Technical Article

The Mystery and Magic of Whitney Elements - An Insight in their Properties and Construction

Introduction

The introduction and extensive application of vector finite elements is considered one of the most important recent advances in electromagnetic field computation. A large number of publications, either theoretical or applied, on this subject, seems to result in some common observations about their advantages over scalar elements. For example, the property of tangential continuity across interface boundaries provides a correct representation of electromagnetic fields, especially when sharp corners or material discontinuities are involved. On the other hand, the property of proper modelling of the nullspace of the curl operator, in other words the consistent modelling of irrotational fields, ensures the elimination of spurious modes, which do not only contaminate the solutions of eigenvalue problems, but are responsible for corruptions (or "vector parasites") in the analysis of deterministic problems as well, when conventional, scalar elements are used. Furthermore, on the level of implementation, the simplicity and clear geometric representation of degrees of freedom, makes it easy to enforce boundary conditions and the property of tangential continuity.

However, the correct topological and geometrical representation of electromagnetic fields via vector finite elements is achieved with the cost of low rates of convergence. Nevertheless, since this drawback can be attributed to the existence of zero eigenvalues in modal electromagnetic field problems, it seems to be an inherent property of Maxwell's equations, rather than a disadvantage of the vector finite element itself.

Since the introduction of edge elements [1], [2], which, from a mathematical point of view, are considered first order Whitney 1-forms, much work has been done to implement them in several electromagnetic field and potential formulations. But despite their extensive application and use, their generalisation from the first order to higher orders has always been an open problem, since there seems to be a lack of a common ground and a straightforward methodology to produce higher order Whitney forms. However, several approaches to the construction of higher order vector finite elements, either tetrahedral [3]-[5], or hexahedral [6]-[8], can be found in the literature. Each approach seems to emphasise on different aspects of the Whitney element theory and results in different element expressions. Sometimes, the proposed scheme is not clearly explained and the real nature of vector finite elements is not evident through its development.

This paper presents a generalised and unified theory of Whitney elements, which results in a systematic methodology for the construction of both tetrahedral and hexahedral vector finite elements. Through the proposed theory, a step-by-step enforcement of the fundamental properties of Whitney elements is adopted, thus providing an insight into their philosophy and nature. For instance, the choice of conforming degrees of freedom, that have a clear geometrical interpretation is very critical, as far as implementation parameters are concerned. Furthermore, the property of decoupling between the degrees of freedom or the associated shape functions contributes to the element's simplicity. Finally, the inherent geometry of electromagnetic fields, as described by certain concepts from Differential Geometry and Geometric Integration Theory is preserved in the discrete domain by taking special care to represent the gradients of scalar vector fields, correctly and consistently.

On the other hand, this paper aims at providing useful, ready-to-use expressions for the resulting higher order Whitney elements and some important guidelines about difficulties in their implementation. Therefore, apart from the underlying theoretical background, it gives to the researcher, as well as to the end-user a useful tool for accurate electromagnetic field computation.

How many degrees of freedom?

The first problem in the generation of Whitney Elements in higher orders is the proper choice of degrees of freedom. The well-founded choice of edge-based degrees of freedom, in the case of edge elements [2], seems to be insufficient when higher order approximations are involved. We will show that in orders higher than one, degrees of freedom defined on the faces or the whole volume of the element are required.

Let's first determine the actual number of degrees of freedom that is required to build an n-th order tetrahedral tangential vector finite element (1-form Whitney element). An important observation is that tangential continuity is automatically obtained, if the field in an n-th order tetrahedral element is expressed by the expansion

$$\mathbf{F} = \sum_{i=1}^{4}\left[\sum_{k=1}^{n}\left(\sum_{i_1=1}^{4}\sum_{i_2=1}^{4}\cdots\sum_{i_k=1}^{4} f^{i}_{i_1 i_2 \cdots i_k}\,\zeta_{i_1}\zeta_{i_2}\ldots\zeta_{i_k}\right)\right]\nabla\zeta_i \quad (1)$$

where ζ_i, i=1,...,4 are the simplex co-ordinates and ζ_i are vectors normal to the face $\{i\}$, provided that the values of degrees of freedom are the same for adjacent elements. However, this primitive form for the vector finite element includes every possible product of simplex co-ordinates, up to the n-th order. Hence, the number of degrees of freedom in (1) is excessively large. To determine the precise number of linearly independent degrees of freedom, which is required, we should focus on the property of correct modelling of the nullspace and the range space of the curl operator, which is considered fundamental in the study of Whitney elements [3].

In order to model the range space of the curl operator correctly, the *curl* of an n-th order approximation should be a complete vector polynomial of order n-1. The number of parameters to built a complete 3D vector polynomial of order n-1 is given by

$$N_c = \frac{n(n+1)(n+2)}{2} \qquad (2)$$

However, since the divergence of the curl of a vector is identically zero, there is a number of linear relations among these parameters. This is proven to be

$$N_d = \frac{(n-1)n(n+1)}{6} \qquad (3)$$

and the actual number of independent coefficients for completeness is N_c-N_d.

Finally, we should add the required number of degrees of freedom to model the nullspace of the curl operator, in other words the irrotational fields. This is the number of independent gradients, N_i, of an n-th order scalar field, which is, in fact, the number of edges of a "gradient tree" (Fig. 1). If the gradients of an irrotational field on the edges of this tree are known, gradients on any other edge can be easily computed. The number of independent edges in a gradient tree is easily proven to be

$$N_i = \frac{n^3 + 6n^2 + 11n}{6} \qquad (4)$$

and the required number of independent degrees of freedom for an n-th order 1-form Whitney element is given by

$$N = N_c - N_d + N_i = \frac{n(n+2)(n+3)}{2} \qquad (5)$$

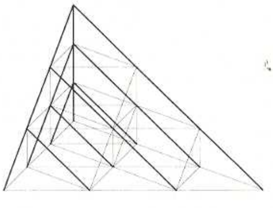


Fig. 1. A gradient tree for a third order element, indicated by the thick lines.

What kind of degrees of freedom?

One of the most obscure aspects of the Whitney element generation methodology is that of the choice of degrees of freedom. What seems apparent in the first order case, i.e. the well known edge element, where the degrees of freedom are the line integrals of the vector field along the tetrahedron's edges, is not enough when dealing with higher orders. On the other hand, it is likely that the tangentially continuous field should be expressed in terms of some kind of tangential projections. The following observations shed light on that issue.

First of all, for an n-th order 1-form Whitney element, n degrees of freedom could be related to each edge. This number accounts for n-th order field variations along the tetrahedron's edges or, in other words, it can represent the n gradients of an n-th order scalar field. Using less than n degrees of freedom on each edge, we could not express n-th order fields along edges, whereas more than n degrees of freedom are not linearly independent. These degrees of freedom can be expressed in terms of field projections on edges. Although we could use point degrees of freedom, in other words tangential projections on specific points of an edge, we will adopt weighted field projections of the form

$$F_{ij}^{p} = \int_{(i)}^{(j)} \mathbf{F} \cdot \hat{\mathbf{t}}_{ij}\, a_p^{n-1} dl \qquad (6)$$

where the nodal shape functions of order n-1 for every node p, on edge $[i,j]$, play the role of the weighting functions. We will show that this choice leads to an elegant definition of the other types of degrees of freedom and a rigorous connection of the 1-form Whitney element to 2-form Whitney elements, i.e. normal vector finite elements. It can be also shown, that any other field projection on edge $[i,j]$ can be expressed as a linear combination of the degrees of freedom in (6). This affine transformation between two arbitrary sets of edge degrees of freedom justifies the fact that all possible choices are, more or less, equivalent, although different choices will result in slightly different shape function expressions.

We now focus on the crucial issue of choosing the remaining degrees of freedom, independent to those given by (6) and to each other, to complete the desired number (5). A convenient approach is to attempt to express the degrees of freedom for the curl of the vector field under consideration, in terms of the degrees of freedom of the vector field itself. This is particularly useful when dealing with Maxwell's equations, because it will provide explicit discrete relations between **E** and **B**, or **H** and **D**. However, we bear in mind that the *curl* of an 1-form (tangentially continuous) field is a 2-form (normally continuous) field, and we should at least comment on how the degrees of freedom for such a kind of field are to be defined.

In a way similar to that of the previous paragraph, an n-th order normally continuous vector field would require $n(n+1)/2$ degrees of freedom for each face, related to normal projections, to describe n-th order field variations on that face. This is also the number of independent curls of an n-th order tangentially continuous field. A reasonable choice for the facial degrees of freedom of an n-th order normally continuous field, similar to (6), is

$$F_{ijk}^{p} = \iint_{\{i,j,k\}} \mathbf{F}\cdot\hat{\mathbf{n}}\, a_p^{n-1} ds \tag{7}$$

where the weighting functions are the nodal shape functions of order n-1 for every node p, on the face $\{i,j,k\}$. Apparently, these degrees of freedom are integrated weighted normal field projections (flows) from the face $\{i,j,k\}$.

In the second order case, the edge degrees of freedom for the field **F** (6) take the form

$$F_{ij}^{i} = \int_{(i)}^{(j)} \mathbf{F}\cdot\hat{\mathbf{t}}_{ij}\,\zeta_i dl, \quad F_{ji}^{j} = \int_{(j)}^{(i)} \mathbf{F}\cdot\hat{\mathbf{t}}_{ji}\,\zeta_j dl \tag{8}$$

To associate degrees of freedom of **F** to those of the *curl* of **F**, we consider the equation

$$\nabla\times(\zeta_2\mathbf{F}) = \nabla\zeta_2\times\mathbf{F} + \zeta_2\nabla\times\mathbf{F} \tag{9}$$

and we apply the Stokes theorem on face $\{1,2,3\}$:

$$\iint_{\{1,2,3\}} \nabla\times(\zeta_2\mathbf{F})\cdot\hat{\mathbf{n}}^{+} ds = \int_{(1)}^{(2)} \zeta_2\mathbf{F}\cdot d\mathbf{l} + \int_{(2)}^{(3)} \zeta_2\mathbf{F}\cdot d\mathbf{l} + \int_{(3)}^{(1)} \zeta_2\mathbf{F}\cdot d\mathbf{l} \tag{10}$$

By combining (9) and (10), we obtain the expression

$$\iint_{\{1,2,3\}} \zeta_2\nabla\times\mathbf{F}\cdot\hat{\mathbf{n}}^{+} ds = -\int_{(2)}^{(1)} \zeta_2\mathbf{F}\cdot d\mathbf{l} + \int_{(2)}^{(3)} \zeta_2\mathbf{F}\cdot d\mathbf{l} - \iint_{\{1,2,3\}} \mathbf{F}\times\hat{\mathbf{n}}^{+}\cdot\nabla\zeta_2 ds \tag{11}$$

In the left side of (11) we have a degree of freedom for the *curl* of **F**, falling into the general category (7). As it can be seen, computation of degrees of freedom for the *curl* of a 2-form vector field involves the edge degrees of freedom of 1-form fields (6) and a new kind of degrees of freedom defined on faces, but related to tangential projections on them. Therefore, it seems reasonable to make the following choice for the facial degrees of freedom of an 1-form field on the face $\{i,j,k\}$:

$$F_{ijk} = \iint_{\{i,j,k\}} \mathbf{F}\times\hat{\mathbf{n}}^{+}\cdot\nabla\zeta_j ds, \quad F_{ikj} = \iint_{\{i,j,k\}} \mathbf{F}\times\hat{\mathbf{n}}^{-}\cdot\nabla\zeta_k ds \tag{12}$$

However, only two out of the three possible degrees of freedom are linearly independent since

$$(\nabla\zeta_i + \nabla\zeta_j + \nabla\zeta_k)\times\hat{\mathbf{n}} = 0 \tag{13}$$

Therefore, we have to define eight facial degrees of freedom, two on each face, which gives rise to an inevitable lack of symmetry. This means that the local numbering of the element will affect the placement of degrees of freedom. We also emphasise, that degrees of freedom on both edges and faces are shared between adjacent elements, therefore we have to place them consistently during the mesh generation procedure. In addition, the unit vectors normal to the surface in the degrees of freedom (12) are assumed to point outwards and inwards, respectively. This also helps to a consistent definition, in the sense that the signs of facial degrees of freedom are the same for adjacent elements. The twenty degrees of freedom for the second order element are shown in Fig. 2.

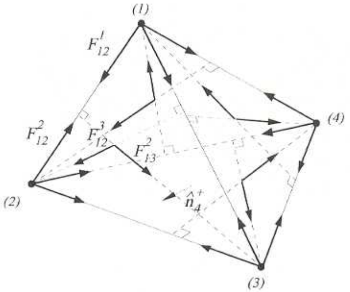


Fig. 2. Degrees of freedom in a second order tetrahedron

In the third order case, our choice of degrees of freedom is justified by a similar procedure. First of all, three degrees of freedom are defined on edge $[i,j]$. According to (6), we define

$$F_{ij}^{ii} = \int_{(i)}^{(j)} \mathbf{F}\cdot\hat{\mathbf{t}}_{ij}\,\zeta_i(2\zeta_i - 1)dl,\; F_{ij}^{ij} = \int_{(i)}^{(j)} \mathbf{F}\cdot\hat{\mathbf{t}}_{ij}\zeta_i\zeta_j dl,$$
$$F_{ij}^{jj} = \int_{(i)}^{(j)} \mathbf{F}\cdot\hat{\mathbf{t}}_{ij}\zeta_j(2\zeta_j - 1)dl \tag{14}$$

Using the Stokes theorem and an approach similar to (9)-(11), we introduce the following facial degrees of freedom on any face $\{i,j,k\}$:

$$F_{pqr}^{q} = \iint_{(i,j,k)} \mathbf{F} \times \hat{\mathbf{n}} \cdot \zeta_q \nabla \zeta_p ds \tag{15}$$

where $(p,q,r) \in \{(i,j,k), (i,k,j), (j,k,i), (j,i,k), (k,i,j), (k,j,i)\}$, in other words any possible combination of indices i, j and k. As a result, we have six independent degrees of freedom for each face. Unlike the second order case, the definition of facial degrees of freedom is symmetric. However, the total number of degrees of freedom, which is 45, is not yet completed. To determine the remaining three of them we should first define a second kind of degrees of freedom for a 2-form (normal) Whitney element. Using Gauss theorem and the same approach as before, we obtain a new kind of degrees of freedom involving volume integrals. For the third order case the three volume degrees of freedom can be defined via

$$F_{ijkl} = \iiint_{(i,j,k,l)} \mathbf{F} \cdot \nabla\zeta_j \times \nabla\zeta_k dv \tag{16}$$

where only three out of the possible combinations of indices (i,j,k,l) should be chosen. We assume that (i,j,k,l) $\in \{(1,2,3,4), (2,3,1,4), (3,1,2,4)\}$. In this case, although we can symmetrically define the facial degrees of freedom, the lack of symmetry is observed in the placement of volume degrees of freedom. Again, since degrees of freedom are shared between neighbouring elements, we should define proper local numberings to place them consistently. The 45 degrees of freedom that have been defined for the third order element are shown in Fig. 3.

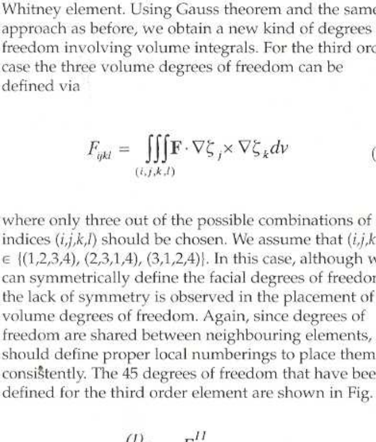


Fig. 3. Degrees of freedom in a third order tetrahedron. Face degrees of freedom are shown only on front face

The analysis can be generalised to orders higher than three, where all categories of degrees of freedom are present. It can be shown that a lack of symmetry, either in facial or in volume degrees of freedom will continue to exist. However, the number of degrees of freedom becomes excessively high and the complexity of expressions makes them have little practical importance.

Properties and construction of shape functions

In the previous paragraph we have introduced the degrees of freedom that will be used to the construction of our higher order Whitney elements. We have clearly stated that this particular choice is not mandatory. Other forms of tangential projections on edges, faces or the whole element's volume could be introduced, either integral- or point-based, but similar to the integrand of (8), (12) and (14)-(16). We emphasise that the types of tangential projections in each kind of degrees of freedom are different and, as it can be shown, this ensures the independence of degrees of freedom, in other words the element's unisolvence.

Let us now proceed to a more formal definition of the properties of tangential vector finite element shape functions. We have seen that even the general form of expansion (1) which has no particular properties, ensures the tangential continuity, on condition that degrees of freedom are consistently defined between two neighbouring elements. Therefore, it seems that the two basic properties of Whitney elements, conformity and unisolvence [1], are almost automatically satisfied. In fact, the introduction of two other properties will determine the exact form of shape functions. As we will see, the importance of those properties is, sometimes, underestimated because they seem to lack a formal definition, although they may seem to be quite obvious.

First of all, we introduce a general expression of the shape functions in terms of some unknown coefficients, which have to be computed. Any shape function of the n-th order 1-form Whitney element is expressed via a vector polynomial expansion. This includes any possible product, of order less than or equal to n, of the simplex co-ordinates that are associated with the 1-, 2- or 3-subsimplex (edge, face or volume, respectively), on which the corresponding degree of freedom is defined. The basis vectors of the expansion are the gradients of the simplex co-ordinates, also associated to the same subsimplex. For instance, a shape function related to an edge degree of freedom, defined on edge $[i,j]$ will be expressed in terms of ζ_i and ζ_j only, whereas the shape function of a facial degree of freedom on face $\{i,j,k\}$ will involve ζ_i, ζ_j and ζ_k. This assumption is by no means restrictive, since the omitted terms are zero on the subsimplex under consideration. A compact algebraic expression for a shape function of any kind and order is

$$\mathbf{w}_{i_1 i_2 \dots i_k}^{j_1 j_2 \dots j_l} = \sum_{m=1}^{k} \left(\sum a_{i_1(n_1)\dots i_k(n_k)}^{i_m} \zeta_{i_1}^{n_1} \dots \zeta_{i_k}^{n_k}\right) \nabla\zeta_{i_m}, \quad n_1 + \dots + n_k \le n \tag{17}$$

where k is the order of the subsimplex, on which the corresponding degree of freedom is defined, i.e. 2, 3 or 4 for edge, face and volume degrees of freedom, respectively. Furthermore, $i_1, i_2, \dots, i_k$ are the indices of the related simplex co-ordinates and the inner summation involves any possible multiplicities $n_1, n_2, \dots, n_k$.

The first property, which has to be imposed on the shape functions is the decoupling of degrees of freedom. This property simply guarantees their "separation", in the sense that any shape function will affect only the corresponding degree of freedom. In terms of a mathematical formulation, every degree of freedom that is computed for a given shape function should be zero, unless it is the one which is directly associated with it. In a more formal interpretation, if we consider the degrees of freedom functionals acting on vector fields, the decoupling property is expressed by

$$\mathcal{F}_{i_1 \ldots i_k}^{j_1 \ldots j_l}(\mathbf{w}_{m_1 \ldots m_k}^{n_1 \ldots n_l}) = \delta_{i_1, m_1} \ldots \delta_{i_k, m_k} \delta_{j_1, n_1} \ldots \delta_{j_k, n_k} \qquad (18)$$

where the arguments of the functionals are the shape functions. We note that (18) includes a normalisation condition. This property is particularly critical when the degrees of freedom of a given field have to be computed. Any 1-form field, **F**, will be approximated by a linear combination of the shape functions,

$$\mathbf{F} = \sum F_{m_1 \ldots m_k}^{n_1 \ldots n_l} \mathbf{w}_{m_1 \ldots m_k}^{n_1 \ldots n_l} \qquad (19)$$

If we apply the functional of (18) on (19) and impose property (18) we have

$$F_{i_1 \ldots i_k}^{j_1 \ldots j_l} = \mathcal{F}_{i_1 \ldots i_k}^{j_1 \ldots j_l}(\mathbf{F}) \qquad (20)$$

which implies that the coefficients in the expansion (19) are, in fact, the degrees of freedom of the vector field. If the decoupling property would not have been imposed, a system of equations would result instead of (20) and the computation of degrees of freedom would not be direct and easy.

Imposition of property (18) on the unknown shape functions (17) results in a set of linear equations in terms of the unknown coefficients of (17). However, this system of equations is underdetermined, which shows that a simple property of decoupling is not enough to produce the exact form of the shape functions. In fact, this property seems to be quite logistic, since it simply prevents shape functions from affecting degrees of freedom irrelevant to them.

To discover what kind of additional constraints should be imposed on the coefficients of (17) we should look back to a property that seems to have been exploited in a previous step of our analysis, the correct modelling of the nullspace of the curl operator. In fact, the true essence of the Whitney element theory is included in this property, since the real source of problems like spurious modes and parasitic vector solutions, when conventional scalar finite elements are used, is, undoubtedly, the poor modelling of irrotational fields. The property of correct nullspace modelling has been used in the derivation of the required number of degrees of freedom (5). However, we have attempted to introduce a very wide class of field variations for the Whitney element expressions (17), and the element may not be able to correctly represent gradients of scalar fields, unless specific constraints are applied.

To find out how this property will practically affect the element construction, we revert to an elegant and formal definition taken from the field of Differential Geometry. Even from the early days of introduction and application of edge elements, the importance of existence of De Rham - Whitney complex,

$$W^0(\tilde{D}) \xrightarrow{grad} W^1(\tilde{D}) \xrightarrow{curl} W^2(\tilde{D}) \xrightarrow{div} W^3(\tilde{D}) \qquad (21)$$

in the discrete domain, has been clearly emphasised [2]. This abstract sequence of Hilbert spaces of scalar or vector fields shows how these spaces are transformed by the vector operators. The four sets in (21) are spaces of the discretised Whitney 0-, 1-, 2- or 3-forms, defined on the discrete tessellation. The meaning of this sequence is that the image of any field belonging to a space to the left of an arrow, when the corresponding operator acts on it, should belong to the space to the right of the arrow. Generally, a De Rham complex is considered the basis for the existence and study of the topological and geometrical properties of spaces. In our case, a corresponding complex exists in the continuous domain, but not in the discrete domain, when nodal finite elements are used.

For the construction of Whitney 1-forms, we concentrate on the first from the three mappings in (21). To interpret this abstract property in terms of algebraic equations, we require that the gradient of any Whitney 0-form, or scalar field defined on a n-th order tetrahedron, will belong to the space of Whitney 1-forms. In other words, we seek additional constraints among the unknown coefficients of (17), to guarantee the existence of solutions to the equations

$$\sum A_{i_1 \ldots i_k}^{j_1 \ldots j_l} \mathbf{w}_{i_1 \ldots i_k}^{j_1 \ldots j_l}(a_{m_1 \ldots m_k}^{n_1 \ldots n_l}) = \nabla \varphi_p^n \qquad (22)$$

where A's are the unknown degrees of freedom, and φ's are the n-th order nodal element shape functions. However, we are not interested in solving the system of equations (22) for the degrees of freedom. This system is a parametric one, since the shape functions are still parameter-dependent, and we search for the constraints among the coefficients, under which the system admits solutions. After some strenuous algebraic manipulation, we can deduce the generic constraints that ensure the existence of solutions for (22). In the second order case the generic constraints are

$$a_{ii}^j + a_{ji}^i = a_{ij}^i + a_{ij}^j = 0 \qquad (23),(24)$$

$$a_{ij}^{k} + a_{jk}^{i} + a_{ki}^{j} = 0 \tag{25}$$

for any i, j, k, whereas for the third order case, these are proven to be

$$a_{iii}^{j} + a_{jii}^{i} = a_{ijj}^{i} + a_{iij}^{j} = 0 \tag{26),(27}$$

$$a_{iij}^{k} + a_{ijk}^{i} + a_{kii}^{j} = 0 \tag{28}$$

$$a_{ijkl} + a_{jkli} + a_{klij} + a_{lijk} = 0 \tag{29}$$

for any i, j, k, l. The coefficients that are involved in (23)-(25) and (26)-(29) are related to the highest order terms in the vector finite element expressions. Hence, it should be emphasised that the n-th order terms cannot vary in an arbitrary way. The property of correct gradient representation requires that their coefficients are related to each other by this kind of cyclic relations. These relations are easily generalised to higher orders.

The decoupling property (18), along with the solvability constraints that have been deduced in the previous paragraph, are combined to form linear systems of equations for the unknown coefficients of the shape functions (17). In the end of this awesome procedure, it may be surprising that the linear systems for the coefficients are neither under- nor overdetermined. The final expressions for the shape functions of a second order 1-form Whitney element are given by

$$\mathbf{w}_{ij}^{i} = (8\zeta_i^2 - 4\zeta_i)\nabla\zeta_j + (-8\zeta_i\zeta_j + 2\zeta_j)\nabla\zeta_i \tag{30}$$

$$\mathbf{w}_{ijk} = 16\zeta_i\zeta_j\nabla\zeta_k - 8\zeta_j\zeta_k\nabla\zeta_i - 8\zeta_k\zeta_i\nabla\zeta_j \tag{31}$$

for edge and facial degrees of freedom, respectively, whereas in the third order case they are given by the following rather complicated expressions,

$$\mathbf{w}_{ij}^{ii} = (45\zeta_i^3 - 45\zeta_i^2 + 9\zeta_i)\nabla\zeta_j + (-45\zeta_i^2\zeta_j + 30\zeta_i\zeta_j - 3\zeta_j)\nabla\zeta_i \tag{32}$$

$$\mathbf{w}_{ij}^{ij} = (45\zeta_i^3 + 180\zeta_i^2\zeta_j + 45\zeta_i\zeta_j^2 - 75\zeta_i^2 - 90\zeta_i\zeta_j + 24\zeta_i)\nabla\zeta_j + (-45\zeta_j^3 - 180\zeta_j^2\zeta_i - 45\zeta_j\zeta_i^2 + 75\zeta_j^2 + 90\zeta_j\zeta_i - 24\zeta_j)\nabla\zeta_i \tag{33}$$

$$\mathbf{w}_{ijk}^{j} = (-270\zeta_i\zeta_j^2 + 90\zeta_i\zeta_j)\nabla\zeta_k + (90\zeta_j^2\zeta_k - 30\zeta_j\zeta_k)\nabla\zeta_i + (180\zeta_i\zeta_j\zeta_k - 30\zeta_i\zeta_k)\nabla\zeta_j \tag{34}$$

$$\mathbf{w}_{ijkl} = 540\zeta_j\zeta_k\zeta_l\nabla\zeta_i - 180\zeta_l\zeta_k\zeta_i\nabla\zeta_j - 180\zeta_l\zeta_i\zeta_j\nabla\zeta_k - 180\zeta_j\zeta_i\zeta_k\nabla\zeta_l \tag{35}$$

for edge, facial and volume degrees of freedom. The edge shape function, corresponding to the third degree of freedom in (14) is also given by (32), but its signs should be inverted.

At last, we should further comment on the term "generic" that has been introduced in the previous paragraph. Constraints (23)-(25) and (26)-(29) are generic, in the sense that they produce the widest possible class of elements. A detailed analysis of (22) will show that there are nongeneric constraints as well. For example, in the second order case we can replace (25) by the equations

$$a_{jk}^{i} = a_{ki}^{j} = 0 \tag{36),(37}$$

Replacement of one constraint by two is definitely more restrictive and leads to an overdetermined system of equations for the unknown coefficients of the shape functions. However, we mention the existence of the nongeneric constraints (36),(37) because a previous approach [4] produces a second order tangential vector finite element that falls into this nongeneric category. Although, in the same approach, shape functions seem to be a priori or heuristically chosen, the fulfilment of constraints (36),(37) is a result of the fact that special care is taken for a correct nullspace modelling, via a different approach, the tree-cotree decompositions [4], [9].

What happens with hexahedral vector finite elements?

Although the construction of hexahedral vector finite elements is considered simpler, compared to the tetrahedral element case, due to the hexahedron's structural simplicity, and various approaches can be found in the literature [5]-[8], we will show that a similar procedure can be used to derive hexahedral Whitney elements. This generalised theory seems to result in wider classes of elements, while it further clarifies some common but, more or less, ad hoc assumptions. We will concentrate on generating second order elements, although any extension is straightforward and easy.

First of all, we have to decide the particular kind of the nodal hexahedral element on which a Whitney form is to be built. We could choose between Lagrangian or Serendipity elements, although there exist other possible node placements, depending on the desired accuracy and number of nodes. This choice will affect the dimension of the nullspace of the discrete curl operator and, consequently, the total number of degrees of freedom, which is proven to be 54, for the second order Lagrangian element and 36 for the Serendipity. In the following example we will build a second order Serendipity element.

The choice of degrees of freedom follows the same rules, as in the case of tetrahedra. Although in the study of Whitney forms in tetrahedra we have used integral degrees of freedom, we could similarly use point degrees of freedom. Although it may be difficult to find explicit relations among point degrees of freedom for different Whitney forms, like (11), they have the advantage of being easier to compute. In the second order 1-form Whitney Serendipity element, the edge-related degrees of freedom, for example along ξ-edges, are defined by

$$\begin{aligned} F^{\xi^+}_{\eta_0,\zeta_0} &= \frac{L_\xi}{2}\mathbf{F}\cdot\hat{\mathbf{t}}_\xi\Big|_{\xi=-1/2,\eta=\eta_0,\zeta=\zeta_0}, \\ F^{\xi^-}_{\eta_0,\zeta_0} &= -\frac{L_\xi}{2}\mathbf{F}\cdot\hat{\mathbf{t}}_\xi\Big|_{\xi=1/2,\eta=\eta_0,\zeta=\zeta_0} \end{aligned} \tag{38}$$

and similarly for η- or ζ-oriented edges. Additionally, the element requires two degrees of freedom in each face. A suitable definition, for example at face ξ= -1, is

$$\begin{aligned} F^{\eta,\zeta}_{-1} &= S\,\mathbf{F}\times\hat{\mathbf{p}}_\xi\cdot\nabla\eta\Big|_{\xi=-1,\eta=0,\zeta=0}, \\ F^{\zeta,\eta}_{-1} &= S\,\mathbf{F}\times\hat{\mathbf{p}}_\xi\cdot\nabla\zeta\Big|_{\xi=-1,\eta=0,\zeta=0} \end{aligned} \tag{39}$$

where S is the area of face ξ= -1 and the p-vector is the unit vector normal to the face. To maintain conformity of degrees of freedom between neighbouring elements, p-vectors are always pointing towards the positive direction of local coordinates.

The derivation of the formulas for the shape functions will be based on the two fundamental properties of Whitney finite elements. However, in this case we could significantly simplify the procedure, if we adopt the restriction that shape functions should have only one covariant component, for example a ξ-edge shape function will be given by

$$\mathbf{w}^{\xi^+}_{\eta_0,\zeta_0} = \Big(\sum_{i,j,k\le n} a_{i,j,k}\xi^i\eta^j\zeta^k\Big)\nabla\xi \tag{40}$$

where n is the order of the approximation and the summation involves, for the moment, every possible polynomial term. This restriction, although simplifying, is not necessary, and a more general treatment would reveal wider classes of elements. In the case of hexahedral elements, it is convenient to enforce the property of correct gradient representation (21), (22), where the gradients of the second order nodal Serendipity element shape functions are involved, before doing anything else. The final result of the analysis requires that most of the coefficients in (40) are null and it is further simplified as follows:

$$\mathbf{w}^{\xi^+}_{\eta_0,\zeta_0} = \Big(\sum_{j,k\le 2} a_{0,j,k}\eta^j\zeta^k + \xi\sum_{j,k\le 1} a_{1,j,k}\eta^j\zeta^k\Big)\nabla\xi \tag{41}$$

This general form, which is also adopted in [5], justifies the term "mixed order elements" which is another commonly used term. In simple words, the variation of any field component on its own direction is of order n-1. The analysis reveals that this assumption is a natural consequence of the correct nullspace modelling property.

The explicit form of the shape functions is finally obtained by enforcing the property of decoupling (20). The expressions for the hexahedral 1-form Whitney Serendipity shape functions, corresponding to degrees of freedom (38), (39) are

$$\mathbf{w}^{\xi^+}_{\eta_0,\zeta_0} = \pm\frac{1}{8}(1+\eta_0\eta)(1+\zeta_0\zeta)(-1+\eta_0\eta+\zeta_0\zeta\mp 2\xi)\nabla\xi \tag{42}$$

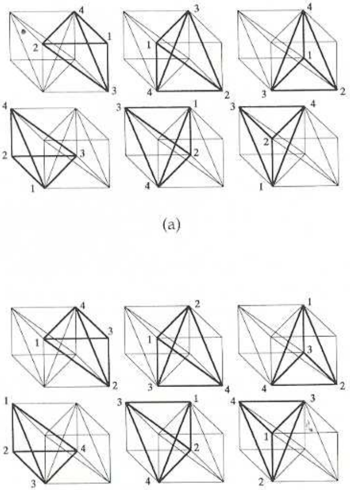
$$\begin{aligned} \mathbf{w}^{\eta,\zeta}_{\xi_0} &= \frac{1}{8}(1+\xi_0\xi)(1-\eta^2)\nabla\zeta, \\ \mathbf{w}^{\zeta,\eta}_{\xi_0} &= -\frac{1}{8}(1+\xi_0\xi)(1-\zeta^2)\nabla\eta \end{aligned} \tag{43}$$

respectively, while the others are obtained by cyclic permutation.

Mesh conformity considerations

The analysis of higher order Whitney 1-forms reveals a new problem in their numerical implementation, the unsymmetric placement of degrees of freedom. In each face of a second order vector finite element there are two degrees of freedom and a fully symmetric arrangement is not possible. When using third order elements, there is no lack of symmetry in face degrees of freedom. However, the three volume degrees of freedom cannot be symmetrically defined. In both cases, special care should be taken to ensure that adjacent elements will have conforming degrees of freedom. In the second order case, this means that two elements sharing the same face should have the same placement of degrees of freedom on it. Similarly, in neighbouring third order elements, the volume degrees of freedom should be consistently placed.

The problem of conforming mesh generation requires the definition of proper local numberings, to ensure conformity of degrees of freedom between adjacent elements. In an arbitrary tetrahedral mesh, we could introduce an appropriate algorithm, which would start from an element of the mesh and define the local numbering from element to element. However, this procedure involves elements of graph theory and it can be very complicated, not to mention that the algorithm may not converge or it may have no solution, unless the mesh is constructed under specific structural criteria. To avoid this kind of complexity we concentrate on the case of structured meshes based on hexahedra. To preserve the property of conformity, we propose a standard local numbering scheme (Fig. 4). Each hexahedron is divided into six tetrahedra and the local numberings are chosen to guarantee conformity, both in inner and outer edges or faces. We emphasise that this particular scheme is valid only if the placement of degrees of freedom in each element is as in Fig. 2 and 3. This scheme is very useful for a successful implementation of higher order vector finite elements. The use of structured meshes is not restrictive, since they can be used as initial meshes in mesh refinement schemes.



(a) (b)

Fig. 4. A local numbering scheme for mesh conformity: (a) the second order case, (b) the third order case

Conclusions

We have presented a generalised theory and a systematic procedure for generating higher order Whitney 1-forms in three-dimensions. The theory is applied in both tetrahedral and hexahedral elements and produces explicit expressions for the finite element shape functions and a clear interpretation of degrees of freedom. The analysis delves into the nature of Whitney forms and vector finite elements and clarifies the importance of their fundamental properties, as well as the means of enforcing them to get the final results. Some ad hoc assumptions about the choice of degrees of freedom are also explained. Finally, we give some important guidelines for their implementation, related to difficulties in mesh generation. The whole analysis, although mathematically oriented, gives a further insight in the fascinating subject of Whitney elements and, hopefully, provides a series of useful tools for the electromagnetic field analyst.

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