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A FINITE ELEMENT METHOD WITH CURRENT CONSERVATION

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SUMMARY

In this paper a new mixed finite element method for device modelling is presented. This discretisation satisfies the usual requirements of current conservation and fitting for the singularly perturbed continuity equation. It is defined for the n-dimensional problem with non-zero recombination and reduces to the Scharfetter-Gummel scheme for one dimension and zero recombination. For recombination unequal to zero a 'stability' problem is encountered with the 'usual' mixed finite element method. For this problem a solution is presented also in this paper. The solution, in principle, is the lumping of the mass matrices involved.

INTRODUCTION

The discretisation methods most used for solving the device modelling equations are some ad hoc generalisation of the so-called Scharfetter-Gummel scheme (see, for example, Polak et al., 1987). This scheme is fully accounted for in the one dimensional case with zero recombination.
A recent publication by F. Brezzi (1987) shows that a certain mixed finite element method reduces to the Scharfetter-Gummel method in the one dimensional zero recombination case. This provides a mathematically well accounted for generalisation of the Scharfetter-Gummel scheme. It thereby satisfies the usual criteria such as current conservation and, moreover, allows (as usual with FEM) a consistent way of interpolating the different quantities involved. However, Brezzi (1987) only treats the zero recombination case. For recombination unequal to zero, or simpler, in applying the method to a problem of the form $\Delta u=u$, an instability is met. In this paper we analyse this problem for the one dimensional case. We also describe the solution for the two dimensional rectangular case and give an example problem. This example shows essentially more accurate currents than achieved with the classical box scheme.

DISCRETISATION REQUIREMENTS

The discretisation of the continuity equation basically should satisfy four requirements:

(1) 'discrete current conservation'
(2) 'upwinding'
(3) interpolation uniquely defined
(4) convergence theory available

We only discuss these topics heuristically and briefly here as a vast literature exists on them.
Most present discretisations used are based on some discrete analogue of Green's theorem (box schemes) and therefore satisfy (1). It is interesting to note that conforming finite element methods with the lowest order basis functions do not satisfy (1). This can be easily understood from the following one dimensional problem: $u_{xx} = 1$ on the interval [0,3], with boundary conditions $u(0) = u(1) = 0$. With one internal node at $x = 1$ we find that $u_x(3) - u_x(0) = 9/4$, which is not equal to the integral of the right hand side over the interval. The explanation for this is the following. In FEM we have performed a partial integration, thus allowing a discontinuity of the u_x-values at internal nodes or interfaces. This in fact is a spurious 'current source'. In mixed FEM we do not perform this partial integration. In fact, continuity of u_x (or, in more than one dimension, the normal component of grad u) is a requirement. So, current conservation is satisfied. More precisely, one of the generalised equations in the mixed finite element formulation of $\Delta u = f$ is $(\text{grad } \sigma, \phi) = (f, \phi)$, where ϕ is the characteristic function of an element. Using Green's theorem on the boundary then shows that

$$\int_{\Gamma} \sigma \cdot dn = \iint_{\Omega} f$$

The concept of 'upwinding' only plays a role if the mesh widths are not sufficiently small. In device modelling this is usually the case (cf. Markowich, 1986). All schemes used for these problems therefore must satisfy this requirement.
In one dimension it is not difficult to define interpolation of the different quantities uniquely. In two (or more) dimensions we meet the following requirement. Suppose (simplified) that $J = \exp(\psi)\ \nabla\Phi$, then $\exp(-\psi)\ J = \nabla\Phi$, so we have that $\nabla \times \{\exp(-\psi)\ J\} = \exp(-\psi)\ \{\nabla \times J - \nabla\psi \times J\} = 0$. For a consistent way of interpolating J and ψ it is therefore necessary that $\nabla \times J = \nabla\psi \times J$. We have not found a way to satisfy this with any of the usual box schemes.
A convergence theory for box schemes in n dimensions with general elements (other than triangles) seems to be extremely difficult to give. For the simplest triangular case it can be

found in Bank and Rose (1987).
Table 1 gives an impression of different methods with respect to the four criteria.

Table 1. Classification of methods

	FEM	upwind FEM	box method	mixed FEM
current conservation	0	0	1	1
upwinding	0	1	1	1
interpolation	1	1	0	0
convergence theory	1	1	0	1

ONE DIMENSIONAL MIXED FEM FOR $(e^{-\Psi} u_x)_x = f(x,u)$

It is advised to consult Brezzi (1987) while reading this section because we shall not repeat the excellent explanations given there. We use the same notation and concentrate here on the problem stemming from $f(x,u) \neq 0$, $f_u(x,u) \neq 0$. In fact, to understand the problem it suffices to take $f(x,u) = \nu u$.
So, let us consider the problem

$$(e^{-\Psi} u_x)_x = \nu u \quad \text{on } [0,1]$$

$$u(0) = u(1) = 1$$

with $\nu \geq 0$. Then, taking the basis functions as in Brezzi (1987), the discretised problem (Lagrange multipliers will be unnecessary !) is given by

$$(1) \qquad \begin{bmatrix} A & B \\ B^T & -\nu D \end{bmatrix} \begin{bmatrix} \sigma \\ u \end{bmatrix} = \begin{bmatrix} r_1 \\ r_2 \end{bmatrix}$$

D is a positive diagonal matrix because u is approximated by piecewise constants. Eliminating σ we get

$$(2) \qquad [-B^T A^{-1} B - \nu D]\, u = r_2 - B^T A^{-1} r_1$$

The solution of this problem (unlike the analytical solution) has negative entries if ν is sufficiently large.
The matrix A is a mass matrix, in the one dimensional case exactly the 'usual' FEM mass matrix. The integrals can be evaluated exactly giving a tridiagonal structure.
In the appendix an even simpler problem is presented to highlight the essence of the situation. It should be stressed that the oscillations which occur in the solution, unlike in conforming FEM, do not come from the matrix D (which is diagonal in this case, and non-diagonal for conforming FEM).
From (2) we find

$$[I + \nu(B^TA^{-1}B)^{-1}D]\ u = (B^TA^{-1}B)^{-1}\ [r_2 - B^TA^{-1}r_1]$$

For $\nu = 0$, although the matrix $B^TA^{-1}B$ is neither an M-matrix nor positive definite, the solution is well-behaved. For large enough ν this is not the case anymore.
A remedy for the stability problems is the lumping of the mass matrix A. This makes $B^TA^{-1}B + \nu D$ an M-matrix, which can easily be proven for the one dimensional case. In the appendix it is shown that this indeed improves the situation for the simple problem.
The lumping has to be performed in a special way to maintain the Scharfetter-Gummel scheme for the zero recombination, 1-d case. Lumping basically means choosing a Lobatto quadrature rule to evaluate the entries of A. This quadrature must have abcissae coinciding with the FEM nodes. In this case we (have to) use

$$\int_{x_i}^{x_{i+1}} e^{-\psi} f(x) \simeq f(x_i) \int_{x_i}^{x_{i+1/2}} e^{-\psi} + f(x_{i+1}) \int_{x_{i+1/2}}^{x_{i+1}} e^{-\psi}$$

With this quadrature rule, only the diagonal elements of A are unequal to zero:

$$a_{ii} = \tau_i(x_i)^2 \int_{x_{i-1/2}}^{x_{i+1/2}} e^{-\psi} = \int_{x_{i-1/2}}^{x_{i+1/2}} e^{-\psi}$$

The resulting one dimensional scheme gives exactly the usual box scheme if the integrals of $e^{-\psi}$ are evaluated exactly, assuming ψ to be piecewise linear.
It may be remarked that, in this scheme, current densities are piecewise linear, not piecewise constant as in the Scharfetter-Gummel scheme. However, an appropriate choice of quadratures for the integral of the recombination over elements exactly gives the Scharfetter-Gummel scheme, so this difference is not essential.

TWO DIMENSIONAL PROBLEM

In 2 dimensions, the situation is less simple. For rectangles we can still use the same lumping technique, giving exactly a diagonal matrix A. The quadrature then is defined by

$$\int_{x_i}^{x_{i+1}} \int_{y_i}^{y_{i+1}} e^{-\psi} f(x,y) \simeq \alpha_{i,i} f(x_i,y_i) + \alpha_{i,i+1} f(x_i,y_{i+1}) + \alpha_{i+1,i} f(x_{i+1},y_i) + \alpha_{i+1,i+1} f(x_{i+1},y_{i+1})$$

with

$$\alpha_{i,i} = \int_{x_i}^{x_{i+1/2}} \int_{y_i}^{y_{i+1/2}} e^{-\psi}$$

and similar definitions for the other α's. When $f(x,y)$ is the inner product of two mixed FEM basis functions τ_i and τ_j, this automatically gives a diagonal matrix A. As in the one-dimensional case, we then have that the Jacobian matrix is an M-matrix when solving $\Delta u = f(x,u)$ with $\partial f/\partial u \geq 0$.
For triangles and non-rectangular quadrilaterals we have not found a method to actually lump the matrix A into diagonal form. However we shall report, in a forthcoming publication, on quadrature rules for the integrals of $e^{-\psi} \tau_i . \tau_j$ that do maintain positive Slotboom variables (and carrier concentrations) for triangles of arbitrary angle, a scheme not yet publised as far as we know. For computational efficiency we then have to introduce Lagrange multipliers as described in Brezzi (1987).
The mixed finite element method with the quadrature described above has been used to simulate a 2-d bipolar transistor, the configuration of which is shown in Figure 1.

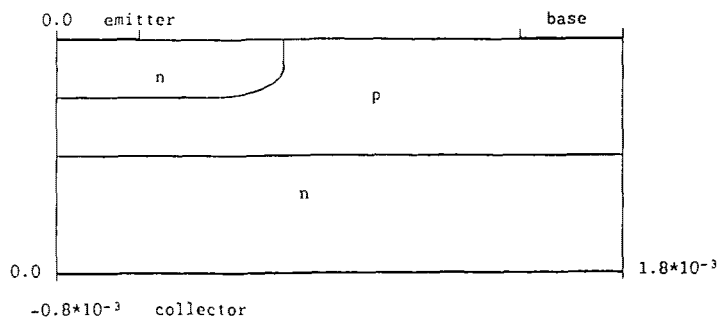

Fig. 1. Configuration of 2-d bipolar transistor

The bias conditions for the collector and base are 1 Volt and 0 Volt, respectively, whereas the emitter bias is stepped from -0.5 to -0.75 Volts. In order to investigate the convergence behaviour, the problem was solved on several grids. In Table 2 we summarize the results obtained, both for the box method and the mixed finite element method. Table 3 contains the relative 'errors' of the collector currents if the solution obtained on the 41 x 37 grid, calculated using the box scheme, is taken as the reference solution (it should be noted that this need not yet be close to the actual solution of the continuous problem).

Table 2. Currents in A/cm at the collector for the box and the mixed scheme.

V_{em}	box			mixed	
	12x10	21x19	41x37	12x10	21x19
-.50	2.099E-05	1.089E-05	1.020E-05	8.197E-06	9.777E-06
-.55	1.409E-04	7.477E-05	7.004E-05	5.661E-05	6.743E-05
-.60	9.323E-04	5.118E-04	4.797E-04	3.909E-04	4.648E-04
-.65	6.004E-03	3.485E-03	3.268E-03	2.696E-03	3.194E-03
-.70	3.644E-02	2.335E-02	2.187E-02	1.842E-02	2.155E-02
-.75	1.959E-01	1.469E-01	1.369E-01	1.182E-01	1.332E-01

Table 3. Relative error from the solution of the finest mesh (41 x 37, box).

V_{em}	box		mixed	
	12x10	21x19	12x10	21x19
-.50	1.059	0.068	0.196	0.041
-.55	1.012	0.068	0.192	0.037
-.60	0.944	0.067	0.185	0.031
-.65	0.837	0.066	0.175	0.023
-.70	0.666	0.068	0.158	0.015
-.75	0.431	0.073	0.137	0.027

From these tables it is clear that the mixed finite element method does produce much more accurate currents than the box method, for this problem. In the near future, it will be investigated whether this also is the case for other devices such as MOS transistors, lateral pnp transistors and thyristors.

CONCLUSION

The result presented in Brezzi (1987) does not yet deal with the zero order term in the device modelling equations (in fact, we have not found any discussion on the inclusion of a zero order term in the literature). In this paper we have shown that a choice of quadrature for the matrix A in the 1-d case and the 2-d rectangular case completely solve this problem. Surprisingly it is not the matrix stemming from the zero order term that causes the problems (this term is already lumped because the potentials are piecewise constant), but the matrix A. For triangles with arbitrary angles we have found a 'stable' scheme which will be reported on in a forthcoming publication.
The advantage of the embedding of the Scharfetter-Gummel scheme in the framework of mixed finite element methods is the fact that it gives a systematic way of dealing with the problems met, e.g. in terms of quadratures or choices of basis and test functions.

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APPENDIX

To illustrate the problems with the mixed finite element method and the necessity for lumping, we consider the following simple 1-d problem:

$$\text{(A1)} \qquad \begin{aligned} & u'' = \nu u \quad \text{on } (0,1) \\ & u(0) = u_l \quad , \quad u(1) = u_r \end{aligned}$$

where $\nu \geq 0$, $u_l \geq 0$, $u_r \geq 0$. We reformulate (A1) as follows:

$$\text{(A2)} \qquad \begin{aligned} & \sigma - u' = 0 \\ & \sigma' - \nu u = 0 \\ & u(0) = u_l \quad , \quad u(1) = u_r \end{aligned}$$

and apply the mixed finite element method for discretising this problem on a simple grid with only 4 nodes (uniformly spaced). Letting $\sigma = (\sigma_1, \sigma_2, \sigma_3, \sigma_4)^T$ be the vector of unknown 'fields' and $u = (u_1, u_2, u_3)^T$ be the vector of unknown 'potentials', we obtain the following system of equations:

$$\begin{bmatrix} A & B \\ B^T & D \end{bmatrix} \begin{bmatrix} \sigma \\ u \end{bmatrix} = \begin{bmatrix} r \\ 0 \end{bmatrix}$$

where:

$$A = \frac{1}{18} \begin{bmatrix} 2 & 1 & 0 & 0 \\ 1 & 4 & 1 & 0 \\ 0 & 1 & 4 & 1 \\ 0 & 0 & 1 & 2 \end{bmatrix} \quad , \quad B = \begin{bmatrix} -1 & 0 & 0 \\ 1 & -1 & 0 \\ 0 & 1 & -1 \\ 0 & 0 & 1 \end{bmatrix}$$

$$D = -\frac{\nu}{3} \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \quad , \quad r = \begin{bmatrix} -u_l \\ 0 \\ 0 \\ u_r \end{bmatrix}$$

Eliminating σ from the first set of equations (i.e. writing

$\sigma = A^{-1}r - A^{-1}Bu)$, we obtain the following system for u:

$$(A3) \qquad [-B^TA^{-1}B + D]\, u = -B^TA^{-1}r$$

We know that for the Laplace-problem, i.e. when $\nu = 0$, the resulting solution is stable. In order to investigate whether this is also the case for $\nu > 0$, we multiply (A3) by the matrix $-(B^TA^{-1}B)^{-1}$, and obtain:

$$(A4) \qquad [I_3 + \frac{\nu}{3}(B^TA^{-1}B)^{-1}]\, u = (B^TA^{-1}B)^{-1}B^TA^{-1}r$$

where I_3 is the 3 x 3 identity matrix. It is easy to check that:

$$B^TA^{-1}r = 18 \begin{bmatrix} 11/15\ u_l + 1/15\ u_r \\ -1/5\ u_l - 1/5\ u_r \\ 1/15\ u_l + 11/15\ u_r \end{bmatrix}$$

and

$$B^TA^{-1}B = \frac{18}{5} \begin{bmatrix} 6 & -3 & 1 \\ -3 & 4 & -3 \\ 1 & -3 & 6 \end{bmatrix}$$

Although $B^TA^{-1}B$ is not an M-matrix, its inverse is positive:

$$(B^TA^{-1}B)^{-1} = \frac{5}{18} \begin{bmatrix} 3/2 & 3/2 & 1/2 \\ 3/2 & 7/2 & 3/2 \\ 1/2 & 3/2 & 3/2 \end{bmatrix}$$

Thus, (A4) becomes:

$$\left[\begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} + \frac{5\nu}{54} \begin{bmatrix} 3/2 & 3/2 & 1/2 \\ 3/2 & 7/2 & 3/2 \\ 1/2 & 3/2 & 3/2 \end{bmatrix} \right] u = \frac{1}{6} \begin{bmatrix} 5\ u_l + u_r \\ 3\ u_l + 3\ u_r \\ u_l + 5\ u_r \end{bmatrix}$$

and it is easily verified that the second component of the solution vector is:

$$u_2 = \frac{1 - \mu}{5\mu^2 + 11\mu + 2}(u_l + u_r) \qquad \text{where} \quad \mu = \frac{5\nu}{54}$$

Thus, for $\nu > 54/5$, u_2 will be negative, and thus the scheme is not stable.
If we now use (lumped) quadrature for the integrals which occur in the matrix A, we obtain:

$$A = \frac{1}{6}\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 2 & 0 & 0 \\ 0 & 0 & 2 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$$

It is straightforward to verify that

$$B^T A^{-1} r = 6\begin{bmatrix} u_l \\ 0 \\ u_r \end{bmatrix}$$

and

$$B^T A^{-1} B = \begin{bmatrix} 9 & -3 & 0 \\ -3 & 6 & -3 \\ 0 & -3 & 9 \end{bmatrix}, \qquad (B^T A^{-1} B)^{-1} = \frac{1}{36}\begin{bmatrix} 5 & 3 & 1 \\ 3 & 9 & 3 \\ 1 & 3 & 5 \end{bmatrix}$$

Thus, in this case, $B^T A^{-1} B$ is an M-matrix. We can now repeat the same procedure as before to obtain the second component of the solution:

$$u_2 = \frac{1}{2}\frac{u_l + u_r}{36\mu^2 + 15\mu + 1} \qquad \text{where} \quad \mu = \frac{\nu}{108}$$

which is always non-negative, thus proving that the scheme is stable in this case.