

Geometrical localisation of the degrees of freedom for Whitney elements of higher order

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Abstract: Low-order Whitney forms are widely used for electromagnetic field problems. Higher-order ones are increasingly applied, but their development is hampered by the complexity of the generation of element basis functions and of the localisation of the corresponding degrees of freedom on the mesh volumes. The paper aims to give a geometrical localisation of the degrees of freedom associated with Whitney forms of a polynomial degree higher than one. A conveniently implementable basis is provided for these elements on simplicial meshes. As for Whitney forms of degree one, the basis is expressed only in terms of the barycentric co-ordinates of the simplex.

1 Introduction and notations

Whitney elements on simplices [1–3] are perhaps the most widely used finite elements in computational electromagnetics. They offer the simplest construction of polynomial discrete differential forms on simplicial complexes. Their associated degrees of freedom (DOF) have a very clear meaning as co-chains and thus give a method for the discretisation of physical balance laws, for example Maxwell equations. Many implementations using Whitney elements of the lowest polynomial degree $k = 1$, exist, and only a few exist for higher orders, $k > 1$. Higher-order extensions of Whitney forms are known and have become an important computational tool. However, in addition to the complexity of the generation of element basis functions, it has remained unclear what kinds of co-chain higher-order Whitney forms should be associated with. The current paper settles this issue, namely, the localisation of the corresponding DOF on the mesh volumes (here, tetrahedra) for higher-order Whitney forms.

Several papers devoted to the construction of (hierarchical or not) high-order shape functions for computational electromagnetics have appeared in the engineering literature, for example [4–6]. Viable sets of basis functions for higher-order Whitney forms in dimension three have been proposed [7], with resulting well-conditioned Galerkin matrices. Boffi *et al.* [8] developed an alternative technique relying on projection-based interpolation, where the high-order space is built by the use of a hierarchical basis, with resulting optimum interpolation error estimates. A parallel approach using the Koszul differential complex has been developed in [9], and a general construction of higher-order discrete differential forms can be found in [10].

In this paper, we shall present a particular construction of Whitney forms of polynomial degree higher than one on

simplices, together with a geometrical localisation of the DOF associated with these forms. We provide a conveniently implementable basis for these elements: at each tetrahedron, this basis is obtained as the product of Whitney forms of degree one by suitable homogeneous polynomials (polynomials whose terms are monomials all having the same total degree) in the barycentric co-ordinate functions of the simplex. There are three key heuristic points underlying this construction

- (i) these higher-order forms should satisfy a partition of unity property
- (ii) being a larger number with respect to those of degree one, they are to be associated with a finer partition in each tetrahedron, the so-called ‘small simplices’, a set of simplices obtained through affine contractions of a mesh simplex
- (iii) the spaces spanned by higher-order forms should constitute an exact sequence.

The proposed higher-order Whitney forms are not linearly independent: a selection procedure has to be specified to produce a valid set of unisolvent local shape functions. The element basis functions are very simple to generate, but the resulting Galerkin matrices are not as well-conditioned as the ones in [7], and preconditioners of the domain decomposition type (see Smith *et al.* [11]) must be used to reduce the condition number.

Let us introduce some notations. Let d be the ambient dimension. Given a domain $\Omega \subset \mathbb{R}^d$, a simplicial mesh \mathfrak{m} in Ω is a tessellation of Ω by d simplices, under the condition that any two of them can intersect along a common $(d - 1)$ face, edge or node, but in no other way, and we denote by $0 \leq p \leq d$ the subsimplex dimension. Labels n, e, f, t are used for nodes, edges and so on, each with its own orientation, and w^n, w^e and so on refer to the corresponding Whitney forms of degree one [2]. Note that e (respectively, f, t) is by definition an ordered couple (respectively, triple, quadruplet) of vertices, not merely a collection. The forms w^e (respectively, w^f, w^t) are indexed over the set of these couples (respectively, triples, quadruplets), and thus we use e (respectively, f, t) also as a label, as it points to the same object in both cases. The sets of nodes, edges, faces, volumes (i.e. tetrahedra) are denoted by $\mathcal{N}, \mathcal{E}, \mathcal{F}, \mathcal{T}$. In short, we denote by S^p the set

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of p simplices of m and by $\#S^p$ its cardinality. The sets of p simplices are linked, as in [2], by the incidence matrices \mathbf{G} , \mathbf{R} , \mathbf{D} (for which the generic notation \mathbf{d} can also be used; the symbol \mathbf{d}_σ^s stands for the incidence matrix entry linking the p simplex s to the $(p+1)$ simplex σ). These matrices are the discrete representation of the exterior derivative operator d that, applied on a $(p-1)$ form, gives a p form.

In what follows, we use multi-index notations: let \mathbf{k} be the array (k_0, \dots, k_d) of integers $k_i \geq 0$, and denote by k its weight $|\mathbf{k}| = \sum_{i=0}^d k_i$. The set of multi-indices \mathbf{k} with $d+1$ components and of weight k is denoted $\mathcal{I}(d+1, k)$, and $\#\mathcal{I}(d+1, k)$ is the binomial coefficient

$$\binom{k+d}{d} = \frac{(k+d)!}{(d!k!)}$$

Let us now recall the notion of barycentric co-ordinates. Let $t = \{n_1, n_2, n_3, n_4\}$ be a tetrahedron of m . Four real numbers, $\lambda_1, \lambda_2, \lambda_3, \lambda_4$, such that $\sum_i \lambda_i = 1$, determine a point x , the barycentre of the n_i s for these weights, uniquely defined by $x - n_0 = \sum_i \lambda_i(n_i - n_0)$, where n_0 is any origin (for example, one of the n_i s). Conversely, any point x has a unique representation of the form $x - n_0 = \sum_i \lambda_i(n_i - n_0)$, and the weights λ_i , considered as functions of x , are the barycentric co-ordinates of x in the affine basis provided by the four vertices n_i s. Note that x belongs to the tetrahedron t if $\lambda_i(x) \geq 0$ for all i . The λ_i s are affine functions of x . Now, consider the mesh m of tetrahedra over Ω . To each node n of the mesh, we attribute a function whose value at point x is 0, if none of the tetrahedra with a vertex in n contains x ; otherwise, it is the barycentric co-ordinate of x with respect to n , in the affine basis provided by the vertices of the tetrahedron to which x belongs. We attribute to this nodal function the symbol w^n . Note that, by construction, $w^n(x) \geq 0$ and $\sum_{n \in \mathcal{N}} w^n(x) = 1$ for all $x \in \Omega$. The w^n s themselves are often called hat functions. Note that, working by restriction to the master d simplex t , w^n and λ_n coincide. Any point x of the meshed domain can be represented as $x = \sum_{n \in \mathcal{N}} w^n(x)n$, where w^n is the only piecewise affine (affine by restriction to each tetrahedron) function that takes value 1 at node n and 0 at all other nodes. Therefore, the weight of x with respect to node n is $w^n(x)$. In the following, when $e = \{m, n\}$ and $f = \{l, m, n\}$, we denote the node l by $f-e$. Thus λ_{f-e} refers, in that case, to λ_l .

Let us denote by $\mathbb{P}_k(\Sigma)$ the vector space of polynomials defined on a domain $\Sigma \subset \mathbb{R}^d$ in d variables of degree $\leq k$ and by $\tilde{\mathbb{P}}_k(\Sigma)$ the subspace of $\mathbb{P}_k(\Sigma)$ of homogeneous polynomials of degree k . A well-known result in algebra states that the dimension of $\mathbb{P}_k(\Sigma)$ is $\binom{k+d}{k}$ and that of $\tilde{\mathbb{P}}_k(\Sigma)$ is $\binom{k+d-1}{k}$.

Definition 1: Let $\mathbf{k} \in \mathcal{I}(d+1, k)$. Then, $\lambda^{\mathbf{k}} = \prod_{i=0}^d (\lambda_i)^{k_i}$.

Homogeneous polynomials of degree k in the $d+1$ barycentric co-ordinates are in one-to-one correspondence with polynomials of degree $\leq k$ in the d Cartesian ones. For this reason, we can say that $\mathbb{P}_k(t) = \text{span}(\lambda^{\mathbf{k}})_{\mathbf{k} \in \mathcal{I}(d+1, k)}$ on each tetrahedron t .

The starting point to present Whitney forms of higher order is the definition of Whitney forms of polynomial degree one given in [12], which we recall hereafter.

Definition 2: The differential $(p+1)$ form w^σ given by $w^\sigma = \sum_{s \in \mathcal{S}_\sigma} \mathbf{d}_\sigma^s \lambda_{\sigma-s} \mathbf{d}w^s$ is the Whitney form of polynomial

degree one associated with a $(p+1)$ simplex σ , $0 \leq p \leq d-1$.

The form w^f , for instance, is itself, like the two-form b associated with the magnetic flux density field, a map from surfaces S to real numbers c^f , whose value we denote by $\int_S w^f$ or by $\langle w^f, S \rangle$. Therefore, w^f is the Whitney form of polynomial degree one associated with f , and the weight c^f (or moment) of S in the chain $\sum_{f \in \mathcal{F}} c^f f$ is $\int_S w^f \equiv \langle w^f, S \rangle$.

For a node n , an edge e , a facet f and a tetrahedron t , definition 2 yields the following scalar or vector functions: $w^n = \lambda_n$, $w^e = \sum_{n \in \mathcal{N}} \mathbf{G}_e^n \lambda_{e-n} \mathbf{d}w^n$, $w^f = \sum_{e \in \mathcal{E}} \mathbf{R}_f^e \lambda_{f-e} \mathbf{d}w^e$, $w^t = \sum_{f \in \mathcal{F}} \mathbf{D}_t^f \lambda_{t-f} \mathbf{d}w^f$.

Remark: The well-known expression of the scalar and vector functions for Whitney elements can be recovered starting from definition 2. For edge functions, it is sufficient to replace d by grad , so that, for the edge $e = \{l, m\}$, the identity $w^e = \sum_{n \in \mathcal{N}} \mathbf{G}_e^n \lambda_{e-n}$ gives $w^e = \lambda_l \mathbf{d}w^m - \lambda_m \mathbf{d}w^l$ and thus the vector function $w^e = \lambda_l \text{grad} \lambda_m - \lambda_m \text{grad} \lambda_l$. For facet and volume functions, some additional properties are necessary, namely

- (a) $d \circ d = 0$
- (b) $d(\alpha w) = d\alpha \wedge w + \alpha dw$, where α is a scalar field, w is a form and \wedge is the exterior product between forms (see [9] for more details)
- (c) ${}^1u \wedge {}^1v = {}^2(u \times v)$, where 1u denotes a one form, 2u denotes a two form and \times is the cross product between ordinary vectors.

To give an application example, let us consider the tetrahedron $t = \{k, l, m, n\}$ and its face $f = \{l, m, n\}$. For all the oriented edges e of t that do not constitute the boundary of f , the quantities \mathbf{R}_f^e are 0, whereas, for $e = \{l, m\}$ or $\{m, n\}$ or $\{n, l\}$, we have $\mathbf{R}_f^e = 1$. In this case, $w^f = \sum_{e \in \mathcal{E}} \mathbf{R}_f^e \lambda_{f-e} \mathbf{d}w^e$ yields $w^f = \lambda_n \mathbf{d}(\lambda_l \mathbf{d}w^m - \lambda_m \mathbf{d}w^l) + \lambda_l \mathbf{d}(\lambda_m \mathbf{d}w^n - \lambda_n \mathbf{d}w^m) + \lambda_m \mathbf{d}(\lambda_n \mathbf{d}w^l - \lambda_l \mathbf{d}w^n)$. Then, using (a) and (b), we obtain, for instance, $\mathbf{d}(\lambda_l \mathbf{d}w^m) = \lambda_l \mathbf{d}dw^m + d\lambda_l \wedge \mathbf{d}w^m = d\lambda_l \wedge d\lambda_m$ (being $w^m = \lambda_m$). We thus obtain $w^f = 2(\lambda_n d\lambda_l \wedge d\lambda_m + \lambda_l d\lambda_m \wedge d\lambda_n + \lambda_m d\lambda_n \wedge d\lambda_l)$. Finally, using (c) and replacing d by grad , we obtain $w^f = 2(\lambda_n \text{grad} \lambda_l \times \text{grad} \lambda_m + \lambda_l \text{grad} \lambda_m \times \text{grad} \lambda_n + \lambda_m \text{grad} \lambda_n \times \text{grad} \lambda_l)$, that is the vector function associated with f .

2 The $\tilde{\mathbf{k}}$ map

We now define a geometrical partition within each mesh tetrahedron t by means of a suitable map. This partition is a key point in the construction of higher-order Whitney forms.

Definition 3: To each $\mathbf{k} \in \mathcal{I}(d+1, k)$ corresponds a map, denoted by $\tilde{\mathbf{k}}$, from t into itself. Let \tilde{k}_i denote the affine function that maps $[0, 1]$ onto $[k_i/(k+1), 1 + k_i/(k+1)]$. If $\lambda_i(x)$ is the i th barycentric co-ordinate of point $x \in t$, its image $\tilde{\mathbf{k}}(x)$ has barycentric co-ordinates $0 \leq \tilde{k}_i(\lambda_i(x)) \leq 1$, with $\tilde{k}_i(\lambda_i(x)) = (\lambda_i(x) + k_i)/(k+1)$.

Geometrically, this map is a homothety or, more precisely, a transformation of space that dilates distances of a factor $1/(k+1)$ with respect to the fixed point of barycentric co-ordinates k_i/k (see Fig. 1 for an example). Note that $\tilde{\mathbf{k}}(t)$, for all possible $\mathbf{k} \in \mathcal{I}(d+1, k)$, are congruent by translation and homothetic to t . They do not pave t , and the holes left are not necessarily homothetic to t . The $\tilde{\mathbf{k}}(x_i)$, for all

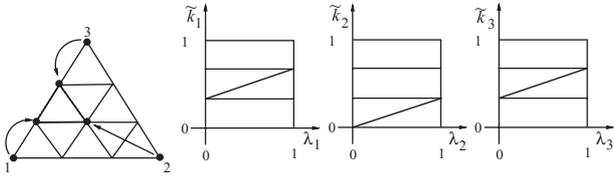


Fig. 1 Mesh triangle t together with principal lattice of order $k+1=3$, mapping $\tilde{\mathbf{k}}$ associated to $\mathbf{k} = (1\ 0\ 1)$ and (dashed) triangle $\tilde{\mathbf{k}}(t)$

possible $\mathbf{k} \in \mathcal{I}(d+1, k)$ and nodes i of t , make the so-called ‘principal lattice of order $k+1$ ’ in t . As an example, take $k=2$: for $d=2$ (see Fig. 2a), the holes left are three small triangles not homothetic to t ; for $d=3$ (see Figs. 2b and c), the holes left are one central small tetrahedron and four octahedra.

Definition 4: The images $\tilde{\mathbf{k}}(S)$, for all simplices $S \in \mathcal{S}^p$, for all $\mathbf{k} \in \mathcal{I}(d+1, k)$, are called small simplices of dimension p and denoted by $s = \{\mathbf{k}, S\}$.

Looking again at Fig. 2, we have six small triangles in 2D and ten small tetrahedra in 3D.

3 High-order Whitney forms

Whitney forms of higher degree in a tetrahedron t are associated with the geometrical partition in t defined by the $\tilde{\mathbf{k}}$ map for all possible multi-indices $\mathbf{k} \in \mathcal{I}(d+1, k)$.

Definition 5: Let $s = \{\mathbf{k}, S\}$ be a small simplex of dimension p . The Whitney p form of degree $k+1$ associated with s is $\lambda^{\mathbf{k}} w^S$, and we denote the span of $\lambda^{\mathbf{k}} w^S$ by W_{k+1}^p .

The method for Whitney p forms of higher polynomial degree is simple: for W_2^p , attach to nodes, edges, faces and so on, products $\lambda_n w^e$, $\lambda_n w^f$ and so on, where n spans \mathcal{N} . For W_3^p , attach to nodes, edges, faces and so on, products $\lambda_n \lambda_m w^e$, $\lambda_n \lambda_m w^f$ and so on, where n, m span \mathcal{N} and so on. DOFs for p forms of degree $k+1$ are localised on small simplices $\{\mathbf{k}, S\}$ of dimension p . As an example, a zero form is represented by its values at the nodes of the principal lattice of order $k+1$ defined in t (as is classical with \mathbb{P}_{k+1} finite elements); the one form h associated with the magnetic field is represented by its circulations along the small edges $\{\mathbf{k}, e\}$ and so on. In [13], the edge element space W_{k+1}^1 of definition 5 is proved to be isomorphic to R_{k+1} defined in [3].

Remark: We would like to make clearer what we mean by ‘geometrical localisation’, the most important point of the

paper that makes it different from what has already been published on the subject of higher Whitney forms. The fact that DOFs for higher Whitney two forms, for example being defined as ‘moments’ as in [3], are not, in an obvious way, integrals over two-dimensional parts, has been used as an argument against calling such forms ‘facet’ elements. In this paper, we have shown that higher-degree p forms are indeed associated with geometric figures of dimension p , even though this association is not as obvious as in the case of lower-degree Whitney forms. Hence, it is legitimate to speak of ‘facet’ elements for two forms, whatever the polynomial degree, and this is related to the fact of having paired DOF with small simplices of dimension 2.

Recall that barycentric functions sum to 1, thus forming a ‘partition of unity’: $\sum_{n \in \mathcal{N}} \lambda_n = 1$. The new forms of definition 5 constitute a partition of unity, as it results from a straightforward generalisation of the same property for Whitney forms of degree one ($k=0$).

Property 1: At all points x , for all ordinary vectors \vec{v} , we have

$$\sum_{e \in \mathcal{E}, \mathbf{k} \in \mathcal{I}(d+1, k)} (\lambda^{\mathbf{k}} w^e(x) \cdot \vec{v}) \vec{e} = \vec{v}$$

$$\sum_{f \in \mathcal{F}, \mathbf{k} \in \mathcal{I}(d+1, k)} (\lambda^{\mathbf{k}} w^f(x) \cdot \vec{v}) \vec{f} = \vec{v}$$

where \vec{e}, \vec{f} are the vector length and vectorial area associated with the edge e and face f .

Proof of Property 1: A vector length associated with an edge e is a vector \vec{e} of modulus length (e) parallel to the edge e , whereas a vectorial area associated with a face f is a vector \vec{f} of modulus area (f) orthogonal to the face f . For $k=0$, the first relationship results from the identity $xy = \sum_{e \in \mathcal{E}} \langle w^e, xy \rangle e$, where xy is the oriented segment from point x to point y . We replace w^e by its proxy, then xy by its vector length \vec{v} and e by its vector length \vec{e} . Then, we multiply both sides by 1, replace the 1 on the left by $\sum_{n \in \mathcal{N}} \lambda_n$ and repeat this k times. Similarly, the second relationship results from the identity $xyz = \sum_{f \in \mathcal{F}} \langle w^f, xyz \rangle f$, where xyz is the oriented surface of vertices x, y and z . We replace w^f by its proxy, then xyz by its vectorial area \vec{v} and f by its vectorial area \vec{f} .

Property 2: For any p simplex, a relationship among the Whitney forms associated with its faces holds. For any

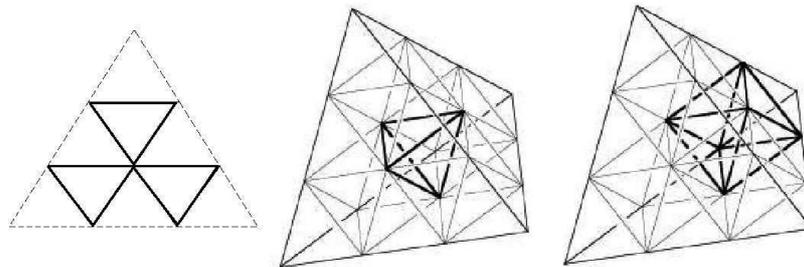


Fig. 2 Images $\tilde{\mathbf{k}}(t)$ for a mesh triangle and tetrahedron t , for $k=2$, and (bold line) examples of ‘holes’ that are (a) triangles, (b) tetrahedra or (c) octahedra not congruent to t

edge e , face f and tetrahedron t , we have, respectively,

$$\begin{aligned}\sum_{n \in \mathcal{N}} \mathbf{G}_e^n \lambda_{e-n} w^n &= 0 \\ \sum_{e \in \mathcal{E}} \mathbf{R}_f^e \lambda_{f-e} w^e &= 0 \\ \sum_{f \in \mathcal{F}} \mathbf{D}_t^f \lambda_{t-f} w^f &= 0\end{aligned}$$

Proof of Property 2: The first identity is evident: we obtain $-\lambda_m \lambda_n + \lambda_n \lambda_m = 0$ for the edge $e = \{n, m\}$. To prove the second identity, we replace w^e by its expression given in Definition 2 and we obtain $\sum_e \mathbf{R}_f^e \lambda_{f-e} w^e = \sum_{n,e} \lambda_{f-e} \lambda_{e-n} \mathbf{R}_f^e \mathbf{G}_e^n d w^n = 0$, as $\mathbf{R}\mathbf{G} = 0$, and $\lambda_{f-e} \lambda_{e-n}$ is the same for all e in ∂f . The third identity can be proved similarly.

Note that the forms $\lambda^{k w^S}$ of definition 5 are generators of W_{k+1}^p but not linearly independent, as results from property 2. For instance, the span of $\lambda^{k w^e}$, $k = 1$, over a tetrahedron has dimension 20 instead of the apparent $24 = 6 \binom{3+1}{1}$, as we have four relationships from property 2. This fact makes the interpretation of DOF difficult with such forms. With standard edge elements, for example, the DOF v_e is the integral of the 1 form $\sum_{e'} v_{e'} w^{e'}$ over edge e . In other words, the square matrix $A_{e e'} = \langle w^e, e' \rangle$ is the identity. This means that edges and forms are in duality. Here, we cannot expect to find a family of simple 1 chains such that each v_{ke} would be the integral of $\sum_{k,e} v_{ke} \lambda^{k w^e}$ over one of them, and have a null integral over all other chains of the family, that is a family of 1 chains in duality with the $\lambda^{k w^e}$. The most natural candidates, that is the ‘small edges’ $\{k, e\}$, fail because the square matrix $A_{\{k,e\} \{k',e'\}} = \langle \lambda^{k w^e}, \{k', e'\} \rangle$ is not the identity. Moreover, the matrix $A_{\{k,e\} \{k',e'\}}$ is not regular; we cannot invert it to find another family of chains, linear combinations of the $\{k, e\}$, in duality with $\lambda^{k w^e}$. We must be content with less: 1 cells such that integrals over them of $\sum_{k,e} v_{ke} \lambda^{k w^e}$ determine the v_{ke} and are in clear one-to-one correspondence with the basis forms $\lambda^{k w^e}$.

For property 3, we introduce some vocabulary. A family of vector spaces X^0, \dots, X^d (all on the same scalar field) and of linear maps A^p from X^{p-1} to X^p , $1 \leq p \leq d$, forms an ‘exact sequence at the level p ’ if $\text{image}(A^p) = \ker(A^{p+1})$ in case $1 \leq p \leq d-1$, if A^1 is injective in case $p = 0$, and if A^d is surjective in case $p = d$. It is customary to discuss sequences with the help of diagrams of the form $\{0\} \rightarrow X^0 \xrightarrow{A^1} X^1 \xrightarrow{A^2} \dots \rightarrow X^{d-1} \xrightarrow{A^d} X^d \rightarrow \{0\}$, where $\{0\}$ is the space of dimension 0. In such diagrams, arrows are labelled with operators, and the image, by any of these operators, of the space to the left of its arrow is in the kernel of the next operator on the right.

Property 3: If the set-union of all tetrahedra in the mesh can be contracted to one of its points by continuous deformation, the sequence $\{0\} \rightarrow W_{k+1}^0 \xrightarrow{\text{grad}} W_{k+1}^1 \xrightarrow{\text{curl}} W_{k+1}^2 \xrightarrow{\text{div}} W_{k+1}^3 \rightarrow \{0\}$ is exact at all levels p except $p = 0$.

Property 3 is quite technical to prove, owing to the difficulty of dealing with the singular matrix $A_{\{k,e\} \{k',e'\}}$. Its proof goes beyond the purpose of this contribution.

Property 4: Let h be the maximum diameter of the mesh tetrahedra and $I_{h,q}$ be the interpolation operator over W_q^p . The

interpolation error $\|u - I_{h,q} u\|$ over a bounded polyhedral domain Ω in the norm defined in W_q^p is $O(h^{\mu-1} q^{1-r})$ where $\mu = \min(r, q+1)$ and r is the regularity of the function u .

If the function u is smooth enough to have bounded derivatives such that $r \geq q+1$, then property 4 states that we can achieve super-algebraic convergence as we increase the polynomial order q and algebraic convergence as we decrease the mesh element size h . This estimate holds even when the weights $\langle \lambda^{k w^S}, \{k', S'\} \rangle$ are numerically computed by means of suitable high-order quadrature formulas. The proof of property 4 is challenging: it can be done theoretically for $p = 0$, whereas only numerically for $p \geq 1$. Preliminary numerical tests have been carried out in 2D with edge elements [14], and results are in agreement with the estimate of property 4.

4 Conclusions

To conclude, we will just recall how important it was, in the 1980s, when edge elements began to be adopted, to realise that gradients of nodal scalar functions were included in the span of edge elements: this is the reason why ‘spurious modes’ do not occur when edge elements are used to solve resonant cavity problems. However, this all important inclusion property is only a part of a larger frame: the ‘exact sequence’ property of Whitney forms. Hence higher-degree Whitney forms, whatever they are, must keep this property. We have shown here that this can be achieved without forfeiting another property of Whitney p forms, which also contributed to the popularity of edge elements: the natural association of degrees of freedom with geometric mesh elements of dimension p , namely the ‘small simplices’ discussed here.

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