

A Finite Element Approximation Theory For The Drift Diffusion Semiconductor Model*

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Abstract

Two-sided estimates are derived for the approximation of solutions to the drift-diffusion steady-state semiconductor device system which are identified with fixed points of Gummel's solution map. The approximations are defined in terms of fixed points of numerical finite element discretization maps. By use of a calculus developed by Krasnosel'skii and his coworkers, it is possible, both to locate approximations near fixed points in an "a priori" manner, as well as fixed points near approximations in an "a posteriori" manner. These results thus establish a nonlinear approximation theory, in the energy norm, with rate keyed to what is possible in a standard linear theory. This analysis provides a convergence theory for typical computational approaches in current use for semiconductor simulation.

1 Introduction

The drift-diffusion model of a steady-state semiconductor device is formed by a system of three coupled partial differential equations (PDEs.) This system of PDEs is solved by a solution vector of three function components. A fixed point mapping $\mathbf{T} : x \mapsto \mathbf{T}x$ can be defined by solving each of these PDEs for its corresponding component and substituting these components in successive PDEs in a Gauss-Seidel fashion. Fixed points of such a mapping \mathbf{T} then coincide with solutions to the drift diffusion model. Iteration with the mapping \mathbf{T} defines an algorithm for the solution of the drift-diffusion model in which the PDEs are decoupled. The mapping \mathbf{T} , termed Gummel's map [5] in the literature, is defined through solution for the potential u , for given electron and hole quasi-Fermi levels v and w , as a fractional step, and subsequently through solution for the electron and hole quasi-Fermi levels. This definition specifies the range of the mapping \mathbf{T} . For the slightly different mapping that operates in the space of the Slotboom variables $V = e^{-v}$, and $W = e^w$, principal properties including

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fixed points and maximum principles, have been studied in increasing generality in [21],[23] and [8]. For this alternative mapping, the Lipschitz constant $L_{\mathbf{T}}$ has been examined in detail in [15],[9],[17],[16]. Employing either quasi-Fermi levels, or Slotboom variables, the appropriate formulation for device applications is the mixed Dirichlet/Neumann boundary value problem, taken over the physical device, \bar{G} , assumed to be a polyhedral domain, with possible solution gradient singularities at boundary transition points [15],[9].

A companion approximation map is induced by piecewise linear finite elements, if the convex minimization, inherent in defining the successive gradient equations, is taken over finite dimensional affine subspaces. The fixed points of the companion map are clearly candidates for approximation of the fixed points of the solution map for the original system of PDEs. In this paper, we deduce an approximation theory, described by two-sided estimates, for this discretization procedure. Our theory is based upon an operator calculus developed by Krasnosel'skii and his collaborators (cf. [20]) in which both the fixed points of the solution map are approximated "a priori" by fixed points of the numerical map, and also fixed points of the solution map are located in an "a posteriori" manner near fixed points or approximate fixed points of the numerical map, so that spurious solutions are not computed. The abstract results are stated as Theorems 4.1 and 4.2 and the semiconductor application as Corollary 4.1. Later in the Introduction, we shall elaborate more fully on these results.

This paper does not deal with the actual algorithms for computing the fixed points of the numerical maps, i.e., for solving the system finite element equations. This issue, or more precisely, the closely related issue of solving the discrete equations which arise by a finite element discretization of the potential equation and a volume element method, based upon exponential fitting and the box method, for the continuity equations, has been intensively studied (cf. [2],[14]). The piecewise linear finite elements of this paper reduce to an approach of this type for properly defined quadrature rules in the finite element equations (cf. [25]). We can distinguish two widely used basic solution methods, either at the operator level or for the discrete system. The oldest approach proceeds by successive substitution, and is known as Gummel's method [5], mentioned above. The more recent algorithm consists of a damped Newton outer iteration, while the Jacobian is formed by linearization of the system of PDEs itself. Newton's equations are then solved either by a sparse direct method, or iteratively, employing preconditioners based on *splittings* of the Jacobian. The numerical approximations introduced in this paper are canonical ones. Therefore our approximation results are valid irrespective of the computational method which is employed for the actual solution of the system. The approximation can equivalently be viewed as defined directly by the weak formulation of the system of differential equations, rather than the fixed point mapping \mathbf{T} . Thus our results apply equally to results obtained through the extensively used computational scheme that is based upon direct application of Newton's method to the discretized system of PDEs. Newton's method for the finite element system will proceed differently, however, if based upon a numerical fixed point map \mathbf{T}_n , rather than the discretized system of PDEs directly. In [19],[11],[10] analytical

and numerical evidence is provided which indicates that to some extent this approach is superior. Thus, although the province of our paper is decidedly a nonlinear approximation theory, we study in detail, in the process, the very maps, including their differential properties, which may well lead to a more effective algorithmic strategy for solving the finite dimensional systems, in such a way that grid independent constants may characterize convergence rates. Linearization based upon the differential map requires smoothing to achieve this (cf. [7]).

We briefly describe now the basis for the major results. Given a fixed point x_0 of a smooth mapping \mathbf{T} , a numerical approximation map \mathbf{T}_n , and a projector map \mathbf{P}_n , a theory is constructed to estimate $\|x_n - \mathbf{P}_n x_0\|$, where $\mathbf{T}_n x_n = x_n$. In fact, the authors of [20] characterize the map $\mathbf{P}_n \mathbf{T}$ as the "Galerkin" approximate map, and \mathbf{T}_n as a "perturbed Galerkin" map. Since x_0 is a fixed point of \mathbf{T} , the estimates represent precisely the dispersion between these two methods. We should stress that the mapping $\mathbf{P}_n \mathbf{T}$ cannot actually be implemented numerically. However, the convergence rate is readily estimated. Now, the "a priori" estimates are derived by deducing a root of the map $\mathbf{A} = \mathbf{I} - \mathbf{T}_n$, in a ball centered at $\mathbf{P}_n x_0$, through construction of an equivalent contraction map: The methodology involves derivative inversion and a mean value calculus. A similar approach is employed for the a posteriori estimates. We shall single out the essential hypotheses which emerge:

1. invertibility of $\mathbf{I} - \mathbf{T}'$;
2. uniform convergence of \mathbf{T}_n to \mathbf{T} and \mathbf{T}'_n to \mathbf{T}' on bounded sets;
3. continuity of \mathbf{T}' ;
4. continuity (uniform in n) of \mathbf{T}'_n ;
5. convergence of \mathbf{P}_n to \mathbf{I} uniformly on appropriate bounded subsets of compactly embedded subspaces.

In our application of this theory, we shall work with energy norms and \mathbf{T} will be compact, so that (i) above reduces to an eigenvalue hypothesis. This is the only "nonverifiable" hypothesis made in the a priori theory, and guarantees that solutions are isolated. The relation to the Babuška–Brezzi inf-sup condition was described in [11]. Hypothesis (v) is related to a regularization hypothesis we must make concerning the solution map for the mixed boundary value problem, i.e., \mathbf{T} and $\mathbf{T}'(z)$ are bounded maps into $H^{1+\theta}$, $\theta = \theta(N) > 0$, for Euclidean dimension N . The usual results in the literature for the mixed boundary value problem are stated in terms of L^p -gradient properties (cf. [22]). The application of this theory to the current continuity equations is discussed in [15]. Our assumption is consistent with these results, though not implied by them. It turns out, however, since \mathbf{T} is defined via decoupling, that the hypothesis is directed toward single linear equations (albeit uniformly) and, at least for $N=2$, asymptotic estimates already exist in the literature (cf. [26],[1]). The verification of (ii)–(iv) is left largely to the appendix because of the heavily detailed

calculations involved. The reader may consult Appendix D for a summary of these properties and the chain of results used for their proof. For reasons of space, we have given only the statements of the technical results employed in Appendices A–C. Proofs can be found in the authors’ monograph [12].

We introduce the discretization in §3, along with a review of the discrete maximum principles derived in [18]. The latter are essential to the interplay between \mathbf{T} and \mathbf{T}_n . A convergence theory for \mathbf{T}_n is also developed in §3, and the major results are stated and derived in §4. Section 2 is devoted to a statement of the continuous problem and a precise development of the map \mathbf{T} . Note that the current continuity equations are discretized in terms of piecewise linear Slotboom variables. However, in the rest of the paper we make use of the quasi-Fermi levels. For the reader’s convenience we have adopted a notational device whereby mappings are indicated in boldface, whereas the images of the mappings are in ordinary italics or upper case. These are the symbols associated with the basic dependent variables of the system.

2 The model and the fixed point map

2.1 The system

The electrostatic potential and the quasi-Fermi levels are scaled by the thermal voltage, $U_T = k_B T/q$, and the length by $l = \sqrt{U_T/n_i q}$, where q denotes the size of the electron charge, T is the temperature which is assumed to be constant, k_B is Boltzmann’s constant. The concentrations n and p of the electron and hole carriers are scaled by the intrinsic concentration n_i and represented in terms of the quasi Fermi levels v and w and the dimensionless electrostatic potential u through the relations $n = e^{u-v}$, $p = e^{w-u}$. Thus we obtain the following steady-state system:

$$\begin{aligned} -\nabla \cdot (\epsilon \nabla u) + e^{u-v} - e^{w-u} &= k_1, \\ -\nabla \cdot (D_n e^{u-v} \nabla v) - R(u, v, w) &= 0, \\ -\nabla \cdot (D_p e^{w-u} \nabla w) + R(u, v, w) &= 0, \end{aligned}$$

where ϵ is the dielectric permittivity. Here, Einstein’s relations have been employed, the bounded function k_1 denotes the net ion impurity concentration, and R denotes a scaled recombination term. In order to expedite the complicated technical analysis, we shall consider the case of vanishing generation-recombination, constant diffusivity (and mobility). in the current continuity equations, The system can then be written

$$-\nabla \cdot (\epsilon \nabla u) + e^{u-v} - e^{w-u} = k_1, \quad (2.1)$$

$$-\nabla \cdot (e^u \nabla e^{-v}) = 0, \quad (2.2)$$

$$-\nabla \cdot (e^{-u} \nabla e^w) = 0, \quad (2.3)$$

subject to mixed Dirichlet/homogeneous Neumann boundary conditions, taken on the Dirichlet part, Σ_D , of the device boundary, and on its complement, Σ_N ,

respectively. These are specified on Σ_D by the traces of appropriate functions \bar{u} , \bar{v} , \bar{w} , where \bar{u} , \bar{v} , \bar{w} are in $C^2(\bar{G})$, and on Σ_N weakly. The analysis to follow admits spatially dependent, positive diffusion and mobility coefficients. It remains to be determined what extensions beyond this are possible.

In [8] a map \mathbf{T}_0 , operating on Slotboom variables is analyzed. The results for \mathbf{T}_0 , operating on Slotboom variables, imply that the map \mathbf{T} , operating on quasi-Fermi levels, is continuous from $K_0 \subset \prod_1^2 L_2(G)$ into $\prod_1^2 H^1(G)$ with bounded range, and acts invariantly on

$$K_0 \equiv \{[v, w] : \inf_{\Sigma_D} \bar{v} \leq v \leq \sup_{\Sigma_D} \bar{v}, \inf_{\Sigma_D} \bar{w} \leq w \leq \sup_{\Sigma_D} \bar{w}\} \quad (2.4)$$

in such a way that fixed points of \mathbf{T} define solutions of the system of boundary-value problems. The map is defined by unfolding: given $[v, w] \in K_0$, the element $u = \mathbf{U}_0(v, w)$ is obtained by solving the weak formulation of the boundary-value problem described by (2.1). The Gauss–Seidel process continues: $\mathbf{V}_0(u)$ and $\mathbf{W}_0(u)$ are the elements computed from the weak formulations of (2.2) and (2.3), respectively, with u determined as above. Altogether,

$$\mathbf{T}_0[v, w] = [v_0, w_0]. \quad (2.5)$$

The invariance, continuity, and compactness properties of \mathbf{T}_0 , taken on $K_0 \subset \prod_1^2 L_2(G)$, are sufficient to deduce the existence of a fixed point $[v_0, w_0]$ via the Schauder theorem, and such defines a solution of the system: $[u_0, v_0, w_0]$.

2.2 The definition of \mathbf{T}

The map \mathbf{T} , required to apply the operator calculus of [20], must be defined on an open set in function space. In this context the suitable space is $\prod_1^2 H^1(G)$. However, the proofs of a number of the results in the appendix require a priori bounds on the extrema of the functions u , v , and w , similar to the a priori bounds, introduced in [8]. In the latter publication the assumption was introduced that the original (V, W) satisfies already the L_∞ bounds specified in (2.4) which the image (V_0, W_0) was shown to satisfy. These L_∞ bounds on the original (V, W) , incorporated into the definition of K_0 for Slotboom variables, on which \mathbf{T}_0 acts, were used to derive a priori L_∞ bounds on the potential function u .

Because the set K_0 is not open, we modify the definition of \mathbf{T} such that the assumption that the original (v, w) lies in K_0 can be removed. To achieve this we compose a \mathbf{T} -like map with a truncation operator \mathbf{Tr} , which leaves (v, w) unaffected within K_0 (where the solution lies), but which restricts the range to a set K (cf. (2.6)) which is only slightly larger than K_0 . By carefully selecting K we achieve that the intermediate function u in the definition of \mathbf{T} satisfies a priori L_∞ bounds which are only slightly wider than those for u in [8]. However, u satisfies these slightly wider bounds as the range of a map defined for all (v, w) in an appropriate open subset of $\prod_1^2 H^1$, and not just on the set K_0 . We introduce $\mathbf{h}_i \in C_0^\infty(\mathbf{R})$, $i = 1, 2$, such that *support* $\mathbf{h}_i = [\alpha_i, \beta_i]$, $\alpha_i > 0$,

and

$$\begin{aligned} h_1(t) &= t, & \inf_{\Sigma_D} \bar{v} \leq t \leq \sup_{\Sigma_D} \bar{v}, \\ h_2(t) &= t, & \inf_{\Sigma_D} \bar{w} \leq t \leq \sup_{\Sigma_D} \bar{w}. \end{aligned}$$

Below we will define an open ball Ω , centered at zero, in $\prod_1^2 H^1$, on which

$$\mathbf{Tr}[v, w] := [\mathbf{h}_1(v), \mathbf{h}_2(w)], \quad [v, w] \in \Omega.$$

Note that the range of \mathbf{Tr} is contained in $K \subset \prod_1^2 L_\infty$, where

$$K = \{[v, w] \in \prod_1^2 L_\infty : \alpha_1 \leq v \leq \beta_1, \alpha_2 \leq w \leq \beta_2\}. \quad (2.6)$$

We consider the extension maps \mathbf{U} of \mathbf{U}_0 , \mathbf{V} of \mathbf{V}_0 , and \mathbf{W} of \mathbf{W}_0 defined as above, with elements in the domain of \mathbf{U} now taken from $K \supset K_0$. In terms of these quantities, \mathbf{T} may be defined by

$$\mathbf{T} = [\mathbf{V} \circ \mathbf{U} \circ \mathbf{Tr}, \mathbf{W} \circ \mathbf{U} \circ \mathbf{Tr}]. \quad (2.7)$$

For reasons related to the technical estimates of the paper, it is essential to identify carefully the domains and ranges of the composition maps used to define \mathbf{T} . Since

$$|\nabla[\mathbf{h}_1(v)]|^2 = |\mathbf{h}'_1(v)\nabla v|^2 \leq c|\nabla v|^2$$

with a similar inequality for $|\nabla[\mathbf{h}_2(w)]|^2$, it follows that the map \mathbf{Tr} has range contained in $K \cap \{C\mu : \mu \in \Omega \subset \prod_1^2 H^1\}$, for some positive constant C . Thus, the domain of \mathbf{U} is $K \cap (C * \Omega)$. Employing the H^1 norm defined below in (2.10), the range of \mathbf{U} is contained in a bounded set Γ in $H^1(G) \cap L_\infty(G)$; indeed this follows from results of [18] (the H^1 bounds will be elaborated in the next section) and, in particular, the following pointwise bounds (maximum principles) hold:

$$\gamma \leq U \leq \delta,$$

$$\begin{aligned} \gamma &= \min(\gamma', \inf_{\Sigma_D} \bar{u}), & \delta &= \max(\delta', \sup_{\Sigma_D} \bar{u}), \\ \gamma' &= \sinh^{-1}[(1/2) \inf_G k_1(\alpha_1 - \alpha_2)/2] + (\alpha_1 + \alpha_2)/2, & (2.8) \\ \delta' &= \sinh^{-1}[(1/2) \sup_G k_1(\beta_1 - \beta_2)/2] + (\beta_1 + \beta_2)/2. \end{aligned}$$

Finally, as part of the mapping \mathbf{T} the joint domain of \mathbf{V} and \mathbf{W} is Γ , while the range of these maps is contained in the intersection of K_0 (not K), defined in (2.4), with the domain Ω , which is now defined. Since, for $U \in \Gamma$ (only the

pointwise bounds are needed),

$$\begin{aligned}
 \int_G |\nabla v|^2 dx &\leq e^{\alpha_1 - \gamma} \int_G e^{U-v} |\nabla v|^2 dx \\
 &= e^{\alpha_1 - \gamma} \int_G e^U \nabla v \cdot \nabla \bar{v} dx \\
 &\leq (1/2) \left[\int_G |\nabla v|^2 dx + e^{2(\delta + \beta_1 - \gamma - \alpha_1)} \int_G |\nabla \bar{v}|^2 dx \right],
 \end{aligned} \tag{2.9}$$

it follows, for $\|\cdot\|_{H^1}^2$ given by

$$\|v\|_{H^1}^2 = \|\nabla v\|_{L^2}^2 + \left(\int_{\Sigma_D} v dx \right)^2, \tag{2.10}$$

that

$$\|v\|_{H^1}^2 < e^{2(\delta + \beta_1 - \gamma - \alpha_1)} \|\bar{v}\|_{H^1}^2 \quad (\text{Note: } v|_{\Sigma_D} = \bar{v}|_{\Sigma_D}),$$

with a similar estimate for $\|w\|_{H^1}^2$. Thus, we choose Ω to contain the open ball centered at 0 of radius $\rho = e^{(\delta + \max\{\beta_i\} - \gamma - \min\{\alpha_i\})} \|[\bar{v}, \bar{w}]\|_{\prod H^1}$. It is evident, from the monotone dependence of γ' and δ' on α_i, β_i , that Ω contains the range of \mathbf{T}_0 as well as that of \mathbf{T} , and hence, that \mathbf{T} is a proper extension of $\mathbf{T}_0|_{\text{range } \mathbf{T}_0}$. However, it is essential for our purposes that Ω also contain the range of \mathbf{T}_n , to be defined in the next section. (cf. (3.2)) This entails an estimation of w_h and w_h . Slight adjustments of (2.10), as well as (3.7) and (3.8) to follow, yield the result that the number ρ just defined need only be perturbed by a term of order $O(h)$. This gives us, finally, the radius of Ω .

2.3 Regularization properties of \mathbf{T}

We now address the hypothesis (v) discussed in the introduction. It may be reduced to the following single statement.

Assumption 1. The solution maps \mathbf{V}, \mathbf{W} are regularizing, i.e., they map Γ boundedly into $H^{1+\theta}(G)$ for some $\theta > 0$, which depends only on the Euclidean dimension N .

Remark 2.1. Note that, under Assumption 1, the mapping \mathbf{T} is compact from Ω into itself. This also holds for \mathbf{T}' by results in the appendix.

We close this section by noting that the maximum principles (2.4) and (2.8) are special cases of the (reduced) bounds

$$\gamma \leq u \leq \delta \tag{2.11}$$

from [18] where γ, δ have the meaning of (2.8), but

$$\gamma' = \inf_{x \in G} f^{-1}(x, \inf_{y \in G} g(y)), \quad \delta' = \sup_{x \in G} f^{-1}(x, \sup_{y \in G} g(y)), \tag{2.12}$$

for the solution u of the gradient equation

$$-\nabla \cdot [a(x) \nabla u(x)] + f(x, u(x)) = g(x). \tag{2.13}$$

Here, $a, g \in L_\infty$, and f is increasing and locally Lipschitz in u for each $x \in G$, with $f^{-1}(x, \cdot)$ the corresponding inverse.

3 The discretized model and the numerical fixed point map

3.1 The finite element maps

In this section we introduce the piecewise linear finite element method which defines the numerical fixed point map. We also describe the associated approximation properties. The finite element equations for the potential equation are given by

$$\langle \epsilon(x) \nabla U_h, \nabla \phi_i \rangle + \langle e^{U_h - v} - e^{w - U_h}, \phi_i \rangle - \langle k_1, \phi_i \rangle = 0 \quad \text{for } i = 1, \dots, M, \quad (3.1)$$

where U_h is a finite element function and the ϕ_i are appropriate test functions comprising a nodal basis of the piecewise linear finite element subspace S_h . According to the assumptions specified regarding \bar{u} , it follows that we may select the piecewise linear interpolant \bar{u}_I of \bar{u} so that $U_h \in \bar{u}_I + S_h$, where the members of S_h vanish on the Dirichlet boundary Σ_D of the polyhedral domain G . The functions of S_h are continuous and are linear in each simplex, S . As usual, $h = \max_S \{\text{diam } S\}$. In (3.1) all integrals can be computed in closed form if piecewise linear approximations to v and w are selected. For reasons of strict symmetry, the domain of \mathbf{U}_h , viewed as a mapping, is chosen to be the same set $K \cap (C * \Omega)$ as the domain of \mathbf{U} described in §2. Prior to discussing the range of \mathbf{U}_h , and hence the joint domain of \mathbf{V}_h and \mathbf{W}_h , we characterize the latter formally in terms of

$$\begin{aligned} \langle e^{U_h} \nabla V_h, \nabla \phi_i \rangle &= 0, & \text{for } i = 1, \dots, M, \\ \langle e^{-U_h} \nabla W_h, \nabla \phi_i \rangle &= 0, & \text{for } i = 1, \dots, M, \end{aligned}$$

and $v_h = -\log(V_h)$, and $w_h = -\log(W_h)$. Thus, the Slotboom variables V and W are approximated by piecewise linear finite elements, rather than the quasi-Fermi levels v and w themselves. As a result, standard linear finite element approximation results are applicable. As before, $\phi_i \in S_h$, and $v_h \in \bar{V}_I + S_h$, $w_h \in \bar{W}_I + S_h$, where we have selected the interpolants for \bar{V} and \bar{W} . The integrals here can be done in closed form as well; however, as noted in the introduction, appropriate upwinding for the current continuity equations is achieved by quadrature rules which are more suitable than exact evaluation.

The range of \mathbf{U}_h is contained in Γ (as is the range of \mathbf{U}), which serves as the joint domain of \mathbf{V}_h and \mathbf{W}_h . Indeed, the fact that U_h satisfies the bounds (2.8) is verified in the authors' paper [18]. Certain mesh restrictions are required, since the proof requires that the matrices corresponding to the Laplacean and the current continuity equations be M-matrices. In order to state these discrete maximum principles in a format applicable both to \mathbf{U}_h , and also \mathbf{V}_h and \mathbf{W}_h , we consider solutions of the gradient equation (2.13). On each element S we have the following definition.

DEFINITION 3.1. Let S be an N -dimensional simplicial finite element such that

- V is the volume,

- \vec{v}_i is a vertex,
- e_{ij} is the edge connecting vertices \vec{v}_i and \vec{v}_j ,
- F_k is the face opposite the vertex k , with measure $|F_k|$,
- h_i is the normal distance of v_i to F_i ,
- γ_{ij} is the angle between the inward normal vectors to the faces F_i and F_j ,
- ϕ_l is the piecewise linear nodal basis function which is 1 at vertex \vec{v}_l ,
-

$$\alpha_{ij} \equiv \int_S a(x) \nabla \phi_i \cdot \nabla \phi_j dx$$

is the ij th entry of the *element* stiffness matrix,

- $\langle a(x) \rangle \equiv \int_S a(x) dx / V$, the average of $a(x)$ over the element S ,
- a_{ij} is the ij th element of the assembled stiffness matrix.

Remark 3.1. It was shown in [18] that

$$\alpha_{ij} \equiv \int_S a(x) \nabla \phi_i \cdot \nabla \phi_j dx = \langle a(x) \rangle \cos(\gamma_{ij}) \frac{1}{h_i h_j} V,$$

or

$$\alpha_{ij} = \langle a(x) \rangle \cos(\gamma_{ij}) \frac{|F_i| |F_j|}{N^2 V}.$$

In [18] it was also shown that L_∞ stability of \mathbf{U}_h follows under the following assumption.

Assumption 2.

- In N dimensions where $N \geq 2$ we require that for every edge jk the off-diagonal element a_{jk} in the matrix satisfies

$$a_{jk} = \sum_{S \text{ adjacent } jk} \langle a(x) \rangle_S \cos(\gamma_{jk}^{(S)}) \frac{V^{(S)}}{h_j h_k} \leq -\frac{\rho}{h_{\max}^2} \sum_{S \text{ adjacent } jk} V^{(S)},$$

with $\rho > 0$. In two dimensions the well-known requirement that for every edge jk in the triangulation we have

$$\frac{1}{2} [\langle a(x) \rangle_{T_1} \cot(\phi_1) + \langle a(x) \rangle_{T_2} \cot(\phi_2)] \geq \rho > 0,$$

where the T_i are the two triangles adjacent to edge jk and the ϕ_i are the two angles opposite to the edge jk , is a slightly more restrictive version of this condition. In higher dimensions we can impose the sufficient condition that the angle between the vectors normal to any two faces of the same polyhedron in the mesh has to be bounded uniformly from above by $\pi/2 - \delta$.

- For all $a, b \in \mathbf{R}$, $a < b$: $|f(x, u) - f(x, v)|/|u - v| \leq D(b, a)$ if $a \leq u, v \leq b$, where $D(\cdot, \cdot)$ is a Lipschitz constant which is a monotonically increasing function of b and a monotonically decreasing function of a .
- The numbers h_i satisfy $h_i \geq h_0 h$, where h_0 does not depend on h .

Remark 3.2. In the application to this paper, the role of a is played for the Poisson equation by $\epsilon(x)$, and for the current continuity equations by e^u, e^{-u} , respectively. The first part of Assumption 2 above is satisfied uniformly in all cases if $\langle a \rangle$ is replaced by the lower bounds expressed in terms of the maximum principles. Under the first part of Assumption 2, it follows from the results of [18] (in the form (2.12)) that U_h satisfies the pointwise estimates expressed in the (partial) definition of Γ (cf. (2.8)) and that \mathbf{V}_h and \mathbf{W}_h have range in K_0 . The function $f(x, u)$ in the respective applications is $e^{u-v(x)} - e^{w(x)-u}$, for Poisson's equation, and $f(x, u) \equiv 0$ for the current continuity equations.

3.2 The numerical fixed point map

If a given finite element space S_h has dimension n , then we may define \mathbf{T}_n , the numerical fixed point map, by

$$\mathbf{T}_n = [\mathbf{V}_h \circ \mathbf{U}_h \circ \mathbf{Tr}, \mathbf{W}_h \circ \mathbf{U}_h \circ \mathbf{Tr}]. \quad (3.2)$$

The only unverified issues related to the definition of \mathbf{T} are the H^1 bounds associated with Γ , containing the range of \mathbf{U}_h and \mathbf{U} , and the related existence question for the finite element solution. By viewing both the solution of the Poisson equation and the finite element equation as resulting from convex minimization, one obtains H^1 bounds common to both, and hence the completion of the definition of Γ .

Thus, define the convex functional,

$$\Phi(u) = \frac{1}{2} \int_G \epsilon |\nabla u|^2 + \int_G H(\cdot, u) - \int_G (k_1 - f(\cdot, 0))u, \quad (3.3)$$

where

$$H(x, \theta) = \int_0^\theta [f(x, s) - f(x, 0)] ds \geq 0, \quad (3.4)$$

$$f(x, s) = e^{s-v(x)} - e^{w(x)-s} \quad (3.5)$$

for a given pair v, w . U and U_h minimize this functional over $\bar{u} + H_{0, \Sigma_D}^1$ and $\bar{u}_I + S_h$, respectively. Here, H_{0, Σ_D}^1 is the completion of $C_0^\infty(G \cup \Sigma_D)$ in the norm defined by (2.10) and $S_h \subset H_{0, \Sigma_D}^1$. In particular,

$$\Phi(U) \leq \Phi(\bar{u}), \quad \Phi(U_h) \leq \Phi(\bar{u}_I). \quad (3.6)$$

H^1 estimates, and hence a proper bound for the definition of Γ , are obtained for $u = U$ and $u = U_h$ from

$$\frac{1}{2} \inf \epsilon \int_G |\nabla u|^2 \leq \Phi(u) - \int_G H(\cdot, u) + \int_G (k_1 - f(\cdot, 0))u$$

$$\leq \max(\Phi(\bar{u}), \Phi(\bar{u}_I)) + \frac{1}{2} \int_G |k_1 - f(\cdot, 0)|^2 + \frac{1}{2} \int_G |u| \quad (3.7)$$

The second and third terms are estimated from the maximum principles, and the assumption $k_1 \in L_\infty(G)$. Now $\Phi(\bar{u}_I) \leq \Phi_0$, independent of h , a fact which follows from (cf. [13, p. 85] and [24]):

$$\begin{aligned} \|\nabla(\bar{u}_I)\|_{L_\infty} &\leq \|\nabla(\bar{u} - \bar{u}_I)\|_{L_\infty} + \|\nabla\bar{u}\|_{L_\infty} \\ &\leq \frac{Ch^2}{\min_{i=1, \dots, M} h_i} |\bar{u}|_{W^{2, \infty}} + \|\nabla\bar{u}\|_{L_\infty}, \end{aligned} \quad (3.8)$$

and the third part of Assumption 2, whereby $\min h_i \geq h_0 h$. It follows that gradient estimates, and hence H^1 estimates, are uniformly obtainable for the continuous and discrete problems. This completes the discussion concerning the definition of \mathbf{T}_n .

3.3 Linear and gradient approximation theory

Prior to describing the approximation properties of \mathbf{T}_n , it is essential to discuss the linear approximation properties of the H_{0, Σ_D}^1 projection \mathbf{Q}_h onto S_h . For $H^{1+\theta}(G) \cap H_{0, \Sigma_D}^1(G)$ functions, with uniform norm bound in this space, interpolation space theory (cf. [3]) gives a uniform h^θ estimate, as measured in H^1 , provided the approximation process is capable of yielding an $O(h)$ estimate for $H^2(G) \cap H_{0, \Sigma_D}^1$. Although detailed results for the latter estimate are not available in the literature, the general procedure is described adequately in [24]: the piecewise linear interpolant of an extension/smoothing process gives the requisite energy upper bound, but the smoothing should be done only in the tangential variables on Σ_D , so that the smoothed function also vanishes on Σ_D . This can be made precise by a decomposition of the polygonal boundary of G , according to edges and internal boundaries of Σ_D , with an accompanying finite partition of unity for G (see [6, §4] for an illustration of how this can be done). The partition of unity sets are then translated and rotated into canonical position. The extension process uses a variant of the Calderón extension operator, applied to cylindrical translation/rotation domains and canonical variables, for Σ_N “cylindrical” cross sections. For Σ_D cross sections, the extension is the trivial zero extension. The entire extended function may be reassembled, via the partition of unity. The smoothing can also be carried out in the canonical variables if desired. The Fourier transform is applied only in the tangential variables for Σ_D cross sections to estimate the smoothing error, via Strang’s argument. In estimating the piecewise linear interpolation error relative to the smoothing, we note that interpolation is *also* specified on Σ_N . It is assumed, in the sense that the arguments require it, that the topology of Σ_D and Σ_N allows for the mechanics sketched above for the extension. This completes the $O(h)$ estimate, and interpolation space theory now applies. Improved estimates, based upon graded meshes as currently employed in the $h-p$ theory, tend not to be uniform over Sobolev classes, and do not appear to be applicable here. We are not aware either, of maximum principles for $p > 1$.

The next result is a generic result for gradient equations which will be used to deduce the approximation properties of U_h .

Proposition 3.1 *Suppose $a(\cdot, \cdot)$ is a continuous symmetric bilinear form on H^1 , L_2 coercive on H_{0,Σ_D}^1 . For $u \in H^1$, let $F(u)$ denote the continuous linear functional on H_{0,Σ_D}^1 defined by*

$$F(u)(v) = \int_G f(\cdot, u)v \quad (3.9)$$

for f increasing in its second argument and $\partial f(\cdot, s)/\partial s \leq C$. Suppose that u and u_h satisfy the gradient relations

$$a(u, v) + F(u)(v) = \langle g, v \rangle \quad \forall v \in H_{0,\Sigma_D}^1, \quad (3.10)$$

$$a(u_h, v_h) + F(u_h)(v_h) = \langle g, v_h \rangle \quad \forall v_h \in S_h, \quad (3.11)$$

where $u \in \bar{u} + H_{0,\Sigma_D}^1$, $u_h \in \bar{u}_I + S_h$, $\bar{u} \in C^2(\bar{G})$. Here, $g \in L_2$ is prescribed. Then there exist constants C_1 and C_2 , independent of h , such that

$$a(u - u_h, u - u_h) \leq C_1 \inf_{v_h \in S_h} a(u - \bar{u}_I - v_h, u - \bar{u}_I - v_h) + C_2 \|\bar{u} - \bar{u}_I\|_{H^1}^2. \quad (3.12)$$

Proof. The first step is the reduction to the case $\bar{u} \mapsto \bar{u}_I$. By this is meant that there is no loss of generality in assuming that the boundary function in (3.10) may be taken to be \bar{u}_I . Denoting the solutions of the corresponding gradient equations with boundary data \bar{u}, \bar{u}_I , respectively, by

$$u_\phi = \phi + \bar{u}, \quad u_\psi = \psi + \bar{u}_I, \quad \phi, \psi \in H_{0,\Sigma_D}^1, \quad (3.13)$$

we obtain, upon subtraction and setting $v = \phi - \psi$,

$$a(\phi - \psi, \phi - \psi) + [F(u_\phi) - F(u_\psi)](u_\phi - u_\psi) = -a(\bar{u} - \bar{u}_I, \phi - \psi) + [F(u_\phi) - F(u_\psi)](\bar{u} - \bar{u}_I).$$

By the continuity and L_2 -coerciveness properties of $a(\cdot, \cdot)$ and the monotonicity and derivative properties of f we deduce that

$$a(\phi - \psi, \phi - \psi) \leq c \|\bar{u} - \bar{u}_I\|_{H^1}^2 \quad (3.14)$$

for some constant c , which depends only on the bound for $\partial f/\partial s$ and the L_2 coerciveness constant of $a(\cdot, \cdot)$.

The second step is the consideration of (3.10) and (3.11) with \bar{u} replaced by \bar{u}_I in (3.10). We shall show that (note that u_ψ above is here identified as u)

$$a(u - u_h, u - u_h) \leq C_1 \inf_{v_h \in S_h} a(u - \bar{u}_I - v_h, u - \bar{u}_I - v_h), \quad (3.15)$$

which, with (3.14), will yield (3.12). We begin with

$$\begin{aligned} & \frac{1}{2}a(u - u_h - v_h, u - u_h - v_h) + F(u)(u - u_h - v_h) - F(u_h)(u - u_h - v_h) \\ &= \frac{1}{2}a(u - u_h, u - u_h) + [F(u) - F(u_h)](u - u_h) + \frac{1}{2}a(v_h, v_h) \\ & - a(u - u_h, v_h) - [F(u) - F(u_h)](v_h) \\ & \geq \frac{1}{2}a(u - u_h, u - u_h), \end{aligned}$$

which follows from the weak relations (3.10, 3.11), the assumed monotonicity of f , and the nonnegativity of $a(v_h, v_h)$. It follows that, for arbitrary $\delta > 0$,

$$a(u - u_h, u - u_h) \leq a(u - u_h - v_h, u - u_h - v_h) + \delta C^2 \|u - u_h\|_{L_2}^2 + \delta^{-1} \|u - u_h - v_h\|_{L_2}^2$$

when C bounds $\partial f / \partial s$. Since $u - u_h$ vanishes on Σ_D , we may choose δ so that (L_2 coerciveness of $a(\cdot, \cdot)$)

$$\delta C^2 \|u - u_h\|_{L_2}^2 \leq \frac{1}{2} a(u - u_h, u - u_h).$$

Since $u - u_h - v_h$ vanishes on Σ_D , it follows that

$$a(u - u_h, u - u_h) \leq C_1 a(u - u_h - v_h, u - u_h - v_h)$$

for all $v_h \in S_h$. The identification $u_h + v_h \mapsto v_h + \bar{u}_I$ now yields (3.15). This concludes the proof.

3.4 Convergence properties of \mathbf{T}_n

On the basis of (3.12), we may assume that there exists an approximation order for U_h, v_h , and w_h :

$$\|U - U_h\|_{H^1} \leq Ch^\theta, \quad \|v - v_h\|_{H^1} \leq Ch^\theta, \quad \|w - w_h\|_{H^1} \leq Ch^\theta, \quad (3.16)$$

for some constant C and $0 < \theta \leq 1$. Here, θ is the regularizing index introduced in Assumption 1 of §2. Note that the second term on the right-hand side of (3.12) is of order h^2 , as remarked earlier.

We may now close this section with a description of the approximation properties of \mathbf{T}_n .

Theorem 3.1 *The estimate*

$$\|(\mathbf{T} - \mathbf{T}_n)[\tilde{v}, \tilde{w}]\| \leq Ch^\theta \quad (3.17)$$

holds for some constant C , uniformly over the domain Ω on which \mathbf{T} and \mathbf{T}_n are defined. The approximation estimates (3.16) are assumed as described in §3.3.

Proof. The proof is a routine application of the triangle inequality:

$$\|(\mathbf{V} \circ \mathbf{U} - \mathbf{V}_h \circ \mathbf{U}_h)[\tilde{v}, \tilde{w}]\| \leq \|(\mathbf{V} - \mathbf{V}_h)U\| + \|\mathbf{V}_h(U - U_h)\|, \quad (3.18)$$

with a similar inequality for the second component.

The estimation of the first of the terms on the right-hand side of (3.18) is governed by (3.16). The estimation of the second term may proceed once an appropriate Lipschitz constant $L_{\mathbf{V}}$ is determined for \mathbf{V} , since \mathbf{V}_h is the composition of a bounded projection with \mathbf{V} . This is discussed at the beginning of Appendix D. Thus, we have

$$\|\mathbf{V}_h U - \mathbf{V}_h U_h\| \leq L_V \|U - U_h\|. \quad (3.19)$$

An application of (3.16)–(3.19) concludes the proof.

4 Existence and convergence of discretized solutions

4.1 The abstract calculus

Let E be a Banach space and \mathbf{T} a mapping from an open set Ω into E . We assume the existence of a fixed point x_0 for \mathbf{T} :

$$\mathbf{T}x_0 = x_0. \quad (4.1)$$

If $\{E_n\}$ denotes a sequence of subspaces of E of dimension $r(n) \geq n$, suppose that $\mathbf{T}_n : \Omega_n \mapsto E_n$, $\Omega_n := \Omega \cap E_n$, has a fixed point:

$$\mathbf{T}_n x_n = x_n. \quad (4.2)$$

Finally, let $\{\mathbf{P}_n\}$ be a family of linear projections onto E_n . We shall describe here the framework of the calculus developed by Krasnosel'skii et al. [20] for the convergence of the solutions of discretizations of fixed point equations (4.2) to the solutions of the original fixed point equation (4.1). First, we demonstrate that for sufficiently small meshwidth h , a solution x_n to the discretized problem (4.2) exists close to all solutions x_0 to the original problem (4.1). Second, we show that for sufficiently small meshwidth h , a solution x_0 to the original problem (4.1) exists close to all solutions x_n to the discretized problem (4.2).

Our first convergence result follows through Theorem 19.1 in [20, Thm. 19.1], as quoted below.

Theorem 4.1 *Let the operators \mathbf{T} and $\mathbf{P}_n \mathbf{T}$ be Fréchet-differentiable in Ω , and \mathbf{T}_n Fréchet-differentiable in Ω_n . Assume that (4.1) has a solution $x_0 \in \Omega$ and the linear operator $\mathbf{I} - \mathbf{T}'(x_0)$ is continuously invertible in E . Let*

$$\|\mathbf{P}_n(x_0) - x_0\| \rightarrow 0,$$

$$\|\mathbf{P}_n \mathbf{T} \mathbf{P}_n x_0 - \mathbf{T} x_0\| \rightarrow 0, \quad \|\mathbf{P}_n \mathbf{T}'(\mathbf{P}_n x_0) - \mathbf{T}'(x_0)\| \rightarrow 0,$$

$$\|[\mathbf{T}_n - \mathbf{P}_n \mathbf{T}] \mathbf{P}_n x_0\| \rightarrow 0, \quad \|[\mathbf{T}'_n - (\mathbf{P}_n \mathbf{T})'](\mathbf{P}_n x_0)\| \rightarrow 0,$$

as $n \rightarrow \infty$. Finally, assume that for any $\epsilon > 0$ there exist n_ϵ and $\delta_\epsilon > 0$ such that

$$\|\mathbf{T}'_n(x) - \mathbf{T}'_n(\mathbf{P}_n x_0)\| \leq \epsilon \quad \text{for } (n \geq n_\epsilon; \|x - \mathbf{P}_n x_0\| \leq \delta_\epsilon, x \in \Omega_n). \quad (4.3)$$

Then there exist n_0 and $\delta_0 > 0$ such that, when $n \geq n_0$, equation (4.2) has a unique solution x_n in the ball $\|x - x_0\| \leq \delta_0$. Moreover,

$$\|x_n - x_0\| \leq \|[\mathbf{I} - \mathbf{P}_n]x_0\| + \|x_n - \mathbf{P}_n x_0\| \rightarrow 0 \quad \text{as } n \rightarrow \infty \quad (4.4)$$

and $\|x_n - \mathbf{P}_n x_0\|$ satisfies the following two-sided estimate ($c_1, c_2 > 0$):

$$c_1 \|\mathbf{P}_n \mathbf{T} x_0 - \mathbf{T}_n \mathbf{P}_n x_0\| \leq \|x_n - \mathbf{P}_n x_0\| \leq c_2 \|\mathbf{P}_n \mathbf{T} x_0 - \mathbf{T}_n \mathbf{P}_n x_0\|. \quad (4.5)$$

Note that in this theorem the actual rate of convergence depends only on the terms in the two sided estimate (4.5). The additional convergence assumptions need not hold with this same rate.

Next, we assert that for sufficiently fine meshwidth h a solution x^* to (4.1) exists close to the solution x_n to the discretized problem (4.2). From [20] we cite Theorem 19.2 as stated in the following theorem.

Theorem 4.2 *Let the operators $\mathbf{T}, \mathbf{P}_n \mathbf{T}$, and \mathbf{T}_n be Fréchet differentiable in some neighborhood of the point $\tilde{x}_n \in \Omega_n$, and $\mathbf{I} - \mathbf{T}'_n(\tilde{x}_n)$ continuously invertible in E_n ,*

$$\|[\mathbf{I} - \mathbf{T}'_n(\tilde{x}_n)]^{-1}\| = \kappa_n.$$

Let

$$\gamma_n \equiv (1 + \kappa_n \|\mathbf{P}_n \mathbf{T}'(\tilde{x}_n)\|) \|[\mathbf{T}' - \mathbf{P}_n \mathbf{T}'](\tilde{x}_n)\| + \kappa_n \|[\mathbf{T}'_n - \mathbf{P}_n \mathbf{T}'](\tilde{x}_n)\| < 1,$$

and for some δ_n and q_n ($\delta_n > 0; 0 < q_n < 1$),

$$\sup_{\|x - \tilde{x}_n\| \leq \delta_n} \|\mathbf{T}'(x) - \mathbf{T}'(\tilde{x}_n)\| \leq \frac{q_n}{\kappa'_n},$$

$$\|\tilde{x}_n - \mathbf{T}\tilde{x}_n\| \leq \frac{\delta_n(1 - q_n)}{\kappa'_n},$$

where

$$\kappa'_n = \frac{1 + \kappa_n \|\mathbf{P}_n \mathbf{T}'(\tilde{x}_n)\|}{1 - \gamma_n}.$$

Then (4.1) has a unique solution x_0 in the ball $\|x - \tilde{x}_n\| \leq \delta_n$, and we have the error estimate

$$\frac{\alpha_n}{1 + q_n} \leq \|\tilde{x}_n - x_0\| \leq \frac{\alpha_n}{1 - q_n}, \quad (4.6)$$

where

$$\alpha_n \equiv \|[\mathbf{I} - \mathbf{T}'(\tilde{x}_n)]^{-1}(\tilde{x}_n - \mathbf{T}\tilde{x}_n)\| \leq \kappa'_n \|\tilde{x}_n - \mathbf{T}\tilde{x}_n\|.$$

Again the actual rate of convergence depends only on the terms in the two sided estimate (4.6) while the additional convergence assumptions need not hold with this same rate.

Also, $\tilde{x}_n = x_n$ is not required.

4.2 The application to the semiconductor problem: General setting

We set $E = \prod_1^2 H^1(G)$ and $E_n = \text{linear span } \{\bar{V}_I, S_h\} \otimes \text{linear span } \{\bar{W}_I, S_h\}$ with \mathbf{P}_n the orthogonal projection onto E_n . The domain Ω of the map \mathbf{T} has been defined in tandem with the composition maps defining \mathbf{T} in §2. \mathbf{T}_n has been defined in §3; for consistency with §4.1 we may wish to consider \mathbf{T}_n as restricted to Ω_n , but this is unimportant. Fixed points of \mathbf{T} were demonstrated

to exist in [8]; parallel arguments yield fixed points of \mathbf{T}_n as well, via an application of Brouwer's fixed point theorem applied to $\bar{\Omega} \cap E_n$. The continuity of this restriction map follows from the continuity of \mathbf{U}_h , since \mathbf{Tr} , \mathbf{V}_h , and \mathbf{W}_h are seen to be continuous from elementary considerations. In turn, the continuity of \mathbf{U}_h follows the proof of the continuity of \mathbf{U} (cf. Lemma 4.3 of [8]). We may assume, then, the existence of fixed points of \mathbf{T}_n .

An important approximation property of \mathbf{P}_n on the union of the convex hull, $\text{co } R_{\mathbf{T}}$, of the range of \mathbf{T} , with $H^{1+\theta}(G) \cap H_{0,\Sigma_D}^1(G)$, is

$$\|\mathbf{P}_n \tau - \tau\|_{H^1} \leq ch^\theta, \quad \|\tau\|_{H^{1+\theta}} \leq 1. \quad (4.7)$$

This is a consequence of Proposition 3.1 and the assumption embodied in (3.16). Note that, in (4.7), τ is a member of the set, $\text{co } R_{\mathbf{T}} \cup (H^{1+\theta} \cap H_{0,\Sigma_{D22}}^1)$. The reason \mathbf{P}_n does not involve affine projection is for consistency with the abstract calculus discussed in §4.1, where linear, not affine, subspaces are employed.

4.3 Verification of the a priori estimates

The following lemma affords a verification of the hypotheses of Theorem 4.1 for the semiconductor application. The properties concerning \mathbf{T}' and \mathbf{T}'_n will be found in the appendix. It is assumed throughout that the Euclidean dimension N satisfies $N \leq 3$.

Lemma 4.1 *For the mapping \mathbf{T} and the piecewise linear finite element projection \mathbf{P}_n*

$$\|\mathbf{P}_n \mathbf{T} \mathbf{P}_n x_0 - \mathbf{T} x_0\| \rightarrow 0, \quad (4.8)$$

$$\|\mathbf{P}_n \mathbf{T}'(\mathbf{P}_n x_0) - \mathbf{T}'(x_0)\| \rightarrow 0, \quad (4.9)$$

$$\|[\mathbf{T}_n - \mathbf{P}_n \mathbf{T}] \mathbf{P}_n x_0\| \rightarrow 0, \quad (4.10)$$

$$\|[\mathbf{T}'_n - (\mathbf{P}_n \mathbf{T})'](\mathbf{P}_n x_0)\| \rightarrow 0, \quad (4.11)$$

while for any $\epsilon > 0$ there exist n_ϵ and $\delta_\epsilon > 0$ such that

$$\|\mathbf{T}'_n(x) - \mathbf{T}'_n(\mathbf{P}_n x_0)\| \leq \epsilon \quad \text{for } (n \geq n_\epsilon; \|x - \mathbf{P}_n x_0\| \leq \delta_\epsilon, x \in \Omega_n). \quad (4.12)$$

Proof. By the triangle inequality,

$$\begin{aligned} \|\mathbf{P}_n \mathbf{T} \mathbf{P}_n x_0 - \mathbf{T} x_0\| &\leq \|\mathbf{P}_n \mathbf{T} \mathbf{P}_n x_0 - \mathbf{P}_n \mathbf{T} x_0\| + \|\mathbf{P}_n \mathbf{T} x_0 - \mathbf{T} x_0\| \\ &= \|\mathbf{P}_n \mathbf{T}(\mathbf{P}_n x_0 - x_0)\| + \|(\mathbf{P}_n - \mathbf{I})\mathbf{T} x_0\| \end{aligned}$$

and both terms tend to zero, the first because $\mathbf{P}_n x_0 \rightarrow x_0$ and \mathbf{P}_n and \mathbf{T} are continuous, the second because $\mathbf{P}_n x_0 \rightarrow x_0$. Thus, (4.8) follows. For the derivative mapping $\mathbf{T}'(x) : f \mapsto g$ we have

$$\begin{aligned} \|[\mathbf{P}_n \mathbf{T}'(\mathbf{P}_n x_0) - \mathbf{T}'(x_0)]f\| &\leq \|[\mathbf{P}_n - \mathbf{I}]\mathbf{T}'(\mathbf{P}_n x_0)f\| + \|[\mathbf{T}'(\mathbf{P}_n x_0) - \mathbf{T}'(x_0)]f\| \\ &\leq c * h^\theta \|\mathbf{T}'(\mathbf{P}_n x_0)f\|_{H^{1+\theta}} + L_{\mathbf{T}'} \|[\mathbf{P}_n - \mathbf{I}]x_0\| \|f\|. \end{aligned}$$

Here we have used (4.7) and the Lipschitz continuity and uniform boundedness in x of the derivative mapping $\mathbf{T}'(x)$ (cf. Appendix D). Relation (4.9) follows from the H^1 convergence of \mathbf{P}_n to \mathbf{I} on $co R_{\mathbf{T}}$. To prove (4.10) we observe that

$$\|[\mathbf{T}_n - \mathbf{P}_n \mathbf{T}] \mathbf{P}_n x_0\| \leq \|[\mathbf{T}_n - \mathbf{T}] \mathbf{P}_n x_0\| + \|[\mathbf{I} - \mathbf{P}_n] \mathbf{T} \mathbf{P}_n x_0\|$$

and the uniform approximation by \mathbf{T}_n on bounded sets as well as the H^1 convergence of \mathbf{P}_n to \mathbf{I} on $co R_{\mathbf{T}}$ imply that the right-hand side tends to zero. The proof of (4.11) proceeds by the addition and subtraction of the term $\mathbf{T}'(\mathbf{P}_n x_0)$, and the application of the triangle inequality. The uniform approximation by \mathbf{T}'_n (cf. Appendix D) and the convergence of \mathbf{P}_n to \mathbf{I} on $H^{1+\theta} \cap H^1_{0,\Sigma_D}$ completes the proof. Note that $(\mathbf{P}_n \mathbf{T})' = \mathbf{P}_n \mathbf{T}'$ is used here. Inequality (4.12) is a restatement of the uniform continuity of \mathbf{T}'_n in n (Appendix D). This concludes the proof.

4.4 Verification of the a posteriori estimates

The following lemma addresses the hypotheses of Theorem 4.2 for the semiconductor application. It is assumed throughout that the Euclidean dimension N satisfies $N \leq 3$.

Lemma 4.2 *Let the operators $\mathbf{T}, \mathbf{P}_n \mathbf{T}$, and \mathbf{T}_n be as defined before. Let $\mathbf{I} - \mathbf{T}'_n(\tilde{x}_n)$ be continuously invertible in E_n at the approximate solution \tilde{x}_n to (4.2), and let*

$$\|[\mathbf{I} - \mathbf{T}'_n(\tilde{x}_n)]^{-1}\| = \kappa_n \leq \kappa. \quad (4.13)$$

Then for a sufficiently small meshwidth h

$$\gamma_n \equiv (1 + \kappa_n \|\mathbf{P}_n \mathbf{T}'(\tilde{x}_n)\|) \|[\mathbf{T}' - \mathbf{P}_n \mathbf{T}'](\tilde{x}_n)\| + \kappa_n \|[\mathbf{T}_n - \mathbf{P}_n \mathbf{T}]'(\tilde{x}_n)\| < 1. \quad (4.14)$$

If $\|\tilde{x}_n - x_n\| \leq Ch^\theta$, where C does not depend on h , then there exist δ_n and q_n ($\delta_n > 0$; $0 < q_n < 1$) such that

$$\sup_{\|x - \tilde{x}_n\| \leq \delta_n} \|\mathbf{T}'(x) - \mathbf{T}'(\tilde{x}_n)\| \leq \frac{q_n}{\kappa'_n}, \quad (4.15)$$

$$\|\tilde{x}_n - \mathbf{T}\tilde{x}_n\| \leq \frac{\delta_n(1 - q_n)}{\kappa'_n} = ch^\theta, \quad (4.16)$$

where

$$\kappa'_n = \frac{1 + \kappa_n \|\mathbf{P}_n \mathbf{T}'(\tilde{x}_n)\|}{1 - \gamma_n}.$$

Proof. The bound on γ_n as stated in (4.14) is proven through

$$\begin{aligned} \gamma_n &\equiv (1 + \kappa_n \|\mathbf{P}_n \mathbf{T}'(\tilde{x}_n)\|) \|[\mathbf{T}' - \mathbf{P}_n \mathbf{T}'](\tilde{x}_n)\| + \kappa_n \|[\mathbf{T}_n - \mathbf{P}_n \mathbf{T}]'(\tilde{x}_n)\| \\ &\leq (1 + \kappa_n \|\mathbf{P}_n \mathbf{T}'(\tilde{x}_n)\|) Ch^\theta \|\mathbf{T}'(\tilde{x}_n)\|_{H^1, H^{1+\theta}} + \kappa_n \|[\mathbf{T}_n - \mathbf{P}_n \mathbf{T}]'(\tilde{x}_n)\| \\ &\leq C * h^\theta. \end{aligned}$$

Here the last inequality follows completely analogously to the bounds in Lemma 4.1 and C is a generic constant.

The existence of a finite δ_n and q_n ($\delta_n > 0$; $0 < q_n < 1$), such that (4.15) and (4.16) hold follows because

$$\sup_{\|x - \tilde{x}_n\| \leq \delta_n} \|\mathbf{T}'(x) - \mathbf{T}'(\tilde{x}_n)\| \leq L_{\mathbf{T}'} \|x - \tilde{x}_n\| \leq L_{\mathbf{T}'} \delta_n,$$

so that we can choose $q_n = L_{\mathbf{T}'} \delta_n \kappa_n'$. On the other hand, x_n is a fixed point of \mathbf{T}_n and therefore

$$\begin{aligned} \|\tilde{x}_n - \mathbf{T}\tilde{x}_n\| &\leq \|\tilde{x}_n - x_n\| + \|\mathbf{T}_n x_n - \mathbf{T}x_n\| + \|\mathbf{T}x_n - \mathbf{T}\tilde{x}_n\| \\ &\leq (1 + L_{\mathbf{T}})\|\tilde{x}_n - x_n\| + \|\mathbf{T}_n - \mathbf{T}\| \|x_n\| \\ &\leq C * h^\theta. \end{aligned}$$

This implies that (4.16) holds provided that

$$\delta_n = C * h^\theta * \frac{\kappa_n'}{(1 - q_n)}.$$

The proof is concluded if we can show that the choices

$$q_n = L_{\mathbf{T}'} \kappa_n' \delta_n, \quad \delta_n = Ch^\theta \kappa_n' / (1 - q_n)$$

are compatible with the requirement $q_n < 1$. Thus, set $\alpha = L_{\mathbf{T}'} \kappa_n'$, $\beta = Ch^\theta \kappa_n'$. We have

$$-\alpha \delta_n^2 + \delta_n - \beta = 0$$

or

$$\alpha \delta_n = \frac{1}{2} (1 \pm \sqrt{1 - 4\alpha\beta}).$$

Provided β is sufficiently small so that $\alpha\beta \leq \frac{1}{4}$, we may choose $\delta_n \leq 1/(2\alpha)$ so that $q_n \leq \frac{1}{2}$. Note that, the bounds for κ_n' and γ_n show that κ_n' remains bounded as h decreases so that the bound $\alpha\beta \leq \frac{1}{4}$ does not depend on h . This concludes the proof.

4.5 Summary of results

The following corollary expresses a summary of the major results in conjunction with the employed hypotheses.

Corollary 4.1 *Assume the regularization hypothesis expressed in Assumption 1 of §2.3. Let x_0 be a fixed point of \mathbf{T} and suppose that $\mathbf{T}'(x_0)$ does not possess 1 as an eigenvalue. Then there exist an index n_0 and a neighborhood of x_0 containing fixed points x_n of \mathbf{T}_n , $n \geq n_0$, satisfying*

$$\|x_0 - x_n\| \leq Ch^\theta. \quad (4.17)$$

Here C is a constant independent of n and h . Conversely, suppose $\{\tilde{x}_n\}$ is a sequence of approximate fixed points of \mathbf{T}_n satisfying $\|\tilde{x}_n - x_n\| \leq ch^\theta$ and (4.13). Then, under the regularity hypothesis, there exists a fixed point x_0 of \mathbf{T} such that

$$\|x_0 - \tilde{x}_n\| \leq Ch^\theta \quad \forall n. \quad (4.18)$$

Here C is a constant independent of n and h . In all cases $N \leq 3$.

Proof. Estimates (4.17) and (4.18) follow from the conjunction of (4.4) with (4.5), and from (4.6), respectively. The former two inequalities must be appropriately combined with the triangle inequality

$$\|\mathbf{P}_n \mathbf{T} x_0 - \mathbf{T}_n \mathbf{P}_n x_0\| \leq \|(\mathbf{P}_n - \mathbf{I}) \mathbf{T} x_0\| + \|\mathbf{T} x_0 - \mathbf{T} \mathbf{P}_n x_0\| + \|(\mathbf{T} - \mathbf{T}_n) \mathbf{P}_n x_0\|,$$

which yields order h^θ convergence upon use of the Lipschitz continuity of \mathbf{T} , and the convergence properties of \mathbf{P}_n and \mathbf{T}_n . Inequality (4.6) must be supplemented by

$$\frac{\alpha_n}{1 - q_n} \leq \left(\frac{\kappa'_n}{1 - q_n} \right) \|\tilde{x}_n - \mathbf{T} \tilde{x}_n\| \leq \delta_n.$$

The choice, $\delta_n = Ch^\theta \kappa'_n / (1 - q_n)$ and the boundedness of κ'_n and $1/(1 - q_n)$ are discussed in the proof of Lemma 4.2. The hypotheses of the corollary absorb those of Theorems 4.1 and 4.2 due to the compactness of $\mathbf{T}'(x_0)$. This concludes the proof. *Remark 4.1.* Estimates of order h^θ follow from Corollary 4.1 for $\|v - v_h\|$ and $\|w - w_h\|$, if $[v, w]$ and $[v_h, w_h]$ are fixed points of \mathbf{T} and \mathbf{T}_n , respectively. Estimates for $\|U - U_h\|$ follow immediately from

$$\|\mathbf{U}(v, w) - U_h\| \leq \|\mathbf{U}(v, w) - \mathbf{U}(v_h, w_h)\| + \|\mathbf{U}(v_h, w_h) - U_h\|,$$

the Lipschitz property of \mathbf{U} , and (3.16), which provides the estimate for the second term on the right-hand side.

Appendix. In Appendices A and B we shall discuss the continuity and compactness properties of \mathbf{U} , \mathbf{V} , \mathbf{W} and their Fréchet derivatives. In Appendix C we shall discuss these for \mathbf{U}_h (\mathbf{V}_h and \mathbf{W}_h are straightforward). Results such as Lemma (B.2), are valid in terms of quasi-Fermi levels but not in terms of Slotboom variables. This is the incentive to define the mapping \mathbf{T} in the space of pairs of quasi-Fermi levels, rather than in the space of pairs of Slotboom variables. L_∞ bounds will be implicit in the various results derived below. As we have noted in the introduction, only the statements of the lemmas are given. For the proofs, the reader may consult the monograph [12].

A The map \mathbf{U}

We begin with a result which is a slight sharpening of Lemma 4.1 of [8]. It will be used in the proof of Lemma A.2. The domain of \mathbf{U} in both of these lemmas is a bounded subset of $\prod_1^2 L_\infty$.

Lemma A.1 *Let $\mathbf{U} : (v, w) \rightarrow u$ be defined through the solution of the boundary value problem*

$$\langle \nabla u, \nabla \phi \rangle + \langle e^{u-v} - e^{w-u} - k_1, \phi \rangle = 0.$$

Then \mathbf{U} is continuous from L_2 into L_2 . In fact, it is Lipschitz continuous into H^1 .

Lemma A.2 *Let $\mathbf{U} : (v, w) \mapsto u$ be the mapping defined implicitly through the solution of the boundary value problem*

$$\langle \nabla u, \nabla \phi \rangle + \langle e^{u-v} - e^{w-u} - k_1, \phi \rangle = 0, \quad (\text{A.1})$$

where $\phi \in H_{0,\Sigma_D}^1$, subject to suitable mixed boundary conditions in N dimensions. Then the derivative $D_{(v,w)}\mathbf{U}(v, w) : (\sigma, \tau) \mapsto \mu$ is defined through the solution of the boundary value problem

$$\langle \nabla \mu, \nabla \phi \rangle + \langle e^{u-v}[\mu - \sigma] + e^{w-u}[\mu - \tau], \phi \rangle = 0, \quad (\text{A.2})$$

where $\mu|_{\Sigma_D} \equiv 0$, $\phi|_{\Sigma_D} \equiv 0$, and for all (v, w) is a uniformly bounded linear mapping from L_2 to H_{0,Σ_D}^1 , and, in particular, compact from L_2 into L_q , $q < [1/2 - 1/N]^{-1}$ if $N \geq 3$ and $q < \infty$ if $N = 2$. The mapping is also uniformly bounded from H^1 to L_∞ if $N \leq 3$. Moreover, the mapping $(v, w) \mapsto D_{(v,w)}\mathbf{U}(v, w)$ is Lipschitz continuous from H^1 to the mappings from L_2 to H_{0,Σ_D}^1 if $N \leq 4$.

This lemma is proven in the Appendix of [12].

B The mappings \mathbf{V} and \mathbf{W}

In [12] it is shown that the mappings \mathbf{V} and \mathbf{W} are continuous from H^1 to itself as stated below.

Lemma B.1 *For $i = 1, 2$, and $u_i \in H^1$ satisfying the maximum principle (2.8), and the boundary conditions, let v_i be the solution to the weak formulation of the mixed boundary value problem*

$$\nabla \cdot (e^{u_i - v_i} \nabla v_i) = 0, \quad (\text{B.1})$$

on G . Then

$$\int_G e^{u_1 - v_1} |\nabla(v_2 - v_1)|^2 dx \leq \int_G e^{u_1 - v_1} |\nabla(u_2 - u_1)|^2 dx, \quad (\text{B.2})$$

and therefore the mapping \mathbf{V} from u to v defined through (B.1) is Lipschitz continuous from H^1 to itself on the range of \mathbf{U} .

Remark. The derivative $D\mathbf{V}(u) : \mu \mapsto \sigma$, is defined through solution of the boundary value problem

$$\langle e^{u-v}[(\mu - \sigma)\nabla v + \nabla \sigma], \nabla \phi \rangle = 0, \quad (\text{B.3})$$

where $\mu \in H^1$, and $\sigma \in H_{0,\Sigma_D}^1$. Here, ϕ is a test function in H_{0,Σ_D}^1 . For smooth v , the standard existence theory (cf. [4, Chap. 8]) yields a solution σ for $N \leq 3$. The proof of the lemma to follow, in which H^1 bounds for σ are determined in terms of μ , allows limits of v and σ , and hence solutions for $v \in H^1 \cap L_\infty$ as specified prior to Appendix A. Finally, the Moser iteration theory (cf. [4]) gives a priori L_∞ bounds on σ in terms of $H^1 \cap L_\infty$ bounds on μ . This is required in the proof of Lemma B.3.

Lemma B.2 *Let $u \in H^1 \cap L_\infty$ be given and, for $N \leq 3$, let v be the solution to the weak formulation of the mixed boundary value problem*

$$\nabla \cdot (e^{u-v} \nabla v) = 0$$

on G . Then the derivative $D\mathbf{V}$ of the mapping \mathbf{V} from u to v defined through this equation is uniformly bounded from H_{0,Σ_D}^1 to itself, and hence for each u , is compact from H_{0,Σ_D}^1 into L_2 .

Lemma B.3 *The derivative $D\mathbf{V}$ as defined by equation (B.3), is a locally Lipschitz continuous mapping from H^1 to the mappings from $H^1 \cap L_\infty$ to H_{0,Σ_D}^1 for Euclidean dimension $N \leq 3$. A similar statement holds for \mathbf{W} .*

C The Mapping \mathbf{U}_h

We begin with a continuity result for \mathbf{U}_h .

Lemma C.1 *The mapping \mathbf{U}_h , defined in §3.1, is Lipschitz continuous on its domain from L_2 to H^1 .*

Proof. The proof follows that of Lemma A.1.

We move now to the differentiability properties of \mathbf{U}_h .

Lemma C.2 *The derivative $D_{(v,w)}\mathbf{U}_h(v,w) : (\sigma, \tau) \mapsto \mu$ is defined through the solution of the projection relation,*

$$\langle \nabla \mu, \nabla \phi \rangle + \langle e^{U_h-v} [\mu - \sigma] + e^{w-U_h} [\mu - \tau], \phi \rangle = 0, \quad (\text{C.1})$$

where μ and ϕ are in S_h . The mapping $(v,w) \mapsto D_{(v,w)}\mathbf{U}_h(v,w)$ is Lipschitz continuous from H^1 to the mappings from L_2 to H^1 , for $N \leq 4$ with Lipschitz constant independent of h .

Proof. The proof follows that of Lemma A.2.

Lemma C.3 *The solutions $D_{(v,w)}\mathbf{U}(v,w)(\sigma, \tau) := \mu$ of (A.2) and $D_{(v,w)}\mathbf{U}_h(v,w)(\sigma, \tau) := \mu_h$ of (C.1) satisfy an estimate of the form*

$$\|\mu - \mu_h\| \leq Ch^\theta \|(\sigma, \tau)\|, \quad (\text{C.2})$$

where C does not depend upon h, v , or w . The norm used here is the H^1 norm.

This lemma is proven in [12].

D Summary of results for \mathbf{T} and \mathbf{T}_n

The mappings \mathbf{V}_h and \mathbf{W}_h are the simple compositions,

$$\mathbf{V}_h = \log \circ \mathbf{t}_{\bar{V}_I}^{-1} \circ \mathbf{Q}_h \circ \mathbf{V} \circ \mathbf{t}_{\bar{V}}, \quad \mathbf{W}_h = \log \circ \mathbf{t}_{\bar{W}_I}^{-1} \circ \mathbf{Q}_h \circ \mathbf{W} \circ \mathbf{t}_{\bar{W}},$$

where \mathbf{Q}_h is the projection of §3.3 and \mathbf{t} denotes the (negative) translation by the subscript variable. The properties of \mathbf{Q}_h , \mathbf{V} , and \mathbf{W} induce results for \mathbf{V}_h and \mathbf{W}_h parallel to those for \mathbf{U}_h as derived in Appendix C. The following results, used in the proofs of Lemmas 4.1 and 4.2, are a direct consequence of Appendices A–C and Assumption 1 of §2.3. $N \leq 3$ is required for the statements.

- \mathbf{T}' is Lipschitz continuous from Ω to the mappings from $\prod_1^2 H^1$ to $\prod_1^2 H_{0,\Sigma_D}^1$

This follows from an application of the chain rule to (2.7) in conjunction with Lemma A.2 and B.3.

- \mathbf{T}' is uniformly bounded over Ω as a linear mapping from $\prod_1^2 H^1$ to $\prod_1^2 (H^{1+\theta} \cap H_{0,\Sigma_D}^1)$.

This follows from Assumption 1 in conjunction with Lemma A.2 and B.2.

- \mathbf{T}'_n converges uniformly to \mathbf{T}'

This follows from Lemma C.3 and the corresponding result for \mathbf{V}_h and \mathbf{W}_h applied to (3.2).

- \mathbf{T}'_n is continuous, uniformly in n and elements of its domain.

This follows from Lemma C.2 and the corresponding result for \mathbf{V}_h and \mathbf{W}_h .

- $\mathbf{T}'(z)$ is compact, for each $z \in \Omega$, as a mapping from $\prod_1^2 H^1$ into $\prod_1^2 H_{0,\Sigma_D}^1$.

This follows from the boundedness assertions of Lemma A.2 and B.2, the regularization hypothesis inherent in Assumption 1 and the compact injection of $H^{1+\theta}$ into H^1 .

References

- [1] A. AZZAM AND E. KREYSZIG, *On solutions of elliptic equations satisfying mixed boundary conditions*, SIAM J. Math. Anal., 13 (1982), pp. 254–262.
- [2] R. E. BANK, D. J. ROSE, AND W. FICHTNER, *Numerical methods for semiconductor device simulation*, SIAM J. Sci. Statist. Comput., 4 (1983), pp. 416–435.
- [3] BERGH AND LÖFSTROM, *Interpolation Spaces*, Springer-Verlag, Berlin, New York, 1986.

- [4] D. GILBARG AND N. S. TRUDINGER, *Elliptic Partial Differential Equations of Second Order*, Springer-Verlag, Berlin, New York, 1983.
- [5] H. GUMMEL, *A self-consistent iterative scheme for one-dimensional steady state transistor calculations*, IEEE Trans. Electron. Devices, ED-11 (1964), pp. 455–465.
- [6] J. W. JEROME, *Asymptotic estimates of the \mathcal{L}_2 n -width*, J. Math. Anal. Appl., 22 (1968), pp. 449–464.
- [7] ———, *An adaptive newton algorithm based on numerical inversion: regularization as postconditioner*, Numer. Math., 47 (1985), pp. 123–138.
- [8] ———, *Consistency of semiconductor modelling: an existence/stability analysis for the stationary van Roosbroeck system*, SIAM J. Appl. Math., 45 (1985), pp. 565–590.
- [9] ———, *The role of semiconductor device diameter and energy-band bending in convergence of Picard iteration for Gummel’s map*, IEEE Trans. Elec. Dev., ED-32 (1985), pp. 2045–2051.
- [10] ———, *Newton’s method for gradient equations based upon the fixed point map*, Numer. Math., 55 (1989), pp. 619–632.
- [11] ———, *Algorithmic aspects of the hydrodynamic and drift-diffusion device models*, in Mathematical Modelling and Simulation of Electrical Circuits and Semiconductor Devices, R.E. Bank, R. Bulirsch and K. Merten, ed., International Series of Numerical Mathematics, Boston, MA, October 1990, Birkhäuser Verlag, Basel, pp. 217–236.
- [12] ———, *Analysis of charge Transport*, Springer, 1996.
- [13] C. JOHNSON, *Numerical Solutions of Partial Differential Equations by the Finite Element Method*, Cambridge University Press, London, 1987.
- [14] T. KERKHOVEN, *Coupled and Decoupled Algorithms for Semiconductor Simulation*, Ph.D. thesis, Yale University, 1985; Tech. report # 429.
- [15] ———, *A proof of convergence of Gummel’s algorithm for realistic boundary conditions*, SIAM J. Numer. Anal., 23 (1986), pp. 1121–1137.
- [16] ———, *A spectral analysis of the decoupling algorithm for semiconductor simulation*, SIAM J. Numer. Anal., 25 (1988), pp. 1299–1312.
- [17] ———, *On the effectiveness of Gummel’s method*, SIAM J. Sci. Statist. Comput., 9 (1988), pp. 48–60.
- [18] T. KERKHOVEN AND J. W. JEROME, *L_∞ Stability of Finite Element Approximations to Elliptic Gradient Equations*, Numer. Math., (1990).

- [19] T. KERKHOVEN AND Y. SAAD, *On Acceleration Methods for Systems of Coupled Nonlinear Partial Differential Equations*, Tech. report UIUCDCS-R-1363, University of Illinois, February 1989.
- [20] M. KRASNOSEL'SKII, G. VAINIKKO, P. ZABREIKO, Y. RUTITSKII, AND V. STETSENKO, *Approximate Solution of Operator Equations*, Wolters-Noordhoff, Groningen, 1972.
- [21] M. MOCK, *On equations describing steady-state carrier distributions in a semiconductor device*, Comm. Pure Appl. Math., 25 (1972), pp. 781–792.
- [22] M. MURTHY AND G. STAMPACCHIA, *A variational inequality with mixed boundary conditions*, Israel J. Math., 13 (1972), pp. 188–224.
- [23] T. I. SEIDMAN, *Steady state solutions of diffusion-reaction systems with electrostatic convection*, Nonlinear Anal. Theory, Methods, Appl., 4 (1980), pp. 623–637.
- [24] G. STRANG, *Approximation in the finite element method*, Numer. Math., 19 (1972), pp. 81–98.
- [25] G.-L. TAN, X.-L. YUAN, Q.-M. ZHANG, W. KU, AND A.-J. SHEY, *Two-dimensional semiconductor device analysis based on new finite-element discretization employing the S-G scheme*, IEEE Trans. on C.A.D., 5 (1989), pp. 468–478.
- [26] N. M. WIGLEY, *Asymptotic expansions at a corner of solutions of mixed boundary value problems*, J. Math. Mech., 13 (1964), pp. 549–576.