Local error indicators for linearized drift-diffusion equations in $H(\text{div}) \times L^2$

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ABSTRACT. *Within the framework of mixed Finite Element Methods, we analyze the numerical analysis of an error indicator. It relies on the residual of a linearized Drift-Diffusion model of the transport equation for electrons in semiconductor devices using Fermi-Dirac statistic. Inf-sup condition, upper and lower bounds are proved. The results are optimal for the natural norms of H(div) and L^2.*

RÉSUMÉ. *Dans le cadre de la méthode des éléments finis mixtes, nous présentons une analyse mathématique des indicateurs d'erreur locale pour l'équation linéarisée de transport des particules chargées. Celle-ci est issue du modèle de Dérive-Diffusion dégénéré pour les semiconducteurs à hétérojonction. La condition inf-sup ainsi que les bornes inférieure et supérieure de l'estimateur sont démontrées. L'estimateur obtenu est optimal pour la norme usuelle de H(div) x L^2.*

KEY WORDS : *a posteriori error estimation, mixed finite elements, linearized electron transport equations.*

MOTS-CLÉS : *estimation d'erreur a posteriori, éléments finis mixtes, équation de transport linéarisée.*

1 Introduction

In computational heterojunction semiconductor devices, as in other problems of fluid dynamics or engineering, one often encounters the difficulty that the overall accuracy of the numerical solution is disturbed by local singularities such as those near heterojunction regions, critical points or boundary layers at ohmic contacts (see [5]).

An obvious solution is to refine the discretization near the critical regions, i.e., to place more grid-points where the solution is less regular. The question then is how to identify these regions automatically and how to guarantee a good balance of the number of grid-points in the refined and un-refined regions so that the overall accuracy is optimal. Another closely related problem is to obtain reliable estimates of the accuracy of the computed numerical solution. A priori error estimates are in general not sufficient since they only yield asymptotic estimates which are not known explicitly. Moreover, they often require regularity assumptions about the solution which, for practical problems, are hardly satisfied.

The problem addressed in this paper is principally to establish an 'a posteriori' error estimator for linearized transport equation for electrons in semiconductor devices. Initially, classical formulation of this equation is considered, then introducing the current density $\vec{u}$ as independent variable, we deduce a mixed formulation for the problem that is later linearized to obtain a linear mixed equations in the variables p (electron quasi-Fermi level) and $\vec{u}$ (current density for electrons). A mixed Raviart-Thomas Finite Element method of minimal order is used to approximate the continuous problem in $H(\text{div}\,) \times L^2$. A priori estimations are also provided. Finally, two theoretical results which guarantee the existence of an isotropic 'a posteriori' local estimator which controls the approximation error are proved. No numerical experiences have been carried out by now. Future works will consider the extensions to anisotropic estimators as well as numerical comparison between isotropic and anisotropic estimators.

2 Continuous problem

Considering the boundary conditions, the transport equation for electrons in semiconductor devices is given by:

$$\left\{ \begin{array}{rcll} -\text{div}\,(\alpha(x,p)\nabla p) + c(x,p) & = & 0 & \Omega, \\ p & = & g_1 & \partial\Omega_D, \\ (\alpha(x,p)\nabla p)\cdot n & = & 0 & \partial\Omega_N, \end{array} \right. \quad (1)$$

where $\Omega \in \mathbb{R}^2$ is a regular domain with $\partial\Omega_D \cup \partial\Omega_N = \partial\Omega$.

2.1 Mixed formulation

Let us consider

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

then the following mixed problem can be derived from equation [1]: *find p and $\vec{u}$, two real value functions such that*

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

with $a(x,p) = \alpha^{-1}(x,p)$.

2.2 Linearization of the continuous model

A linear version of the problem [2] in a neighborhood of a point $(\vec{u}^0, p^0)$ is given by the following equations:

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

with

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

The problem [3] is going to be solved by a mixed variational method, thus, the functions $a(.)$, $\vec{b}(.)$, $c(.)$, f, g and g_1 and the domain Ω are supposed to be regular enough so that the mixed variational formulation to be well posed in the function spaces $L^2(\Omega)$ and $H(\mathrm{div}\,,\Omega)$ and to guarantee the existence, uniqueness and regularity of the weak solution.

2.3 Mixed variational formulation of the linear model equations

Let us define

$$X = X(\Omega) = H(\mathrm{div}\,,\Omega),$$

$$X_0 = X_0(\Omega) = H_{0,N}(\mathrm{div}\,,\Omega),$$

$$Y = Y(\Omega) = L^2(\Omega),$$

where

$$H(\mathrm{div}\,,\Omega) = \{\vec{v} \in (L^2(\Omega))^2 : \ \mathrm{div}\,(\vec{v}) \in L^2(\Omega)\},$$
$$H^1_{0,D}(\Omega) = \{\vec{v} \in H^1(\Omega) : \ \vec{v}|_{\partial\Omega} = 0 \text{ over } \partial\Omega_D\},$$
$$H_{0,N}(\mathrm{div}\,,\Omega) = \{\vec{v} \in H(\mathrm{div}\,,\Omega) : \ \langle \vec{v}\cdot n, \vec{w}\rangle = 0 \ \ \forall \vec{w} \in H^1_{0,D}(\Omega)\}.$$

The following mixed variational problem is considered:
find $(\vec{u}, p) \in X_0 \times Y$ *so that:*

$$\left\{\begin{array}{lcll} \int_\Omega a(x)\vec{u}\cdot\vec{v}\,dx + \int_\Omega p\,div\,(\vec{v})\,dx & & & \\ \qquad - \int_\Omega \vec{b}(x)p\cdot\vec{v}\,dx & = & \langle f,\vec{v}\rangle + \langle \vec{v}\cdot n, g_1\rangle & \forall \vec{v}\in X_0, \\ \int_\Omega div\,(\vec{u})q\,dx - \int_\Omega c(x)pq\,dx & = & -\int_\Omega gq\,dx & \forall q \in Y \end{array}\right. \quad (4)$$

Now, we note

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

Let $\mathcal{A}$ be defined as

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

by adding the two equations of problem [4]. The same process is applied to define the continuous linear form

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

Therefore, the mixed variational problem [4] is equivalent to the following problem: *find* $U \in Z_0$ *so that:*

$$\mathcal{A}(U,V) = \langle \mathcal{F}, V\rangle \qquad\qquad \forall V \in Z_0. \quad (5)$$

Let us consider an arbitrary $F = (f,g) \in Z_0'$, with $f \in X_0'$ and $g \in Y$. The second equation of [4] is equivalent to

$$\int_\Omega c(x)pq\,dx = \int \mathrm{div}\,(\vec{u})q\,dx + \langle g, q\rangle. \quad (6)$$

Let us define $C\colon L^2(\Omega) \longrightarrow L^2(\Omega)$ as

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

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

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

Let us define $B: H(\text{div}\,,\Omega) \longrightarrow L^2(\Omega)$ as

$$\int_\Omega B(\vec{u})q\,dx = \int_\Omega \text{div}\,(\vec{u})q\,dx,$$

i.e., $\langle B(\vec{u}), q\rangle = \langle \text{div}\,(\vec{u}), q\rangle$. Thus, the equation [6] can be written as

$$C(p) = B(\vec{u}) + g \Leftrightarrow p = C^{-1}(B(\vec{u}) + g). \tag{7}$$

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

$$\int_\Omega A(\vec{u}) \cdot \vec{v}\,dx = \int_\Omega a(x)\vec{u} \cdot \vec{v}\,dx, \tag{8}$$

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

$$\langle A(\vec{u}), \vec{v}\rangle + \langle B(\vec{v}), p\rangle - \langle p, \vec{b} \cdot \vec{v}\rangle = \langle f, \vec{v}\rangle \tag{9}$$

but $p = C^{-1}(B(\vec{u}) + g)$, therefore

$$\langle A(\vec{u}), \vec{v}\rangle + \langle B(\vec{v}) - \vec{b} \cdot \vec{v}, C^{-1}(B(\vec{u}) + g)\rangle = \langle f, \vec{v}\rangle, \quad \forall\vec{v} \in X_0, \tag{10}$$

and this expression is equivalent to

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

$$\langle f, \vec{v}\rangle - \langle C^{-1}g, B(\vec{v})\rangle + \langle C^{-1}g, \vec{b} \cdot \vec{v}\rangle, \quad \forall\vec{v} \in X_0.$$

Let us define the application

$$\vec{v} \mapsto \langle f, \vec{v}\rangle - \langle C^{-1}g, B(\vec{v})\rangle + \langle C^{-1}g, \vec{b} \cdot \vec{v}\rangle = l(\vec{v}), \tag{11}$$

for which the following inequality holds:

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

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

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

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

To prove the ellipticity of the bilinear form $a(\cdot,\cdot)$ note that

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

and

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

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

Imposing $\epsilon = \gamma$, we obtain

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

Finally, the following expression can be derived,

$$a(\vec{v},\vec{v}) \geq \left(\alpha - \frac{||\vec{b}||^2_{L^\infty}}{2\gamma}\right)||\vec{v}||^2_{L^2} + \frac{\gamma}{2}||C^{-1}B(\vec{v})||^2_{L^2}, \tag{12}$$

supposing that $||\vec{b}||_{L^\infty}$ is sufficiently small to verify

$$\alpha - \frac{||\vec{b}||^2_{L^\infty}}{2\gamma} \geq \delta \geq 0, \tag{13}$$

then,

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

Therefore, under the hypothesis:

1. $a \in L^\infty$, $a(x) \geq \alpha > 0$, $\forall x \in \Omega$,
2. $c \in L^\infty$, $c(x) \geq \gamma > 0$, $\forall x \in \Omega$,
3. $\vec{b} \in L^\infty$, with $||\vec{b}||_{L^\infty}$ verifying equation [13],

the mixed problem [5] is well possed, i.e., for all $f \in X_0'$, $g \in L^2$, the mixed problem [5] has an unique solution $(\vec{u}, p)$ and continuous dependence of the solution with respect to data.

Remark 2.1 *It is easy to verify that the application $\tilde{f}$ defined by*

$$\langle \tilde{f}, \vec{v} \rangle = \int_\Omega \vec{f} \cdot \vec{v}\, dx + \langle g_1, \vec{v} \cdot \vec{n} \rangle$$

is a linear form in X_0'.

As the mixed problem is well posed, then the bilinear form $\mathcal{A}(U, V)$ verifies the *inf–sup* condition, i.e., there exists a constant $\beta > 0$ so that:

$$\inf_{U,V \neq 0} \sup \frac{\mathcal{A}(U, V)}{||U||_Z ||V||_Z} \geq \beta > 0, \tag{14}$$

3 Internal approximation by a mixed F.E.M of minimal order

The mixed variational problem [4] is discretized using the Raviart-Thomas F.E. of minimal order. Let us consider a regular family of triangulations $\mathcal{T}_h$ of Ω, $0 < h \leq 1$, that is, there exists a constant σ independent of h so that $\frac{h_K}{\rho_K} < \sigma$, for all triangle $K \in \mathcal{T}_h$, where h_K is the diameter of a triangle K and ρ_K is the diameter of the circumscript circle to K. Geometrically speaking, the previous conditions is equivalent to 'minimal angles of triangles bounded from below'. Let us consider

$$RT_0(K) = (P_0(K))^2 + xP_0(K); \quad x \in \mathbb{R}^2,$$

$$R_0(\partial K) = \{q : \ q \in L^2(\partial K), \ q|_{F_i} \in P_0(F_i), \ i = 1, 2, 3\},$$

where F_i, $i = 1, 2, 3$ are the three edges of K and $\dim RT_0(K) = 3$. The degrees of freedom for a triangle K are

$$\sum_K = \{(l_i)_{i=1,3} : RT_0(K) \to \mathbb{R}\}$$

where l_i is a linear form defined by

$$l_i(\vec{v}) = \int_{\partial K} \vec{v} \cdot \vec{n}\, q\, ds; \quad \forall q \in R_0(\partial K); \quad \forall \vec{v} \in RT_0(K). \tag{15}$$

Definition 3.1 $(K, \sum_K, RT_0(K))$ *is a F.E. of Raviart-Thomas.*

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

$$W(K) = \{\vec{v}_K \in (L^s(K))^2 : \; div\, \vec{v}_K \in L_2(K)\}, \tag{16}$$

for s fixed > 2*, then such a construction is possible. In that case the interpolation operator* $\pi_K : W(K) \mapsto RT_0(K)$ *is defined by*

$$\int_{\partial K} (\vec{v}_K - \pi_K(\vec{v}_K)) \cdot \vec{n}\, ds = 0. \tag{17}$$

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

$$X_h = \{\vec{v} \in X : \; \vec{v}|_K \in RT_0(K) \; \forall K \in \mathcal{T}_h\},$$

and

$$Y_h = \{q \in Y : \; q|_K \in P_0(K) \; \forall K \in \mathcal{T}_h\},$$

a global interpolation operator from

$$W(\Omega) = H(\mathrm{div}, \Omega) \cap (L^s(\Omega))^2, \tag{18}$$

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

$$(\Pi_h \vec{v})|_K = \pi_K(\vec{v}|_K). \tag{19}$$

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

Now, due to boundary conditions, the following spaces are considered:

$$X_{0h} = X_0 \cap X_h,$$

$$Z_h = X_h \times Y_h \text{ and } Z_{0h} = Z_0 \cap Z_h.$$

The discretization of the mixed variational problem [4] is given by:

$$\begin{cases} \textit{Find } U_h = (\vec{u}_h, p_h) \in Z_{0h} \textit{ so that:} \\ \mathcal{A}(U_h, V_h) = \langle \mathcal{F}, V_h \rangle_{Z',Z} \quad \forall V_h \in Z_{0h}. \end{cases} \tag{20}$$

The proof of existence and uniqueness of the previous discrete problem and the following convergence results are given in [3].

Theorem 3.1 *Let $(\vec{u}_h, p_h)$ be the solution of the mixed continuous problem [4]. Then, the approximation error can be estimated by the inequalities*

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

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

$$(iii) \quad ||div(\vec{u} - \vec{u}_h)||_{L^2(\Omega)} \leq Ch^s||p||_{H^{s+2}(\Omega)}, \quad 0 \leq s \leq 1.$$

Remark 3.2 *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 estimator for the linear equations

As problem [5] is well-posed, that is, there exists a unique solution for it and the suitable choice of approximation spaces imply the existence of a constant, independent of h, $\beta > 0$ so that:

$$\sup_{V \neq 0} \frac{A(U - U_h, V)}{||V||_Z} \geq \beta(||\vec{u} - \vec{u}_h||_X + ||p - p_h||_Y) \tag{21}$$

$$\begin{aligned}
A(U - U_h, V) &= \int_\Omega a(x)(\vec{u} - \vec{u}_h) \cdot \vec{v}\, dx + \int_\Omega \operatorname{div} \vec{v}(p - p_h) dx \\
&- \int_\Omega \vec{b}(x) \cdot \vec{v}(p - p_h)\, dx + \int_\Omega \operatorname{div}(\vec{u} - \vec{u}_h) q\, dx \\
&- \int_\Omega c(x)(p - p_h) q\, dx \\
&= \sum_K \left(\int_K a(x)(\vec{u} - \vec{u}_h) \cdot \vec{v}\, dx + \int_K \operatorname{div} \vec{v}(p - p_h)\, dx \right. \\
&- \int_K \vec{b}(x) \cdot v(p - p_h)\, dx + \int_K \operatorname{div}(\vec{u} - \vec{u}_h) q\, dx \\
&- \left. \int_K c(x)(p - p_h) q\, dx \right).
\end{aligned}$$

Applying now the Green's formula to the term:

$$\int_K \operatorname{div} \vec{v}(p - p_h)\, dx,$$

and using the boundary conditions, we obtain

$$
\begin{aligned}
A(U-U_h,V) &= \sum_K \Big(\int_K a(x)(\vec{u}-\vec{u}_h)\cdot\vec{v}\,dx - \int_K \vec{v}\cdot\nabla(p-p_h)\,dx \\
&+ \langle \vec{v}\cdot\vec{n}, p-p_h\rangle_{\partial K} - \int_K \vec{b}(x)\cdot\vec{v}(p-p_h)\,dx \\
&+ \int_K \operatorname{div}(\vec{u}-\vec{u}_h)q\,dx - \int_K c(x)(p-p_h)q\,dx \Big)
\end{aligned}
$$

Let us define $S(K)$ as the set of edges of K, F_i, $i=1,2,3$, so that $F_i \not\subset \partial\Omega$. Then, the following expression is obtained:

$$
\begin{aligned}
A(U-U_h,V) &= \sum_K \Big(\int_K (\vec{f}-a(x)\vec{u}_h+\nabla p_h+\vec{b}(x)p_h)\cdot\vec{v}\,dx \\
&+ \int_K (-g-\operatorname{div}\vec{u}_h+c(x)p_h)q\,dx \\
&+ \sum_{F\in S(K)} \langle -p_h, \vec{v}\cdot\vec{n}\rangle_F + \sum_{F\subset\partial K\cap\partial\Omega_D} \langle g_1-p_h, \vec{v}\cdot\vec{n}\rangle_F \Big).
\end{aligned}
$$

Thus, for all $V \neq 0 \in Z_0$, the following estimation is derived:

$$
\begin{aligned}
\frac{A(U-U_h,V)}{||V||_{Z_0}} &\leq \sum_K \Big(||\vec{f}-a(x)\vec{u}_h+\nabla p_h+\vec{b}(x)p_h||_{L^2(K)} \\
&+ ||-g-\operatorname{div}\vec{u}_h+c(x)p_h||_{L^2(K)} \\
&+ \frac{1}{2}\sum_{F\in S(K)} h_K^{-\frac{1}{2}}||[p_h]||_{L^2(F)} + \sum_{F\subset\partial K\cap\partial\Omega_D} h_K^{-\frac{1}{2}}||g_1-p_h||_{L^2(F)} \Big).
\end{aligned}
$$

Noting

$$
\begin{aligned}
\eta(K) &= ||\vec{f}-a(x)\vec{u}_h+\nabla p_h+\vec{b}(x)p_h||_{L^2(K)} \\
&+ ||-g-\operatorname{div}\vec{u}_h+c(x)p_h||_{L^2(K)} \qquad (22) \\
&+ \frac{1}{2}\sum_{F\in S(K)} h_K^{-\frac{1}{2}}||[p_h]||_{L^2(F)} + \sum_{F\subset\partial K\cap\partial\Omega_D} h_K^{-\frac{1}{2}}||g_1-p_h||_{L^2(F)}
\end{aligned}
$$

the following result is obtained:

Proposition 4.1 *Let $(\vec{u},p)$ be the solution of the problem [4] and $(\vec{u}_h,p_h)$ be the solution of the discrete problem [20], then the following 'a posteriori' estimation is obtained:*

$$
||\vec{u}-\vec{u}_h||_X + ||p-p_h||_Y \leq C\Big(\sum_{K\in\mathcal{T}_h} \eta(K)^2\Big)^{\frac{1}{2}}, \qquad (23)
$$

where C is a positive constant depending on β.

Remark 4.1 *If we note*

$$\eta = \Big(\sum_{K \in \mathcal{T}_h} \eta(K)^2 \Big)^{\frac{1}{2}},$$

then η is named an 'a posteriori' estimator computed with the residual of the equation and it can be used in isotropic mesh adaptation procedures.

In practice, equation [22] is replaced by

$$\begin{aligned} \eta_R(K) &= ||\vec{f}_{mh} - a(x)\vec{u}_h + \nabla p_h + \vec{b}(x)p_h||_{L^2(K)} \\ &+ ||-g_{mh} - \operatorname{div}\vec{u}_h + c(x)p_h||_{L^2(K)} \\ &+ \frac{1}{2}\sum_{F \in S(K)} h_K^{-\frac{1}{2}}||[p_h]||_{L^2(F)} + \sum_{F \in \partial K \cap \partial\Omega_D} h_K^{-\frac{1}{2}}||i_h(g_1) - p_h||_{L^2(F)} \end{aligned} \tag{24}$$

where g_{mh} (respectively $\vec{f}_{mh}$) is an approximation of g (respectively $\vec{f}$), i_h is an interpolation operator and m is an integer greater than zero. Trivially, an analogous estimation to [23] can be derived:

Proposition 4.2 *Let us consider the same hypotheses as in proposition [4.1], then the following estimation is obtained:*

$$\begin{aligned} ||\vec{u} - \vec{u}_h||_X + ||p - p_h||_Y &\leq C\Big(\sum_{K \in \mathcal{T}_h} \eta_R(K)^2 + ||g - g_{mh}||^2_{L^2(K)} \\ &+ ||\vec{f} - \vec{f}_{mh}||^2_{L^2(K)} \\ &+ \sum_{F \in \partial K \cap \partial\Omega_D} h_K^{-1}||g_1 - i_h(g_1)||^2_{L^2(F)}\Big)^{\frac{1}{2}} \end{aligned} \tag{25}$$

Remark 4.2 *We are principally interested in deducing an 'a posteriori' error estimation for the initial non linear problem. Thus, the error indicator $\eta(K)$ given in equation [22] can be considered as an approximation of first order of the following estimator*

$$\begin{aligned} \eta(K) &= ||-a(x,p_h)\vec{u}_h + \nabla p_h||_{L^2(K)} \\ &+ ||-div\,\vec{u}_h + c(x,p_h)||_{L^2(K)} \\ &+ \frac{1}{2}h_K^{-\frac{1}{2}}\sum_{F \in S(K)} ||[p_h]||_{L^2(F)} + h_K^{-\frac{1}{2}}\sum_{F \in \partial K \cap \partial\Omega_D} ||g_1 - p_h||_{L^2(F)}. \end{aligned} \tag{26}$$

Up to now, no theoretical proof of this estimator has been done. It will be considered in future works.

Interpretation: *The two first terms of estimator [22] correspond to the residuals of the two equations of the discretized mixed variational problem. Thus, if the equations are assumed to be numerically well-solved, then these* *two quantities must be small. The third term controls the discontinuity of the primal variable p across the mesh edges. Finally, the last term controls if the imposition of the boundary condition over the device ohmic contacts is verified. The first and the two last terms cannot be estimated in an optimal way. This is due to the anisotropy of $H(div, \Omega)$. Moreover, the traces of $H(div, \Omega)$-functions are only in $H^{-1/2}(\partial\Omega)$. In order to avoid the negative exponent, different norms must be used (in particular mesh-dependent norms).*

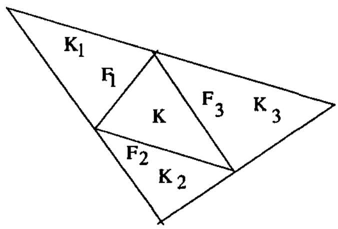

Figure 1: *Definition of* ω_K

Let us proof a reciprocal result to proposition [4.1].

Proposition 4.3 *With the definition [22], there is a constant C, which only depends on the minimal angle in the triangulation such that*

$$\eta(K) \leq C(||\vec{u} - \vec{u}_h||_{H(div,\omega_K)} + h_K^{-1}||p - p_h||_{L^2(\omega_K)}), \qquad (27)$$

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

Proof
The proof of this proposition is quite technique and it is based on the study of a function $\mathcal{E}$ defined by

$$\mathcal{E}(V) = \mathcal{A}(U - U_h, V), \quad \forall V \in Z_0,$$

then

$$\begin{aligned} \mathcal{E}(V) &= \sum_K \int_K (\vec{f} - a(x)\vec{u}_h + \nabla p_h + \vec{b}(x)p_h) \cdot \vec{v}\, dx \\ &+ \int_K (-g - \operatorname{div} \vec{u}_h + c(x)p_h)q\, dx \\ &+ \sum_{F \in S(K)} \langle -p_h, \vec{v} \cdot \vec{n} \rangle_F + \sum_{F \in \partial K \cap \partial\Omega_D} \langle g_1 - p_h, \vec{v} \cdot \vec{n} \rangle_F. \end{aligned}$$

Let us introduce the following notations:

$$\begin{aligned}
\mathrm{I} &= \|\vec{f} - a(x)\vec{u}_h + \nabla p_h + \vec{b}(x)p_h\|_{L^2(K)},\\
\mathrm{II} &= \| - g - \operatorname{div}\vec{u}_h + c(x)p_h\|_{L^2(K)},\\
\mathrm{III} &= \frac{1}{2}h_K^{-\frac{1}{2}} \sum_{F\in S(K)} \|[p_h]\|_{L^2(F)},\\
\mathrm{IV} &= h_K^{-\frac{1}{2}} \sum_{F\in\partial K\cap\partial\Omega_D} \|g_1 - p_h\|_{L^2(F)}.
\end{aligned}$$

For all triangle $K \in \mathcal{T}_h$, let us consider a function φ_K defined as:

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

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

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

Clearly, for all $K \in \mathcal{T}_h$ and for all $\vec{v}_K$ element of a finite dimensional subspace of $L^2(K)$, using the fact that norms are equivalent in finite dimentional spaces and passing through the reference element $\hat{K}$, we obtain

$$C_0\|\vec{v}_K\|_{L^2(K)} \le \|\vec{v}_K\varphi_K(x)^{\frac{1}{2}}\|_{L^2(K)} \le C_1\|\vec{v}_K\|_{L^2(K)}, \tag{28}$$

where C_0 and C_1 are independent of K and $\vec{v}_K$. We can also obtain that

$$\|\vec{v}_K\varphi_K(x)\|_{L^2(K)} \le \|\vec{v}_K\|_{L^2(K)} \tag{29}$$

Majoration of I: Let us consider the following test function

$$\vec{v}_K = \varphi_K(x)(\vec{f}(x) - a(x)\vec{u}_h + \nabla p_h + \vec{b}(x)p_h).$$

From its definition $\vec{v}_K$ is an element of $H(\operatorname{div},\Omega)$ ($\vec{v}_K \in H(\operatorname{div},K)$ and we have the continuity of the normal component $\vec{v}_K\cdot\vec{n}_{F_i}$, where F_i are the interior edges of K, in fact their are all 0). Denoting by $V = (\vec{v}_K, 0)$ then

$$\begin{aligned}
\mathcal{E}(V) &= \int_K (\vec{f} - a(x)\vec{u}_h + \nabla p_h + \vec{b}(x)p_h)^2\varphi_K\,dx\\
&= \|(\vec{f} - a(x)\vec{u}_h + \nabla p_h + \vec{b}(x)p_h)\varphi_K^{\frac{1}{2}}\|_{L^2(K)}^2\\
&\ge C_1^I\|\vec{f} - a(x)\vec{u}_h + \nabla p_h + \vec{b}(x)p_h\|_{L^2(K)}^2,
\end{aligned}$$

thus,

$$\begin{aligned}
(\mathrm{I})^2 &\le \mathcal{E}(V)\\
&\le C_2^I\|U - U_h\|_{Z(K)}\|V\|_{Z(K)}\\
&\le C_2^I(\|\vec{u} - \vec{u}_h\|_{H(\operatorname{div},K)} + \|p - p_h\|_{L^2(K)})\\
&\qquad \|(\vec{f} - a(x)\vec{u}_h + \nabla p_h + \vec{b}(x)p_h)\varphi_K\|_{H(\operatorname{div},K)},
\end{aligned}$$

now, using the equivalence of norms in finite dimentional spaces in the reference configuration and an inverse inequality for the div-norm we obtain

$$\mathrm{I} \leq C_3^I(1+h_K^{-1})(\|\vec{u}-\vec{u}_h\|_{H(\mathrm{div}\,,K)}+\|p-p_h\|_{L^2(K)}).$$

Majoration of II: Let us consider the following test function

$$q_K = \varphi_K(-g - \mathrm{div}\,\vec{u}_h + c(x)p_h).$$

As in the previous estimation, it is clear that q_K is an element of $L^2(\Omega)$. Noting by $V=(0,q_K)$ then

$$\begin{aligned} \mathcal{E}(V) &= \int_K (-g-\mathrm{div}\,\vec{u}_h+c(x)p_h)^2\varphi_K\,dx \\ &= \|(-g-\mathrm{div}\,\vec{u}_h+c(x)p_h)\varphi_K^{\frac{1}{2}}\|_{L^2(K)}^2 \\ &\geq C_1^{II}\|-g-\mathrm{div}\,\vec{u}_h+c(x)p_h\|_{L^2(K)}^2, \end{aligned}$$

therefore,

$$\begin{aligned} (\mathrm{II})^2 &\leq \mathcal{E}(V) \\ &\leq C_2^{II}\|U-U_h\|_{Z(K)}\|V\|_{Z(K)} \\ &\leq C_2^{II}(\|\vec{u}-\vec{u}_h\|_{H(\mathrm{div}\,,K)}+\|p-p_h\|_{L^2(K)}) \\ &\quad \|(-g-\mathrm{div}\,\vec{u}_h+c(x)p_h)\varphi_K\|_{L^2(K)} \\ &\leq C_3^{II}(\|\vec{u}-\vec{u}_h\|_{H(\mathrm{div}\,,K)}+\|p-p_h\|_{L^2(K)}) \\ &\quad \|-g-\mathrm{div}\,\vec{u}_h+c(x)p_h\|_{L^2(K)}, \end{aligned}$$

thus, II is upper bounded by

$$\mathrm{II} \leq C_3^{II}(\|\vec{u}-\vec{u}_h\|_{H(\mathrm{div}\,,K)}+\|p-p_h\|_{L^2(K)}).$$

Remark 4.3 *To stablish similar the majorations of I and II, we can also work with polynomial interpolations f_h, g_h, c_h, a_h and b_h of f, g, c, a and b.*

Majoration of III: Let F be an internal edge, therefore, there exists two triangles K_1^F and K_2^F so that $F = K_1^F \cap K_2^F$. Let us define $\omega_F = K_1^F \cup K_2^F$ (see fig. [2]). Observing that $[p_h]|_F$ is constant, then a suitable function P_F is constructed by:

$$P_F([p_h])(x) = \begin{cases} \vec{v}_1^F(x) & \text{if } x \in K_1^F \\ \vec{v}_2^F(x) & \text{otherwise} \end{cases} \tag{30}$$

where $\vec{v}_1^F$ (respectively $\vec{v}_2^F$) is the unique polynomial defined over K_1^F (respectively K_2^F) in RT_0 so that each degree of freedom is 0 except the one in F that it is imposed to be $[p_h]$. It is clear from the definition of $P_F([p_h])$ that it belongs to $H(\mathrm{div}\,,\omega_K)$. Similar constructions can be considered if $[p_h]$ is

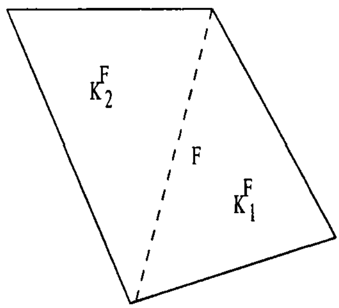

Figure 2. *Definition of* $\omega_F = K_1^F \cup K_2^F$

polynomial over F using the appropriated generalized Raviart-Thomas F.E. It is not very difficult to prove that P_F is linear and verifies

$$||P_F([p_h])||_{H(\text{div},\omega_F)} \leq Ch_F^{\frac{1}{2}}||[p_h]||_{L^2(F)},$$

Let us consider the test function

$$V = (P_F([p_h], 0),$$

then

$$||[p_h]||^2_{L^2(F)} \leq \left| \begin{array}{ll} \mathcal{E}(V)- & \sum_{K \subset K_1^F \cup K_2^F} \int_K (\vec{f} - a(x)\vec{u}_h \\ & +\nabla p_h + \vec{b}(x)p_h)P_F([p_h])\, dx \end{array} \right|,$$

thus

$$\begin{array}{rcl} ||[p_h]||^2_{L^2(F)} & \leq & ||A||||U - U_h||_{Z(\omega_F)}||P_F([p_h])||_{Z(\omega_F)} \\ & + & ||\vec{f} - a(x)\vec{u}_h + \nabla p_h + \vec{b}(x)p_h||_{L^2(\omega_F)}||P_F([p_h])||_{L^2(\omega_F)}, \end{array}$$

using now the majoration of P_F we obtain

$$h_F^{-\frac{1}{2}}||[p_h]||_{L^2(F)} \leq C_h^{III}||U - U_h||_{Z(\omega_F)}.$$

Majoration of IV. Finally, let F be a boundary edge satisfying $F \in \partial\Omega_D$ and let K_1^F be the triangle containing F. For the sake of simplicity, let us suppose g_1 constant over F. In this case the function P_F is constructed:

$$P_F(g_1 - p_h)(x) = \vec{v}_1^F(x) \tag{31}$$

where $\vec{v}_1^F$ is the unique polynomial defined over K_1^F in RT_0 so that each degree of freedom are 0 except the one in F that it is imposed to be $g_1 - p_h$. As in previous case, P_F is linear and verifies

$$||P_F(g_1 - p_h)||_{H(\text{div},K_1^F)} \leq Ch_F^{\frac{1}{2}}||g_1 - p_h||_{L^2(F)},$$

Let us consider the test function

$$V = (P_F(g_1 - p_h), 0),$$

then

$$||g_1 - p_h||^2_{L^2(F)} \leq \left| \begin{array}{c} \mathcal{E}(V) - \displaystyle\int_{K_1^F} (\vec{f} - a(x)\vec{u}_h + \nabla p_h + \vec{b}(x)p_h) \\ P_F(g_1 - p_h)\, dx \end{array} \right|,$$

thus

$$\begin{array}{rcl} ||g_1 - p_h||^2_{L^2(F)} & \leq & ||A||\,||U - U_h||_{Z(K_1^F)}||P_F(g_1 - p_h)||_{Z(K_1^F)} \\ & + & ||\vec{f} - a(x)\vec{u}_h + \nabla p_h + \vec{b}(x)p_h||_{L^2(K_1^F)} \\ & & ||P_F(g_1 - p_h)||_{L^2(k_1^F)}, \end{array}$$

using the majoration of P_F we obtain

$$h_F^{-\frac{1}{2}}||g_1 - p_h||_{L^2(F)} \leq C_h^{IV}||U - U_h||_{Z(K_1^F)}.$$

In the general case, where g_1 is not constant over F, then a suitable polynomial approximation g_{1_s} is considered. In that case the following estimation is obtained:

$$h_F^{-\frac{1}{2}}||g_1 - p_h||_{L^2(F)} \leq C_h^{IV}(||U - U_h||_{Z(K_1^F)} + h^{-\frac{1}{2}}||g_1 - g_{1s}||_{L^2(F)}).$$

Finally, if the estimator given by the equation [24] is considered, then the following proposition can be derived:

Proposition 4.4 *With the definition [24] the following estimation is obtained*

$$\begin{array}{rll} \eta_R(K) & \leq C & (||\vec{u} - \vec{u}_h||_{H(div,\omega_K)} + h_K^{-1}||p - p_h||_{L^2(\omega_K)}) \\ + & & ||\vec{f} - \vec{f}_{mh}||_{L^2(\omega_K)} + ||g - g_{mh}||_{L^2(\omega_K)} + h_K^{-\frac{1}{2}}||g_1 - i_h(g_1)||_{L^2(\partial K \cap \partial\Omega_D)} \end{array} \quad (32)$$

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]).*

5 Conclusion

The paper has outlined an 'a posteriori' local error estimator based on the residual of the linearized transport equation for electrons. Two theoretical results gives an idea about the efficacity of the error estimator. Future works will consider the construction of an anisotropic estimator based on local corrections of numerical solution as well as numerical experiences comparing the isotropic and anisotropic estimators.

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References

[1] A. EL BOUKILI, *Analyse mathématique et simulation numérique bidimensionnelle des dispositifs semiconducteurs à hétérojonctions par l'approche éléments finis mixtes.* Thèse de Doctorat de l'Université Paris VI, (1995).

[2] C. BERNARDI, B. MÉTIVET AND R. VERFÜRTH, *'Analyse numérique d'indicateurs d'erreur'.* *Publications du Laboratoire d'Analyse Numerique U.P.M.C (Paris VI)*, (1993).

[3] A. EL BOUKILI, *'Analyse mathématique d'un problème non linéaire et non standard issu des équations de semiconducteurs à hétérojonctions en statistique de Fermi-Dirac'. To appear as Report INRIA*, (1995).

[4] C. BREZZI, M. FORTIN, *Mixed and Hybrid Finite Element Methods.* Springer-Verlag, Berlin, Heidelberg, 1991.

[5] F. HECHT, A. MARROCCO, *Mixed finite element simulation of heterojunction structures including a boundary layer model for the quasi-fermi levels.* Presented in NASECODE X, Dublin, 1994.

[6] J. POUSIN, J. RAPPAZ, *'Consistency, stability a priori and a posteriori erros for Petrov-Galerkin methods applied to nonlinear problems'. Publications of École Polytechnique Fédérale de Lausanne*, (1992).

[7] R. VERFÜRTH, *'A Posteriori Error Estimation and Adaptive Mesh-Refinement Techniques', J. Comput. Appl. Math.*, (1993).

[8] R. VERFÜRTH, *'A posteriori error estimators and adaptive mesh-refinement techniques for the Navier-Stokes equations'. Incompressible Computational Fluid Dynamics, Trends and Advances.* M.D. Gunzburger and R.A. Nicolaides eds., Cambridge University Press, pp. 447-477, (1993).

[9] R. VERFÜRTH, *'A review of a posteriori error estimation and adaptive mesh-refinement techniques'. (internal publication) Institut für Angewandte Mathematik.* Unversität Zürich, (1993).

[10] R. VERFÜRTH, *'A Posteriori Error estimates for non-linear problems. Finite element discretizations of elliptic equations', To appear in Math. Comput.*, (1994).

[11] I. Babuska, J. Osborn, and J. Pitkäranta, *Analysis of mixed methods using mesh dependent norms.* Math. Comput. 35, pp. 1039-1062, 1980.

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