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Well-conditioned Orthonormal Hierarchical $\mathcal{L}_2$ Bases on $\mathbb{R}^n$ Simplicial Elements

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Abstract We construct well-conditioned orthonormal hierarchical bases for simplicial $\mathcal{L}_2$ finite elements. The construction is made possible via classical orthogonal polynomials of several variables. The basis functions are orthonormal over the reference simplicial elements in two and three dimensions. The mass matrices M are identity while the conditioning of the stiffness matrices S grows as $\mathcal{O}(p^3)$ with respect to the order p. The diagonally normalized stiffness matrices are well conditioned. The diagonally normalized composite matrices $\zeta M + S$ are also well conditioned for a wide range of ζ. For the mass, stiffness and composite matrices, the bases in this study have much better conditioning than existing high-order hierarchical bases.

Keywords Hierarchical bases · Simplicial $\mathcal{L}_2$-conforming elements · Matrix conditioning

1 Introduction

In 1973 Reed and Hill [19] introduced the discontinuous Galerkin (DG) method as a technique to solve neutron transport problems. The first numerical analysis of the DG method was carried out by Lasaint and Raviart [17] for a linear advection equation. The DG method has been dormant for quite a few years, and nowadays has become a popular method to solve a variety of problems. A recent review [11] on the DG method is done for convection-dominated problems.

Unlike the classical continuous Galerkin method [8] where a $\mathcal{C}^0$ continuity requirement on the solution space has to be maintained across inter-element boundaries, there is no such restriction for the DG method. Thus, the DG method allows for a more flexible basis construction and mesh configurations, e.g., non-conforming and hybrid meshes. In the work of Cockburn and Shu [10] which initiated much recent DG research, piecewise linear and quadratic finite elements were used on rectangular and triangular meshes. For the triangular

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element with quadratic polynomial approximation, six degrees of freedom for each element have been associated with the geometrical identities on the triangle, viz., three at the mid-points of the edges and three on the vertexes [10]. It has been shown that for the resulting DG discretization, the local mass matrix is not diagonal but a dense matrix [10]. Applying the Gram-Schmidt process, Remacle et al. [20] have constructed an orthogonal polynomial basis out of the monomials on a 2-simplex, and applied the DG method for compressible flow problems, i.e., the double Mach reflection and the Rayleigh-Taylor instability. However, the explicit formula for the shape function is not given in [20]. Furthermore, it is noted that the choice of a different initial non-orthogonal basis will result in a different orthogonal basis after the Gram-Schmidt process. Targeting on solving the Maxwell equations with the DG method and based on previous works, Cockburn et al. [9] have proposed the locally divergence-free polynomials. On a rectangular mesh, improved results have been shown relative to those based on the classical piecewise polynomials [9]. However, the *global* divergence-free property is lost with the locally divergence-free approximation [9]. It should be pointed out that the shape functions with the locally divergence-free property have to be carefully designed [9], and it is not clear how to extend the technique directly to non-rectangular meshes, e.g., triangular and tetrahedral meshes.

In this study we focus our attention on constructing orthonormal hierarchical polynomial bases on reference simplicial elements, viz., triangular and tetrahedral elements with the DG method. In particular, with increasing orders of approximation, we are concerned with the growth rate of the condition numbers of the stiffness matrices from the variational formulation of second-order elliptic problems [5, 6]. As in the cases for the $\mathcal{H}^1$-conforming [1, 7, 24] and $\mathcal{H}(\mathbf{curl})$-conforming [2, 21–23] hierarchical bases, the conditioning of the stiffness matrices could be problematic with improperly constructed high-order hierarchical bases for the DG methods. Such an issue has not been sufficiently addressed. Our effort in constructing orthonormal hierarchical bases with well-conditioned stiffness matrices for simplicial elements seems to be the first of such attempts, which is motivated by a recent study of Dunkl and Xu [13] on orthogonal polynomials of several variables over standard domains, e.g., cube, unit ball, and simplex. It should be noted that early in 1975 Koornwinder has already constructed orthogonal polynomials over several types of domain in two dimensions, e.g., a disk, a triangle, and a region bounded by two straight lines and a parabola [16]. Independently, Dubiner [12] has obtained different orthogonal bases on a triangle and on a triangular pyramid (a tetrahedron) for spectral methods (see the Remark 2.1 in Sect. 2). For the two-dimensional case on the reference 2-simplex, our formula differs from the one by Koornwinder [16], and the basis in this study is also different from the one obtained by Remacle et al. via the Gram-Schmidt process [20].

The rest of the paper is organized as follows. The construction of orthonormal and hierarchical basis functions is given in Sect. 2. Numerical results of matrix conditioning are reported in Sect. 3. Discussion and conclusion are presented in Sect. 4. The proof of Theorem 2.1 is given in the Appendix.

2 Construction of Orthonormal Hierarchical Basis Functions

We construct orthonormal hierarchical basis functions for the $\mathcal{L}_2$-conforming elements on the reference simplicial elements. Let K^n be the simplex in $\mathbb{R}^n$, i.e.,

$$K^n := \left\{ \mathbf{x} \in \mathbb{R}^n : 0 \le x_i;\ \sum_{i=1}^{n} x_i \le 1 \right\}. \tag{1}$$

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

$$|\mathbf{x}| = \sum_{i=1}^{n} |x_i|. \tag{2}$$

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

$$\mathbf{x}_0 := 0, \qquad \mathbf{x}_i := (x_1, x_2, \ldots, x_i), \quad 1 \le i \le n. \tag{3}$$

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

$$\vec{\alpha}^i := (\alpha_i, \alpha_{i+1}, \ldots, \alpha_n), \quad 1 \le i \le n. \tag{4}$$

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

$$\vec{\tau}^i := (\tau_i, \tau_{i+1}, \ldots, \tau_{n+1}), \quad 1 \le i \le n+1. \tag{5}$$

It is shown [13] that the weight function associated with the classical orthogonal polynomials on K^n takes the form

$$W_{\vec{\tau}}^{(K^n)}(\mathbf{x}) = (1 - |\mathbf{x}|)^{\tau_{n+1} - \frac{1}{2}} \prod_{i=1}^{n} x_i^{\tau_i - \frac{1}{2}}, \quad \mathbf{x} \in K^n, \ \tau_i \ge -\frac{1}{2}, \ i = 1, 2, \ldots, n+1. \tag{6}$$

The basis functions are constructed with the help of the following theorem on orthogonal polynomials over an n-simplex K^n [13].

Theorem 2.1 *The polynomials*

$$P_{\vec{\alpha}}\left(W_{\vec{\tau}}^{(K^n)}; \mathbf{x}\right) = \left[h_{\vec{\alpha}}^{(K^n)}\right]^{-1} \prod_{i=1}^{n} \left(\frac{1 - |\mathbf{x}_i|}{1 - |\mathbf{x}_{i-1}|}\right)^{|\vec{\alpha}^{i+1}|} p_{\alpha_i}^{(\rho_i^1, \rho_i^2)}\left(\frac{2x_i}{1 - |\mathbf{x}_{i-1}|} - 1\right), \tag{7a}$$

where $p_{\alpha_i}^{(\rho_i^1, \rho_i^2)}$ *is the classical orthonormal Jacobi polynomials of one variable,* $\rho_i^1 = 2|\vec{\alpha}^{i+1}| + |\vec{\tau}^{i+1}| + (n - i - 1)/2$ *and* $\rho_i^2 = \tau_i - 1/2$, *are orthonormal, the normalization constant* $h_{\vec{\alpha}}^{(K^n)}$ *is given by*

$$\left[h_{\vec{\alpha}}^{(K^n)}\right]^{-2} = \prod_{i=1}^{n} 2^{\rho_i^1 + \rho_i^2 + 1}, \tag{7b}$$

and the weight function takes the form in (6).

The proof of Theorem 2.1 can be found in [13]. However, the normalization constant $h_{\vec{\alpha}}^{(K^n)}$ given in [13] is wrong. The fallacious [13] normalization constant has been corrected in our formula (7b). For the sake of completeness of this work, a concise proof is given in the Appendix.

Using the result in Theorem 2.1, the orthonormal hierarchical shape functions on the reference element in 2-D and 3-D dimensions are given as follows:

- *Orthonormal Hierarchical Basis in 2-D Simplex*

$$\Phi_{i,j}^{K^2} = \sqrt{2(i+j+1)(2j+1)}(1-x_1)^j P_i^{(2j+1,0)}(2x_1-1)\, P_j^{(0,0)}\left(\frac{2x_2}{1-x_1}-1\right),$$
$$0 \le i, j;\ i+j \le p. \tag{8}$$

- *Orthonormal Hierarchical Basis in 3-D Simplex*

$$\Phi_{i,j,k}^{K^3} = \lambda(1-x_1)^j(1-x_1-x_2)^k P_i^{(2j+2k+2,0)}(2x_1-1)\, P_j^{(2k+1,0)}\left(\frac{2x_2}{1-x_1}-1\right)$$
$$\times\, P_k^{(0,0)}\left(\frac{2x_3}{1-x_1-x_2}-1\right) \tag{9}$$

with the scaling coefficient

$$\lambda = \sqrt{(2k+1)(2j+2k+2)(2i+2j+2k+3)}, \quad 0 \le i, j, k;\ i+j+k \le p. \tag{10}$$

Again, from Theorem 2.1, we have the following orthonormal conditions of the basis functions:

$$M_{\ell_1,\ell_2} := \langle \Phi_{\ell_1}, \Phi_{\ell_2} \rangle|_{K^d} = \delta_{\ell_1,\ell_2} \tag{11}$$

where $\ell = (i, j)$ in 2-D and $\ell = (i, j, k)$ in 3-D.

In deriving the above formula (8), the parameter τ_i in Theorem 2.1 takes the value of $\frac{1}{2}$. The function $P_n^{(\alpha,\beta)}(x)$ is the classical *un-normalized* Jacobi polynomials of a single variable [18].

Theorem 2.2 *Let $p \in \mathbb{N}_0$. The bases for the spaces $\mathbb{P}_p(K^n)$, $n = 2, 3$ of polynomials of total degree at most p are given by*

$$\mathbb{P}_p(K^2) = \text{span}\{\Phi_{i,j}^{K^2} : 0 \le i, j;\ i+j \le p\}, \tag{12a}$$
$$\mathbb{P}_p(K^3) = \text{span}\{\Phi_{i,j,k}^{K^3} : 0 \le i, j, k;\ i+j+k \le p\}. \tag{12b}$$

Proof First, for each shape function, we have $\Phi_{i,j}^{K^2} \in \mathbb{P}_p(K^2)$ and $\Phi_{i,j,k}^{K^3} \in \mathbb{P}_p(K^3)$. Further, it is noticed that with different indexes the shape functions given in (8) and in (9) are linearly independent. Second, the numbers of independent shape functions are $\frac{(p+1)(p+2)}{2}$ and $\frac{(p+1)(p+2)(p+3)}{6}$ for two and three dimensions, respectively, which coincide with their respective dimensions of $\mathbb{P}_p(K^2)$ and $\mathbb{P}_p(K^3)$. □

Remark 2.1 The formulas of orthonormal basis functions above are different from Dubiner bases proposed in [12]. In fact, the Dubiner bases [12] are special cases of the more general result in Theorem 2.1. The parameter of the weight function in equation (6) takes the particular value $\tau_i = 0$ [13] for the Dubiner basis [12], whereas in our construction this parameter has the value $\tau_i = \frac{1}{2}$.

3 Conditioning of Matrices

We check the conditioning of the mass M and stiffness S matrices on the reference element. The stiffness matrix comes from the variational formulation of the Laplacian in a second-order elliptic problem, e.g., the Poisson's equation in potential theory [15]

$$-\Delta u = f. \tag{13}$$

The components of each matrix are defined as

$$M_{\ell_1,\ell_2} := \langle \Phi_{\ell_1}, \Phi_{\ell_2} \rangle|_{K^d}, \quad S_{\ell_1,\ell_2} := \langle \nabla\Phi_{\ell_1}, \nabla\Phi_{\ell_2} \rangle|_{K^d}, \quad d = 2, 3. \tag{14}$$

In view of the construction of the shape functions, the mass matrix M is an *identity matrix* with condition number of one (1). The stiffness matrix S is real, symmetric and semi-positive definite, and therefore has non-negative real eigenvalues.

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

$$\kappa(A) = \frac{\lambda_{\max}}{\lambda_{\min}}, \tag{15}$$

where $\lambda_{\max}$ and $\lambda_{\min}$ are the maximum and minimum eigenvalues of the matrix A, respectively. For the stiffness matrix S, only positive eigenvalues are counted. We also consider the diagonally *normalized* mass and stiffness matrices, viz.

$$\widetilde{M} := \Lambda_M^{-\frac{1}{2}} M \Lambda_M^{-\frac{1}{2}}, \qquad \widetilde{S} := \Lambda_S^{-\frac{1}{2}} S \Lambda_S^{-\frac{1}{2}}, \tag{16}$$

where Λ_M and Λ_S are the diagonal matrices of the mass M and stiffness matrices S, respectively.

3.1 Conditioning of Mass Matrix M and Stiffness Matrix S

3.1.1 2-D Case

The condition numbers of the original and normalized mass and stiffness matrices are shown in Tables 1 and 2, respectively. As a comparison, the condition numbers generated with the basis by Ainsworth and Coyle [4] are recorded. The ratios of the condition numbers between the A-C basis [4] and the new basis are shown in each table as well.

From Table 1 two observations on the conditioning for the original *un-normalized* matrices can be made.

- For the mass matrix M, starting from order three, the conditioning with the basis in this study is at least three orders better than the basis by Ainsworth and Coyle [4]. The higher the order of approximation, the greater the advantage with the new basis. Indeed, starting from order ten, the conditioning with the new basis is at least twelve orders better relative to the one in [4].
- For the stiffness matrix S, starting from order six, the conditioning with the basis in this study is at least three order better than the basis by Ainsworth and Coyle [4]. The higher the order of approximation, the greater the advantage with the new basis. For example, starting from order ten, the conditioning with the new basis has been at least seven orders better relative to the one in [4].

Table 1 Two-dimensional case: condition numbers of the mass matrix M and stiffness matrix S from the new basis and the basis in [4], denoted 'A-C'

Order	Mass		Stiffness		Ratio	
p	New	A-C	New	A-C	Mass	Stiff-
0	1.000e00	1.000e00	1.000e00	1.000e00	1.000e00	1.000e00
1	1.000e00	1.200e01	3.000e00	9.000e00	1.200e01	3.000e00
2	1.000e00	2.180e02	9.899e00	4.678e01	2.180e02	4.726e00
3	1.000e00	2.483e03	4.055e01	3.254e02	2.483e03	8.025e00
4	1.000e00	3.557e04	8.641e01	3.066e03	3.557e04	3.548e01
5	1.000e00	5.155e05	8.120e01	3.652e04	5.155e05	4.498e02
6	1.000e00	7.889e06	2.819e02	4.963e05	7.889e06	1.761e03
7	1.000e00	1.568e08	2.285e02	7.353e06	1.568e08	3.218e04
8	1.000e00	3.022e09	7.049e02	1.155e08	3.022e09	1.639e05
9	1.000e00	5.735e10	1.042e03	1.931e09	5.735e10	1.853e06
10	1.000e00	1.064e12	1.490e03	3.433e10	1.064e12	2.304e07

Table 2 Two-dimensional case: condition numbers of the diagonally normalized mass matrix $\widetilde{M}$ and stiffness matrix $\widetilde{S}$ from the new basis and the basis in [4], denoted 'A-C'

Order	Mass		Stiffness		Ratio	
p	New	A-C	New	A-C	Mass	Stiff-
0	1.000e00	1.000e00	1.000e00	1.000e00	1.000e00	1.000e00
1	1.000e00	3.000e00	2.618e00	9.000e00	3.000e00	3.438e00
2	1.000e00	4.121e01	4.795e00	2.783e01	4.121e01	5.804e00
3	1.000e00	4.459e02	6.893e00	2.019e02	4.459e02	2.929e01
4	1.000e00	6.787e03	1.125e01	1.917e03	6.787e03	1.704e02
5	1.000e00	8.615e04	1.618e01	2.168e04	8.615e04	1.340e03
6	1.000e00	1.353e06	2.280e01	3.092e05	1.353e06	1.356e04
7	1.000e00	2.776e07	3.087e01	4.347e06	2.776e07	1.408e05
8	1.000e00	4.720e08	4.058e01	7.065e07	4.720e08	1.741e06
9	1.000e00	8.688e09	5.208e01	1.151e09	8.688e09	2.210e07
10	1.000e00	1.459e11	6.530e01	2.022e10	1.459e11	3.096e08

Similarly, by examining the figures in Table 2 and by comparing the figures in Tables 1 and 2, one can make a couple of remarks.

- For the normalized mass matrix $\widetilde{M}$, starting from order four, the new basis is at least three order better relative to the one in [4], and starting from order ten, the basis in this study has begun to show eleven orders better than the Ainsworth-Coyle basis [4]. The higher the order of approximation, the greater the advantage with the proposed new basis.
- For the normalized stiffness matrix $\widetilde{S}$, the conditioning is *not* a problem with the new basis: the matrix is *well conditioned*. In contrast, the condition number with the basis in [4] still grows *exponentially* with polynomial degree p. Indeed, starting from order five, the new basis is at least three order better relative to the one in [4], and starting from order ten, the conditioning of the new basis has been at least eight orders better relative

Table 3 Three-dimensional case: condition numbers of the mass matrix M and stiffness matrix S from the new basis and the basis in [4], denoted 'A-C'

Order	Mass		Stiffness		Ratio	
p	New	A-C	New	A-C	Mass	Stiff-
0	1.000e00	1.000e00	1.000e00	1.000e00	1.000e00	1.000e00
1	1.000e00	2.000e01	4.000e00	1.600e01	2.000e01	4.000e00
2	1.000e00	8.399e02	2.019e01	1.215e02	8.399e02	6.018e00
3	1.000e00	3.936e04	4.195e01	4.715e03	3.936e04	1.124e02
4	1.000e00	8.142e05	1.118e02	5.104e04	8.142e05	4.565e02
5	1.000e00	2.532e07	2.063e02	1.457e06	2.532e07	7.063e03
6	1.000e00	6.181e08	3.505e02	2.562e07	6.181e08	7.310e04
7	1.000e00	1.885e10	5.597e02	7.087e08	1.885e10	1.266e06
8	1.000e00	5.728e11	8.511e02	1.675e10	5.728e11	1.968e07
9	1.000e00	1.948e13	1.244e03	5.068e11	1.948e13	4.074e08
10	1.000e00	6.207e14	1.759e03	1.332e13	6.207e14	7.572e09

Table 4 Three-dimensional case: condition numbers of the diagonally normalized mass matrix $\widetilde{M}$ and stiffness matrix $\widetilde{S}$ from the new basis and the basis in [4], denoted 'A-C'

Order	Mass		Stiffness		Ratio	
p	New	A-C	New	A-C	Mass	Stiff-
0	1.000e00	1.000e00	1.000e00	1.000e00	1.000e00	1.000e00
1	1.000e00	4.000e00	3.912e00	1.600e01	4.000e00	4.090e00
2	1.000e00	2.465e02	9.460e00	6.594e01	2.465e02	6.970e00
3	1.000e00	2.957e03	1.356e01	1.393e03	2.957e03	1.027e02
4	1.000e00	1.356e05	1.994e01	1.812e04	1.356e05	9.087e02
5	1.000e00	2.627e06	2.842e01	4.181e05	2.627e06	1.471e04
6	1.000e00	1.378e08	3.868e01	9.835e06	1.378e08	2.543e05
7	1.000e00	2.427e09	5.170e01	2.596e08	2.427e09	5.021e06
8	1.000e00	1.355e11	6.658e01	7.697e09	1.355e11	1.156e08
9	1.000e00	2.768e12	8.415e01	2.051e11	2.768e12	2.437e09
10	1.000e00	1.245e14	1.042e02	6.402e12	1.245e14	6.144e10

to the Ainsworth-Coyle basis [4]. The higher the order of approximation, the greater the advantage with the newly constructed basis.

3.1.2 3-D Case

The conditioning results of the original and normalized mass and stiffness matrices are shown in Tables 3 and 4, respectively. Similar to the two-dimensional case, from Table 3 two observations on the conditioning for the original *un-normalized* matrices can be made.

- For the mass matrix M, starting from order three, the conditioning with the basis in this study is at least four orders better than the basis by Ainsworth and Coyle [4]. The higher the order of approximation, the greater the advantage with the new basis. Indeed, starting

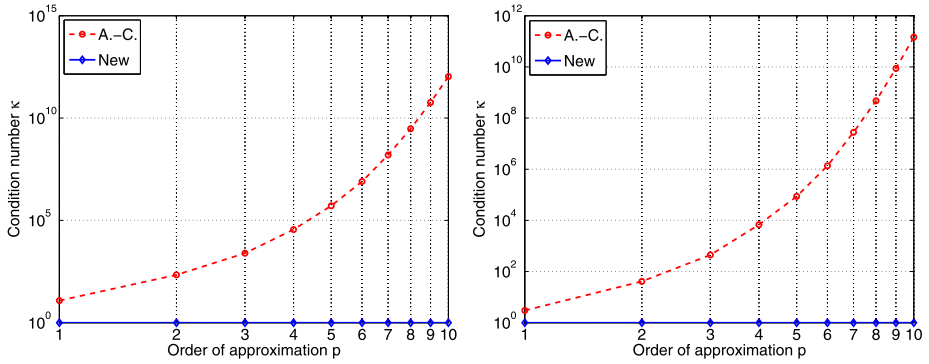

Fig. 1 Two-dimensional case: condition numbers of the mass matrices: original (*left*) and diagonally normalized (*right*)

from order nine, the conditioning with the new basis is at least thirteen orders better relative to the one in [4].

- For the stiffness matrix S, starting from order six, the conditioning with the basis in this study is at least four orders better than the basis by Ainsworth and Coyle [4]. The higher the order of approximation, the greater the advantage with the new basis. For instance, starting from order nine, the conditioning with the new basis has been at least eight orders better relative to the one in [4].

Similar to its two-dimensional counterpart, by examining the figures in Table 4 and by comparing the figures in Tables 3 and 4, one can make a couple of remarks.

- For the normalized mass matrix $\widetilde{M}$, starting from order four, the new basis is at least five order better relative to the one in [4], and starting from order nine, the basis in this study has begun to show twelve orders better than the Ainsworth-Coyle basis [4]. The higher the order of approximation, the greater the advantage with the new basis.
- For the normalized stiffness matrix $\widetilde{S}$, the conditioning again is *not* a problem with the new basis: the matrix is *well conditioned*. In contrast, the condition number with the basis in [4] still grows *exponentially* with polynomial degree p. Indeed, starting from order five, the new basis is at least four order better relative to the one in [4], and starting from order nine, the new basis has begun to show nine orders better than the Ainsworth-Coyle basis [4]. The higher the order of approximation, the greater the advantage with the newly constructed basis.

3.1.3 $\mathcal{O}(p^3)$ Growth Rate of Conditioning Number

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 for the two-dimensional case are shown in Figs. 1 and 2 for the mass and stiffness matrices, respectively. Similarly, results for the three-dimensional case are shown in Figs. 3 and 4 for the mass and stiffness matrices, respectively.

From Figs. 1 and 3 obviously one can see that for the Ainsworth-Coyle basis [4] the condition numbers grow exponentially vs. order of approximation for both the original and diagonally normalized mass matrices. In contrast, the new bases have a perfect condition number of one.

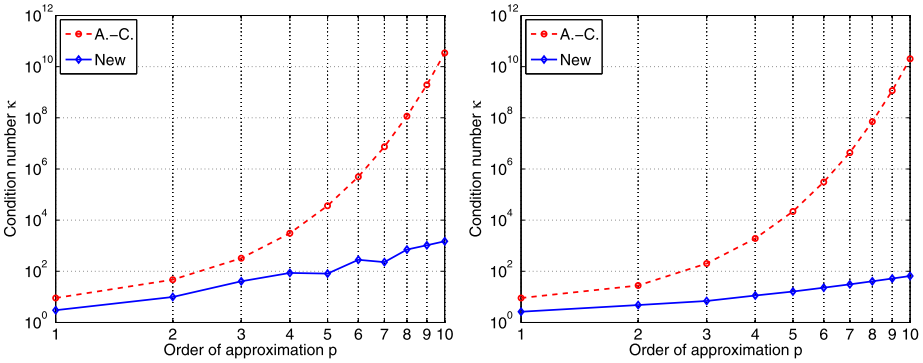

Fig. 2 Two-dimensional case: condition numbers of the stiffness matrices: original (*left*) and diagonally normalized (*right*)

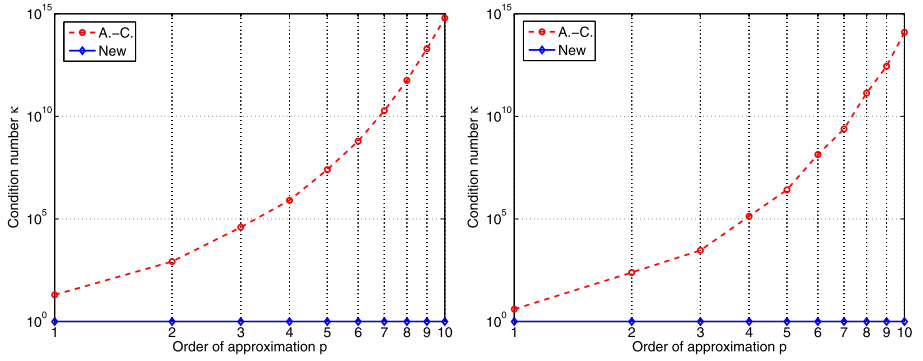

Fig. 3 Three-dimensional case: condition numbers of the mass matrices: original (*left*) and diagonally normalized (*right*)

Similarly, from Figs. 2 and 4 one concludes that for the Ainsworth-Coyle basis [4] the condition numbers grow exponentially vs. order of approximation for both the original and diagonally normalized stiffness matrices. For the new bases, the condition numbers grow linearly vs. order of approximation. Since the diagonally normalized stiffness matrices are well conditioned and the condition numbers of which are rather small, we concentrate on the study of the growth rate of the original *un-normalized* stiffness matrices.

From Figs. 2 and 4, and on a logarithmic scale, the condition number κ_d grows linearly vs. order of approximation p

$$\log \kappa_d(p) \approx \mu + \nu \log p, \quad d = 2,\ 3. \tag{17}$$

From the figures in Tables 1 and 3, asymptotically one can compute the growth rate. For the bases in two and three dimensions, qualitatively one finds such a relation

$$\kappa_d(p) \approx \lambda_d\, p^3, \quad d = 2,\ 3, \tag{18}$$

where the constant $\lambda_d = 10^{\mu}$ is independent of the order of approximation p. So the condition number grows on the order of $\mathcal{O}(p^3)$, i.e., a cubic growth with order of approximation

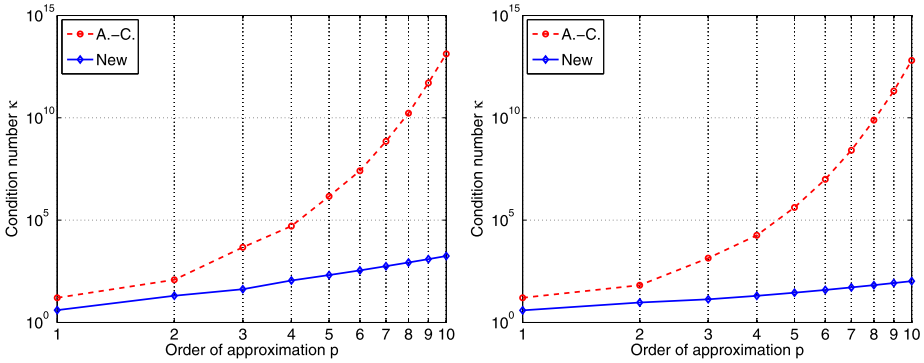

Fig. 4 Three-dimensional case: condition numbers of the stiffness matrices: original (*left*) and diagonally normalized (*right*)

and independent of approximation dimension. For the moment a rigorous proof of this assertion still lacks. In this aspect, we should mention the work by Hu and collaborators [14] on establishing the bounds of the condition numbers from the bases for the $\mathcal{H}^1$-conforming finite elements, and the similar work by Ainsworth and Coyle [3] for the Nédélec elements. The shape functions in both works [3, 14] are essentially constructed by the tensor product of Legendre polynomials for *rectangular* elements, whereas in our case, the shape functions are constructed via the *non-degenerate* Jacobi polynomials for the *simplicial* elements.

The scaling constant λ_d is different in each dimension and we find $\lambda_2 \approx 1.18$ and $\lambda_3 \approx 1.68$. So quantitatively we establish the relation between the condition number κ_d of the original un-normalized stiffness matrix S and the order of approximation p

$$\kappa_2(p) \approx 1.18 p^3, \quad \text{for two dimensions,} \tag{19a}$$

$$\kappa_3(p) \approx 1.68 p^3, \quad \text{for three dimensions.} \tag{19b}$$

The difference between the two scaling coefficients λ_3 and λ_2 is about $\frac{1}{2}$. It might be a coincidence for such a difference.

3.2 Conditioning of the Composite Matrix $\zeta M + S$

In reality after discretization with the DG method, one needs to solve a linear system which involves the following composite matrix as a building block

$$K(M, S; \zeta) := \zeta M + S, \quad \zeta > 0. \tag{20}$$

We study the conditioning of the composite matrix K for a few different values of the parameter ζ, viz., $\zeta = \{0.01, 1, 100\}$. For the two- and three-dimensional bases, the comparison results are recorded in Tables 5–10. The two columns with the common heading 'Ratio' list the ratio of the condition numbers from the bases by Ainsworth and Coyle [4] and from our newly derived bases.

Upon a careful examination of the figures in Tables 5–10, several observations are in place.

- For all values of the parameter ζ studied and, for both the newly derived two- and three-dimensional bases, the diagonally normalized composite matrix $\widetilde{K}(M, S; \zeta)$ is well conditioned for all orders of approximation up to $p = 10$. Moreover, the condition number

Table 5 Two-dimensional case: condition numbers of the composite matrix: original $K(M, S; \zeta)$ and normalized $\widetilde{K}(M, S; \zeta)$ from the new basis and the basis in [4], denoted 'A-C', where $\zeta = 0.01$

Order	Original		Normalized		Ratio	
p	New	A-C	New	A-C	Original	Normal.
0	1.000e00	1.000e00	1.000e00	1.000e00	1.000e00	1.000e00
1	3.601e03	9.003e02	2.617e00	8.995e00	2.500e-1	3.437e00
2	1.571e04	1.259e03	4.793e00	2.783e01	8.014e-2	5.806e00
3	4.004e04	1.964e03	6.890e00	2.019e02	4.905e-2	2.930e01
4	8.531e04	3.323e03	1.124e01	1.917e03	3.895e-2	1.706e02
5	1.605e05	3.652e04	1.618e01	2.168e04	2.275e-1	1.340e03
6	2.782e05	5.007e05	2.280e01	3.093e05	1.800e00	1.357e04
7	4.510e05	7.353e06	3.086e01	4.347e06	1.630e01	1.409e05
8	6.957e05	1.161e08	4.057e01	7.065e07	1.669e02	1.741e06
9	1.028e06	1.931e09	5.207e01	1.151e09	1.878e03	2.210e07
10	1.470e06	3.433e10	6.529e01	2.022e10	2.335e04	3.097e08

Table 6 Two-dimensional case: condition numbers of the composite matrix: original $K(M, S; \zeta)$ and normalized $\widetilde{K}(M, S; \zeta)$ from the new basis and the basis in [4], denoted 'A-C', where $\zeta = 1$

Order	Original		Normalized		Ratio	
p	New	A-C	New	A-C	Original	Normal.
0	1.000e00	1.000e00	1.000e00	1.000e00	1.000e00	1.000e00
1	3.700e01	9.25e00	2.498e00	8.538e00	2.500e-1	3.418e00
2	1.581e02	4.926e01	4.596e00	2.782e01	3.116e-1	6.053e00
3	4.014e02	3.245e02	6.629e00	2.025e02	8.084e-1	3.055e01
4	8.541e02	3.108e03	1.088e01	1.926e03	3.639e00	1.770e02
5	1.606e03	3.639e04	1.583e01	2.176e04	2.266e01	1.375e03
6	2.783e03	4.993e05	2.239e01	3.107e05	1.794e02	1.388e04
7	4.511e03	7.336e06	3.045e01	4.368e06	1.626e03	1.434e05
8	6.958e03	1.159e08	4.014e01	7.101e07	1.666e04	1.769e06
9	1.029e04	1.928e09	5.162e01	1.157e09	1.874e05	2.241e07
10	1.470e04	3.431e10	6.483e01	2.032e10	2.334e06	3.134e08

$\kappa(\widetilde{K})$ decreases with the increase of the parameter ζ for each order of approximation, which is understandable since the mass matrix M is perfectly conditioned with a condition number of one.

- For each fixed value of the parameter ζ, and for both the newly derived two- and three-dimensional bases, the condition number of the original un-normalized composite matrix $K(M, S; \zeta)$ grows mildly with the approximation order p. Furthermore, for each order of approximation, the condition number $\kappa(K)$ reduces roughly by an order with a tenfold increase in the parameter ζ.
- For a fixed value of the parameter ζ and for a particular order of approximation, the condition number with the newly constructed three-dimensional basis is a little larger than its corresponding one with the two-dimensional basis, which holds for both the diagonally normalized composite matrix $\widetilde{K}$ and the original un-normalized matrix K. Such a

Table 7 Two-dimensional case: condition numbers of the composite matrix: original $K(M, S; \zeta)$ and normalized $\widetilde{K}(M, S; \zeta)$ from the new basis and the basis in [4], denoted 'A-C', where $\zeta = 100$

Order	Original		Normalized		Ratio	
p	New	A-C	New	A-C	Original	Normal.
0	1.000e00	1.000e00	1.000e00	1.000e00	1.000e00	1.000e00
1	1.360e00	1.071e01	1.183e00	3.643e00	7.875e00	3.079e00
2	2.571e00	1.347e02	1.725e00	3.407e01	5.239e01	1.975e01
3	5.004e00	9.820e02	2.704e00	2.518e02	1.962e02	9.312e01
4	9.531e00	8.857e03	4.320e00	2.770e03	9.293e02	6.412e02
5	1.705e01	8.764e04	6.877e00	2.850e04	5.140e03	4.144e03
6	2.882e01	1.004e06	1.079e01	4.141e05	3.484e04	3.838e04
7	4.610e01	1.250e07	1.612e01	5.777e06	2.711e05	3.584e05
8	7.057e01	1.692e08	2.308e01	9.709e07	2.398e06	4.207e06
9	1.038e02	2.517e09	3.179e01	1.689e09	2.425e07	5.313e07
10	1.480e02	3.880e10	4.240e01	2.867e10	2.622e08	6.762e08

Table 8 Three-dimensional case: condition numbers of the composite matrix: original $K(M, S; \zeta)$ and normalized $\widetilde{K}(M, S; \zeta)$ from the new basis and the basis in [4], denoted 'A-C', where $\zeta = 0.01$

Order	Original		Normalized		Ratio	
p	New	A-C	New	A-C	Original	Normal.
0	1.000e00	1.000e00	1.000e00	1.000e00	1.000e00	1.000e00
1	8.001e03	1.600e03	3.910e00	1.599e01	2.000e-1	4.090e00
2	3.145e04	1.614e03	9.456e00	6.593e01	5.132e-2	6.972e00
3	7.823e04	4.778e03	1.355e01	1.393e03	6.108e-2	1.028e02
4	1.616e05	5.104e04	2.019e01	1.812e04	3.158e-1	8.975e02
5	2.979e05	1.462e06	2.853e01	4.181e05	4.908e00	1.465e04
6	5.062e05	2.562e07	3.909e01	9.837e06	5.061e01	2.517e05
7	8.084e05	7.102e08	5.174e01	2.596e08	8.785e02	5.017e06
8	1.229e06	1.675e10	6.674e01	7.698e09	1.363e04	1.153e08
9	1.797e06	5.074e11	8.415e01	2.051e11	2.824e05	2.437e09
10	2.541e06	1.332e13	1.042e02	6.403e12	5.242e06	6.145e10

fact resonates with the common agreement that three-dimensional problems are generally harder to solve than two-dimensional ones. We are short of the definite reason for this fact. However, a phenomenological explanation is due to the dimensional difference.

- As a performance comparison with the bases by Ainsworth and Coyle [4], the new bases have a better conditioning for the diagonally normalized composite matrix $\widetilde{K}$ for each order of approximation and for all values of the parameter ζ in this study. The higher the order of approximation, the more striking difference between the two sets of bases. For example, with the modest order $p = 5$ and $\zeta = 0.01$, the ratios are 1.340×10^3 and 1.465×10^4 for the two- and three-dimensional bases, respectively, and with the higher order $p = 10$ and $\zeta = 100$, the ratios increase to 6.762×10^8 and 1.576×10^{11} for the two- and three-dimensional bases, respectively.

Table 9 Three-dimensional case: condition numbers of the composite matrix: original $K(M, S; \zeta)$ and normalized $\widetilde{K}(M, S; \zeta)$ from the new basis and the basis in [4], denoted 'A-C', where $\zeta = 1$

Order	Original		Normalized		Ratio	
p	New	A-C	New	A-C	Original	Normal.
0	1.000e00	1.000e00	1.000e00	1.000e00	1.000e00	1.000e00
1	8.100e01	1.620e01	3.770e00	1.543e01	2.000e-1	4.093e00
2	3.155e02	1.205e02	9.047e00	6.494e01	3.819e-1	7.178e00
3	7.833e02	4.741e03	1.323e01	1.390e03	6.053e00	1.051e02
4	1.617e03	5.120e04	1.963e01	1.811e04	3.166e01	9.226e02
5	2.980e03	1.467e06	2.804e01	4.195e05	4.923e02	1.496e04
6	5.063e03	2.569e07	3.855e01	9.992e06	5.074e03	2.592e05
7	8.085e03	7.122e08	5.120e01	2.608e08	8.809e04	5.094e06
8	1.229e04	1.679e10	6.618e01	7.787e09	1.366e06	1.177e08
9	1.797e04	5.086e11	8.358e01	2.060e11	2.830e07	2.465e09
10	2.541e04	1.335e13	1.036e02	6.460e12	5.254e08	6.236e10

Table 10 Three-dimensional case: condition numbers of the composite matrix: original $K(M, S; \zeta)$ and normalized $\widetilde{K}(M, S; \zeta)$ from the new basis and the basis in [4], denoted 'A-C', where $\zeta = 100$

Order	Original		Normalized		Ratio	
p	New	A-C	New	A-C	Original	Normal.
0	1.000e00	1.000e00	1.000e00	1.000e00	1.000e00	1.000e00
1	1.800e00	1.667e01	1.480e00	6.000e00	9.261e00	4.054e00
2	4.145e00	4.447e02	2.728e00	1.500e02	1.073e02	5.499e01
3	8.823e00	1.218e04	4.998e00	1.463e03	1.380e03	2.927e02
4	1.716e01	1.625e05	8.416e00	3.806e04	9.470e03	4.522e03
5	3.079e01	3.519e06	1.305e01	6.230e05	1.143e05	4.774e04
6	5.162e01	6.299e07	1.986e01	2.089e07	1.220e06	1.052e06
7	8.184e01	1.525e09	2.897e01	3.727e08	1.863e07	1.287e07
8	1.239e02	3.604e10	4.050e01	1.459e10	2.909e08	3.602e08
9	1.807e02	9.959e11	5.458e01	3.109e11	5.511e09	5.696e09
10	2.551e02	2.627e13	7.144e01	1.126e13	1.030e11	1.576e11

- For the Ainsworth and Coyle bases [4], as with each component study on the mass and stiffness matrices, the condition number of the composite matrix K and of the diagonally normalized matrix $\widetilde{K}$ grows exponentially with the order of approximation for each specific value of the parameter ζ considered. We refrain from further comments on the 'A-C' bases [4].

4 Discussion and Conclusion

New orthonormal hierarchical bases for simplicial $\mathcal{L}_2$-conforming elements in two and three dimensions have been proposed with the goal of improving the conditioning of the mass and stiffness matrices. The basis functions are orthonormal in $\mathcal{L}_2$ norm over the reference ele-

ments, and are given explicitly by the formula (8). The construction of the new basis is motivated by the study of orthogonal polynomials of several variables [13] over an n-simplex. This is achieved by appropriately exploiting classical Jacobi polynomials over simplicial elements.

On the reference element the mass matrix is an identity matrix, thus, is perfectly conditioned with a condition number of one. In contrast, the condition number of the Ainsworth-Coyle bases [4] grows exponentially. For both the original and diagonally *normalized* mass matrices, in terms of matrix conditioning and starting from order four of approximation, the bases in this study are at least three and five orders better than the bases in [4] for two and three dimensions, respectively.

The conditioning of the original un-normalized stiffness matrix follows a cubic law, viz., the condition number grows cubically vs. order of approximation, and is *independent* of dimension. To the best of our knowledge, such facts have never been established before. The latter fact of *dimension-independence* comes as a surprise. Furthermore, the diagonally *normalized* stiffness matrix is well conditioned. As a comparison, for the bases proposed by Ainsworth and Coyle [4], the condition number of the stiffness matrices grows exponentially vs. order of approximation. In particular, for both the original and diagonally *normalized* stiffness matrices, in terms of matrix conditioning and starting from order six of approximation, the proposed bases are at least three and four orders better than the bases in [4] for two and three dimensions, respectively.

The conditioning of the composite matrix $K(M, S; \zeta) = \zeta M + S$ has also been studied in terms of several distinct values of the parameter ζ which has the dynamical range of 10^4. It is found that the diagonally normalized composite matrix $\widetilde{K}$ is well conditioned. Moreover, starting from order five of approximation and with all the values of the parameter ζ studied, the new bases are at least three and four orders better than the bases in [4] for two and three dimensions, respectively. The higher the order of approximation, the greater the advantage of the proposed new bases, which rightfully fulfill the goal of hierarchical bases.

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Appendix: Proof of Theorem 2.1

To prove Theorem 2.1, we first establish a lemma.

Lemma A.1 *For the integral of a scalar function $f(\mathbf{x}) \in \mathcal{L}_1(K^n)$, the following holds*

$$I^{(K^n)}[f(\mathbf{x})] := \int_{K^n} f(\mathbf{x}) d\mathbf{x} \tag{21}$$

$$= \int_{K^{n-1}} \left(\int_0^{1-|\mathbf{x}_{n-1}|} f\left(\mathbf{x}_{n-1}, (1-|\mathbf{x}_{n-1}|)s\right) ds \right) \cdot (1-|\mathbf{x}_{n-1}|) \cdot d\mathbf{x}_{n-1}. \tag{22}$$

Proof By definition we have

$$I^{(K^n)}[f(\mathbf{x})] := \int_0^1 dx_1 \int_0^{1-x_1} dx_2 \cdots \int_0^{1-x_1-\cdots-x_{n-1}} f(x_1, \ldots, x_{n-1}, x_n) dx_n \tag{23a}$$

$$= \int_0^1 dx_1 \int_0^{1-x_1} dx_2 \cdots \int_0^{1-|\mathbf{x}_{n-1}|} f\left(\mathbf{x}_{n-1}, (1-|\mathbf{x}_{n-1}|)s\right) ds \cdot (1-|\mathbf{x}_{n-1}|) \tag{23b}$$

$$= \int_{K^{n-1}} \left(\int_0^{1-|\mathbf{x}_{n-1}|} f\left(\mathbf{x}_{n-1}, (1-|\mathbf{x}_{n-1}|)s\right) ds \right) \cdot (1-|\mathbf{x}_{n-1}|) \cdot d\mathbf{x}_{n-1}. \tag{23c}$$

□

The substitution $x_n = (1-|\mathbf{x}_{n-1}|)s$ has been used in the proof. A formal proof of Theorem 2.1 follows.

Proof It is clear and easy to show that the polynomials $P_{\vec{\alpha}}(W_{\vec{\tau}}^{(K^n)}; \mathbf{x})$ are pairwise orthogonal with respect to the weight function $W_{\vec{\tau}}^{(K^n)}(\mathbf{x})$, thus, the proof is omitted. We need to show the normality property of the orthogonal polynomials $P_{\vec{\alpha}}(W_{\vec{\tau}}^{(K^n)}; \mathbf{x})$. Using the Lemma A.1 repeatedly we can reduce the integral on K^n to a multiple of n integrals of a single variable. In specific, we have

$$\int_{K^n} W_{\vec{\tau}}^{(K^n)}(\mathbf{x}) \left[P_{\vec{\alpha}} \left(W_{\vec{\tau}}^{(K^n)}; \mathbf{x} \right) \right]^2 d\mathbf{x} \tag{24a}$$

$$= \left[h_{\vec{\alpha}}^{(K^n)} \right]^{-2} \prod_{i=1}^n \int_0^1 (1-s)^{\rho_i^1} s^{\rho_i^2} \left[p_{\alpha_i}^{(\rho_i^1, \rho_i^2)}(2s-1) \right]^2 ds \tag{24b}$$

$$= \left[h_{\vec{\alpha}}^{(K^n)} \right]^{-2} \prod_{i=1}^n \frac{1}{2^{\rho_i^1+\rho_i^2+1}} \int_{-1}^1 (1-\sigma)^{\rho_i^1} (1+\sigma)^{\rho_i^2} \left[p_{\alpha_i}^{(\rho_i^1, \rho_i^2)}(\sigma) \right]^2 d\sigma \tag{24c}$$

$$= \left[h_{\vec{\alpha}}^{(K^n)} \right]^{-2} \prod_{i=1}^n \frac{1}{2^{\rho_i^1+\rho_i^2+1}} \times 1 \tag{24d}$$

$$= 1. \tag{24e}$$

□

The change of variable $s = \frac{x_i}{1-|\mathbf{x}_{i-1}|}$ has been used in the second line (24b) for $i = 1, 2, \ldots, n$. A further change of variable $\sigma = 2s - 1$ has been applied in the third line (24c). The fourth line (24d) is obtained by the orthonormal property of the classical Jacobi polynomials of one variable [18]. And the last line is true in view of the formula $[h_{\vec{\alpha}}^{(K^n)}]^{-2}$ given in (7b).

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