Basis Functions matching Tangential Components on Element Edges

J.S. van Welij

Nederlandse Philips Bedrijven BV

SUMMARY

This article describes a way to construct a vector function which matches given constant tangential components on all the edges of a finite element mesh. For this purpose, a set of vector basis functions is defined, each belonging to an edge of the mesh. The formulae are given for hexahedra, tetrahedra, quadrilaterals and triangles.

The idea is applied to the continuity equations of the semiconductor model, here formulated as div(a grad u) = R. The result is a method which reduces in 1-D to the Scharfetter-Gummel method. For the special case a = constant, a normal finite element method is obtained. In the limit for vanishing element size, the method converges to standard FEM.

The observation is used that it has definite advantages to consider J = a grad u rather than grad u as constant between two mesh points. This allows to express the tangential component along each mesh edge accurately in the coefficients and unknowns at the ends of the edge. Existing methods of the pipe space type express the equation div J = 0 in these discrete edge values. This leads to severe restrictions on the shapes of the allowed elements.

After forming a function for J which matches the edge values and is defined in the wole element, the condition on the divergence can be formulated in its standard variational form.

1. INTRODUCTION

The continuity equations of the semiconductor model, can be formulated in the form:

$$\mathrm{div}(a \ \mathrm{grad}\ u) = R$$

The function a(x) may vary rapidly, but is positive for any x. For the 1-D case it has been pointed out [1] that it is better to approximate J = a grad u as constant between two mesh points, than grad u, as would follow from standard linear finite elements.
Assuming that log(a) can be well approximated by a linear function, J can be evaluated without having to approximate grad u accurately. This allows a relatively coarse mesh to be used.

In more dimensions, there is not an immediate extension. Ideally the 1-D approach should be applied in the direction of the vector grad a [2,3]. However, since this leads to practical problems, the general approach is to apply the idea to the tangential components of J on the edges in the mesh [4].

One approach is to leave the value of J undefined inside the elements and consider the so called pipe space, consisting of all edges in the mesh, each of which has an associated width. The condition on the divergence of such a discretely defined J is formulated as a weighted sum of all edges ending in a vertex. This leads to unpleasant restrictions on the element shape. It seems that for triangles all angles must be sharp and for quadrilaterals the vertices of each one must lie on a circle [5].

Another proposition [6] is to define the current inside the element differently for each test function. Although this can be shown to converge, it leaves an uneasy feeling.

The following sections show the full vector J can be interpolated, such that the tangential components match exactly the ones formulated through 1-D integration along each edge. The divergence condition can then weakly be imposed in the normal way. As weighting functions, the normal nodal functions are used and integration by parts is performed. A box scheme is also possible [3], but not considered here.

For the interpolation, vector basis functions are needed, defined within an element, which have a constant tangential component along one edge and which are normal to all other edges in the element.
The construction of the functions is such that gradients of the nodal functions can be represented exactly. Actually the gradients of the nodal basis functions are just the sum of the basis functions for the edges that end in the node, with a possible minus sign if they are oriented away from the node.

It will be shown that in 3-D not only on the edges, but actually on the whole surfaces, the tangential components are continuous across element boundaries. Normal components are not continuous, but this is not worse than for standard finite elements.

The functions will be defined for hexahedra, tetrahedra, quadrilaterals, and triangles. A more theoretical background to the idea of partially continuous elements is given in [7]. The formulae for the functions on tetrahedra can be found in [8]. The extension to hexahedra and an application of the elements to the calculation of eddy currents can be found in [9].

In the present article, basis functions are considered with constant components along edges. An immediate extension is to have linearly varying components.

Along the same lines as done here for given tangential components on the edges, a set of vector basis functions can be constructed to match given currents passing through the faces in normal direction. The form is given as a remark at the end.

2. THE FORMULATION

To complete the basics for the formulation, set $v = \ln a$. With a subscript i and j to denote the various values at the end points of the 1-D interval, the approximation of J by a constant and v by a linear function results in:

$$\exp\left(v_i + \frac{x - x_i}{x_j - x_i} (v_j - v_i) \right) (\text{grad } u) = J$$

Division by the exponential, integration from x_i to x_j and some rearranging gives:

$$J = - \frac{v_j - v_i}{\exp(-v_j) - \exp(-v_i)} \quad \frac{u_j - u_i}{x_j - x_i}$$

Here only values at the end points of the interval occur and the transition to 2-D or 3-D can be made. When reading for J its tangential component on an element edge and interpreting $x_j - x_i$ as the length of the edge, this formula remains valid.

Now for each edge, a constant A_{ij} is defined, where this time i and j stand for the end points of the edge:

$$A_{ij} = - \frac{v_j - v_i}{\exp(-v_j) - \exp(-v_i)} = \frac{- \ln(a_j/a_i)}{1/a_j - 1/a_i}$$

It can be shown that the value of A_{ij} is always between a_i and a_j and that $A_{ij} = A_{ji}$. The value can be extended by continuity if $a_i = a_j$, in which case $A_{ij} = a_i = a_j$.

In the next section, for each edge a basis function W_{ij} is defined, which has a constant tangential component on the edge in question and a tangential component 0 on all other edges in the mesh. Using these functions, write:

$$J(x) = \sum_{\text{edges}} (A_{ij} \; W_{ij}(x) \; (u_j - u_i))$$

The division by the length of the edge is taken care of by the normalisation of the functions W_{ij}, which is such that they integrate to one along their edge. The definition of the edge basis function orientates the edge. Taking the reversed direction, changes the sign, so: $W_{ji} = -W_{ij}$.

Now the equation left is just div J = R. After multiplying by the standard weighting functions w_i, belonging to the vertices in the mesh, and a formal integration by parts, this becomes:

$$\int J \cdot \text{grad } w_i \, dV = \int R \, w_i \, dV$$

For each w_i, this is an expression in the u_j at the nodes.

If the A_{ij} and R are really known, this leads to a linear system. The resulting matrix is generally not symmetric. Because of the implicit upwind character of the formulation, this is not surprising.

In the full semiconductor model, the functions a and R may depend on the field, the currents or the concentrations. In that case a set of non linear equations is obtained. If the A_{ij} are determined simultaneously from the field equation, a coupled system arises.

For the 1-D case this formulation becomes the same as the well known Gummel-Scharfetter scheme.

For the case a = constant, A_{ij} = a for all edges, and the sum can be rearranged:

$$\sum_{\text{edges}} (W_{ij}\,(u_j - u_i)) = \sum_{\text{vertices}} (u_j \sum_{\substack{\text{edges of}\\ \text{vertex}}} W_{ij})$$

The last sum runs over all edges ending in the vertex and by definition $W_{ij} = -W_{ji}$. As shown in the next section, it so happens that the last sum is precisely grad w_j, where w_j is the normal basis function for the vertex in question. As a consequence J is the sum of u_j grad w_j for this special case, which is the standard finite element form.

Also, if the mesh size goes to zero, every A_{ij} approaches the local value of a, and the method converges to the standard finite element method.

3. THE VECTOR BASIS FUNCTIONS FOR EDGES

3.1 Hexahedra

3.1a Definition

Consider isoparametric hexahedra, that is, each element is seen as the image of the unit cube under a trilinear mapping x(s), where $x = (x_1, x_2, x_3)$ and $s = (s_1, s_2, s_3)$ are three dimen sional vectors (Fig. 1). The mapping is defined by means of functions wi belonging to the corners. The point (1,1,1) on the unit cube has:

$$w_8(s) = s_1\ s_2\ s_3$$

The others are obtained by forming all combinations under replacement of some s_i by $(1-s_i)$. If $P_1,\ldots,P_8$ are the corners of the hexahedron, the actual mapping is written as:

$$x(s) = \sum (w_i(s)\ P_i)$$

Restricted to the element, also the inverse mapping $s(x)$ exists. The surface $s_3 = 1$ for example is the top of the element. So evidently grad s_3 is normal to the top face.

First define the vectors:

$$V_i = dx(s)/ds_i$$

Since the functions $x(s)$ are trilinear polynomials in s, the V_i are bilinear and are readily calculated. Strictly speaking, they are defined on the unit cube, but the mapping allows to interpret them on the hexahedron.

Geometrically the vectors V_i can be interpreted as connecting the points on the opposite faces $s_i = 0$ and $s_i = 1$, which have the both other s_j the same. In every point on an edge of the element in direction s_i, V_i is the vector describing that edge.

The Jacobian matrix ds/dx, which has grad s_i as rows, is the inverse of dx/ds, which has V_j as columns, so:

$$V_j.(\text{grad } s_i) = \delta_{i,j}$$

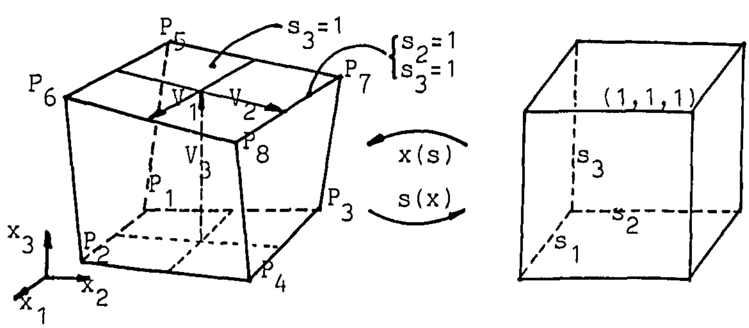

Fig. 1. The mapping $x(s)$ transforms the unit cube into the hexahedron. Its inverse $s(x)$ is a vector function on the original space. The equation $s_3(x) = 1$ describes the top face.

This delivers an explicit expression for grad s_i. For example, with "x" standing for the vector cross product and "." for the vector inner product:

$$\text{grad } s_1 = (V_2 \times V_3)/((V_2 \times V_3).V_1)$$

Cyclic permutation gives the others. The validity of these expressions is easily checked. Note that the denominator is actually the Jacobian of the transformation and has, in any point the same value for all three gradients.

The vector basis functions belong to the edges. The tangential component of the function for a certain edge must vanish on all other edges. The normalisation is chosen such that the integral of the function along the edge is one.
Now the basis function for the edge where $s_2 = 1$ and $s_3 = 1$, so running along s_1, is defined as:

$$W(x) = s_2(x)\, s_3(x) \text{ grad } s_1(x)$$

On both faces $s_1 = 0$ (front) and $s_1 = 1$ (back) this vector function is normal to the face, so it does no contribute to the tangential components there; this includes all edges not running in direction s_1. On the edges in direction s_1 to which this function does not belong, the product $s_2\, s_3$ is always zero, so the whole function vanishes. On its own edge, $s_2\, s_3 = 1$ and the tangential component is found by multiplication by $V_1/||V_1||$. The denominator in the expression for grad s_1 is cancelled and the result is $1/||V_1||$, which is constant along the edge.

3.1b Continuity across element faces

With the help of the above, the proof of continuity across element faces follows easily. On all faces not containing the edge in question, the tangential components have been shown to vanish. From the remaining two faces, take for example the top face and the same W as before. The unit normal is parallel to grad s_3:

$$n = (V_1 \times V_2)/||V_1 \times V_2||$$

Strictly speaking, the decomposition of a vector into normal and tangential components is given by $W = n(W.n) + n x (W x n)$. As usual just Wxn is interpreted here as tangential component. This is justified by the observation that continuity of nx(Wxn) across a surface is equivalent to continuity of Wxn. Substitution gives:

$$Wxn = s_2\, s_3 \frac{(V_2 \times V_3)}{(V_2 \times V_3)\cdot V_1} \times \frac{(V_1 \times V_2)}{||V_1 \times V_2||}$$

$$= s_2\, s_3 \frac{((V_2 \times V_3)\cdot V_2)V_1 - ((V_2 \times V_3)\cdot V_1)V_2}{((V_2 \times V_3)\cdot V_1)\ ||V_1 \times V_2||}$$

$$= -\ s_2\, s_3\, V_2 \ /\ ||V_1 \times V_2||$$

All quantities appearing in this expression are continuous going through the top face to the next element. By simple symmetry all the other cases follow immediately.

3.1c The relation between scalar and edge basis functions

The notation used makes it surprisingly easy to establish the relation between the standard nodal basis functions and the edge basis functions.

The ordinary scalar test function for the point $s_1 = s_2 = s_3 = 1$ is given by $w_8(x) = s_1(x)\ s_2(x)\ s_3(x)$. Its gradient is:

$$\begin{aligned} \text{grad } w_8 &= s_2\, s_3 \text{ grad } s_1 + s_1\, s_3 \text{ grad } s_2 + s_1\, s_2 \text{ grad } s_3 \\ &= W_{78} + W_{68} + W_{48} \end{aligned}$$

where W_{78}, W_{68} and W_{48} belong to the three edges ending in the point considered. The definition of the W orientates the edges. Edges beginning in a point appear with a minus sign.

3.2 Tetrahedra

Because all occurring functions are linear, they can be described directly in the real coordinates. All reasoning for consistency is straightforward in the vectorial notation used. The definition of the functions for this case as well as for triangles, can also be found in [8].

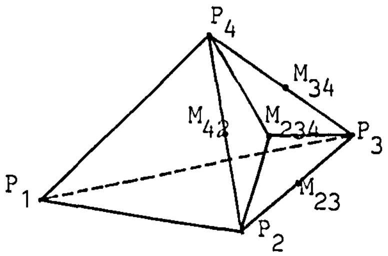

Fig 2. A tetrahedron, with some notations; P_i are the corners, V_{ij} the edge vectors, M_{ij} the midpoints of the edges and M_{ijk} the centres of the faces.

The corners of the tetrahedron are denoted by P_1,P_2,P_3,P_4 and the position where the functions are evaluated by X. Some more notation is used to make the formulae look symmetric (Fig. 2). They are the centres of gravity of the edges and faces, the edge vectors and the volume:

$$M_{ij} = (P_i + P_j) / 2 \qquad M_{ijk} = (P_i + P_j + P_k) / 3$$

$$V_{ij} = P_j - P_i \qquad V = V_{12} \times V_{23} \cdot V_{34} / 6$$

The basis function for the edge from point 1 to 2 is:

$$W_{12} = V_{34} \times (X - M_{34}) / 6V$$

The others are similar, where V_{ij} or V_{ji} has to be chosen to determine the orientation correctly. By definition $W_{ij} = -W_{ji}$.

For the proof of the demanded properties consider W_{12} for the edge from point P_1 to point P_2. For any point X in the faces (P_1,P_3,P_4) and (P_2,P_3,P_4) the cross product delivers a vector normal to the face. This includes all edges but (P_1,P_2), where the tangential component times the length of the edge is:

$$W_{12} \cdot V_{12} = V_{34} \times (X - M_{34}) \cdot V_{12} / 6V$$

For any X on edge (P_1,P_2) this is 1.

The scalar basis function for node 1 and its gradient can be written as:

$$w_1 = (X - M_{234}) \cdot V_{23} \times V_{34} / 6V$$

$$\text{grad } w_1 = V_{23} \times V_{34} / 6V = W_{21} + W_{31} + W_{41}$$

The proof of the last equality is most easily seen by geometric interpretation. The length of $V_{23} \times V_{34}$ is just twice the area of face (P_2,P_3,P_4). This triangle can be split by connecting the centre to the corners. The double area becomes:

$$V_{23} \times (M_{234} - M_{23}) + V_{34} \times (M_{234} - M_{34}) + V_{42} \times (M_{234} - M_{42})$$

Now realise that $V_{23} + V_{34} + V_{42} = 0$, and add this sum multiplied by $X - M_{234}$ to the previous expression, effectively replacing M_{234} by X.

3.3 Quadrilaterals

The functions for quadrilaterals can be produced from the ones for hexahedra by simply setting $s_3 = 1$ and $V_3 = e_3$, the unit vector perpendicular to the plane. The forms and their relations are written out completely here. The four corners and the edges are counted cyclically, although in a program it would probably be simpler to orientate all edges along the parametric main directions.

$$\begin{array}{lll}
W_{12} = (1-s_2)\text{grad } s_1 & w_1 = (1-s_1)(1-s_2) & \text{grad } w_1 = W_{41} - W_{12} \\
W_{23} = s_1 \text{ grad } s_2 & w_2 = s_1 (1-s_2) & \text{grad } w_2 = W_{12} - W_{23} \\
W_{34} = -s_2 \text{ grad } s_1 & w_3 = s_1 s_2 & \text{grad } w_3 = W_{23} - W_{34} \\
W_{41} = -(1-s_1)\text{grad } s_2 & w_4 = (1-s_1) s_2 & \text{grad } w_4 = W_{34} - W_{41}
\end{array}$$

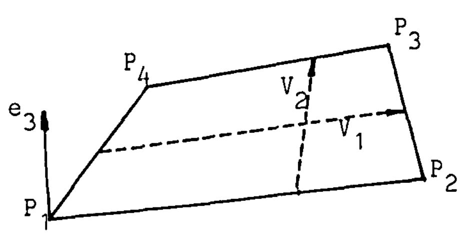

Fig 3. A quadrilateral with the vectors V_1 and V_2 in a generic point. The edges are counted cyclically. E_3 is the unit normal to the plane.

3.4 Triangles

Here the corners and edges are counted cyclically. With E the unit vector normal to the triangle, A its area and the same notation as for tetrahedra, the function for the edge from point P_1 to P_2 is:

$$W_{12} = E \times (X - P_3) / 2A$$

The standard basis function for node 1 and its gradient are:

$$w_1 = (X - M_{23}) \cdot E \times V_{23} / 2A$$

$$\text{grad } w_1 = E \times V_{23} / 2A = - W_{12} + W_{31}$$

The proofs of all properties are trivial.

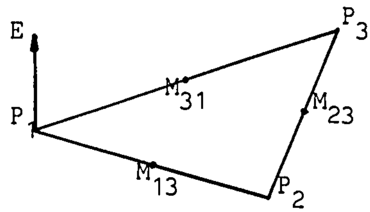

Fig 3. A triangle, with some notations; P_i are the corners, V_{ij} the edge vectors, M_{ij} the midpoints of the edges. E denotes the unit normal to the plane.

The complete form for J within an element is for this simplest case:

$$J = A_{12} W_{12} (u_2-u_1) + A_{23} W_{23} (u_3-u_2) + A_{31} W_{31} (u_1-u_3)$$

The separate coefficients for u_1, u_2 and u_3 are:

$$A_{31} W_{31} - A_{12} W_{12}, \quad A_{12} W_{12} - A_{32} W_{32}, \quad A_{23} W_{23} - A_{31} W_{31}$$

The gradients of the weighting functions w_1, w_2 and w_3 are:

$$W_{31} - W_{12}, \qquad W_{12} - W_{32}, \qquad W_{23} - W_{31}$$

From this example can be seen that generally the matrix is only symmetric if all three A_{ij} are equal.

4. FURTHER REMARKS

Making some vertices of a hexahedron coincide, other shapes, such as prisms and pyramids can be created. In this process the mapping x(s) becomes singular at those vertices. However, the integrals in the variational formulation are still defined and by using internal integration points, such as the Gauss points, practical problems are circumvented. This can also be applied to the edge elements. All functions associated with edges that have been reduced to length 0 must be dropped.

A direct extension to higher order exists. Instead of a constant component along each edge, a linealy varying component is taken. Each edge basis function is split into two, belonging to both ends of the edge. For hexahedra or quadrilaterals, they are obtained from the simple edge function by multiplication by s_i and $1 - s_i$, where i is the applicable mesh direction. For tetrahedra or triangles the multipliers are the scalar basis functions for both ends.

Following the same lines of reasoning as used before for tangential components on edges, another set of vector basis functions can be defined for normal components on the faces of the element.

For the hexahedron top face, where $s_3 = 1$, using the same notation as in section 3.1, the function is:

$$W = s_3 \text{ (grad } s_1 \times \text{grad } s_2)$$

$$= s_3 V_3 / ((V_1 \times V_2) . V_3)$$

The integral of the normal component over the face to which the function belongs is just 1. A geometric interpretation is that the vector is just in the direction of the isoparametric coordinate line from a point on one face to the corresponding point on the opposite face and the length diminishes linearly from one to the other.

If six net currents are defined on the faces with zero sum, the composition appears to be exactly non divergent in the whole volume.

5. REFERENCES

[1] SCHARFETTER, D.L. and GUMMEL, H.K.
"Large-signal analysis of a silicon Read diode oscillator"
IEEE Transactions on Electronic Devices, 1969 ED-16 p64.

[2] POLAK, S.J. and SCHILDERS, W.
"A Characteristics Box Scheme for the Singularly perturbed Continuity Equation"
Simulation of Semiconductor Devices and Processes, Pineridge press, 1984 p240.

[3] POLAK, S.J., DEN HEIJER, C., SCHILDERS, W., MARKOWICH, P.
"Semiconductor Device Modelling from the Numerical Point of View"
Int. Journal on Numerical Methods in Engineering, to appear.

[4] MOCK, M.S.
"Analysis of a Discretization Algorithm for Stationary Continuity Equations in Semiconductor Device Models, II"
Compel, 1984 vol 3 no 3 p 137.

[5] MOCK, M.S.
"Quadrilateral Elements and the Scharfetter-Gummel Method"
Simulation of Semiconductor Devices and Processes, 1984, p298.

[6] ZLAMAL, M.
"A Finite Element Solution of the Fundamental Equations of Semiconductor Devices, I"
Mathematics of Computation, to appear.

[7] NEDELEC, J.C.
"Mixed Finite Elements in R3"
Numerische Mathematik, 1980.

[8] BOSSAVIT, A.
"Two Dual Formulations of the 3-D Eddy Current Problem"
Compel, 1985 vol 4 nr 2 p 103.

[9] VAN WELIJ, J.S.
"Calculations of Eddy Currents in terms of H on hexahedra"
IEEE Transactions on Magnetics, 1985 vol 21 nr 6 p2239.