

GENERATION OF HIGHER-ORDER POLYNOMIAL BASIS OF NÉDÉLEC H(CURL) FINITE ELEMENTS FOR MAXWELL'S EQUATIONS

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Abstract

The goal of this study is the automatic construction of a vectorial polynomial basis for Nédélec mixed finite elements [7], particular, the generation of finite elements without the expression of the polynomial basis functions, using symbolic calculus: the exhibition of basis functions has no practical interest.

Key words: Higher-order H(curl) Nédélec finite element, symbolic calculation.
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Introduction

This article addresses the need to increase the order of finite element methods in electromagnetism [3],[6],[9].

The important points in this presentation are:

- The option for the use of symbolic calculus which represents roughly 300 lines of Maple language, the use of which consists of:
 - . writing the general form of the polynomials
 - . writing the degrees of freedom
 - . solving the unisolvence system
 - . writing the masses and stiffness matrices analytically integrated

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- Characterization and determination of the polynomial spaces associated with the mixed finite elements of $H(\text{curl})$ in \mathbb{R}^3 , also called Nédélec finite elements.
- A new, algebraic characterization of the $H(\text{curl})$ conforming, respecting the continuity of the degrees of freedom and base functions. Taking account of these matricial relationships takes up roughly 500 lines in Fortran 90 language.

The results are presented conventionally with finite elements [7]. The value of this approach lies in the naturalness and simplicity of the formulation compared, for example, to [1],[2],[4],[5],[10], insofar as the approach extends the original text of Nédélec without introducing any polynomial functions other than those contained in this paper [7]. The only datum is the order of the finite element. Extension to quadrangles or to hexahedra can be made in a similar manner.

The algebraic answer to the problem of orientation, which is fundamental in mixed finite elements, is presented. It must be understood that with mixed finite elements the essential datum, in addition to the nodes and the connectivity of the meshes (triangles or tetrahedra) is the orientation. An orientation of the edges and faces (for tetrahedra) must be given *a priori*. Taking account of that orientation - whatever it is - is performed here in a matricial, algebraic manner, which is an important result of this study.

The aim here is to determine polynomial basis functions of triangular and tetrahedral elements for any order k . For that purpose, must first be expressed the polynomial space of start R^k for any order k then the mathematical expression of the degrees of freedom must be given and finally the unisolvance system must be solved. For all those steps, a symbolic mathematical program is used.

1 Finite elements of order k in \mathbb{R}^3 on tetrahedra

Let x, y, z be the current coordinates in \mathbb{R}^3 . Notations of certain polynomial spaces used to define Nédélec finite elements are recalled:

\mathbb{P}_k linear space of polynomials of degree $\leq k$,

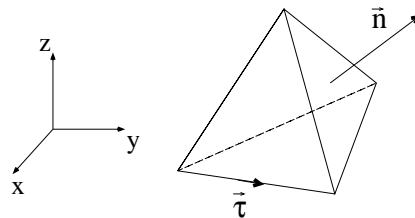


Fig. 1. Tetrahedron notations

$\tilde{\mathbb{P}}_k$ linear space of homogeneous polynomials of degree k ,

$$S^k = \{u \in (\tilde{\mathbb{P}}_k)^3, u_1x + u_2y + u_3z = 0\}.$$

Consider a tetrahedron K , with six edges Γ_i and unitary tangent vector $\vec{\tau}_i$, for

$i = 1, \dots, 6$, with four faces f_j and a unitary normal vector \vec{n}_j , for $j = 1, \dots, 4$. The finite element defined on K is considered, by the following linear space of polynomials of order k and class $H(curl)$:

$$R^k = (\mathbb{P}_{k-1})^3 \oplus S^k, \quad (1)$$

and according to figure 1 and the definition above, the set of linear forms as degrees of freedom (d.o.f.), first d.o.f. based on edges,

$$\int_{\Gamma_i} (\vec{p} \cdot \vec{\tau}_i) q(s) ds, \text{ for } q(s) \in \mathbb{P}_{k-1}, \quad (2)$$

then d.o.f. based on faces,

$$\int_{f_j} (\vec{p} \wedge \vec{n}_j) \cdot \vec{q} d\gamma, \text{ for } \vec{q} \in (\mathbb{P}_{k-2})^2, \quad (3)$$

and finally d.o.f. based on volumes,

$$\int_K \vec{p} \cdot \vec{r} dx dy dz, \text{ for } \vec{r} \in (\mathbb{P}_{k-3})^3. \quad (4)$$

The dimension of this finite element is given by [7]:

$$\dim R^k = \frac{(k+3)!}{2(k-1)!(k+1)}$$

2 Space of polynomials and degrees of freedom of k-order $H(curl)$ finite elements

The subject of interest is the k-order finite element built on a tetrahedron (see figure 1). In the sequel classical notations of finite elements are used: \hat{K} is the reference tetrahedron with nodes $(0, 0, 0)$, $(1, 0, 0)$, $(0, 1, 0)$, $(0, 0, 1)$, K is any tetrahedron of the mesh, \hat{f} a face of \hat{K} , f a face of K , etc. For each of the four faces \hat{f} with number $i \in \{1, 3, 5, 7\}$, the normal vectors $\vec{\hat{n}}_i$ are defined, with the notation $\vec{\hat{n}}_{i+1} = \vec{\hat{n}}_i$ for convenience, by (see figure 2):

$$\vec{\hat{n}}_1 = \begin{pmatrix} 0 \\ 0 \\ -1 \end{pmatrix}, \vec{\hat{n}}_3 = \begin{pmatrix} 0 \\ -1 \\ 0 \end{pmatrix}, \vec{\hat{n}}_5 = \begin{pmatrix} -1 \\ 0 \\ 0 \end{pmatrix}, \vec{\hat{n}}_7 = \frac{1}{\sqrt{3}} \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}.$$

To define these d.o.f., the following eight vectors are used (see figure 2):

$$\vec{\hat{q}}_1 = \vec{\hat{q}}_6 = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, \quad \vec{\hat{q}}_2 = \vec{\hat{q}}_3 = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}$$

$$\vec{\hat{q}}_4 = \vec{\hat{q}}_5 = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}, \quad \vec{\hat{q}}_7 = \begin{pmatrix} -1 \\ 1 \\ 0 \end{pmatrix}, \quad \vec{\hat{q}}_8 = \begin{pmatrix} -1 \\ -1 \\ 2 \end{pmatrix}.$$

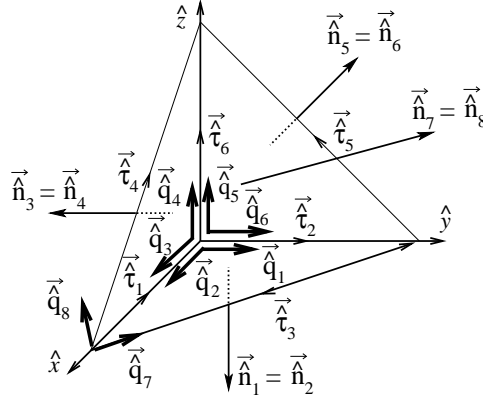


Fig. 2. k-order reference tetrahedron

2.1 Characterizing and determining S^k

To build R^k , the set S^k must first be explicitly determined. Monomials base functions were determined and chosen as weight functions. Any other choice of base to generate R^k is acceptable. For example, Legendre polynomials can be used as barycentric coordinates that can be employed as in the reference [1]. We prove that S^k is entirely described by the following polynomials vectors:

$$\text{for } 0 \leq m + n \leq k, m \neq 0 \text{ and } n \neq k : \begin{pmatrix} \hat{x}^{m-1} \hat{y}^n \hat{z}^{k-m-n+1} \\ 0 \\ -\hat{x}^m \hat{y}^n \hat{z}^{k-m-n} \end{pmatrix}, \quad (5)$$

$$\text{for } 0 \leq m + n \leq k, m \neq k \text{ and } n \neq 0 : \begin{pmatrix} 0 \\ \hat{x}^m \hat{y}^{n-1} \hat{z}^{k-m-n+1} \\ -\hat{x}^m \hat{y}^n \hat{z}^{k-m-n} \end{pmatrix}, \quad (6)$$

$$\text{for } m + n = k + 1, m \neq 0 \text{ and } n \neq 0 : \begin{pmatrix} \hat{x}^{m-1} \hat{y}^n \\ -\hat{x}^m \hat{y}^{n-1} \\ 0 \end{pmatrix}. \quad (7)$$

PROOF. Let d be the dimension of space. $\mathcal{N}_{k,d}$ is noted as the cardinal of polynomials S^k (in the sense of [7]). $\mathcal{N}_{k,d}^1$ is noted as the cardinal of polynomials given by (5) and (6). It is clear that this gives, with here, $d = 3$:

$$\mathcal{N}_{k,3} = 2\mathcal{N}_{k,3}^1 + \mathcal{N}_{k,2}$$

therefore:

$$\mathcal{N}_{k,3} = 2\mathcal{N}_{k,3}^1 + \mathcal{N}_{k,2}$$

and we have:

$$\mathcal{N}_{k,d}^1 = \frac{(d+k-2)!}{(d-1)!(k-1)!}$$

that is:

$$\mathcal{N}_{k,2}^1 = k \text{ and } \mathcal{N}_{k,3}^1 = \frac{(k+1)k}{2}$$

so that finally:

$$\mathcal{N}_{k,3} = k(k+2)$$

which is the dimension of S^k .

2.2 Definition of the degrees of freedom

A symbolic program is essentially used to create and solve the unisolvance system, thanks to which the polynomials in $\text{span}\{\vec{q}_i\}$ generating R^k and the degrees of freedom σ_i are defined. The symbolic calculus is then used to solve and find the $\vec{p}_i \in \text{span}\{\vec{q}_i\}$ which verify $\sigma_i(\vec{p}_i) = \delta_{ij}$.

$$\text{Let : } \vec{\hat{p}} = \begin{pmatrix} \hat{p}_1(\hat{x}, \hat{y}, \hat{z}) \\ \hat{p}_2(\hat{x}, \hat{y}, \hat{z}) \\ \hat{p}_3(\hat{x}, \hat{y}, \hat{z}) \end{pmatrix} \in R^k,$$

where $\hat{p}_i(\hat{x}, \hat{y}, \hat{z})$ are polynomials of order k in the variables \hat{x}, \hat{y} and \hat{z} defined by linear combination of monomials (5),(6) and (7).

The classic degrees of freedom are then chosen, namely those introduced by Nédélec, and based on the edges, the faces and the volume moments.

Degrees of freedom of edge type

If k is the order of the element, the number of edge d.o.f. is $n_e = 6k$ and following figure 2 with a parametrization on each edge $\hat{\Gamma}$ with tangent vector $\vec{\hat{\tau}}_i$, they are:
for $m = 1, \dots, k$

$$\int_0^1 -\hat{p}_1(1 - \hat{s}, 0, 0) \hat{s}^{m-1} d\hat{s} \quad (8)$$

$$\int_0^1 \hat{p}_2(0, \hat{s}, 0) \hat{s}^{m-1} d\hat{s} \quad (9)$$

$$\int_0^1 (\hat{p}_1(\hat{s}, 1 - \hat{s}, 0) - \hat{p}_2(\hat{s}, 1 - \hat{s}, 0)) \hat{s}^{m-1} d\hat{s} \quad (10)$$

$$\int_0^1 (-\hat{p}_1(1 - \hat{s}, 0, \hat{s}) + \hat{p}_3(1 - \hat{s}, 0, \hat{s})) \hat{s}^{m-1} d\hat{s} \quad (11)$$

$$\int_0^1 (\hat{p}_2(0, \hat{s}, 1 - \hat{s}) - \hat{p}_3(0, \hat{s}, 1 - \hat{s})) \hat{s}^{m-1} d\hat{s} \quad (12)$$

$$\int_0^1 \hat{p}_3(0, 0, \hat{s}) \hat{s}^{m-1} d\hat{s} \quad (13)$$

Volume type degrees of freedom

For k the element order, $n_v = k(k-1)(k-2)/2$ the number of volume degrees of freedom, these d.o.f. are, for $m + n + l \leq k - 3$:

$$\int_0^1 \int_0^{1-\hat{x}} \int_0^{1-\hat{x}-\hat{y}} \hat{p}_1(\hat{x}, \hat{y}, \hat{z}) \hat{x}^m \hat{y}^n \hat{z}^l d\hat{x}d\hat{y}d\hat{z} \quad (14)$$

$$\int_0^1 \int_0^{1-\hat{x}} \int_0^{1-\hat{x}-\hat{y}} \hat{p}_2(\hat{x}, \hat{y}, \hat{z}) \hat{x}^m \hat{y}^n \hat{z}^l d\hat{x}d\hat{y}d\hat{z} \quad (15)$$

$$\int_0^1 \int_0^{1-\hat{x}} \int_0^{1-\hat{x}-\hat{y}} \hat{p}_3(\hat{x}, \hat{y}, \hat{z}) \hat{x}^m \hat{y}^n \hat{z}^l d\hat{x}d\hat{y}d\hat{z} \quad (16)$$

Face type degrees of freedom

If k is the order of the element, $n_f = 4k(k-1)$ the number of faces degrees of freedom, we define according to figure 2, for $m + n \leq k - 2$:

$$\int_0^1 \int_0^{1-\hat{u}} (\vec{\hat{p}}(\hat{v}, \hat{u}, 0) \wedge \vec{\hat{n}}_1) \cdot \vec{\hat{q}}_1 \hat{u}^m \hat{v}^n d\hat{u}d\hat{v} \quad (17)$$

$$\int_0^1 \int_0^{1-\hat{u}} (\vec{\hat{p}}(\hat{v}, \hat{u}, 0) \wedge \vec{\hat{n}}_2) \cdot \vec{\hat{q}}_2 \hat{u}^m \hat{v}^n d\hat{u}d\hat{v} \quad (18)$$

$$\int_0^1 \int_0^{1-\hat{u}} (\vec{\hat{p}}(\hat{u}, 0, \hat{v}) \wedge \vec{\hat{n}}_3) \cdot \vec{\hat{q}}_3 \hat{u}^m \hat{v}^n d\hat{u}d\hat{v} \quad (19)$$

$$\int_0^1 \int_0^{1-\hat{u}} (\vec{\hat{p}}(\hat{u}, 0, \hat{v}) \wedge \vec{\hat{n}}_4) \cdot \vec{\hat{q}}_4 \hat{u}^m \hat{v}^n d\hat{u}d\hat{v} \quad (20)$$

$$\int_0^1 \int_0^{1-\hat{u}} (\vec{\hat{p}}(0, \hat{v}, \hat{u}) \wedge \vec{\hat{n}}_5) \cdot \vec{\hat{q}}_5 \hat{u}^m \hat{v}^n d\hat{u}d\hat{v} \quad (21)$$

$$\int_0^1 \int_0^{1-\hat{u}} (\vec{\hat{p}}(0, \hat{v}, \hat{u}) \wedge \vec{\hat{n}}_6) \cdot \vec{\hat{q}}_6 \hat{u}^m \hat{v}^n d\hat{u}d\hat{v} \quad (22)$$

$$\int_0^1 \int_0^{1-\hat{u}} (\vec{\hat{p}}(1-\hat{u}-\hat{v}, \hat{u}, \hat{v}) \wedge \vec{\hat{n}}_7) \cdot \vec{\hat{q}}_7 \hat{u}^m \hat{v}^n d\hat{u}d\hat{v} \quad (23)$$

$$\int_0^1 \int_0^{1-\hat{u}} (\vec{\hat{p}}(1-\hat{u}-\hat{v}, \hat{u}, \hat{v}) \wedge \vec{\hat{n}}_8) \cdot \vec{\hat{q}}_8 \hat{u}^m \hat{v}^n d\hat{u}d\hat{v} \quad (24)$$

3 Change of bases for the degrees of freedom to preserve $H(\text{curl})$ continuity

The second part of this work concerns the transformations of the reference element into a mesh element, and the problem of orientation. This is covered in this paragraph. The transformations of the reference element into any cell are independent of the basis functions but dependent upon the degrees of freedom and of course on the order, in other words on the orientation chosen in the mesh.

As the $H(\text{curl})$ finite elements are invariant by affine transformation if a given (3×3) matrice B , is used :

$$\vec{p} = B^{*-1} \vec{\hat{p}}$$

affine equivalent finite elements can be defined [6],[7].

3.1 Change of bases for edge degree of freedom

For all numbers i of an edge $\hat{\Gamma}$, $\vec{\hat{p}}_j$ must be found, such that $\hat{\sigma}_i(\vec{\hat{p}}_j) = \delta_{ij}$, where δ_{ij} is the kronecker symbol and where for these degrees of freedom, for $i = 1, \dots, k$:

$$\hat{\sigma}_i(\vec{\hat{p}}_j) = \int_{\hat{\Gamma}} \vec{\hat{p}}_j \cdot \vec{\hat{\tau}} \hat{s}^{i-1} d\hat{s}$$

We define:

$$\vec{\tilde{p}}_j = B^{*-1} \vec{\hat{p}}_j$$

We suppose that the degrees of freedom for each edge Γ of a tetrahedron K are, for $i = 1, \dots, k$:

$$\tilde{\sigma}_i(\vec{\tilde{p}}_j) = \int_{\Gamma} \vec{\tilde{p}}_j \cdot \vec{\tau} s^{i-1} ds$$

Then $\tilde{\sigma}_i$ verifies: $\tilde{\sigma}_i(\vec{\tilde{p}}_j) = \hat{\sigma}_i(\vec{\hat{p}}_j) = \delta_{ij}$.

We define: $\sigma_i(\vec{p}) = \tilde{\sigma}_i(\vec{\tilde{p}})$ when the edge Γ is covered in the same way as $\hat{\Gamma}$. If this

edge is covered in the opposite way, we define, with reference to a parametrization of Γ on the interval $[0, 1]$:

$$\sigma_i(\vec{p}) = - \int_{\Gamma} \vec{p} \cdot \vec{\tau} (1-s)^{i-1} ds$$

Then the matrix: $A_e = (a_{il}^e)$ is formally defined, where $a_{il}^e = (-1)^{l+1} \binom{i-1}{l}$, if $(i-1) \geq l$ and $a_{il}^e = 0$ otherwise. This gives:

$$\begin{pmatrix} \sigma_1 \\ \dots \\ \sigma_i \\ \dots \\ \sigma_k \end{pmatrix} = A_e \begin{pmatrix} \tilde{\sigma}_1 \\ \dots \\ \tilde{\sigma}_i \\ \dots \\ \tilde{\sigma}_k \end{pmatrix} \quad (25)$$

Then as $H(curl)$ compatible basis $\text{Span}\{\vec{p}_i\}$ related to the edges, must be chooses the following:

$$\begin{pmatrix} \vec{p}_1 \\ \dots \\ \vec{p}_i \\ \dots \\ \vec{p}_k \end{pmatrix} = {}^t A_e \begin{pmatrix} \vec{p}_1 \\ \dots \\ \vec{p}_i \\ \dots \\ \vec{p}_k \end{pmatrix}. \quad (26)$$

3.2 Change of bases for faces degree of freedom

As for the edges, the $H(curl)$ continuity at the faces interfaces must be formulated. This study is restricted to the second order case; the k-order general case will be presented in a paper to be published.

For all numbers i of a face \hat{f} , \vec{p}_j must be found such that $\hat{\sigma}_i(\vec{p}_j) = \delta_{ij}$, where for these degrees of freedom:

$$\hat{\sigma}_i(\vec{p}_j) = \frac{1}{|\hat{f}|} \int_{\hat{f}} (\vec{p}_j \wedge \vec{n}) \cdot \vec{q}_i d\gamma$$

This gives:

$$\hat{\sigma}_i(\vec{p}_j) = \tilde{\sigma}_i(\vec{p}_j) = \frac{1}{|f|} \int_f (\vec{p}_j \wedge \vec{n}) \cdot \vec{u}_i d\gamma$$

where: $\vec{p}_j = B^{*-1} \vec{\hat{p}}_j$ and $\vec{u}_i = B(\vec{\hat{n}} \wedge \vec{\hat{q}}_i) \wedge \vec{n}$. The degree of freedom for a face f in the mesh is defined by:

$$\sigma_i(\vec{p}) = \frac{1}{|f|} \int_f (\vec{p} \wedge \vec{n}) \cdot \vec{q}_i d\gamma$$

where $\vec{q}_i = \frac{B\vec{\hat{q}}_i}{|B\vec{\hat{q}}_i|}$ and $\vec{q}_{i+1} = \vec{q}_i^\perp, \vec{q}_{i+1} \subset f$, for $i \in \{1, 3, 5, 7\}$. Then basis functions \vec{p}_j related to faces are sought verifying:

$$\sigma_i(\vec{p}_j) = \tilde{\sigma}_i(B^{*-1} \vec{\hat{p}}_j) = \delta_{ij}$$

To that end - according to the figure - the \vec{u}_i on each orthonormal vector base face $(\vec{q}_i, \vec{q}_{i+1})$ is decomposed, so that:

$$\vec{u}_i = \alpha_i \vec{q}_i + \beta_i \vec{q}_{i+1}$$

$$\vec{u}_{i+1} = \alpha_{i+1} \vec{q}_i + \beta_{i+1} \vec{q}_{i+1}$$

For the degrees of freedom, this gives:

$$\tilde{\sigma}_i = \alpha_i \sigma_i + \beta_i \sigma_{i+1}$$

$$\tilde{\sigma}_{i+1} = \alpha_{i+1} \sigma_i + \beta_{i+1} \sigma_{i+1}$$

or with the (2×2) matrix $A_f = \begin{pmatrix} \alpha_i & \beta_i \\ \alpha_{i+1} & \beta_{i+1} \end{pmatrix}$.

$$\begin{pmatrix} \sigma_i \\ \sigma_{i+1} \end{pmatrix} = A_f^{-1} \begin{pmatrix} \tilde{\sigma}_i \\ \tilde{\sigma}_{i+1} \end{pmatrix} \quad (27)$$

finally the effective vectorial basis on face f is taken to be:

$$\begin{pmatrix} \vec{p}_j \\ \vec{p}_{j+1} \end{pmatrix} = {}^t A_f \begin{pmatrix} \vec{\hat{p}}_j \\ \vec{\hat{p}}_{j+1} \end{pmatrix}. \quad (28)$$

4 Obtention of mass and stiffness matrices

Finally, the symbolic program is again used to form the mass matrix and elementary stiffness, such that the expression of the elementary matrices of the linearized problem is totally automatic and the final form of the basis functions is determined solely by the choice of the degrees of freedom. In particular, the polynomials are not presented in their explicit form as only the calculation of the matricial terms matters.

Let Ω be a simply connected polyhedron domain in \mathbb{R}^3 and τ_h a conformal and regular partition of Ω into tetrahedra $\{K\}$. On the reference element \hat{K} the mass and stiffness matrices can be defined:

$$\hat{M} = (\hat{m}_{ij})$$

$$\hat{K} = (\hat{k}_{ij})$$

where

$$\hat{m}_{ij} = \int_{\hat{K}} \vec{\hat{p}}_i \cdot \vec{\hat{p}}_j d\hat{x}d\hat{y}d\hat{z} \quad (29)$$

$$\hat{k}_{ij} = \int_{\hat{K}} \text{curl } \vec{\hat{p}}_i \cdot \text{curl } \vec{\hat{p}}_j d\hat{x}d\hat{y}d\hat{z} \quad (30)$$

For that purpose, a symbolic program (Maple) is used to make an exact integration of these integrals with a simplification by the 6 factors of the symmetric matrix $(BB^*)^{-1}$.

In fact, taking $\vec{\hat{p}}_i = B^{*-1} \vec{\hat{p}}_i$, the integral (29) and (30) are algebraically computed, with respectively 6 real coefficients μ_l and κ_l and the results may be simplified under the simple form:

$$m_{ij} = \sum_{1 \leq l \leq 6} \mu_l b_l$$

$$k_{ij} = \sum_{1 \leq l \leq 6} \kappa_l b_l$$

with :

$$(B^*B)^{-1} = \begin{pmatrix} b_1 & b_4 & b_6 \\ b_4 & b_2 & b_5 \\ b_6 & b_5 & b_3 \end{pmatrix} \quad (31)$$

Conclusion

The systems $\hat{\sigma}_i(\vec{\hat{p}}_j) = \delta_{ij}$ with relations (1) to (20) and equations (25)-(26), are solved with symbolic calculus (see the appendix). Although polynomial vector bases are effectively produced by these equations, their contents never appear. The genericity of the finite element (calculation starting from an domain of reference) must be completed, i.e. corrected, to take account of the orientation. The orientation is *a priori* data on the given mesh, expressed by an algebraic modification of the elementary matrix for those of the d.o.f. the orientation of which is nil in conformity with the reference domain. It is at the same time necessary to consider for each element the numbering of the d.o.f. to assign the terms of the matrices and it is necessary next for each element to consider the change in orientation between the reference element and the element in the mesh:

- affine transformation point by point for integration with appropriate numbering of the mesh,

- transformation of the orientations taken into account for each element.

The main effort will then be devoted to the $H(\text{curl})$ compatibility equations (25) through (28) that must be processed with a small but not easy to handle program. The practical process presented here is at the same time traditional and general. Its main properties are:

- it uses calculation symbolic system (dynamic mathematics),
- it never presents, whatever the order, the explicit polynomial vector functions form.

This method can be extended to the $H(\text{div})$ conforming finite elements [8], and more generally to any mixed finite elements using such degrees of freedom.

APPENDIX: a basis polynomial functions construction Maple program, can be found in [11]

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