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A triangular mixed finite element method for the stationary semiconductor device equations


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A TRIANGULAR MIXED FINITE ELEMENT METHOD
FOR THE STATIONARY SEMICONDUCTOR DEVICE EQUATIONS (*)

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Abstract — A Petrov-Galerkin mixed finite element method based on triangular elements for
a self-adjoint second order elliptic system arising from a stationary model of a semiconductor
device is presented. This method is based on a novel formulation of the corresponding discrete
problem and can be regarded as a natural extension to two dimensions of the well-known
Scharfetter-Gummel one-dimensional scheme. Existence, uniqueness and stability of the
approximate solution are proved for an arbitrary triangular mesh and an error estimate is given
for an arbitrary Delaunay triangulation and its Dirichlet tesselation. No restriction is required on
the angles of the triangles in the mesh. The associated linear system has the same form as that
obtained from the conventional box method with an exponentially fitted approximation to the
coefficient function on each element. The evaluation of the terminal currents associated with the
method is also discussed and it is shown that the computed terminal currents are convergent and
conservative.

Résumé — On présente ici une méthode d'éléments fins mixte, de type Petrov-Galerkin,
basée sur des éléments triangulaires, pour un système elliptique auto-adjoint du second ordre,
émanant d'un modèle stationnaire pour des semiconducteurs. Cette méthode est basée sur une
nouvelle formulation du problème discret correspondant et peut être considérée comme une
extension bidimensionnelle naturelle de la méthode bien connue de Scharfetter-Gummel.
L'existence, l'unicité et la stabilité de la solution approchée sont établies pour un maillage
triangulaire arbitraire et une estimation de l'erreur est donnée pour une triangulation de Delaunay
arbitraire et sa tesselation de Dirichlet. Aucune restriction n'est imposée sur les angles des
triangles du maillage. Le système associé a la même forme que celle obtenue par la traditionnelle
« box-method » avec une approximation du coefficient de type exponentiel sur chaque élément.
On discute aussi l'évaluation des courants à travers les terminaux associés à cette méthode et on
démontre que les courants calculés sont convergents et conservatifs.

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1. INTRODUCTION

The stationary behaviour of semiconductor devices in two dimensions can be described by the following coupled system of nonlinear second-order elliptic partial differential equations [24].

\[ \varepsilon \nabla^2 \psi = \eta e^\psi - \rho e^{-\phi} - N \]  
(1.1)

\[ \nabla \cdot (\mu_n e^\phi \nabla \eta) = R(\psi, \eta, \rho) \]  
(1.2)

\[ \nabla \cdot (\mu_p e^{-\psi} \nabla \rho) = R(\psi, \eta, \rho) \]  
(1.3)

with appropriate interface and boundary conditions. Using Gummel's method [13] and Newton's method we can decouple and linearise the equations of this nonlinear system so that at each iteration step we have to solve a set of three linear equations of the form

\[ - \nabla \cdot (a(x) \nabla u) + G(x) u = F(x) \text{ in } \Omega \]  
(1.4)

with the boundary conditions \( u|_{\partial \Omega_D} = \gamma(x) \) and \( \nabla u \cdot n|_{\partial \Omega_N} = 0 \), where \( \Omega \subset \mathbb{R}^2 \), \( \partial \Omega = \partial \Omega_D \cup \partial \Omega_N \) is the boundary of \( \Omega \), \( \partial \Omega_D \cap \partial \Omega_N = \emptyset \), \( n \) denotes the unit outward normal vector on \( \partial \Omega \), \( a \in C^0(\overline{\Omega}) \), \( a_1 \equiv a(x) \equiv a_0 > 0 \), \( G \in H^1(\Omega) \cap C^0(\overline{\Omega}) \), \( G_1 \equiv G(x) \equiv G_0 \equiv 0 \) and \( F \in L^2(\Omega) \). Here \( a_0 \), \( a_1 \), \( G_0 \) and \( G_1 \) are constants.

In what follows we consider only homogeneous Dirichlet boundary conditions \( \gamma(x) \equiv 0 \). For the inhomogeneous case we can subtract a special function satisfying the boundary conditions and reduce the problem to a homogeneous one. We assume for simplicity that \( \partial \Omega \) is polygonal.

To solve (1.4) with the given boundary conditions the box method [17, 8, 19] is often used. Analyses of this method can be found for example in [21, 4, 16 and 14]. More recently Markowich and Zlătăleşcu [18], presented a triangular finite element method for the solution of (1.4). Brezzi et al. [5, 6, 7] also presented some mixed finite element methods for the solution of (1.4). However, their methods are based on triangulations having acute angles only. In this paper we present a triangular finite element method for (1.4) under milder restrictions on the triangles. This method is based on a novel discrete formulation. The formulation of the method is discussed in the next section. The existence and uniqueness of the discrete solution are proved for an arbitrary triangular mesh in Section 3. In Section 4 we give an error estimate for the approximate solution under mild restrictions on the mesh. Finally, in Section 5 it is shown that the terminal currents computed by the method are convergent and conservative.

In what follows \( L^2(\Omega) \) and \( W^{m,p}(\Omega) \) denote the usual Sobolev Spaces with norms \( \| \cdot \|_0 \) and \( \| \cdot \|_{W^{m,p}} \) respectively (cf. for example [1]). The inner
product on $L^2(\Omega)$ and $(L^2(\Omega))^2$ is denoted by $(\cdot, \cdot)$ and the $k$-th order seminorm on $W^{m,p}(\Omega)$ is denoted by $| \cdot |_{k,p}$. The Sobolev space $W^{m,2}(\Omega)$ is denoted by $H^m(\Omega)$ and the corresponding norm and seminorm is denoted respectively by $\| \cdot \|_m$ and $\| \cdot \|_k$. We put $L^2(\Omega) = (L^2(\Omega))^2$ and $H_D^1(\Omega) = \{ v \in H^1(\Omega) : v|_{\partial \Omega} = 0 \}$. We use $| \cdot |$ to denote absolute value, Euclidean length or area, depending on the context.

2. THE PETROV-GALERKIN MIXED FINITE ELEMENT FORMULATION

As in Miller et al. [20], by the introduction of a new variable $\mathbf{v} = a \nabla u$, we get from (1.4) a first order system of PDEs in the variables $[f, u]$

\begin{align*}
\nabla u - a^{-1} f &= 0 \quad (2.1) \\
- \nabla \cdot f + Gu &= F. \quad (2.2)
\end{align*}

The corresponding variational problem is

**Problem 2.1:** Find a pair $[f, u] \in L^2(\Omega) \times H_D^1(\Omega)$ such that for all $[q, v] \in L^2(\Omega) \times H_D^1(\Omega)$

\begin{align*}
(\nabla u, q) - \left( a^{-1} f, q \right) &= 0 \quad (2.3) \\
(f, \nabla v) + (Gu, v) &= (F, v). \quad (2.4)
\end{align*}

The existence and uniqueness of the solution to Problem 2.1 have been proved (see, for example, [22]).

To discuss the finite element approximation to Problem 2.1 we first define some meshes on $\Omega$. Let $\mathcal{C}$ denote a family of triangulations of $\Omega$

$$
\mathcal{C} = \{ T_h : 0 < h \leq h_0 \}
$$

where $T_h$ denotes a triangulation of $\Omega$ with each triangle $t$ having diameter $h_t$ less than or equal to $h$ and $h_0$ is a positive constant which is smaller than the diameter of $\Omega$. For each $T_h \in \mathcal{C}$, let $X_h = \{ x_i \}_{i=1}^N$ denote the set of all vertices of $T_h$ and $E_h = \{ e_i \}_{i=1}^N$ the set of all edges of $T_h$. We denote by $p_t$ the diameter of the incircle of $t$.

**Definition 2.1:** The family of meshes $\mathcal{C}$ is regular if there exists a constant $\sigma_1 > 0$, independent of $h$, such that

$$
\max_{t \in T_h} \frac{h_t}{p_t} \leq \sigma_1 \quad \forall h \in (0, h_0].
$$

We assume henceforth that $\mathcal{C}$ is regular.
DEFINITION 2.2: $T_h$ is a Delaunay triangulation if, for every $t \in T_h$, the circumcircle of $t$ contains no other vertices in $X_h$ (cf. [10]).

DEFINITION 2.3: The Dirichlet tessellation $D_h$ corresponding to the triangulation $T_h$ is defined by $D_h = \{ D_i \}_{i=1}^{N}$ where

$$D_i = \{ x : |x - x_i| < |x - x_j|, x_j \in X_h, j \neq i \} \quad (2.5)$$

for all $x_i \in X_h$ (cf. [11]).

We now construct two new meshes associated with the triangulation $T_h$. For each $x_i \in X_h$ we define the open region $\Omega(x_i)$ consisting of the union of all the triangles $t \in T_h$ with the common vertex $x_i$ and an open region $b(x_i) \subset \Omega(x_i)$ constructed as follows: for each $t \in \Omega(x_i)$, choose a point $p \in t$ arbitrarily and connect it to the midpoints of the two edges of $t$ sharing $x_i$, as shown in figure 2.1. (We remark that $p \in t$ is not necessary. However, for simplicity, we assume it does. We also assume that the same $p \in t$ is chosen for each vertex of $t$.) The domain within the resulting polygon is $b(x_i)$. For the sake of convenience, we sometimes denote $b(x_i)$ simply by $b$. The set of all such $b(x_i)$ is denoted by $B^V_h$ which we regard as a dual mesh to $T_h$. We put $B^V = \{ B^V_h : 0 < h \leq h_0 \}$.

![Figure 2.1. — The regions $\Omega(x)$, $b(x)$ and $\Omega(e)$ for the vertex $x$ and edge $e$.](image)

We remark that $B^V_h$ is determined uniquely by $B^F_h$, and vice versa, and that $B^E_h$ divides each $t \in T_h$ into three triangles $t_1$, $t_2$, $t_3$. We put $B^E = \{ B^E_h : 0 < h \leq h_0 \}$.
DEFINITION 2.4: The family of meshes $E$ is regular if there exists a positive constant $\sigma_2$, independent of $h$, such that for any $i, j \in \{1, 2, 3\}$, $i \neq j$

$$\max_{t \in T_h} \frac{|t_i| + |t_j|}{|t|} \geq \sigma_2 \quad \forall h \in (0, h_0].$$ \tag{2.6}

Regularity of $E$ is equivalent to the condition that for all $t \in T_h$ and the chosen point $p \in t$, the minimal distance between $p$ and the vertices of $t$ has a positive lower bound. Note also that regularity of $E$ implies that there is a positive constant $\sigma_3$ independent of $h$, such that

$$\min_{x \in x_h} \frac{|b(x_i)|}{\Omega(x_i)} \geq \sigma_3 \quad \forall h \in (0, h_0].$$ \tag{2.7}

We remark that if $T_h$ is a Delaunay triangulation and the point $p \in t$ is chosen to be the circumcentre of $t$, for each $t \in T_h$, then the corresponding mesh $B_h^V$ coincides with the Dirichlet tessellation dual to $T_h$, i.e. $B_h^V = D_h$.

Corresponding to the three meshes $B_h^E$, $T_h$ and $B_h^V$, we now construct three finite-dimensional spaces $L_h \subset L^2(\Omega)$, $H_h \subset H^1_D(\Omega)$ and $L_h \subset L^2(\Omega)$ as follows. Without loss of generality, we assume that the edges and vertices are numbered so that $\{e_i\}_{i=1}^M$ is the set of all edges in $E_h$ not on $\partial \Omega_D$ and $\{x_i\}_{i=1}^N$ is the set of all nodes in $X_h$ not on $\partial \Omega_D$.

For the mesh corresponding to $B_h^E$ we define, for each $i = 1, 2, \ldots, N_E$, a piecewise constant vector-valued function with domain $\bar{\Omega}$ by

$$q_i(x) = \begin{cases} e_i & \text{if } x \in \Omega(e_i) \\ 0 & \text{otherwise} \end{cases}$$

where $e_i$ is the unit tangential vector along the edge $e_i$. Obviously we have $(q_i, q_j) = \delta_{ij}|\Omega(e_i)|$, where $\delta_{ij}$ is the Kronecker notation. We take $L_h = \text{span} \{q_i\}_{i=1}^M$.

Next, letting $\{\phi_i\}_{i=1}^N$ be the conventional piecewise linear basis functions for $T_h$, we define $H_h = \text{span} \{\phi_i\}_{i=1}^N$.

Finally, to construct $L_h$ we define a set of piecewise constant basis functions $\psi_i$, $(i = 1, 2, \ldots, N)$ corresponding to the mesh $B_h^V$ as follows:

$$\psi_i(x) = \begin{cases} 1 & \text{if } x \in b(x_i) \\ 0 & \text{otherwise} \end{cases}$$

We then define $L_h = \text{span} \{\psi_i\}_{i=1}^N$. 
We introduce the mass lumping operator \( L : C^0(\Omega) \to L^2(\Omega) \) such that for any \( u \in C^0(\Omega) \)
\[
L(u)(x) = \sum_{x_i \in x_h} u(x_i) \psi_i(x) \quad \forall x \in \bar{\Omega} .
\]  
(2.8)

Using the three finite dimensional spaces we now define the following discrete Petrov-Galerkin problem.

**PROBLEM 2.2:** Find a pair \([f_h, u_h] \in L_h \times H_h\) such that for all \([q_h, v_h] \in L_h \times L_h\)
\[
(\nabla u_h, q_h) - (a^{-1} f_h, q_h) = 0 \quad \text{ (2.9)}
\]
\[
A(f_h, v_h) + (L(G u_h), v_h) = (\hat{F}, v_h) \quad \text{ (2.10)}
\]

where \(\hat{F}\) is a (quadrature) approximation to \(F\) and \(A(\cdot, \cdot)\) denotes the bilinear form on \(L_h \times L_h\) defined by
\[
A(f_h, v_h) = - \sum_{b \in B_h} \int_{\partial b} f_h \cdot n_{\partial b} \gamma_0(v_h|_b) \, ds . \quad \text{ (2.11)}
\]

Here \(v_h|_b\) denotes the restriction of \(v_h\) to \(b\), \(\gamma_0(v|_b)\) denotes the continuous extension of \(v|_b\) to \(\partial b\) and \(n_{\partial b}\) is the unit outward normal vector on \(\partial b\).

Let \(f_h = \sum_{i=1}^M f_i, q_i, u_h = \sum_{i=1}^N u_i, \phi_i\), where \(\{f_i\}_1^M\) and \(\{u_i\}_1^N\) are two sets of constants. Substituting these into (2.9) and taking \(q_h = q_j\), we get
\[
\sum_{i=1}^M f_i (a^{-1} q_i, q_j) - \sum_{i=1}^N u_i (\nabla \phi_i, q_j) = 0
\]
for each \(j = 1, 2, ..., M\). This linear system of equations has the solution
\[
f_j = \frac{1}{a_j^{-1}} u_{j2} - u_{j1} \quad j = 1, 2, ..., M
\]
where \(a_j^{-1} = \frac{1}{|\Omega(e_j)|} \int_{\Omega(e_j)} a^{-1} \, dx\) and \(u_{jk} = u_h(x_{jk}), k = 1, 2\) (see fig. 2.2a).

For the evaluation of \(a_j^{-1}\) we refer to the Appendix. Thus we have
\[
f_h = \sum_{i=1}^M \frac{1}{a_i^{-1}} \frac{u_{i2} - u_{i1}}{|e_i|} q_i . \quad \text{ (2.12)}
\]
Substituting (2.12) into (2.10) and letting $v_h = \psi_j$, we obtain

$$
- \sum_{i=1}^{M} \frac{1}{a_i^{-1}} u_{i2} - u_{i1} \int_{\partial b(\gamma_j)} q_i \cdot n_{\partial b(\gamma_j)} ds + (L(Gu_h), \psi_j) = (\tilde{F}, \psi_j) \tag{2.13}
$$

for each $j = 1, 2, ..., M$. From its definition (see fig. 2.1) we know that $\partial b(\gamma_j)$ consists of a finite number of segments. Clearly $\partial b(\gamma_j) \cap \Omega(e_i)$ consists of at most two segments which we denote by $\partial b_{ij,1}$ and $\partial b_{ij,2}$ if $\gamma_j$ is an end-point of $e_i$. Therefore, from (2.13), we have for $j = 1, 2, ..., N$

$$
- \sum_{i=1}^{M} \frac{1}{a_i^{-1}} u_{i2} - u_{i1} \sum_{k=1}^{2} e_i \cdot n_{ij,k} |\partial b_{ij,k}| + (L(Gu_h), \psi_j) = (\tilde{F}, \psi_j) \tag{2.14}
$$

where $n_{ij,k}$ denotes the unit vector normal to $\partial b_{ij,k}$. It is easy to see that $|e_i \cdot n_{ij,k}| |\partial b_{ij,k}|$ is equal to the length of the projection of $\partial b_{ij,k}$ onto the line perpendicular to $e_i$. This length is actually the distance from the chosen point $p \in t_k$ to $e_i$, i.e. the height of the triangle $\Omega(e_i) \cap t_k$ with base $e_i$, where $t_k$ denotes the triangle having $e_i$ as one edge and containing $\partial b_{ij,k}$. From the formulae for evaluating the area of a triangle we have

$$
\sum_{i=1}^{2} |e_i \cdot n_{ij,k}| |\partial b_{ij,k}| = \frac{2 |\Omega(e_i)|}{|e_i|}. \tag{2.15}
$$

Finally, with the notation in figure 2.2b, taking into account the sign of each $e_i \cdot n_{ij,k}$ and using (2.14) and (2.15) we find that for all $j = 1, 2, ..., N$

$$
\sum_{k \in I_j} \frac{1}{a_{jk}^{-1}} \frac{2 |\Omega(e_{jk})|}{|e_{jk}|} \frac{u_j - u_k}{|e_{jk}|} + G_j u_j |b(x_j)| = (\tilde{F}, \psi_j) \tag{2.16}
$$

where $I_j = \{k : e_{jk} \in E_h \}$ is the index set of neighbouring nodes of $x_j$ and $G_j = G(x_j)$. 

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The coefficient matrix of (2.16) is a symmetric, positive definite $M$-matrix. The latter property follows from the fact that it is a diagonally dominant matrix with all diagonal elements positive and all nonzero off-diagonal elements negative (see, for example, [25, § 3.5]). When $T_h$ is a Delaunay triangulation and $B_h^V$ is the Dirichlet tessellation dual to $T_h$, the term $2\frac{\Omega(e_{jk})}{|e_{jk}|}$ in (2.16) is the length between the circumcentres of the two triangles sharing $e_{jk}$ and $|b(x_j)| = |D_j|$, where $D_j$ is defined in (2.7). Therefore the expression (2.16) coincides with that obtained from the conventional box method with an inverse-average approximation to the coefficient function $a$.

3. EXISTENCE, UNIQUENESS AND STABILITY OF DISCRETE SOLUTIONS

In this section we prove that Problem 2.2 has a unique solution and that the solution is stable. Instead of proving directly that the mixed Problem 2.2 has a unique solution we consider an equivalent problem for which the existence and uniqueness of the solution can be established by standard finite element analysis.

Let $\Pi_a$ be the operator from $\nabla H_h = \{\nabla u_h : u_h \in H_h\}$ to $L_h$ determined by (2.9) with $a$ as a parameter. Introducing the bilinear forms $\tilde{A}(u_h, v_h) = A(\Pi_a \nabla u_h, v_h)$ and $B(u_h, v_h) = \tilde{A}(u_h, v_h) + (L(Gu_h), v_h)$ on $H_h \times L_h$, we define the following problem:

**PROBLEM 3.1:** Find $u_h \in H_h$ such that for all $v_h \in L_h$

$$B(u_h, v_h) = (\tilde{F}, v_h).$$

We say that problem 2.2 is equivalent to Problem 3.1 if the following two conditions hold:

(i) If $[f_h, u_h]$ is a solution of Problem 2.2, then $u_h$ is a solution of Problem 3.1.

(ii) If $u_h$ is a solution of problem 3.1, then $[\Pi_a \nabla u_h, u_h]$ is a solution of Problem 2.2.

**THEOREM 3.1:** Problem 2.2 is equivalent to Problem 3.1.

**Proof:** Assume that $u_h$ is a solution of Problem 3.1. From (2.8) and the choice of $L_h$ we know that there is an $f_h \in L_h$ such that for all $q_h \in L_h$

$$(\nabla u_h, q_h) - (a^{-1} f_h, q_h) = 0$$

i.e. $f_h = \Pi_a \nabla u_h$. Making use of the definition of $B(u_h, v_h)$ and the above equality we know that (3.1) reduces to (2.10) and therefore $[\Pi_a \nabla u_h, u_h]$ is a solution of Problem 2.2.
Conversely, if \( [f_h, u_h] \) is a solution of Problem 2.2, elimination of \( f_h \) in Problem 2.2 yields Problem 3.1, as shown in the previous section. □

**Lemma 3.2**: Assume that that \( \mathcal{B}^E \) is regular. Then there exist constants \( C_1, C_2 > 0 \), independent of \( h \), such that for any \( u_h \in H_h \)

\[
C_1 \| \nabla u_h \|_0 \leq \| \Pi_1 \nabla u_h \|_0 \leq C_2 \| \nabla u_h \|_0 .
\]

**Proof**: From Section 2 we know that for any \( u_h \in H_h \), \( \Pi_1 \nabla u_h = \sum_{i=1}^M (\nabla u_h \cdot e_i) |_e q_i \). Thus

\[
\| \nabla u_h - \Pi_1 \nabla u_h \|_0^2 = \sum_{i=1}^M \int_{\Omega(e_i)} | \nabla u_h - (\nabla u_h \cdot e_i) e_i |^2 dx
\]

\[
= \sum_{i=1}^M \int_{\Omega(e_i)} | \nabla u_h \cdot e_i^\perp |^2 dx
\]

\[
= \sum_{i=1}^M \int_{\Omega(e_i)} | \nabla u_h |^2 \cos^2 \theta_{h,i} dx
\]

where \( e_i^\perp \) denotes the unit normal vector to \( e_i \) such that \( \nabla u_h \cdot e_i^\perp \equiv 0 \) and \( \cos \theta_{h,i} = \frac{\nabla u_h \cdot e_i^\perp}{|\nabla u_h|} \). Since \( \nabla u_h \) is constant in each \( t \in T_h \), summing over \( t \in T_h \) we have

\[
\| \nabla u_h - \Pi_1 \nabla u_h \|_0^2 = \sum_{i \in T_h} | \nabla u_h |^2 \left[ \cos^2 \theta_{h,1} | t_1 | + \cos^2 \theta_{h,2} | t_2 | + \cos^2 \theta_{h,3} | t_3 | \right]
\]

\[
\leq \alpha \| \nabla u_h \|_0^2
\]

where \( t_1, t_2 \) and \( t_3 \) are the three triangles which form a partition of \( t \), \( e_1, e_2 \) and \( e_3 \) are the three edges of \( t \) and

\[
\alpha = \max_{t \in T_h} \frac{\cos^2 \theta_{h,1} | t_1 | + \cos^2 \theta_{h,2} | t_2 | + \cos^2 \theta_{h,3} | t_3 |}{|t|}.
\]

Since \( \mathcal{B}^E \) is regular, from (2.6) we know that, for all \( t \in T_h \), the \( t_1, t_2, t_3 \) satisfy \( |t| = |t_1| + |t_2| + |t_3| \) and

\[
\max_t \frac{|t_i|}{|t|} = \sigma < 1
\]

where \( \sigma \) is a positive constant, independent of \( h \). Furthermore, since for each \( i = 1, 2, 3 \)

\[
\cos^2 \theta_{h,i} \leq \gamma
\]

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where $0 \leq \gamma \leq 1$ is a constant, independent of $h$, and $\gamma < 1$ for at least one $i \in \{1, 2, 3\}$, it is easy to see that $\alpha < 1$. Thus (3.3) implies (3.2).

When restricted to $H_h$, the lumping operator $L$ and its inverse $L^{-1}$ are linear and bounded. This is established in the following lemma.

**Lemma 3.3**: Assume that $\mathcal{B}^E$ is regular. Then there exist positive constants $C_1$ and $C_2$, independent of $h$, such that for all $u_h \in H_h$

$$C_1 \| u_h \|_0 \leq \| L(u_h) \|_0 \leq C_2 \| u_h \|_0.$$  

(3.4)

**Proof**: See [15, p. 23] or [4].

Define a functional on $L_h$ by $\| v_h \|_{1,L} = \| \nabla L^{-1}(v_h) \|_0$ for all $v_h \in L_h$. We have the following lemma.

**Lemma 3.4**: Assume that $\mathcal{B}^E$ is regular. Then $\| \cdot \|_{1,L}$ is a norm on $L_h$ and there exists a positive constant $C$, independent of $h$, such that $\| v_h \|_0 \leq C \| v_h \|_{1,L}$ for all $v_h \in L_h$.

**Proof**: It is easy to see that the triangle inequality is satisfied by $\| \cdot \|_{1,L}$ and $\| \alpha v_h \|_{1,L} = |\alpha| \| v_h \|_{1,L}$ for all $v_h \in L_h$ and all $\alpha \in \mathbb{R}$. We now prove that if $\| v_h \|_{1,L} = 0$, then $v_h = 0$. In fact, if $\| v_h \|_{1,L} = 0$ for a $v_h \in L_h$, from its definition we have $\| \nabla L^{-1}(v_h) \|_0 = 0$. Since $L^{-1}(v_h) \in H_h$, we have $\| L^{-1}(v_h) \|_1 = 0$ (generalised Friedrichs' inequality, see, for example, [12, p. 25]) and so $\| L^{-1}(v_h) \|_0 = 0$. Using (3.4) we obtain $\| v_h \|_0 = 0$ and thus $v_h = 0$. Thus $\| \cdot \|_{1,L}$ is a norm.

Furthermore, since $L^{-1}(v_h) \in H_h$ for all $v_h \in L_h$, we have

$$\| v_h \|_{1,L} = \| \nabla L^{-1}(v_h) \|_0 \geq C \| L^{-1}(v_h) \|_1 \geq C \| L^{-1}(v_h) \|_0 \geq C \| v_h \|_0$$

where $C$ denotes a generic positive constant, independent of $h$. In the above we used the generalised Friedrichs' inequality and Lemma 3.3.

The existence and uniqueness of the solution to Problem 3.1 is contained in the following theorem:

**Theorem 3.5**: Assume that $\mathcal{B}^E$ is regular. Then Problem 3.1 has a unique solution and the solution is stable.

**Proof**: In fact the existence and uniqueness of the solution to Problem 3.1 has already been established since we have shown that the coefficient matrix of (2.16) is a symmetric and positive definite $M$-matrix. To prove the stability, we need to verify only the following coercivity inequality (see, for example [2])

$$\sup_{v_h \in L_h, \| v_h \|_{1,L} = 1} |B(u_h, v_h)| \geq a_0 \alpha \| u_h \|_1 \quad \forall u_h \in H_h$$

(3.5)
where $\alpha$ is a positive constant, independent of $h$, $u_h$, $v_h$ and $a$, and constant $a_0$ is the lower bound of $a$ defined in Section 1. In what follows we use $C$ to denote a generic positive constant, independent of $h$, $u_h$, $v_h$ and $a$.

If $u_h = 0$ then clearly (3.5) holds. When $u_h \neq 0$ we put $\bar{v}_h = L(u_h)/\gamma_{u_h}$, where $\gamma_{u_h} = \|\nabla u_h\|_{1,L}$. Then $\|\bar{v}_h\|_{1,L} = 1$ and

$$\tilde{A}(u_h, \bar{v}_h) = \tilde{A}\left(u_h, \frac{L(u_h)}{\gamma_{u_h}}\right)$$

$$= \frac{1}{\gamma_{u_h}} \sum_{b \in \mathcal{E}_h} \int_{\partial b} \Pi_a \nabla u_h \cdot n_{ab} \frac{L(u_h)}{\gamma_{u_h}} \, ds$$

$$= \frac{1}{\gamma_{u_h}} \sum_{b \in \mathcal{E}_h} u_h(x_b) \int_{\partial b} \Pi_a \nabla u_h \cdot n_{ab} \, ds \quad (3.8)$$

where $x_b$ is the mesh node contained in $b$. Summing (3.8) over $\partial b_i = \bigcup (\partial b \cap \Omega(e_i))$ we obtain, using arguments similar to those in the derivation of (2.16)

$$\tilde{A}(u_h, \bar{v}_h) = \frac{1}{\gamma_{u_h}} \sum_{i=1}^{M} (u_{i2} - u_{i1}) \int_{\partial b_i} \Pi_a \nabla u_h \cdot n_{ib} \, ds$$

$$= \frac{1}{\gamma_{u_h}} \sum_{i=1}^{M} a_i^{-1} \left(\left|\frac{u_{i2} - u_{i1}}{|e_i|}\right|^2 \frac{2|\Omega(e_i)|}{|e_i|}\right)$$

$$\equiv 2 a_0 \sum_{i=1}^{M} \left(\left|\frac{u_{i2} - u_{i1}}{|e_i|}\right|^2 \frac{1}{|\Omega(e_i)|}\right)$$

$$= \frac{2 a_0}{\gamma_{u_h}} \left\|\Pi_1 \nabla u_h\right\|_0^2$$

$$\equiv 2 a_0 C \left\|\nabla u_h\right\|_0^2$$

$$\equiv a_0 \alpha \left\|u_h\right\|_1$$

where $n_{ib}$ denotes the unit vector normal to $\partial b_i$, chosen so that the angle between $n_{ib}$ and $e_i$ is smaller than $\pi/2$. In the above we used (3.2) and the generalised Friedrichs’ inequality (see, for example [12, p. 25]). It follows that for all $u_h \in H_h$

$$\sup_{v_h \in L_h, \|v_h\|_0 = 1} |B(u_h, v_h)| \geq \tilde{A}(u_h, \bar{v}_h) + (L(Gu_h), \bar{v}_h) \geq a_0 \alpha \|u_h\|_1$$
since $G \geq 0$ and
\[
(L(G u_h), \bar{v}_h) = \frac{1}{\gamma_{u_h}} (L(G u_h), L(u_h)) = \frac{1}{\gamma_{u_h}} \sum_{i=1}^{N} G_i u_i^2 |b_i| \geq 0
\]
where $u_i = u_h(x_i)$ This completes the proof of the theorem \(\square\)

From Theorems 3.1 and 3.5 we have

**COROLLARY 3.3** Assume that $\mathcal{B}^E$ is regular Then Problem 2.2 has a unique solution

We comment that Problem 3.1 can be regarded as a generalised finite element method which is closely related to a mixed finite element method For details, we refer the reader to, for example [3]

**4 ERROR ESTIMATE**

In this section we give an error estimate for the approximate solution to Problem 2.2 We first state the following lemma

**LEMMA 4.1** Assume that $T_h$ is a Delaunay triangulation and that $B_h^\nu$ is the corresponding Dirichlet tessellation Then there exist positive constants $C_1$ and $C_2$, independent of $h$, such that for all $w_h \in H_h$ and all $v_h \in L_h$
\[
\|L(w_h) - w_h\|_0 \leq C_1 h |w_h|_1 \tag{4.1}
\]
and
\[
|G(w_h) - L(G w_h), v_h| \leq C_2 h \|v_h\|_0 \left(\|G w_h\|_1 + \|G w_h\|_1 + \|G\|_{W_2} \|w_h\|_1\right) \tag{4.2}
\]
where $(G w_h)\ell$ denotes the $H_h$-interpolant of $G w_h$

**Proof** For the proof of (4.1) we refer to [9] or [15, p 23] We now prove (4.2)

For any $w_h \in H_h$, we have
\[
|G(w_h) - L(G w_h), v_h| = |G(w_h) - G w_h, v_h) + L((G w_h)\ell) - L(G w_h), v_h)| + |((G w_h)\ell - L((G w_h)\ell), v_h)|
\]
for all $v_h \in L_h$ Since $(G w_h)(x_i) = (G w_h)\ell (x_i), \forall x_i \in X,$ using (4.1) we have from the above equality
\[
|G(w_h) - L(G w_h), v_h| \leq C h \|v_h\|_0 \left|\|G w_h\|_1 + \|G w_h - (G w_h)\ell, v_h\|_1\right| \tag{4.3}
\]
Using Cauchy-Schwarz inequality we have

\[
\left| (Gw_h - (Gw_h)_I, v_h) \right| = \left| \sum_{t \in T_h} \int_t (Gw_h - (Gw_h)_I) v_h \, dx \right| \\
\leq \sum_{t \in T_h} \left( \int_t |Gw_h - (Gw_h)_I|^2 \, dx \right)^{1/2} \left( \int v_h^2 \, dx \right)^{1/2} \\
= Ch \left( \sum_{t \in T_h} \left| Gw_h - (Gw_h)_I \right|^2 \right)^{1/2} \left\| v_h \right\|_0 \\
\leq Ch \left( \sum_{t \in T_h} \left( |Gw_h|_{1,t}^2 + |Gw_h|_{2,t}^2 \right) \right)^{1/2} \left\| v_h \right\|_0 \\
\leq Ch \left( |Gw_h|, |Gw_h|_2 \right) \left\| v_h \right\|_0.
\] (4.4)

In the above we used the estimate

\[
|Gw_h - (Gw_h)_I|_{0,t} \leq Ch (|Gw_h|_{1,t} + |Gw_h|_{2,t}) \quad \forall t \in T_h.
\]

For any \( w_h \in H_h \) we have \( |Gw_h|_2 \leq \| G \|_{L^\infty} \| w_h \|_1 \). Substituting this estimate into (4.4) and then the result into (4.3) we obtain (4.2). \( \square \)

Let \( \bar{f} \) and \( a_A \) be defined for each \( e_i \in E_h \) by

\[
\bar{f} \mid_{\Omega(e_i)} = \frac{1}{|\partial b_i|} \int_{\partial b_i} f \, ds, \quad \partial b_i = \Omega(e_i) \cap \left( \bigcup_{b \in B_h^V} \partial b \right)
\]

(4.5)

\[
a_A \mid_{\Omega(e_i)} = \left( \frac{1}{|\Omega(e_i)|} \int_{\Omega(e_i)} a^{-1} \, dx \right)^{-1}.
\]

(4.6)

Define the norm \( \| \cdot \|_a = (a^{-1}, \cdot, \cdot)^{1/2} \). The error estimate for the solution to Problem 3.1 is given in the following theorem:

**THEOREM 4.3:** Let \( u \) and \( u_h \) be the solutions of Problems 1.1 and 3.1 respectively. Assume that \( T_h \) is a Delaunay triangulation and that \( B_h^V \) is the corresponding Dirichlet tessellation. Then there exists a positive constant \( C = C (|\Omega|) \), independent of \( h \), such that

\[
\| u_h - u \|_1 \leq C \left( \| \bar{f} - a_A \nabla u_I \|_0 + G_1 \| u - u_I \|_0 + \| \bar{f} - F \|_0 \right.
\]

\[
+ h (|Gu_I|_1 + (Gu_I)_I|_1 + \| G \|_{L^\infty} \| u_I \|_1) \right)
\]

(4.7)

\[
\| f - f_h \|_a \leq 2 \| f - f' \|_a + \| a \nabla (u - u_h) \|_a
\]

(4.8)
where $u_I$ is the $H_h$-interpolant of $u$, $f'$ is the interpolant of $f$ in $L_h$ and $a_0$ and $G_1$ are respectively the lower bound of $a$ and the upper bound of $G$, as defined in Section 1.

Proof: In what follows we let $C = C(|\Omega|)$ denote a generic positive constant, independent of $h$. Take $v_h \in L_h$ such that $\|v_h\|_{L^1} \leq 1$. Multiplying (2.2) by $v_h$ and integrating by parts we get

$$A(f, v_h) + (Gu, v_h) = (F, v_h). \quad (4.9)$$

Letting $f_I = \Pi_a(\nabla u_I)$, where $\Pi_a$ is the operator defined in the previous section, we have from (2.10) and (4.9)

$$A(f_h - f_I, v_h) + (L(Gu_h) - L(Gu_I), v_h) = A(f - f_I, v_h) + (Gu - L(Gu_I), v_h) + (\hat{F} - F, v_h)$$

$$= A(f - f_I, v_h) + (Gu - Gu_I, v_h)$$

$$+ (Gu_I - L(Gu_I), v_h) + (\hat{F} - F, v_h). \quad (4.10)$$

By the definition of $B(., .)$, from (4.10), using the Cauchy-Schwarz inequality we obtain

$$|B(u_h - u_I, v_h)| \leq |A(f - f_I, v_h)| + |(Gu - Gu_I, v_h)|$$

$$+ |(Gu_I - L(Gu_I), v_h)| + \|\hat{F} - F\|_0.$$

In the above we used Lemma 3.4. The first term on the right side of (4.11) can be written in the form

$$A(f - f_I, v_h) = - \sum_{d \in \partial_h^I} \int_{\partial d} (f - f_I) \cdot n_{\partial d} v_h \, ds.$$

Summing over $\partial d_i$ we get

$$A(f - f_I, v_h) = - \sum_{i=1}^{M} (v_{i2} - v_{i1}) \int_{\partial d_i} (f - f_I) \cdot n_{\partial d_i} \, ds$$

$$= - \sum_{i=1}^{M} (v_{i2} - v_{i1}) (\bar{f} - f_I) \big|_{\Omega(e_i)} \cdot n'_{\partial d_i} |\partial d_i|. \quad (4.12)$$

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where \( \mathbf{n}'_{\partial b_i} \) denotes the unit normal vector on \( \partial b_i \) such that \( \mathbf{e}_i \cdot \mathbf{n}'_{\partial b_i} > 0 \) and \( v_{ij} \) (\( j = 1, 2 \)) denote the nodal values of \( v_h \) at the two end-points of the edge \( e_i \), as shown in figure 2.2(a). Since \( T_h \) is a Delaunay triangulation and \( B_{\partial}^T \) is the corresponding Dirichlet tessellation we have \( \mathbf{n}'_{\partial b_i} = \mathbf{e}_i \). We get from (4.12)

\[
A(\mathbf{f} - \mathbf{f}_T, v_h) = - \sum_{i=1}^{M} \left( v_{i2} - v_{i1} \right) (\mathbf{f} - \mathbf{f}_T) \left| \mathbf{e}_i \cdot \frac{2|\Omega(e_i)|}{|e_i|} \right| \Omega(e_i).
\]

Using Hölder's inequality we obtain

\[
|A(\mathbf{f}_h - \mathbf{f}_T, v_h)| \leq \frac{1}{2} \left( \sum_{i=1}^{M} \left( \frac{v_{i2} - v_{i1}}{|e_i|} \right)^2 |\Omega(e_i)| \right)^{1/2} \times
\]

\[
\times \left( \sum_{i=1}^{M} \left( (\mathbf{f}_T - \mathbf{f}_T) \left| \mathbf{e}_i \right| \cdot \frac{2|\Omega(e_i)|}{|e_i|} \right)^2 |\Omega(e_i)| \right)^{1/2}
\]

\[
= 2 \| \Pi_1 \nabla L^{-1}(v_h) \|_0 \| \Pi_1 (\mathbf{f}_T - a_A \nabla u_f) \|_0
\]

\[
\leq C \| v_h \|_{1,L} \| \mathbf{f}_T - a_A \nabla u_f \|_0
\]

\[
\leq C \| \mathbf{f}_T - a_A \nabla u_f \|_0 \quad (4.13)
\]

since \( \mathbf{f}_T = \Pi_a(\nabla u_f) = \Pi_1(a_A \nabla u_f) \). In the above we have made use of Lemmas 3.2 and 3.3. Substituting (4.13) into (4.11) and using Lemma 4.2 we obtain

\[
|B(u_h - u_T, v_h)| \leq C \left( \| \mathbf{f}_T - a_A \nabla u_f \|_0 + G_1 \| u - u_T \|_0 + \| F - \hat{F} \|_0 \right.
\]

\[
+ \left. \frac{h(\| G u_f \|_1 + \| G \|_{\mathcal{W}, \infty} \| u_f \|_1)}{\| v_h \|_{1,L}} \right).
\]

(4.14)

Since (4.14) holds for all \( v_h \in L_h, \| v_h \|_{1,L} \leq 1 \), using the inf-sup condition (3.5) we finally obtain

\[
a_0 \alpha \| u_h - u_T \|_1 \leq \sup_{v_h \in L_h, \| v_h \|_{1,L} \leq 1} |B(u_h - u_T, v_h)|
\]

\[
\leq C \left( \| \mathbf{f}_T - a_A \nabla u_f \|_0 + G_1 \| u - u_T \|_0 + \| F - \hat{F} \|_0 \right.
\]

\[
+ \left. \frac{h(\| G u_f \|_1 + \| G \|_{\mathcal{W}, \infty} \| u_f \|_1)}{\| v_h \|_{1,L}} \right).
\]

From the above inequality (4.7) follows immediately.
Since $f_h - f^l \in L_h$, using (2.3) and (2.9) we have

$$(a^{-1}(f_h - f^l), f_h - f^l) = (a^{-1}(f^h - f), f^h - f^l) + (a^{-1}(f - f^l), f_h - f^l) + \nabla(u_h - u), f^h - f^l).$$

Using Cauchy-Schwarz inequality we obtain from the above equation

$$\|f_h - f^l\|_a \leq \|f - f^l\|_a + \|\nabla(u - u_h)\|_a. \quad (4.15)$$

Finally, (4.8) follows from the triangular inequality and (4.15). We thus have proved the theorem. \(\Box\)

We comment that (4.8) tell us nothing about the convergence of $f_h$ to $f$. This is because even $f$ is constant, the first term on the right side of (4.8) becomes

$$\|f - f^l\|_a \geq a_0^{-1} \sum_{i=1}^{M} \|f - (f \cdot e_i) e_i\|_0^2 = a_0^{-1} \sum_{i=1}^{M} (f \cdot e_i^\perp)^2 |\Omega(e_i)|$$

where $e_i^\perp$ denotes a unit vector perpendicular to $e_i$. Thus, clearly, $\|f - f^l\|_a$ does not converge to zero as $h \to 0$. This shows that (4.8) does not imply that $\|f - f_h\|_a$ converges to zero as $h \to 0$. Nevertheless, as we will see in the next section, the computed terminal currents are convergent.

5. EVALUATION OF TERMINAL CURRENTS

The evaluation of terminal currents is of importance in practice. It is often the final goal of device modelling. We now discuss a method for evaluating terminal currents with the finite element method presented previously. Since in this section we are concerned only with the current continuity equations we have $G \equiv 0$. Furthermore, for simplicity, we restrict our attention to a device with a finite number of ohmic contacts and so $\partial \Omega_h$ is a finite set of separated segments.

For any $c \in \partial \Omega_D$, let $\{x_i^c\}_{i=1}^{N_c}$ denote the nodes on $c$. In what follows it is necessary to make some assumptions about the construction of the meshes $T_h$ and $B_h^V$. These are contained in the following assumption.

**Assumption 5.1**: Assume that $T_h$ is a Delaunay triangulation such that for each contact $c \in \partial \Omega_D$, the end-points of $c$ belong to the set of vertices $X_h$ of $T_h$ and $B_h^V$ is the Dirichlet tessellation dual to $T_h$.

Let $\psi^c$ be a piecewise constant function satisfying

$$\psi^c(x) = \begin{cases} 
1 & x \in \bigcup_{i=1}^{N_c} h(x_i^c) \\
0 & \text{otherwise}.
\end{cases} \quad (5.1)$$
Multiplying (2.2) by $\Psi^c$ and integrating by parts we have

$$- \int_c f \cdot n \, ds - \sum_{b \in B^c_k} \int_{\partial b \setminus (\partial b \cap c)} \Psi^c f \cdot n \, ds = (F, \Psi^c).$$

Thus the outflow current through $c$ is

$$J_c = \int_c f \cdot n \, ds = - \sum_{b \in B^c_k} \int_{\partial b \setminus (\partial b \cap c)} \Psi^c f \cdot n \, ds - (F, \Psi^c). \quad (5.2)$$

Replacing $f$ by the finite element solution $f_h$ and $F$ by the quadrature approximation $\tilde{F}$ in (5.2), we obtain the following approximate outflow current through $c$

$$J^h_c = \int_c f_h \cdot n \, ds = - \sum_{b \in B^c_k} \int_{\partial b \setminus (\partial b \cap c)} \Psi^c f_h \cdot n \, ds - (\tilde{F}, \Psi^c). \quad (5.3)$$

From (5.3), (5.1) and the argument used in the derivation of (2.14), we obtain

$$J^h_c = \frac{1}{|I_j|} \sum_{j=1}^{N_c} \left[ \int_{\partial b(x_j)} f_h \cdot n \, ds - \int_{b(x_j)} \tilde{F} \, dx \right]$$

$$= \frac{1}{|I_j|} \sum_{j=1}^{N_c} \left[ \sum_{k \in I_j} \frac{2}{a^j_k} \frac{1}{|e^j_k|} \frac{1}{|e^j_k|} - \frac{1}{|b(x_j)|} \int_{b(x_j)} \tilde{F} \, dx \right] \quad (5.4)$$

where $I_j$ is the index set of neighbouring nodes of $x_j$ as defined in Section 2.

The convergence and the conservation of the computed terminal currents are established in the following theorem.

**Theorem 5.1:** Let $[f, u]$ and $[f_h, u_h]$ be the solutions of Problems 2.1 and 2.2 respectively. Let $J_c$ and $J^h_c$ be respectively the exact and the computed outflow currents through $c \in \partial \Omega_D$. Under Assumption 5.1, there exists a constant $\gamma > 0$, independent of $h$, such that

$$|J_c - J^h_c| \leq \gamma \|\Psi^c\|_{1,L} \left( \|\bar{F} - a_A \nabla u_h\|_0 + \|F - \tilde{F}\|_0 \right) \quad (5.5)$$

where $\bar{F}$ and $a_A$ are defined in (4.5) and (4.6) respectively. Furthermore

$$\sum_{c \in \partial \Omega_D} J^h_c = - \int_\Omega \tilde{F} \, dx. \quad (5.6)$$
Proof : The following proof of (5.5) is similar to that of (4.7). Let $\gamma$ denote a generic positive constant, independent of $h$. From (5.2-3) we have

$$J_c - J^h_c = - \sum_{b \in B_h^Y} \int_{\partial b \setminus (\partial b \cap c)} \psi^c (f - f_h) \cdot n \, ds + (\hat{F} - F, \psi^c). \quad (5.7)$$

Since $\psi^c$ is constant on $c$, summing over $\partial b$, we obtain (5.5) as follows:

$$|J_c - J^h_c| \leq \sum_{b \in B_h^Y} \int_{\partial b \setminus (\partial b \cap c)} \psi^c (f - f_h) \cdot n \, ds + |(\hat{F} - F, \psi^c)|$$

$$= \left| \sum_{i=1}^{M} (\phi_i^c - \phi_i^c) (\hat{f} - f_h) \right|_{\Omega(e_i)} \cdot e_i 2 \frac{|\Omega(e_i)|}{|e_i|} + |(\hat{F} - F, \psi^c)|$$

$$\approx 2 \left[ \sum_{i=1}^{M} \left( \frac{(\phi_i^c - \phi_i^c)}{|e_i|} \right)^2 \frac{1}{|\Omega(e_i)|} \right]^{1/2} \times$$

$$\left[ \sum_{i=1}^{M} \left( (\hat{f} - f_h) \right|_{\Omega(e_i)} \cdot e_i \right)^2 \frac{1}{|\Omega(e_i)|} \right]^{1/2}$$

$$+ \|F - \hat{F}\|_0 \|\psi^c\|_0$$

$$= 2 \left\| \Pi_1(\nabla L^{-1}(\psi^c)) \right\|_0 \left\| \Pi_1(\hat{f} - a_A \nabla u_h) \right\|_0 + \|F - \hat{F}\|_0 \|\psi^c\|_0$$

$$\leq 2 \gamma \|\psi^c\|_{1,L} \left\{ \|\hat{f} - a_A \nabla u_h\|_0 + \|F - \hat{F}\|_0 \right\}.$$

In the above we used Hölder’s inequality and Lemmas 3.2, 3.3 and 3.4.

To prove (5.6), we first notice that

$$A(f_{h,1}) = \sum_{b \in B_h^Y} \int_{\partial b \setminus (\partial b \cap \partial \Omega_D)} f_h \cdot n \, ds = 0 \quad (5.8)$$

since, for all $e_i \in \Omega(h), f_h$ is constant in each subregion $\Omega(e_i)$. Summing (5.3) over all the contacts we have

$$\sum_{c \in \partial \Omega_D} J^h_c = - \sum_{c \in \partial \Omega_D} \left[ \sum_{b \in B_h^Y} \int_{\partial b \setminus (\partial b \cap c)} \psi^c f_h \cdot n \, ds - (\hat{F}, \psi^c) \right]$$

$$= - \sum_{b \in B_h^Y} \int_{\partial b \setminus (\partial b \cap c)} \psi^c f_h \cdot n \, ds - (\hat{F}, \psi)$$

$$= A(f_h, \psi) - (\hat{F}, \psi) \quad (5.9)$$

where $\psi = \sum_{c \in \partial \Omega_D} \psi^c$ and $A(., .)$ is the bilinear form defined in Section 2.
From (5.8) and (5.9) we obtain
\[ \sum_{c \in \partial \Omega_D} J_c^h = A(f_h, \psi - 1) - (\hat{F}, \psi - 1) - (\hat{F}, 1) \]
\[ = - \int_{\Omega} \hat{F} \, dx. \]

In the above we used (2.10) with \( G = 0 \) since \( \psi - 1 \in L_h \). \( \square \)

6. CONCLUSION

A Petrov-Galerkin mixed finite element approach based on a novel formulation was used to approximate the self-adjoint system of second order elliptic PDEs describing a semiconductor device. The existence, uniqueness and stability of the approximate solution were proved for an arbitrary triangular mesh and an error estimate was obtained for an arbitrary Delaunay triangulation and corresponding Dirichlet tessellation. No restrictions need to be imposed on the angles of the triangles in the mesh. The resulting linear system coincides with that obtained from the conventional box scheme with an inverse-average approximation to the coefficient function. In the case of the semiconductor continuity equations this is in fact an exponentially fitted approximation to the coefficient functions. The evaluation of the approximate terminal currents associated with the method was discussed and the computed terminal currents were shown to be convergent and conservative. This method may be applied to the case of non-Delaunay triangulations if we introduce areas and lengths with negative weights. However the coefficient matrices of the resulting linear systems may not be \( M \)-matrices. We will discuss this further in a forthcoming paper.

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Evaluation of the coefficients in the linear systems arising from the discretisation of the continuity equations

In this appendix we discuss in detail the evaluation of $a_{jk}^{-1}$ in (2.16). From the definition we have

$$I(e_{jk}) = a_{jk}^{-1} = \frac{1}{|\Omega(e_{jk})|} \int_{\Omega(e_{jk})} a^{-1} \, dx$$

(A.1)

where, by definition, $\Omega(e_{jk})$ is the union of the two triangles obtained from the construction of the mesh $B^p$ in Section 2 (cf. fig. 2.1). We omit the subscript $jk$ in (A.1) and assume that $\Omega(e) = t_1 \cup t_2$, where $e \in E_h$ is an edge of the mesh and $t_1$ and $t_2$ are two triangles. Thus we have

$$I(e) = \frac{1}{|\Omega(e)|} \int_{\Omega(e)} a^{-1}(x) \, dx$$

(A.2)

where $x = (x_1, x_2)$ and $dx = dx_1 \, dx_2$. In the case of the continuity equations (1.2-3) $a(x)$ is equal to $\mu_n e^{\psi(x)}$ and $\mu_p e^{-\psi(x)}$ respectively. Therefore, if we assume that $\mu_n$ and $\mu_p$ are constant, from (A.2) we see that we need only to evaluate integrals of the form

$$I(t) = \frac{1}{|t|} \int_t e^{\psi(x)} \, dx$$

(A.3)

where $t$ is a triangle with vertices $x_i$ ($i = 1, 2, 3$) and $\psi(x) = \pm \psi(x)$. Since $\psi$ is the computed solution to the Poisson equation, we assume that $\psi$ is linear on $t$ and $\psi(x_i) = \psi_i$ ($i = 1, 2, 3$). Let $s = s(x)$ be the linear transformation from $t$ to the reference triangle $\hat{t}$ with vertices $(0, 0), (1, 0)$ and $(0, 1)$ in the $(s_1, s_2)$. Using this transformation (A.3) can be written in the form

$$I(t) = \frac{1}{|\hat{t}|} \int_{\hat{t}} \det(J) e^{\psi(s)} \, ds_1 \, ds_2$$

$$= \frac{1}{|\hat{t}|} \int_{\hat{t}} e^{\psi(s)} \, ds_1 \, ds_2$$

(A.4)

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where \( J = \frac{\partial(x_1, x_2)}{\partial(s_1, s_2)} \) is the Jacobian of the transformation which is a matrix with constant entries and \( \det(\cdot) \) denotes the determinant. Since \( \phi(x) \) is linear, \( \phi(s) \) is also linear and

\[
\phi(s) = \alpha_0 + \alpha_1 s_1 + \alpha_2 s_2 \tag{A.5}
\]

for some constants \( \alpha_i \) (\( i = 1, 2, 3 \)). Substituting this into (A.4) we obtain

\[
I(\dot{t}) = \int_0^1 ds_1 \int_0^{1-s_1} e^{\alpha_0 + \alpha_1 s_1 + \alpha_2 s_2} ds_2
\]

\[
= \frac{e^{\alpha_0}}{\alpha_2} \int_0^1 e^{\alpha_1 s_1} (e^{\alpha_2 (1-s_1)} - 1) ds_1
\]

\[
= \frac{e^{\alpha_0}}{\alpha_2} \left( e^{\alpha_1 \alpha_2 - 1} - \frac{e^{\alpha_1}}{\alpha_1} \right)
\]

\[
= \frac{e^{\alpha_0}}{\alpha_2} \left( e^{\alpha_2} B^{-1}(\alpha_1 - \alpha_2) - B^{-1}(\alpha_1) \right) \tag{A.6}
\]

where \( B(x) \) is the Bernoulli function defined by

\[
B(x) = \begin{cases} x/(e^x - 1) & x \neq 0 \\ 1 & x = 0 \end{cases}.
\]

Since \( \psi(x) \) is linear and \( \psi(x_i) = \psi_i \) (\( i = 1, 2, 3 \)) we have

\[
\psi(s) = \psi_1 + (\psi_2 - \psi_1) s_1 + (\psi_3 - \psi_1) s_2. \tag{A.7}
\]

Furthermore, since \( |\dot{t}| = 1/2 \), from (A.3)-(A.7) we obtain

\[
\frac{1}{|\dot{t}|} \int_t e^{\psi(x)} dx = \frac{2}{(\psi_3 - \psi_1)} \left( e^{\psi_2} B^{-1}(\psi_2 - \psi_3) - e^{\psi_1} B^{-1}(\psi_2 - \psi_1) \right) \tag{A.8}
\]

\[
\frac{1}{|\dot{t}|} \int_t e^{-\psi(x)} dx = \frac{2}{(\psi_1 - \psi_3)} \left( e^{-\psi_2} B^{-1}(\psi_3 - \psi_2) - e^{-\psi_1} B^{-1}(\psi_1 - \psi_2) \right). \tag{A.9}
\]

Substituting (A.8) (or (A.9)) into (A.2) we obtain an expression for the coefficient \( a^{-1}_{jk} \) in the linear system arising from the electron (or hole) continuity equation. This expression is a function of the nodal values of \( \psi \). We remark that when the absolute values of the differences between the nodal values \( \psi_i \) (\( i = 1, 2, 3 \)) are small, it is necessary to use Taylor expansions about zero to obtain accurate evaluations of the right-hand sides of (A.8)-(A.9).
REFERENCES


