On some numerical problems in semiconductor device simulation

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ABSTRACT - We recall in the introduction the main features of the drift-diffusion model for semiconductor devices, pointing out its physical meaning, its possible derivation, and its limits. Then, in Section 2, we present a mixed finite element method for the discretization of this model. Finally, using asymptotic analysis techniques, we compare the qualitative behaviour of the mixed method with other methods (classical conforming Galerking method and harmonic average methods). This asymptotic analysis provides some indication of the advantages of the mixed method.

1. Introduction

The most commonly used model for charge transport in semiconductors is the so called drift-diffusion model, which - in an appropriate system of units - reads

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

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

Here, p denotes the position density of the positively charged holes, $\underline{J}$ the hole current density, and ψ the electrostatic potential. $\underline{E} = -\underline{\nabla}_x \psi$ 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. The equations (1.1), (1.2) hold for all values of the position variable x in the semiconductor domain $\Omega \subset \mathbf{R}^3$, and for the time $t \geq 0$ (in the sequel we shall skip the subscript x when denoting the gradient and the divergence taken with respect to the position variable).

The drift-diffusion equations are supplemented by mixed Neumann Dirichlet boundary conditions for p on $\partial\Omega$, and by an initial condition at $t = 0$. The Dirichlet segments model contacts, where a voltage is applied to the device, and the Neumann segments represent insulating boundaries or so called artificial boundary segments introduced to separate the device under consideration from neighbouring devices in the chip. For details on the boundary and initial conditions we refer to [9], [10].

The corresponding drift-diffusion model for the position density n of the negatively charged conduction electrons is obtained by making the obvious sign changes in (1.1),(1.2), taking into account the opposite flow direction of the electrons in the electric field $\underline{E}$. The potential ψ is usually modelled self-consistently as Coulomb potential generated by the space charge of the semiconductor, i.e., it is obtained as solution of a Poisson equation whose right-hand side represents the charge density determined by $p,\ n$, and by the density of impurity ions implanted into the semiconductor in order to control its electrical performance (see [16]). Then, after modelling the recombination-generation rate and the carrier mobilities as functions of $n,\ p$, and $\underline{E}$ and after inserting the current relation (1.2) into the continuity equation (1.1), a system of two parabolic equations (for n and p respectively) coupled to the Poisson equation for ψ is obtained. The mathematical analysis and the numerical treatment of this highly non linear pde system is a formidable task and has received a lot of attention in the mathematical, physical, and engineering literature so far (see [9], [10], [16] and the references therein). In this paper we shall focus on a particular issue, namely on the discretization of the steady-state drift-diffusion equation in the two dimensional case, i.e., we shall assume $\frac{\partial p}{\partial t} \equiv 0$, and $\Omega \subset \mathbf{R}^2$. Before going into the details of the numerical analysis (Sections 2 and 3), we now discuss the physical background of the drift-diffusion model.

Obviously, the equation (1.1) is a standard conservation law (continuity equation) for the hole current density, analogous to fluid dynamics. The source term R describes the loss and, respectively, gain of charged particles due to the recombination-generation of electron-hole carrier pairs (see [16] for an account of the most important recombination-generation mechanisms in semiconductor).

The current relation (1.2) also has a simple phenomenological interpretation. Ob-

viously, the term $\underline{J}_{diff} := -\mu\underline{\nabla}p$ represents a diffusion current, and $\underline{J}_{drift} := \mu p\underline{E}$ a drift current caused by the electric field $\underline{E}$. Thus, (1.2) postulates that the total hole current in the semiconductor is the sum of a diffusive current and of an electric field driven convection current. This intriguing but purely phenomenological reasoning however does not explain the equality of the diffusion and convection coefficients. Moreover, a more rigorous derivation which illuminates the limits of validity of the drift-diffusion model is desirable. Both these issues are dealt with in a satisfactory way by taking the semiclassical Boltzmann equation for semiconductors (see [10], [13]) as a basis for deriving (1.1),(1.2). The Boltzmann equation, whose solution is the phase space density of holes, models the convection of the electric field by a hyperbolic differential operator in the phase space and the collisions (scattering events) of particles with each other and with their environment by a non local non linear operator. It turns out that the drift-diffusion model can be derived from the Boltzmann equation by taking the limit of the normed mean free path (i.e., the average length travelled by a particle between two consecutive scattering events divided by the characteristic length of the device) going to zero, when a linearized scattering operator is used (see [10], [14]). The equality of the diffusion and drift coefficients comes out automatically in this approach. Also, information on the validity of (1.1),(1.2) can be deduced from this limiting procedure. First, the considered physical situation must be such that the performed linearization of the scattering kernel is valid, i.e., the particle density must be reasonably small. This requires a non-degenerate semiconductor (the density of the implanted impurity ions is reasonably low, i.e., at most $\simeq 10^{19}$ particles per cubic centimeter in silicon). Also, the semiconductor has to be operated under moderate electric field strengths. Second, the normed mean free path of the device must be small in order for the limiting procedure to make sense. This means that the caracteristic length of the considered device must be large in comparison with the mean free path of the semiconductor. While this condition is usually satisfied for modern silicon technology, it fails for other semiconductors which have a larger mean free path. However, it is certainly also going to be a problem for the next generation of even higher integrated silicon devices (technology with the characteristic device length of less than 0.5 micron).

We remark that a lot of research on other charge transport models for semiconductors is currently going on. Quantum transport models (Wigner equation) are investigated for ultra integrated semiconductor devices, semiclassical Boltzmann-type models for semiconductors other than silicon and, most recently,the so called hydrodynamic semiconductor transport model,which is an extension of the drift-diffusion model not based on the mean free path limit, is under extensive scrutiny (see [10]).

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, [9], [16]) is often used. Then, at each iteration, one has to solve a problem of the type

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

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 refer to [8] for the treatment of the more general case $c \geq 0$. 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

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

equation (2.1) can be written in the symmetric form

$$\begin{cases} \textit{Find } \rho \in H^1(\Omega) \textit{ such that} & \\ \qquad -div(\mathrm{e}^{-\psi}\underline{\nabla}\rho) = f & \textit{in } \Omega \\ \qquad \rho = \chi := \mathrm{e}^{\psi} g & \textit{on } \Gamma_0 \\ \qquad \dfrac{\partial \rho}{\partial n} = 0 & \textit{on } \Gamma_1 \end{cases} \tag{2.3}$$

and the hole current density is now given by

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

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 [15]) 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 [15], we define, for all T$\in T_h$, the following set of polynomial vectors

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

Then, we construct our finite element spaces as follows

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

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

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

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

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

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

It is clear that $\widetilde{\rho}_h$ will be an approximation of the solution ρ of (2.3), and $\underline{\widetilde{J}}_h$ 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

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

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

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

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

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

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

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

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):

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

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

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

The transformation (2.20) amounts to multiplying the matrix M columnwise by the value of $(\mathrm{e}^{\psi})^I$ 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.

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

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

where the change of variable is now

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

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 $\xi \in C^0(\overline{\Gamma}_D)$

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

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

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

Conforming method with harmonic average

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

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:

$$\int_\mathrm{T} \mathrm{e}^{\phi/\lambda} dxdy \simeq \lambda^2 |\mathrm{T}| \mathrm{e}^{\phi^\mathrm{T}_{max}/\lambda}, \tag{3.7}$$

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

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 $\overline{\mathrm{T}}$ 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

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

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 e_i $(i = 1, 2, 3)$ are the edges of T, and $\chi^{(i)}$ are the piecewise linear non-conforming basis functions, that is,

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

In (3.15) δ_{ij} is the Kronecker's symbol, and the harmonic average (3.6,*iv*) is used. From (3.14), (3.6,*iv*), (3.7), and (3.8) we have then

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

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

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

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], [12], [11] 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 $\psi_{|\overline{\mathrm{T}}}$ 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 $\psi_{|\overline{\mathrm{T}}}$ 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.

4. References

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