Adaptive Techniques for Semiconductor Equations with a Raviart-Thomas Element

A. El Boukili[*] A. Madrane[†] R. Vaillancourt[‡]

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[*]SILVACO International, 4701 Patrick Henry Drive, Bldg. 2, Santa Clara, CA 95054, U.S.A.

[†]German Aerospace Center,DLR Inst. of Design Aerodynamics, Lilienthalplatz 7, 38108 Braunschweig, Germany, Aziz.Madrane@dlr.de

[‡]University of Ottawa, Department of Mathematics and Statistics, Ottawa, On, Canada K1N 6N5, remi@uottawa.ca

Abstract

Efficient and reliable *a posteriori* local error indicators are considered for a Raviart-Thomas element in the solution of convection-dominated semiconductor transport equations. Numerical results for a realistic semiconductor device show that an unstructured mesh adaptation based on these estimators leads to an efficient and robust algorithm.

Keywords: Mesh optimization; Raviart-Thomas element; Semiconductor equations.

Résumé

Dans le cadre de la méthode des éléments finis mixtes de Raviart–Thomas, on présente une analyse mathématique des indicateurs d'erreur pour l'équation de transport des particules chargées pour les semiconducteurs à hétérojonction. Les résultats numériques montrent que le maillage adaptatif non structuré basé sur ces estimateurs assure l'efficacité et la robustesse de l'algorithme.

1 Introduction

Numerical modeling of microelectronic devices is an integrated part of Computer Aided Design of integrated microsystems. This paper emphasizes the development of an advanced automatic mesh adaptation technique to optimize the cost-effective design of electronic devices. The linearized convection-dominated transport equations are considered for electron and hole flow coupled with Poisson's equation, where current densities and quasi-Fermi levels are taken as variables. An efficient and reliable a posteriori error estimator is presented for the adaptive mesh generation in the Raviart–Thomas finite element approach. To the authors' knowledge, local refinement of the mesh in Raviart–Thomas discretization with the indicated variables has not been used for the drift-diffusion equations. Verfürth [5], [6], and Hoppe and colleagues [2], [3] have used similar methods for a standard diffusion equation as Poisson's equation. The lower and upper bounds reported here for the estimator are obtained in El Boukili et al. [4]. Numerical results are presented for a realistic Heterojunction Bipolar Transistor (HBT).

2 Mixed formulation

The linear advection-dominated transport equation for electron flow in semiconductor devices in mixed form is

$$\begin{array}{rcll} a(x)\vec{u} - \nabla p - \vec{b}(x)p &=& \vec{f}(x) & \text{in } \Omega, \\ -\operatorname{div}\vec{u} + c(x)p &=& g(x) & \text{in } \Omega, \\ p &=& g_1 & \text{on } \partial\Omega_D, \\ \vec{u}\cdot\vec{n} &=& 0 & \text{on } \partial\Omega_N, \end{array} \tag{1}$$

where Ω stands for a bounded polygonal domain in $\mathbb{R}^2$ with Dirichlet and Neumann boundary conditions on $\partial\Omega_D$ and $\partial\Omega_N$, respectively.

Problem (1) will be solved by a mixed variational method in the spaces $H(\operatorname{div},\Omega)$ and $L^2(\Omega)$. In El Boukili [1], sufficient regularity conditions on the functions a, $\vec{b}$, c, $\vec{f}$, g and g_1, and the domain Ω are detailed for the problem to be well defined.

This variational formulation leads to the following nonstandard saddle point problem: Find $(\vec{u},p) \in X_0 \times Y$ such that

$$\begin{array}{rcl} a(\vec{u},p) + b_1(\vec{v},p) - b_2(\vec{v},p) &=& (\vec{f},\vec{v}) + \langle \vec{v}\cdot\vec{n}, g_1\rangle \qquad \forall \vec{v} \in X_0, \\ b_1(\vec{u},q) - c(p,q) &=& -(g,q) \qquad \forall q \in Y, \end{array} \tag{2}$$

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

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

In this analysis, $< \cdot,\cdot >$ and $(\cdot,\cdot)$ represent the $L^2(\Omega)$ duality and inner products, respectively. We let $Z = X \times Y$, $Z_0 = X_0 \times Y$, $U = (\vec{u},p)$, and $V = (\vec{v},q)$. We define $\mathcal{A}$ as

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

by adding the two equations of problem (2). The same process is applied to define the continuous linear form

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

It is shown in El Boukili [1] that the mixed variational problem (2) is equivalent to the following well-posed problem: Find $U \in Z_0$ such that

$$\mathcal{A}(U,V) = \langle \mathcal{F}, V\rangle \qquad \forall V \in Z_0. \tag{3}$$

3 Mixed discretization

For the Raviart–Thomas element, as in El Boukili [1], let $\mathcal{T}_h$ be a regular triangulation of Ω and consider the expression

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

Then, the approximation spaces are given by

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

The following spaces take care of the boundary conditions:

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

The discretization of problem (2) is given by

$$\text{Find } U_h = (\vec{u}_h, p_h) \in Z_{0h} \text{ such that } \mathcal{A}(U_h, V_h) = \langle \mathcal{F}, V_h\rangle_{Z',Z} \quad \forall V_h \in Z_{0h}. \tag{4}$$

Theorem 1 (El Boukili [1]) *The discrete problem (4) has a unique solution $(\vec{u}_h, p_h)$ verifying the following a priori error estimates:*

$$\begin{array}{ll} (i) & \|p - p_h\|_{L^2(\Omega)} \le Ch\|p\|_{H^2(\Omega)}, \\ (ii) & \|\vec{u} - \vec{u}_h\|_{L^2(\Omega)} \le Ch\|p\|_{H^2(\Omega)}, \\ (iii) & \|div(\vec{u} - \vec{u}_h)\|_{L^2(\Omega)} \le Ch^s\|p\|_{H^{s+2}(\Omega)}, \qquad 0 \le s \le 1. \end{array}$$

A posteriori error estimates for the Raviart–Thomas element involves additional difficulties which cannot be resolved by direct application of well established methods for other mixed methods as done by Verfürth [5], [6] for the Navier–Stokes equations. 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 $H(\mathrm{div}, \Omega)$-functions are contained only in $H^{-1/2}(\partial\Omega)$. On the one hand, the $H(\mathrm{div}, \Omega)$-norm is an anisotropic norm, and, as in El Boukili et al. [4],there is no interpolation operator for $H(\mathrm{div}, \Omega)$-functions as the Clément oparator for $H^1(\Omega)$-functions.

To overcome these difficulties one has to argue on the discrete level where traces are meaningful in an $L^2(\Omega)$ sense. To this end, we shall use the solvability and stability of the discrete problem and the following saturation assumption.

Saturation Assumption. There exists a number $\gamma < 1$ such that

$$\|\vec{u} - \vec{u}_{h/2}\|_{X_h} + \|p - p_{h/2}\|_{Y_h} \le \gamma[\|\vec{u} - \vec{u}_h\|_{X_h} + \|p - p_h\|_{Y_h}]. \tag{5}$$

Let $S(K) = \{F_1, F_2, F_3\}$ denote the set of internal edges of K, and set

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

where $[p_h]$ denotes the jump of p_h across the edge F.

The a priori error estimates given in Theorem 1, in general, implies that refining the grid and reducing h improve the global error of the finite element solutions. Therefore, we assume that we can exclude the exceptional cases where the improvement is very small.

The saturation assumption leads to the following reliability and efficiency results.

Theorem 2 (El Boukili et al. [4])

$$\|\vec{u}_{h/2} - \vec{u}_h\|_X + \|p_{h/2} - p_h\|_Y \leq C\left[\sum_{K\in\mathcal{T}_h} \eta(K)^2\right]^{1/2}, \tag{6}$$

$$\|\vec{u} - \vec{u}_h\|_X + \|p - p_h\|_Y \leq \frac{C}{1-\gamma}\left[\sum_{K\in\mathcal{T}_h} \eta(K)^2\right]^{1/2}, \tag{7}$$

Theorem 3 (El Boukili et al. [4]) *By definition (6), there is a constant C depending only on the minimal angle in the triangulation such that*

$$\eta(K) \leq C\Big[\|\vec{u} - \vec{u}_h\|_{H(div,\omega_K)} + (1 + h_F^{-1})\|p - p_h\|_{L^2(\omega_K)}\Big], \tag{8}$$

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

4 Numerical results for a HBT

We present the performance of the mesh adaptation technique using an isotropic metric based on the a posteriori error estimator (6). We consider the drift-diffusion model for an industrial heterojunction bipolar transistor described in El Boukili [1].

Figure 1 shows the initial coarse triangulation at step 1 and the optimal mesh at step 8. A significant adaptive refinement is observed in the neighborhood of the heterojunction interfaces due to the large variation in electron densities and in the neighborhood of the Ohmic contacts due to the boundary layers.

Figure 2 shows the total current lines and the current lines for electrons and holes, when the transistor effect is significant (the applied voltage is -1.4 volts at emitter (E) and 0 volts at base (B) and collector (C)).

Figure 3 shows the number of nodes of the successive meshes as the coupled Solver/Adaptation cycle proceeds. Spurious oscillations in the graph are due to a few ill-adapted initial meshings. Initially, we notice a mesh over-refinement, but, as the solution improves, the mesher gradually reduces the number of nodes and reaches an optimal mesh and accuracy in the solutions, thus implying convergence of the mesh adaptive process.

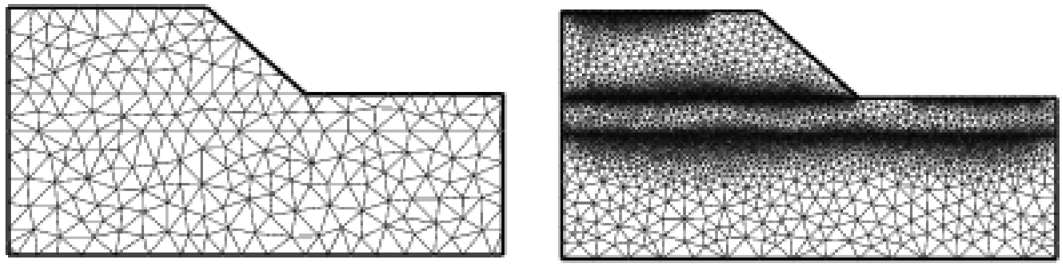

Figure 1: Initial mesh: 397 vertices, and final mesh : 6750 vertices.

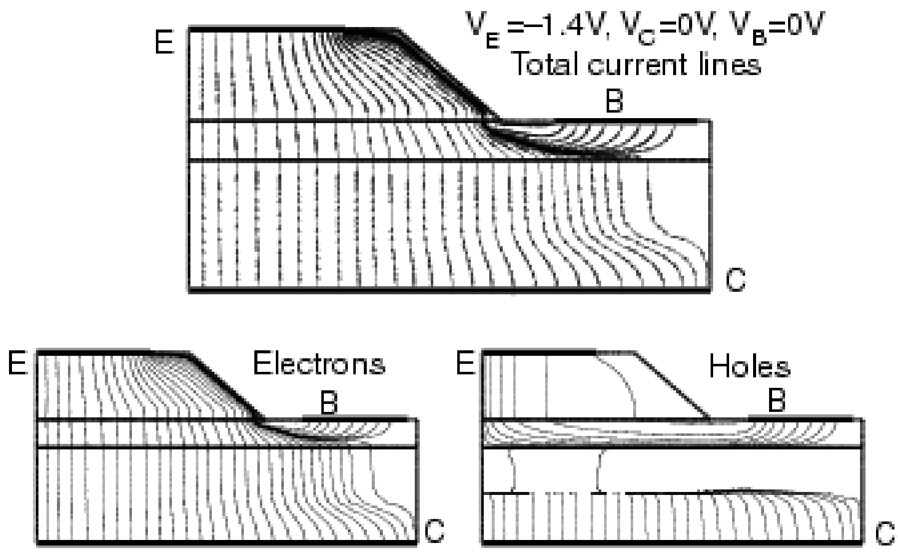

Figure 2: Current lines in HBT, when transistor effect is significant.

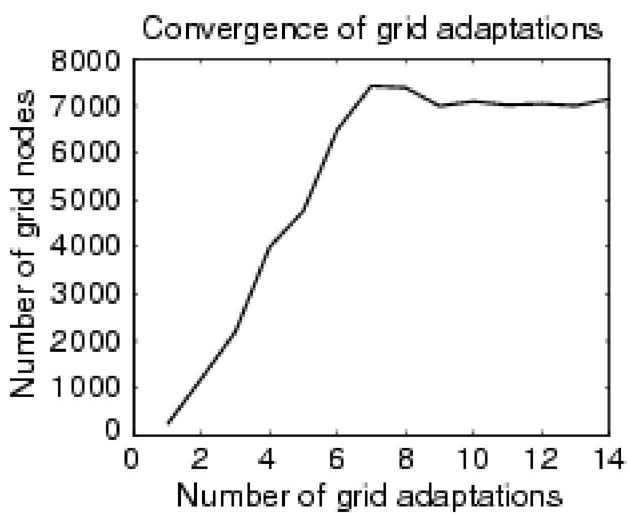

Figure 3: Number of nodes versus number of adaptation cycles for HBT device.

5 Conclusion

This paper has outlined an a posteriori local error estimator based on the residual of the linearized transport equation for electrons in semiconductor devices. Two theoretical results prove the reliability and the effeciency of the error estimator. Numerical results show the robustness and the efficiency of the mesh adaptive process.

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