

ON THE CONSTRUCTION OF WELL-CONDITIONED HIERARCHICAL BASES FOR TETRAHEDRAL $\mathcal{H}(\mathbf{curl})$ -CONFORMING NÉDÉLEC ELEMENT*

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Abstract

A partially orthonormal basis is constructed with better conditioning properties for tetrahedral $\mathcal{H}(\mathbf{curl})$ -conforming Nédélec elements. The shape functions are classified into several categories with respect to their topological entities on the reference 3-simplex. The basis functions in each category are constructed to achieve maximum orthogonality. The numerical study on the matrix conditioning shows that for the mass and quasi-stiffness matrices, and in a logarithmic scale the condition number grows linearly vs. order of approximation up to order three. For each order of approximation, the condition number of the quasi-stiffness matrix is about one order less than the corresponding one for the mass matrix. Also, up to order six of approximation the conditioning of the mass and quasi-stiffness matrices with the proposed basis is better than the corresponding one with the Ainsworth-Coyle basis *Internat. J. Numer. Methods. Engrg.*, 58:2103–2130, 2003. except for order four with the quasi-stiffness matrix. Moreover, with the new basis the composite matrix $\mu M + S$ has better conditioning than the Ainsworth-Coyle basis for a wide range of the parameter μ .

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Key words: Hierarchical bases, Tetrahedral $\mathcal{H}(\mathbf{curl})$ -conforming elements, Matrix conditioning.

1. Introduction

The Nédélec elements [20] are the natural choices when problems in electromagnetism are solved by the conforming finite element methods. Hierarchical bases are more convenient to use when the p -refinement technique is applied with the finite element methods [7]. Webb [28] constructed hierarchical vector bases of arbitrary order for triangular and tetrahedral finite elements. It was shown [12] that the basis functions in [28] indeed span the true Nédélec space defined in [20]. A basis in terms of the affine coordinates was also given [12]. Inspired by

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Nédélec's foundational work [20] and following Webb [28], many researchers had constructed various hierarchical bases for several commonly known elements in 2D and 3D [1, 3–5, 15, 16, 21, 25, 27]. From the perspective of differential forms, Hiptmair [13] laid a general framework for canonical construction of $\mathcal{H}(\mathbf{curl})$ - and $\mathcal{H}(\text{div})$ -conforming finite elements. In this respect, the reader is referred to the works [14, 22–24] and the monograph [9].

One problem with hierarchical bases is the matrix ill-conditioning when higher-order bases are applied [2, 28, 31, 32]. For a hierarchical basis to be useful, the issue of ill-conditioning has to be resolved. Using Gram-Schmidt orthogonalization procedure Webb [28] gave the explicit formulas of the basis functions up to order three for triangular and tetrahedral elements. Following the same line of development [28], i.e., decomposing the basis functions into rotational and irrotational groups, Sun and collaborators [27] investigated the conditioning issue more carefully and also gave the basis functions up to the third order. Ainsworth and Coyle [3] studied both the dispersive and conditioning issues for the hierarchical basis on the hybrid quadrilateral/triangular meshes. With the aid of Jacobi polynomials, the interior bubble functions are made orthogonal over an equilateral reference triangle [3]. With this partial orthogonality it was shown that the condition numbers of both the mass matrix and the stiffness matrix could be reduced significantly [3]. Using Legendre polynomials Jørgensen et al. constructed a near-orthogonal basis for the quadrilaterals and suggested that the same procedure could be applied for the triangles with the help of collapsed coordinate system [17]. Partially addressing the conditioning issue, Schöberl and Zaglmayr [25] created bases for high-order Nédélec elements with the property of local complete sequence. The key components in their construction [25] are using (i) the gradients of scalar basis functions and, (ii) scaled and integrated Legendre polynomials. However, the ill-conditioning issue was pronounced with higher-order approximation and moderate growth of the condition number was reported [25]. A new hierarchical basis with uncommon orthogonality properties was constructed by Ingelström [15] for tetrahedral meshes. It is shown that higher-order basis functions vanished if they were projected onto the relatively lower-order $\mathcal{H}(\mathbf{curl})$ -conforming spaces [15] using the Nédélec interpolation operator [20], and [15] such a basis was well suited for multi-level solvers. Using the orthogonalization procedure by Sheshevskii [26] and conforming to the Nédélec [20] condition, Abdul-Rahman and Kasper proposed a new hierarchical basis for the tetrahedral element [1].

The Gram-Schmidt scheme used by Webb [28] or the orthogonalization method applied by Abdul-Rahman and Kasper [1] involves a linear system of equations to be solved, and the coefficients associated with the basis functions in general cannot be expressed in closed forms. The focus of the current work is to investigate the possibility of constructing a well-conditioned hierarchical basis for the tetrahedral $\mathcal{H}(\mathbf{curl})$ -conforming elements without recourse to the Gram-Schmidt orthogonalization. The construction is made possible by the results of orthogonal polynomials of several variables on an n -simplex [11]. The basis functions of any approximation order are given explicitly in closed form. Our work is based upon the studies by Ainsworth and Coyle [5], and by Schöberl and Zaglmayr [25]. The main goal of this study is to try to resolve the conditioning issue or at least partially, which was missed in the study by Ainsworth and Coyle [5].

The rest of this paper is organized as follows. The construction of basis functions is given in Section 2. Numerical results of matrix conditioning and sparsity are shown in Section 3. Concluding remarks are included in Section 4.

2. Construction of Basis Functions

We construct basis functions for the $\mathcal{H}(\mathbf{curl})$ -conforming elements on the reference 3-simplex. The construction is based upon the work [5, 25, 30].

2.1. Preliminary Results

Let K^n be the simplex in \mathbb{R}^n , i.e.,

$$K^n := \left\{ \mathbf{x} \in \mathbb{R}^n : 0 \leq x_i; \sum_{i=1}^n x_i \leq 1 \right\}. \quad (2.1)$$

The notation $|\mathbf{x}|$ means the discrete ℓ^1 norm for a generic point $\mathbf{x} \in K^n$, i.e.,

$$|\mathbf{x}| = \sum_{i=1}^n |x_i|. \quad (2.2)$$

Denote \mathbf{x}_i the truncation or projection of the point \mathbf{x} in the first i -dimensions, viz.,

$$\mathbf{x}_0 := 0, \quad \mathbf{x}_i := (x_1, x_2, \dots, x_i), \quad 1 \leq i \leq n. \quad (2.3)$$

For a point $\vec{\alpha} \in \mathbb{N}_0^n$, denote $\vec{\alpha}^i$ the truncation or projection of the point $\vec{\alpha}$ from the i -th dimension, i.e.,

$$\vec{\alpha}^i := (\alpha_i, \alpha_{i+1}, \dots, \alpha_n), \quad 1 \leq i \leq n. \quad (2.4)$$

For a point $\vec{\tau} \in \mathbb{R}^{n+1}$, the notation $\vec{\tau}^i$ is similarly defined as in $\vec{\alpha}^i$, viz.,

$$\vec{\tau}^i := (\tau_i, \tau_{i+1}, \dots, \tau_{n+1}), \quad 1 \leq i \leq n+1. \quad (2.5)$$

It is shown [11] that the weight function associated with the classic orthogonal polynomials on K^n takes the form

$$W_{\vec{\tau}}^{(K^n)}(\mathbf{x}) = (1 - |\mathbf{x}|)^{\tau_{n+1} - \frac{1}{2}} \prod_{i=1}^n x_i^{\tau_i - \frac{1}{2}}, \quad \mathbf{x} \in K^n, \quad \tau_i \geq -\frac{1}{2}, \quad i = 1, 2, \dots, n+1. \quad (2.6)$$

The basis functions are constructed with the aid of the following theorem on orthogonal polynomials over an n -simplex K^n [11].

Theorem 2.1. *The polynomials*

$$P_{\vec{\alpha}} \left(W_{\vec{\tau}}^{(K^n)}; \mathbf{x} \right) = \left[h_{\vec{\alpha}}^{(K^n)} \right]^{-1} \prod_{i=1}^n \left(\frac{1 - |\mathbf{x}_i|}{1 - |\mathbf{x}_{i-1}|} \right)^{|\vec{\alpha}^{i+1}|} p_{\alpha_i}^{(\rho_i^1, \rho_i^2)} \left(\frac{2x_i}{1 - |\mathbf{x}_{i-1}|} - 1 \right), \quad (2.7a)$$

where $p_{\alpha_i}^{(\rho_i^1, \rho_i^2)}$ is the classic orthonormal Jacobi polynomials of one variable,

$$\rho_i^1 = 2|\vec{\alpha}^{i+1}| + |\vec{\tau}^{i+1}| + \frac{1}{2}(n - i - 1), \quad \rho_i^2 = \tau_i - \frac{1}{2},$$

are orthonormal, the normalization constant $h_{\vec{\alpha}}^{(K^n)}$ is given by

$$\left[h_{\vec{\alpha}}^{(K^n)} \right]^{-2} = \prod_{i=1}^n 2^{\rho_i^1 + \rho_i^2 + 1}, \quad (2.7b)$$

and the weight function takes the form in Eq. (2.6).

The proof of Theorem 2.1 can be found in [11]. However, the normalization constant $h_{\vec{\alpha}}^{(K^n)}$ given in [11] is wrong, which has been corrected by formula (2.7b). For details, please refer to [30].

2.2. Construction on the 3-simplex

Using the result in Theorem 2.1, we construct shape functions for the $\mathcal{H}(\mathbf{curl})$ -conforming element. The shape functions are grouped into several categories based upon their topological entities on the reference 3-simplex. If possible, the basis functions in each category are constructed so that they are orthonormal on the reference element.

Any point in the 3-simplex is uniquely located in terms of the local coordinate system (ξ, η, ζ) . The vertexes are numbered as $\mathbf{v}_0(0, 0, 0), \mathbf{v}_1(1, 0, 0), \mathbf{v}_2(0, 1, 0), \mathbf{v}_3(0, 0, 1)$. The barycentric coordinates are given as

$$\lambda_0 = 1 - \xi - \eta - \zeta, \quad \lambda_1 = \xi, \quad \lambda_2 = \eta, \quad \lambda_3 = \zeta. \quad (2.8)$$

The directed tangent on a generic edge $\mathbf{e}_j = [j_1, j_2]$ is defined as

$$\tau^{\mathbf{e}_j} := \tau^{[j_1, j_2]} = \mathbf{v}_{j_2} - \mathbf{v}_{j_1}, \quad j_1 < j_2. \quad (2.9)$$

The edge is parametrized as

$$\gamma_{\mathbf{e}_j} := \lambda_{j_2} - \lambda_{j_1}, \quad j_1 < j_2. \quad (2.10)$$

2.2.1. Edge functions

A generic edge can be uniquely identified with

$$\mathbf{e}_j = [j_1, j_2], \quad j_1 = 0, 1, 2, \quad j_1 < j_2 \leq 3, \quad j = j_1 + j_2 + \text{sgn}(j_1). \quad (2.11)$$

Lowest order:

The shape functions for the lowest order, also called the Whitney element [9, 29], are given as

$$\Phi_0^{\mathbf{e}_j} = |\tau^{\mathbf{e}_j}| (\lambda_{j_2} \nabla \lambda_{j_1} - \lambda_{j_1} \nabla \lambda_{j_2}). \quad (2.12)$$

The tangential component of the function $\Phi_0^{\mathbf{e}_j}$ on its associated edge is unit and vanishes on other five edges, viz., it has the property

$$\mathbf{e}_k \cdot (\Phi_0^{\mathbf{e}_j}) = \delta_{jk}, \quad \{j, k\} = 1, \dots, 6. \quad (2.13)$$

where δ_{jk} is the Kronecker delta. Further, the shape functions are divergence-free, viz.,

$$\nabla \cdot \Phi_0^{\mathbf{e}_j} = 0, \quad j = 1, \dots, 6. \quad (2.14)$$

Higher order:

The shape functions for higher-order of approximation are constructed so that they are curl-free. The explicit formula is given by

$$\Phi_i^{\mathbf{e}_j} = \sqrt{\frac{2i+1}{2}} P_i(\gamma_{\mathbf{e}_j}) \frac{\nabla \gamma_{\mathbf{e}_j}}{|\gamma_{\mathbf{e}_j}|}, \quad i = 1, \dots, p, \quad j = 1, \dots, 6. \quad (2.15)$$

In addition to the curl-free property of these functions, viz.,

$$\nabla \times \Phi_i^{\mathbf{e}_j} = \mathbf{0}, \quad i = 1, \dots, p, \quad j = 1, \dots, 6, \quad (2.16)$$

the trace of which on the associated edge is orthonormal, viz.,

$$\langle \Phi_i^{\mathbf{e}_j}, \Phi_k^{\mathbf{e}_j} \rangle|_{\mathbf{e}_j} = \delta_{ik}, \quad \{i, k\} = 1, \dots, p, \quad j = 1, \dots, 6. \quad (2.17)$$

Property (2.16) follows from the fact that the shape function $\Phi_i^{\mathbf{e}_j}$ can be written as the gradient of a certain function. Property (2.17) can be proved by the orthogonality of the Legendre polynomials.

2.2.2. Face functions

Each face on the 3-simplex is uniquely defined as

$$\mathbf{f}_{j_1} = [j_2, j_3, j_4], \quad 0 \leq \{j_1, j_2, j_3, j_4\} \leq 3, \quad j_2 < j_3 < j_4. \quad (2.18)$$

The face functions are further grouped into two categories [5] - edge-based face functions and face bubble functions.

Edge-based face functions:

These functions are associated with the three edges of a certain face \mathbf{f}_{j_1} , and have non-zero tangential components only on the associated face \mathbf{f}_{j_1} . Using the results in Theorem 2.1, the orthonormal shape functions are give as

$$\Phi_{\mathbf{e}=[k_1, k_2]}^{\mathbf{f}_{j_1}, i} = C_i \lambda_{k_1} \lambda_{k_2} (1 - \lambda_{k_1})^i P_i^{(1,2)} \left(\frac{2\lambda_{k_2}}{1 - \lambda_{k_1}} - 1 \right) \frac{\nabla \lambda_{k_3}}{|\nabla \lambda_{k_3}|}, \quad (2.19a)$$

where

$$C_i = (i+3) \sqrt{\frac{(2i+4)(2i+5)(2i+7)}{i+1}}, \quad 0 \leq i \leq p-2, \quad (2.19b)$$

$$k_1 = \{j_2, j_3\}, \quad k_2 = \{j_3, j_4\}, \quad k_1 < k_2, \quad k_3 = \{j_2, j_3, j_4\} \setminus \{k_1, k_2\}. \quad (2.19c)$$

In the formula (2.19a), the function $P_i^{(1,2)}(\bullet)$ is the classic *un-normalized* Jacobi polynomial of degree i with a single variable [19]. Again, by the results in Theorem 2.1, one can prove the orthonormal property of edge-based face functions

$$\left\langle \Phi_{\mathbf{e}=[k_1, k_2]}^{\mathbf{f}_{j_1}, m}, \Phi_{\mathbf{e}=[k_1, k_2]}^{\mathbf{f}_{j_1}, n} \right\rangle_{K^3} = \delta_{mn}, \quad \{m, n\} = 0, 1, \dots, p-2. \quad (2.20)$$

Face bubble functions:

The face bubble functions, which belong to each specific set and are associated with a particular face \mathbf{f}_{j_1} , vanish on all other three faces. In view of the results in Theorem 2.1, the explicit formula is given as

$$\begin{aligned} \Phi_{m,n}^{\mathbf{f}_{j_1}, j_3} &= \Upsilon (1 - \lambda_{j_2})^m (1 - \lambda_{j_2} - \lambda_{j_3})^n \\ &\times P_m^{(2n+3,2)} \left(\frac{2\lambda_{j_3}}{1 - \lambda_{j_2}} - 1 \right) P_n^{(0,2)} \left(\frac{2\lambda_{j_4}}{1 - \lambda_{j_2} - \lambda_{j_3}} - 1 \right) \frac{\tau^{[j_2, j_3]}}{|\tau^{[j_2, j_3]}|}, \end{aligned} \quad (2.21a)$$

$$\begin{aligned} \Phi_{m,n}^{\mathbf{f}_{j_1}, j_4} &= \Upsilon (1 - \lambda_{j_2})^m (1 - \lambda_{j_2} - \lambda_{j_3})^n \\ &\times P_m^{(2n+3,2)} \left(\frac{2\lambda_{j_3}}{1 - \lambda_{j_2}} - 1 \right) P_n^{(0,2)} \left(\frac{2\lambda_{j_4}}{1 - \lambda_{j_2} - \lambda_{j_3}} - 1 \right) \frac{\tau^{[j_2, j_4]}}{|\tau^{[j_2, j_4]}|}, \end{aligned} \quad (2.21b)$$

where

$$\Upsilon = C_m^{n,1} C_m^{n,2} \lambda_{j_2} \lambda_{j_3} \lambda_{j_4}, \quad (2.21c)$$

$$C_m^{n,1} = \sqrt{(2n+3)(m+n+3)(m+2n+4)(m+2n+5)}, \quad (2.21d)$$

$$C_m^{n,2} = \frac{\sqrt{(2m+2n+7)(2m+2n+8)(2m+2n+9)}}{\sqrt{(m+1)(m+2)}}, \quad (2.21e)$$

$$0 \leq \{m, n\}, m+n \leq p-3. \quad (2.21f)$$

The face bubble functions again share the orthonormal property on the reference 3-simplex

$$\left\langle \Phi_{m_1,n_1}^{\mathbf{f}_{j_1},j_3}, \Phi_{m_2,n_2}^{\mathbf{f}_{j_1},j_3} \right\rangle_{K^3} = \delta_{m_1 m_2} \delta_{n_1 n_2}, \\ 0 \leq \{m_1, m_2, n_1, n_2\}, m_1 + n_1, m_2 + n_2 \leq p - 3, \quad (2.22a)$$

$$\left\langle \Phi_{m_1,n_1}^{\mathbf{f}_{j_1},j_4}, \Phi_{m_2,n_2}^{\mathbf{f}_{j_1},j_4} \right\rangle_{K^3} = \delta_{m_1 m_2} \delta_{n_1 n_2}, \\ 0 \leq \{m_1, m_2, n_1, n_2\}, m_1 + n_1, m_2 + n_2 \leq p - 3. \quad (2.22b)$$

2.2.3. Interior functions

The interior functions are also classified into two categories: face-based interior functions and interior bubble functions.

Face-based interior functions:

The face-based interior functions which are associated with a particular face \mathbf{f}_{j_1} have non-zero normal components only on the associated face, and have no contribution to the tangential components on all four faces. Utilizing the results in Theorem 2.1, the formulas of these functions are given as

$$\Phi_{m,n}^{\mathbf{t},\mathbf{f}_{j_1}} = \Upsilon (1 - \lambda_{j_2})^m (1 - \lambda_{j_2} - \lambda_{j_3})^n \\ \times P_m^{(2n+3,2)} \left(\frac{2\lambda_{j_3}}{1-\lambda_{j_2}} - 1 \right) P_n^{(0,2)} \left(\frac{2\lambda_{j_4}}{1-\lambda_{j_2}-\lambda_{j_3}} - 1 \right) \frac{\nabla \lambda_{j_1}}{|\nabla \lambda_{j_1}|}, \quad (2.23a)$$

where

$$\Upsilon = C_m^{m,1} C_m^{n,2} \lambda_{j_2} \lambda_{j_3} \lambda_{j_4}, \quad (2.23b)$$

$$0 \leq \{m, n\}, m + n \leq p - 3. \quad (2.23c)$$

The face-based interior functions enjoy the orthonormal property on the reference 3-simplex

$$\left\langle \Phi_{m_1,n_1}^{\mathbf{t},\mathbf{f}_{j_1}}, \Phi_{m_2,n_2}^{\mathbf{t},\mathbf{f}_{j_1}} \right\rangle_{K^3} = \delta_{m_1 m_2} \delta_{n_1 n_2}, \quad 0 \leq \{m_1, m_2, n_1, n_2\}, m_1 + n_1, m_2 + n_2 \leq p - 3. \quad (2.24)$$

Interior bubble functions:

The interior bubble functions have both vanishing tangential and normal components on all four faces of the reference 3-simplex. Similarly, by using the results in Theorem 2.1, the formulas of these functions are given as

$$\Phi_{\ell,m,n}^{\mathbf{t},\vec{e}_d} = \Psi P_\ell^{(2m+2n+8,2)} (2\lambda_1 - 1) \\ \times P_m^{(2n+5,2)} \left(\frac{2\lambda_2}{1-\lambda_1} - 1 \right) P_n^{(2,2)} \left(\frac{2\lambda_3}{1-\lambda_1-\lambda_2} - 1 \right) \vec{e}_d, \quad (2.25a)$$

where

$$\Psi = C_{\ell,m,n} \lambda_0 \lambda_1 \lambda_2 \lambda_3 (1 - \lambda_1)^m (1 - \lambda_1 - \lambda_2)^n, \quad (2.25b)$$

$$C_{\ell,m,n} = C_{\ell,m,n}^1 C_{\ell,m,n}^2, \quad (2.25c)$$

$$C_{\ell,m,n}^1 = \sqrt{\frac{(\ell + 2m + 2n + 9)(\ell + 2m + 2n + 10)(2\ell + 2m + 2n + 11)(m + 2n + 6)}{(\ell + 1)(m + 1)(n + 1)}}, \quad (2.25d)$$

$$C_{\ell,m,n}^2 = \sqrt{\frac{(m + 2n + 7)(2m + 2n + 8)(n + 3)(n + 4)(2n + 5)}{(\ell + 2)(m + 2)(n + 2)}}, \quad (2.25e)$$

$$0 \leq \{\ell, m, n\}, \ell + m + n \leq p - 4, \quad d = 1, 2, 3. \quad (2.25f)$$

Again, one can show the orthonormal property of the interior bubble functions

$$\langle \Phi_{\ell_1, m_1, n_1}^{\mathbf{t}, \vec{e}_{d_1}}, \Phi_{\ell_2, m_2, n_2}^{\mathbf{t}, \vec{e}_{d_2}} \rangle|_{K^3} = \delta_{\ell_1 \ell_2} \delta_{m_1 m_2} \delta_{n_1 n_2}, \quad (2.26a)$$

where

$$0 \leq \{\ell_1, \ell_2, m_1, m_2, n_1, n_2\}, \ell_1 + m_1 + n_1, \ell_2 + m_2 + n_2 \leq p - 4, \{d_1, d_2\} = 1, 2, 3. \quad (2.26b)$$

Following the same manner as in [5], it can be shown that the newly constructed basis is indeed a hierarchical one for tetrahedral $\mathcal{H}(\mathbf{curl})$ -conforming elements. The global basis functions for a physical element can be constructed through a covariant transformation [5].

3. Conditioning and Sparsity of Matrices

As in [3], we check the conditioning of the mass M , quasi-stiffness S matrices and their composite $K(\mu; M, S)$ on the reference element. The components of each matrix are defined as

$$M_{i,j} := \langle \Phi_i, \Phi_j \rangle|_{K^3}, \quad S_{i,j} := \langle \nabla \times \Phi_i, \nabla \times \Phi_j \rangle|_{K^3}. \quad (3.1)$$

Both the mass and quasi-stiffness matrices have particular sparsity structure due to the unique construction of the basis.

3.1. The Case of the Mass and Quasi-stiffness Matrices

3.1.1. Sparsity of the matrices

We first study the sparsity of the mass and quasi-stiffness matrices for each approximation order. We calculate the percentage of nonzero entries in each particular matrix. As a performance comparison with the basis by Ainsworth and Coyle [5], we also record the calculation from their basis. The comparison result is listed in Table 3.1, where the last two columns keep record of the ratios of the percentage between the Ainsworth-Coyle basis and the newly constructed basis.

Some observations can be made from Table 3.1. For the lowest order $p = 0$, the performance of the two bases is the same. For the approximation order $p = \{1, 2, 3, 5, 6\}$, the mass matrix is relatively more sparse with the new basis. For the approximation order $p = 4$, the mass matrix from the Ainsworth-Coyle basis [5] is a little more sparse - with 0.24% more sparsity. For the approximation order $p = \{2, 3, 4, 5\}$, the quasi-stiffness matrix is relatively more sparse with the new basis, and the performance is the same with order $p = 1$. For the approximation order $p = 6$,

Table 3.1: Sparsity of the mass matrix M and quasi-stiffness matrix S from the new basis and the basis in [5], denoted ‘A-C’.

Order p	Mass		Quasi-stiffness		Ratio	
	New	A-C	New	A-C	Mass	Q.-S.
0	50.00%	50.00%	66.67%	66.67%	1.000	1.000
1	54.17%	79.17%	16.67%	16.67%	1.462	1.000
2	67.33%	78.00%	24.67%	44.67%	1.158	1.811
3	61.11%	66.17%	36.11%	48.11%	1.083	1.332
4	57.68%	57.44%	48.01%	52.35%	0.996	1.090
5	51.02%	55.80%	56.09%	57.69%	1.094	1.029
6	46.01%	53.87%	63.22%	56.25%	1.171	0.890

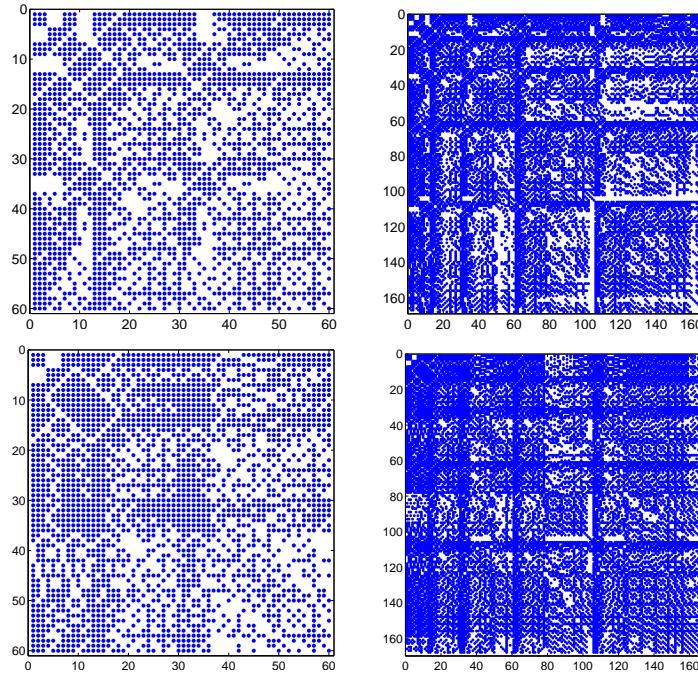


Fig. 3.1. Sparsity profiles of the mass matrices from the new basis (top) and the basis in [5] (bottom): $p = 3$ (left) and $p = 5$ (right).

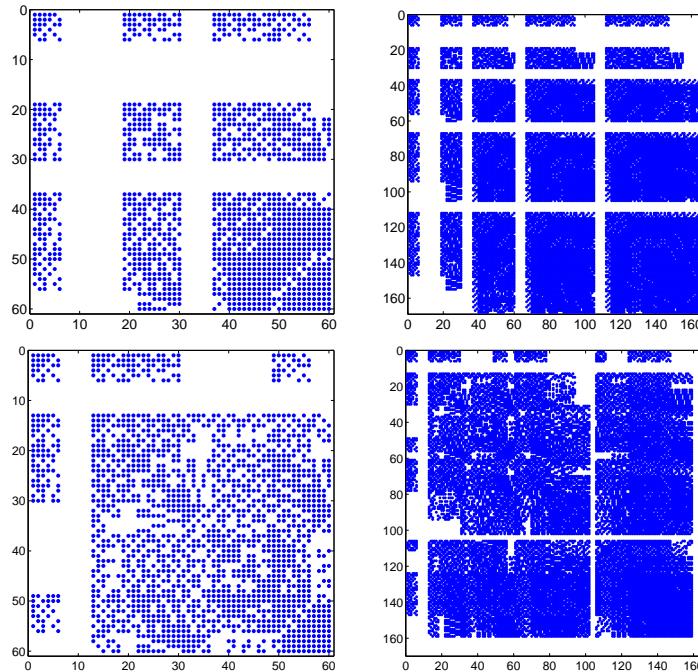


Fig. 3.2. Sparsity profiles of the quasi-stiffness matrices from the new basis (top) and the basis in [5] (bottom): $p = 3$ (left) and $p = 5$ (right).

the quasi-stiffness matrix from the Ainsworth-Coyle basis [5] is more sparse. Starting from order $p = 2$ and with the new basis, the mass matrix becomes more sparse as the approximation order p increases. The sparsity trend is just opposite for the quasi-stiffness matrix. Starting from order $p = 1$, the matrix is relatively denser with the increase of approximation order.

In Figs. 3.1 and 3.2 we respectively show the sparsity profiles of the mass and quasi-stiffness matrices for the approximation orders $p = 3$ and $p = 5$.

3.1.2. Condition numbers of the matrices

The mass matrix M is real, symmetric and positive definite, and thus its eigenvalues are all positive. The quasi-stiffness matrix S is real, symmetric and semi-positive definite, and therefore has non-negative eigenvalues.

The condition number of a matrix A is calculated by the formula

$$\kappa(A) = \frac{\lambda^{\max}}{\lambda^{\min}}, \quad (3.2)$$

where λ^{\max} and λ^{\min} are the maximum and minimum eigenvalues of the matrix A , respectively. For the quasi-stiffness matrix S , only positive eigenvalues are considered. The condition numbers of the mass and quasi-stiffness matrices are shown in Table 3.2. As a comparison, the condition numbers generated with the basis by Ainsworth and Coyle [5] are also recorded. The ratios of the condition numbers between the A-C basis [5] and the new basis are shown in the table as well.

Table 3.2: Condition numbers of the mass matrix M and quasi-stiffness matrix S from the new basis and the basis in [5], denoted ‘A-C’.

Order p	Mass		Quasi-stiffness		Ratio	
	New	A-C	New	A-C	Mass	Q.-S.
0	5.000e00	1.000e01	2.500e0	4.000e0	2.000e0	1.600e0
1	2.227e01	5.741e01	2.500e0	4.000e0	2.578e0	1.600e0
2	2.571e03	4.162e03	1.630e2	2.803e2	1.618e0	1.720e0
3	2.028e04	2.467e05	9.701e2	2.059e3	1.216e1	2.122e0
4	2.790e05	1.852e07	3.745e4	3.260e4	6.638e1	0.870e0
5	4.073e07	6.329e08	1.171e6	7.716e7	1.554e1	6.589e1
6	7.334e09	2.335e10	3.195e7	5.885e9	3.184e0	1.842e2

From Table 3.2 several observations on the conditioning for the mass and quasi-stiffness matrices can be made.

- For the mass matrix M and for each order of approximation, the condition number from the new basis is always lower than the corresponding one from the basis by Ainsworth and Coyle [5]. Indeed for the orders $p = 3$, $p = 4$, and $p = 5$, the new basis is at least one order better in terms of matrix conditioning with the most striking case for $p = 4$.
- For the quasi-stiffness matrix S , with the exception for order $p = 4$, for which the condition numbers from both bases are very close to each other, the condition number from the new basis is lower than the corresponding one from the Ainsworth-Coyle (A-C) basis [5]. The most pronounced case is with the order of approximation $p = 6$, for which the proposed basis is at least two orders better than the A-C basis [5] in terms of matrix conditioning.

- For both bases, the conditioning of the mass matrix is more severe than the quasi-stiffness matrix.

In order to see the trend of the growth with the condition numbers for both matrices, we plot the condition numbers vs. the order of approximation on a logarithmic scale. The results are shown in Figs. 3.3 and 3.4 for the mass and quasi-stiffness matrices, respectively.

From Fig. 3.3 and for both bases, the condition number increases *super-linearly* vs. order of approximation on a logarithmic scale. For the newly constructed basis and for the first three orders of approximation shown in Fig. 3.3, the condition number grows linearly vs. order of approximation; and starting from order four (4), the condition number begins to increase *super-linearly*. By examining the trend shown in Fig. 3.3 and data in Table 3.2, one concludes that there is no reason to apply a high-order basis which is beyond order six (6). For the later case, the numerical result with such a high-order basis does not seem to be trustable due to the consideration of matrix conditioning. In fact, with the new basis and for order $p = 7$, the condition number of the mass matrix has increased up to 1.534×10^{12} . It is noted the theoretical results [4] on the condition numbers cannot be applied to this study since they are intended for the quadrilateral and hexahedral elements.

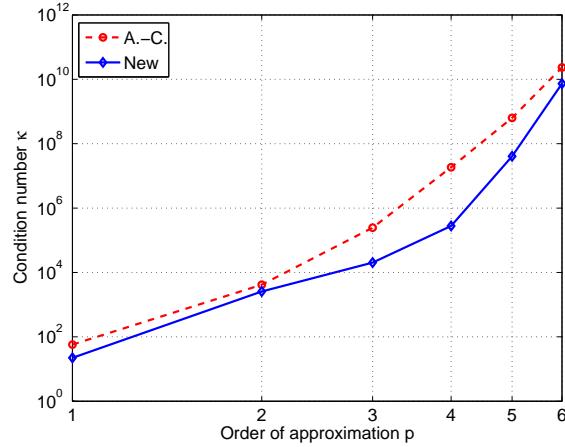


Fig. 3.3. Condition numbers of the mass matrices.

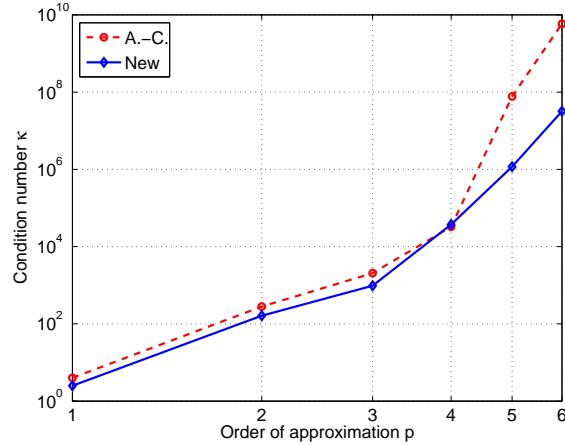


Fig. 3.4. Condition numbers of the quasi-stiffness matrices.

Similar remarks can be made for the quasi-stiffness matrices. From Fig. 3.4 and for the two bases, the condition number grows *super-linearly* vs. order of approximation on a logarithmic scale. For the new basis, the curve in Fig. 3.4 seems to be connected by two straight lines with the common point for the order of approximation $p = 3$. Again, it is not advised to use a relatively higher-order basis, e.g., beyond order six in view of the matrix conditioning. The growth rates of the condition numbers for the quasi-stiffness matrices shown in Fig. 3.4 do not conform to the theoretical study [4] either.

3.2. The case of the composite matrix

In solving the Helmholtz equation by the Nédélec element, one needs to consider the composite matrix

$$K(\mu; M, S) = \mu M + S, \quad \mu > 0, \quad (3.3)$$

where $\mu = k^2$, and k is the wave number. We study the conditioning and sparsity of the composite matrix for a wide range of the parameter μ . In particular, we consider four cases with $\mu = \{1, 10, 100, 1000\}$ for the approximation order from zero up to six.

3.2.1. Sparsity of the composite matrix

For each approximation order and for both bases, we record the percentage of nonzero entries in the composite matrix and calculate the ratio. The result is shown in Table 3.3. Note that for all the values of the parameter μ , the sparsity does not change for each specific order of approximation.

Table 3.3: Sparsity of the composite matrix K from the new basis and the basis in [5], denoted by ‘A-C’.

Order	New	A-C	Ratio
0	83.33%	83.33%	1.000
1	62.50%	87.50%	1.400
2	72.00%	83.33%	1.157
3	73.61%	78.06%	1.060
4	80.79%	73.39%	0.908
5	82.67%	76.21%	0.922
6	85.49%	75.33%	0.881

It is clear from Table 3.3 that for the relatively lower orders of approximation $p = \{1, 2, 3\}$, the composite matrix is more sparse with our new basis. However, for relatively higher orders of approximation $p = \{4, 5, 6\}$, the composite matrix is more dense with our new basis. For the lowest order $p = 0$, the performance is the same.

From Fig. 3.5 to Fig. 3.10 we show the sparsity profiles of the composite matrices with both bases for the approximation order from one up to six.

3.2.2. Condition numbers of the composite matrices

The comparison results with the basis by Ainsworth and Coyle [5] are shown from Table 3.4 to Table 3.7.

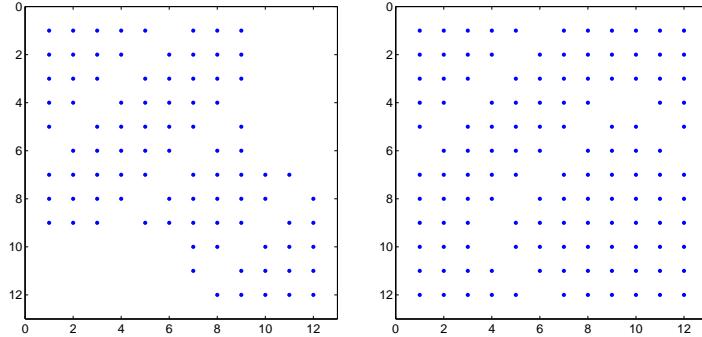


Fig. 3.5. Sparsity profiles of the composite matrix from the new basis (left) and the basis in [5] (right) with approximation order $p = 1$.

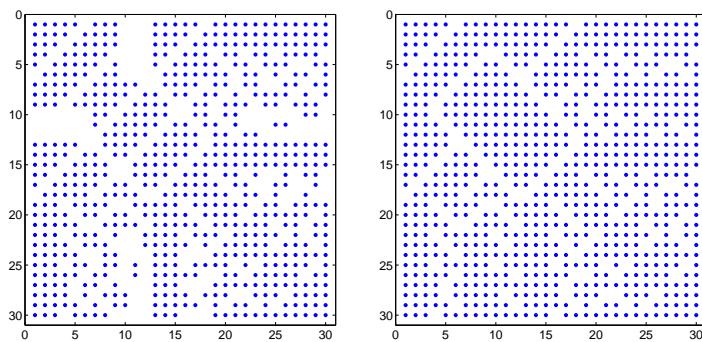


Fig. 3.6. Sparsity profiles of the composite matrix from the new basis (left) and the basis in [5] (right) with approximation order $p = 2$.

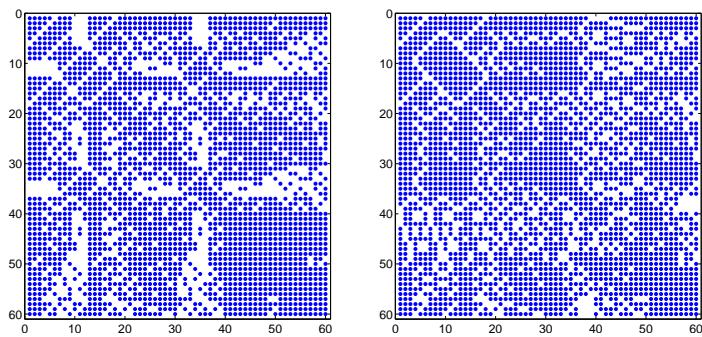


Fig. 3.7. Sparsity profiles of the composite matrix from the new basis (left) and the basis in [5] (right) with approximation order $p = 3$.

A few remarks are in place based upon the results shown in these four tables. For the approximation order from zero up to six and for each value of the parameter μ considered, the condition number of the composite matrix is always lower for the newly constructed basis. In particular, with the fifth order of approximation, the conditioning of the composite matrix has been improved at least by an order relative to the Ainsworth-Coyle basis [5]. For the case with the parameter $\mu = 1000$ and with order $p = 5$, the condition number has decreased by about 586 times. For each specific value of the parameter μ and with both bases, the condition

number grows with the increase of approximation order. Due to such a growth, in practice it is not advisable to apply a much higher order of approximation, for example, $p > 6$. It is worthwhile to note that Ledger et al. [18] have applied the highest approximation order $p = 4$ for a bistatic electromagnetic scattering problem. The maximum approximation order $p = 5$ has been considered in [6] for the study of a benchmark Maxwell eigenvalue problem. In [10] the authors have utilized the greatest approximation order $p = 6$ to demonstrate the exponential convergence in the computation of Maxwell eigenvalues.

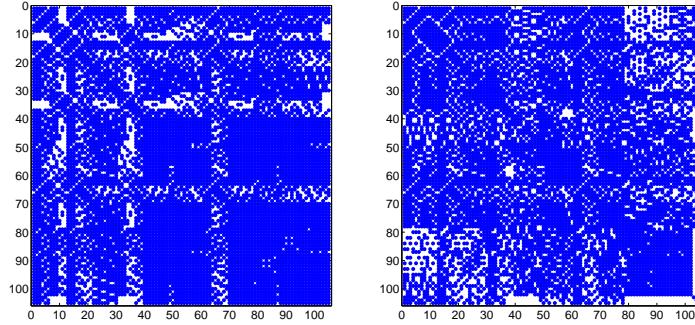


Fig. 3.8. Sparsity profiles of the composite matrix from the new basis (left) and the basis in [5] (right) with approximation order $p = 4$.

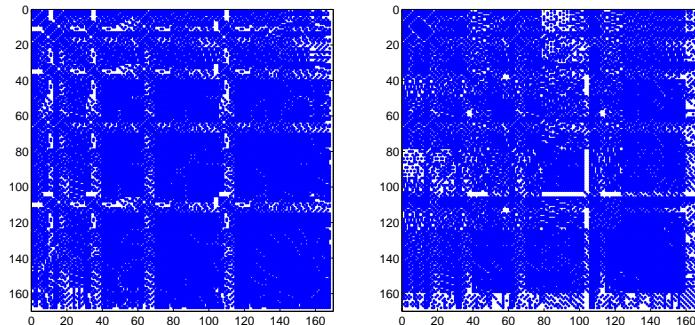


Fig. 3.9. Sparsity profiles of the composite matrix from the new basis (left) and the basis in [5] (right) with approximation order $p = 5$.

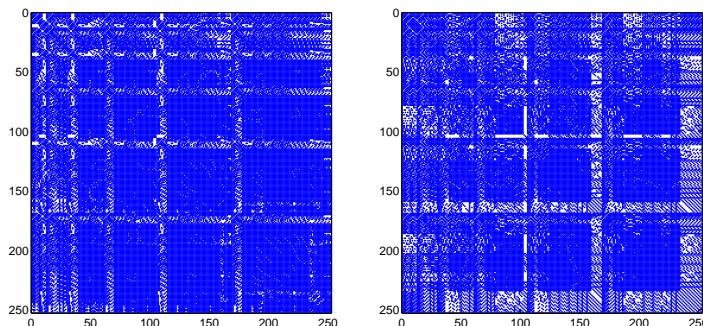


Fig. 3.10. Sparsity profiles of the composite matrix from the new basis (left) and the basis in [5] (right) with approximation order $p = 6$.

Table 3.4: Condition number of the composite matrix K from the new basis and the basis in [5], denoted by ‘A-C’. $\mu = 1$.

Order	New	A-C	Ratio
0	5.097e00	6.500e00	1.275e0
1	2.726e02	6.004e02	2.202e0
2	2.934e04	3.541e04	1.207e0
3	4.019e05	1.538e06	3.826e0
4	1.050e07	5.118e07	4.874e0
5	3.217e09	3.355e10	1.043e1
6	7.408e11	1.604e12	2.164e0

Table 3.5: Condition number of the composite matrix K from the new basis and the basis in [5], denoted by ‘A-C’. $\mu = 10$.

Order	New	A-C	Ratio
0	6.009e00	7.400e00	1.231e0
1	3.290e01	6.877e01	2.090e0
2	3.274e03	4.017e03	1.227e0
3	4.342e04	1.762e05	4.057e0
4	1.110e06	6.018e06	5.419e0
5	3.336e08	4.058e09	1.217e1
6	7.543e10	4.437e11	5.883e0

Table 3.6: Condition number of the composite matrix K from the new basis and the basis in [5], denoted by ‘A-C’. $\mu = 100$.

Order	New	A-C	Ratio
0	3.571e00	7.143e00	2.000e0
1	1.725e01	5.741e01	3.329e0
2	1.321e03	3.428e03	2.595e0
3	1.012e04	1.829e05	1.806e1
4	1.828e05	6.920e06	3.785e1
5	4.584e07	2.356e09	5.140e1
6	9.786e09	4.252e10	4.345e0

Table 3.7: Condition number of the composite matrix K from the new basis and the basis in [5], denoted by ‘A-C’. $\mu = 1000$.

Order	New	A-C	Ratio
0	4.808e00	9.615e00	2.000e0
1	2.131e01	5.741e01	2.695e0
2	2.203e03	3.814e03	1.731e0
3	1.585e04	2.196e05	1.385e1
4	1.783e05	1.202e07	6.742e1
5	2.180e07	1.280e10	5.872e2
6	3.864e09	1.921e11	4.973e1

4. Discussion and Conclusion

A new set of hierarchical basis for tetrahedral $\mathcal{H}(\mathbf{curl})$ -conforming elements has been proposed with the goal of improving the conditioning of the mass and quasi-stiffness matrices. The basis functions are given analytically. The construction of the new basis is motivated by the study of orthogonal polynomials of several variables [11], and based upon the work by Ainsworth and Coyle [5], and by Schöberl and Zaglmayr [25], thus combines the advantage of both works. The idea is to make each sub-set of shape functions, grouped and associated with a topological entity on the 3-simplex, have maximum orthonormality over the reference element. This is achieved by appropriately exploiting classic orthogonal polynomials, viz., Legendre and Jacobi polynomials over simplicial elements. The result of such a construction is that the basis functions are *partially* orthonormal over the 3-simplex but not completely. One is tempted to use the standard Gram-Schmidt orthogonalization procedure to make the entire basis functions orthonormal. However, such an effort will destroy the unique features of each category to which a particular set of basis functions belong. In this sense, explicit construction of a hierarchical and complete orthonormal basis for tetrahedral $\mathcal{H}(\mathbf{curl})$ -conforming elements does not exist.

The sparsity pattern of the mass and quasi-stiffness matrices has been studied numerically, and the opposite trend of percentage of nonzero entries in both matrices has been identified. Compared with the Ainsworth-Coyle basis [5] and in general, both the mass and quasi-stiffness matrices are relatively more sparse.

The numerical experiment has shown that the conditioning of the mass matrix is relatively more pronounced, i.e., one order higher than that with the quasi-stiffness matrix. For both the mass and quasi-stiffness matrices and on the logarithmic scale, the condition number grows linearly vs. the order of approximation up to order three. It does not make too much sense if a rather high-order basis, e.g., beyond order six is applied due to the quick growth of the condition numbers of the mass and quasi-stiffness matrices. The so-called “curse of dimensionality” [8] manifests in this context. In contrast to the two-dimensional case, for which we have constructed a well-conditioned hierarchical basis for the *triangular* $\mathcal{H}(\mathbf{curl})$ -conforming elements up to a relatively higher order [30], e.g., order twelve, we cannot construct beyond a relatively lower order a well-conditioned hierarchical basis for tetrahedral $\mathcal{H}(\mathbf{curl})$ -conforming elements using the same technique as in [30]. The main reason is due to the coupling of the non-orthogonal face modes from different groups, to the coupling of the non-orthogonal interior modes from different categories, and to the coupling of the face and interior modes [2, 32].

For the composite matrix $\mu M + S$ and with a dynamical range of $\mu = 1000$, the newly constructed basis shows better conditioning relative to the Ainsworth-Coyle basis [5] for the approximation order from zero up to six. For the fifth order of approximation, the conditioning of the composite matrix has been improved at least one order. With the proposed basis and for the approximation order $p = \{1, 2, 3\}$, the composite matrix is relatively more sparse.

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