

TWO-DIMENSIONAL EXPONENTIAL FITTING AND APPLICATIONS TO DRIFT-DIFFUSION MODELS*

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This paper is dedicated to Jim Douglas, Jr., on the occasion of his 60th birthday.

Abstract. A class of methods is introduced that generalizes the so-called exponential fitting method to two-dimensional problems and, more specifically, to equations of the type $\operatorname{div}(\nabla u + u \nabla \psi) = f$, with ψ given and $|\nabla \psi|$ big in a part of the domain. The basic idea is the following: (i) write the equation as $\operatorname{div}(e^{-\psi} \nabla \rho) = f$ through the change of variables $u = \rho e^{-\psi}$; (ii) discretize the symmetric equation by means of a method that uses some kind of harmonic average for the coefficient $e^{-\psi}$ (mixed, hybrid, etc.); (iii) write the discrete scheme in terms of the nodal values of $u = e^{-\psi} \rho$. This produces an M -matrix.

Key words. exponential fitting, upwind, mixed finite element method, semiconductors

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1. Introduction. The aim of this paper is to present some new discretization schemes that generalize to the two-dimensional case the so-called exponential fitting method (Allen and Southwell [1]; see also [20]), better known among electrical engineers as the “Scharfetter–Gummel method” [23], [15]. Our scheme will apply to equations of the type:

$$(1.1) \quad \begin{aligned} &\text{Find } u \in H^1(\Omega) \text{ such that} \\ &\operatorname{div}(\nabla u + u \nabla \psi) = f \quad \text{in } \Omega \subset \mathbb{R}^2, \\ &u = g \quad \text{on } \Gamma_0 \subset \partial\Omega, \\ &\frac{\partial u}{\partial n} + u \frac{\partial \psi}{\partial n} = 0 \quad \text{on } \Gamma_1 = \partial\Omega \setminus \Gamma_0. \end{aligned}$$

In the applications to semiconductor device equations, ψ represents the electric potential after a suitable scaling, and u represents the concentration of positive charges. The function f takes into account the possible “birth” and “death” of positive charges, so that (1.1) is a classical conservation law. Note that, in the actual device simulation problems, the potential ψ is itself an unknown and (1.1) is coupled with (at least) two other equations: one describing the conservation law for negative charges (similar to (1.1)) and another relating the electric potential ψ to the charge density (basically, Maxwell’s first law). Moreover, f is some (unclear) nonlinear function of $|\nabla \psi|$ and of the concentration of positive and negative charges. We refer to Mock [18] or Markowich [15] for a much more detailed description of the various physical aspects of these problems. Here, we will deal only with problem (1.1), assuming that ψ , f , and g are known. We point out that the electric field $\nabla \psi$ appearing in (1.1) (after scaling) can be fairly big in some parts of Ω , so that (1.1) will be advection dominated. This obviously requires some special care in the choice of the discretization. The methods that we are proposing here are based on the following structure. We consider the classical change of variables

$$(1.2) \quad u = \rho e^{-\psi}.$$

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In the new unknown ρ , problem (1.1) becomes

$$(1.3) \quad \begin{aligned} &\text{Find } \rho \in H^1(\Omega) \text{ such that} \\ &\operatorname{div}(e^{-\psi} \nabla \rho) = f \quad \text{in } \Omega, \\ &\rho = \chi := e^{\psi} g \quad \text{on } \Gamma_0, \\ &\frac{\partial \rho}{\partial n} = 0 \quad \text{on } \Gamma_1. \end{aligned}$$

We then discretize (1.3) by means of some method that produces, in the unknown ρ , a symmetric positive-definite M -matrix. For reasons that will be clearer later on, it is also convenient to choose a method that makes use of some type of harmonic average of the coefficient $e^{-\psi}$ appearing in (1.3). Finally, we express the nodal values of ρ through the nodal values of u :

$$(1.4) \quad \rho_i = e^{\psi_i} u_i$$

and we write the discretized version of (1.3) in terms of the nodal values of u . We therefore obtain an M -matrix acting on the nodal values of u .

In the following sections we describe some of these methods in more detail, assuming, for the sake of simplicity, $f=0$. As we shall see, one of the basic features of the methods is that they are current-preserving, (current $= \underline{J} = \nabla u + u \nabla \psi$) either in a strong sense (mixed methods) or in some weaker sense (hybrid methods). This is particularly important in the applications, as the current is possibly the most relevant unknown of the problem. The current conservation property is the main novelty (in a finite-element context) of our schemes. As we will see, they are based on the choice of nonstandard methods for the discretization of (1.3) in contrast with the classical methods used before. The advantage of these methods is to introduce harmonic average of the coefficient $e^{-\psi}$ in (1.3) instead of the usual average, thus reproducing in the two-dimensional case some of the good features of the Scharfetter–Gummel scheme. Other methods were introduced before in attempts to extend the Scharfetter–Gummel scheme to two-dimensional problems (see, e.g., Mock [18], [19], Markowich and Zlámal [16], Bank, Rose, and Fichtner [4]), but they all used (in one way or another) some sort of one-dimensional harmonic average on suitably chosen lines (boundaries of the triangles, lines normal to the edges at midpoints, etc.), which makes the methods more ad hoc and the analysis more difficult. With our choice, instead, the scheme is set into a much more classical framework. This can also be seen from our error analysis, which is a suitable modification (with only minor changes for the mixed methods and with heavier changes for hybrid methods) of the classical ones. Indeed, our error estimates (see Theorems 2.1 and 3.1) reproduce easily the classical ones with optimal error estimates for a smooth ψ with $|\nabla \psi|$ small, and still retain some meaning for bigger $|\nabla \psi|$. Although our error estimates compare favorably with the ones in the literature, nevertheless we consider them rather unsatisfactory, since we lack knowledge of regularity results for the current that are independent of the size of $|\nabla \psi|$. However, it is a common belief (see Mock [18], Markowich [15]) that in the applications the current \underline{J} is reasonably smooth.

As expected, the discrete schemes that we obtain in this way provide some sort of natural upwinding, related to other upwinding schemes like that of Tabata [24], but different from them. In the numerical experiments performed so far, the methods show an artificial diffusion of order h (mesh size) in the crosswind direction, unless the mesh is suitably related to $\nabla \psi$ (in which case the effect of the artificial diffusion is negligible).

Some of the methods presented here were previously announced in [11].

2. Hybrid methods. Let us consider (see [12]) a regular sequence $\{T_h\}_h$ of decompositions of Ω into triangles T (for the sake of simplicity we shall assume that Ω is a polygon). For each T_h in the sequence and for every function $\xi \in C^0(\Gamma_0)$ we consider the sets

$$(2.1) \quad \Phi_{h,\xi} = \{\phi \in C^0(\bar{\Omega}), \phi = \xi \text{ at the nodes on } \Gamma_0, \phi|_T \in P_1 \forall T \in T_h\},$$

$$(2.2) \quad \Sigma_h = \{\tau \in [L^2(\Omega)]^2, \tau|_T \in (P_0)^2 \forall T \in T_h\}$$

and the corresponding discretization of (1.3) (with $f=0$):

$$(2.3) \quad \begin{aligned} &\text{Find } \sigma_h \in \Sigma_h \text{ and } \rho_h \in \Phi_{h,\chi} \text{ such that} \\ &\int_{\Omega} e^{\psi} \sigma_h \cdot \tau \, dx - \int_{\Omega} \nabla \rho_h \cdot \tau \, dx = 0 \quad \forall \tau \in \Sigma_h, \\ &\int_{\Omega} \nabla \phi \cdot \sigma_h \, dx = 0 \quad \forall \phi \in \Phi_{h,0}. \end{aligned}$$

It is clear that ρ_h will be an approximation of the solution ρ of (1.3) while σ_h will be an approximation of the current

$$(2.4) \quad \sigma = e^{-\psi} \nabla \rho = \nabla u + u \nabla \psi.$$

In particular, the first equation of (2.3) is a discretized version of (2.4), and the second equation of (2.3) is a discretized version of $\operatorname{div} \sigma = 0$. In the computations we usually assume that ψ is *piecewise linear* in each T , so that the integrals in (2.3) can be computed exactly.

PROPOSITION 2.1. *Problem (2.3) has a unique solution.*

Proof. It is easy to check that the abstract theory of [5] applies immediately to this case. In particular, the inf-sup condition holds trivially since $\nabla(\Phi_{h,0}) \subset \Sigma_h$. \square

Remark 2.1. Introducing the piecewise constant function $\bar{\psi}$ defined by

$$(2.5) \quad e|_T = \frac{\int_T e^{\psi} \, dx}{|T|},$$

the first equation of (2.3) gives

$$(2.6) \quad e^{\bar{\psi}} \sigma_h = \nabla \rho_h.$$

Substituting (2.6) into the second equation of (2.3), we find that (2.3) can be rewritten as

$$(2.7) \quad \begin{aligned} &\text{Find } \rho_h \in \Phi_{h,\chi} \text{ such that} \\ &\int_{\Omega} e^{-\bar{\psi}} \nabla \rho_h \cdot \nabla \phi \, dx = 0 \quad \forall \phi \in \Phi_{h,0}, \end{aligned}$$

that is, a *conforming discretization* of (1.3) in which we take the *harmonic average* $e^{-\bar{\psi}}$ of the coefficient $e^{-\psi}$ instead of the usual average.

The following proposition expresses the *weak continuity* of the current σ_h . In order to state it, we introduce first the jumps of $\sigma_h \cdot \underline{n}$ on an edge of T_h . If l is an internal edge, belonging to two triangles T_1 and T_2 and if $\underline{n}^i (i=1,2)$ are the unit outward normals to l , we define the jump of $\sigma_h \cdot \underline{n}$ across l as

$$(2.8) \quad [\sigma_h \cdot \underline{n}]_l = |l| (\sigma_{h|_{T_1}} \cdot \underline{n}^1 + \sigma_{h|_{T_2}} \cdot \underline{n}^2).$$

If instead l is a boundary edge belonging to a triangle T and \underline{n}^T is the unit outward normal to l , we set

$$(2.9) \quad [\sigma_h \cdot \underline{n}]_l = |l| \sigma_h|_T \cdot \underline{n}^T.$$

PROPOSITION 2.2. Let (σ_h, ρ_h) be the solution of (2.3), let P be a vertex of T_h belonging to $\Omega \cup \Gamma_1$, and let $l_i (i=1, \dots, r)$ be the edges having P in common. Then

$$(2.10) \quad \sum_{i=1}^r [\sigma_h \cdot \underline{n}]_{l_i} = 0.$$

Proof. Integrating the second equation of (2.3) by parts in every triangle T we get

$$(2.11) \quad \sum_T \int_{\partial T} \sigma_h \cdot \underline{n} \phi \, dl = 0 \quad \forall \phi \in \Phi_{h,0}.$$

Now, taking $\phi = 1$ at P and $\phi = 0$ at the other nodes, we obtain (2.10) easily from (2.11) and (2.8) or (2.9). \square

As we have seen, in the applications the function ψ (or, rather, $\psi_{\max} - \psi_{\min}$) might be fairly big. Therefore, it is inconvenient to implement (2.3) or (2.7) on the computer, since $e^{-\bar{\psi}}$ and $\chi (= e^{\psi} g)$ can be a considerable source of problems. Besides, the variable ρ itself has very little physical interest. Therefore, we go back to the original variable u via (1.4). For this, we define, for every function z in $C^0(\bar{\Omega})$, its piecewise linear interpolant z^I verifying $z^I = z$ at every vertex in T_h . Then, problem (2.3) (or rather (2.7)) can be rewritten as

Find $u_h \in \Phi_{h,g}$ such that

$$(2.12) \quad \int_{\Omega} e^{-\bar{\psi}} \nabla (e^{\psi} u_h)^I \cdot \nabla \phi \, dx = 0 \quad \forall \phi \in \Phi_{h,0}.$$

PROPOSITION 2.3. If the triangulation T_h is of weakly acute type (every angle of every $T \in T_h$ is less than or equal to $\pi/2$) then the matrix associated with (2.12) is an M -matrix.

Proof. It is easy to see that the matrix associated with (2.7) is symmetric and positive definite. Moreover, if the triangulation T_h is of weakly acute type, then all the off-diagonal coefficients are less than or equal to zero. Hence we have an M -matrix. On the other hand, the change of variable “ $\rho_h = e^{\psi} u_h$ at the nodes” corresponds to multiplying every column of the matrix associated with (2.7) by e^{ψ_i} (ψ_i being the value of ψ at the corresponding vertex). This does not change the M -character of the matrix. Indeed, the properties of (i) being nonsingular; (ii) having the off-diagonal coefficients less than or equal to zero, and (iii) having all the coefficients of the inverse matrix greater than or equal to zero still hold when multiplying to the right by a positive diagonal matrix. \square

Remark 2.2. Looking at the contributions of every triangle T to the stiffness matrix of (2.12), we see that the order of magnitude of the terms $\nabla (e^{\psi} u_h)^I$ is at most $e^{\psi_M^T}$, where ψ_M^T is the maximum of ψ in T . On the other hand, $e^{\bar{\psi}}$ is also of order $e^{\psi_M^T}$ so that the coefficients of (2.12) are of reasonable size or possibly very small. Problems can arise only if we have a row or a column, in the matrix, which contains only very small coefficients. This can happen to a row only if the decomposition is of weakly acute type and the gradient of ψ is very specially oriented with respect to the mesh. On the contrary, this happens to a column whenever a node P is such that $\psi(P) \ll \psi_M^T$ for every triangle T having a vertex in P . However, this will not be true in the interior of Ω , if we assume that ψ does not have very deep minima (compared with the local mesh size). Under the same assumptions for $\nabla \psi$ this will not be true on Γ_1 either, since, in the applications, $\partial \psi / \partial n$ will be small on Γ_1 .

On the other hand, the average of $e^{-\psi}$ in T will have the order of magnitude of $e^{-\psi_m^T}$ (where ψ_m^T is the minimum value of ψ in T). Therefore, the use of the average of $e^{-\psi}$ instead of the harmonic average $e^{-\bar{\psi}}$ in (2.12) will produce contributions to the coefficients of size $e^{\psi_M^T - \psi_m^T}$, which is a potential source of troubles. Nevertheless a solid theoretical argument showing the superiority of the harmonic average is still to be found, in our opinion, except for the obvious one-dimensional case where (2.12) coincides with the Scharfetter–Gummel method and gives the exact solution (at the nodes) for a piecewise linear ψ . For other considerations on the use of the harmonic average in one dimension (although in a different context), see [3].

Now we will present another scheme that perhaps better deserves the name “hybrid.” To simplify the presentation we will assume that Ω is a square which has been subdivided into N^2 subsquares Q of side h . We introduce the spaces

$$(2.13) \quad \Phi_{h,\xi} = \{\phi \in C^0(\bar{\Omega}), \phi = \xi \text{ at the nodes on } \Gamma_0, \phi|_Q \in Q_1 \forall Q\},$$

$$(2.14) \quad \Sigma_h = \{\tau \in [L^2(\Omega)]^2, \tau|_Q \in (\nabla Q_1) \forall Q\}.$$

In (2.13) and (2.14), Q_1 is the set of polynomials of degree less than or equal to 1 in each variable, and ∇Q_1 is clearly the set of pairs of polynomials of the type $(a + by, c + bx)$, $a, b, c \in \mathbb{R}$. The hybrid discretization of (1.3) will now be

$$(2.15) \quad \begin{aligned} &\text{Find } \underline{\sigma}_h \in \Sigma_h \text{ and } \rho_h \in \Phi_{h,\chi} \text{ such that} \\ &\int_{\Omega} e^{\psi} \underline{\sigma}_h \cdot \tau \, dx - \int_{\Omega} \nabla \rho_h \cdot \tau \, dx = 0 \quad \forall \tau \in \Sigma_h, \\ &\int_{\Omega} \nabla \phi \cdot \underline{\sigma}_h \, dx = 0 \quad \forall \phi \in \Phi_{h,0}. \end{aligned}$$

It is now less immediate to write (2.15) in the form (2.7), that is, as a conforming method with harmonic average. However, we can still go back to the unknown u_h and obtain the following problem:

$$(2.16) \quad \begin{aligned} &\text{Find } \underline{\sigma}_h \in \Sigma_h \text{ and } u_h \in \Phi_{h,g} \text{ such that} \\ &\int_{\Omega} e^{\psi} \underline{\sigma}_h \cdot \tau \, dx - \int_{\Omega} \nabla (e^{\psi} u_h)^I \cdot \tau \, dx = 0 \quad \forall \tau \in \Sigma_h, \\ &\int_{\Omega} \nabla \phi \cdot \underline{\sigma}_h \, dx = 0 \quad \forall \phi \in \Phi_{h,0}, \end{aligned}$$

with obvious meaning for $(\)^I$ in this new case.

PROPOSITION 2.4. *Problem (2.15) (and then (2.16)) has a unique solution.*

The proof is identical to that of Proposition 2.1. \square

We can also see that $\underline{\sigma}_h$ has a weak conservation property similar to that of Proposition 2.2.

We remark now that the matrix associated with (2.15) has the structure

$$(2.17) \quad \begin{pmatrix} A & B \\ B^T & 0 \end{pmatrix}$$

with A block-diagonal (each block corresponding to a single element). Therefore $\underline{\sigma}_h$ can be eliminated by static condensation. The resulting matrix $B^T A^{-1} B$, acting on the nodal values of ρ_h , will be a symmetric positive-definite M -matrix. With an argument similar to that of Proposition 2.3 we can therefore prove the following result.

PROPOSITION 2.5. *If we eliminate $\underline{\sigma}_h$ in (2.16) by static condensation, the resulting matrix, acting on the nodal values of u_h , is an M -matrix.*

Remark 2.3. In a more general case, for a polygon Ω divided into quadrilaterals, we can use the spaces Q_1 and ∇Q_1 on the reference element, and define the local spaces via an isoparametric mapping. Note, however, that it will be more convenient to use a contravariant mapping for the vector variables in Σ_h , in order to preserve the zero-divergence property. All this is classical, but the notation would still be a little cumbersome. This is the reason why we decided to present the method in the simplified case.

We will now present some unsatisfactory error bounds for the current σ . Since it is clear that the two simple examples presented here do not span the whole range of possible hybrid discretizations, we will present a more abstract result, including both cases presented here plus some others. For more information on the mathematical treatment of hybrid methods (although in different contexts) see, e.g., [6], [10], [25], [17], [9].

Assume therefore that the spaces Σ_h and Φ_h are either the ones introduced in (2.1), (2.2) or the ones introduced in (2.13), (2.14). We set $(\cdot, \cdot) = \text{inner product in } [L^2(\Omega)]^2$, $a(\sigma, \tau) = (e^\psi \sigma, \tau)$, and $\|\sigma\|_a^2 = a(\sigma, \sigma)$. Finally, we consider our discrete problems in their common form:

$$(2.18) \quad \begin{aligned} &\text{Find } \sigma_h \in \Sigma_h \text{ and } u_h \in \Phi_{h,g} \text{ such that} \\ &a(\sigma_h, \tau) = (\nabla(e^\psi u_h)^I, \tau) \quad \forall \tau \in \Sigma_h, \\ &(\nabla \phi, \sigma_h) = 0 \quad \forall \phi \in \Phi_{h,0}. \end{aligned}$$

We have the following theorem.

THEOREM 2.1. *Let u be the solution of (1.1) (always with $f=0$) and let $\sigma := e^{-\psi} \nabla(e^\psi u) = \nabla u + u \nabla \psi$. Let (σ_h, u_h) be the solution of (2.18) and let σ^I and $\tilde{\sigma}$ be the approximations of σ defined by*

$$(2.19) \quad \sigma^I \in \Sigma_h \quad \text{and} \quad (\sigma - \sigma^I, \tau) = 0 \quad \forall \tau \in \Sigma_h,$$

$$(2.20) \quad \tilde{\sigma} = e^{-\psi} \nabla(e^\psi u)^I.$$

Then

$$(2.21) \quad \|\sigma - \sigma_h\|_a \leq 2\{\|\sigma - \sigma^I\|_a + \|\sigma - \tilde{\sigma}\|_a\}.$$

Proof. We have

$$(2.22) \quad \begin{aligned} \|\sigma - \sigma_h\|_a^2 &= a(\sigma - \sigma_h, \sigma - \sigma_h) \\ &= a(\sigma - \sigma_h, \sigma - \sigma^I) + a(\sigma - \sigma_h, \sigma^I - \sigma_h) \\ &= I + II, \end{aligned}$$

$$(2.23) \quad \begin{aligned} II &= a(\sigma - \sigma_h, \sigma^I - \sigma_h) \\ &= (\nabla(e^\psi u) - \nabla(e^\psi u_h)^I, \sigma^I - \sigma_h) \\ &= (\nabla(e^\psi u) - \nabla(e^\psi u)^I, \sigma^I - \sigma_h) + (\nabla(e^\psi u)^I - \nabla(e^\psi u_h)^I, \sigma^I - \sigma_h) \\ &= a(\sigma - \tilde{\sigma}, \sigma^I - \sigma_h) + (\nabla(e^\psi u)^I - \nabla(e^\psi u_h)^I, \sigma - \sigma_h) \\ &= a(\sigma - \tilde{\sigma}, \sigma^I - \sigma_h), \end{aligned}$$

where in the last step we use the fact that $(e^\psi u)^I - (e^\psi u_h)^I \in \Phi_{h,0}$. From (2.22) and (2.23) we have, via the Cauchy-Schwarz inequality,

$$(2.24) \quad \begin{aligned} \|\sigma - \sigma_h\|_a^2 &\leq \|\sigma - \sigma_h\|_a \|\sigma - \sigma^I\|_a + \|\sigma - \tilde{\sigma}\|_a \|\sigma^I - \sigma_h\|_a \\ &\leq \|\sigma - \sigma_h\|_a (\|\sigma - \sigma^I\|_a + \|\sigma - \tilde{\sigma}\|_a) + \|\sigma - \tilde{\sigma}\|_a \|\sigma - \sigma^I\|_a, \end{aligned}$$

from which (2.21) follows easily. \square

3. Mixed methods. We consider now another class of nonstandard methods for dealing with problem (1.3), namely, the class of so-called mixed methods. For this, we start, as before, with the simplest element of the family. Again let $\{T_h\}_h$ be a family of regular decompositions of Ω into triangles T [12]. According to [22], we define the following set of polynomial vectors:

$$(3.1) \quad RT(T) = \{\tau = (\tau_1, \tau_2), \tau_1 = a + bx, \tau_2 = c + by, a, b, c \in \mathbb{R}\},$$

and, for every triangulation T_h , we set

$$(3.2) \quad \Sigma_h = \{\tau \in [L^2(\Omega)]^2, \operatorname{div} \tau \in L^2(\Omega), \tau \cdot n = 0 \text{ on } \Gamma_1, \tau|_T \in RT(T) \quad \forall T \in T_h\},$$

$$(3.3) \quad \Phi_h = \{\phi \in L^2(\Omega): \phi|_T \in P_0(T) \quad \forall T \in T_h\},$$

and we consider the discretized version of (1.3) defined as follows:

$$(3.4) \quad \begin{aligned} &\text{Find } \sigma_h \in \Sigma_h \text{ and } \rho_h \in \Phi_h \text{ such that} \\ &\int_{\Omega} e^{\psi} \sigma_h \cdot \tau \, dx = - \int_{\Omega} \rho_h \operatorname{div} \tau \, dx + \int_{\Gamma_0} \chi \tau \cdot n \, d\Gamma \quad \forall \tau \in \Sigma_h, \\ &\int_{\Omega} \phi \operatorname{div} \sigma_h \, dx = 0 \quad \forall \phi \in \Phi_h. \end{aligned}$$

The interpretation of the two equations of (3.4) is again very easy, and is the same as we had for the two equations of (2.3). We now recall a basic result on mixed methods, in the form introduced by Douglas and Roberts [13]. To do that, we first introduce some notation. First of all, let $p > 2$ be such that for every function $f \in L^2(\Omega)$ the solution w of the auxiliary problem

$$(3.5) \quad \begin{aligned} \Delta w &= f \quad \text{in } \Omega, \\ w &= 0 \quad \text{on } \Gamma_0, \\ \frac{\partial w}{\partial n} &= 0 \quad \text{on } \Gamma_1 \end{aligned}$$

belongs to $W^{1,p}(\Omega)$ and

$$(3.6) \quad \|w\|_{W^{1,p}(\Omega)} \leq c \|f\|_{L^2(\Omega)},$$

with c independent of f . Such a p always exists since we assume that Ω is a polygon. Then we set

$$(3.7) \quad \begin{aligned} \Sigma &= \{\tau \in [L^p(\Omega)]^2; \operatorname{div} \tau \in L^2(\Omega); \tau \cdot n = 0 \text{ on } \Gamma_1\}, \\ \|\tau\|_{\Sigma} &= \|\tau\|_{[L^p(\Omega)]^2} + \|\operatorname{div} \tau\|_{L^2(\Omega)} \end{aligned}$$

and we define, for every triangulation T_h , the operators $\Pi_h: \Sigma \rightarrow \Sigma_h$ and $P_h: L^2(\Omega) \rightarrow \Phi_h$ as follows:

$$(3.8) \quad \int_l (\Pi_h \tau - \tau) \cdot n \, dl = 0 \quad \forall \tau \in \Sigma, \quad \forall l \text{ edge of } T_h,$$

$$(3.9) \quad \int_T (P_h \phi - \phi) \, dx = 0 \quad \forall \phi \in L^2(\Omega), \quad \forall T \in T_h.$$

A few remarks are in order regarding (3.8). First, a little functional analysis will show that the integral of $\tau \cdot n$ on an edge l makes sense. This is due to the fact that we assumed $p > 2$ and $\operatorname{div} \tau \in L^2(\Omega)$. Second, it is not difficult to show that the knowledge

of $\Pi_{h\tau} \cdot \eta$ on every edge will characterize $\Pi_{h\tau} \in \Sigma_h$ in a unique way (see [22]). Hence the operator Π_h is well defined. Moreover, we have

$$(3.10) \quad \|\Pi_{h\tau}\|_{[L^2(\Omega)]^2} \leq c \|\tau\|_{\Sigma},$$

with c independent of τ and h . On the other hand, P_h is a simple L^2 -projection and does not need any comment. The commutative diagram property of Douglas and Roberts [13] can then be expressed in the following way.

PROPOSITION 3.1.

$$(3.11) \quad \begin{array}{ccc} \Sigma & \xrightarrow{\text{div}} & L^2(\Omega) \\ \Pi_h \downarrow & & \downarrow P_h \\ \Sigma_h & \xrightarrow{\text{div}} & \Phi_h \longrightarrow 0 \end{array}$$

Remark 3.1. Proposition 3.1 means, in other words, that for every $\tau \in \Sigma$ we have

$$(3.12) \quad \text{div}(\Pi_{h\tau}) = P_h \text{div } \tau,$$

and besides, the divergence operator from Σ to $L^2(\Omega)$ is surjective (this can be easily checked through the auxiliary problem (3.5) and setting $\tau := \nabla w \in \Sigma$) and the divergence operator from Σ_h to Φ_h is also surjective (this is an easy consequence of (3.12) and of the above result). Moreover, from (3.6), (3.10), and (3.12) we get

$$(3.13) \quad \begin{aligned} \exists c > 0: \quad \forall h \quad \forall \phi \in \Phi_h, \exists \tau \in \Sigma_h \text{ such that} \\ \text{div } \tau = \phi \quad \text{and} \quad \|\tau\|_{[L^2(\Omega)]^2} \leq c \|\phi\|_{L^2(\Omega)}, \end{aligned}$$

which is a stronger form of the inf-sup condition.

In particular, (3.13) implies immediately the following well-known result.

PROPOSITION 3.2. Problem (3.4) has a unique solution.

As far as the continuity of the current is concerned, we remark that the condition $\text{div } \tau \in L^2(\Omega)$ in definition (3.2) of Σ_h implies that every τ in Σ_h has a continuous normal component when passing from one element to another. This, on one hand, is very satisfactory since the solution σ_h itself will have a continuous normal component (strong continuity property for the current). On the other hand, we have a serious drawback: the matrix associated with (3.4) has again the structure (2.17), but now the submatrix A will no longer be block-diagonal, due to the continuity properties of the elements of Σ_h . Hence, the a priori elimination of σ_h by static condensation will not be possible anymore. This is particularly bad since the matrix (of the type (2.17)) associated with (3.4) is only symmetric, but it is neither positive-definite nor an M -matrix. A clever escape from this dead end was found by Fraeij de Veubeke [14] for a similar problem (and the philosophy has then been extended to a number of similar cases). In his terminology, it amounts to assuming the stresses (here, the current) to be totally discontinuous and to forcing the continuity of the normal components by means of interelement Lagrange multipliers. Here we need a more detailed description of the procedure. For this we first set

$$(3.14) \quad \tilde{\Sigma}_h = \{\tau \in [L^2(\Omega)]^2; \tau|_T \in RT \quad \forall T \in \mathcal{T}_h\}.$$

Then, calling E_h the set of edges of T_h , we set, for every function $\xi \in L^2(\Gamma_0)$

$$(3.15) \quad \Lambda_{h,\xi} = \left\{ \mu \mid \mu \in L^2(E_h); \mu|_l \in P_0 \quad \forall l \in E_h; \int_l (\mu - \xi) dl = 0 \quad \forall l \subset \Gamma_0 \right\}.$$

Now we consider the “extended” discretized problem

$$\begin{aligned}
 &\text{Find } \tilde{\sigma}_h \in \tilde{\Sigma}_h, \tilde{\rho}_h \in \Phi_h, \tilde{\lambda}_h \in \Lambda_{h,\chi} \text{ such that} \\
 &\int_{\Omega} e^{\psi} \tilde{\sigma}_h \cdot \underline{\tau} \, dx + \sum_T \int_T \tilde{\rho}_h \operatorname{div} \underline{\tau} \, dx = \sum_T \int_{\partial T} \tilde{\lambda}_h \underline{\tau} \cdot \underline{n} \, dl \quad \forall \underline{\tau} \in \tilde{\Sigma}_h, \\
 &\sum_T \int_T \phi \operatorname{div} \tilde{\sigma}_h \, dx = 0 \quad \forall \phi \in \Phi_h, \\
 &\sum_T \int_{\partial T} \mu \tilde{\sigma}_h \cdot \underline{n} \, dl = 0 \quad \forall \mu \in \Lambda_{h,0}.
 \end{aligned}
 \tag{3.16}$$

The following proposition can be found in [2].

PROPOSITION 3.3. *Problem (3.16) has a unique solution. Moreover, if $(\tilde{\sigma}_h, \tilde{\rho}_h, \tilde{\lambda}_h)$ is the solution of (3.16) and (σ_h, ρ_h) is the solution of (3.4) we have*

$$\tilde{\sigma}_h = \sigma_h \quad \text{and} \quad \tilde{\rho}_h = \rho_h.
 \tag{3.17}$$

We remark now that the matrix associated with (3.16) has the structure

$$\begin{bmatrix} A & B & C \\ B^T & 0 & 0 \\ C^T & 0 & 0 \end{bmatrix}
 \tag{3.18}$$

but now A is block-diagonal. In other words, $\tilde{\sigma}_h$ can be eliminated, element by element, by static condensation. This leaves us with the matrix

$$\begin{bmatrix} B^T A^{-1} B & B^T A^{-1} C \\ C^T A^{-1} B & C^T A^{-1} C \end{bmatrix},
 \tag{3.19}$$

where $B^T A^{-1} B$ is block-diagonal (actually, in the present case, diagonal) and nonsingular. Hence $\tilde{\rho}_h$ can also be eliminated, at the element level, by static condensation. This leaves us, finally, with a matrix (acting only on the interelement multiplier $\tilde{\lambda}_h$) which can be proved to be a symmetric positive-definite matrix, which is an M -matrix if T_h is of weakly acute type. It is also possible to prove (see [2]) that $\tilde{\lambda}_h$ will also be an approximation of ρ .

We are therefore ready to introduce an approximation of our original unknown u . For this we define, for every $\zeta \in L^2(E_h)$, ζ^I to now be the L^2 -projection of ζ onto Λ_h , that is

$$\zeta_{|l}^I = \frac{1}{|l|} \int_l \zeta \, dl \quad \forall l \in E_h.
 \tag{3.20}$$

Now, using the change of variable $\tilde{\lambda}_h = (e^{\psi})^I u_h$, we can rewrite (3.16) in the form

$$\begin{aligned}
 &\text{Find } \sigma_h \in \tilde{\Sigma}_h, \rho_h \in \Phi_h, u_h \in \Lambda_{h,g} \text{ such that} \\
 &\int_{\Omega} e^{\psi} \sigma_h \cdot \underline{\tau} \, dx + \sum_T \int_T \rho_h \operatorname{div} \underline{\tau} \, dx = \sum_T \int_{\partial T} e^{\psi} u_h \underline{\tau} \cdot \underline{n} \, dl \quad \forall \underline{\tau} \in \tilde{\Sigma}_h, \\
 &\sum_T \int_T \phi \operatorname{div} \sigma_h \, dx = 0 \quad \forall \phi \in \Phi_h, \\
 &\sum_T \int_{\partial T} \mu \sigma_h \cdot \underline{n} \, dl = 0 \quad \forall \mu \in \Lambda_{h,0},
 \end{aligned}
 \tag{3.21}$$

where we go back to the original names for the variables σ_h and ρ_h in virtue of (3.17).

The following proposition can now be easily proved, under the assumption that T_h is of weakly acute type.

PROPOSITION 3.4. *If we eliminate σ_h and ρ_h in (3.21) by static condensation, the resulting matrix, acting on the unknown u_h only, is an M -matrix.*

Proof. The matrix that we have to analyze can be obtained from the matrix corresponding to (3.16) by multiplying each column by the value of $(e^\psi)^l$ on the corresponding edge. \square

Remark 3.2. In the particular case that we are considering, the unknown ρ_h can actually be eliminated a priori. In fact, considering definitions (3.1) and (3.14), the second equation of (3.21) tells us from the beginning that σ_h must be constant in each triangle. We might therefore set the problem in the space Σ_h as defined in (3.2) (let us call it Σ_h^0 now, to avoid confusion) and drop ρ_h from the beginning:

Find $\sigma_h \in \Sigma_h^0$, $u_h \in \Lambda_{h,g}$ such that

$$(3.22) \quad \begin{aligned} \int_{\Omega} e^{\psi} \sigma_h \cdot \underline{n} \, dx &= \sum_T \int_{\partial T} e^{\psi} u_{hT} \cdot \underline{n} \, dl \quad \forall T \in \Sigma_h^0, \\ \sum_T \int_{\partial T} \mu \sigma_h \cdot \underline{n} \, dl &= 0 \quad \forall \mu \in \Lambda_{h,0}. \end{aligned}$$

This, with some minor adjustment (see [11]), can also be done when f (in (1.1)) is not zero. We only have to write σ_h in (3.21) as

$$(3.23) \quad \sigma_h = \sigma_h^0 + \sigma_h^f,$$

with σ_h^0 unknown belonging to Σ_h^0 and σ_h^f given, in any triangle T , by

$$(3.24) \quad \sigma_h^f = (\bar{f}/2)(x - x_T, y - y_T),$$

where \bar{f} is the mean value of f in T and (x_T, y_T) are the coordinates of the barycenter of T . On the other hand, the reduction to the form (3.22) is not possible for a more general mixed discretization of (1.3) (while (3.21) is fairly general).

Remark 3.3. Proposition 3.4 states that the final matrix (associated with (3.21)) in the unknown u_h is always an M -matrix. However (as we saw in Remark 2.2 for the hybrid methods) particular choices of $\nabla \psi$ and of the mesh might generate a column of very small coefficients (we can check that, in the present case, we never have a row of very small coefficients, even for decompositions of weakly acute type or for “nasty” $\nabla \psi$). A column (corresponding to an edge l_i of T_h) can be made of very small coefficients if $\max_{x \in l_i} \psi(x) \ll \max_{x \in l_j} \psi(x)$ for all edges l_j ($j \neq i$) sharing a triangle with l_i . This will not happen in the interior if $\nabla \psi$ is not too wild, and will not happen at the boundary edges on Γ_1 if $\partial \psi / \partial n$ is not too big.

As in the previous section, we consider here another possible choice of mixed finite-element discretizations of (1.3). Again, in order to avoid the technicalities connected with isoparametric elements and contravariant transformations, we consider a decomposition of Ω into squares Q . We now set

$$(3.25) \quad RTS = \{T \mid \tau_1 = a + bx; \tau_2 = c + dy; a, b, c, d \in \mathbb{R}\},$$

$$(3.26) \quad \tilde{\Sigma}_h = \{T \in [L^2(\Omega)]^2; T|_Q \in RTS \, \forall Q\},$$

$$(3.27) \quad \Sigma_h = \tilde{\Sigma}_h \cap \Sigma,$$

$$(3.28) \quad \Phi_h = \{\phi \in L^2(\Omega); \phi|_Q \in P_0 \, \forall Q\}$$

and for every $\xi \in L^2(\Gamma_0)$

$$(3.29) \quad \Lambda_{h,\xi} = \left\{ \mu \in L^2(E_h); \mu|_l \in P_0 \quad \forall l \in E_h: \int_l (\mu - \xi) dl = 0 \quad \forall l \subset \Gamma_0 \right\},$$

where E_h is now the set of the edges of the decomposition into squares. Problems (3.4), (3.16), and (3.21) can now be rewritten, formally unchanged, but with the new meaning (3.26)–(3.29) for the discrete spaces (and using Q instead of T in (3.16) and in (3.21)). Propositions 3.1–3.3 still hold formally unchanged for the new discretization. Note that the definitions (3.8) and (3.9) (of Π_h and P_h , respectively) can also be left formally unchanged. To preserve the M -matrix property stated in Proposition 3.4 we must modify the space (3.25) choosing, e.g., vectors of the form $\tau_1 = a + b(x - \frac{2}{3}x^3)$, $\tau_2 = c + d(y - \frac{2}{3}y^3)$ on the reference square $(-1, 1) \times (-1, 1)$. In this case, it will be convenient to approximate e^ψ as in (2.5), to simplify the evaluation of integrals of the type $\int e^\psi x^6 dx$.

More information on mixed methods can be found, for instance, in [22], [21], [25], [13], [7]–[9].

As we did in § 2, we now present an error bound for the approximation of the current. As we shall see, this can be done here on the formulation (3.4) directly, and therefore standard techniques apply. For the sake of completeness, we report nevertheless the simple proof. For this, let again Σ_h and Φ_h be either the spaces defined in (3.2), (3.3) (for triangular decompositions) or the ones defined in (3.27), (3.28) (for squares). Using the same notation as in Theorem 2.1, we rewrite the discrete problem (3.4) as

$$(3.30) \quad \begin{aligned} &\text{Find } \underline{\sigma}_h \in \Sigma_h, \rho_h \in \Phi_h \text{ such that} \\ &a(\underline{\sigma}_h, \underline{\tau}) + (\operatorname{div} \underline{\tau}, \rho_h) = \int_{\Gamma_0} \chi \underline{\tau} \cdot \underline{n} d\Gamma \quad \forall \underline{\tau} \in \Sigma_h, \\ &(\operatorname{div} \underline{\sigma}_h, \phi) = 0 \quad \forall \phi \in \Phi_h. \end{aligned}$$

Then we have the following theorem.

THEOREM 3.1. *Let u be the solution of (1.1) (always with $f = 0$), let $\underline{\sigma} := e^{-\psi} \nabla(e^\psi u) = \nabla u + u \nabla \psi$ and $(\underline{\sigma}_h, \rho_h)$ be the solution of (3.30). Then*

$$(3.31) \quad \|\underline{\sigma} - \underline{\sigma}_h\|_a \leq \|\underline{\sigma} - \Pi_h \underline{\sigma}\|_a,$$

where $\Pi_h \underline{\sigma}$ is defined as in (3.8).

Proof. We have

$$(3.32) \quad \begin{aligned} \|\underline{\sigma} - \underline{\sigma}_h\|_a^2 &= a(\underline{\sigma} - \underline{\sigma}_h, \underline{\sigma} - \underline{\sigma}_h) \\ &= a(\underline{\sigma} - \underline{\sigma}_h, \underline{\sigma} - \Pi_h \underline{\sigma}) + a(\underline{\sigma} - \underline{\sigma}_h, \Pi_h \underline{\sigma} - \underline{\sigma}_h). \end{aligned}$$

Note that

$$(3.33) \quad \begin{aligned} a(\underline{\sigma} - \underline{\sigma}_h, \Pi_h \underline{\sigma} - \underline{\sigma}_h) &= (\rho_h - \rho, \operatorname{div}(\Pi_h \underline{\sigma} - \underline{\sigma}_h)) \\ &= (\rho_h - \rho, P_h \operatorname{div} \underline{\sigma} - \operatorname{div} \underline{\sigma}_h) = 0, \end{aligned}$$

using (3.12) and $\operatorname{div} \underline{\sigma} = \operatorname{div} \underline{\sigma}_h = 0$. Hence (3.31) follows immediately from (3.32), (3.33). \square

We point out that, thanks to Proposition 3.3, the estimate (3.31) actually holds for the solution of (3.16), and hence of (3.21).

4. Numerical results. We present in this section some numerical results obtained using the methods described in the previous sections over triangular decompositions.

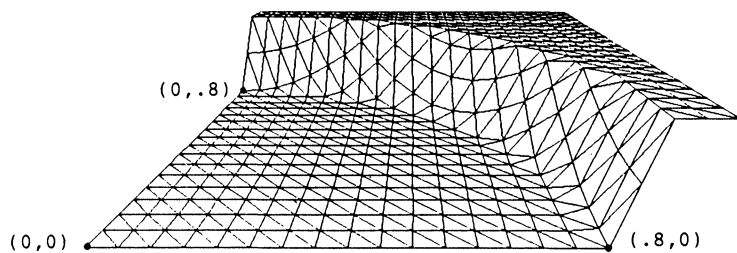


FIG. 1

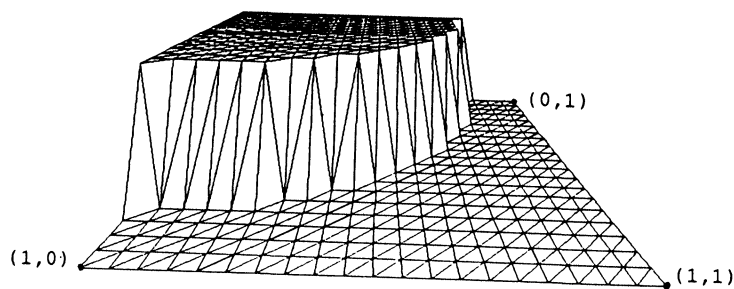


FIG. 2

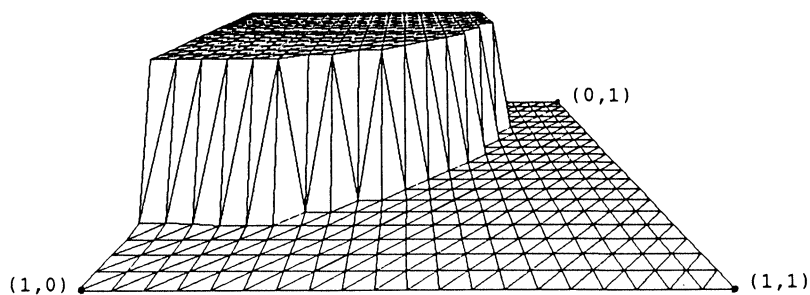


FIG. 3

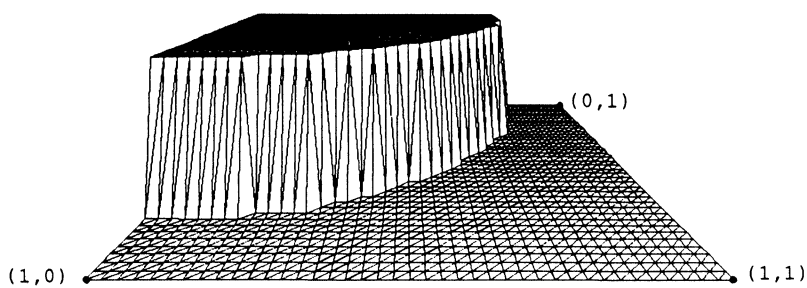


FIG. 4

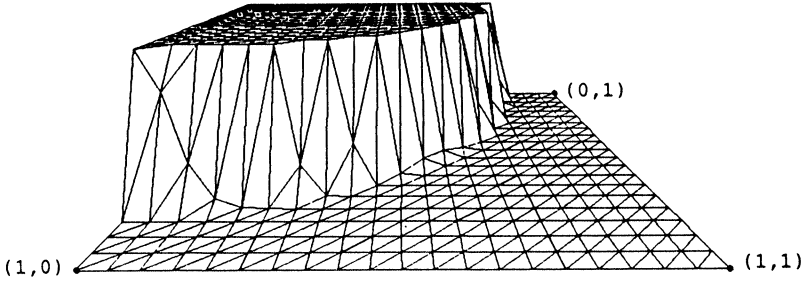


FIG. 5

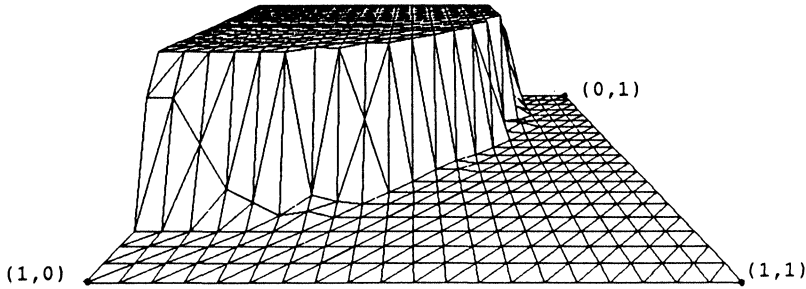


FIG. 6

The domain Ω is the unit square: the function $\psi(x)$ is given by $\psi(x) = \psi_0(x)/\lambda$, where $\psi_0(x)$ in its turn has the expression

$$\psi_0(x) = \begin{cases} 0 & \text{if } 0 \leq \rho \leq .8, \\ 2(\rho - .8) & \text{if } .8 \leq \rho \leq .9, \\ .2 & \text{if } .9 \leq \rho, \end{cases}$$

and $\rho = (x_1^2 + x_2^2)^{1/2}$ (see Fig. 1). The boundary conditions for u are: $u = .3$ on $\{x_1 = 0, x_2 \leq .25\}$ and on $\{x_2 = 0, x_1 \leq .25\}$, $u = 0$ on $\{x_1 = 1, x_2 \geq .75\}$ and on $\{x_2 = 1, x_1 \geq .75\}$. Homogeneous Neumann boundary conditions are assumed elsewhere. In Figs. 2–4 we show u_h as computed with, respectively, hybrid methods (2.12) on a 20×20 mesh, and mixed methods (3.21) on a 10×10 and 20×20 mesh. In all these cases, $\lambda = 10^{-4}$ was used. In Figs. 5–6 we report the results for $\lambda = 10^{-2}$ for hybrid methods on a 20×20 mesh, and for mixed methods on a 10×10 mesh, respectively.

Remark 4.1. The methods presented in the previous sections exhibit upwinding features that show up when $|\nabla \psi|$ is large with respect to the mesh size. As already pointed out in Remark 2.2 for the hybrid scheme, and in Remark 3.3 for the mixed scheme, the coefficients of the stiffness matrices include exponentials of the difference of nodal values of ψ . In the i th row, the coefficients corresponding to nodes downwind (with respect to the i th node) decrease exponentially as $|\nabla \psi|$ increases. Then the upwinding effect is not present if $|\nabla \psi|$ is small (i.e., if the problem is not advection dominated). Instead, whenever $|\nabla \psi|$ is large, the schemes adapt automatically to the changed nature of the problem and choose the upwind nodes with no extra computational cost. Hence we can say that, in a natural and automatic way, the more $|\nabla \psi|$ is large, the more upwind the schemes.

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