

### 3-D Mixed Finite Element Schemes for Charge Transport Equations

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**Abstract.** We use the Raviart-Thomas-Nédélec space to discretize the current continuity equations of the drift-diffusion semiconductor models with Mixed Finite Element methods in  $\mathbb{R}^3$ . An asymptotic analysis of the behaviour of the scheme when the potential is very large is given.

#### 1. INTRODUCTION

We extend to 3-D problems the mixed approach introduced in [1-2] to discretize the current continuity equations arising in the drift-diffusion model for semiconductors. For simplicity, we shall deal only with the equation for positive charges, i.e., we want to find a solution  $p \in H^1(\Omega)$  such that:

$$\begin{cases} -\operatorname{div}(\nabla p + p\nabla\psi) = f & \text{in } \Omega \subset \mathbb{R}^3 \\ p = g & \text{on } \Gamma_0 \subset \partial\Omega \\ \frac{\partial p}{\partial n} + p \frac{\partial \psi}{\partial n} = 0 & \text{on } \Gamma_1 = \partial\Omega \setminus \Gamma_0. \end{cases} \quad (1)$$

The first equation of (1) describes the stationary behaviour of a semiconductor when the concentration of positive charges is  $p$  and the electrical potential, coming from the solution of the Poisson's equation, is  $\psi$ . For a complete description of a stationary semiconductor problem one needs another equation for the negative charges and a Poisson equation for  $\psi$ . All the quantities are conveniently scaled in order to avoid numerical problems due to the different orders of magnitude of the physical quantities. See [3] for more details.

We assume that  $\psi$ ,  $f$  and  $g$  are known. In general, the right-hand side in (1) is a nonlinear function of the negative and positive charge concentration. Here, we shall assume that some linearization has been introduced, so that  $f$  is independent of the actual  $p$ . Following [1-2], we use the Slotbloom change of variables for  $p$ :

$$p = u e^{-\psi} \quad (2)$$

giving us a new problem in the  $u$  variable:

$$\begin{cases} -\operatorname{div}(e^{-\psi}\nabla u) = f & \text{in } \Omega \\ u = e^{\psi}g = \chi & \text{on } \Gamma_0 \\ \frac{\partial u}{\partial n} = 0 & \text{on } \Gamma_1. \end{cases} \quad (3)$$

#### 2. MIXED SCHEME

To introduce the mixed scheme, we define the following spaces:

$$\begin{aligned} \Sigma &= \{\tau \in H(\operatorname{div}; \Omega), \tau \cdot n = 0 \text{ on } \Gamma_1\}, \\ \Phi &= L^2(\Omega). \end{aligned}$$

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The current  $\underline{J} = -e^{-\psi} \nabla u = -(\nabla p + p \nabla \psi)$  is now a new variable and the mixed formulation of (3) is:

$$\begin{cases} \text{Find } \underline{J} \in \Sigma \text{ and } u \in \Phi \text{ such that:} \\ \int_{\Omega} e^{\psi} \underline{J} \cdot \underline{\tau} dx + \int_{\Omega} u \operatorname{div} \underline{\tau} dx = \int_{\Gamma_0} \chi \underline{\tau} \cdot \underline{n} ds & \forall \underline{\tau} \in \Sigma \\ \int_{\Omega} \phi \operatorname{div} \underline{J} dx = \int_{\Omega} \phi f dx & \forall \phi \in \Phi \end{cases} \quad (4)$$

where  $\underline{n}$  is the outward unit normal to  $\Gamma_0$ . Now we discretize equation (4) introducing a regular sequence  $\{T_h\}_h$  of decompositions of  $\Omega$  into tetrahedrons  $T$  (see [4]), assuming for simplicity that  $\Omega$  is a polyhedron. We introduce the Raviart-Thomas-Nédélec [5] set of polynomial vectors on  $T \in T_h$ , with  $\Omega = \cup T \subset \mathbb{R}^3$ :

$$RTN(T) = \operatorname{span} \{(1, 0, 0), (0, 1, 0), (0, 0, 1), (x, y, z)\}.$$

Next, we construct our finite element spaces as follows:

$$\begin{aligned} \Sigma_h &= \{\underline{\tau}_h \in (L^2(\Omega))^3 : \underline{\tau}_h|_T \in RTN(T) \forall T \in T_h\}, \\ \Phi_h &= \{\phi_h \in L^2(\Omega) : \phi_h \in P_0(T) \forall T \in T_h\}. \end{aligned}$$

Notice that no continuity requirement on the normal component of  $\underline{\tau}_h \in \Sigma_h$  at the interelement boundaries is made, so that  $\Sigma_h \not\subset \Sigma$ . Actually, we relax this continuity via Lagrange multipliers, by introducing the ‘Lagrange multiplier space’  $\Lambda_{h,\chi}$  in the following way:

$$\Lambda_{h,\chi} = \{\mu_h \in L^2(E_h) : \mu_h|_l \in P_0(l), \forall l \in E_h, \int_l (\mu_h - \chi) d\sigma = 0 \forall l \subset \Gamma_0\},$$

where  $l$  is a face of the tetrahedron and  $E_h$  is the set of faces of  $T_h$ . The continuity of the normal components of the current at the interelements is then forced by the Lagrange multipliers. In this way, the discretization of (4) gives us the new problem:

$$\begin{cases} \text{Find } \underline{J}_h \in \Sigma_h, u_h \in \Phi_h, \lambda_h \in \Lambda_{h,\chi} \text{ such that:} \\ \int_{\Omega} e^{\psi} \underline{J}_h \cdot \underline{\tau}_h dx + \Sigma_T \int_T u_h \operatorname{div} \underline{\tau}_h dx - \Sigma_T \int_{\partial T} \lambda_h \underline{\tau}_h \cdot \underline{n} ds = 0 & \forall \underline{\tau}_h \in \Sigma_h \\ \Sigma_T \int_T \phi_h \operatorname{div} \underline{J}_h dx = \int_{\Omega} f \phi_h dx & \forall \phi_h \in \Phi_h \\ \Sigma_T \int_{\partial T} \mu_h \underline{J}_h \cdot \underline{n} ds = 0 & \forall \mu_h \in \Lambda_{h,0}. \end{cases} \quad (5)$$

In the computation  $\psi$  is assumed piecewise linear in each tetrahedron so that the integral of  $e^{\psi}$  can be computed exactly. Then we introduce the piecewise constant function  $\bar{\psi}$  defined in each  $T \in T_h$  as:

$$e^{\bar{\psi}}|_T = \frac{\int_T e^{\psi} dx}{|T|}. \quad (6)$$

Hence, the system (5) can be written, with obvious notation, as the linear system:

$$\begin{cases} e^{\bar{\psi}} A \underline{J} + B \underline{u} - C \underline{\lambda} = 0 \\ B^* \underline{J} = \underline{F} \\ C^* \underline{J} = 0. \end{cases} \quad (7)$$

In (7),  $\underline{J}$  can be easily eliminated by static condensation,  $A$  being a block-diagonal matrix (each block being a  $4 \times 4$  matrix):

$$\underline{J} = e^{-\bar{\psi}} A^{-1} (C \underline{\lambda} - B \underline{u})$$

leading to the new system:

$$\begin{cases} -e^{-\bar{\psi}} B^* A^{-1} B \underline{u} + e^{-\bar{\psi}} B^* A^{-1} C \underline{\lambda} = \underline{F} \\ -e^{-\bar{\psi}} C^* A^{-1} B \underline{u} + e^{-\bar{\psi}} C^* A^{-1} C \underline{\lambda} = 0. \end{cases}$$

Also  $\underline{u}$  can be eliminated by static condensation,  $B^* A^{-1} B$  being block-diagonal (actually diagonal in our case):

$$\underline{u} = e^{-\bar{\psi}} (B^* A^{-1} B)^{-1} (e^{-\bar{\psi}} B^* A^{-1} C \underline{\lambda} - \underline{F}). \quad (8)$$

The final system is then:

$$e^{-\bar{\psi}} M \underline{\lambda} = D \underline{F} \quad (9)$$

where:  $D = -(C^* A^{-1} B)(B^* A^{-1} B)^{-1}$

and:  $M = C^* A^{-1} C - C^* A^{-1} B (B^* A^{-1} B)^{-1} B^* A^{-1} C$ .

It can be checked that the matrix  $M$  is an M-matrix, if the triangles of the tetrahedrons have each angle  $\leq \pi/2$ . It can be proved [6] that  $\underline{\lambda}$  is an approximation of  $\underline{u}$ . Then, following [1-2], to go back to the original variable  $p$ , we use the following discrete version of transformation (2):

$$\lambda_h|_l = e^{\bar{\psi}}|_l p_h,$$

with:

$$e^{\bar{\psi}}|_l = \frac{\int_l e^{\bar{\psi}} d\sigma}{|l|} \quad \forall l \in E_h. \quad (10)$$

That is, each column of the matrix  $M$  has now to be multiplied by  $e^{\bar{\psi}}$  on the corresponding face. Although the resulting matrix is not anymore symmetric, it is still an M-matrix.

### 3. ASYMPTOTIC BEHAVIOUR OF THE FINAL MATRIX

We will now study the asymptotic behaviour of the numerical scheme when the potential becomes very large. For that, let us write:

$$\psi = \frac{\psi^0}{\varepsilon} \quad (11)$$

where  $\psi^0$  is a piecewise linear function with smooth gradient,  $\varepsilon$  a small real parameter and we want to analyze the behaviour of the scheme for  $\varepsilon$  going to zero. It is easy to check that the contributions  $m_{ij}^T$  of an element  $T$  to the final matrix have the form:

$$m_{ij}^T = e^{-\bar{\psi}}|_T L_{ij}^T e^{\bar{\psi}}|_{l_j} \quad (12)$$

where  $L_{ij}^T$  is a matrix depending on the basis functions.

The function  $\psi^0$  on a tetrahedron could have its maximum on a vertex, on an edge or on a face. It could also be constant.

We shall first analyze the asymptotic behaviour of  $e^{-\bar{\psi}}|_T$  in the different cases:

a)  $\psi_{\max} = \psi(V)$ , that is, the maximum of  $\psi$  is reached on a vertex:

$$e^{\bar{\psi}}|_T \simeq \varepsilon^3 e^{\psi_{\max}}$$

b)  $\psi_{\max} = \psi(V_1) = \psi(V_2)$ , that is,  $\psi$  has its maximum on the  $V_1 V_2$  edge:

$$e^{\bar{\psi}}|_T \simeq \varepsilon^2 e^{\psi_{\max}}$$

c)  $\psi_{\max} = \psi(\text{face})$  that is  $\psi$  has its maximum on a face:

$$e^{\bar{\psi}}|_T \simeq \varepsilon e^{\psi_{\max}}$$

d)  $\psi_{\max} = \text{const}(T)$ ,  $\psi$  is constant on each tetrahedron:

$$e^{\bar{\psi}}|_T = e^{\psi_{\max}}$$

On each face  $l_j$ ,  $\psi$  is a linear function in two variables, and we also have to examine 3 cases:

a')  $\psi$  has its maximum at one vertex:

$$e^{\tilde{\psi}}|_{l_j} \simeq \varepsilon^2 e^{\psi_{\max}|_{l_j}}$$

b')  $\psi$  has its maximum on an edge:

$$e^{\tilde{\psi}}|_{l_j} \simeq \varepsilon e^{\psi_{\max}|_{l_j}}$$

c')  $\psi = \text{const}$

$$e^{\tilde{\psi}}|_{l_j} = e^{\psi_{\max}|_{l_j}}$$

Consequently, since:  $\psi_{\max} = \varepsilon^{-1}\psi_{\max}^0$ , and:  $\psi_{\max}|_{l_j} = \varepsilon^{-1}\psi_{\max}^0|_{l_j}$ , we have:

$$m_{ij}^T = C(\varepsilon, L_{ij}^T) e^{(\psi_{\max}|_{l_j} - \psi_{\max})} \simeq \begin{cases} C(\varepsilon, L_{ij}^T) & \text{if } \psi_{\max}|_{l_j} \equiv \psi_{\max} \\ 0 & \text{otherwise} \end{cases}$$

Hence, we are interested to study  $C(\varepsilon, L_{ij}^T)$  when  $\psi_{\max}|_{l_j} \equiv \psi_{\max}$ . It is then immediate to see that case a) on  $T$  will imply case a') on  $l_j$ . Similarly, b) implies that b') holds, and c) implies c'). Consequently, if one of these cases holds, we have:

$$m_{ij}^T \simeq \begin{cases} \varepsilon^{-1} \frac{\nu_i \nu_j}{|T|} & \text{if } \psi_{\max}|_{l_j} \equiv \psi_{\max} \\ 0 & \text{otherwise} \end{cases}$$

(where:  $\nu_i = |l_i| \underline{n}_i$ ).

Therefore, as in the 2-D case, the asymptotic behaviour of the scheme fits the structure of the continuous problem (1):

$$-\nabla p + \frac{\psi^0}{\varepsilon} p = f.$$

As a final remark, let us point out that if case d) holds, then  $\nabla \psi \equiv 0$  in  $T$ , and the scheme fits again the structure of problem (1), which reduces in this case to:  $-\nabla p = f$ .

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