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ON SOME RECENT RESULTS ON THE NUMERICAL PROBLEMS IN SEMICONDUCTOR DEVICE SIMULATION

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1. Introduction

We shall deal in this paper with the so-called drift-diffusion model for semiconductor device simulation:

$$\frac{\partial p}{\partial t} + div\underline{J} = -R \tag{1.1}$$

$$\underline{J} = -\mu(\underline{\nabla} p + p\underline{\nabla}\psi) . \tag{1.2}$$

Here, p denotes the position density of the positively charged holes, $\underline{J}$ the hole current density, and ψ the electrostatic potential. $\underline{E} = -\underline{\nabla}\psi$ is the electric field, and the source term R is the recombination-generation rate of charged carrier pairs. The coefficient $\mu >$ 0 stands for the hole mobility. Equations (1.1)-(1.2) are usually coupled with another pair of equations (very similar to (1.1)-(1.2)) describing the motion of negatively charged electrons n, plus a Poisson equation for the electrical potential ψ. Basic references on the various physical and mathematical aspects of the whole system of equations as well as on other ways of discretizing it are listed at the end of the paper. Here, we recall a mixed finite element method for the discretization of (1.1)-(1.2) recently introduced in [4],[5],[8]. Using asymptotic analysis techniques, we compare the qualitative behaviour of the mixed method with other methods (classical conforming Galerkin method and harmonic average methods). This asymptotic analysis provides some indication of the advantages of the mixed method.

2. Mixed approximation of the continuity equation

We shall describe in this section a mixed approximation to the continuity equation (1.1), (1.2). For simplicity, we shall consider the stationary two-dimensional case and a constant mobility coefficient $\mu \equiv 1$. In the solution of the coupled system of three equations (for ψ, n, and p), a linearization method of Gummel type (approximate Newton decoupling method, [10], [17]) is often used. Then, at each iteration, one has to solve a problem of the type

$$\left\{\begin{array}{l} \textit{Find } p \in H^1(\Omega) \textit{ such that} \\ -div(\underline{\nabla} p + p\underline{\nabla}\psi) \;+\; cp \;=\; f \quad \textit{in } \Omega \subset \mathbf{R}^2 \\ \qquad\qquad\qquad\qquad p \;=\; g \quad \textit{on } \Gamma_0 \subset \partial\Omega \\ \qquad\qquad\qquad\qquad \dfrac{\partial p}{\partial n} \;=\; 0 \quad \textit{on } \Gamma_1 = \partial\Omega \backslash \Gamma_0 \;, \end{array}\right. \tag{2.1}$$

where ψ is assumed to be known and piecewise linear (coming from a discretization of the Poisson equation). In the equation (2.1) f is a function independent of p, and c a non negative function independent of p, which can be assumed piecewise constant. To simplify the exposition, we shall assume here $c = 0$. We recall that, since $|\underline{\nabla}\psi|$ is quite large in some parts of the domain, equation (2.1) is an advection dominated equation, for which classical discretization methods may fail. Using the classical change of variable from the charge density p to the Slotboom variable ρ

$$p \;=\; \rho e^{-\psi} \;, \tag{2.2}$$

equation (2.1) can be written in the symmetric form

$$\left\{\begin{array}{l} \textit{Find } \rho \in H^1(\Omega) \textit{ such that} \\ \qquad -div(e^{-\psi}\underline{\nabla}\rho) \;=\; f \qquad \textit{in } \Omega \\ \qquad\qquad \rho \;=\; \chi := e^{\psi} g \quad \textit{on } \Gamma_0 \\ \qquad\qquad \dfrac{\partial \rho}{\partial n} \;=\; 0 \qquad \textit{on } \Gamma_1 \end{array}\right. \tag{2.3}$$

and the hole current density is now given by

$$\underline{J} \;=\; -e^{-\psi}\underline{\nabla}\rho \;. \tag{2.4}$$

Note that in (2.3) homogeneous Neumann conditions come from the usually made assumption that $-\underline{E}\cdot\underline{n} \equiv \frac{\partial\psi}{\partial n}$ vanishes on Γ_1. The idea is to discretize equation (2.3) with mixed finite element methods, go back to the original variable p by using a discrete version of the transformation (2.2), and then solve for p. For the case $c = 0$, a mixed scheme (based on the lowest order Raviart-Thomas element [16]) has been introduced and extensively discussed in [4] for the case $f = 0$, and in [5] for $f \neq 0$. The scheme provides an approximate current with continuous normal component at the interelement boundaries. Moreover, the matrix associated with the scheme can be proved to be an M-matrix, if a weakly acute triangulation is used (every angle of every triangle is $\leq \pi/2$). This property guarantees a discrete maximum principle and, in particular, a non-negative solution if the boundary data are non-negative. Moreover, when going back to the variable p, this structure property of the matrix is retained.

Let us recall the mixed scheme. For that, let $\{T_h\}$ be a regular decomposition of Ω into triangles T ([6]) (Ω is assumed to be a polygonal domain). According to [16], we define, for all $T \in T_h$, the following set of polynomial vectors

$$RT(T) = \{\underline{\tau} = (\tau_1, \tau_2),\ \tau_1 = \alpha + \beta x,\ \tau_2 = \gamma + \beta y,\ \alpha, \beta, \gamma \in \mathbf{R}\} . \tag{2.5}$$

Then, we construct our finite element spaces as follows

$$\widetilde{V}_h = \{\underline{\tau} \in [L^2(\Omega)]^2 :\ div\underline{\tau} \in L^2(\Omega),\ \underline{\tau} \cdot \underline{n} = 0\ on\ \Gamma_1,\ \underline{\tau}_{|T} \in RT(T),\ \forall T \in T_h\} \tag{2.6}$$

$$W_h = \{\phi \in L^2(\Omega) : \phi_{|T} \in P_0(T)\ \forall T \in T_h\}. \tag{2.7}$$

As usual, $P_0(T)$ denotes the space of constants on T. The mixed discretization of (2.3) is then the following

$$\begin{cases} \textit{Find } \widetilde{\underline{J}}_h \in \widetilde{V}_h\ ,\ \widetilde{\rho}_h \in W_h \textit{ such that :} \\ \displaystyle\int_\Omega e^{\overline{\psi}} \widetilde{\underline{J}}_h \cdot \underline{\tau} dxdy - \int_\Omega div\ \underline{\tau}\ \widetilde{\rho}_h\ dxdy = 0 \quad \underline{\tau} \in \widetilde{V}_h, \\ \displaystyle\int_\Omega div\ \widetilde{\underline{J}}_h\ \phi\ dxdy = \int_\Omega f\phi dxdy \qquad\qquad \phi \in W_h. \end{cases} \tag{2.8}$$

In the first equation of (2.8) $\overline{\psi}$ denotes the piecewise constant function defined in each triangle T by

$$e^{\overline{\psi}}{}_{|T} = (\int_T e^{\psi} dxdy)/|T| . \tag{2.9}$$

It is clear that $\widetilde{\rho}_h$ will be an approximation of the solution ρ of (2.3), and $\widetilde{\underline{J}}_h$ will be an approximation of the current $\underline{J}$. In particular, the first equation of (2.8) is a discretized version of (2.4), and the second equation of (2.8) is a discretized version of $div\underline{J} = f$. Uniqueness results for (2.8) follow from the general theory of [3].

We remark that the condition $div\underline{\tau} \in L^2(\Omega)$ in the definition (2.6) implies that *every* $\underline{\tau} \in \widetilde{V}_h$ *has a continuous normal component* when going from one element to another. This means, in particular, that the current is preserved.

The algebraic treatment of system (2.8) needs some care. Actually, the matrix associated with (2.8) has the form

$$\begin{pmatrix} \widetilde{A} & -\widetilde{B} \\ -\widetilde{B}^* & 0 \end{pmatrix} \tag{2.10}$$

and is not positive-definite (H^* denotes the transpose of the matrix H). A way to avoid this inconvenience is to relax the continuity requirement in the space definition (2.6) and to enforce it back by using interelement Lagrange multipliers. (See [7] where this idea was first introduced). The procedure is the following. First we set

$$V_h = \{\underline{\tau} \in [L^2(\Omega)]^2 : \underline{\tau}_{|T} \in RT(T)\ \forall T \in T_h\}. \tag{2.11}$$

Then, denoting by E_h the set of edges e of T_h, we define, for any function $\xi \in L^2(\Gamma_0)$

$$\Lambda_{h,\xi} = \{\mu \in L^2(E_h) : \mu_{|e} \in P_0(e)\ \forall e \in E_h\ ;\ \int_e (\mu - \xi) ds = 0\ \forall e \subset \Gamma_0\}\ , \tag{2.12}$$

where $P_0(e)$ denotes the space of constants on e. The mixed-equilibrium discretization of (2.3) is then

$$\begin{cases} \textit{Find } \underline{J}_h \in V_h\ ,\ \rho_h \in W_h\ ,\ \lambda_h \in \Lambda_{h,\chi} \textit{ such that :} \\ \int_\Omega e^{\overline{\psi}} \underline{J}_h \cdot \underline{\tau} dxdy - \sum_T \int_T div\ \underline{\tau}\ \rho_h dxdy + \sum_T \int_{\partial T} \lambda_h \underline{\tau} \cdot \underline{n}\ ds = 0 \quad \underline{\tau} \in V_h, \\ \sum_T \int_T div\ \underline{J}_h\ \phi dxdy = \int_\Omega f \phi dxdy \qquad \phi \in W_h, \\ \sum_T \int_{\partial T} \mu \underline{J}_h \cdot \underline{n}\ ds = 0 \qquad \mu \in \Lambda_{h,0}. \end{cases} \tag{2.13}$$

It is easy to see that problem (2.13) has a unique solution and that

$$\underline{J}_h \equiv \widetilde{\underline{J}}_h\ ,\ \rho_h \equiv \widetilde{\rho}_h\ . \tag{2.14}$$

Moreover, λ_h is a good approximation of ρ at the interelements. (See [1] for detailed proofs). The linear system associated with (2.13) can be written in matrix form as

$$\begin{pmatrix} A & -B & C \\ -B^* & 0 & 0 \\ C^* & 0 & 0 \end{pmatrix} \begin{pmatrix} \underline{J}_h \\ \rho_h \\ \lambda_h \end{pmatrix} = \begin{pmatrix} 0 \\ -F \\ 0 \end{pmatrix}\ . \tag{2.15}$$

In (2.15) the notation $\underline{J}_h, \rho_h, \lambda_h$ is used also for the vectors of the nodal values of the corresponding functions. The matrix in (2.15) is not positive definite. However, A is block- diagonal (each block being a 3x3 matrix corresponding to a single element T) and can be easily inverted at the element level. Hence, the variable $\underline{J}_h$ can be eliminated by static condensation, leading to the new system

$$\begin{pmatrix} B^*A^{-1}B & -B^*A^{-1}C \\ -C^*A^{-1}B & C^*A^{-1}C \end{pmatrix} \begin{pmatrix} \rho_h \\ \lambda_h \end{pmatrix} = \begin{pmatrix} F \\ 0 \end{pmatrix}\ . \tag{2.16}$$

The matrix in (2.16) is symmetric and positive definite. Moreover, $B^*A^{-1}B$ is a diagonal matrix, so that the variable ρ_h can also be eliminated by static condensation. This leads to a final system, acting on the unknown λ_h only, of the form

$$M\ \lambda_h = G\ , \tag{2.17}$$

where M and G are given by:

$$M = C^*A^{-1}C - C^*A^{-1}B(B^*A^{-1}B)^{-1}B^*A^{-1}C\ , \tag{2.18}$$

$$G = C^*A^{-1}B(B^*A^{-1}B)^{-1}F\ , \tag{2.19}$$

and M is symmetric and positive definite. In order to go back to the original unknown p we recall that λ_h is an approximation of ρ and we can use a discrete version of the inverse transform of (2.2):

$$\lambda_h = (e^{\psi})^I p_h. \tag{2.20}$$

In (2.20) $(e^{\psi})^I$ is given edge by edge by the meanvalue of e^{ψ}:

$$e^{\psi^I}{}_{|e} = (\int_e e^{\psi} ds)/|e| . \tag{2.21}$$

The transformation (2.20) amounts to multiplying the matrix M columnwise by the value of $(e^{\psi})^I$ on the corresponding edge. The final system in the unknown p_h will be of the type

$$\widetilde{M} p_h = G . \tag{2.22}$$

The matrix $\widetilde{M}$ is not symmetric anymore, but it is an M-matrix if the matrix (2.18) is an M-matrix, which holds true if the triangulation is of weakly acute type.

Remark We are considering here, for the sake of simplicity, the case $c = 0$ only (for (2.1)). The general case $c(x) \geq 0$ can also be treated along the same lines. However, it can be seen that the choice (2.5)-(2.7), (2.11), (2.12) produces, as a final matrix M, a matrix that is not monotone. A cure for that has been proposed in [8], [9] with the use of more sophisticated choices of local polinomial vectors instead of (2.5).

3. Asymptotic behaviour of the numerical scheme

We already pointed out in the previous sections that the electric field $\underline{E}$ $(= -\underline{\nabla}\psi)$ can be, in most applications, very large in some parts of the domain Ω. The aim of this section is to perform a (rough) analysis of the mixed exponential fitting scheme (and of some other possible schemes for (2.3)) when the electric field becomes larger and larger. This will show why the choice of a mixed method for discretizing (2.3) seems to be preferable, apart from the obvious reason that it is strongly current-preserving.

In order to perform our asymptotic analysis we shall make the simplifying assumption that we are dealing with a given potential ψ, piecewise linear, of "moderate size", and that our equation is

$$-div(\underline{\nabla} p + p\underline{\nabla}(\frac{\psi}{\lambda})) = f, \tag{3.1}$$

where λ is a real valued parameter. We are obviously interested in the behaviour of numerical schemes for (3.1) when λ becomes smaller and smaller. The symmetric form of (3.1) reads then

$$-div(e^{-(\psi/\lambda)}\underline{\nabla}\rho) = f, \tag{3.2}$$

where the change of variable is now

$$p = \rho e^{-(\psi/\lambda)} . \tag{3.3}$$

We shall analyze the asymptotic **behaviour** (as $\lambda \to 0$) of three different schemes, all based on the idea of discretizing (3.2) first, and then use (3.3) to obtain a numerical scheme in the unknown p (and hence a scheme for (3.1)). In particular, we will consider the following discretization methods for (3.2): *a)* classical conforming piecewise linear methods, *b)* conforming piecewise linear mothods with harmonic average (as pointed out in [4], [5] they can be regarded as a discretization of (3.2) by means of hybrid methods), and *c)* mixed methods as described in the previous section.

We recall that, calling Z_h the space of continuous piecewise linear functions on Ω and setting, for all function $\xi \in C^0(\overline{\Gamma}_D)$

$$Z_{h,\xi} = \{v \in Z_h,\ v = \xi \text{ at nodes } \in \overline{\Gamma}_D\}\ , \tag{3.4}$$

the methods *a)* and *b)* can be written in the following way.

Classical method

$$\begin{cases} (i) & \rho_h \in Z_{h,\chi}\ , \\ (ii) & \displaystyle\int_\Omega e^{-(\psi/\lambda)} \underline{\nabla}\rho_h \cdot \underline{\nabla} v dxdy = \int_\Omega f v dxdy \quad \forall v \in Z_{h,0}\ , \\ (iii) & p_h = e^{-(\psi/\lambda)}\rho_h \quad \text{at the nodes}\ . \end{cases} \tag{3.5}$$

Conforming method with harmonic average

$$\begin{cases} (i) & \rho_h \in Z_{h,\chi}\ , \\ (ii) & \displaystyle\int_\Omega \overline{e^{-(\psi/\lambda)}} \underline{\nabla}\rho_h \cdot \underline{\nabla} v dxdy = \int_\Omega f v dxdy \quad \forall v \in Z_{h,0}\ , \\ (iii) & p_h = e^{-(\psi/\lambda)}\rho_h \quad \text{at the nodes}\ , \\ (iv) & \displaystyle\overline{e^{-(\psi/\lambda)}}_{|T} = \frac{|T|}{\left(\int_T e^{\psi/\lambda} dxdy\right)} \ \forall T \in T_h \quad (\text{harmonic average}). \end{cases} \tag{3.6}$$

In order to analyze the behaviour of the schemes (3.5), (3.6) and of the mixed scheme of Section 2, we shall need the following asymptotic formulae, valid as $\lambda \to 0$ for a function ϕ linear on a triangle T:

$$\int_T e^{\phi/\lambda} dxdy \simeq \lambda^2 |T| e^{\phi^T_{max}/\lambda}, \tag{3.7}$$

$$\int_e e^{\phi/\lambda} ds \simeq \lambda |e| e^{\phi^e_{max}/\lambda}, \tag{3.8}$$

In (3.7), (3.8) T is a triangle, e is an edge of T, and ϕ^T_{max}, ϕ^e_{max} represent the maximum value of ϕ over $\overline{T}$ and over $\overline{e}$, respectively. Formulae (3.7), (3.8) can be easily checked by direct computation. They hold in the *generic* case where the values ϕ^T_{max} and ϕ^e_{max} are assumed only at one point.

We are now able to analyze the limit behaviour of the various schemes. For this, let us just look at the contributions of a single triangle T to the final matrix. Denoting by $\phi^{(i)}$ $(i = 1, 2, 3)$ the basis functions on T, we have, for the classical method

$$\int_{\mathrm{T}} \mathrm{e}^{-(\psi/\lambda)} \underline{\nabla}\phi^{(i)} \cdot \underline{\nabla}\phi^{(j)} dxdy \simeq \lambda^2 L_{ij}^{\mathrm{T}} \mathrm{e}^{-(\phi_{min}^{\mathrm{T}}/\lambda)}, \tag{3.9}$$

where L_{ij}^{T} are the contributions of the conforming approximation of the Laplace operator, that is

$$L_{ij}^{\mathrm{T}} := \int_{\mathrm{T}} \underline{\nabla}\phi^{(i)} \cdot \underline{\nabla}\phi^{(j)} dxdy, \tag{3.10}$$

and ψ_{min}^{T} is obviously the minimum value of ψ over $\overline{\mathrm{T}}$. Taking into account transformation (3.5,*iii*), the contributions to the final matrix, acting on p_h are given by

$$M_{ij}^{\mathrm{T}} \simeq \lambda^2 L_{ij}^{\mathrm{T}} \mathrm{e}^{(\psi_j - \psi_{min}^{\mathrm{T}})/\lambda}, \tag{3.11}$$

(where ψ_j= value of ψ at the node j). Hence, for the classical method, some coefficients of the matrix blow up exponentially when $\lambda \to 0$.

Let us now consider the case (3.6) where the harmonic average is used. From (3.6,*iv*) and (3.7) we have

$$\int_{\mathrm{T}} \overline{\mathrm{e}^{-(\psi/\lambda)}} \underline{\nabla}\phi^{(i)} \cdot \underline{\nabla}\phi^{(j)} dxdy \simeq \frac{1}{\lambda^2} L_{ij}^{\mathrm{T}} \mathrm{e}^{-(\psi_{max}^{\mathrm{T}})/\lambda}, \tag{3.12}$$

where the coefficients L_{ij}^{T} are defined in (3.10). Then, combining (3.12) and (3.6 ,*iii*), the contributions of the triangle T to the final matrix are

$$M_{ij}^{\mathrm{T}} \simeq \frac{1}{\lambda^2} L_{ij}^{\mathrm{T}} \mathrm{e}^{(\psi_j - \psi_{max}^{\mathrm{T}})/\lambda}. \tag{3.13}$$

We see that, when using the harmonic average, some contributions can become very small, but this can be regarded as a natural upwinding effect which is rather desirable than disturbing. However, it is also clear that the contributions which are not exponentially small have order of magnitude $1/\lambda^2$, while from (3.1) one would expect coefficients of order $1/\lambda$. As discussed in [5] in the framework of hybrid methods, this is clearly not disturbing if $f = 0$, but it can be a source of inconsistency for $f \neq 0$ and λ small, as shown in [5] on simple practical experiments. (We refer to [5] for possible remedies for this method). We point out that this drawback is not present in the mixed formutation (2.13), (2.9), (2.21). Actually, one can easily see that the contributions of a triangle T to the final matrix, acting on p_h, for mixed methods are given by

$$M_{ij}^{\mathrm{T}} = \int_{\mathrm{T}} \overline{\mathrm{e}^{-(\psi/\lambda)}} \underline{\nabla}\chi^{(i)} \cdot \underline{\nabla}\chi^{(j)} dxdy \left(\int_{e_j} \mathrm{e}^{\psi/\lambda} ds\right) |e_j|^{-1}, \tag{3.14}$$

where the harmonic average (3.6,*iv*) is used. In (3.14) e_i $(i = 1, 2, 3)$ are the edges of T, and $\chi^{(i)}$ are the piecewise linear non-conforming basis functions, that is,

$$\chi^{(i)} \in P_1(T) \ ; \ \int_{e_j} \chi^{(i)} ds \ = \ |e_j| \delta_{ij}, \tag{3.15}$$

where δ_{ij} is the Kronecker's symbol. From (3.14), (3.6,*iv*), (3.7), and (3.8) we have then

$$M_{ij}^T \ \simeq \ \frac{1}{\lambda} \widetilde{L}_{ij}^T e^{(\psi_{mes}^{*j} - \psi_{mes}^T)/\lambda}, \tag{3.16}$$

where $\widetilde{L}_{ij}^T$ are the coefficients of the elementary stiffness matrix coming from a piecewise linear non-conforming approximation of the Laplace operator, that is,

$$\widetilde{L}_{ij}^T \ := \ \int_T \underline{\nabla} \chi^{(i)} \cdot \underline{\nabla} \chi^{(j)} dx dy. \tag{3.17}$$

It is now clear what the advantages of mixed methods are: 1) exponential blow-up of the coefficients is avoided, 2) some contributions will go exponentially to zero, corresponding to a natural upwinding effect, 3) the order of magnitude of the non vanishing coefficients is $1/\lambda$, as expected from (3.1).

The above considerations shed, in our opinion, a better light on several common choices for finite element approximations of the continuity equations, motivating the use of *one-dimensional harmonic averages* which are common in semiconductor device applications ([2], [15], [12] etc.). In the context of mixed methods we can use two-dimensional harmonic averages (which is, in a sense, more natural), since we compensate a factor λ from (3.8), due to the different change of variable from ρ_h to p_h (average on an edge instead of point value).

Remark. We discussed so far the generic case where $\psi_{|\overline{T}}$ reaches its maximum at one point only. However, one can easily see that the "automatic adjustment" provided by mixed methods works as well for the non generic case where $\psi_{|\overline{T}}$ reaches its maximum on a whole edge. Finally, for $\psi = constant$ on T, we are just dealing with the Laplace operator, for which usual and harmonic average coincide and both give rise to the standard conforming scheme for Laplace operator. Similarly, the mixed approach above described produces the usual mixed approximation of the Laplace operator.

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