded connected region $D \subset R^n$, we consider the system

$$\kappa \Delta \psi + N + \rho e^{-\psi} - \zeta e^{\psi} = 0, \quad (1.1)$$

$$\nabla \cdot (e^{\psi} \nabla \zeta) = 0, \quad (1.2)$$

$$\nabla \cdot (e^{-\psi} \nabla \rho) = 0, \quad (1.3)$$

for the three real scalar functions ψ, ζ, ρ of $x = (x_1, \dots, x_n)$. In (1.1) κ is a positive constant and N is a given smooth function of x , defined in D . We assume boundary conditions of the form

$$\zeta(x) = \rho(x) = 1, \quad \psi(x) \text{ specified}, \quad x \in \partial D_1, \quad (1.4a)$$

$$\zeta(x) = b, \quad \rho(x) = 1/b, \quad \psi(x) \text{ specified}, \quad x \in \partial D_2, \quad 0 < b < 1, \quad (1.4b)$$

$$v \cdot \nabla \zeta(x) = v \cdot \nabla \rho(x) = v \cdot \nabla \psi(x) = 0, \quad x \in \partial D_3, \quad (1.4c)$$

where the boundary ∂D is the union of the three segments $\partial D_1, \partial D_2, \partial D_3$, and where v is the outward unit vector normal to the boundary.

The variables in the system (1.1–1.3) admit the following physical interpretation [13]: $\psi, \zeta e^{\psi}, \rho e^{-\psi}$ are the electrostatic potential, electron density, and hole density, respectively; κ is the dielectric constant, N the ionized impurity concentration, and the quantities $e^{\psi} \nabla \zeta, e^{-\psi} \nabla \rho$ are proportional to the electron and hole current densities, respectively. In obtaining eqs. (1.1–1.3) we are assuming the applicability of Boltzmann statistics and constant carrier mobilities, and are neglecting recombination of mobile carriers. A system of units is adopted in which the Boltzmann voltage, the electronic charge, and the intrinsic carrier density have magnitude unity.

Numerous numerical investigations of systems of equations of this form have been reported [2, 4, 8, 9, 15, 16], based on finite difference approximations. Many of these investigations do not include computations of the current characteristics of the devices considered.

In this paper we derive estimates of the errors in such numerical approximations of the solution of the system (1.1–1.4), and in particular the errors in the computed values of the device currents, which are of particular physical interest.

Our method of analysis is a variation of the Rayleigh–Ritz–Galerkin method, as applied to

nonlinear boundary value problems [3]. We first obtain the desired error estimates in terms of norms of the right sides of (1.1–1.3), when the solution functions ψ, ζ, ρ , are replaced in these equations by sufficiently smooth approximating functions. Schemes for constructing suitable approximations from finite-dimensional function sets are then presented. This approach allows the order of magnitude of the errors to be estimated, even when the mesh is of moderate size. For the one-dimensional problem, a particularly simple finite-element scheme can be used, even if the discrete equations are not solved to high accuracy. The two-dimensional problem is much more complicated, and we simply show how suitable numerical schemes can be constructed.

The present results depend on an existence-uniqueness theory for the system (1.1–1.4) which appeared in [11].

We note that the system (1.1–1.4) is invariant under the interchange $\psi \rightarrow -\psi, N \rightarrow -N, \zeta \rightarrow \rho, \rho \rightarrow \zeta$. For this reason, it is sufficient to write out the analysis only for the electron-related terms, as the corresponding terms for holes are obtainable by the above interchange.

Except where noted otherwise, our estimates can be made computible and *a priori*. However, in this form the estimates are so crude as to be useless from a practical viewpoint. For this reason, we denote several multiplicative constants by C , with the understanding that such constants will be determined empirically as required.

2. Assumptions, definitions and notation

We denote by ψ, ζ, ρ , the exact solution functions satisfying (1.1–1.4), and by ψ', ζ', ρ' the computed numerical approximations, which are assumed to satisfy the boundary conditions (1.4). We set

$$r_1 = \kappa \Delta \psi' + N + \rho' e^{-\psi'} - \zeta' e^{\psi'} \tag{2.1a}$$

$$r_2 = \nabla \cdot (e^{\psi'} \nabla \zeta') \tag{2.1b}$$

$$r_3 = \nabla \cdot (e^{-\psi'} \nabla \rho') \tag{2.1c}$$

where the r_i are, in general, distributions of x in D . We also define the functions ζ', ρ' to be the solutions of

$$\nabla \cdot (e^{\psi'} \nabla \zeta') = 0, \quad x \in D, \tag{2.2a}$$

$$\nabla \cdot (e^{-\psi'} \nabla \rho') = 0, \quad x \in D, \tag{2.2b}$$

respectively, also satisfying the prescribed boundary conditions for ζ and ρ .

The electron current J is defined as

$$J = \int_{\partial D_1} e^{\psi} v \cdot \nabla \zeta \, dx = - \int_{\partial D_2} e^{\psi} v \cdot \nabla \zeta \, dx ; \tag{2.3}$$

we also set

$$J' = \int_{\partial D_1} e^{\psi'} v \cdot \nabla \zeta' \, dx = - \int_{\partial D_2} e^{\psi'} v \cdot \nabla \zeta' \, dx \tag{2.4}$$

and choose for the numerical approximation,

$$J' = (1-b)^{-1} \left(\int_{\partial D_1} e^{\psi'} v \cdot \nabla \zeta' \, dx + b \int_{\partial D_2} e^{\psi'} v \cdot \nabla \zeta' \, dx \right). \tag{2.5}$$

We use the following scalar product and norm notation:

$$(u, v) = \int_D u(x) v(x) \, dx, \quad \|u\| = \text{Sup}_{x \in D} |u(x)|,$$

$$\|u\|_p = \left(\int_D |u(x)|^p \, dx \right)^{1/p}; \quad \|u\|_{m,p} = \left(\int_D \sum_{|\alpha|=m} |\partial_x^\alpha u|^p \, dx \right)^{1/p}.$$

It is assumed that the boundary segments $\partial D_1, \partial D_2$ are sufficiently large that the integrals (2.3–2.5) are defined, and an estimate of the form

$$\|u\|_2 \leq C \|u\|_{1,2} \tag{2.6}$$

holds for all functions equal to zero on $\partial D_1 \cup \partial D_2$. From [11] we will infer the existence of uniform bounds on ψ, ψ' , and the estimate

$$\|\psi - \psi'\|_{1,2} \leq C \|\kappa \Delta \psi' + N + \dot{\rho} e^{-\psi} - \dot{\zeta} e^{\psi'}\|_2 \tag{2.7}$$

which is essential in the following analysis. We note that uniform bounds on ζ, ρ are immediate from (1.2, 1.3) and the maximum principle; in the following, we also assume ζ', ρ' uniformly bounded.

3. Basic analysis

In this section we relate norms of the errors in the approximating functions ψ', ζ', ρ' to the magnitude of the error terms r_1, r_2, r_3 in (2.1). Our results are contained in the following theorem.

Theorem 1. *Suppose the functions ψ', ζ', ρ' satisfy the boundary conditions (1.4), and in (2.1), $r_1, r_2, r_3 \in L_2(D)$. Then there exists a constant C depending on $D, \|N\|, b$, and the boundary data for ψ such that*

$$\begin{aligned} E &= \|\psi' - \psi\|_{1,2} + \|\zeta' - \zeta\|_{1,2} + \|\rho' - \rho\|_{1,2} + |J' - J| + |J'_* - J_*| \\ &\leq C (\|r_1\|_2 + \|r_2\|_2 + \|r_3\|_2) \end{aligned} \tag{3.1}$$

where J_* is the expression for the hole current, analogous to (2.3), and J'_* is the computed approximation to J_* , analogous to (2.5).

Proof: We write out the proof only for the electron terms, as noted above. From the triangle inequality, we have

$$\|\zeta' - \zeta\|_{1,2} \leq \|\zeta' - \dot{\zeta}\|_{1,2} + \|\dot{\zeta} - \zeta\|_{1,2} \tag{3.2}$$

$$|J' - J| \leq |J' - \dot{J}| + |\dot{J} - J|. \tag{3.3}$$

Integrating by parts, and using (2.1–2.5) we obtain

$$(e^{\psi'}, |\nabla \dot{\zeta}|^2) = (1 - b) \dot{J} \tag{3.4}$$

$$(e^{\psi}, |\nabla \zeta|^2) = (1 - b) J \tag{3.5}$$

$$(e^{\psi'}, |\nabla \zeta'|^2) = (1 - b) J' - (\zeta', r_2). \tag{3.6}$$

For some constant c , since ψ' is assumed uniformly bounded, we have also

$$\begin{aligned} c \|\zeta' - \dot{\zeta}\|_{1,2}^2 &\leq (e^{\psi'}, |\nabla (\zeta' - \dot{\zeta})|^2) \\ &= (e^{\psi'}, |\nabla \zeta'|^2) - (e^{\psi'}, |\nabla \dot{\zeta}|^2) \\ &= (\dot{\zeta} - \zeta', r_2) \end{aligned} \tag{3.7a}$$

$$= (1 - b)(J' - \dot{J}) - (\zeta', r_2) \tag{3.7b}$$

so that

$$(1 - b)(J' - \dot{J}) = (\dot{\zeta}, r_2) \quad \text{or} \quad |J' - \dot{J}| \leq C \|r_2\|_1. \tag{3.8}$$

Next suppose $J \geq \dot{J}$, then

$$\begin{aligned}
 (1-b)(J-j) &= (e^\psi, |\nabla\zeta|^2) - (e^{\psi'}, |\nabla\zeta|^2) \\
 &= (e^\psi, |\nabla\zeta|^2) - (e^\psi, |\nabla(\zeta - \zeta')|^2) - (e^{\psi'}, |\nabla\zeta|^2) \\
 &\leq (e^\psi - e^{\psi'}, |\nabla\zeta|^2) = (e^{\psi - \psi'} - 1, e^{\psi'} |\nabla\zeta|^2) \\
 &= -(\zeta' e^{\psi'}, \nabla\zeta \cdot \nabla(e^{\psi - \psi'} - 1)) \\
 &= -(\zeta' e^\psi, \nabla\zeta \cdot \nabla(\psi - \psi')) \\
 &\leq C \|\zeta'\|_{1,2} \|\psi - \psi'\|_{1,2} \leq C (J)^\frac{1}{2} \|\psi - \psi'\|_{1,2} \leq C \|\psi - \psi'\|_{1,2}
 \end{aligned} \tag{3.9}$$

since ψ' is assumed uniformly bounded, and therefore J is from (2.2a, 3.4).

Similarly for $J \leq \hat{J}$, we obtain

$$\begin{aligned}
 (1-b)(\hat{J} - J) &= (e^{\psi'}, |\nabla\zeta|^2) - (e^\psi, |\nabla\zeta|^2) \\
 &= (e^{\psi'}, |\nabla\zeta|^2) - (e^{\psi'}, |\nabla(\zeta - \zeta')|^2) - (e^\psi, |\nabla\zeta|^2) \\
 &\leq (e^{\psi'} - e^\psi, |\nabla\zeta|^2) \\
 &\leq C \|\psi - \psi'\|_{1,2}
 \end{aligned} \tag{3.10}$$

by reasoning entirely analogous to that used to obtain (3.9). In addition

$$\begin{aligned}
 c \|\zeta' - \zeta\|_{1,2}^2 &\leq (e^{\psi'}, |\nabla(\zeta' - \zeta)|^2) = (\zeta' - \zeta, \nabla \cdot (e^{\psi'} \nabla \zeta)) \\
 &= (\zeta' - \zeta, \nabla \cdot (e^{\psi' - \psi} (e^\psi \nabla \zeta))) = (\zeta' - \zeta', e^{\psi'} \nabla \zeta \cdot \nabla(\psi' - \psi)) \\
 &\leq C \|\zeta' - \zeta\|_2 \|\psi' - \psi\|_{1,2} \leq C \|\zeta' - \zeta\|_{1,2} \|\psi' - \psi\|_{1,2}
 \end{aligned}$$

where we have assumed the boundary ∂D sufficiently regular that $\|\nabla\zeta\|$ exists [11]. Thus

$$\|\zeta' - \zeta\|_{1,2} \leq C \|\psi' - \psi\|_{1,2} \tag{3.11}$$

Collecting these results, we have from (3.7a, 3.8, 3.9, 3.10, 3.11)

$$\|\zeta - \zeta'\|_{1,2} \leq C(\zeta - \zeta', r_2) + C \|\psi - \psi'\|_{1,2} \tag{3.12}$$

$$|J - J'| \leq C \|r_2\|_1 + C \|\psi - \psi'\|_{1,2} \tag{3.13}$$

and similar expressions for the hole terms. To estimate $\|\psi - \psi'\|_{1,2}$, we use (2.7) and the triangle inequality to obtain

$$\begin{aligned}
 \|\psi' - \psi\|_{1,2} &\leq C(\|r_1\|_2 + \|\zeta' - \zeta\|_2 + \|\rho' - \rho\|_2) \\
 &\leq C(\|r_1\|_2 + (\zeta' - \zeta', r_2)^\frac{1}{2} + (\rho - \rho', r_3)^\frac{1}{2}).
 \end{aligned} \tag{3.14}$$

From (3.12, 3.13, 3.14) and the corresponding estimates for the hole terms, we have the left side of (3.1), denoted by E , estimated as follows:

$$E \leq C(\|r_1\|_2 + \|r_2\|_1 + \|r_3\|_1 + (\zeta' - \zeta', r_2)^\frac{1}{2} + (\rho - \rho', r_3)^\frac{1}{2}). \tag{3.15}$$

Finally, we estimate the scalar products in (3.15) using the Schwarz inequality,

$$\begin{aligned}
 (\zeta' - \zeta', r_2) &\leq \|\zeta' - \zeta'\|_2 \|r_2\|_2 \\
 &\leq C \|\zeta' - \zeta'\|_{1,2} \|r_2\|_2 \\
 &\leq C(\zeta' - \zeta', r_2)^\frac{1}{2} \|r_2\|_2
 \end{aligned} \tag{3.16}$$

using (3.7a). Then (3.16) becomes

$$(\zeta' - \zeta', r_2) \leq C \|r_2\|_2^2 ; \tag{3.17}$$

using (3.17) and the corresponding estimate for $(\rho - \rho', r_3)$ in (3.15), the result (3.1) follows. This concludes the proof of Theorem 1.

Corollary: For the case $n=1$ (D an interval, $\partial D_1, \partial D_2$ the end points) the right side of (3.1) may be replaced by

$$C(\|r_1\|_2 + \|r_2\|_1 + \|r_3\|_1). \tag{3.18}$$

Proof: Instead of (3.16), we use in (3.15) the estimate

$$\begin{aligned} (\xi - \zeta', r_2) &\leq \|\xi - \zeta'\| \|r_2\|_1 \\ &\leq C \|\xi - \zeta'\|_{1,2} \|r_2\|_1 \\ &\leq C (\xi - \zeta', r_2)^{\frac{1}{2}} \|r_2\|_1 \end{aligned}$$

so that

$$(\xi - \zeta', r_2) \leq C \|r_2\|_1^2 \tag{3.19}$$

from which the result follows immediately.

4. Discretization error in one-dimensional problems

The use of suitable finite-element schemes, in the construction of the approximating functions ψ', ζ', ρ' , allows the terms of the form $\|r_i\|_p$ in (3.1) or (3.18) to be readily estimated. In this section we carry out such estimates for the one-dimensional problem, in which case a particularly simple numerical scheme can be used. In addition, our estimates allow for the generally inexact solution of the discrete equations, and allow the asymptotic order of magnitude of the errors to be achieved, using a rather coarse mesh. Such restrictions on practical computations are commonly encountered in this type of problem.

We set $D = (0, L)$, with $\partial D_1, \partial D_2$ the respective endpoints, $L = Mh$, and $x_m = mh, m = 0, 1, \dots, M$. The functions $\psi', \zeta',$ and ρ' are specified by a set of parameters $\psi_m, \zeta_m, \rho_m, m = 0, 1, \dots, M$. For $m = 0$ and $m = M$, the parameters ψ_m, ζ_m, ρ_m are assigned their respective boundary values; for other values of m , they are obtained from the difference equations presented below. The functions ψ', ζ', ρ' are defined as follows, in each interval $x_m \leq x \leq x_{m+1}$:

$$\psi'(x) = \hat{\psi}(x) + \gamma(x) \tag{4.1a}$$

$$\hat{\psi}(x) = \left(\frac{x-x_m}{h}\right) \psi_{m+1} + \left(\frac{x_{m+1}-x}{h}\right) \psi_m \tag{4.1b}$$

$$\gamma(x) = \left(\frac{x_{m+1}-x}{h}\right)^3 \frac{\Delta_m \psi}{6} + \left(\frac{x-x_m}{h}\right)^3 \frac{\Delta_{m+1} \psi}{6} \tag{4.1c}$$

$$\frac{d}{dx} \left(e^{\psi} \frac{d\zeta'}{dx} \right) = 0, \quad x \in (x_m, x_{m+1}); \quad \zeta'(x_m) = \zeta_m, \quad \zeta'(x_{m+1}) = \zeta_{m+1} \tag{4.2}$$

$$\frac{d}{dx} \left(e^{-\psi} \frac{d\rho'}{dx} \right) = 0, \quad x \in (x_m, x_{m+1}); \quad \rho'(x_m) = \rho_m, \quad \rho'(x_{m+1}) = \rho_{m+1} \tag{4.3}$$

where in (4.1c) we use the abbreviation

$$\Delta_m \psi = \psi_{m+1} - 2\psi_m + \psi_{m-1}, \quad m = 1, 2, \dots, M-1; \quad \Delta_m \psi = 0, \quad m = 0, M. \tag{4.4}$$

The function ψ' as given in (4.1) is also obtained by cubic spline interpolation [1] between the point values

$$\begin{aligned} \psi'(x_m) &= \psi_m + \frac{1}{6} \Delta_m \psi = \frac{1}{6} (\psi_{m-1} + 4\psi_m + \psi_{m+1}), \quad m = 1, 2, \dots, M-1; \\ \psi'(0) &= \psi_0, \quad \psi'(L) = \psi_M. \end{aligned} \tag{4.5}$$

The parameters ψ_m, ζ_m, ρ_m are obtained by the approximate solution of the system

$$R_1^m = R_2^m = R_3^m = 0, \quad m = 1, 2, \dots, M-1, \tag{4.6}$$

where

$$R_1^m = \kappa \frac{\Delta_m \psi}{h^2} + N(x_m) + \rho_m \exp\left(-\frac{\psi_{m-1} + 4\psi_m + \psi_{m+1}}{6}\right) - \zeta_m \exp\left(\frac{\psi_{m-1} + 4\psi_m + \psi_{m+1}}{6}\right), \tag{4.7}$$

$$h^2 R_2^m = \left(\frac{\psi_{m+1} - \psi_m}{e^{-\psi_m} - e^{-\psi_{m+1}}} \right) (\zeta_{m+1} - \zeta_m) - \left(\frac{\psi_m - \psi_{m-1}}{e^{-\psi_{m-1}} - e^{-\psi_m}} \right) (\zeta_m - \zeta_{m-1}), \tag{4.8}$$

$$h^2 R_3^m = \left(\frac{\psi_{m+1} - \psi_m}{e^{\psi_{m+1}} - e^{\psi_m}} \right) (\rho_{m+1} - \rho_m) - \left(\frac{\psi_m - \psi_{m-1}}{e^{\psi_m} - e^{\psi_{m-1}}} \right) (\rho_m - \rho_{m-1}); \tag{4.9}$$

the factors in parentheses in (4.8, 4.9) are defined continuously at $\psi_m = \psi_{m \pm 1}$. The system (4.6) possesses a solution [11]; however, in the following we allow for nonzero values of the R_i^m . We note that if $R_1^m = 0$ for some m , the approximating functions actually satisfy eq. (1.1) at the point x_m . Eqs. (1.2, 1.3) are satisfied by these approximating functions except at the interior mesh points.

The electron current J' is readily computed from (2.5, 4.1, 4.2), and is given by

$$J' = (1-b)^{-1} \left[(1-\zeta_1) \int_0^h e^{-\psi'(x)} dx - b(\zeta_{M-1} - b) \int_{L-h}^L e^{-\psi'(x)} dx \right]. \tag{4.10}$$

In the following, it is convenient to employ the following notation:

$$u(x) = \zeta'(x) e^{\psi'(x)}, \quad v(x) = \rho'(x) e^{-\psi'(x)}, \quad w(x) = N(x) + v(x) - u(x), \quad 0 \leq x \leq L; \tag{4.11}$$

$$\left. \begin{aligned} \hat{u}(x) &= \left(\frac{x-x_m}{h} \right) u(x_{m+1}) + \left(\frac{x_{m+1}-x}{h} \right) u(x_m) \\ \hat{v}(x) &= \left(\frac{x-x_m}{h} \right) v(x_{m+1}) + \left(\frac{x_{m+1}-x}{h} \right) v(x_m) \\ \hat{N}(x) &= \left(\frac{x-x_m}{h} \right) N(x_{m+1}) + \left(\frac{x_{m+1}-x}{h} \right) N(x_m) \end{aligned} \right\} x_m \leq x \leq x_{m+1}, m=0, 1, \dots, M-1 \tag{4.12}$$

In addition, it follows from (4.1) that

$$\psi'_{xx}(x) = \left(\frac{x-x_m}{h} \right) \frac{\Delta_{m+1}\psi}{h^2} + \left(\frac{x_{m+1}-x}{h} \right) \frac{\Delta_m\psi}{h^2}, \quad x_m \leq x \leq x_{m+1}, \quad m=0, 1, \dots, M-1. \tag{4.13}$$

A first integral of (4.2) gives

$$\zeta'_x(x) = a_m e^{-\psi'(x)}, \quad x_m < x < x_{m+1}; \quad a_m = (\zeta_{m+1} - \zeta_m) \int_{x_m}^{x_{m+1}} e^{-\psi'(x)} dx, \tag{4.14}$$

$m = 0, 1, \dots, M-1;$

we also set

$$b_m = (\zeta_{m+1} - \zeta_m) \int_{x_m}^{x_{m+1}} e^{-\psi(x)} dx = (\zeta_{m+1} - \zeta_m) (\psi_{m+1} - \psi_m) / [h(e^{-\psi_m} - e^{-\psi_{m+1}})], \tag{4.15}$$

$m = 0, 1, \dots, M-1.$

Our estimates of the discretization error associated with this scheme are contained in the following two lemmas:

Lemma 1: *In the above difference scheme, suppose ψ_m, ζ_m, ρ_m are bounded, independently of m and h ; then there exists a constant C , independent of h , such that*

$$\|r_1\|_2 \leq \left(h \sum_{m=1}^{M-1} (R_1^m)^2 \right)^{\frac{1}{2}} + \|N - \hat{N}\|_2 + Ch^2 \left[1 + \sup_{1 \leq m \leq M-1} |R_1^m| + h \sum_{m=1}^{M-1} (|R_2^m| + |R_3^m|) + h^2 \left(\sum_{m=1}^{M-1} |R_1^m| \right) \left(\sum_{m=1}^{M-1} (|R_1^m| + |R_2^m| + |R_3^m|) \right) \right]. \tag{4.16}$$

Proof: We estimate $\|r_1\|_2$ from (2.1a), using the triangle inequality and (4.7), (4.12), (4.13),

$$\begin{aligned} \|r_1\|_2 &= \|\kappa\psi'_{xx} + N + v - u\|_2 \\ &\leq \|\kappa\psi'_{xx} + \hat{N} + \hat{v} - \hat{u}\|_2 + \|N - \hat{N}\|_2 + \|v - \hat{v}\|_2 + \|u - \hat{u}\|_2 \\ &\leq \left(h \sum_{m=1}^{M-1} (R_1^m)^2 \right)^{\frac{1}{2}} + \|N - \hat{N}\|_2 + \|v - \hat{v}\|_2 + \|u - \hat{u}\|_2 . \end{aligned}$$

From (4.12) it follows that in any interval $x_m \leq x \leq x_{m+1}$,

$$u(x) - \hat{u}(x) = - \left(\frac{x_{m+1} - x}{h} \right) \int_{x_m}^x (y - x_m) u_{xx}(y) dy - \left(\frac{x - x_m}{h} \right) \int_x^{x_{m+1}} (x_{m+1} - y) u_{xx}(y) dy ; \tag{4.17}$$

from (4.2, 4.11, 4.14), we have for $x_m < x < x_{m+1}$

$$\begin{aligned} u_{xx} &= (e^{\psi'} \zeta'_x + e^{\psi'} \zeta \psi_x)_x = e^{\psi'} (\zeta'_x \psi'_x + \zeta' \psi'_{xx} + \zeta' (\psi'_x)^2) \\ &= a_m \psi'_x + u (\psi'_{xx} + (\psi'_x)^2) . \end{aligned} \tag{4.18}$$

In (4.18) the boundedness of u (independently of h) follows from (4.1, 4.2) and the hypotheses on the parameters ψ_m, ζ_m . From (4.13, 4.7) we have

$$|\psi'_{xx}| \leq C(1 + |R_1^m| + |R_1^{m+1}|) , \tag{4.19}$$

so that

$$|\psi'_x| \leq C \left(1 + h \sum_{m=1}^{M-1} |R_1^m| \right) . \tag{4.20}$$

From (4.1, 4.14, 4.15) it follows that $|a_m| \leq C|b_m|$; we rewrite (4.8) in the form

$$hR_2^m = b_m - b_{m-1} \tag{4.21}$$

and note that

$$\sum_{m=0}^{M-1} b_m \int_{x_m}^{x_{m+1}} e^{-\hat{\psi}(x)} dx = b - 1 , \tag{4.22}$$

using the boundary conditions (1.4) for ζ . From (4.21, 4.22) and the boundedness of $\hat{\psi}$, it follows that

$$|b_m| \leq C \left(1 + h \sum_{i=1}^{M-1} |R_2^i| \right) . \tag{4.23}$$

Combining (4.18, 4.19, 4.20, 4.23) we have

$$|u_{xx}(x)| \leq C \left[1 + \sup_{1 \leq m \leq M-1} |R_1^m| + h \sum_{m=1}^{M-1} |R_2^m| + h^2 \left(\sum_{m=1}^{M-1} |R_1^m| \right) \left(\sum_{m=1}^{M-1} (|R_1^m| + |R_2^m|) \right) \right] \tag{4.24}$$

for $x \in (x_j, x_{j+1})$, $j=0, 1, \dots, M-1$. Then from (4.17) we obtain

$$\|u - \hat{u}\| \leq C \left[1 + \sup_{1 \leq m \leq M-1} |R_1^m| + h \sum_{m=1}^{M-1} |R_2^m| + h^2 \left(\sum_{m=1}^{M-1} |R_1^m| \right) \left(\sum_{m=1}^{M-1} (|R_1^m| + |R_2^m|) \right) \right] ; \tag{4.25}$$

by analogous methods, a similar estimate is obtained for $\|v - \hat{v}\|$, which establishes the result (4.16).

Lemma 2: *Under the same hypotheses as for lemma 1, there exists a constant C independent of h such that*

$$\begin{aligned} \|r_2\|_1 &\leq C \left\{ h \sum_{m=1}^{M-1} |R_2^m| + \left(1 + h \sum_{m=1}^{M-1} |R_2^m| \right) \left| \sum_{m=0}^{M-1} |A_{m+1} \psi - A_m \psi| \right. \right. \\ &\quad \left. \left. + \sum_{m=1}^{M-1} (e^{\frac{1}{2}|A_m \psi|} - 1)(e^{\frac{3}{2}|A_m \psi|} - 1) \right| \right\} \tag{4.26} \end{aligned}$$

Proof: From (4.14) we have

$$\|r_2\|_1 = \sum_{m=1}^{M-1} |a_m - a_{m-1}| \tag{4.27}$$

it follows from (4.14, 4.15) that

$$a_m = b_m \int_{x_m}^{x_{m+1}} e^{-\hat{\psi}} dx \Big/ \int_{x_m}^{x_{m+1}} e^{-\psi'} dx$$

so that

$$\begin{aligned} a_m - a_{m-1} &= (b_m - b_{m-1}) \int_{x_{m-1}}^{x_m} e^{-\hat{\psi}} dx \Big/ \int_{x_{m-1}}^{x_m} e^{-\psi'} dx \\ &\quad + b_m \int_{x_m}^{x_{m+1}} \int_{x_{m-1}}^{x_m} e^{-\hat{\psi}(x) - \hat{\psi}(y)} (e^{-\gamma(x)} - e^{-\gamma(y)}) dy dx \Big/ \\ &\quad \int_{x_m}^{x_{m+1}} \int_{x_{m-1}}^{x_m} e^{-\psi'(x) - \psi'(y)} dy dx . \end{aligned} \tag{4.28}$$

In (4.28) we use (4.21) and the boundedness of $\gamma(x)$ to estimate the first term, and (4.23) to estimate the factor b_m in the second term. Again using the boundedness of γ , and substituting $s = (x - x_m)/h, t = (y - x_{m-1})/h$, it follows that the ratio of the double integrals in (4.28) is estimated by

$$\begin{aligned} &C \int_0^1 \int_0^1 e^{-(\psi_{m+1} - \psi_m)s} e^{-(\psi_m - \psi_{m-1})t} (e^{-\gamma(x)} - e^{-\gamma(y)}) ds dt \\ &= C \int_0^1 \int_0^1 \exp \left(-\frac{1}{2}(\psi_{m+1} - \psi_{m-1})(s+t) - \frac{\Delta_m \psi}{2}(s-t) \right) \left[\exp \left(-\frac{s^3}{6} \Delta_{m+1} \psi - \frac{(1-s)^3}{6} \Delta_m \psi \right) \right. \\ &\quad \left. - \exp \left(-\frac{t^3}{6} \Delta_m \psi - \frac{(1-t)^3}{6} \Delta_{m-1} \psi \right) \right] ds dt \\ &= C \int_0^1 \int_0^1 \exp \left(-\frac{1}{2}(\psi_{m+1} - \psi_{m-1})(s+t) - \frac{\Delta_m \psi}{2}(s-t) - \frac{\Delta_m \psi}{6}(1-s)^3 \right) \left[\exp \left(-\frac{\Delta_{m+1} \psi}{6} s^3 \right) \right. \\ &\quad \left. - \exp \left(-\frac{\Delta_m \psi}{6} t^3 \right) \right] ds dt \\ &\quad + C \int_0^1 \int_0^1 \exp \left(-\frac{1}{2}(\psi_{m+1} - \psi_{m-1})(s+t) - \frac{\Delta_m \psi}{2}(s-t) - \frac{\Delta_m \psi}{6} t^3 \right) \left[\exp \left(-\frac{\Delta_m \psi}{6} (1-s)^3 \right) \right. \\ &\quad \left. - \exp \left(-\frac{\Delta_{m-1} \psi}{6} (1-t)^3 \right) \right] ds dt . \end{aligned} \tag{4.29}$$

The two expressions in (4.29) are estimated similarly; the first term can be rewritten

$$\begin{aligned} &C \int_0^1 \int_0^1 \exp \left(-\frac{1}{2}(\psi_{m+1} - \psi_{m-1})(s+t) - \frac{\Delta_m \psi}{2}(s-t - \frac{1}{3}(1-s)^3) \right) \\ &\quad \left[\exp \left(-\frac{\Delta_{m+1} \psi}{6} s^3 \right) - \exp \left(-\frac{\Delta_m \psi}{6} s^3 \right) \right] ds dt \\ &\quad + C \int_0^1 \int_0^1 \exp \left(-\frac{1}{2}(\psi_{m+1} - \psi_{m-1})(s+t) - \frac{\Delta_m \psi}{2}(s-t - \frac{1}{3}(1-s)^3) \right) \\ &\quad \left[\exp \left(-\frac{\Delta_m \psi}{6} s^3 \right) - \exp \left(-\frac{\Delta_m \psi}{6} t^3 \right) \right] ds dt . \end{aligned} \tag{4.30}$$

The first term in (4.30) is $\leq C|\Delta_{m+1}\psi - \Delta_m\psi|$, using the mean value theorem and the boundedness of the discrete variables. To estimate the second term, we note that

$$\int_0^1 \int_0^1 \exp\left(-\frac{1}{2}(\psi_{m+1} - \psi_m)(s+t)\right) \left[\exp\left(-\frac{\Delta_m\psi}{6}s^3\right) - \exp\left(-\frac{\Delta_m\psi}{6}t^3\right) \right] ds dt = 0$$

by symmetry; thus the second term is equal to

$$C \int_0^1 \int_0^1 \exp\left(-\frac{1}{2}(\psi_{m+1} - \psi_{m-1})(s+t)\right) \left[\exp\left(-\frac{\Delta_m\psi}{2}\left(s-t - \frac{1}{3}(1-s)^3\right)\right) - 1 \right] \left[\exp\left(-\frac{\Delta_m\psi}{6}(s^3 - t^3)\right) - 1 \right] \exp\left(-\frac{\Delta_m\psi}{6}t^3\right) ds dt \leq C(\exp(\frac{2}{3}|\Delta_m\psi|) - 1)(\exp(\frac{1}{6}|\Delta_m\psi|) - 1) \tag{4.31}$$

since for $0 \leq s, t \leq 1, |s - t - \frac{1}{3}(1-s)^3| \leq \frac{4}{3}$ and $|s^3 - t^3| \leq 1$. The same estimate is readily obtained for the second term in (4.29), which establishes (4.26).

Based on the estimates (4.16, 4.26), and a similar estimate for $\|r_3\|_1$, we obtain the following:

Theorem 2: Suppose that h is chosen sufficiently small, and the difference equations (4.6–4.9) are solved to sufficient accuracy, that the following are valid, with constants independent of h :

- (a) $\|N - \hat{N}\|_2 = O(h^2)$;
- (b) $\sum_{m=1}^{M-2} |w_{m+1} - w_m|$ is bounded (depending on the particular problem, this bound may or may not be known a priori) ;
- (c) $h^2 w(x_m) \leq 1, \quad m = 1, 2, \dots, M-1$;
- (d) ψ_m, ζ_m, ρ_m are bounded independently of m and h ;
- (e) $\left(h \sum_{m=1}^{M-1} (R_1^m)^2\right)^{\frac{1}{2}}, \quad h \sum_{m=1}^{M-1} (|R_2^m| + |R_3^m|) = O(h^2)$;

then

$$\|\psi - \psi'\|_{1,2} + \|\zeta - \zeta'\|_{1,2} + \|\rho - \rho'\|_{1,2} + |J - J'| + |J_* - J'_*| = O(h^2). \tag{4.32}$$

Proof: Using hypotheses (a, d, e) in lemma 1, we have $\|r_1\|_2 = O(h^2)$ from (4.16). From (4.7, 4.11) we have

$$\Delta_m\psi = \kappa h^2 R_1^m - \kappa h^2 w(x_m) ; \tag{4.33}$$

using (4.33) and hypotheses (c, e) in lemma 2 give

$$\|r_2\|_1 \leq C \left[h^2 + h^2 \sum_{m=1}^{M-2} |w(x_{m+1}) - w(x_m)| + \sum_{m=1}^{M-1} (\Delta_m\psi)^2 \right] = O(h^2) + Ch^2 \sum_{m=1}^{M-2} |w(x_{m+1}) - w(x_m)| \tag{4.34}$$

again using (4.33). From hypothesis (b), the sum in (4.34) is bounded independently of h , so $\|r_2\|_1 = O(h^2)$. A similar estimate holds for $\|r_3\|_1$, and establishes the result (4.32) from (3.1). This concludes the proof of theorem 2.

We note that under the hypotheses of theorem 2, the order of magnitude of the error in the computed current J' is not changed if eq. (4.10) is replaced by the simpler expression

$$J' = (-b_0 + b b_{M-1}) / (1 - b). \tag{4.35}$$

By using more elaborate discrete equations, one may obtain a numerical scheme which is superior to the one described above, in the sense that hypotheses (b, c) of theorem 2 may be

dropped. From (4.1, 4.14) it follows that the a_m can be computed to arbitrary accuracy, in terms of the discrete variables. The conclusion of theorem 2 depends only on the boundedness of the a_m , as applied to (4.18), and an estimate of the form

$$\sum_{m=1}^{M-1} |a_m - a_{m-1}| = O(h^2) \tag{4.36}$$

to replace lemma 2.

5. Two-dimensional problems

In this section we are concerned with obtaining estimates of the error terms in (3.1) for a two-dimensional domain D . The methods of Section 4 unfortunately cannot be generalized to higher dimensional domains.

For simplicity, we specialize the domain D to be a rectangle, with boundary segments oriented as shown in fig. 1. As in the preceding analysis, we consider the case where the relative variations in $e^{\pm\psi}$, ζ , ρ' between mesh points are large, but we assume that the relative variations in ψ , ζe^ψ , $\rho e^{-\psi}$, $e^\psi \nabla \zeta$, $e^{-\psi} \nabla \rho$ are $O(h)$. As the detailed analysis for two-dimensional problems is quite lengthy, compared with that given above for the one-dimensional problem, we simply show here how suitable computation schemes may be constructed. As in the preceding sections, we carry out the analysis only for the electron terms.

The essential problem is the solution of (2.1b) for ζ' in terms of ψ' , in such a manner that $\|r_2\|_2$ as determined from (2.1b) can be made small. The following approach is proposed: instead of trying to approximate (1.2) directly, we describe the current density components by a "stream function" denoted by θ , defined in D and satisfying the boundary conditions shown in fig. 1,

$$(e^\psi \zeta_x)(x, y) = J\theta_y(x, y), \quad (e^\psi \zeta_y)(x, y) = -J\theta_x(x, y), \quad (x, y) \in D \tag{5.1}$$

where J is the total electron current, given in (2.3). From (1.4, 5.1) it is clear that θ , as a function of (x, y) , satisfies the equation

$$\nabla \cdot (e^{-\psi} \nabla \theta) = e^{-\psi} (\Delta \theta - \nabla \psi \cdot \nabla \theta) = 0, \quad (x, y) \in D, \tag{5.2}$$

and the boundary conditions as shown in fig. 1.

The advantage of introducing θ is that in view of our hypotheses on the relative variations in ψ and $e^\psi \nabla \zeta$, we can apply standard numerical techniques to the solution of equation (5.2). Our computed approximation to θ is denoted by θ' , and satisfies

$$\Delta \theta' - \nabla \psi' \cdot \nabla \theta' = r_4 \tag{5.7}$$

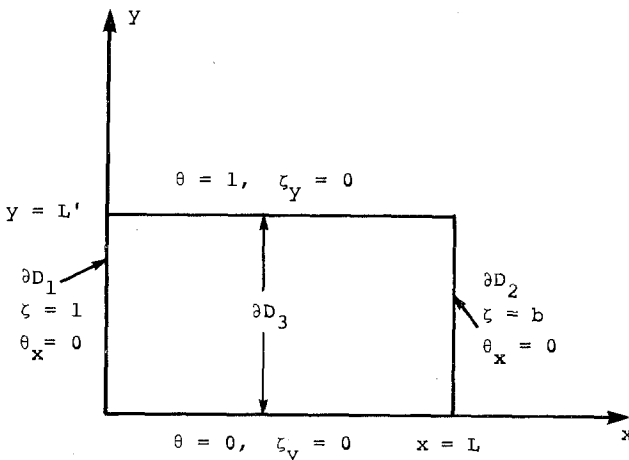


Figure 1. Orientation of boundary segments for two-dimensional problem.

for some error term r_4 ; as previously, we assume that θ' satisfies the prescribed boundary conditions exactly. To compute an approximation ζ' , we use (5.1) and the boundary conditions to obtain

$$\zeta'(x, y) = 1 - j(y) \int_0^x e^{-\psi'(z,y)} \theta'_y(z, y) dz \tag{5.4a}$$

$$= b + j(y) \int_x^L e^{-\psi'(z,y)} \theta'_y(z, y) dz, \quad (x, y) \in D, \tag{5.4b}$$

where

$$j(y) = (1 - b) / \int_0^L e^{-\psi'(z,y)} \theta'_y(z, y) dz. \tag{5.5}$$

From (2.5, 5.4, 5.5), we obtain an expression for the approximation to the total electron current, which is given by

$$J' = \int_0^{L'} j(y) (\theta'_y(0, y) - b \theta'_y(L, y)) dy / (1 - b). \tag{5.6}$$

For this computation scheme, we have the following estimate:

Lemma 3: *Suppose the quantities $\psi', \psi'_y, \theta'_x, \theta'_y, \theta'_{yy}$ are uniformly bounded for $(x, y) \in D$, and $j(y)$ uniformly bounded for $y \in [0, L]$; then there exists a constant C , depending on D and the bounds for these quantities, such that*

$$\|r_2\|_2 \leq C [\|r_4\|_2 + \|r_4\|_{1,2} + \|r_4\|_2^2 + \|r_4\|_{1,2}^2]. \tag{5.7}$$

Proof: We differentiate (5.4) with respect to x , to obtain

$$\zeta'_x(x, y) = -e^{-\psi'(x,y)} j(y) \theta'_y(x, y); \tag{5.8}$$

rewriting (5.3) in the form

$$(e^{-\psi'} \theta'_x)_x + (e^{-\psi'} \theta'_y)_y = e^{-\psi'} r_4 \tag{5.9}$$

and differentiating (5.4a) with respect to y , we obtain, using (5.9) and the boundary conditions for θ' ,

$$\begin{aligned} \zeta'_y(x, y) &= j_y(y) \int_0^x e^{-\psi'(z,y)} \theta'_y(z, y) dz + j(y) \int_0^x (e^{-\psi'} \theta'_y)_y(z, y) dz \\ &= j_y(y) \int_0^x e^{-\psi'(z,y)} \theta'_y(z, y) dz + j(y) \int_0^x (-e^{-\psi'} \theta'_x)_x(z, y) dz \\ &\quad + j(y) \int_0^x e^{-\psi'(z,y)} r_4(z, y) dz \\ &= j_y(y) \int_0^x e^{-\psi'(z,y)} \theta'_y(z, y) dz - j(y) e^{-\psi'(x,y)} \theta'_x(x, y) \\ &\quad + j(y) \int_0^x e^{-\psi'(z,y)} r_4(z, y) dz. \end{aligned}$$

Differentiating (5.5) with respect to y , we obtain similarly

$$j_y(y) = -(j(y))^2 \int_0^L e^{-\psi'(z,y)} r_4(z, y) dz / (1 - b). \tag{5.11}$$

From (5.8–5.10) we have

$$(e^{\psi'} \zeta'_x)_x(x, y) = j(y) \theta'_{xy}(x, y) \tag{5.12}$$

and

$$\begin{aligned}
 (e^{\psi'} \zeta')_y(x, y) &= -j(y) \theta'_{xy}(x, y) - j_y(y) \theta'_x(x, y) \\
 &+ \frac{\partial}{\partial t} \left(e^{\psi'(x,t)} \int_0^x e^{-\psi'(z,t)} (j_y(t) \theta'_y(z, t) + j(t) r_4(z, t)) dz \right)_{t=y}; \tag{5.13}
 \end{aligned}$$

thus

$$\begin{aligned}
 r_2(x, y) &= -j_y(y) \theta'_x(x, y) \\
 &+ \frac{\partial}{\partial t} \left(e^{\psi'(x,t)} \int_0^x e^{-\psi'(z,t)} (j_y(t) \theta'_y(z, t) + j(t) r_4(z, t)) dz \right)_{t=y} \tag{5.14}
 \end{aligned}$$

From the boundedness of $j(y)$ as a function of y , we infer from (5.11)

$$\int_0^{L'} |j_y(y)|^2 dy \leq C \|r_4\|_2^2; \tag{5.15}$$

performing the indicated differentiations in (5.14) and taking the L_2 norm, using (5.13, 5.15), the boundedness of ψ', ψ'_y , and the derivatives of θ' , and the Schwarz inequality repeatedly, we obtain an estimate for $\|r_2\|_2$ of the form

$$\|r_2\|_2 \leq C [\|r_4\|_2 + \|r_4\|_4^2 + \|r_4\|_{1,2}], \tag{5.16}$$

for which (5.7) follows by the Sobolev inequality. This concludes the proof of lemma 3.

We note that the term $\|r_1\|_2$ in (3.1) can be estimated by methods similar to those used for the one-dimensional problem in Section 4. Under suitable additional hypotheses, bounds for the second derivatives of ζ' may be obtained from (5.12, 5.13).

In general it will not be possible to perform the indicated integrals in (5.4, 5.5, 5.6) exactly. We assume that the additional error introduced in the approximation ζ' can be represented by adding an error term $r_5 = r_5(x, y)$ to $e^{-\psi'} \theta'_y$ in the integrands of (5.4, 5.5). Under these conditions, lemma 3 remains valid if the additional terms $\|r_5\|_2 + \|r_5\|_{1,2} + \|r_5\|_{2,2} + \|r_5\|_2^2 + \|r_5\|_{1,2}^2 + \|r_5\|_{2,2}^2$ are inserted in the brackets in (5.7). The method of proving lemma 3 is essentially unchanged.

Finally, we note that uniform bounds for $\psi - \psi', \zeta - \zeta', \rho - \rho'$ may be obtained from the bounds in the norm $\|\cdot\|_{1,2}$ and the inequality [10]

$$\|\cdot\| \leq C |\log \delta| (\|\cdot\|_{1,2} + \delta \|\cdot\|_{2,2}) \tag{5.17}$$

which is valid for any function in $H_2^2(D)$ equal to zero on $\partial D_1 \cup \partial D_2$. If we obtain convergence of order h^p in the norm $\|\cdot\|_{1,2}$, setting $\delta \sim h^p$, we have uniform convergence of order $h^p |\log h|$, since from (3.1) we are assured of the square integrability of the second derivatives of ψ', ζ', ρ' .

6. Discussion and summary

Although the above analysis is not sharp with respect to multiplicative constants, it may be of practical value in the construction of suitable computation schemes for this type of problem.

This is particularly true of the one-dimensional analysis of Section 4, where sufficient conditions for attainment of the asymptotic convergence rate are obtained, and where the effects of inexact solution of the discrete equations can be appraised. The difference scheme (4.6–4.9) does not require that the variations in ψ, ζ, ρ between mesh points be small, and allows for a finite number of “depletion layer” edges, where abrupt variations in the charge density w , as given by (4.11), may occur. This scheme can readily be generalized to the case of nonuniform mesh point spacing, with theorem 2 remaining valid. Hypothesis (e) of theorem 2 may provide an effective criterion for terminating the iterative solution of the discrete equations, when relatively slowly converging methods are used for their solution [6, 12].

In addition, equations (2.5, 4.10) provide an unambiguous expression for the computed value of the electron current. In the general case, one has $b \ll 1$, and the current is essentially

evaluated at the boundary ∂D_1 ; for bipolar or field-effect devices in their normal operating conditions, this is the emitter or source contact, respectively.

To the best of our knowledge, the scheme (4.6–4.9) has not been employed in an actual computation. A similar scheme, however, in which the averages $(\psi_{m-1} + 4\psi_m + \psi_{m+1})/6$ are replaced by ψ_m in (4.7) has been used, both in one dimension [14], and in two-dimensional models of the insulated-gate field-effect transistor [7, 12]. In this device, the current flow is essentially one-dimensional, and thus the analysis of Section 4 at least relevant, if not rigorously applicable. It is readily shown that theorem 2 remains true for the numerical scheme so obtained.

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