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Generalisations of the box method using the mixed finite element method

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In this paper we present the box method as a mixed finite element method with a suitable quadrature. This interpretation provides a way of defining a continuous current density for the box method. Also, in this way, higher order box methods can be derived which are suitable for application to the discretisation of the semiconductor device problem.

Introduction

The box method is the most widely used discretisation method for the semiconductor device problem. The main reason for this is that it yields discrete current conservation and utilizes 'upwinding' by using the Scharfetter-Gummel expressions for the current densities. Another reason for its use is that solutions of the resulting discrete systems satisfy the maximum principle (positive carrier concentrations !) if the underlying triangular mesh is of Delauney-type. A drawback of the method is that it does not yield a continuous expression for the electric field and the current densities: only components along the edges of the meshes are given. Because of the latter, one could be tempted to think about the application of finite element methods to the discretisation of the semiconductor problem. Unfortunately, it is wellknown that ordinary finite element methods, although frequently used in other disciplines, do not possess any of the properties listed above (although 'upwinding' can be achieved, for example, by using the streamline upwind methods proposed by Hughes and Brooks; cf. [1]).
Recently, mixed finite element methods have been proposed for the discretisation of the semiconductor device problem (cf. [2]). These methods differ from ordinary finite element methods in several respects but, most importantly, they yield Scharfetter-Gummel type expressions for the current densities in a natural way and resulting solutions satisfy discrete current conservation. Unfortunately, the mixed finite element methods proposed have been shown to be rather unstable (cf. [3]). For example, the solution of Poisson's equation will lead to unphysical oscillations in the electric potential ψ, even for triangulations without any obtuse angle. The same holds for the solutions of the continuity equations whenever a non-zero recombination term is present. Furthermore, if obtuse angles occur, the method will always be unstable, even when the underlying mesh is of

Delauney-type. Although attempts have been undertaken to remedy this situation (cf. [3] where quadrature rules are suggested, and [4] where new elements are introduced), the latter problem has not been resolved so far.
In the following sections we present a class of mixed finite element methods which can be used on Delauney-type triangular meshes. The box method is shown to be equivalent to the lowest-order element in this class. Because of this, a recipe can be given for producing a continuous expression for the electric field and the current densities from the solutions obtained with the box discretisation. Furthermore, higher order extensions of the box method are immediate consequences of this new class of mixed finite element methods.

Mixed finite element formulation of the semiconductor problem

In this paper we consider the following system of equations:

$$\nabla \cdot \mathbf{J} = R(u) \tag{1}$$

$$\mathbf{J} = a\nabla u \tag{2}$$

on the region $\Omega \subset R^2$, with suitable boundary conditions. Remark that Poisson's equation as well as the continuity equations for holes and electrons can be written in the above form. The mixed variational formulation of the problem (1)-(2) is: find $(u, \mathbf{J}) \in L^2(\Omega) \times H(div;\Omega)$ such that

$$\int\int_\Omega \phi\nabla \cdot \mathbf{J} dO = \int\int_\Omega \phi R(u) dO \qquad \forall \phi \in L^2(\Omega) \tag{3}$$

$$\int\int_\Omega a^{-1}\mathbf{J} \cdot \tau dO = -\int\int_\Omega u\nabla \cdot \tau dO \qquad \forall \tau \in H(div;\Omega) \tag{4}$$

where

$$H(div;\Omega) = \{\tau \in (L^2(\Omega))^2 | \nabla \cdot \tau \in L^2(\Omega)\}$$

It is wellknown that the problem (3)-(4) has a unique solution $(u, \mathbf{J}) \in L^2(\Omega) \times H(div;\Omega)$, which is the weak solution of (1)-(2).
The mixed discretisation now consists of choosing suitable finite dimensional subspaces $V_h \subset L^2(\Omega)$ and $W_h \subset H(div;\Omega)$ and to restrict the problem (3)-(4) to these subspaces: find $(u_h, \mathbf{J}_h) \in V_h \times W_h$ such that

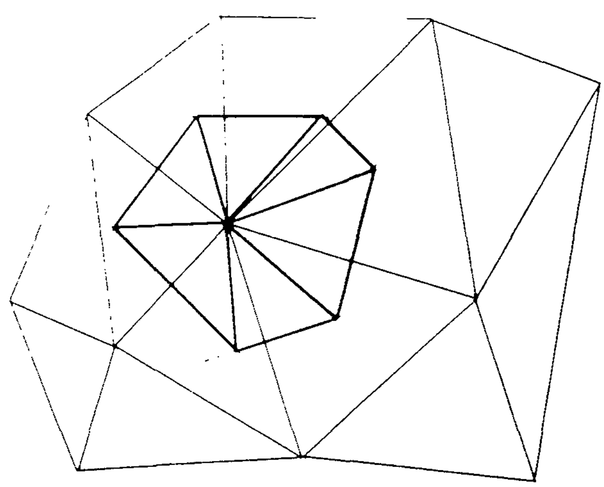
$$\int\int_\Omega \phi_h\nabla \cdot \mathbf{J}_h dO = \int\int_\Omega \phi_h R(u_h) dO \qquad \forall \phi_h \in V_h \tag{5}$$

$$\int\int_\Omega a^{-1}\mathbf{J}_h \cdot \tau_h dO = -\int\int_\Omega u_h\nabla \cdot \tau_h dO \qquad \forall \tau_h \in W_h \tag{6}$$

The remaining problem is to construct suitable subspaces V_h and W_h. The Brezzi-Babuska conditions (cf. [5]) give sufficient (but not necessary) conditions on these subspaces in order to guarantee uniqueness of the solution of (5)-(6). For triangular meshes, a class of finite element spaces have been proposed which satisfy these conditions: the so-called *Raviart-Thomas elements* (cf. [6]). The latter are widely used in the context of mixed finite element discretisations.

Equivalence of the box method and a low-order mixed finite element method

In view of the foregoing we now assume that the region Ω has been triangulated and that the mesh is of Delauney-type. Because of the latter assumption we can associate, with each mesh point, a so-called *box* which is constructed by intersecting the midperpendiculars of the edges of the triangles. These boxes are sometimes termed the *Voronoi polygons.* Using these we construct a new triangulation Π_h of the domain Ω: divide each of the Voronoi-polygons into triangles in such a way that the vertices of these triangles are the centre of the polygon and two neighbouring extremal points on the boundary of the polygon. Thus, two of the three vertices of these new triangles are points of intersection of midperpendiculars. Figure 1 explains the construction graphically.



New triangulation

We now consider the mixed finite element method which makes use of the lowest-order RT-elements for the approximation of the fields and current densities on the triangulation Π_h, and of the piecewise constant approximations of the potentials on a box. In order to analyse this method, we introduce the following notation. For each mesh point (x_i, y_i) we let B_i be the box around it and T_i^k, $k = 1, ..., n_i$ the triangles of Π_h which are contained in B_i. Thus, we have that $\Pi_h = \cup_i \cup_{k=1}^{n_i} T_i^k$.
We define

$$V_h = \{u_h \text{ is constant on each box}\}$$

This space is spanned by the basis functions ϕ_i, which are 1 on B_i and 0 on all other boxes. Remark that these functions are not continuous over the box edges. Furthermore, we let W_h be the space of lowest-order Raviart-Thomas elements on the triangles of Π_h, i.e. W_h is the space spanned by the vector basis functions τ_j, which have a constant normal component equal to 1 along edge j of a triangle in Π_h and zero normal component along each of the other edges. Thus, the support of τ_j extends over two triangles. On each of these triangles, τ_j is of the form

$$\tau_j(x, y) = \frac{\pm l_j}{2area(T)} \begin{pmatrix} x - x_{i(j)} \\ y - y_{i(j)} \end{pmatrix}$$

in which $(x_{i(j)}, y_{i(j)})$ is the vertex of the triangle T opposite the edge j, and l_j the length of edge j.

We will now show that the box method is equivalent to this mixed finite element method when a suitable quadrature is chosen. To this end, set up the mixed FEM equation of the form (5) for the box B_i:

$$\int\int_{B_i} \nabla \cdot \mathbf{J}_h dO - \int\int_{B_i} R(u_h) dO \tag{7}$$

Using Green's theorem, the fact that $u_h = u_i$ on B_i, and the property of the lowest-order RT-elements that their normal components along an arbitrary line are constant, we obtain:

$$\sum_{k=1}^{n_i} l_i^k J_i^{k,out} - area(B_i) R(u_i) \tag{8}$$

where l_i^k is the length of the edge of T_i^k which coincides with the outer edge of the box B_i and $J_i^{k,out}$ is the normal component of $\mathbf{J}_h$ along that edge.
Next we use equation (6) for the τ_j which correspond to edges which coincide with the outer edges of B_i. For each triangle $T_i^k \in B_i$ there is (except at the boundary) another triangle $T_{i'}^{k'} \in B_{i'}$ which, together, form the support of τ_j. Then we have:

$$\int\int_{\Omega} a^{-1} \mathbf{J}_h \cdot \tau_j dO = \int\int_{T_i^k \cup T_{i'}^{k'}} a^{-1} \mathbf{J}_h \cdot \tau_j dO$$

$$\sim \frac{1}{dist(i,i')} \{ \int_{(x_i,y_i)}^{(x_{i'},y_{i'})} a^{-1} ds \} \; \mathbf{J}_h(\frac{x_i + x_{i'}}{2}, \frac{y_i + y_{i'}}{2}) \cdot \int\int_{T_i^k \cup T_{i'}^{k'}} \tau_j dO$$

The latter integral can be shown to be equal to

$$\frac{\pm l_j}{3} \begin{pmatrix} x_{i'} - x_i \\ y_{i'} - y_i \end{pmatrix}$$

Since T_i^k and $T_{i'}^{k'}$ are congruent, it then follows that

$$\int\int_{\Omega} a^{-1} \mathbf{J}_h \cdot \tau_j dO \sim \pm \{ \int_{(x_i,y_i)}^{(x_{i'},y_{i'})} a^{-1} ds \} \; \frac{l_i^k}{3} J_i^{k,out}$$

The treatment of the right hand side of (6) is slightly more complicated. Since the τ_j have constant divergence on each triangle, we may replace the right hand side of the weak formulation:

$$\int\int_{T_i^k \cup T_{i'}^{k'}} u \nabla \cdot \tau_j dO \sim l_i^k \; (u(z_i^k) - u(z_{i'}^{k'}))$$

where z_i^k and $z_{i'}^{k'}$ are the centres of gravity of T_i^k and $T_{i'}^{k'}$, respectively. Using interpolation we obtain:

$$\int\int_{T_i^k \cup T_{i'}^{k'}} u \nabla \cdot \tau_j dO \sim \frac{l_i^k}{3} \; (u(x_i, y_i) - u(x_{i'}, y_{i'}))$$

Thus, the right hand side of (6) can be approximated by

$$\frac{l_i^k}{3}(u_{i'} - u_i)$$

Combining the obtained approximations, we finally get:

$$J_i^{k,out} = \frac{u_{i'} - u_i}{\int_{(x_i,y_i)}^{(x_{i'},y_{i'})} a^{-1} ds} \tag{9}$$

Equations (8) and (9) yield the box scheme discretisation ! Thus, we have shown that the latter can be obtained by approximating the integrals in the lowest order RT-method described above.

Interpolations for the fields and current densities obtained using the box method

The equivalence of the box method and a low-order mixed finite element method opens possibilities for obtaining expressions for the fields and current densities inside the elements (remember that the box method only provides components of these on the edges). We will describe two ways of doing this.

We can use equations (5) and (6) for the test functions which have not yet been used in the above. More specifically: for each box B_i, we can set up a system of n_i equations for the n_i remaining unknowns, namely the normal components of $\mathbf{J}_h$ along the inner edges of the box. In the resulting set of equations, the values of the components of $\mathbf{J}_h$ along the outer edges of B_i occur, for which we can substitute expression (9), as well as the values u_i which have already been determined. Remark that these calculations can all be done *locally*, i.e. this can be considered as a postprocessing exercise. Having obtained the values for the n_i remaining unknowns for the box B_i, we can give an expression for $\mathbf{J}_h$ inside the box: thus we have produced an $H(div;\Omega)$-function (with continuous normal components over the edges of the triangles T_i^k). This is important for adaptive runs, or for applications in which the fields and/or the current densities are coefficients in another equation (e.g. the temperature equation, or the hydrodynamic equations). In the lecture we will give an example of this.

The method just described for obtaining the fields and current densities inside the box does guarantee current conservation on the boxes, but not on the triangles of Π_h. The latter can be achieved by considering a mixed finite element method on each box B_i, in which we now introduce piecewise constant potentials on the triangles of Π_h. Thus, there are $2n_i$ remaining unknowns per box. In order to have a well-determined system of equations for these, we impose the extra restriction that the average of the newly introduced u_i^k (value of potential on T_i^k) is equal to the value u_i calculated in the centre of the box:

$$u_i = \frac{\sum_{i=1}^{n_i} area(T_i^k) u_i^k}{area(B_i)}$$

This second way of interpolating the results obtained by the box method does guarantee current conservation on the triangles of Π_h, and yields another approximation for the potentials.

Higher order (box) methods

In the previous sections we have shown how the box method may be considered as a mixed finite element method with a suitable quadrature rule. This can be exploited further to develop higher-order box methods: the spaces V_h and W_h may be chosen to contain higher order basis functions. Because the space V_h will always contain the piecewise constant functions, current conservation is guaranteed for all higher order mixed FEM of this type. This will be discussed in more detail in the lecture.

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