Unstructured grid adaptation for convection-dominated semiconductor equations*

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Abstract

A Raviart–Thomas mixed finite element is used to develop new *a posteriori* local error indicators for convection-dominated semiconductor transport equations. Lower and upper bounds of the estimators are established. These bounds differ by a negative power, $h^{-1/2}$, of the mesh size. Existence and uniqueness of the solution in the continuous and discrete cases are proven. The anisotropy of the $H(\mathrm{div})$ norm and the poor regularity of $H(\mathrm{div})$ functions prevent a direct application of frequently used arguments. An optimal estimator is obtained using a rigorous nonstandard analysis. Numerical results in the case of a realistic device show that an unstructured grid adaptation based on these estimators leads to an efficient and robust algorithm.

Keywords. A posteriori error estimators, Raviart–Thomas element, adaptive grid generation, semiconductor equations, discretization of nonsymmetric operators

Mathematical Subject Classification. 65N30, 65N12, 82D37

Résumé

On développe de nouveaux estimateurs *a posteriori* de l'erreur locale au moyen d'un élément fini mixe de Raviart–Thomas pour les équations de transport à convection dominante pour semiconducteurs. On obtient des bornes inférieures et supérieures des estimateurs. Ces bornes diffèrent par une puissance négative, $h^{-1/2}$, du pas du maillage. On démontre l'existence et l'unicité de la solution dans les cas continu et discret. L'anisotropie de la norme $H(\mathrm{div})$ et la piètre régularité des fonctions de $H(\mathrm{div})$ barrent l'application des arguments usuels. Une analyse rigoureuse produit un estimateur optimal. Les résultats numériques dans une situation réaliste montre qu'un maillage adapté basé sur ces estimateurs donne lieu à un algorithme efficace et robuste.

1 Introduction

The numerical solution of microelectronic devices is an integrated part of the Computer Aided Design of integrated microsystems. In this paper the emphasis is on the development of an advanced automatic grid (mesh) adaptation technique that can be used to optimize the cost-effective design of electronic devices by simulating the fabrication processes, the electric behavior of the devices, and the global network of electric circuits.

We consider the linearized convection-dominated transport equations for electron and hole flows coupled with Poisson's equation as a model of fluid drift-diffusion (El Boukili [8]) where current densities and quasi-Fermi levels are used as variables.

Error estimations in computational processes have been a subject of interest for more than two decades since the pioneering work of Babuška and Rheinboldt [2]. An extended account of this subject is found in Ainsworth and Oden [1], Rappaz [15], Verfürth [20], Fortin [9, 10], and Nithiarasu and Zienkiewicz [14].

The originality of this paper consists, firstly, in the proof of the existence and uniqueness of the solution to the linearized convection-dominated transport equations of the drift-diffusion model for semiconductor devices, in the continuous case, using mixed variational formulation in $H(\text{div}) \times L^2$; secondly, in the development of new *a posteriori* error estimators, which depends on a negative power, $h^{-1/2}$, of the mesh size, for the adaptive grid generation within the Raviart–Thomas finite element approach. The authors do not know how to remove this negative power with method they use. Some work has been done on symmetric equations (standard diffusion equation) as Poisson's equation in Verfürth [4, 20] and Hoppe *et al.* [11, 12]. But, to our knowledge, no work has been done on local mesh refinement within the Raviart–Thomas discretization for second-order nonsymmetric operators as the linearized semiconductor transport equations (or drift-diffusion model equations) with the indicated variables. Our analysis in deriving the error indicators could be seen as an extension to a nonsymmetric problem of the work by Braess and Verfürth [4].

The mesh adaptation technique is a mechanism that enriches the grid or the interpolation space under the guidance of an error indicator in view of improving the computed solution. Adaptive strategies can be classified into five categories: node-moving schemes (r-method), mesh refinement/coarsening schemes (h-method), subspace enrichment schemes (p-method), remeshing methods, and combined methods. These strategies cannot be applied blindly but need the guidance of local error estimators. One can distinguish between residual-based estimators and interpolation-based estimators, see Verfürth [20] for a complete literature. Here we focus attention on residual-based *a posteriori* error estimators which, recently, benefitted from a strong mathematical foundation.

In section 2, we present the mixed formulation in the continuous case and we establish existence and uniqueness results. In section 3, we introduce the discretization method, existence results for the discrete problem and *a priori* error estimates. In section 4, which is the main part of this paper, we develop *a posteriori* error estimators and establish two theoretical results that guarantee the efficiency and reliability of these estimators. Finally, in section 5, we demonstrate the benefit of the grid adaptation approaches based on these estimators by means of numerical results for a realistic *Heterojunction Bipolar Transistor* (HBT) working as a high frequency amplifier (used in mobile phones), see El Boukili [8]. The mesh adaptive technique is based on a remeshing at each step using the Delaunay algorithm.

2 Continuous problem

The semiconductor transport equation for the electron flow using the quasi-Fermi level variable p, with Dirichlet and Neumann boundary conditions, is

$$\begin{cases} -\text{div}(\alpha(x,p)\nabla p) + c(x,p) &= 0 \quad \text{in } \Omega, \\ p &= g_1 \quad \text{on } \partial\Omega_D, \\ (\alpha(x,p)\nabla p)\cdot \mathrm{n} &= 0 \quad \text{on } \partial\Omega_N, \end{cases} \tag{1}$$

where $\Omega \subset \mathbb{R}^2$ is a regular domain with boundary $\partial\Omega = \partial\Omega_D \cup \partial\Omega_N$, such that $\partial\Omega_D \cap \partial\Omega_N = \emptyset$ and meas $(\partial\Omega_D) \neq 0$, and n is the outward normal vector to $\partial\Omega$.

2.1 Mixed formulation

Substituting the vector-valued function

$$\mathrm{u} = \alpha(x,p)\nabla p$$

into equation (1), one can derive the following mixed problem:

Find two real-valued functions, p *and* u*, such that*

$$\left\{\begin{array}{rcll} a(x,p)\mathrm{u} &=& \nabla p & \text{in } \Omega, \\ -\operatorname{div}\mathrm{u} + c(x,p) &=& 0 & \text{in } \Omega, \\ p &=& g_1 & \text{on } \partial\Omega_D, \\ \mathrm{u}\cdot\mathrm{n} &=& 0 & \text{on } \partial\Omega_N, \end{array}\right. \tag{2}$$

with $a(x,p) = 1/\alpha(x,p)$*.*

2.2 Linearization of the continuous model

Problem (2) is linearized in a neighborhood of a point (u^0, p^0) as follows:

$$\left\{\begin{array}{rcll} a(x)\mathrm{u} - \nabla p - \mathrm{b}(x)p &=& \mathrm{f}(x) & \text{in } \Omega, \\ -\operatorname{div}\mathrm{u} + c(x)p &=& g(x) & \text{in } \Omega, \\ p &=& g_1 & \text{on } \partial\Omega_D, \\ \mathrm{u}\cdot\mathrm{n} &=& 0 & \text{on } \partial\Omega_N, \end{array}\right. \tag{3}$$

where

$$\begin{array}{rcl} a(x) &=& a(x,p^0(x)), \\ \mathrm{b}(x) &=& -a'_p(x,p^0(x))\mathrm{u}^0(x), \\ \mathrm{f}(x) &=& a'_p(x,p^0(x))\mathrm{u}^0(x)p^0(x), \\ c(x) &=& c'_p(x,p^0(x)), \\ g(x) &=& c'_p(x,p^0(x))p^0(x) - c(x,p^0(x)). \end{array}$$

2.3 Mixed variational formulation and preprocessing

We shall use the following notation to denote three three spaces,

$$X = H(\operatorname{div},\Omega), \qquad X_0 = H_{0,N}(\operatorname{div},\Omega), \qquad Y = L^2(\Omega),$$

where

$$\begin{array}{rcl} H(\operatorname{div},\Omega) &=& \{\mathrm{v}\in (L^2(\Omega))^2 :\ \operatorname{div}\mathrm{v}\in L^2(\Omega)\}, \\ H^1_{0,D}(\Omega) &=& \{\mathrm{v}\in H^1(\Omega) :\ \mathrm{v}|_{\partial\Omega} = 0 \text{ over } \partial\Omega_D\}, \\ H_{0,N}(\operatorname{div},\Omega) &=& \{\mathrm{v}\in H(\operatorname{div},\Omega) :\ \langle \mathrm{v}\cdot\mathrm{n}, w\rangle_{\partial\Omega_N} = 0 \qquad \forall\, w\in H^1_{0,D}(\Omega)\}. \end{array}$$

In this analysis, $< \cdot,\cdot >$ and $(\cdot,\cdot)$ represent the duality and inner products, respectively. The natural norm of v in $H(\operatorname{div},\Omega)$ is defined by

$$\|\mathrm{v}\|^2_{H(\operatorname{div},\Omega)} = \|\mathrm{v}\|^2_{L^2(\Omega)} + \|\operatorname{div}\mathrm{v}\|^2_{L^2(\Omega)}. \tag{4}$$

We note that the restriction of the normal trace of $H(\operatorname{div},\Omega)$ functions is not defined. This explains why we defined $H_{0,N}(\operatorname{div},\Omega)$ as the polar space of $H_{0,D}(\Omega)$.

The following **mixed variational problem** is considered:
Find $(\mathrm{u},p)\in X_0\times Y$ *such that*:

$$\left\{\begin{array}{rcll} \displaystyle\int_\Omega a(x)\mathrm{u}\cdot\mathrm{v}\,dx + \int_\Omega \operatorname{div}\mathrm{v}\,p\,dx && & \\ \displaystyle -\int_\Omega \mathrm{b}(x)\cdot\mathrm{v}p\,dx &=& \langle \mathrm{f},\mathrm{v}\rangle + \langle \mathrm{v}\cdot\mathrm{n}, g_1\rangle & \forall \mathrm{v}\in X_0, \\ \displaystyle\int_\Omega \operatorname{div}\mathrm{u}\,q\,dx - \int_\Omega c(x)pq\,dx &=& \displaystyle -\int_\Omega gq\,dx & \forall\, q\in Y. \end{array}\right. \tag{5}$$

The following notation will be used:

$$Z = X\times Y, \qquad Z_0 = X_0\times Y, \qquad U = (\mathrm{u},p), \qquad V = (\mathrm{v},q).$$

We define the bilinear form $\mathcal{A}$ on $Z_0 \times Z_0$ as the sum of the two left-hand sides of equation (5):

$$\begin{aligned}\mathcal{A}(U,V) &= \int_\Omega a(x)\mathrm{u}\cdot \mathrm{v}\, dx + \int_\Omega \operatorname{div} \mathrm{v}\, p\, dx - \int_\Omega \mathrm{b}(x)\cdot \mathrm{v}\, p\, dx \\ &\quad + \int_\Omega \operatorname{div} \mathrm{u}\, q\, dx - \int_\Omega c(x) pq\, dx,\end{aligned}$$

The same process is applied in defining the continuous linear form

$$\mathcal{F}(V) = \int_\Omega \mathrm{f}\cdot \mathrm{v}\, dx + \langle \mathrm{v}\cdot \mathrm{n}, g_1\rangle - \int_\Omega gq\, dx.$$

Therefore, problem (5) is equivalent to the following problem:
Find $U \in Z_0$ such that

$$\mathcal{A}(U,V) = \mathcal{F}(V) \qquad \forall V \in Z_0. \tag{6}$$

The existence and uniqueness of the solution to this problem and the final result will be collected in Theorem 2.1 at the end of this section. Towards this goal, we consider an arbitrary $F = (\mathrm{f}, g) \in Z_0'$, with $\mathrm{f} \in X_0'$ and $g \in Y$. The second equation of (5) is equivalent to

$$\int_\Omega c(x) pq\, dx = \int_\Omega \operatorname{div} \mathrm{u}\, q\, dx + \langle g, q\rangle. \tag{7}$$

We define the mapping $C\colon L^2(\Omega) \longrightarrow L^2(\Omega)$ as

$$\int_\Omega C(p) q\, dx = \int_\Omega c(x) pq\, dx,$$

that is, $\langle C(p), q\rangle = (c(x)p, q)$, and assume that the following hypothesis holds: there exists $\gamma > 0$ such that $c(x) \geq \gamma$ for all $x \in \Omega$. In that case, C is invertible and

$$\|C^{-1}\| \leq \frac{1}{\gamma}.$$

We note that the definition of C is valid when c is bounded.

We define the mapping $B\colon H(\operatorname{div}, \Omega) \longrightarrow L^2(\Omega)$ as

$$\int_\Omega B(\mathrm{u}) q\, dx = \int_\Omega \operatorname{div} \mathrm{u}\, q\, dx,$$

that is, $\langle B(\mathrm{u}), q\rangle = (\operatorname{div} \mathrm{u}, q)$. Thus, equation (7) can be written as

$$C(p) = B(\mathrm{u}) + g \quad\Longleftrightarrow\quad p = C^{-1}(B(\mathrm{u}) + g). \tag{8}$$

Let us consider the following hypothesis on $a(x)$: there exists $\alpha > 0$ such that for all $x \in \Omega$, $a(x) \geq \alpha$, and define $A\colon \left(L^2(\Omega)\right)^2 \longrightarrow \left(L^2(\Omega)\right)^2$ as

$$\int_\Omega A(\mathrm{u})\cdot \mathrm{v}\, dx = \int_\Omega a(x)\mathrm{u}\cdot \mathrm{v}\, dx, \tag{9}$$

that is, $\langle A(\mathrm{u}), \mathrm{v}\rangle = (a(x)\mathrm{u}, \mathrm{v})$. With this notation, the first equation of the mixed formulation (5) can be written as:

$$\langle A(\mathrm{u}), \mathrm{v}\rangle + \langle B(\mathrm{v}), p\rangle - \langle p, \mathrm{b}\cdot \mathrm{v}\rangle = \langle \mathrm{f}, \mathrm{v}\rangle. \tag{10}$$

Since $p = C^{-1}(B(\mathrm{u}) + g)$, then

$$\langle A(\mathrm{u}), \mathrm{v}\rangle + \langle B(\mathrm{v}) - \mathrm{b}\cdot \mathrm{v}, C^{-1}(B(\mathrm{u}) + g)\rangle = \langle \mathrm{f}, \mathrm{v}\rangle, \qquad \forall \mathrm{v} \in X_0, \tag{11}$$

and this expression is equivalent to

$$\begin{aligned}&\langle A(\mathrm{u}), \mathrm{v}\rangle + \langle C^{-1}B(\mathrm{u}), B(\mathrm{v})\rangle - \langle C^{-1}B(\mathrm{u}), \mathrm{b}\cdot \mathrm{v}\rangle \\ &= \langle \mathrm{f}, \mathrm{v}\rangle - \langle C^{-1}g, B(\mathrm{v})\rangle + \langle C^{-1}g, \mathrm{b}\cdot \mathrm{v}\rangle, \qquad \forall \mathrm{v} \in X_0.\end{aligned}$$

In the sequel, usual norms, unless explicitly denoted otherwise, will be as follows: $\|\cdot\|_{p,S}$ will denote the norms $\|\cdot\|_{L^p(S)}$ or $\|\cdot\|_{(L^p(S))^2}$.

We define the application

$$\mathrm{v} \mapsto \langle \mathrm{f}, \mathrm{v}\rangle - \langle C^{-1}g, B(\mathrm{v})\rangle + \langle C^{-1}g, \mathrm{b}\cdot \mathrm{v}\rangle =: l(\mathrm{v}) \tag{12}$$

for which the following inequality holds:

$$\begin{aligned} |l(\mathrm{v})| &\leq \|\mathrm{f}\|_{X_0'}\|\mathrm{v}\|_{X_0} + \|C^{-1}g\|_{2,\Omega}\|B(\mathrm{v})\|_{2,\Omega} + \|C^{-1}g\|_{2,\Omega}\|\mathrm{b}\cdot\mathrm{v}\|_{2,\Omega} \\ &\leq C\left[\|\mathrm{f}\|_{X_0'} + \frac{1}{\gamma}\|g\|_{2,\Omega} + \frac{1}{\gamma}\|g\|_{2,\Omega}\|\mathrm{b}\|_{\infty,\Omega}\right]\|\mathrm{v}\|_{X_0}, \end{aligned}$$

that is, $l \in X_0'$. Let us study the properties of the bilinear form $a(\cdot,\cdot)$ defined as

$$a(\mathrm{u},\mathrm{v}) = \langle A(\mathrm{u}), \mathrm{v}\rangle + \langle C^{-1}B(\mathrm{u}), B(\mathrm{v})\rangle - \langle C^{-1}B(\mathrm{u}), \mathrm{b}\cdot\mathrm{v}\rangle.$$

Firstly,

$$\begin{aligned} |a(\mathrm{u},\mathrm{v})| &\leq \|A(\mathrm{u})\|_{2,\Omega}\|\mathrm{v}\|_{2,\Omega} + \|C^{-1}B(\mathrm{u})\|_{2,\Omega}\|B(\mathrm{v})\|_{2,\Omega} \\ &\quad + \|C^{-1}B(\mathrm{u})\|_{2,\Omega}\|\mathrm{b}\cdot\mathrm{v}\|_{2,\Omega} \\ &\leq \|a\|_{\infty,\Omega}\|\mathrm{u}\|_{2,\Omega}\|\mathrm{v}\|_{2,\Omega} + \|C^{-1}\|\,\|\operatorname{div}\mathrm{u}\|_{2,\Omega}\|\operatorname{div}\mathrm{v}\|_{2,\Omega} \\ &\quad + \|C^{-1}\|\,\|\operatorname{div}\mathrm{u}\|_{2,\Omega}\|\mathrm{b}\|_{\infty,\Omega}\|\mathrm{v}\|_{2,\Omega} \\ &\leq \left[\|a\|_{\infty,\Omega} + \|C^{-1}\|(1+\|\mathrm{b}\|_{\infty,\Omega})\right]\|\mathrm{u}\|_{H(\mathrm{div},\Omega)}\|\mathrm{v}\|_{H(\mathrm{div},\Omega)}. \end{aligned}$$

To prove the ellipticity of $a(\cdot,\cdot)$ note that the two inequalities:

$$\langle C^{-1}B(\mathrm{v}), B(\mathrm{v})\rangle = \langle C^{-1}B(\mathrm{v}), C\,C^{-1}B(\mathrm{v})\rangle \geq \gamma|C^{-1}B(\mathrm{v})\|^2_{2,\Omega}$$

and

$$-\langle C^{-1}B(\mathrm{v}), \mathrm{b}\cdot\mathrm{v}\rangle \geq -\frac{1}{2}\left(\epsilon\|C^{-1}B(\mathrm{v})\|^2_{2,\Omega} + \frac{1}{\epsilon}\|\mathrm{b}\cdot\mathrm{v}\|^2_{2,\Omega}\right), \qquad \epsilon > 0,$$

imply

$$a(\mathrm{v},\mathrm{v}) \geq \alpha\|\mathrm{v}\|^2_{2,\Omega} + \gamma\|C^{-1}B(\mathrm{v})\|^2_{2,\Omega} - \frac{1}{2}\left(\epsilon\|C^{-1}B(\mathrm{v})\|^2_{2,\Omega} + \frac{1}{\epsilon}\,\|\mathrm{b}\cdot\mathrm{v}\|^2_{2,\Omega}\right).$$

Setting $\epsilon = \gamma$, we obtain

$$\frac{1}{\epsilon}\,\|\mathrm{b}\cdot\mathrm{v}\|^2_{2,\Omega} = \frac{1}{\gamma}\,\|\mathrm{b}\cdot\mathrm{v}\|^2_{2,\Omega} \leq \frac{1}{\gamma}\,\|\mathrm{b}\|^2_{\infty,\Omega}\|\mathrm{v}\|^2_{2,\Omega},$$

Finally, the following inequality

$$a(\mathrm{v},\mathrm{v}) \geq \left(\alpha - \frac{\|\mathrm{b}\|^2_{\infty,\Omega}}{2\gamma}\right)\|\mathrm{v}\|^2_{2,\Omega} + \frac{\gamma}{2}\|C^{-1}B(\mathrm{v})\|^2_{2,\Omega}, \tag{13}$$

can be derived, and if we suppose that $\|\mathrm{b}\|_{\infty,\Omega}$ is sufficiently small to verify

$$\alpha - \frac{\|\mathrm{b}\|^2_{\infty,\Omega}}{2\gamma} \geq \delta \geq 0, \tag{14}$$

then,

$$\begin{aligned} a(\mathrm{v},\mathrm{v}) &\geq \delta\|\mathrm{v}\|^2_{2,\Omega} + \frac{\gamma}{2}\|C^{-1}B(\mathrm{v})\|^2_{2,\Omega} \\ &\geq \delta\|\mathrm{v}\|^2_{2,\Omega} + \frac{\gamma}{2\|c\|^2_{\infty,\Omega}}\,\|\operatorname{div}\mathrm{v}\|^2_{2,\Omega}. \end{aligned}$$

Collecting the above result we have the following existence and uniqueness theorem.

Theorem 2.1 *Under the following hypotheses:*

(i) $a \in L^\infty, \quad a(x) \geq \alpha > 0, \quad \forall\, x \in \Omega,$

(ii) $c \in L^\infty, \quad c(x) \geq \gamma > 0, \quad \forall\, x \in \Omega,$

(iii) $\mathrm{b} \in (L^\infty)^2$, *with* $\|\mathrm{b}\|_{\infty,\Omega}$ *verifying equation* (14), *the mixed problem* (6) *has a unique solution* (u, p), *for all* $\mathrm{f} \in X_0'$ *and* $g \in Y$.

Since the mixed problem is well posed, the bilinear form $\mathcal{A}(U,V)$ verifies the inf-sup condition, that is, there exists a constant $\beta > 0$ such that:

$$\inf_{U \neq 0} \sup_{V \neq 0} \frac{A(U,V)}{\|U\|_Z \|V\|_Z} \geq \beta > 0. \tag{15}$$

Remark 2.1 *Conditions (i), (ii), and (iii) of Theorem 2.1 are realistic, and the data, which come from the devices studied here, fit the theoretical framework.*

3 Raviart–Thomas discretization

The mixed variational problem (5) is discretized by means of the Raviart–Thomas finite element of minimal order. A family of triangulations $\mathcal{T}_h$ of Ω, $0 < h \leq 1$, is *regular* if there exists a constant σ independent of h such that $h_K/\rho_K < \sigma$ for all triangles $K \in \mathcal{T}_h$, where h_K is the diameter of the triangle K and ρ_K is the diameter of the circumscribed circle to K. Geometrically speaking, regularity is equivalent to the fact that the minimal angles of all triangles are bounded from below. For regular $\mathcal{T}_h$, consider

$$\begin{aligned} RT_0(K) &= (P_0(K))^2 + xP_0(K), \qquad x \in \mathbb{R}^2, \\ R_0(\partial K) &= \{q : \ q \in L^2(\partial K), \ q|_{F_i} \in P_0(F_i), \ i = 1,2,3\}, \end{aligned}$$

where $P_0(K)$ is the set of polynomials of degree zero, that is, constants, F_i, $i = 1,2,3$, are the three edges of K and $\dim RT_0(K) = 3$. The *degrees of freedom* of a triangle K are

$$\Sigma_K = \{(l_i)_{i=1,2,3} : RT_0(K) \to \mathbb{R}\}; \tag{16}$$

here l_i is the linear form defined by

$$l_i(\mathrm{v}) = \int_{F_i} \mathrm{v} \cdot \mathrm{n} \, ds, \qquad \forall \, \mathrm{v} \in RT_0(K). \tag{17}$$

Definition 3.1 *The triple* $(K, \Sigma_K, RT_0(K))$ *is a Raviart–Thomas finite element.*

Remark 3.1 *Using the degrees of freedom* (16)*, it is possible to define a local interpolation operator* $\pi_K(\mathrm{v}_K)$ *for all* $\mathrm{v}_K \in H(\mathrm{div}, K)$ *provided* v_K *is slightly smoother than merely belonging to* $H(\mathrm{div}, K)$ *[5]. In general, it is not possible to compute expressions like* $\int_{\partial K} \mathrm{v}_K \cdot \mathrm{n} \, w \, ds$*, where* $w \in R_0(\partial K)$*, since* $\mathrm{v}_K \cdot \mathrm{n}$ *is only defined in* $H^{-1/2}(\partial K)$*. However, it is easy to check that if* v_K *belongs to the space*

$$W(K) = \{\mathrm{v}_K \in (L^s(K))^2 : \ \mathrm{div}\, \mathrm{v}_K \in L^2(K)\} \tag{18}$$

for fixed $s > 2$*, then such a construction is possible, see [5].*

It is clear that the spaces defined previously can be used to define an internal approximation of $H(\mathrm{div}, \Omega)$. At this point, let us consider the two sets X_h and Y_h:

$$\begin{aligned} X_h &= \{\mathrm{v} \in X : \ \mathrm{v}|_K \in RT_0(K) \ \ \forall \, K \in \mathcal{T}_h\}, \\ Y_h &= \{q \in Y : \ q|_K \in P_0(K) \ \ \forall \, K \in \mathcal{T}_h\}. \end{aligned}$$

A global interpolation operator from

$$W(\Omega) = H(\mathrm{div}, \Omega) \cap (L^s(\Omega))^2 \tag{19}$$

(for fixed $s > 2$) into X_h can be defined simply by setting

$$(\Pi_h \mathrm{v})|_K = \pi_K(\mathrm{v}|_K). \tag{20}$$

Clearly $\mathrm{div}\, X_h = Y_h$.

Next, to handle the boundary conditions, the following three spaces are considered:

$$X_{0h} = X_0 \cap X_h, \qquad Z_h = X_h \times Y_h, \qquad Z_{0h} = Z_0 \cap Z_h.$$

The discretization of the mixed variational problem (5) is as follows:

$$\begin{cases} \textit{Find } U_h = (\mathrm{u}_h, p_h) \in Z_{0h} \textit{ such that:} \\ \\ \mathcal{A}(U_h, V_h) = \mathcal{F}(V_h) \qquad \forall\, V_h \in Z_{0h}. \end{cases} \tag{21}$$

To establish the existence and uniqueness of the solution to problem (21) in Theorem 3.1 below we shall use the following duality lemma.

Lemma 3.1 (Duality Lemma, [7]) *Let $2 \le \theta < +\infty$, $\boldsymbol{\omega} \in X$, and $\mathrm{q} \in [L^2(\Omega)]^2$. If $\tau \in Y_h$ satisfies*

$$(a\boldsymbol{\omega}, \mathrm{v}) - (\operatorname{div} \mathrm{v}, \tau) + (\mathrm{b}\tau, \mathrm{v}) \;=\; (\mathrm{q}, \mathrm{v}), \qquad \mathrm{v} \in X_{0h}, \tag{22}$$

$$(\operatorname{div} \boldsymbol{\omega}, w) - (c\tau, w) \;=\; (r, w), \qquad w \in Y_h, \tag{23}$$

then, for h sufficiently small, there exists a constant $C = C(\theta, a, \mathrm{b}, c, \Omega) > 0$ such that

$$\|\tau\|_{\theta,\Omega} \le C\left[h^{2/\theta}\|\boldsymbol{\omega}\|_{\theta,\Omega} + h\|\operatorname{div} \boldsymbol{\omega}\|_{2,\Omega} + \|\mathrm{q}\|_{2,\Omega} + \|r\|_{2,\Omega}\right]. \tag{24}$$

Theorem 3.1 *For h sufficiently small, the nonstandard mixed discrete problem (21) has a unique solution in $X_{0h} \times Y_h$.*

Proof. The proof employs arguments similar to those used by Douglas and Roberts [7] in the case of Dirichlet boundary conditions. Here, we are working with mixed boundary conditions which require an additional effort. Let (u_{h1}, p_{h1}) and (u_{h2}, p_{h2}) be two solutions and write $u_{h0} = u_{h1} - u_{h2}$ and $p_{h0} = p_{h1} - p_{h2}$. Then (u_{h0}, p_{h0}) satisfies the following homogeneous system:

$$(a\mathrm{u}_{h0}, \mathrm{v}) - (\operatorname{div} \mathrm{v}, p_{h0}) + (\mathrm{b}p_{h0}, \mathrm{v}) \;=\; 0, \qquad \mathrm{v} \in X_{0h}, \tag{25}$$

$$(\operatorname{div} \mathrm{u}_{h0}, w) - (cp_{h0}, w) \;=\; 0, \qquad w \in Y_h. \tag{26}$$

Using inequality (24) with $\theta = 2$, we obtain

$$\|p_{h0}\|_{2,\Omega} \le Ch\left[\|\mathrm{u}_{h0}\|_{2,\Omega} + \|\operatorname{div} \mathrm{u}_{h0}\|_{2,\Omega}\right].$$

For $w = \operatorname{div} \mathrm{u}_{h0}$, we have

$$(\operatorname{div} \mathrm{u}_{h0}, \operatorname{div} \mathrm{u}_{h0}) = (cp_{h0}, \operatorname{div} \mathrm{u}_{h0})$$

and, by applying the Cauchy–Schwartz inequality, we get

$$\|\operatorname{div} \mathrm{u}_{h0}\|_{2,\Omega} \le \|p_{h0}\|_{2,\Omega},$$

which implies the inequality

$$\|p_{h0}\|_{2,\Omega} \le Ch\|\mathrm{u}_{h0}\|_{2,\Omega}.$$

Therefore, by (25) with $v = u_{h0}$, we obtain

$$(a\mathrm{u}_{h0}, \mathrm{u}_{h0}) = (\operatorname{div} \mathrm{u}_{h0}, p_{h0}) - (\mathrm{b}p_{h0}, \mathrm{u}_{h0}).$$

The Cauchy–Schwartz inequality and the duality lemma imply that

$$\|\mathrm{u}_{h0}\|_{2,\Omega} \le Ch\left[\|\operatorname{div} \mathrm{u}_{h0}\|_{2,\Omega} + \|p_{h0}\|_{2,\Omega}\right].$$

Thus, for h sufficiently small, we have

$$\|\mathrm{u}_{h0}\|_{2,\Omega} \le C'\|p_{h0}\|_{2,\Omega},$$

where C' is a constant. Finally, we obtain

$$\|\mathrm{u}_{h0}\|_{2,\Omega} \le C'\|p_{h0}\|_{2,\Omega} \le Ch\|\mathrm{u}_{h0}\|_{2,\Omega}.$$

We conclude that for h sufficiently small

$$\|\mathrm{u}_{h0}\|_{2,\Omega} = \|p_{h0}\|_{2,\Omega} = 0;$$

hence, $\mathrm{u}_{h0} = p_{h0} = 0$. This assures the solvability of the discrete problem. □

Remark 3.2 *No coercivity is required to prove the existence and uniqueness of the discrete mixed problem. In some way, this condition is replaced by the assumption on the mesh size h. In our case the coercivity is not satisfied. On the other hand, the duality lemma 3.1 can be viewed as a generalization of the* inf-sup *condition (or LBB condition) used in the analysis (see [5] among others).*

The optimal rate of convergence of the discrete solution with respect to the mesh is guaranteed by the following result, which was established in the doctoral thesis [8].

Theorem 3.2 *Let (u_h, p_h) be the solution of the mixed discrete problem (21). Then, the approximation error can be estimated by the inequalities:*

(i) $\|p - p_h\|_{2,\Omega} \leq Ch\|p\|_{H^2(\Omega)}$,

(ii) $\|\mathrm{u} - \mathrm{u}_h\|_{2,\Omega} \leq Ch\|p\|_{H^2(\Omega)}$,

(iii) $\|\operatorname{div}(\mathrm{u} - \mathrm{u}_h)\|_{2,\Omega} \leq Ch^s\|p\|_{H^{s+2}(\Omega)}, \qquad 0 \leq s \leq 1,$

where C is a strictly positive constant independent of h.

Remark 3.3 *We observe that the former theorem proves convergence in $X_0 \times Y$ at an optimal rate and with minimal smoothness requirements on the solution.*

4 A posteriori error estimators

To derive the *a posteriori* error estimations for the Raviart–Thomas element (that is, in $H(\operatorname{div}, \Omega) \times L^2(\Omega)$), many mathematical difficulties arise, and there is no direct application of the well established methods for other mixed methods as Stokes' or Navier-Stokes' problems [17], [20], [3]. These difficulties are not caused by the fact that this element refers to a mixed method, but are due to the fact that the traces of $H(\operatorname{div}, \Omega)$ functions are only in $H^{-1/2}(\partial\Omega)$ and, hence, are not in $L^2(\partial\Omega)$. Moreover, the traces of the functions in the Raviart–Thomas spaces are not contained in $H^{1/2}(\partial\Omega)$, because they are only piecewise polynomials. Likewise, we loose a factor h in the *a posteriori* estimator for the Raviart–Thomas element in comparison with other elements. This is due to the fact that the $H(\operatorname{div}, \Omega)$ norm is anisotropic, that is, it refers to differential operators of different orders. On the other hand, we do not have an interpolation operator for $H(\operatorname{div}, \Omega)$ functions as the Clément operator for $H^1(\Omega)$ functions (see [3]).

There are two ways to overcome the difficulties related to the regularity of the traces of $H(\operatorname{div}, \Omega)$ functions. One way is to use Helmholtz' decomposition as in [6] or [13]. But, the estimator obtained in this case does not involve the jump of p_h which one wants to control in practice. The second way is to use a saturation assumption as in [4]. In this case, one argues on the discrete level where the traces are meaningful in the $L^2(\partial\Omega)$ sense. In our analysis, we shall consider the latter way.

We note that the *a priori* error estimates given in Theorem 3.2 imply that, in general, a refinement of the grid and a reduction of h will lead to a reduction of the global error in the finite element solutions. However, these estimates provide no information on the reduction of the local errors. Therefore, we shall assume that we can exclude the exceptional cases in which the improvement is very small.

Assumption 4.1 (Saturation Assumption) *There exists a number $\gamma < 1$ such that*

$$\|\mathrm{u} - \mathrm{u}_{h/2}\|_{X_h} + \|p - p_{h/2}\|_{Y_h} \leq \gamma\big[\|\mathrm{u} - \mathrm{u}_h\|_{X_h} + \|p - p_h\|_{Y_h}\big]. \tag{27}$$

The following inequality follows from the saturation assumption:

$$\|\mathrm{u} - \mathrm{u}_h\|_{X_h} + \|p - p_h\|_{Y_h} \leq \frac{1}{1-\gamma}\big[\|\mathrm{u}_{h/2} - \mathrm{u}_h\|_{X_h} + \|p_{h/2} - p_h\|_{Y_h}\big]. \tag{28}$$

Therefore, it suffices to establish an upper bound for

$$\|\mathrm{u}_{h/2} - \mathrm{u}_h\|_{X_h} + \|p_{h/2} - p_h\|_{Y_h}. \tag{29}$$

This is the content of Theorem 4.1 below. Define

$$\begin{aligned} A_1(U_{h/2} - U_h, \mathrm{V}_{h/2}) \quad := \quad & (a(x)(\mathrm{u}_{h/2} - \mathrm{u}_h), \mathrm{v}_{h/2}) + (p_{h/2} - p_h, \operatorname{div}\mathrm{v}_{h/2}) \\ & -(\mathrm{b}(p_{h/2} - p_h), \mathrm{v}_{h/2}) \end{aligned} \tag{30}$$

and

$$A_2(U_{h/2}-U_h,\mathrm{V}_{h/2}):=(\operatorname{div}(\mathrm{u}_{h/2}-\mathrm{u}_h),w_{h/2})-(c(p_{h/2}-p_h),w_{h/2}). \tag{31}$$

Then, the solvability and the stability of the discrete problem (21) with respect to the natural $H(\operatorname{div},\Omega)$ norm (4) implies that there exists a constant C, independent of h, such that

$$\begin{aligned}&\|\mathrm{u}_{h/2}-\mathrm{u}_h\|_{X_h}+\|p_{h/2}-p_h\|_{Y_h}\\ &\quad\le\ C\sup_{\substack{V_{h/2}\in Z_{h/2}\\ \|V_{h/2}\|_Z=1}}\left[A_1(U_{h/2}-U_h,\mathrm{V}_{h/2})+A_2(U_{h/2}-U_h,\mathrm{V}_{h/2})\right].\end{aligned}$$

We have

$$\begin{aligned}A_1(U_{h/2}-U_h,\mathrm{V}_{h/2})\ &=\ \int_\Omega a(x)(\mathrm{u}_{h/2}-\mathrm{u}_h)\cdot\mathrm{v}_{h/2}\,dx+\int_\Omega\operatorname{div}\mathrm{v}_{h/2}(p_{h/2}-p_h)dx\\ &\quad-\int_\Omega\mathrm{b}(x)\cdot\mathrm{v}_{h/2}(p_{h/2}-p_h)\,dx\\ &=\ \sum_K\Big[\int_K a(x)(\mathrm{u}_{h/2}-\mathrm{u}_h)\cdot\mathrm{v}_{h/2}\,dx+\int_K\operatorname{div}\mathrm{v}_{h/2}(p_{h/2}-p_h)\,dx\\ &\quad-\int_K\mathrm{b}(x)\cdot\mathrm{v}_{h/2}(p_{h/2}-p_h)\,dx\Big].\end{aligned}$$

Applying Green's formula to the integral

$$\int_K\operatorname{div}\mathrm{v}_{h/2}(p_{h/2}-p_h)\,dx$$

and using the boundary conditions, we obtain

$$\begin{aligned}&A_1(U_{h/2}-U_h,\mathrm{V}_{h/2})\\ &=\ \sum_K\Big[\int_K a(x)(\mathrm{u}_{h/2}-\mathrm{u}_h)\cdot\mathrm{v}_{h/2}\,dx-\int_K\mathrm{v}_{h/2}\cdot\nabla(p_{h/2}-p_h)\,dx\\ &\quad+\langle\mathrm{v}_{h/2}\cdot\mathrm{n},p_{h/2}-p_h\rangle_{\partial K}-\int_K\mathrm{b}(x)\cdot\mathrm{v}_{h/2}(p_{h/2}-p_h)\,dx\Big].\end{aligned} \tag{32}$$

Let $S(K)=\{F_1,F_2,F_3\}$ denote the set of edges of K, where $F_i\not\subset\partial\Omega$. Then, (32) becomes

$$\begin{aligned}&A_1(U_{h/2}-U_h,V_{h/2})+A_2(U_{h/2}-U_h,V_{h/2})\\ &=\ \sum_K\Big[\int_K(\mathrm{f}_{mh}-a_{mh}(x)\mathrm{u}_h+\nabla p_h+\mathrm{b}_{mh}(x)p_h)\cdot\mathrm{v}_{h/2}\,dx\\ &\quad+\int_K(-g_{mh}-\operatorname{div}\mathrm{u}_h+c(x)p_h)q_{h/2}\,dx\\ &\quad+\sum_{F\in S(K)}\langle -p_h,\mathrm{v}_{h/2}\cdot\mathrm{n}\rangle_F+\sum_{F\subset\partial K\cap\partial\Omega_D}\langle i_h(g_1)-p_h,\mathrm{v}_{h/2}\cdot\mathrm{n}\rangle_F\Big],\end{aligned} \tag{33}$$

where f_{mh}, a_{mh}, b_{mh}, and g_{mh} are polynomial approximations of order m ($m>0$) to f, a, b, and g, respectively, and i_h is an interpolation operator.

Remark 4.1 *The standard derivation of a local a posteriori error estimator in other functional spaces such as $H^1(\Omega)$ suggests to estimate $\|\mathrm{u}-\mathrm{u}_h\|_X+\|p-p_h\|_Y$ directly and to replace $(u_{h/2},p_{h/2})$ by (u,p) and $\mathrm{v}_{h/2}$ by an arbitrary function $\mathrm{v}\in H(\operatorname{div})$. This would avoid the saturation assumption. But unfortunately, the passage from $\langle -p_h,\mathrm{v}_{h/2}\cdot\mathrm{n}\rangle_{\partial K}$ in equation (32) to $\sum_{F\in S(K)}\langle -p_h,\mathrm{v}_{h/2}\cdot\mathrm{n}\rangle_F$ does not make sense when $\mathrm{v}_{h/2}$ is replaced by $\mathrm{v}\in H(\operatorname{div})$, because the traces of $H(\operatorname{div},K)$ functions are not in $L^2(\partial K)$.*

Thus, for all $V_{h/2}\in Z_{0h/2}$ with $\|V_{h/2}\|_Z=1$, the following estimate is derived:

$$\begin{aligned}A(U_{h/2}-U_h,V_{h/2})\ &\le\ C\sum_K\Big[\|\mathrm{f}-a(x)\mathrm{u}_h+\nabla p_h+\mathrm{b}(x)p_h\|_{2,K}\\ &\quad+\|-g-\operatorname{div}\mathrm{u}_h+c(x)p_h\|_{2,K}\\ &\quad+\frac12\sum_{F\in S(K)}h_K^{-1/2}\|[p_h]\|_{2,F}+\sum_{F\subset\partial K\cap\partial\Omega_D}h_K^{-1/2}\|g_1-p_h\|_{2,F}\Big].\end{aligned}$$

In this estimate, C is a positive constant independent of h, and the *jump* $[p_h]$ on each interior edge F is defined in the direction of the positive normal to the edge F. The negative power of h comes from the use of the inverse estimate given by inequality (40). If $F = K_i \cap K_j$ and the positive normal to F is oriented from K_i to K_j, the jump $[p_h]$ is defined as $[p_h] = p_h\big|_{K_i} - p_h\big|_{K_j}$.

We set

$$\begin{aligned}\eta_R(K) \quad := \quad & \|\mathrm{f}_{mh} - a_{mh}(x)\mathrm{u}_h + \nabla p_h + \mathrm{b}_{mh}(x)p_h\|_{2,K} \\ & + \| - g_{mh} - \operatorname{div} \mathrm{u}_h + c_{mh}(x)p_h\|_{2,K} \\ & + \frac{1}{2}\sum_{F\in S(K)} h_K^{-1/2}\|[p_h]\|_{2,F} + \sum_{F\subset \partial K\cap\partial\Omega_D} h_K^{-1/2}\|i_h(g_1) - p_h\|_{2,F}.\end{aligned} \tag{34}$$

By combining the above estimations and using the saturation assumption, we obtain the following *a posteriori* error estimation.

Theorem 4.1 *The following a posteriori error estimation holds:*

$$\begin{aligned}& \|\mathrm{u} - \mathrm{u}_h\|_X + \|p - p_h\|_Y \\ & \leq \quad C\Big[\sum_{K\in\mathcal{T}_h} \eta_R(K)^2 + \|g - g_{mh}\|_{2,K}^2 + \|\mathrm{f} - \mathrm{f}_{mh}\|_{2,K}^2 \\ & \qquad + \|a - a_{mh}\|_{2,K}^2\|\mathrm{b} - \mathrm{b}_{mh}\|_{2,K}^2 + \sum_{F\in\partial K\cap\partial\Omega_D} h_K^{-1}\|g_1 - i_h(g_1)\|_{2,F}^2\Big]^{1/2},\end{aligned} \tag{35}$$

where C is a positive constant.

This theorem establishes the reliability of the estimator (34).

Remark 4.2 *The number $\eta_R(K)$ is called a residual a posteriori error estimator. It is a powerful and fundamental tool in an isotropic mesh adaptation procedure. This fact will be confirmed by the numerical results presented in Section 5.*

Remark 4.3 *We are mainly interested in deriving an a posteriori error estimator for the initial nonlinear problem. Thus, the error indicator $\eta_R(K)$ in (34) can be considered as a first-order approximation to the following estimator:*

$$\begin{aligned}\eta_R(K) \quad = \quad & \| - a_{mh}(x, p_h)\mathrm{u}_h + \nabla p_h\|_{2,K} + \| - \operatorname{div} \mathrm{u}_h + c_{mh}(x, p_h)\|_{2,K} \\ & + \frac{1}{2}\sum_{F\in S(K)} h_K^{-1/2}\|[p_h]\|_{2,F} + \sum_{F\in\partial K\cap\partial\Omega_D} h_K^{-1/2}\|i_h(g_1) - p_h\|_{2,F}.\end{aligned} \tag{36}$$

A theoretical proof of this estimator will be considered in future work.

Interpretation: *The first two terms on the right-hand side of estimator (34) correspond to the residuals of the two equations of the discretized mixed variational problem. Thus, if these equations are assumed to be numerically well solved, then these two quantities will be small. The third term controls the discontinuity (or the variation) of the primal variable p across the mesh edges. So, this term can localize the internal layer problems related to large gradients (or shocks). These problems are present, in particular, at the heterojunction interfaces of the device in hand and at its Ohmic contacts. Finally, the last term controls the imposition of the boundary condition over the device Ohmic contacts. Thus, this term can localize the boundary layer problems.*

To guarantee the efficiency of the estimator (34), we need the following theorem which is a reciprocal result to Theorem 4.1.

Theorem 4.2 *There exits a constant C, depending only on the minimal angle in the triangulation such that*

$$\begin{aligned}\eta_R(K) \quad \leq \quad & C\Big[\|\mathrm{u} - \mathrm{u}_h\|_{H(\mathrm{div},\omega_K)} + (1 + h_K^{-1})\|p - p_h\|_{2,\omega_K} \\ & + \|g - g_{mh}\|_{2,K} + \|\mathrm{f} - \mathrm{f}_{mh}\|_{2,K} + \|a - a_{mh}\|_{2,K} \\ & + \|\mathrm{b} - \mathrm{b}_{mh}\|_{2,K} + h_K^{-1/2}\|i_h(g_1) - g_1\|_{2,F}\Big].\end{aligned} \tag{37}$$

where $\omega_K = \{K_0 \in \mathcal{T}_h :\ K_0 \cap K = F_i$ edges of $K,\ i = 1, 2, 3\}$ (see Fig. 1).

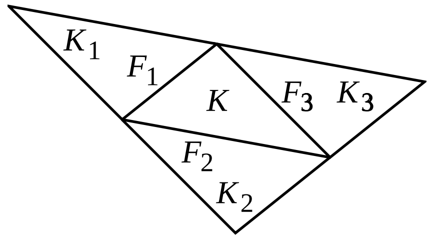

Figure 1: Definition of ω_K.

Proof. We introduce the following notation:

$$\begin{aligned}
\text{I} &:= \|\mathrm{f}_{mh} - a_{mh}(x)\mathrm{u}_h + \nabla p_h + \mathrm{b}_{mh}(x)p_h\|_{2,K},\\
\text{II} &:= \| - g_{mh} - \operatorname{div}\mathrm{u}_h + c_{mh}(x)p_h\|_{2,K},\\
\text{III} &:= \frac{1}{2}h_K^{-1/2}\sum_{F\in S(K)}\|[p_h]\|_{2,F},\\
\text{IV} &:= h_K^{-1/2}\sum_{F\in\partial K\cap\partial\Omega_D}\|i_h(g_1) - p_h\|_{2,F}.
\end{aligned}$$

For each triangle $K \in \mathcal{T}_h$, define the function φ_K by

$$\varphi_K(x) := \begin{cases} \widehat{\varphi}_{\widehat{K}} \circ F_K^{-1}(x) & \text{if } x \in \widehat{K},\\ 0 & \text{otherwise,}\end{cases}$$

where $\widehat{K}$ is the reference element and $\widehat{\varphi}_{\widehat{K}}$ is a real function verifying:

- $0 \le \widehat{\varphi}_{\widehat{K}}(\hat{x}) \le 1$, for all $\hat{x} \in \widehat{K}$, with $\widehat{\varphi}_{\widehat{K}}(\hat{x}) = 0$, for all $\hat{x} \in \partial\widehat{K}$, and
- $\widehat{\varphi}_{\widehat{K}} \in C^1(\widehat{K})$ and $\nabla\widehat{\varphi}_{\widehat{K}} \in L^\infty(\widehat{K})^2$.

Clearly, for all $K \in \mathcal{T}_h$ and all elements v_K of a finite dimensional subspace of $L^2(K)$, using the fact that norms are equivalent in finite dimensional spaces and passing through the reference element $\widehat{K}$, we obtain the norm-equivalent inequalities

$$C_0\|\mathrm{v}_K\|_{2,K} \le \|\mathrm{v}_K\varphi_K(x)^{1/2}\|_{2,K} \le C_1\|\mathrm{v}_K\|_{2,K}, \tag{38}$$

where C_0 and C_1 are independent of K and v_k. We can also obtain the inequality

$$\|\mathrm{v}_K\varphi_K(x)\|_{2,K} \le \|\mathrm{v}_K\|_{2,K}. \tag{39}$$

Estimation of I. Let us introduce the following function:

$$\mathrm{v}_K := [\mathrm{f}_{mh}(x) - a_{mh}(x)\mathrm{u}_h + \nabla p_h + \mathrm{b}_{mh}(x)p_h]\,\varphi_K(x).$$

By definition, v_K is an element of $H(\operatorname{div},\Omega)$ with continuous normal component $\mathrm{v}_K\cdot\mathrm{n}_{F_i}$, where F_i are the interior edges of K. Using the equivalence of the norms given by equation (38), we get

$$\begin{aligned}
I^2 &\le \|(\mathrm{f}_{mh} - a_{mh}(x)\mathrm{u}_h + \nabla p_h + \mathrm{b}_{mh}(x)p_h)\varphi_K^{1/2}(x)\|_{2,K}^2\\
&= \int_K \big(\mathrm{f}_{mh} - a_{mh}(x)\mathrm{u}_h + \nabla p_h + \mathrm{b}_{mh}(x)p_h\big)^2\cdot\varphi_K(x)\,dx\\
&= \int_K \big(\mathrm{f}_{mh} - a_{mh}(x)\mathrm{u}_h + \nabla p_h + \mathrm{b}_{mh}(x)p_h\big)\cdot\mathrm{v}_K\,dx\\
&= \int_K \big(\mathrm{f} - \mathrm{f} + a\mathrm{u}_h - a\mathrm{u}_h + \mathrm{b}p_h - \mathrm{b}p_h\\
&\quad + \mathrm{f}_{mh} - a_{mh}(x)\mathrm{u}_h + \nabla p_h + \mathrm{b}_{mh}(x)p_h\big)\cdot\mathrm{v}_K\,dx\\
&= \int_K [-(\mathrm{f} - \mathrm{f}_{mh}) + (a - a_{mh})\mathrm{u}_h - (\mathrm{b} - \mathrm{b}_{mh})p_h]\cdot\mathrm{v}_K\,dx\\
&\quad + \int_K [a(\mathrm{u} - \mathrm{u}_h) - \mathrm{b}(p - p_h)]\cdot\mathrm{v}_K\,dx - \int_K \nabla(p - p_h)\cdot\mathrm{v}_K\,dx,
\end{aligned}$$

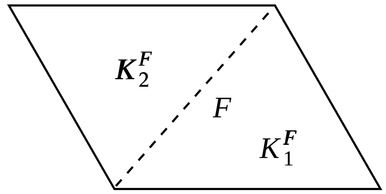

Figure 2: Definition of ω_F.

where the first equation, for f, in (3) has been used in the last equality. Using Green's formula and the definition of v_K, we get

$$\begin{aligned} I^2 &\leq C_1 I \left[\|\mathrm{f} - \mathrm{f}_{mh}\|_{2,K} + \|a - a_{mh}\|_{2,K} + \|\mathrm{b} - \mathrm{b}_{mh}\|_{2,K}\right] \\ &\quad + C_2 I \left[\|\mathrm{u} - \mathrm{u}_h\|_{2,K} + \|p - p_h\|_{2,K}\right] \\ &\quad + \|p - p_h\|_{2,K} \|\operatorname{div}(\mathrm{v}_K)\|_{2,K}. \end{aligned}$$

Using the equivalence of norms in finite dimensional spaces in the reference configuration and an inverse inequality for the divergence operator, we can prove the inequality (see Lemma 4.1 of [18] for the details):

$$\|\operatorname{div} \mathrm{v}_K\|_{2,K} \leq \sqrt{2}\,\|\nabla \mathrm{v}_K\|_{2,K} \leq C_2 h_K^{-1} \|\mathrm{v}_K\|_{2,K}, \tag{40}$$

and obtain the final estimate for I:

$$\begin{aligned} I &\leq C_0 \left[\|\mathrm{u} - \mathrm{u}_h\|_{H(\operatorname{div},K)} + (1 + h_K^{-1})\|p - p_h\|_{2,K}\right] \\ &+ C_{00} \left[\|\mathrm{f} - \mathrm{f}_{mh}\|_{2,K} + \|a - a_{mh}\|_{2,K} + \|\mathrm{b} - \mathrm{b}_{mh}\|_{2,K}\right]. \end{aligned}$$

Estimation of II. The estimation of II is straightforward:

$$\begin{aligned} II &= \|g - g + c_{mh} p - c_{mh} p - g_{mh} - \operatorname{div}(\mathrm{u}_h) + c_{mh} p_h\|_{2,K} \\ &\leq \|g - g_{mh}\|_{2,K} + C_2 \|c - c_{mh}\|_{2,K} + \|\mathrm{u} - \mathrm{u}_h\|_{H(\operatorname{div},K)} + C_3 \|p - p_h\|_{2,K}, \end{aligned}$$

where the second equation, for g, in (3) has been used in the last inequality.

Estimation of III. Let F be an internal edge; thus, there exist two triangles K_1^F and K_2^F such that $F = K_1^F \cap K_2^F$. Set $\omega_F = K_1^F \cup K_2^F$ (see Fig. 2).

Observing that $[p_h]|_F$ is constant, we can construct a suitable function P_F by

$$P_F([p_h])(x) := \begin{cases} \mathrm{v}_1^F(x) & \text{if } x \in K_1^F, \\ \mathrm{v}_2^F(x) & \text{if } x \in K_2^F, \\ 0 & \text{otherwise}, \end{cases} \tag{41}$$

where v_1^F and v_2^F are the unique polynomials defined over K_1^F and K_2^F, respectively, in RT_0 such that each degree of freedom is 0 except the one in F which has to be $[p_h]$ (that is, $\mathrm{v}_1^F \cdot \mathrm{n}_1^F = [p_h]$, $\mathrm{v}_2^F \cdot \mathrm{n}_2^F = -[p_h]$, and $\mathrm{v}_{1,2}^F \cdot \mathrm{n}_e = 0$, where e is an edge different from F). By definition, it is clear that $P_F([p_h])$ belongs to $H(\operatorname{div}, \omega_K)$. Similar constructions can be considered if $[p_h]$ is a polynomial over F by means of an appropriate generalized Raviart–Thomas finite element. It is not very difficult to prove that P_F is linear and verifies the following lemma, whose proof is a direct consequence of Lemma 4 in [18].

Lemma 4.1 *The function P_F satisfies the inequality*

$$\|P_F([p_h])\|_{H(\operatorname{div},\omega_F,h)} \leq C h_K^{1/2} \|[p_h]\|_{2,F},$$

where

$$\|\mathrm{v}\|_{H(\operatorname{div},\omega_F,h)} = \|\mathrm{v}\|_{L^2(\omega_F)} + h\|\operatorname{div} \mathrm{v}\|_{L^2(\omega_F)}, \qquad \forall\, \mathrm{v} \in X_{0h}.$$

By construction of P_F and the fact that $[p]=0$, we get

$$\begin{aligned}\|[p_h]\|_{2,F}^2 &= \int_F [p_h]P_h([p_h])\cdot \mathrm{n}\, ds\\ &= \int_F [p-p_h]P_h([p_h])\cdot \mathrm{n}\, ds\\ &= \int_{\omega_F} (p-p_h)\operatorname{div}(P_h([p_h]))\, dx + \int_{\omega_F} \nabla(p-p_h)\cdot P_h([p_h])\, dx.\end{aligned}$$

On the other hand, we have

$$\int_{\omega_F} \nabla(p-p_h)\cdot P_h([p_h])\, dx = \int_{\omega_F} a(\mathrm{u}-\mathrm{u}_h)\cdot P_h([p_h])\, dx + \int_{\omega_F} \mathrm{b}(p-p_h)\cdot P_h([p_h])\, dx$$

and

$$\begin{aligned}\|[p_h]\|_{2,F} &\le C_4\Big[\|\mathrm{u}-\mathrm{u}_h\|_{2,\omega_F} + \|p-p_h\|_{2,\omega_F}\|P_h([p_h])\|_{2,\omega_F}\Big]\\ &\quad + \|p-p_h\|_{2,\omega_F}\|\operatorname{div}(P_h([p_h]))\|_{2,\omega_F}.\end{aligned}$$

Using Lemma 4.1, we obtain

$$\begin{aligned}\|[p_h]\|_{2,F} &\le C_4\Big[\|\mathrm{u}-\mathrm{u}_h\|_{2,\omega_F} + \|p-p_h\|_{2,\omega_F}\Big]h_K^{1/2}\|[p_h]\|_{2,F}\\ &\quad + C_5 h_K^{-1}\|p-p_h\|_{2,\omega_F}h_K^{1/2}\|[p_h]\|_{2,F}.\end{aligned}$$

Finally, we get the desired estimate:

$$h_K^{-1/2}\|[p_h]\|_{2,F} \le C\Big[\|\mathrm{u}-\mathrm{u}_h\|_{H(\operatorname{div},\omega_F)} + (1+h_K^{-1})\|p-p_h\|_{2,\omega_F}\Big].$$

Estimation of IV. The estimation of IV is based on the same arguments as those used for III. Let F be a boundary edge satisfying $F\in\partial\Omega_D$ and let K_1^F be the triangle containing F. For simplicity, suppose that $i_h(g_1)$ is constant over F. In this case, the function P_F is constructed in the form

$$P_F(i_h(g_1)-p_h)(x) = \mathrm{v}_1^F(x), \tag{42}$$

where v_1^F is the unique polynomial defined over K_1^F in RT_0 such that all degrees of freedom are 0 except the one in F which is taken to be $i_h(g_1)-p_h$. As in the previous case, P_F is linear and verifies the inequality

$$\|P_F(i_h(g_1)-p_h)\|_{H(\operatorname{div},K_1^F,h)} \le C h_K^{1/2}\|i_h(g_1)-p_h\|_{2,F}, \tag{43}$$

with

$$\begin{aligned}\|i_h(g_1)-p_h\|_{2,F}^2 &= \int_F (i_h(g_1)-p_h)P_h(i_h(g_1)-p_h)\cdot\mathrm{n}\, ds\\ &= \int_F ((p-p_h)+i_h(g_1)-g_1)P_h(i_h(g_1)-p_h)\cdot\mathrm{n}\, ds\\ &= \int_F P_h(i_h(g_1)-p_h)\cdot\mathrm{n}(p-p_h)\, ds + \int_F (i_h(g_1)-g_1)^2\, ds.\end{aligned}$$

Using inequality (43) and the same analysis as for the estimation of III, we get

$$\begin{aligned}h_K^{-1/2}\|i_h(g_1)-p_h\|_{2,F} &\le C\Big[\|\mathrm{u}-\mathrm{u}_h\|_{H(\operatorname{div},\omega_F)} + (1+h_K^{-1})\|p-p_h\|_{2,\omega_F}\Big]\\ &\quad + h_K^{-1/2}\|i_h(g_1)-p_h\|_{2,F}.\end{aligned}$$

This ends the rather technical proof of Theorem 4.2. □

Remark 4.4 *All the terms of the estimator are optimally estimated in the natural norm of $H(\operatorname{div},\Omega)$ (4) and one cannot do better using this norm. A comparison with the upper bound (35) shows that the estimate in Theorem 4.2 involves a negative power of h. The reason is the anisotropy of the natural norm of $H(\operatorname{div},\Omega)$ (that is, $\|\operatorname{div}\mathrm{v}\|_{2,K}\le Ch_K^{-1}\|v\|_{2,K}$).*

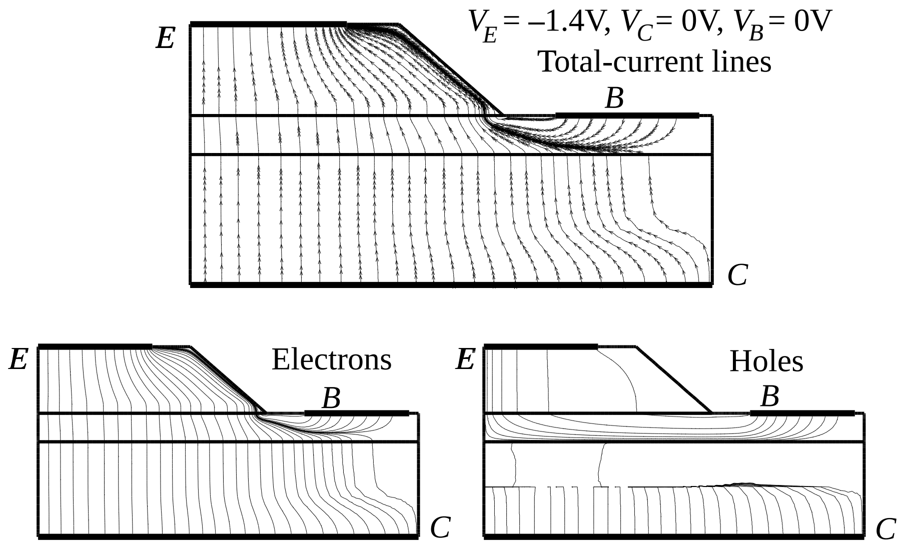

Figure 3: Current lines of solution at optimal mesh when the transistor effect is significant.

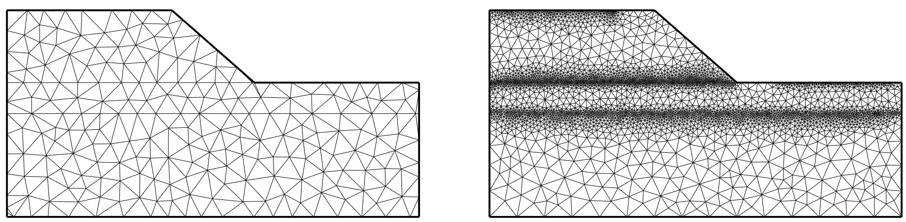

Figure 4: Initial coarse grid: 230 vertices (left). Adapted grid after 4 steps: 2911 vertices (right).

5 Numerical results for an HBT

The mesh adaptive algorithm is based on a remeshing at each step using the Delaunay algorithm. The performance of this adaptive technique is presented using an isotropic metric which is based on the *a posteriori* error estimators obtained above.

We consider the drift-diffusion model in the case of an industrial heterojunction bipolar transistor whose structure is described in El Boukili [8].

Figure 3 shows the current lines (the quantities of interest) when the transistor effect is significant. The applied voltage at emitter E is -1.4 volts, and it is 0 volt at base B and collector C.

Figure 4 shows the initial coarse grid and the adapted grid at step 4. Figure 5 illustrates the adapted grid at steps 5 and 9. We should notice that the adapted grid at step 9 is in a sense optimal (see Fig. 6 described below) for the considered device. The refinement process is stopped when the estimated error is less than a certain tolerance. We observe a significant adaptive refinement in the neighborhood of the heterojunction interfaces due to the large variation of the electron densities and the neighborhood of the Ohmic contacts where the boundary layer problems are present.

Figure 6 illustrates the convergence of the coupled Solver/Adaptation cycle by showing the number of nodes of the successive meshes as the overall loop proceeds. An indication of convergence is the leveling off of the number of nodes after a certain number of remeshing steps. Indeed, we observe an initial increase in the number of nodes, followed by a gradual decrease to the asymptotic value. The first few meshing steps being not well adapted, the solutions are polluted with spurious oscillations. This explains an over-refinement of the meshes at the beginning, but, as the solution improves, the mesher gradually reduces the number of nodes to reach an optimal mesh and optimal accuracy of the solutions.

Figures 7 shows the mesh obtained at convergence of the adaptation cycle (after 4 iterations) when starting from a fine grid. We observe that this mesh has the same overall aspect and nearly the same number of vertices as the

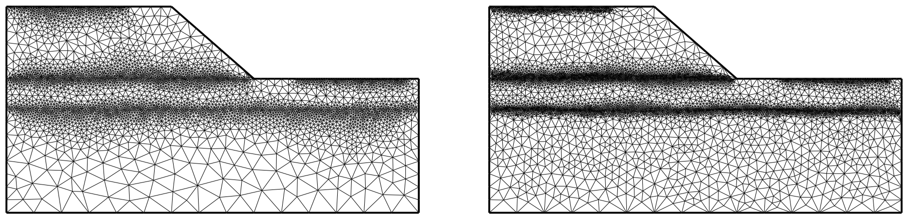

Figure 5: Adapted grid after 5 and 9 iterations: 4007 vertices (left), and 8159 vertices (right).

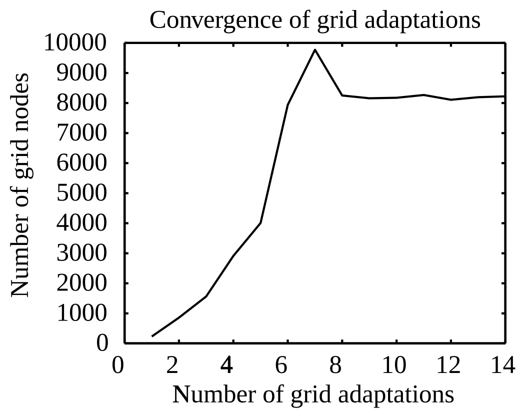

Figure 6: Total number of vertices versus adaptation cycles for a heterojunction bipolar transistor.

mesh obtained at convergence (after 9 iterations, see Fig. 5) when starting from a coarse mesh, thus supporting the conjecture that the adapted mesh (or optimal mesh) could be unique [10] and would solve the problem with optimal accuracy. Similarly, we notice that the solution obtained at convergence of the mesher-solver loop starting from a coarse or fine mesh is the same as the one shown in Fig. 3. This illustrates the mesh-independent solution. This may lead to user-independent solutions as the gridding decisions are taken away from the user, who may have no *a priori* knowledge about the best grid for a given geometry for various problems. This fact is the fundamental goal of any mesh adaptation technique. We should note that many numerical experiments for different structures have been performed and the same behavior of the adaptive procedure was observed.

6 Conclusion

A posteriori error estimators, coupled with a powerful mesh adaptation algorithm, have been proposed, analyzed mathematically, and successfully implemented within a Raviart–Thomas mixed finite element for drift-diffusion semiconductor equations. The adaptative iteration proceeds by successive local alterations of the previous grid. The adaptive process and its coupling with the solver are both shown to converge to an optimal mesh and optimal solution.

Future work will consider the construction of anisotropic estimators ([16]) for a domain decomposition with nonmatching grids at the interface of heterojunctions to reduce strong refinement on both sides of the interfaces due to strong continuity requirements.

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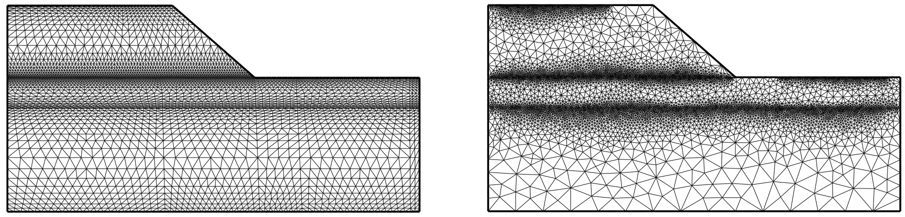

Figure 7: Initial fine grid: 3784 vertices (left). Adapted grid at convergence: 8120 vertices (right).

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