HEXAHEDRAL H(DIV) AND H(CURL) FINITE ELEMENTS

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Abstract. We study the approximation properties of some finite element subspaces of $\boldsymbol{H}(\mathrm{div};\Omega)$ and $\boldsymbol{H}(\mathbf{curl}\,;\Omega)$ defined on hexahedral meshes in three dimensions. This work extends results previously obtained for quadrilateral $\boldsymbol{H}(\mathrm{div};\Omega)$ finite elements and for quadrilateral scalar finite element spaces. The finite element spaces we consider are constructed starting from a given finite dimensional space of vector fields on the reference cube, which is then transformed to a space of vector fields on a hexahedron using the appropriate transform (e.g., the Piola transform) associated to a trilinear isomorphism of the cube onto the hexahedron. After determining what vector fields are needed on the reference element to insure $O(h)$ approximation in $\boldsymbol{L}^2(\Omega)$ and in $\boldsymbol{H}(\mathrm{div};\Omega)$ and $\boldsymbol{H}(\mathbf{curl}\,;\Omega)$ on the physical element, we study the properties of the resulting finite element spaces.

Introduction

In the series of papers [1], [2], and [3], the approximation properties of finite elements on quadrilateral meshes in $\mathbb{R}^2$ was considered. Papers [1] and [3] examine the case of scalar approximation and paper [2] the approximation of vector functions in the space $\boldsymbol{H}(\mathrm{div};\Omega) = \{\boldsymbol{v} \in \boldsymbol{L}^2(\Omega) : \mathrm{div}\,\boldsymbol{v} \in L^2(\Omega)\}$ (see also [10]).

For scalar problems, the finite element spaces are constructed in the standard way, starting with a given finite dimensional space of functions on a square reference element $\hat{K}$ which is then transformed to a space of functions on each convex quadrilateral element K via a bilinear isomorphism of the square onto the element. It was well known that for affine isomorphisms, a necessary and sufficient condition for approximation of order $r+1$ in L^2 and order r in H^1 is that the given space of functions on the reference element contain $\mathcal{P}_r(\hat{K})$, all polynomial functions of total degree at most r on $\hat{K}$. In the case of bilinear isomorphisms, it was also well known that the same estimates hold if the function space contains $\mathcal{Q}_r(\hat{K})$, all polynomial functions of separate degree r on $\hat{K}$. In [1], it is shown by means of a simple and non-pathological counterexample, that this latter condition is also necessary. This result was then used to show that various methods that are successful on rectangular meshes lose accuracy when applied on quadrilateral meshes. This includes the use of serendipity finite element spaces, the combination of bilinearly mapped piecewise continuous quadratic elements for the two components of velocity and bilinearly mapped piecewise linear elements for the pressure in the approximation of the Stokes problem, and certain nonconforming finite elements defined on quadrilateral meshes.

In [2], results were obtained on the approximation properties of quadrilateral finite element spaces of vector-valued functions defined by the Piola transform, extending the results

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described above for scalar approximation. These finite element spaces are also constructed in the standard way, starting with a given finite dimensional space of vector-valued functions on a square reference element, which is then transformed to a vector-valued space of functions on each convex quadrilateral element via a Piola transform associated to a bilinear isomorphism of the square onto the element. Such spaces are important in defining finite element approximations of $\boldsymbol{H}(\mathrm{div};\Omega)$. In [2], it is shown that for optimal order L^2 approximation, the space of functions on the reference element must contain the space $\boldsymbol{S}_r$, generated by the standard basis functions for the local Raviart-Thomas space of degree r, but replacing the basis functions $(\hat{x}^{r+1}\hat{y}^r, 0)$ and $(0, \hat{x}^r\hat{y}^{r+1})$ by the single basis function $(\hat{x}^{r+1}\hat{y}^r, -\hat{x}^r\hat{y}^{r+1})$. Additional functions must be added to obtain optimal approximation of the divergence. A consequence of the results obtained is that while the Raviart–Thomas space of index r achieves order $r+1$ approximation in L^2 for quadrilateral meshes as for rectangular meshes, the order of approximation of the divergence is only of order r in the quadrilateral case (but of order $r+1$ for rectangular meshes). Thus, in the case $r = 0$, there is no convergence in $\boldsymbol{H}(\mathrm{div};\Omega)$. For the Brezzi–Douglas–Marini and Brezzi–Douglas–Fortin–Marini spaces, the order of convergence is severely reduced on general quadrilateral meshes not only for $\mathrm{div}\,\boldsymbol{u}$ but also for $\boldsymbol{u}$ itself. Also contained in [2] is a construction of a new quadrilateral finite element space that provides optimal order approximation in $\boldsymbol{H}(\mathrm{div};\Omega)$. As a further application of these results, it is established that despite the loss of accuracy in the approximation of the divergence, one still retains optimal order approximation in L^2 to both the vector and scalar variable when the standard mixed method is applied to the solution of the Dirichlet problem for Poisson's equation using mapped Raviart-Thomas elements of index r to approximate the vector variable and mapped discontinuous piecewise polynomials of degree r to approximate the scalar variable. Of course, there is a degradation in the approximation of the divergence. By contrast, it is demonstrated in numerical computations that when such elements are used in a least-squares formulation in which the functional $J(q,\boldsymbol{v}) = \|\boldsymbol{v} - \mathbf{grad}\, q\|^2_{L^2(\Omega)} + \|\,\mathrm{div}\,\boldsymbol{v} + f\|^2_{L^2(\Omega)}$ is minimized over $\boldsymbol{v}$ in the lowest order Raviart-Thomas space and q in the space of mapped piecewise bilinear elements, the loss of accuracy in the approximation of the divergence results in lack of convergence for both the scalar and vector variable.

In this paper, we consider the extension of these results to hexahedral meshes in three dimensions. In this case, in addition to the space $\boldsymbol{H}(\mathrm{div};\Omega)$, there is another important space $\boldsymbol{H}(\mathbf{curl}\,;\Omega) = \{\boldsymbol{v} \in \boldsymbol{L}^2(\Omega) : \mathbf{curl}\;\boldsymbol{v} \in \boldsymbol{L}^2(\Omega)\}$, that arises naturally in many applications (e.g., Maxwell's equations). The finite element spaces studied are defined on irregular hexahedral elements obtained by trilinear mappings from a reference cube. These maps are considerably more complicated than bilinear maps in two dimensions, since a general trilinear map of the unit cube produces a solid that can have hyperboloid as well as planar faces. Recent progress has been made on the questions of invertibility of these maps and positivity of their Jacobians on the reference element (e.g., see [17], [18],[19]). Although there has been a fairly extensive study of tetrahedral finite elements, most elements defined on cubes have not been studied to determine if they maintain key approximation properties when mapped to general hexahedrons, despite the fact that this is implicitly assumed, since meshes of regular hexahedrons are quite restrictive in their use. One exception is the case of almost affine elements, (nearly parallelepipeds) which can result from nested refinement strategies, and which have the same approximation properties as elements defined on parallelepipeds (e.g., see [16], [5]). For the reader interested in additional background material, a set of hierarchical basis functions for the spaces $\boldsymbol{H}(\mathrm{div})$ and $\boldsymbol{H}(\mathbf{curl})$ of arbitrary order for the most commonly used reference domains in two and three dimensions can be found in [14].

Following the approach of [1] and [2], we shall consider the question of what functions are necessary on the reference element to guarantee optimal order approximation by finite element subspaces of $\boldsymbol{H}(\mathrm{div};\Omega)$ and $\boldsymbol{H}(\mathbf{curl};\Omega)$. In particular, we will show that the space obtained by a general trilinear mapping of the Raviart-Thomas-Nédélec element of lowest degree defined on a cube, i.e., a space defined locally by vectors of the form $(a_1 + b_1\hat{x}, a_2 + b_2\hat{y}, a_3 + b_3\hat{z})$ does not contain constants, and hence does not have good approximation properties. We then seek to construct the simplest space that does have this property. As we shall see, the resulting space is already quite complicated (a 21 dimensional subspace of the dimension 36 second lowest degree Raviart-Thomas-Nédélec space $\boldsymbol{RT}_1$), even in the lowest order case, and hence we restrict the paper only to this case. We then ask a similar question about what functions are needed to produce an $O(h)$ approximation to $\mathrm{div}\,\boldsymbol{u}$.

The fact that mapped linears do not approximate well is noted in [12] and [13]. In these papers, an alternative approximation is constructed which gives good approximations in the case when the primary (boundary) faces and also appropriately defined "secondary faces," (internal to the element) are planar. The approach taken is to seek a space on the physical element so that $\boldsymbol{u}\cdot\boldsymbol{n}$ is constant on each boundary face, where $\boldsymbol{n}$ denotes the face normal. The advantage of this approach is that the local dimension of the spaces (6) is the same as for the lowest order Raviart-Thomas space on cubes. The disadvantage is that the standard use of the reference element to simplify computations is lost.

In the case of $\boldsymbol{H}(\mathbf{curl};\Omega)$, a natural place to begin is to consider mappings of the lowest order Nédélec space $\boldsymbol{N}_0 = \{a_1 + b_1\hat{y} + c_1\hat{z} + d_1\hat{y}\hat{z}, a_2\hat{x} + b_2 + c_2\hat{z} + d_2\hat{x}\hat{z}, a_3\hat{x} + b_3\hat{y} + c_3 + d_3\hat{x}\hat{y})$ defined on the reference cube. For $\hat{\boldsymbol{u}}$ of this form, we define $\boldsymbol{u}(\boldsymbol{F}_K(\hat{\boldsymbol{x}})) = D\boldsymbol{F}_K^{-T}(\hat{\boldsymbol{x}})\hat{\boldsymbol{u}}(\hat{\boldsymbol{x}})$, where $\boldsymbol{F}_K(\hat{\boldsymbol{x}})$ is a trilinear map taking the reference cube to the physical element and $D\boldsymbol{F}_K$ is the matrix of first partial derivatives of $\boldsymbol{F}_K$. We show that this procedure produces a space which contains constant vectors, and hence provides an $O(h)$ approximation in L^2. However, the $\mathbf{curl}$ of the space does not contain constant vectors, so one no longer has optimal order approximation of $\mathbf{curl}\,\boldsymbol{u}$. Thus, we construct a new space that does have optimal order convergence.

An outline of the paper is as follows. In the next section, we introduce the notation to be used and collect some preliminary results. In § 2, we consider the case of uniform meshes, and state the three dimensional analogue of results obtained in [1] and [2] in two dimensions. In § 3, we consider what function space is necessary on the reference element in order to produce a mapped $\boldsymbol{H}(\mathrm{div};\Omega)$ finite element space providing $O(h)$ approximations in $\boldsymbol{L}^2(\Omega)$, and then derive such as space. We then consider in the following section what additional functions must be added to also produce an $O(h)$ approximation to the divergence. In § 5, we combine these results to derive an $\boldsymbol{H}(\mathrm{div};\Omega)$ finite element space that also produces an $O(h)$ approximation to the divergence. Analogous results for the lowest order mapped $\boldsymbol{H}(\mathbf{curl};\Omega)$ space are derived in § 6. In § 7, we show that the discrete de Rham diagram involving these spaces commutes, a key property in the analysis of finite element methods, and then use these results in § 8 to obtain error estimates for the finite element $\boldsymbol{H}(\mathrm{div};\Omega)$ and $\boldsymbol{H}(\mathbf{curl};\Omega)$ spaces derived in the previous sections. In § 9, we make some remarks about the application of these spaces to mixed finite element methods. Since the spaces we construct involve a substantial number of degrees of freedom, we consider in the final section whether there are simpler spaces that give optimal order approximation for special classes of hexahedrons.

1. Notation and preliminaries

Throughout the paper, we suppose that Ω is a polyhedron and that it is covered by a hexahedral mesh $\mathcal{T}_h$ consisting of elements K of maximum diameter h obtained from a single reference element $\hat{K} = [0,1]^3$ by the application of a trilinear diffeomorphism $\boldsymbol{F}_K : \hat{K} \to \mathbb{R}^3$ such that $K = \boldsymbol{F}_K(\hat{K})$. To simplify notation, we shall often drop the subscript K on $\boldsymbol{F}_K$ when only a single element is under consideration.

For functions in $\boldsymbol{H}(\mathrm{div};\Omega)$, the natural way to transform functions from $\hat{K}$ to K is via the *Piola transform*. Namely, given a function $\hat{\boldsymbol{u}} : \hat{K} \to \mathbb{R}^3$, we define $\boldsymbol{u} = \boldsymbol{P}_F \hat{\boldsymbol{u}} : K \to \mathbb{R}^3$ by

$$\boldsymbol{u}(\boldsymbol{x}) = J\boldsymbol{F}(\hat{\boldsymbol{x}})^{-1} D\boldsymbol{F}(\hat{\boldsymbol{x}})\hat{\boldsymbol{u}}(\hat{\boldsymbol{x}}), \tag{1.1}$$

where $\hat{\boldsymbol{x}} \in \hat{K}$, $\boldsymbol{x} = \boldsymbol{F}(\hat{\boldsymbol{x}})$, and $D\boldsymbol{F}(\hat{\boldsymbol{x}})$ is the Jacobian matrix of the mapping $\boldsymbol{F}$ and $J\boldsymbol{F}(\hat{\boldsymbol{x}})$ its determinant. We shall assume that $\mathrm{sgn}(J\boldsymbol{F}(\hat{\boldsymbol{x}})) > 0$. The transform has the property that if $\boldsymbol{u} = \boldsymbol{P}_F \hat{\boldsymbol{u}}$, $p = \hat{p} \circ \boldsymbol{F}^{-1}$ for some $\hat{p} : \hat{K} \to \mathbb{R}$, and $\boldsymbol{n}$ and $\hat{\boldsymbol{n}}$ denote the unit outward normals on faces f and $\hat{f}$ of K and $\hat{K}$, respectively, then

$$\int_K \mathrm{div}\, \boldsymbol{u}\, p \, d\boldsymbol{x} = \int_{\hat{K}} \hat{\mathrm{div}}\, \hat{\boldsymbol{u}}\, \hat{p}\, d\hat{\boldsymbol{x}}, \quad \int_f \boldsymbol{u} \cdot \boldsymbol{n}\, p\, dA = \int_{\hat{f}} \hat{\boldsymbol{u}} \cdot \hat{\boldsymbol{n}}\, \hat{p}\, d\hat{A}, \tag{1.2}$$

where we have used the fact that

$$\boldsymbol{n}(\boldsymbol{x}) = \frac{[D\boldsymbol{F}(\hat{\boldsymbol{x}})]^{-T}\hat{\boldsymbol{n}}(\hat{\boldsymbol{x}})}{|[D\boldsymbol{F}(\hat{\boldsymbol{x}})]^{-T}\hat{\boldsymbol{n}}(\hat{\boldsymbol{x}})|}.$$

Since continuity of $\boldsymbol{u} \cdot \boldsymbol{n}$ is necessary for finite element subspaces of $\boldsymbol{H}(\mathrm{div};\Omega)$, use of the Piola transform facilitates the definition of finite element subspaces of $\boldsymbol{H}(\mathrm{div};\Omega)$ by mapping from a reference element.

Using the Piola transform, a standard construction of a finite element subspace proceeds as follows. Let $\hat{\boldsymbol{V}} \subset \boldsymbol{H}(\mathrm{div}, \hat{K})$ be a finite dimensional space of vector fields on $\hat{K}$, typically polynomial, the space of reference *shape functions*. Now suppose we are given a mesh $\mathcal{T}_h$ consisting of elements K of maximum diameter h, each of which is the image of $\hat{K}$ under some given diffeomorphism: $K = \boldsymbol{F}_K(\hat{K})$. We assume the mesh family is shape-regular and non-degenerate in the following sense:

(SR-ND1): There exists a constant σ independent of h and K such that the shape constants $\sigma_K := h_K/\rho_K \le \sigma$, where h_K denotes the diameter of K and ρ_K is the diameter of the largest ball B_K contained in K such that K is star-shaped with respect to B_K.

(SR-ND2): There exists a constant $\gamma > 0$ independent of h and K, such that $J\boldsymbol{F}_K(\hat{\boldsymbol{x}}) \ge \gamma h_K^3$ for all $\hat{x} \in \hat{K}$.

Remarks. 1) The parameter σ_K in (SR-ND1) is termed the "chunkiness" of the element. A uniform bound on chunkiness implies that certain constants in the Bramble-Hilbert lemma are independent of the domain (see [9], [6]). We shall use this fact when we prove interpolation error estimates. Assumption (SR-ND2) guarantees that various estimates for $\boldsymbol{F}_K$ and its derivatives can be proved.

2) In the case when $\boldsymbol{F}_K$ is an affine map, condition (SR-ND2) follows from (SR-ND1). In two dimensions, when $\boldsymbol{F}_K$ is a bilinear map, condition (SR-ND1) is not enough to guarantee (SR-ND2). In that case, one may follow [11](pp 105), and instead define shape-regularity as condition (SR-ND1) with a modified definition of $\rho_K = 2\min_{1\le i\le 4}$ {diameter of circle inscribed in S_i}, where S_i is the subtriangle of K connecting the vertices a_{i-1}, a_i and a_{i+1}. This modified definition implies (SR-ND2). The authors of this paper are not aware of a simple geometric condition guaranteeing (SR-ND2) in the case of a hexahedron in three dimensions. Some results in this direction that indicate some of the complexity and other references on the subject can be found in [19]. It is also possible to weaken (SR-ND1) so that K is only assumed to be a finite union of star-shaped domains (see [9]).

Via the Piola transform, we then obtain the space $\boldsymbol{V}(K) = \boldsymbol{P}_{F_K}\hat{\boldsymbol{V}}$ of shape functions on K. Finally we define the finite element space as

$$\boldsymbol{V}_h = \{\, \boldsymbol{v} \in \boldsymbol{H}(\mathrm{div};\Omega) : \boldsymbol{v}|_K \in \boldsymbol{V}(K),\ \forall K \in \mathcal{T}_h \,\}.$$

Recall that $\boldsymbol{V}_h$ may be characterized as the subspace of

$$\tilde{\boldsymbol{V}}_h := \{\, \boldsymbol{v} \in \boldsymbol{L}^2(\Omega) : \boldsymbol{v}|_K \in \boldsymbol{P}_{F_K}\hat{\boldsymbol{V}},\ \forall K \in \mathcal{T}_h \,\},$$

consisting of vector fields whose normal component is continuous across interelement faces.

An analogous approach is used for functions in $\boldsymbol{H}(\mathbf{curl}\,;\Omega)$. In this case, given a function $\hat{\boldsymbol{u}} : \hat{K} \mapsto \mathbb{R}^3$, we define $\boldsymbol{u} = \boldsymbol{R}_F\hat{\boldsymbol{u}} : K \mapsto \mathbb{R}^3$ by

$$\boldsymbol{u}(\boldsymbol{x}) = \boldsymbol{R}_F\hat{\boldsymbol{u}} \equiv (D\boldsymbol{F})^{-T}(\hat{\boldsymbol{x}})\,\hat{\boldsymbol{u}}(\hat{\boldsymbol{x}}), \tag{1.3}$$

where again, $\boldsymbol{x} = \boldsymbol{F}(\hat{\boldsymbol{x}})$. The transform has the property that if $\boldsymbol{u} = \boldsymbol{R}_F\,\hat{\boldsymbol{u}}$, $\boldsymbol{w} = \boldsymbol{R}_F\hat{\boldsymbol{w}}$, $p = \hat{p}\circ\boldsymbol{F}^{-1}$, $\boldsymbol{q} = \boldsymbol{P}_F\,\hat{\boldsymbol{q}}(\hat{\boldsymbol{x}})$, and $\boldsymbol{t}$ and $\hat{\boldsymbol{t}}$ denote unit tangent vectors in the direction of an edge e and $\hat{e}$ of K and $\hat{K}$, respectively, then

$$\int_e \boldsymbol{u}\cdot\boldsymbol{t}\,p\,ds = \int_{\hat{e}} \hat{\boldsymbol{u}}\cdot\hat{\boldsymbol{t}}\ \hat{p}\,d\hat{s}, \quad \int_f \boldsymbol{u}\times\boldsymbol{n}\cdot\boldsymbol{w}\,dA = \int_{\hat{f}} \hat{\boldsymbol{u}}\times\hat{\boldsymbol{n}}\cdot\hat{\boldsymbol{w}}\,d\hat{A}, \quad \int_K \boldsymbol{u}\cdot\boldsymbol{q}\,d\boldsymbol{x} = \int_{\hat{K}} \hat{\boldsymbol{u}}\cdot\hat{\boldsymbol{q}}\,d\hat{\boldsymbol{x}}, \tag{1.4}$$

where we have used the fact that

$$\boldsymbol{t}(\boldsymbol{x}) = \frac{[D\boldsymbol{F}(\hat{\boldsymbol{x}})]^T\hat{\boldsymbol{t}}(\hat{\boldsymbol{x}})}{|[D\boldsymbol{F}(\hat{\boldsymbol{x}})]^T\hat{\boldsymbol{t}}(\hat{\boldsymbol{x}})|}.$$

The above results are used to establish continuity of the tangential components of $\boldsymbol{u}$, necessary for finite element subspaces of $\boldsymbol{H}(\mathbf{curl}\,;\Omega)$.

Using the transform (1.3), a standard construction of a finite element subspace of the space $\boldsymbol{H}(\mathbf{curl}\,;\Omega)$ proceeds in the same manner as for $\boldsymbol{H}(\mathrm{div};\Omega)$. Let $\hat{\boldsymbol{U}} \subset \boldsymbol{H}(\mathbf{curl}\,,\hat{K})$ be a finite dimensional space of vector fields on $\hat{K}$. Using the given mesh $\mathcal{T}_h$ consisting of elements K, each of which is the image of $\hat{K}$ under some given diffeomorphism: $K = \boldsymbol{F}_K(\hat{K})$, we define $\boldsymbol{U}(K) = \boldsymbol{R}_{F_K}\hat{\boldsymbol{U}}$ and the finite element space as

$$\boldsymbol{U}_h = \{\, \boldsymbol{u} \in \boldsymbol{H}(\mathbf{curl}\,;\Omega) \mid \boldsymbol{u}|_K \in \boldsymbol{R}_{F_K}\hat{\boldsymbol{U}},\ \forall K \in \mathcal{T}_h \,\}.$$

Similarly to divergence conforming elements, $\boldsymbol{U}_h$ may be characterized as the subspace of

$$\tilde{\boldsymbol{U}}_h := \{\, \boldsymbol{u} \in \boldsymbol{L}^2(\Omega) \mid \boldsymbol{u}|_K \in \boldsymbol{R}_{F_K}\hat{\boldsymbol{U}},\ \forall K \in \mathcal{T}_h \,\},$$

consisting of vector fields whose tangential components are continuous across interelement faces.

2. Approximation theory of vector fields on uniform meshes

In this preliminary section of the paper, we state the three dimensional analogue of some results obtained in [1] and [2] for approximation of scalar functions and vector fields on rectangular meshes.

Let K be any cube with edges parallel to the axes, i.e., $K = \boldsymbol{D}_K(\hat{K})$ with

$$\boldsymbol{D}_K(\hat{\boldsymbol{x}}) = \boldsymbol{x}_K + h_K\hat{\boldsymbol{x}},$$

where $\boldsymbol{x}_K \in \mathbb{R}^3$ is the corner of K with smallest (x, y, z) coordinates and $h_K > 0$ is its side length. The Piola transform (1.1) of $\hat{\boldsymbol{u}} \in \boldsymbol{L}^2(\hat{K})$ is easily seen to be $(\boldsymbol{P}_{D_K}\hat{\boldsymbol{u}})(\boldsymbol{x}) = h_K^{-2}\hat{\boldsymbol{u}}(\hat{\boldsymbol{x}})$, where $\boldsymbol{x} = \boldsymbol{D}_K(\hat{\boldsymbol{x}})$. We also have that $\operatorname{div}(\boldsymbol{P}_{D_K}\hat{\boldsymbol{u}})(\boldsymbol{x}) = h_K^{-3}\hat{\operatorname{div}}\hat{\boldsymbol{u}}(\hat{\boldsymbol{x}})$. If we apply the transform (1.3) to $\hat{\boldsymbol{u}} \in \boldsymbol{L}^2(\hat{K})$, then $(\boldsymbol{R}_{D_K}\hat{\boldsymbol{u}})(\boldsymbol{x}) = h_K^{-1}\hat{\boldsymbol{u}}(\hat{\boldsymbol{x}})$ and $\mathbf{curl}\,(\boldsymbol{R}_{D_K}\hat{\boldsymbol{u}})(\boldsymbol{x}) = h_K^{-2}\hat{\mathbf{curl}}\ \hat{\boldsymbol{u}}(\hat{\boldsymbol{x}})$.

We denote the unit cube by both Ω (when we think of it as a domain) and $\hat{K}$ (when we think of it as a reference element). For n a positive integer, we let $\mathcal{U}_h$ be the uniform mesh of Ω consisting of n^3 subcubes of side length $h = 1/n$. Given a subspace $\hat{\boldsymbol{V}}$ of $\boldsymbol{L}^2(\hat{K})$, we define, as in the previous section, $\boldsymbol{V}(K) = \boldsymbol{P}_{D_K}\hat{\boldsymbol{V}}$, $\boldsymbol{U}(K) = \boldsymbol{R}_{D_K}\hat{\boldsymbol{U}}$,

$$\tilde{\boldsymbol{V}}_h = \{\boldsymbol{v} \in \boldsymbol{L}^2(\Omega) : \boldsymbol{v}_K \in \boldsymbol{V}(K), \forall K \in \mathcal{U}_h\}, \tag{2.1}$$

$$\tilde{\boldsymbol{U}}_h = \{\boldsymbol{v} \in \boldsymbol{L}^2(\Omega) : \boldsymbol{v}_K \in \boldsymbol{U}(K), \forall K \in \mathcal{U}_h\}. \tag{2.2}$$

Then the analogue of Theorems 2.1 and 2.2 of [2] for the space $\boldsymbol{H}(\operatorname{div};\Omega)$ is as follows. Since we only consider a simple special case, we include the proof of the first theorem. The second is proved in in a similar manner.

Theorem 2.1. *Let $\hat{\boldsymbol{V}}$ be a finite dimensional subspace of $\boldsymbol{L}^2(\hat{K})$. The following conditions are equivalent:*
(i) There is a constant C such that $\inf_{\boldsymbol{v}\in\tilde{\boldsymbol{V}}_h} \|\boldsymbol{u}-\boldsymbol{v}\|_{\boldsymbol{L}^2(\Omega)} \le Ch\|\nabla\boldsymbol{u}\|_{\boldsymbol{L}^2(\Omega)}$ for all $\boldsymbol{u} \in \boldsymbol{H}^1(\Omega)$.
(ii) $\inf_{\boldsymbol{v}\in\tilde{\boldsymbol{V}}_h} \|\boldsymbol{u}-\boldsymbol{v}\|_{\boldsymbol{L}^2(\Omega)} = o(1)$ for all $\boldsymbol{u} \in \boldsymbol{\mathcal{P}}_0(\Omega)$.
(iii) $\hat{\boldsymbol{V}} \supseteq \boldsymbol{\mathcal{P}}_0(\hat{K})$.

Proof. Clearly (i) implies (ii) since if $\boldsymbol{u} \in \boldsymbol{\mathcal{P}}_0(\Omega)$, then the right hand side of (i) equals zero. By the Bramble-Hilbert lemma, (iii) implies (i). Thus, we need only show that (ii) implies (iii). We have

$$\inf_{\boldsymbol{v}\in\tilde{\boldsymbol{V}}_h} \|\boldsymbol{u}-\boldsymbol{v}\|^2_{\boldsymbol{L}^2(\Omega)} = \sum_{K\in\mathcal{U}_h} \inf_{\boldsymbol{v}_K\in\boldsymbol{V}_K} \|\boldsymbol{u}-\boldsymbol{v}_K\|^2_{\boldsymbol{L}^2(K)} = h^3 \sum_{K\in\mathcal{U}_h} \inf_{\hat{\boldsymbol{v}}\in\hat{\boldsymbol{V}}} \|h^{-2}[\hat{\boldsymbol{u}}-\hat{\boldsymbol{v}}]\|^2_{\boldsymbol{L}^2(\hat{K})},$$

where we have used the Piola transform and the fact that the mesh is uniform to make the change of variable $\boldsymbol{u}(\boldsymbol{x}) = h^{-2}\hat{\boldsymbol{u}}(\hat{\boldsymbol{x}})$ and $\boldsymbol{v}_K = h^{-2}\hat{\boldsymbol{v}}$ in the last step. In particular, for $\boldsymbol{u} = \boldsymbol{e}_i$, where $\boldsymbol{e}_i$ is any one of the three unit vectors, $\hat{\boldsymbol{u}} = h^2\boldsymbol{e}_i$. If we set $\hat{\boldsymbol{w}} = h^2\hat{\boldsymbol{v}}$, then the quantity

$$c_i := \inf_{\hat{\boldsymbol{w}}\in\hat{\boldsymbol{V}}} \|\boldsymbol{e}_i - \hat{\boldsymbol{w}}\|^2_{\boldsymbol{L}^2(\hat{K})}$$

is also independent of K. Hence,

$$\inf_{\boldsymbol{v}\in\tilde{\boldsymbol{V}}_h} \|\boldsymbol{e}_i-\boldsymbol{v}\|^2_{\boldsymbol{L}^2(\Omega)} = h^3 \sum_{K\in\mathcal{U}_h} \inf_{\hat{\boldsymbol{w}}\in\hat{\boldsymbol{V}}} \|\boldsymbol{e}_i-\hat{\boldsymbol{w}}\|^2_{\boldsymbol{L}^2(\hat{K})} = h^3 \sum_{K\in\mathcal{U}_h} c_i = c_i.$$

The hypothesis that this quantity is $o(1)$ implies that $c_i = 0$, i.e., that the constant functions belong to $\hat{\boldsymbol{V}}$. □

Theorem 2.2. *Let $\hat{\boldsymbol{V}}$ be a finite dimensional subspace of $\boldsymbol{L}^2(\hat{K})$. The following conditions are equivalent:*
(i) There is a constant C such that $\inf_{\boldsymbol{v}\in\tilde{\boldsymbol{V}}_h} \|\operatorname{div}\boldsymbol{u} - \operatorname{div}\boldsymbol{v}\|_{L^2(\Omega)} \le Ch\|\nabla\operatorname{div}\boldsymbol{u}\|_{\boldsymbol{L}^2(\Omega)}$ for all $\boldsymbol{u}\in\boldsymbol{H}^1(\Omega)$ with $\operatorname{div}\boldsymbol{u}\in H^1(\Omega)$.
(ii) $\inf_{\boldsymbol{v}\in\tilde{\boldsymbol{V}}_h} \|\operatorname{div}\boldsymbol{u} - \operatorname{div}\boldsymbol{v}\|_{L^2(\Omega)} = o(1)$ for all $\boldsymbol{u}$ with $\operatorname{div}\boldsymbol{u}\in\mathcal{P}_0(\Omega)$.
(iii) $\hat{\operatorname{div}}\hat{\boldsymbol{V}} \supseteq \mathcal{P}_0(\hat{K})$.

Since we do not impose interelement continuity in the definition of $\tilde{\boldsymbol{V}}_h$, we interpret $\operatorname{div}\boldsymbol{v}$ as the elementwise divergence of $\boldsymbol{v}$. Analogous results hold for the space $\boldsymbol{H}(\mathbf{curl};\Omega)$, and are stated below.

Theorem 2.3. *Let $\hat{\boldsymbol{U}}$ be a finite dimensional subspace of $\boldsymbol{L}^2(\hat{K})$. The following conditions are equivalent:*
(i) There is a constant C such that $\inf_{\boldsymbol{v}\in\tilde{\boldsymbol{U}}_h} \|\boldsymbol{u}-\boldsymbol{v}\|_{\boldsymbol{L}^2(\Omega)} \le Ch\|\nabla\boldsymbol{u}\|_{\boldsymbol{L}^2(\Omega)}$ for all $\boldsymbol{u}\in\boldsymbol{H}^1(\Omega)$.
(ii) $\inf_{\boldsymbol{v}\in\tilde{\boldsymbol{U}}_h} \|\boldsymbol{u}-\boldsymbol{v}\|_{\boldsymbol{L}^2(\Omega)} = o(1)$ for all $\boldsymbol{u}\in\boldsymbol{\mathcal{P}}_0(\Omega)$.
(iii) $\hat{\boldsymbol{U}} \supseteq \boldsymbol{\mathcal{P}}_0(\hat{K})$.

Theorem 2.4. *Let $\hat{\boldsymbol{U}}$ be a finite dimensional subspace of $\boldsymbol{L}^2(\hat{K})$. The following conditions are equivalent:*
(i) There is a constant C such that $\inf_{\boldsymbol{v}\in\tilde{\boldsymbol{U}}_h} \|\mathbf{curl}\,\boldsymbol{u}-\mathbf{curl}\,\boldsymbol{v}\|_{\boldsymbol{L}^2(\Omega)} \le Ch\|\nabla\mathbf{curl}\,\boldsymbol{u}\|_{\boldsymbol{L}^2(\Omega)}$ for all $\boldsymbol{u}\in\boldsymbol{H}^1(\Omega)$ with $\mathbf{curl}\,\boldsymbol{u}\in\boldsymbol{H}^1(\Omega)$.
(ii) $\inf_{\boldsymbol{v}\in\tilde{\boldsymbol{U}}_h} \|\mathbf{curl}\,\boldsymbol{u}-\mathbf{curl}\,\boldsymbol{v}\|_{\boldsymbol{L}^2(\Omega)} = o(1)$ for all $\boldsymbol{u}$ with $\mathbf{curl}\,\boldsymbol{u}\in\boldsymbol{\mathcal{P}}_0(\Omega)$.
(iii) $\hat{\mathbf{curl}}\,\hat{\boldsymbol{U}} \supseteq \boldsymbol{\mathcal{P}}_0(\hat{K})$.

3. Necessary conditions for optimal $\boldsymbol{L}^2(\Omega)$ approximation of $\boldsymbol{H}(\operatorname{div};\Omega)$ elements on hexahedral meshes

In this section, we consider finite element spaces defined by the mapping (1.1) and determine necessary necessary conditions for $O(h)$ approximation of a vector field on shape-regular/non-degenerate hexahedral meshes. We begin by letting $\boldsymbol{F}$ be a general trilinear mapping from the unit cube $\hat{K}$ to a general hexahedron K. Hence $\boldsymbol{F}$ is defined by

$$\begin{aligned}
F_1 &= a_1 + b_1\hat{x} + c_1\hat{y} + d_1\hat{z} + e_1\hat{x}\hat{y} + f_1\hat{y}\hat{z} + g_1\hat{z}\hat{x} + h_1\hat{x}\hat{y}\hat{z},\\
F_2 &= a_2 + b_2\hat{x} + c_2\hat{y} + d_2\hat{z} + e_2\hat{x}\hat{y} + f_2\hat{y}\hat{z} + g_2\hat{z}\hat{x} + h_2\hat{x}\hat{y}\hat{z},\\
F_3 &= a_3 + b_3\hat{x} + c_3\hat{y} + d_3\hat{z} + e_3\hat{x}\hat{y} + f_3\hat{y}\hat{z} + g_3\hat{z}\hat{x} + h_3\hat{x}\hat{y}\hat{z}.
\end{aligned}$$

It follows from the results of the previous section that if we consider a sequence $\mathcal{T}_h = \mathcal{U}_h$ of uniform meshes of the unit cube into subcubes of side $h = 1/n$, then the approximation estimate

$$\inf_{\boldsymbol{v}\in\tilde{\boldsymbol{V}}_h} \|\boldsymbol{u}-\boldsymbol{v}\|_{L^2(\Omega)} = o(1), \quad \forall\boldsymbol{u}\in\boldsymbol{\mathcal{P}}_0(\Omega) \tag{3.1}$$

is valid only if $\hat{\boldsymbol{V}} \supseteq \boldsymbol{\mathcal{P}}_0(\hat{K})$. In this section, we show that for this estimate to hold for more general hexahedral meshes $\mathcal{T}_h$, stronger conditions on $\hat{\boldsymbol{V}}$ are required.

Following the arguments presented in [2], which we shall transfer to the present setting, the key condition needed to determine the set $\hat{\boldsymbol{V}}$ is that after mapping by the Piola transform associated to the mapping of the cube to an arbitrary hexahedron, the resulting functions on the hexahedron contain the constant vectors $(1,0,0)$, $(0,1,0)$, and $(0,0,1)$. To determine these functions, we apply the inverse Piola transform to these constant vectors, i.e.,

$$\hat{\boldsymbol{u}}(\hat{\boldsymbol{x}}) = \boldsymbol{P}_F^{-1}\boldsymbol{u}(\boldsymbol{x}) = J\boldsymbol{F}(\hat{\boldsymbol{x}})D\boldsymbol{F}^{-1}(\hat{\boldsymbol{x}})\boldsymbol{u}(\boldsymbol{x}).$$

Now

$$D\boldsymbol{F} = \begin{pmatrix} b_1 + e_1\hat{y} + g_1\hat{z} + h_1\hat{y}\hat{z} & c_1 + e_1\hat{x} + f_1\hat{z} + h_1\hat{x}\hat{z} & d_1 + f_1\hat{y} + g_1\hat{x} + h_1\hat{x}\hat{y} \\ b_2 + e_2\hat{y} + g_2\hat{z} + h_2\hat{y}\hat{z} & c_2 + e_2\hat{x} + f_2\hat{z} + h_2\hat{x}\hat{z} & d_2 + f_2\hat{y} + g_2\hat{x} + h_2\hat{x}\hat{y} \\ b_3 + e_3\hat{y} + g_3\hat{z} + h_3\hat{y}\hat{z} & c_3 + e_3\hat{x} + f_3\hat{z} + h_3\hat{x}\hat{z} & d_3 + f_3\hat{y} + g_3\hat{x} + h_3\hat{x}\hat{y} \end{pmatrix}. \tag{3.2}$$

Hence, when $\boldsymbol{u}(\boldsymbol{x}) = (1,0,0)^T$,

$$\begin{aligned} \hat{u}_1(\hat{\boldsymbol{x}}) &= (c_2 + e_2\hat{x} + f_2\hat{z} + h_2\hat{x}\hat{z})(d_3 + f_3\hat{y} + g_3\hat{x} + h_3\hat{x}\hat{y}) \\ &\quad - (d_2 + f_2\hat{y} + g_2\hat{x} + h_2\hat{x}\hat{y})(c_3 + e_3\hat{x} + f_3\hat{z} + h_3\hat{x}\hat{z}), \\ \hat{u}_2(\hat{\boldsymbol{x}}) &= -(b_2 + e_2\hat{y} + g_2\hat{z} + h_2\hat{y}\hat{z})(d_3 + f_3\hat{y} + g_3\hat{x} + h_3\hat{x}\hat{y}) \\ &\quad + (d_2 + f_2\hat{y} + g_2\hat{x} + h_2\hat{x}\hat{y})(b_3 + e_3\hat{y} + g_3\hat{z} + h_3\hat{y}\hat{z}), \\ \hat{u}_3(\hat{\boldsymbol{x}}) &= (b_2 + e_2\hat{y} + g_2\hat{z} + h_2\hat{y}\hat{z})(c_3 + e_3\hat{x} + f_3\hat{z} + h_3\hat{x}\hat{z}) \\ &\quad - (c_2 + e_2\hat{x} + f_2\hat{z} + h_2\hat{x}\hat{z})(b_3 + e_3\hat{y} + g_3\hat{z} + h_3\hat{y}\hat{z}). \end{aligned}$$

If we define

$$\begin{aligned} &A_1^1 = c_2d_3 - d_2c_3, && A_2^1 = d_2b_3 - b_2d_3, && A_3^1 = b_2c_3 - c_2b_3, \\ &B_1^1 = f_2b_3 - f_3b_2, && B_2^1 = g_2b_3 - b_2g_3, && B_3^1 = b_2e_3 - e_2b_3, \\ &C_1^1 = c_2f_3 - f_2c_3, && C_2^1 = g_2c_3 - c_2g_3, && C_3^1 = e_2c_3 - c_2e_3, \\ &D_1^1 = f_2d_3 - d_2f_3, && D_2^1 = d_2g_3 - g_2d_3, && D_3^1 = e_2d_3 - e_3d_2, \\ &E_1^1 = h_2b_3 - h_3b_2, && E_2^1 = h_2c_3 - h_3c_2, && E_3^1 = h_2d_3 - h_3d_2, \\ &G_1^1 = e_2g_3 - g_2e_3, && G_2^1 = f_2e_3 - e_2f_3, && G_3^1 = g_2f_3 - f_2g_3, \\ &H_1^1 = f_2h_3 - h_2f_3, && H_2^1 = h_3g_2 - h_2g_3, && H_3^1 = e_2h_3 - h_2e_3, \end{aligned} \tag{3.3}$$

then $\boldsymbol{P}_F^{-1}(1,0,0)^T$ will have the form:

(3.4)
$$\begin{aligned} &A_1^1 + (D_3^1 - C_2^1)\hat{x} + C_1^1\hat{y} + D_1^1\hat{z} - (E_2^1 + G_2^1)\hat{x}\hat{y} + (E_3^1 - G_3^1)\hat{x}\hat{z} + G_1^1\hat{x}^2 + H_3^1\hat{x}^2\hat{y} - H_2^1\hat{x}^2\hat{z}, \\ &A_2^1 + B_2^1\hat{x} + (B_1^1 - D_3^1)\hat{y} + D_2^1\hat{z} + (E_1^1 - G_1^1)\hat{y}\hat{x} - (E_3^1 + G_3^1)\hat{y}\hat{z} + G_2^1\hat{y}^2 - H_3^1\hat{x}\hat{y}^2 + H_1^1\hat{y}^2\hat{z}, \\ &A_3^1 + B_3^1\hat{x} + C_3^1\hat{y} + (C_2^1 - B_1^1)\hat{z} - (E_1^1 + G_1^1)\hat{z}\hat{x} + (E_2^1 - G_2^1)\hat{z}\hat{y} + G_3^1\hat{z}^2 + H_2^1\hat{x}\hat{z}^2 - H_1^1\hat{y}\hat{z}^2. \end{aligned}$$

Vectors of identical forms with coefficients $A_1^2, A_2^2, \cdots$ and $A_1^3, A_2^3, \cdots$, defined analogously, are obtained for the choices $(0,1,0)$ and $(0,0,1)$. If we consider the coefficients A_i, B_i, C_i, etc. as arbitrary, rather than as functions of the 14 coefficients defined above, then this is a linear space involving 20 independent parameters, which we denote by $\hat{\boldsymbol{S}}_0^-$. Note that although there are 21 coefficients in the above expressions, the three coefficients B_1^1, C_2^1, D_3^1 only appear in equation (3.4) in the terms $(D_3^1 - C_2^1)$, $(B_1^1 - D_3^1)$, and $(C_2^1 - B_1^1)$, and these three terms sum to zero. Hence, there are only two linearly independent coefficients in these three terms, so the linear space $\hat{\boldsymbol{S}}_0^-$ involves 20 independent parameters, rather than 21.

In fact, defining mappings $\boldsymbol{F}^1(\hat{x},\hat{y},\hat{z}),\cdots,\boldsymbol{F}^{11}(\hat{x},\hat{y},\hat{z})$ by

$$\boldsymbol{F}^1=[\hat{x}+\hat{y}\hat{x},\hat{y},\hat{z}],\qquad \boldsymbol{F}^2=[\hat{x},\hat{y}+\hat{y}\hat{z},\hat{z}],\qquad \boldsymbol{F}^3=[\hat{x},\hat{y},\hat{z}+\hat{x}\hat{z}],$$
$$\boldsymbol{F}^4=[\hat{x}+\hat{x}\hat{z},\hat{y}+\hat{y}\hat{z},\hat{z}],\qquad \boldsymbol{F}^5=[\hat{x}+\hat{x}\hat{y},\hat{y},\hat{z}+\hat{y}\hat{z}],\qquad \boldsymbol{F}^6=[\hat{x},\hat{y}+\hat{x}\hat{y},\hat{z}+\hat{x}\hat{z}],$$
$$\boldsymbol{F}^7=[\hat{x}+\hat{x}\hat{y}\hat{z},\hat{y},\hat{z}],\qquad \boldsymbol{F}^8=[\hat{x},\hat{y}+\hat{x}\hat{y}\hat{z},\hat{z}],$$
$$\boldsymbol{F}^9=[\hat{x}+\hat{x}\hat{y}\hat{z},\hat{y}+\hat{y}\hat{z},\hat{z}],\qquad \boldsymbol{F}^{10}=[\hat{x},\hat{y}+\hat{x}\hat{y}\hat{z},\hat{z}+\hat{x}\hat{z}],\qquad \boldsymbol{F}^{11}=[\hat{x}+\hat{x}\hat{y},\hat{y},\hat{z}+\hat{x}\hat{y}\hat{z}],$$

we can establish the following result, analogous to Lemma 3.3 of [2].

Lemma 3.1. *Let $\hat{\boldsymbol{V}}$ be a space of vectorfields on $\hat{K}$ such that $\boldsymbol{P}_F\hat{\boldsymbol{V}}\supseteq\boldsymbol{\mathcal{P}}_0(\boldsymbol{F}(\hat{K}))$, where $\boldsymbol{F}$ is any one of the trilinear isomorphisms $\boldsymbol{F}^1,\cdots,\boldsymbol{F}^{11}$. Then $\hat{\boldsymbol{V}}\supseteq\hat{\boldsymbol{S}}_0^-$.*

Proof. Since $\boldsymbol{P}_F\hat{\boldsymbol{V}}\supseteq\boldsymbol{\mathcal{P}}_0(\boldsymbol{F}(\hat{K}))$, we have that $\hat{\boldsymbol{V}}\supseteq\boldsymbol{P}_F^{-1}\boldsymbol{\mathcal{P}}_0(\boldsymbol{F}(\hat{K}))$. Thus, it is sufficient to prove that $\hat{\boldsymbol{S}}_0^-\subseteq\sum_{i=1}^{11}\boldsymbol{P}_{F^i}^{-1}\boldsymbol{\mathcal{P}}_0(\boldsymbol{F}(\hat{K}))$. Applying the first three mappings to the unit vectors $[1,0,0],[0,1,0],[0,0,1]$ gives the vectors

$$[1,0,0],\quad[-\hat{x},1+\hat{y},0],\quad[0,0,1+\hat{y}],\quad[1+\hat{z},0,0],\quad[0,1,0],$$
$$[0,-\hat{y},1+\hat{z}],\quad[1+\hat{x},0,-\hat{z}],\quad[0,1+\hat{x},0],\quad[0,0,1],$$

from which we can generate the vectors

$$[1,0,0],\ [0,1,0],\ [0,0,1],\ [0,\hat{x},0],\ [0,0,\hat{y}],\ [\hat{z},0,0],\ [-\hat{x},\hat{y},0],\ [0,-\hat{y},\hat{z}],\ [\hat{x},0,-\hat{z}].$$

Applying the second three mappings to these unit vectors gives the vectors

$$[1+\hat{z},0,0],\qquad[0,1+\hat{z},0],\qquad[-\hat{x}-\hat{x}\hat{z},-\hat{y}-\hat{y}\hat{z},1+2\hat{z}+\hat{z}^2],$$
$$[1+\hat{y},0,0],\qquad[-\hat{x}-\hat{x}\hat{y},1+2\hat{y}+\hat{y}^2,-\hat{z}-\hat{y}\hat{z}],\qquad[0,0,1+\hat{y}],$$
$$[1+2\hat{x}+\hat{x}^2,-\hat{y}-\hat{x}\hat{y},-\hat{z}-\hat{x}\hat{z}],\qquad[0,1+\hat{x},0],\qquad[0,0,1+\hat{x}],$$

from which we can generate the additional vectors

$$[0,0,\hat{x}],\ [\hat{y},0,0],\ [0,\hat{z},0],\ [\hat{x}^2,-\hat{x}\hat{y},-\hat{x}\hat{z}],\ [-\hat{x}\hat{y},\hat{y}^2,-\hat{y}\hat{z}],\ [-\hat{x}\hat{z},-\hat{y}\hat{z},\hat{z}^2].$$

Applying the third set of mappings to these unit vectors gives the vectors

$$[1,0,0],\qquad[-\hat{x}\hat{z},1+\hat{y}\hat{z},0],\qquad[-\hat{x}\hat{y},0,1+\hat{y}\hat{z}],$$
$$[1+\hat{x}\hat{z},-\hat{y}\hat{z},0],\qquad[0,1,0],\qquad[0,-\hat{x}\hat{y},1+\hat{x}\hat{z}],$$

from which we can generate the additional vectors

$$[-\hat{x}\hat{z},\hat{y}\hat{z},0],\qquad[-\hat{x}\hat{y},0,\hat{y}\hat{z}],\qquad[0,-\hat{y}\hat{x},\hat{x}\hat{z}].$$

Applying the final set of mappings gives the vectors

$$[1+\hat{z},0,0],\qquad[-\hat{x}\hat{z},1+\hat{y}\hat{z},0],\qquad[-\hat{x}\hat{y},-\hat{y}-\hat{y}^2\hat{z},1+\hat{z}+\hat{y}\hat{z}+\hat{y}\hat{z}^2],$$
$$[1+\hat{x}+\hat{x}\hat{z}+\hat{x}^2\hat{z},-\hat{y}\hat{z},-\hat{z}-\hat{x}\hat{z}^2],\qquad[0,1+\hat{x},0],\qquad[0,-\hat{x}\hat{y},1+\hat{x}\hat{z}],$$
$$[1+\hat{x}\hat{y},0,-\hat{y}\hat{z}],\qquad[-\hat{x}-\hat{x}^2\hat{y},1+\hat{y}+\hat{x}\hat{y}+\hat{x}\hat{y}^2,-\hat{x}\hat{z}],\qquad[0,0,1+\hat{y}],$$

from which we can generate the additional vectors

$$[0,-\hat{y}^2\hat{z},\hat{y}\hat{z}^2],\qquad[\hat{x}^2\hat{z},0,-\hat{x}\hat{z}^2],\qquad[-\hat{x}^2\hat{y},\hat{x}\hat{y}^2,0].$$

These vectors span $\hat{\boldsymbol{S}}_0^-$. □

There are other choices of mappings that we could have made to achieve this result. These choices will simplify the construction of special meshes, when we use this lemma below to establish the following necessary condition (the analogue of Theorem 3.1 of [2]) on the choice of $\hat{\boldsymbol{V}}$ to ensure the approximation result (3.1).

Theorem 3.2. *Suppose that the estimate* (3.1) *holds whenever* $\mathcal{T}_h$ *is a sequence of shape-regular/non-degenerate hexahedral meshes of a three dimensional domain* Ω*. Then* $\hat{\boldsymbol{V}} \supseteq \hat{\boldsymbol{S}}_0^-$.

Proof. To establish the theorem, we follow the proof of Theorem 3.1 of [2]), and assume that $\hat{\boldsymbol{V}} \not\supseteq \hat{\boldsymbol{S}}_0^-$. We then exhibit a sequence $\mathcal{T}_h$ of shape-regular/non-degenerate meshes $(h = 1, 1/2, 1/3, \cdots)$ of the unit square for which the estimate (3.1) does not hold. We know by Lemma 3.1, that for at least one of the mappings $\boldsymbol{F}^i$, $i = 1, \cdots, 11$, $\boldsymbol{P}_{F^i}\hat{\boldsymbol{V}}$ does not contain $\boldsymbol{\mathcal{P}}_0(\boldsymbol{F}^i(\hat{K}))$. We assume, without loss of generality, that for either $i = 1$, $i = 4$, $i = 7$, or $i = 9$,

$$\boldsymbol{P}_{F^i}\hat{\boldsymbol{V}} \not\supseteq \boldsymbol{\mathcal{P}}_0(\boldsymbol{F}^i(\hat{K})). \tag{3.5}$$

To define the mesh $\mathcal{T}_h$, we first define for each of the maps $\boldsymbol{F}^i$, a mesh $\mathcal{T}_h^1$ of the unit cube, consisting of eight elements $K_1, \cdots, K_8$. This is done by specifying the vertices of K_1 and then showing that a trilinear map of the form $\boldsymbol{E} \circ \boldsymbol{F}$ maps the unit cube onto K_1, where the map $\boldsymbol{E}$ is a linear isomorphism. To obtain the other elements, we note that for each map $\boldsymbol{F}$, exactly four vertices of $\boldsymbol{F}(\hat{K})$ will have x coordinate equal to zero, exactly four vertices will have y coordinate equal to zero, and exactly four vertices will have z coordinate equal to zero. We then define K_2 as the element in which the the zero x coordinates are set to one, K_3 as the element in which the the zero y coordinates are set to one, and K_4 as the element in which both the zero x coordinates and y coordinates are set to one. The remaining four elements are obtained from these by changing the zero z coordinates to one.

For the map $\boldsymbol{F}^1$, we define K_1 to be the element with vertices $(0, 0, 0)$, $(1/3, 0, 0)$, $(0, 1/2, 0)$, $(2/3, 1/2, 0)$, $(0, 0, 1/2)$, $(1/3, 0, 1/2)$, $(0, 1/2, 1/2)$, $(2/3, 1/2, 1/2)$, and define $\boldsymbol{E}^1(x, y, z) = (x/3, y/2, z/2)$. We then note that $\boldsymbol{E}^1 \circ \boldsymbol{F}^1$ is a trilinear map from the unit cube onto the element K_1. Although we will not write them explicitly, we can then use the description of the vertices of K_i, $i = 2, \cdots, 8$ given above to also find trilinear maps from the unit cube onto each of these elements. In this case, all these elements will be congruent to K_1, but this will not be the case for the other choices of the map $\boldsymbol{F}$.

For $h = 1/n$, we then construct the mesh $\mathcal{T}_h$ by partitioning the unit cube into n^3 subcubes K, and meshing each subcube K with the mesh obtained by applying the mapping $\boldsymbol{D}_K(\hat{\boldsymbol{x}}) \equiv \boldsymbol{x}_K + h_K\hat{\boldsymbol{x}}$, where $\boldsymbol{x}_K$ is the corner of K with smallest x, y, z coordinates and h_K is the side length of K. Combining these steps, we see that for each element T of the mesh $\mathcal{T}_h$, there is a natural way to construct a trilinear mapping $\boldsymbol{F}$ from the unit cube onto T based on the mapping $\boldsymbol{F}^1$. The first step is to compose $\boldsymbol{F}^1$ with the linear isomorphism $\boldsymbol{E}^1(x) = (x/3, y/2, z/2)$ to obtain a trilinear map $\boldsymbol{E}^1 \circ \boldsymbol{F}^1$ from the unit cube onto the element K_1. We then obtain, as described above, trilinear maps from the unit cube onto the elements $K_2, \cdots, K_8$. Finally, further composition with the map $\boldsymbol{D}_K$ (consisting of dilation and translation), taking the unit cube onto the subsquare K containing T, defines a trilinear isomorphism of the unit cube onto T.

For the mapping $\boldsymbol{F}^4$, the vertices of K_1 are chosen to be $(0,0,0)$, $(1/3,0,0)$, $(0,1/3,0)$, $(1/3,1/3,0)$, $(0,0,1/2)$, $(2/3,0,1/2)$, $(0,2/3,1/2)$, $(2/3,2/3,1/2)$. The mapping $\boldsymbol{E}^2\circ\boldsymbol{F}^4$, where $\boldsymbol{E}^2=(x/3,y/3,z/2)$, then gives a trilinear map from the unit cube onto the element K_1. For the mapping $\boldsymbol{F}^7$, the vertices of K_1 are chosen to be $(0,0,0)$, $(1/3,0,0)$, $(0,1/2,0)$, $(1/3,1/2,0)$, $(0,0,1/2/)$, $(1/3,0,1/2)$, $(0,1/2,1/2)$, $(2/3,1/2,1/2)$, and $\boldsymbol{E}^1\circ\boldsymbol{F}^7$ gives a trilinear map from the unit cube onto the element K_1. For the mapping $\boldsymbol{F}^9$, the vertices of K_1 are chosen to be $(0,0,0)$, $(1/3,0,0)$, $(0,1/3,0)$, $(1/3,1/3,0)$, $(0,0,1/2)$, $(1/3,0,1/2)$, $(0,2/3,1/2)$, $(2/3,2/3,1/2)$, and $\boldsymbol{E}^2\circ\boldsymbol{F}^9$ gives a trilinear map from the unit cube onto the element K_1. Four choices of the mesh $\mathcal{T}_h^1$, corresponding to these four cases, are shown in Figure 1.

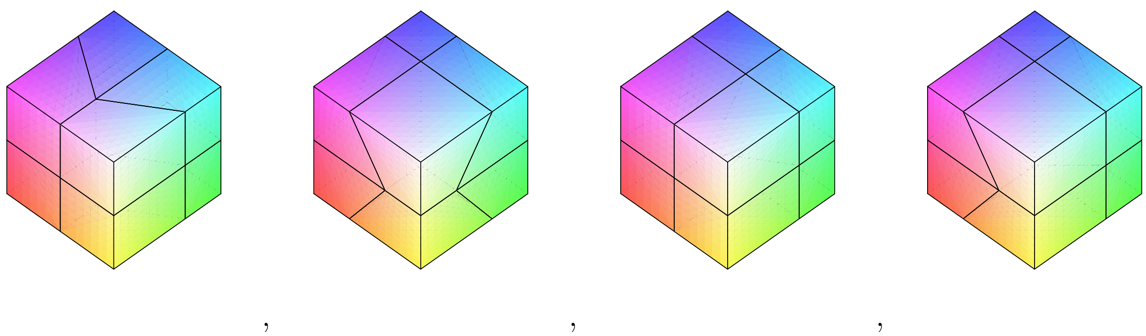

FIGURE 1. The mesh $\mathcal{T}_h^1$.

Having specified the mesh $\mathcal{T}_h$ and a trilinear map from the unit cube onto each element of the mesh, we have determined a space $\tilde{\boldsymbol{V}}(\mathcal{T}_h)$ based on the shape functions in $\hat{\boldsymbol{V}}$. We need to show that estimate (3.1) does not hold. To do so,we observe that $\tilde{\boldsymbol{V}}(\mathcal{T}_h)$ coincides precisely with the space

$$\{\boldsymbol{u}:\boldsymbol{u}|_K=\boldsymbol{P}_{D_K}\hat{\boldsymbol{V}}(\mathcal{T}_h^1),\forall K\in\mathcal{U}_h\},$$

where $\mathcal{U}_h$ is the uniform mesh partitioning Ω into n^3 subcubes of side length $h=1/n$ and

$$\hat{\boldsymbol{V}}(\mathcal{T}_h^1)=\{\hat{\boldsymbol{v}}:\hat{\boldsymbol{v}}|_{K_i}\in\hat{\boldsymbol{V}}\}.$$

Thus, we may apply Theorem 2.1 to conclude that (3.1) does not hold if we can show that $\hat{\boldsymbol{V}}(\mathcal{T}_h^1)\not\supseteq\boldsymbol{\mathcal{P}}_0(\hat{K})$. We do this for the first case corresponding to the map $\boldsymbol{F}^1$ since the argument is similar in the other cases. Now, by construction, the functions in $\hat{\boldsymbol{V}}(\mathcal{T}_h^1)$ restrict to functions in $\boldsymbol{P}_F\hat{\boldsymbol{V}}$ on $K_1=\boldsymbol{F}(\hat{K})$, where $\boldsymbol{F}=\boldsymbol{E}^1\circ\boldsymbol{F}^1$. Hence, it is enough to show that $\boldsymbol{P}_F\hat{\boldsymbol{V}}\not\supseteq\boldsymbol{\mathcal{P}}_0(K_1)$. Now by the composition property of the Piola transform, $\boldsymbol{P}_F\hat{\boldsymbol{V}}=\boldsymbol{P}_{E^1}(\boldsymbol{P}_{F^1}\hat{\boldsymbol{V}})$. Since $\boldsymbol{E}^1$ is a linear isomorphism of $\boldsymbol{F}^1(\hat{K})$ onto K_1, $\boldsymbol{P}_{E^1}$, is a linear isomorphism of $\boldsymbol{\mathcal{P}}_0(\boldsymbol{F}^1(\hat{K})$ onto $\boldsymbol{\mathcal{P}}_0(K_1)$. Thus, $\boldsymbol{P}_F\hat{\boldsymbol{V}}\supseteq\boldsymbol{\mathcal{P}}_0(K_1)$ only if $\boldsymbol{P}_{F^1}\hat{\boldsymbol{V}}\supseteq\boldsymbol{\mathcal{P}}_0(\boldsymbol{F}^1(\hat{K}))$. But from (3.5), we have that $\boldsymbol{P}_{F^1}\hat{\boldsymbol{V}}\not\supseteq\boldsymbol{\mathcal{P}}_0(\boldsymbol{F}^1(\hat{K}))$ and so $\boldsymbol{P}_F\hat{\boldsymbol{V}}\not\supseteq\boldsymbol{\mathcal{P}}_0(K_1)$. Hence, (3.1) does not hold. ☐

We end this section by determining an appropriate set of degrees of freedom for the space $\boldsymbol{V}_h$. Instead of choosing $\hat{\boldsymbol{V}}$ to be the 20 dimensional linear space $\hat{\boldsymbol{S}}_0^-$ determined above, we take $\hat{\boldsymbol{V}}$ to be a slightly larger 21 dimensional subspace $\hat{\boldsymbol{S}}_0$ of $\boldsymbol{RT}_1$ (dimension = 36) that includes $\boldsymbol{RT}_0$, consisting of all vectors $\hat{\boldsymbol{u}}$ of the form:

$$\hat{\boldsymbol{u}}_1 = A_1 + B_1\hat{x} + C_1\hat{y} + D_1\hat{z} - (E_2 + G_2)\hat{x}\hat{y} + (E_3 - G_3)\hat{x}\hat{z} + G_1\hat{x}^2 + H_3\hat{x}^2\hat{y} - H_2\hat{x}^2\hat{z},$$
$$\hat{\boldsymbol{u}}_2 = A_2 + B_2\hat{x} + C_2\hat{y} + D_2\hat{z} + (E_1 - G_1)\hat{y}\hat{x} - (E_3 + G_3)\hat{y}\hat{z} + G_2\hat{y}^2 - H_3\hat{x}\hat{y}^2 + H_1\hat{y}^2\hat{z},$$
$$\hat{\boldsymbol{u}}_3 = A_3 + B_3\hat{x} + C_3\hat{y} + D_3\hat{z} - (E_1 + G_1)\hat{z}\hat{x} + (E_2 - G_2)\hat{z}\hat{y} + G_3\hat{z}^2 + H_2\hat{x}\hat{z}^2 - H_1\hat{y}\hat{z}^2,$$

where again the coefficients A_i, B_i, C_i, etc. are considered arbitrary. The reason for slightly enlarging the space is to be able to find degrees of freedom that will insure continuity of $\hat{\boldsymbol{u}} \cdot \boldsymbol{n}$ across elements sharing a common face, a necessary condition to have the global finite element space a subspace of $\boldsymbol{H}(\mathrm{div};\Omega)$.

Since for $\hat{\boldsymbol{u}} \in \hat{\boldsymbol{S}}_0$, $\hat{\boldsymbol{u}} \cdot \hat{\boldsymbol{n}}$ is a polynomial of degree ≤ 1 on each face, we can insure continuity of $\hat{\boldsymbol{u}} \cdot \hat{\boldsymbol{n}}$ by specifying 3 degrees of freedom on each face, i.e.,

$$\int_{\hat{F}} (\hat{\boldsymbol{u}} \cdot \hat{\boldsymbol{n}})\, \hat{p}\, d\hat{s}, \quad \hat{p} \in \mathcal{P}_1(\hat{F}).$$

We then define the final 3 degrees of freedom by

$$\int_{\hat{K}} \hat{\boldsymbol{u}} \cdot \hat{\boldsymbol{r}}\, d\hat{x}, \quad \hat{\boldsymbol{r}} \in \hat{\boldsymbol{R}}, \tag{3.6}$$

where $\hat{\boldsymbol{R}}$ denotes the span of the vectors

$$\hat{\boldsymbol{r}}_1 := (0, 1/2 - \hat{z}, \hat{y} - 1/2), \qquad \hat{\boldsymbol{r}}_2 := (1/2 - \hat{z}, 0, \hat{x} - 1/2), \qquad \hat{\boldsymbol{r}}_3 := (1/2 - \hat{y}, x - 1/2, 0).$$

We now show that these choices give a unisolvent set of degrees of freedom for $\hat{\boldsymbol{S}}_0$. We first observe that if $\hat{\boldsymbol{u}}_1 \cdot \hat{\boldsymbol{n}}_1 = 0$ on the face $\hat{x} = 0$, then $A_1 = C_1 = D_1 = 0$. A similar argument using the corresponding normals on the faces $\hat{y} = 0$ and $\hat{z} = 0$ gives $A_2 = B_2 = D_2 = 0$ and $A_3 = B_3 = C_3 = 0$. The conditions $\hat{\boldsymbol{u}} \cdot \hat{\boldsymbol{n}} = 0$ on the remaining three faces give the equations

$$\begin{aligned} &B_1 + G_1 = 0, && -E_2 - G_2 + H_3 = 0, && E_3 - G_3 - H_2 = 0,\\ &C_2 + G_2 = 0, && E_1 - G_1 - H_3 = 0, && -E_3 - G_3 + H_1 = 0,\\ &D_3 + G_3 = 0, && -E_1 - G_1 + H_2 = 0, && E_2 - G_2 - H_1 = 0. \end{aligned}$$

These are easily solved, giving

$$\begin{aligned} &E_1 = (H_3 + H_2)/2, && E_2 = (H_1 + H_3)/2, && E_3 = (H_1 + H_2)/2,\\ &G_1 = (H_2 - H_3)/2, && G_2 = (H_3 - H_1)/2, && G_3 = (H_1 - H_2)/2,\\ &B_1 = (H_3 - H_2)/2, && C_2 = (H_1 - H_3)/2, && D_3 = (H_2 - H_1)/2. \end{aligned}$$

Hence, if the 18 face degrees of freedom of $\hat{\boldsymbol{u}}$ are equal to zero, then $\hat{\boldsymbol{u}}$ will have the form

$$\begin{aligned} \hat{\boldsymbol{u}}_1 &= \hat{x}(1 - \hat{x})[H_2(z - 1/2) - H_3(y - 1/2)],\\ \hat{\boldsymbol{u}}_2 &= \hat{y}(1 - \hat{y})[H_3(\hat{x} - 1/2) - H_1(\hat{z} - 1/2)],\\ \hat{\boldsymbol{u}}_3 &= \hat{z}(1 - \hat{z})[H_1(\hat{y} - 1/2) - H_2(\hat{x} - 1/2)]. \end{aligned} \tag{3.7}$$

Then, setting the final three degrees of freedom equal to zero, we see that $H_1 = H_2 = H_3 = 0$.

4. Necessary conditions for optimal approximation of the divergence

We next consider the issue of what additional functions, if any, must be added to the space on the reference element to also insure an optimal $O(h)$ approximation of the divergence. It follows from the results of § 2 that if we consider a sequence $\mathcal{T}_h = \mathcal{U}_h$ of uniform meshes of the unit cube into subcubes of side $h = 1/n$, then the approximation estimate

$$\inf_{\boldsymbol{v}\in\tilde{\boldsymbol{V}}_h} \|\operatorname{div}(\boldsymbol{u}-\boldsymbol{v})\|_{L^2(\Omega)} = o(1) \tag{4.1}$$

is valid only if $\hat{\operatorname{div}}\hat{\boldsymbol{V}} \supseteq \mathcal{P}_0(\hat{K})$. We show in this section that for this estimate to hold for more general hexahedral meshes, we will need much stronger conditions on $\hat{\boldsymbol{V}}$.

Again following the arguments presented in [2], the key condition needed is that after mapping by the Piola transform associated to the mapping of the cube to an arbitrary hexahedron, the divergence of the resulting functions on the hexahedron must contain constants. To determine these functions, we use the fact that

$$\hat{\operatorname{div}}\,\hat{\boldsymbol{u}} = J\boldsymbol{F}(\hat{\boldsymbol{x}})\operatorname{div}\boldsymbol{u}.$$

Thus, if the divergence of the space on the physical element contains constants, the original space must contain the function $J\boldsymbol{F}(\hat{\boldsymbol{x}})$ for any choice of the constants b_i, c_i, etc. An explicit computation gives the formula

$$\begin{aligned} J\boldsymbol{F}(\hat{\boldsymbol{x}}) &= [\det(\boldsymbol{b}|\boldsymbol{c}|\boldsymbol{d})]1 + [\det(\boldsymbol{b}|\boldsymbol{c}|\boldsymbol{g}) - \det(\boldsymbol{b}|\boldsymbol{d}|\boldsymbol{e})]\hat{x} + [\det(\boldsymbol{b}|\boldsymbol{c}|\boldsymbol{f}) + \det(\boldsymbol{c}|\boldsymbol{d}|\boldsymbol{e})]\hat{y} \\ &+ [\det(\boldsymbol{c}|\boldsymbol{d}|\boldsymbol{g}) - \det(\boldsymbol{b}|\boldsymbol{d}|\boldsymbol{f})]\hat{z} + [-\det(\boldsymbol{c}|\boldsymbol{e}|\boldsymbol{g}) + \det(\boldsymbol{b}|\boldsymbol{c}|\boldsymbol{h}) + \det(\boldsymbol{b}|\boldsymbol{e}|\boldsymbol{f})]\hat{x}\hat{y} \\ &+ [\det(\boldsymbol{b}|\boldsymbol{f}|\boldsymbol{g}) - \det(\boldsymbol{b}|\boldsymbol{d}|\boldsymbol{h}) - \det(\boldsymbol{d}|\boldsymbol{e}|\boldsymbol{g})]\hat{x}\hat{z} + [\det(\boldsymbol{c}|\boldsymbol{f}|\boldsymbol{g}) + \det(\boldsymbol{c}|\boldsymbol{d}|\boldsymbol{h}) + \det(\boldsymbol{d}|\boldsymbol{e}|\boldsymbol{f})]\hat{y}\hat{z} \\ &+ \det(\boldsymbol{b}|\boldsymbol{e}|\boldsymbol{g})\hat{x}^2 - \det(\boldsymbol{c}|\boldsymbol{e}|\boldsymbol{f})\hat{y}^2 - \det(\boldsymbol{d}|\boldsymbol{f}|\boldsymbol{g})\hat{z}^2 + 2\det(\boldsymbol{e}|\boldsymbol{f}|\boldsymbol{g})\hat{x}\hat{y}\hat{z} \\ &+ \det(\boldsymbol{b}|\boldsymbol{e}|\boldsymbol{h})\hat{x}^2\hat{y} - \det(\boldsymbol{b}|\boldsymbol{g}|\boldsymbol{h})\hat{x}^2\hat{z} - \det(\boldsymbol{c}|\boldsymbol{e}|\boldsymbol{h})\hat{y}^2\hat{x} + \det(\boldsymbol{c}|\boldsymbol{f}|\boldsymbol{h})\hat{y}^2\hat{z} + \det(\boldsymbol{d}|\boldsymbol{g}|\boldsymbol{h})\hat{z}^2\hat{x} \\ &- \det(\boldsymbol{d}|\boldsymbol{f}|\boldsymbol{h})\hat{z}^2\hat{y} - \det(\boldsymbol{e}|\boldsymbol{g}|\boldsymbol{h})\hat{x}^2\hat{y}\hat{z} + \det(\boldsymbol{e}|\boldsymbol{f}|\boldsymbol{h})\hat{x}\hat{y}^2\hat{z} + \det(\boldsymbol{f}|\boldsymbol{g}|\boldsymbol{h})\hat{x}\hat{y}\hat{z}^2. \end{aligned} \tag{4.2}$$

Viewing this as a linear polynomial space, and assuming the coefficients are all independent, this is a 20 dimensional subspace of $\mathcal{Q}_2 \cap \mathcal{P}_4$, which we denote by R_0 (note the monomials $\hat{x}^2\hat{y}^2$, $\hat{x}^2\hat{z}^2$, and $\hat{y}^2\hat{z}^2$ are not present). Since the divergence of our original 21 dimensional space already contained constants, we remove constants from this 20 dimensional space, and denote by $\hat{Q}$ the span of the remaining 19 monomials:

$$\hat{x}, \hat{y}, \hat{z}, \hat{x}\hat{y}, \hat{x}\hat{z}, \hat{y}\hat{z}, \hat{x}^2, \hat{y}^2, \hat{z}^2, \hat{x}^2\hat{y}, \hat{x}^2\hat{z}, \hat{y}^2\hat{x}, \hat{y}^2\hat{z}, \hat{z}^2\hat{x}, \hat{z}^2\hat{y}, \hat{x}\hat{y}\hat{z}, \hat{x}^2\hat{y}\hat{z}, \hat{y}^2\hat{x}\hat{z}, \hat{z}^2\hat{x}\hat{y}.$$

Thus, $R_0 = \operatorname{span}\{1, \hat{Q}\}$. In fact, defining mappings $\boldsymbol{G}^1(\hat{x},\hat{y},\hat{z}), \cdots, \boldsymbol{G}^8(\hat{x},\hat{y},\hat{z})$ by

$$\begin{aligned} &\boldsymbol{G}^1 = [\hat{x}, \hat{y}, \hat{z} + \hat{x}\hat{y}\hat{z}], && \boldsymbol{G}^2 = [\hat{x} + \hat{x}\hat{y}\hat{z}, \hat{y}, \hat{z} + \hat{y}\hat{z}], \\ &\boldsymbol{G}^3 = [\hat{x} + \hat{x}\hat{z}, \hat{y} + \hat{x}\hat{y}\hat{z}, \hat{z}], && \boldsymbol{G}^4 = [\hat{x}, \hat{y} + \hat{x}\hat{y}, \hat{z} + \hat{x}\hat{y}\hat{z}], \\ &\boldsymbol{G}^5 = [\hat{x}(1+\hat{y}), \hat{y}(1+\hat{z}), \hat{z}(1+\hat{x})], && \boldsymbol{G}^6 = [\hat{x}(1+\hat{y}), \hat{y}(1+\hat{z}), \hat{z}(1+\hat{x}\hat{y})], \\ &\boldsymbol{G}^7 = [\hat{x}(1+\hat{y}), \hat{y}(1+\hat{x}\hat{z}), \hat{z}(1+\hat{x})], && \boldsymbol{G}^8 = [\hat{x}(1+\hat{y}\hat{z}), \hat{y}(1+\hat{z}), \hat{z}(1+\hat{x})], \end{aligned}$$

we can establish the following result, analogous to Lemma 3.4 of [2].

Lemma 4.1. *Let $\hat{\boldsymbol{V}}$ be a space of vectorfields on $\hat{K}$ such that* $\operatorname{div} \boldsymbol{P}_F \hat{\boldsymbol{V}} \supseteq \mathcal{P}_0$*, where F is any one of the trilinear isomorphisms $\boldsymbol{F}^0 = [\hat{x}, \hat{y}, \hat{z}]$, $\boldsymbol{F}^1, \cdots, \boldsymbol{F}^{11}$ or $\boldsymbol{G}^1, \cdots, \boldsymbol{G}^8$. Then* $\operatorname{div} \hat{\boldsymbol{V}} \supseteq R_0$.

Proof. Now $J\boldsymbol{F}^0(\hat{\boldsymbol{x}}) = 1$, and using (4.2), we easily obtain the following expressions for $J\boldsymbol{F}$ corresponding to the choices $\boldsymbol{F}^1, \cdots, \boldsymbol{F}^{11}$.

$$\begin{aligned}
\boldsymbol{F}^1, \boldsymbol{F}^2, \boldsymbol{F}^3: &\qquad J\boldsymbol{F} = 1 + \hat{y}, \quad 1 + \hat{z}, \quad 1 + \hat{x},\\
\boldsymbol{F}^4, \boldsymbol{F}^5, \boldsymbol{F}^6: &\qquad J\boldsymbol{F} = 1 + 2\hat{z} + \hat{z}^2, \quad 1 + 2\hat{y} + \hat{y}^2, \quad 1 + 2\hat{x} + \hat{x}^2,\\
\boldsymbol{F}^7, \boldsymbol{F}^8: &\qquad J\boldsymbol{F} = 1 + \hat{y}\hat{z}, \quad 1 + \hat{\hat{x}z},\\
\boldsymbol{F}^9, \boldsymbol{F}^{10}, \boldsymbol{F}^{11}: &\qquad J\boldsymbol{F} = 1 + \hat{z} + \hat{y}\hat{z} + \hat{z}^2\hat{y}, \quad 1 + \hat{x} + \hat{x}\hat{z} + \hat{x}^2\hat{z}, \quad 1 + \hat{y} + \hat{x}\hat{y} + \hat{y}^2\hat{x}.
\end{aligned}$$

In a similar manner, we find $J\boldsymbol{G}^1(\hat{\boldsymbol{x}}) = 1 + \hat{x}\hat{y}$, and the following expressions for $J\boldsymbol{G}(\hat{\boldsymbol{x}})$ corresponding to the choices $\boldsymbol{G}^2, \cdots, \boldsymbol{G}^8$.

$$\begin{aligned}
\boldsymbol{G}^2, \boldsymbol{G}^3, \boldsymbol{G}^4: &\quad J\boldsymbol{G}(\hat{\boldsymbol{x}}) = 1 + \hat{y} + \hat{y}\hat{z} + \hat{y}^2\hat{z}, \quad 1 + \hat{z} + \hat{x}\hat{z} + \hat{z}^2\hat{x}, \quad 1 + \hat{x} + \hat{x}\hat{y} + \hat{x}^2\hat{y},\\
\boldsymbol{G}^5: &\quad J\boldsymbol{G}(\hat{\boldsymbol{x}}) = 1 + \hat{x} + \hat{y} + \hat{z} + \hat{x}\hat{y} + \hat{x}\hat{z} + \hat{y}\hat{z} + 2\hat{x}\hat{y}\hat{z},\\
\boldsymbol{G}^6, \boldsymbol{G}^7, \boldsymbol{G}^8: &\quad J\boldsymbol{G}(\hat{\boldsymbol{x}}) = 1 + \hat{y} + \hat{z} + \hat{x}\hat{y} + \hat{y}\hat{z} + \hat{y}^2\hat{x} + \hat{x}\hat{y}^2\hat{z},\\
&\qquad 1 + \hat{x} + \hat{y} + \hat{x}\hat{y} + \hat{x}\hat{z} + \hat{x}^2\hat{z} + \hat{x}^2\hat{y}\hat{z}, \qquad 1 + \hat{x} + \hat{z} + \hat{x}z + \hat{y}\hat{z} + \hat{z}^2\hat{y} + \hat{x}\hat{y}\hat{z}^2.
\end{aligned}$$

Taking appropriate linear combinations, we can recover all the elements in R_0. □

Using this lemma, we can now establish the following necessary condition (the analogue of Theorem 3.2 of [2]) on the choice of $\hat{\boldsymbol{V}}$ to ensure the approximation result (4.1).

Theorem 4.2. *Suppose that the estimate* (4.1) *holds whenever $\mathcal{T}_h$ is a sequence of shape-regular/non-degenerate sequence of hexahedral meshes of a three dimensional domain Ω. Then* $\hat{\operatorname{div}} \hat{\boldsymbol{V}} \supseteq R_0$.

Proof. The proof is essentially identical to the proof of Theorem 3.2, except that Lemma 4.1 and Theorem 2.2 are used in place of Lemma 3.1 and Theorem 2.1. However, in addition to the basic mappings $\boldsymbol{F}^1, \cdots, \boldsymbol{F}^{11}$ used in Theorem 3.2, we have also defined the maps $\boldsymbol{G}^1, \cdots, \boldsymbol{G}^8$, and we need to check that if any of these is used to define the element K_1, then we can find additional maps onto elements $K_2, \cdots, K_8$, such that the eight elements fit together to form a unit cube. Since the elements $\boldsymbol{G}^1, \cdots, \boldsymbol{G}^4$ are of the same type as those defined previously, and $\boldsymbol{G}^6, \cdots, \boldsymbol{G}^8$ are symmetric versions of the same map, we can restrict ourselves to considering only the maps $\boldsymbol{G}^5$ and $\boldsymbol{G}^8$. For the map $\boldsymbol{G}^5$, the vertices of K_1 are chosen to be $(0,0,0)$, $(1/3,0,0)$, $(0,1/3,0)$, $(2/3,1/3,0)$, $(0,0,1/3)$, $(1/3,0,2/3)$, $(0,2/3,1/3)$, $(2/3,2/3,2/3)$. The mapping $\boldsymbol{E}^3 \circ \boldsymbol{G}^5$, where $\boldsymbol{E}^3 = (x/3, y/3, z/3)$ then gives a trilinear map from the unit cube onto the element K_1. For the mapping $\boldsymbol{G}^8$, the vertices of K_1 are chosen to be $(0,0,0)$, $(1/3,0,0)$, $(0,1/3,0)$, $(1/3,1/3,0)$, $(0,0,1/3)$, $(1/3,0,2/3)$, $(0,2/3,1/3)$, $(2/3,2/3,2/3)$, and $\boldsymbol{E}^3 \circ \boldsymbol{G}^8$ gives a trilinear map from the unto cube onto the element K_1. In both these cases, the elements $K_2, \cdots, K_8$ are determined as before. The two choices of the mesh $\mathcal{T}_h^1$ corresponding to these maps are shown in Figure 2. □

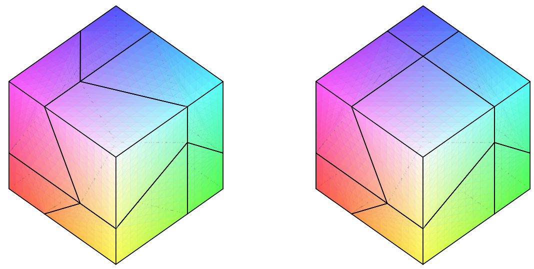

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FIGURE 2. The mesh $\mathcal{T}_h^1$ for the maps $\boldsymbol{G}^5$ and $\boldsymbol{G}^8$.

5. An optimal order $\boldsymbol{H}(\mathrm{div};\Omega)$ space and its properties

As a consequence of Theorem 4.2, a necessary condition for an optimal order approximation of the divergence is that we add to $\hat{\boldsymbol{S}}_0$ a space of dimension 19, whose divergence gives the space $\hat{Q}$. We do this in a way so that any element in this space will have the property that $\hat{\boldsymbol{q}} \cdot \hat{\boldsymbol{n}} = 0$ on $\partial\hat{K}$. It is easy to check that adding vector functions of the form $[\hat{x}(1-\hat{x})g_1, \hat{y}(1-\hat{y})g_2, \hat{z}(1-\hat{z})g_3]$ will satisfy the desired requirements if

$$\begin{aligned} g_1 &= \tilde{A}_1 + \tilde{B}_1\hat{x} + \tilde{B}_2\hat{y} + \tilde{B}_3\hat{z} + \tilde{H}\hat{y}\hat{z} + \tilde{F}_1\hat{x}\hat{z} + \tilde{G}_1\hat{x}\hat{y} + \tilde{I}_1\hat{x}\hat{y}\hat{z}, \\ g_2 &= \tilde{A}_2 + \tilde{B}_2\hat{x} + \tilde{C}_2\hat{y} + \tilde{C}_3\hat{z} + \tilde{E}_2\hat{y}\hat{z} + \tilde{H}\hat{x}\hat{z} + \tilde{G}_2\hat{x}\hat{y} + \tilde{I}_2\hat{x}\hat{y}\hat{z}, \\ g_3 &= \tilde{A}_3 + \tilde{B}_3\hat{x} + \tilde{C}_3\hat{y} + \tilde{D}_3\hat{z} + \tilde{E}_3\hat{y}\hat{z} + \tilde{F}_3\hat{x}\hat{z} + \tilde{H}\hat{x}\hat{y} + \tilde{I}_3\hat{x}\hat{y}\hat{z}. \end{aligned} \tag{5.1}$$

Here the coefficients $\tilde{A}_i, \tilde{B}_i$, etc., are considered arbitrary with no relation to the constants used previously. If we denote this space by $\hat{\boldsymbol{T}}_0$, then vector functions in the 40 dimensional space $\hat{\boldsymbol{V}}_0 \equiv \hat{\boldsymbol{S}}_0 \oplus \hat{\boldsymbol{T}}_0$ will have the form:

$$\begin{aligned} \hat{\boldsymbol{u}}_1 &= A_1 + B_1\hat{x} + C_1\hat{y} + D_1\hat{z} + E_1\hat{x}\hat{y} + F_1\hat{x}\hat{z} \\ &\quad + \hat{x}(1-\hat{x})(G_1 + H_1\hat{x} + I_1\hat{y} + J_1\hat{z} + K\hat{y}\hat{z} + L_1\hat{x}\hat{y} + M_1\hat{x}\hat{z} + N_1\hat{x}\hat{y}\hat{z}) \\ \hat{\boldsymbol{u}}_2 &= A_2 + B_2\hat{x} + C_2\hat{y} + D_2\hat{z} + E_2\hat{y}\hat{x} + F_2\hat{y}\hat{z} \\ &\quad + \hat{y}(1-\hat{y})(G_2 + H_2\hat{x} + I_2\hat{y} + J_2\hat{z} + K\hat{x}\hat{z} + L_2\hat{x}\hat{y} + M_2\hat{y}\hat{z} + N_2\hat{x}\hat{y}\hat{z}) \\ \hat{\boldsymbol{u}}_3 &= A_3 + B_3\hat{x} + C_3\hat{y} + D_3\hat{z} + E_3\hat{z}\hat{x} + F_3\hat{z}\hat{y} \\ &\quad + \hat{z}(1-\hat{z})(G_3 + H_3\hat{x} + I_3\hat{y} + J_3\hat{z} + K\hat{x}\hat{y} + L_3\hat{x}\hat{z} + M_3\hat{y}\hat{z} + N_3\hat{x}\hat{y}\hat{z}). \end{aligned}$$

Here again all constants are considered arbitrary with no relation to the constants defined previously. Note there are some simple computations needed to verify this. For example, in the original 21 dimensional space $\hat{\boldsymbol{S}}_0$, we allowed vectors of the form $(0, \hat{y}\hat{x}, -\hat{z}\hat{x})$ and $(\hat{x}^2, -\hat{y}\hat{x}, -\hat{z}\hat{x})$. By adding the vector $(\hat{x}^2, 0, 0)$, we then recover the vectors $(0, \hat{y}\hat{x}, 0)$ and $(0, 0, \hat{z}\hat{x})$. Similarly, in $\hat{\boldsymbol{S}}_0$, we allowed vectors of the form $(\hat{x}^2\hat{y}, -\hat{x}\hat{y}^2, 0)$. By adding the vector $(-\hat{x}^2\hat{y}, -\hat{x}\hat{y}^2, 0)$, we then recover the vectors $(\hat{x}^2\hat{y}, 0, 0)$ and $(0, \hat{x}\hat{y}^2, 0)$. The subspace constructed above is a subspace of $\boldsymbol{RT}_2$, ($\dim \boldsymbol{RT}_2 = 108$). Note that although the dimension of $\hat{\boldsymbol{V}}_0$ is greater than the dimension of $\boldsymbol{RT}_1$, $\boldsymbol{RT}_1$ is not a subspace of $\hat{\boldsymbol{V}}_0$, so it does not suffice to simply use $\boldsymbol{RT}_1$ to obtain optimal order convergence on a general hexahedral mesh.

We then choose degrees of freedom for $\hat{\boldsymbol{V}}_0$ to be:

$$\int_{\hat{F}} (\hat{\boldsymbol{q}} \cdot \hat{\boldsymbol{n}}) \hat{p} \, ds, \quad \hat{p} \in \mathcal{P}_1(F), \tag{5.2}$$

$$\int_{\hat{K}} \hat{\boldsymbol{q}} \cdot \hat{\boldsymbol{r}} \, dx, \quad \hat{\boldsymbol{r}} \in \hat{\boldsymbol{R}} \oplus \boldsymbol{\mathcal{P}}_0, \tag{5.3}$$

$$\int_{\hat{K}} \hat{\operatorname{div}} \, \hat{\boldsymbol{q}} \, \hat{p} \, dx, \quad \hat{p} \in \hat{Q} \setminus \mathcal{P}_1. \tag{5.4}$$

We first show these are a unisolvent set of degrees of freedom for $\hat{\boldsymbol{V}}_0$, and that the resulting finite element space $\boldsymbol{V}_h$ will be a subspace of $\boldsymbol{H}(\operatorname{div}; \Omega)$.

Lemma 5.1. *The degrees of freedom (5.2)-(5.3) are divergence conforming and unisolvent using the space of vector polynomials $\hat{\boldsymbol{V}}_0$ on $\hat{K}$.*

Proof. It is easy to see that these degrees of freedom are unisolvent. Setting them all to zero, we first observe $\hat{\boldsymbol{q}} \cdot (0, 0, -1)$ on the face $\hat{z} = 0$ is of the form $A_3 + B_3\hat{x} + C_3\hat{y}$. The conditions on the degrees of freedom on this face then imply $A_3 = B_3 = C_3 = 0$. Hence, $\hat{\boldsymbol{q}} \cdot \hat{\boldsymbol{n}} = 0$ on this face, which establishes that the element is divergence conforming on this face, i.e., that the degrees of freedom on the face $\hat{z} = 0$ uniquely determine $\hat{\boldsymbol{q}} \cdot \hat{\boldsymbol{n}} = 0$ on this face. On the face $\hat{z} = 1$, the condition $\hat{\boldsymbol{q}} \cdot (0, 0, 1) = 0$ then implies $D_3 = E_3 = F_3 = 0$. Thus $\hat{\boldsymbol{q}} \cdot \hat{\boldsymbol{n}} = 0$ on this face, and the element is also divergence conforming on the face $\hat{z} = 1$.

By similar reasoning on the other faces, $A_i = B_i = C_i = D_i = E_i = F_i = 0$, $i = 1, 2$, and thus the element will be divergence conforming on all faces. Using the divergence theorem, and the degrees of freedom (5.2)-(5.3) we also have for all $\hat{p} \in \mathcal{P}_1$,

$$\int_{\hat{K}} \hat{\operatorname{div}} \hat{\boldsymbol{q}} \, \hat{p} \, d\hat{x} = \int_{\partial \hat{K}} \hat{\boldsymbol{q}} \cdot \hat{\boldsymbol{n}} \, \hat{p} \, d\hat{s} - \int_{\hat{K}} \hat{\boldsymbol{q}} \cdot \hat{\nabla} p \, d\hat{x} = 0.$$

Hence, together with (5.4), we get

$$\int_{\hat{K}} \hat{\operatorname{div}} \, \hat{\boldsymbol{q}} \, \hat{p} \, d\hat{x} = 0,$$

for all $\hat{p} \in R_0$. Since $\hat{\operatorname{div}} \, \hat{\boldsymbol{q}}$ belongs to this space, we find that $\hat{\operatorname{div}} \, \hat{\boldsymbol{q}} = 0$. Thus, $\hat{\boldsymbol{q}}$ has the form given by (3.7). It then easily follows from the second set of degrees of freedom that $\hat{\boldsymbol{q}} = 0$. □

The next lemma shows that the degrees of freedom are unchanged when mapped by the trilinear map $\boldsymbol{F}$.

Lemma 5.2. *The degrees of freedom of a function $\boldsymbol{u}$ on K and for $\hat{\boldsymbol{u}}$ on $\hat{K}$ are identical provided $\boldsymbol{u}$ and $\hat{\boldsymbol{u}}$ are related by (1.1) and $\boldsymbol{R} \oplus \boldsymbol{\mathcal{P}}_0$ is transformed using (1.3).*

Proof. This result follows by using the usual change of variables formulae together with the relationship between volume and surface Jacobians in equation (1.34) of [7] and summarized in (1.2). □

6. Necessary conditions for optimal $\boldsymbol{L}^2(\Omega)$ approximation of $\boldsymbol{H}(\mathbf{curl};\Omega)$ elements on hexahedral meshes

In this section, we consider finite element spaces defined by the mapping (1.3) from a reference element and determine necessary conditions for $O(h)$ approximation of a vector field on shape-regular/non-degenerate hexahedral meshes. Following the previous approach, we first determine what shape functions $\hat{\boldsymbol{U}}$ are needed on the reference cube, so that after application of the mapping (1.3), the resulting functions contain the constant vectors $(1,0,0)$, $(0,1,0)$, and $(0,0,1)$. This is done by applying the inverse of the mapping (1.3) to these constant vectors, i.e., the mapping

$$\hat{\boldsymbol{u}}(\hat{\boldsymbol{x}}) = (D\boldsymbol{F})^T(\hat{\boldsymbol{x}})\,\boldsymbol{u}(\boldsymbol{x}). \tag{6.1}$$

When $\boldsymbol{u}(\boldsymbol{x})$ is the unit vector with i^{th} component equal to one, we find

$$\begin{aligned} \hat{u}_1(\boldsymbol{x}) &= b_i + e_i\hat{y} + g_i\hat{z} + h_i\hat{y}\hat{z}, \\ \hat{u}_2(\boldsymbol{x}) &= c_i + e_i\hat{x} + f_i\hat{z} + h_i\hat{x}\hat{z}, \\ \hat{u}_3(\boldsymbol{x}) &= d_i + f_i\hat{y} + g_i\hat{x} + h_i\hat{x}\hat{y}. \end{aligned}$$

Hence, the curl conforming finite element space must contain the span of the following functions

$$\begin{pmatrix}1\\0\\0\end{pmatrix}, \begin{pmatrix}0\\1\\0\end{pmatrix}, \begin{pmatrix}0\\0\\1\end{pmatrix}, \begin{pmatrix}\hat{y}\\\hat{x}\\0\end{pmatrix}, \begin{pmatrix}\hat{z}\\0\\\hat{x}\end{pmatrix}, \begin{pmatrix}0\\\hat{z}\\\hat{y}\end{pmatrix}, \begin{pmatrix}\hat{y}\hat{z}\\\hat{x}\hat{z}\\\hat{x}\hat{y}\end{pmatrix}.$$

This is $\hat{\nabla}\mathcal{P}_{1,1,1}$, where $\mathcal{P}_{1,1,1}$ denotes the tensor product of linear polynomials in each variable. Since the lowest order Nédélec space, denoted by $\boldsymbol{N}_0$, is given by $\boldsymbol{N}_0 = \mathcal{P}_{0,1,1}\times\mathcal{P}_{1,0,1}\times\mathcal{P}_{1,1,0}$, we see that $\boldsymbol{N}_0$ contains the necessary functions. If we apply (6.1) to the space $\boldsymbol{\mathcal{P}}_1$, then using the expressions for $\boldsymbol{F}$ and $D\boldsymbol{F}$, it is easy to check that the resulting space of vectors $\in \boldsymbol{N}_1 = \mathcal{P}_{1,2,2}\times\mathcal{P}_{2,1,2}\times\mathcal{P}_{2,2,1}$. By arguments analogous to those used previously, $\boldsymbol{N}_1$ satisfies the necessary conditions for second order accuracy in $\boldsymbol{L}^2$.

We next consider the issue of what additional functions, if any, must be added to the space on the reference cube to also insure optimal approximation of $\mathbf{curl}\ \boldsymbol{u}$. For this, we use the fact that

$$\hat{\mathbf{curl}}\ \hat{\boldsymbol{u}}(\boldsymbol{x}) = J\boldsymbol{F}(\hat{\boldsymbol{x}})(D\boldsymbol{F})^{-1}(\hat{\boldsymbol{x}})\,\mathbf{curl}\ \boldsymbol{u}(\boldsymbol{x}).$$

Thus, we are back to the question of $\boldsymbol{L}^2$ approximation in $\boldsymbol{H}(\text{div};\Omega)$, where $\boldsymbol{q} = \mathbf{curl}\ \boldsymbol{u}$. Now

$$\hat{\mathbf{curl}}\ \boldsymbol{N}_0 = \text{span}\left\{\begin{pmatrix}1\\0\\0\end{pmatrix}, \begin{pmatrix}0\\1\\0\end{pmatrix}, \begin{pmatrix}0\\0\\1\end{pmatrix}, \begin{pmatrix}\hat{x}\\\hat{-y}\\0\end{pmatrix}, \begin{pmatrix}\hat{-x}\\0\\\hat{z}\end{pmatrix}\right\}.$$

Thus, we need to add 15 basis functions to $\boldsymbol{N}_0$, whose curls give the remaining vectors in the 20-dimensional space $\boldsymbol{S}_0^-$. A good choice is the following, whose span we denote by $\boldsymbol{M}_0$.

$$
\begin{aligned}
\hat{\boldsymbol{\phi}}_1 &= [0,(1-\hat{z})\hat{x}(1-\hat{x}),0]^T, & \hat{\boldsymbol{\phi}}_2 &= [0,\hat{z}\hat{x}(1-\hat{x}),0]^T,\\
\hat{\boldsymbol{\phi}}_3 &= [0,0,(1-\hat{y})\hat{x}(1-\hat{x})]^T, & \hat{\boldsymbol{\phi}}_4 &= [0,0,\hat{y}\hat{x}(1-\hat{x})^T,\\
\hat{\boldsymbol{\phi}}_5 &= [(1-\hat{z})\hat{y}(1-\hat{y}),0,0]^T, & \hat{\boldsymbol{\phi}}_6 &= [\hat{z}\hat{y}(1-\hat{y}),0,0]^T,\\
\hat{\boldsymbol{\phi}}_7 &= [0,0,(1-\hat{z})\hat{y}(1-\hat{y})]^T, & \hat{\boldsymbol{\phi}}_8 &= [0,0,\hat{z}\hat{y}(1-\hat{y})]^T,\\
\hat{\boldsymbol{\phi}}_9 &= [(1-\hat{y})\hat{z}(1-\hat{z}),0,0]^T, & \hat{\boldsymbol{\phi}}_{10} &= [\hat{y}\hat{z}(1-\hat{z}),0,0]^T,\\
\hat{\boldsymbol{\phi}}_{11} &= [0,(1-\hat{x})\hat{z}(1-\hat{z})]^T, & \hat{\boldsymbol{\phi}}_{12} &= [0,\hat{x}\hat{z}(1-\hat{z})]^T,\\
\hat{\boldsymbol{\phi}}_{13} &= [\hat{y}(1-\hat{y})\hat{z}(1-\hat{z}),0,0]^T, & \hat{\boldsymbol{\phi}}_{14} &= [0,\hat{x}(1-\hat{x})\hat{z}(1-\hat{z}),0]^T,\\
\hat{\boldsymbol{\phi}}_{15} &= [0,0,\hat{x}(1-\hat{x})\hat{y}(1-\hat{y})]^T.
\end{aligned}
$$

To see that $\mathbf{curl}\ \boldsymbol{M}_0 + \mathbf{curl}\ \boldsymbol{N}_0$ spans $\boldsymbol{S}_0^-$, we note that

$$
\begin{gathered}
\mathbf{curl}\,(\hat{\boldsymbol{\phi}}_1+\hat{\boldsymbol{\phi}}_2) = [0,0,1-2\hat{x}]^T, \qquad \mathbf{curl}\,(\hat{\boldsymbol{\phi}}_3+\hat{\boldsymbol{\phi}}_4) = [0,1-2\hat{x},0]^T,\\
\mathbf{curl}\,(\hat{\boldsymbol{\phi}}_2+\hat{\boldsymbol{\phi}}_4) = [0,-\hat{y}+2\hat{x}\hat{y},\hat{z}-2\hat{x}\hat{z}]^T = [0,-\hat{y},\hat{z}]^T + 2[0,\hat{x}\hat{y},-\hat{x}\hat{z}]^T,\\
\mathbf{curl}\,(\hat{\boldsymbol{\phi}}_1-\hat{\boldsymbol{\phi}}_2) = [2\hat{x}(1-\hat{x}),0,(1-2\hat{x})(1-2\hat{z})]^T = -2[\hat{x}^2,-\hat{x}\hat{y},-\hat{x}\hat{z}]^T\\
-2[0,\hat{x}\hat{y},-\hat{x}\hat{z}]^T + 2[\hat{x},0,-\hat{z}]^T - 2[0,0,\hat{x}]^T + [0,0,1]^T,\\
\mathbf{curl}\ \hat{\boldsymbol{\phi}}_{13} = [0,2\hat{y}^2\hat{z}-\hat{y}^2-2\hat{y}\hat{z}+\hat{y},-2\hat{y}\hat{z}^2+\hat{z}^2+2\hat{y}\hat{z}-\hat{z}]^T\\
= 2[0,\hat{y}^2\hat{z},-\hat{y}\hat{z}^2]^T + [\hat{x}\hat{y},-\hat{y}^2,\hat{z}\hat{y}]^T + [-\hat{x}\hat{z},-\hat{y}\hat{z},\hat{z}^2]^T\\
+[-\hat{x}\hat{y},0,\hat{z}\hat{y}]^T + [\hat{x}\hat{z},-\hat{y}\hat{z},0]^T + [0,\hat{y},-\hat{z}]^T.
\end{gathered}
$$

Using these formulas, together with analogous formulas for the other $\hat{\boldsymbol{\phi}}_i$, the desired result is easily established.

These basis functions all have the property that their edge degrees of freedom are zero, i.e., $\hat{\boldsymbol{\phi}}\cdot\hat{\boldsymbol{t}} = 0$ along each of the 12 edges of the cube $\hat{K}$, where $\hat{\boldsymbol{t}}$ is the tangent vector to that edge. In addition, the tangential component of each $\hat{\boldsymbol{\phi}}$ vanishes on all except at most one face of $\hat{K}$, and for three of the basis functions, the tangential component vanishes on all faces.

Setting $\hat{\boldsymbol{U}}_0 = \boldsymbol{N}_0 + \boldsymbol{M}_0$, we now show that

$$\int_{\hat{e}} \hat{\boldsymbol{u}}\cdot\hat{\boldsymbol{t}}\,p\,d\hat{s}, \quad p\in\mathcal{P}_0 \text{ for all edges } \hat{e} \text{ with unit tangent } \hat{\boldsymbol{t}}, \tag{6.2}$$

$$\int_{\hat{f}} (\hat{\nabla}\times\hat{\boldsymbol{u}})\cdot\hat{\boldsymbol{n}}\,p\,d\hat{x}, \quad p\in\mathcal{P}_1\setminus\mathcal{P}_0, \text{ for all faces } \hat{f} \text{ with normal } \hat{\boldsymbol{n}}, \tag{6.3}$$

$$\int_{\hat{K}} (\hat{\nabla}\times\hat{\boldsymbol{u}})\cdot\hat{\boldsymbol{r}}\,d\hat{x}, \quad \hat{\boldsymbol{r}}\in\hat{\boldsymbol{R}}, \tag{6.4}$$

are a unisolvent set of degrees of freedom for the 27-dimensional space $\hat{\boldsymbol{U}}_0$, and the finite element space defined from these degrees of freedom is curl-conforming.

We start by proving that the degrees of freedom are invariant under the appropriate change of variables.

Lemma 6.1. *The degrees of freedom of a function* $\boldsymbol{u}$ *on* K *and for* $\hat{\boldsymbol{u}}$ *on* $\hat{K}$ *are identical provided* $\boldsymbol{u}$ *and* $\hat{\boldsymbol{u}}$ *are related by (1.3) and* $\hat{\boldsymbol{R}}$ *is transformed in the same way.*

Proof. This result follows by using the usual change of variables formulae together with the relationship between volume and surface Jacobians in equation (1.34) of [7] (summarized in (1.4)). ☐

Lemma 6.2. *The finite element constructed using* $\hat{\boldsymbol{U}}_0$ *together with the degrees of freedom (6.2)-(6.4) is curl-conforming and unisolvent.*

Proof. Using Lemma 6.1, we need only prove unisolvence and conformance on the reference element. On $\hat{K}$, the general basis function in $\hat{\boldsymbol{U}}_0$ can be written $\hat{\boldsymbol{u}} = (\hat{u}_1, \hat{u}_2, \hat{u}_3)$ where

$$\begin{aligned}
\hat{u}_1 &= a_1 + a_6\hat{y} + a_8\hat{z} + a_{10}\hat{y}\hat{z} + a_{15}(1-\hat{z})\hat{y}(1-\hat{y}) + a_{18}\hat{z}(1-\hat{z})(1-\hat{y}) \\
&\quad + a_{21}\hat{z}(1-\hat{z})\hat{y} + a_{24}\hat{y}(1-\hat{y})\hat{z} + a_{27}\hat{y}(1-\hat{y})\hat{z}(1-\hat{z}), \\
\hat{u}_2 &= a_2 + a_4\hat{x} + a_9 z + a_{11}\hat{x}\hat{z} + a_{13}\hat{x}(1-\hat{x})(1-\hat{z}) + a_{17}(1-\hat{x})\hat{z}(1-\hat{z}) \\
&\quad + a_{19}\hat{x}(1-\hat{x})\hat{z} + a_{22}\hat{z}(1-\hat{z})\hat{x} + a_{26}\hat{z}(1-\hat{z})\hat{x}(1-\hat{x}), \\
\hat{u}_3 &= a_3 + a_5\hat{x} + a_7\hat{y} + a_{12}\hat{x}\hat{y} + a_{14}\hat{x}(1-\hat{x})(1-\hat{y}) + a_{16}(1-\hat{x})\hat{y}(1-\hat{y}) \\
&\quad + a_{20}\hat{x}(1-\hat{x})\hat{y} + a_{23}\hat{y}(1-\hat{y})\hat{x} + a_{25}\hat{y}(1-\hat{y})\hat{x}(1-\hat{x}).
\end{aligned}$$

Consider a face $\hat{f}$. Suppose the degrees of freedom (6.2) vanish for all edges $\hat{e}$ of $\hat{f}$ and that the degrees of freedom (6.3) also vanish for $\hat{f}$. With no loss of generality, we can assume the face is $\hat{z} = 0$. On this face, the tangential components of $\hat{\boldsymbol{u}}$ are

$$\hat{u}_1 = a_1 + a_6\hat{y} + a_{15}\hat{y}(1-\hat{y}), \qquad \hat{u}_2 = a_2 + a_4\hat{x} + a_{13}\hat{x}(1-\hat{x}).$$

The degrees of freedom (6.2) applied on the edges along ($\hat{x} = 0$, $\hat{z} = 0$), ($\hat{x} = 1$, $\hat{z} = 0$), ($\hat{y} = 0$, $\hat{z} = 0$) and ($\hat{y} = 1$, $\hat{z} = 0$) show that $a_1 = a_6 = a_2 = a_4 = 0$. But on the face $\hat{z} = 0$,

$$\hat{\nabla} \times \hat{\boldsymbol{u}} \cdot \hat{\boldsymbol{n}} = a_4 + a_{13}(1-2\hat{x}) - a_6 - a_{15}(1-2\hat{y}).$$

Using the fact that $a_4 = a_6 = 0$, the vanishing of the degrees of freedom (6.3) on this face (choosing successively $\hat{p} = \hat{x}$ and then $\hat{p} = \hat{y}$) shows that $a_{13} = a_{15} = 0$. Thus $\hat{u}_1 = \hat{u}_2 = 0$ on this face. This proves that the element is curl conforming.

To show unisolvence, note that if all the degrees of freedom vanish, then all tangential components vanish on the surface of $\hat{K}$, and so

$$\hat{\boldsymbol{u}} = a_{25}\begin{pmatrix} 0 \\ 0 \\ \hat{y}(1-\hat{y})\hat{x}(1-\hat{x}) \end{pmatrix} + a_{26}\begin{pmatrix} 0 \\ \hat{z}(1-\hat{z})\hat{x}(1-\hat{x}) \\ 0 \end{pmatrix} + a_{27}\begin{pmatrix} \hat{y}(1-\hat{y})\hat{z}(1-\hat{z}) \\ 0 \\ 0 \end{pmatrix}.$$

Using $\hat{\boldsymbol{r}}_3 = (1/2 - \hat{y}, \hat{x} - 1/2, 0)$ we have

$$\int_{\hat{K}} \hat{\nabla} \times \hat{\boldsymbol{u}} \cdot \hat{\boldsymbol{r}}_3 \, dV = 2a_{25}\int_{\hat{K}} [(1/2-\hat{y})^2\hat{x}(1-\hat{x}) + (1/2-\hat{x})^2\hat{y}(1-\hat{y})]\, dV = \frac{1}{18}a_{25},$$

so the vanishing of the interior degrees of freedom (6.4) shows that $a_{25} = 0$, and similarly that $a_{26} = a_{27} = 0$. This completes the proof. ☐

The space we have constructed is first order convergent in both the $\boldsymbol{H}(\mathbf{curl}\,;\Omega)$ norm and $\boldsymbol{L}^2$ norm. We note that all the basis functions in $\hat{\boldsymbol{U}}_0$ are contained in $\boldsymbol{N}_1 = \mathcal{P}_{1,2,2} \times \mathcal{P}_{2,1,2} \times \mathcal{P}_{2,2,1}$. Hence $\boldsymbol{N}_1$ is first order convergent in the $\boldsymbol{H}(\mathbf{curl}\,;\Omega)$ norm and second order convergent in the $\boldsymbol{L}^2$ norm.

7. Projection operators and the discrete de Rham complex

Associated to the degrees of freedom of the space $\hat{\boldsymbol{V}}_0$ on the reference element, there is a natural bounded projection operator $\hat{\boldsymbol{\pi}}^{\hat{\boldsymbol{V}}} : \boldsymbol{H}^1(\hat{K}) \to \hat{\boldsymbol{V}}_0$. We then define the corresponding projector operator $\boldsymbol{\pi}_K^{\boldsymbol{V}} : \boldsymbol{H}^1(K) \to \boldsymbol{P}_F \hat{\boldsymbol{V}}_0$ by $\boldsymbol{\pi}_K^{\boldsymbol{V}} = \boldsymbol{P}_F \hat{\boldsymbol{\pi}}^{\hat{\boldsymbol{V}}} \boldsymbol{P}_F^{-1}$. A global projection operator $\boldsymbol{\pi}_h^{\boldsymbol{V}} : \boldsymbol{H}^1(\Omega) \to \boldsymbol{V}_h$ is defined piecewise, i.e., $(\boldsymbol{\pi}_h^{\boldsymbol{V}} \boldsymbol{u})_K = \boldsymbol{\pi}_K^{\boldsymbol{V}}(\boldsymbol{u}|_K)$. Similarly, associated to the degrees of freedom of the space $\hat{\boldsymbol{U}}_0$ on the reference element, there is a natural bounded projection operator $\hat{\boldsymbol{\pi}}^{\hat{\boldsymbol{U}}} : \boldsymbol{H}^1(\mathbf{curl}\,, \hat{K}) \to \hat{\boldsymbol{U}}_0$, where

$$\boldsymbol{H}^1(\mathbf{curl}\,, \hat{K}) = \{\boldsymbol{v} \in \boldsymbol{H}^1(\hat{K}) : \mathbf{curl}\,\boldsymbol{v} \in \boldsymbol{H}^1(\hat{K})\}.$$

Since it is not at all obvious, we note that a demonstration that the edge degrees of freedom are well defined for the space $\boldsymbol{H}^1(\mathbf{curl}\,, \hat{K})$ can be found in the proof of Theorem 3.2 in [8]. We then define the corresponding projector operator $\boldsymbol{\pi}_K^{\boldsymbol{U}} : \boldsymbol{H}^1(\mathbf{curl}\,, K) \to \boldsymbol{R}_F \hat{\boldsymbol{U}}_0$ by $\boldsymbol{\pi}_K^{\boldsymbol{U}} = \boldsymbol{R}_F \hat{\boldsymbol{\pi}}^{\hat{\boldsymbol{U}}} \boldsymbol{R}_F^{-1}$. A global projection operator $\boldsymbol{\pi}_h^{\boldsymbol{U}} : \boldsymbol{H}^1(\mathbf{curl}\,, \Omega) \to \boldsymbol{U}_h$ is defined piecewise, i.e., $(\boldsymbol{\pi}_h^{\boldsymbol{U}} \boldsymbol{u})_K = \boldsymbol{\pi}_K^{\boldsymbol{U}}(\boldsymbol{u}|_K)$.

To describe our discrete de Rham complex, we need to first define some additional spaces. On $\hat{K}$, we define $\hat{S} = \mathcal{P}_{1,1,1}$, the tensor product of linear polynomials in each variable. We then define in the usual way $S_K = \{p : p(\boldsymbol{F}_K(\hat{\boldsymbol{x}})) = \hat{p}(\hat{\boldsymbol{x}}),\ \hat{\boldsymbol{x}} \in \hat{K},\ \hat{p} \in \hat{S}\}$, and then

$$S_h = \{p \in H^1(\Omega) : p|_K \in S_K, \forall K \in \mathcal{T}_h\}.$$

We next define the space $\hat{W} = \hat{\operatorname{div}}\,\hat{V}$, i.e., $\hat{W} = \operatorname{span} R_0$ and then a space of shape functions on K by

$$W_K = \{w : w(\boldsymbol{F}_K(\hat{\boldsymbol{x}})) = (J\boldsymbol{F})^{-1}(\hat{\boldsymbol{x}})\hat{w}(\hat{\boldsymbol{x}}),\ \hat{\boldsymbol{x}} \in \hat{K},\ \hat{w} \in \hat{W}\}.$$

Finally, we define

$$W_h = \{w \in L^2(\Omega) : w|_K \in W_K, \forall K \in \mathcal{T}_h\}.$$

For the space $\hat{S}$, we let $\hat{\pi}^{\hat{S}}$ be the usual Lagrange interpolation operator (interpolating at the vertices of the set $\hat{K}$). For the space $\hat{W}$, we let $\hat{\pi}^{\hat{W}}$ denote the L^2 projection. Associated to these projections, we then define projection operators on the element K in the usual way, i.e.,

$$\pi_K^S p(\boldsymbol{x}) = \hat{\pi}^{\hat{S}} \hat{p} \circ \boldsymbol{F}_K^{-1}(\boldsymbol{x}) = \hat{\pi}^{\hat{S}} \hat{p}(\hat{\boldsymbol{x}}), \qquad \pi_K^W w(\boldsymbol{x}) = (J\boldsymbol{F})^{-1} \hat{\pi}^{\hat{W}}\, \hat{w} \circ \boldsymbol{F}_K^{-1}(\boldsymbol{x}) = (J\boldsymbol{F})^{-1} \hat{\pi}^{\hat{W}}\, \hat{w}(\hat{\boldsymbol{x}}).$$

We now show that the following discrete de Rham diagram commutes

$$\begin{array}{ccccccc}
H^1(\Omega) & \xrightarrow{\mathbf{grad}} & \boldsymbol{H}(\mathbf{curl}\,;\Omega) & \xrightarrow{\mathbf{curl}} & \boldsymbol{H}(\mathrm{div};\Omega) & \xrightarrow{\mathrm{div}} & L^2(\Omega) \\
\cup & & \cup & & \cup & & \\
H^2(\Omega) & & \boldsymbol{H}^1(\mathbf{curl}\,,\Omega) & & \boldsymbol{H}^1(\Omega) & & \\
\pi_h^S \downarrow & & \boldsymbol{\pi}_h^{\boldsymbol{U}} \downarrow & & \boldsymbol{\pi}_h^{\boldsymbol{V}} \downarrow & & \pi_h^W \downarrow \\
S_h & \xrightarrow{\mathbf{grad}} & \boldsymbol{U}_h & \xrightarrow{\mathbf{curl}} & \boldsymbol{V}_h & \xrightarrow{\mathrm{div}} & W_h
\end{array}$$

We note that the above diagram is directly related to a similar diagram on the reference element. This follows easily from the relationships below.

$$\pi_K^S p = \hat{\pi}^{\hat{S}} \hat{p}, \quad \boldsymbol{\pi}_K^{\boldsymbol{U}} \boldsymbol{u} = \boldsymbol{R}_F \hat{\boldsymbol{\pi}}^{\hat{\boldsymbol{U}}} \boldsymbol{R}_F^{-1} \boldsymbol{u}, \quad \boldsymbol{\pi}_K^{\boldsymbol{V}} \boldsymbol{v} = \boldsymbol{P}_F \hat{\boldsymbol{\pi}}^{\hat{\boldsymbol{V}}} \boldsymbol{P}_F^{-1} \boldsymbol{v}, \quad \pi_K^W w = (J\boldsymbol{F})^{-1} \hat{\pi}^{\hat{W}} (J\boldsymbol{F} w),$$
$$\mathbf{grad}\; p = \boldsymbol{R}_F \hat{\mathbf{grad}}\; \hat{p}, \qquad \mathbf{curl}\; \boldsymbol{u} = \boldsymbol{P}_F \hat{\mathbf{curl}}\; \boldsymbol{R}_F^{-1} \boldsymbol{u}, \qquad \mathrm{div}\; \boldsymbol{v} = (J\boldsymbol{F})^{-1} \hat{\mathrm{div}}\, \boldsymbol{P}_F^{-1} \boldsymbol{u}.$$

Then for example, if we know that $\boldsymbol{\pi}^{\hat{\boldsymbol{V}}} \hat{\mathbf{curl}}\; \hat{\boldsymbol{u}} = \hat{\mathbf{curl}}\; \hat{\boldsymbol{\pi}}^{\hat{\boldsymbol{U}}}\, \hat{\boldsymbol{u}}$, we have

$$\begin{aligned}
\boldsymbol{\pi}_K^{\boldsymbol{V}} \mathbf{curl}\; \boldsymbol{u} = \boldsymbol{P}_F \hat{\boldsymbol{\pi}}^{\hat{\boldsymbol{V}}} \boldsymbol{P}_F^{-1} \boldsymbol{P}_F\, \hat{\mathbf{curl}}\; \boldsymbol{R}_F^{-1} \boldsymbol{u} = \boldsymbol{P}_F \hat{\boldsymbol{\pi}}^{\hat{\boldsymbol{V}}} \hat{\mathbf{curl}}\; \hat{\boldsymbol{u}} = \boldsymbol{P}_F \hat{\mathbf{curl}}\; \hat{\boldsymbol{\pi}}^{\hat{\boldsymbol{U}}}\, \boldsymbol{R}_F^{-1} \boldsymbol{u} \\
= \boldsymbol{P}_F \hat{\mathbf{curl}}\; \boldsymbol{R}_F^{-1} \boldsymbol{\pi}_K^{\boldsymbol{U}} \boldsymbol{u} = \boldsymbol{P}_F \boldsymbol{P}_F^{-1} \mathbf{curl}\, \boldsymbol{\pi}_K^{\boldsymbol{U}} \boldsymbol{u} = \mathbf{curl}\, \boldsymbol{\pi}_K^{\boldsymbol{U}} \boldsymbol{u}.
\end{aligned}$$

To check that the diagram commutes, we shall instead use the relationships given in Lemmas 5.2 and 6.1 between the degrees of freedom on the element K and the element $\hat{K}$.

Lemma 7.1. *For all sufficiently smooth vector functions* $\boldsymbol{u}$, $\boldsymbol{\pi}_h^{\boldsymbol{V}} \nabla \times \boldsymbol{u} = \nabla \times \boldsymbol{\pi}_h^{\boldsymbol{U}} \boldsymbol{u}$.

Proof. Since $\nabla \times \boldsymbol{U}_h \subset \boldsymbol{V}_h$ we see that the lemma is proved if we can show that $\boldsymbol{\pi}_h^{\boldsymbol{V}}(\nabla \times (I - \boldsymbol{\pi}_h^{\boldsymbol{U}})\boldsymbol{u} = 0$. Thus it suffices to show that $\boldsymbol{\pi}_h^{\boldsymbol{U}} \nabla \times \boldsymbol{w} = 0$ for any smooth function $\boldsymbol{w}$ having the property that the degrees of freedom (6.2)-(6.4) vanish on every element. To do this, we need to show that the degrees of freedom (5.2)-(5.4) for $\nabla \times \boldsymbol{w}$ vanish, and we can restrict ourselves to the reference element via Lemma 5.2. It is obvious that the degrees of freedom (5.4) vanish, since $\hat{\nabla} \cdot \hat{\nabla} \times \hat{\boldsymbol{w}} = 0$. For the degrees of freedom (5.3), we see that for $\hat{\boldsymbol{r}} \in \hat{\boldsymbol{R}}$,

$$\int_{\hat{K}} \hat{\nabla} \times \hat{\boldsymbol{w}} \cdot \hat{\boldsymbol{r}}\, d\hat{x} = 0,$$

since this is just (6.4). For $\hat{\boldsymbol{r}} \in \boldsymbol{\mathcal{P}}_0$ we see that $\hat{\boldsymbol{r}} = \hat{\nabla} \hat{p}$ for some $\hat{p} \in \mathcal{P}_1 \setminus \mathcal{P}_0$ and so, using integration by parts,

$$\int_{\hat{K}} \hat{\nabla} \times \hat{\boldsymbol{w}} \cdot \hat{\boldsymbol{r}}\, d\hat{x} = \int_{\hat{K}} \hat{\nabla} \times \hat{\boldsymbol{w}} \cdot \hat{\nabla} \hat{p}\, d\hat{x} = -\int_{\hat{K}} \hat{\nabla} \cdot \hat{\nabla} \times \hat{\boldsymbol{w}}\, \hat{p}\, d\hat{x} + \int_{\partial \hat{K}} (\hat{\nabla} \times \hat{\boldsymbol{w}}) \cdot \hat{\boldsymbol{n}}\, \hat{p}\, d\hat{s}.$$

The first term on the right hand side vanishes trivially and the second term vanishes because the degrees of freedom (6.3) vanish.

It remains to show that the face degrees of freedom (5.2) vanish. This is implied by (6.3) if $p \in \mathcal{P}_1 \setminus \mathcal{P}_0$. In the case $p \in \mathcal{P}_0$, using integration by parts, and the vector and scalar surface curls,

$$\int_{\hat{f}} (\hat{\nabla} \times \hat{\boldsymbol{w}}) \cdot \hat{\boldsymbol{n}}\, \hat{p}\, d\hat{s} = \int_{\hat{f}} \hat{\nabla}_{\hat{f}} \times \hat{\boldsymbol{w}}_T\, \hat{p}\, d\hat{s} = \int_{\hat{f}} \hat{\boldsymbol{w}}_T \vec{\hat{\nabla}}_{\hat{f}} \times \hat{p}\, d\hat{s} + \int_{\partial \hat{f}} \hat{\boldsymbol{w}} \cdot \boldsymbol{t}\, \hat{p}\, d\hat{s},$$

where $\hat{\boldsymbol{w}}_T$ denotes the tangential component of $\hat{\boldsymbol{w}}$ on $\hat{f}$. The first term on the right hand side vanishes because p is constant and the second due to the vanishing of the degrees of freedom (6.2). Thus all the degrees of freedom for $\nabla \times \boldsymbol{w}$ vanish and so $\boldsymbol{\pi}_h^{\boldsymbol{V}} \nabla \times \boldsymbol{w} = 0$. □

Lemma 7.2. *For all sufficiently smooth functions p, $\boldsymbol{\pi}_h^{\boldsymbol{U}} \nabla p = \nabla \times \pi_h^S p$.*

Proof. Since $\nabla S_h \subset \boldsymbol{U}_h$, we see that the lemma is proved if we can show that $\boldsymbol{\pi}_h^{\boldsymbol{U}} \nabla (I - \pi_h^S) p = 0$. Thus it suffices to show that $\boldsymbol{\pi}_h^{\boldsymbol{U}} \nabla q = 0$ for any smooth function q that vanishes at the nodes of every element. To do this we need to show that the degrees of freedom (6.2)-(6.4) for ∇q vanish, and we can restrict ourselves to the reference element via Lemma 6.1. It is obvious that the degrees of freedom (6.3)-(6.4) vanish since $\hat{\nabla} \times \hat{\nabla} \hat{q} = 0$. For the edge degrees of freedom in (6.2), we see that for $\hat{p} \in \mathcal{P}_0$

$$\int_{\hat{e}} \hat{\nabla} \hat{q} \cdot \boldsymbol{t} \, \hat{p} \, d\hat{s} = \hat{p} \int_{\hat{e}} \frac{\partial}{\partial \hat{s}} \hat{q} \, d\hat{s} = 0.$$

Thus all the degrees of freedom for $\hat{\nabla} \hat{q}$ vanish and so $\boldsymbol{\pi}_h^{\boldsymbol{U}} \nabla q = 0$. □

Lemma 7.3. *For all sufficiently smooth vector functions $\boldsymbol{v}$, $\pi_h^W \nabla \cdot \boldsymbol{v} = \nabla \cdot \boldsymbol{\pi}_h^{\boldsymbol{V}} \boldsymbol{v}$.*

Proof. Since $\nabla \cdot \boldsymbol{V}_h \subset W_h$, we see that the lemma is proved if we can show that $\pi_h^W \nabla \cdot (I - \boldsymbol{\pi}_h^{\boldsymbol{V}}) \boldsymbol{v} = 0$. Thus it suffices to show that $\pi_h^W \nabla \cdot \boldsymbol{w} = 0$ for any smooth vector function $\boldsymbol{w}$ such that the degrees of freedom (5.2)-(5.4) vanish. Using (5.4), we have on the reference element $\hat{K}$ that

$$\int_{\hat{K}} \hat{\nabla} \cdot \hat{\boldsymbol{w}} \, \hat{p} \, d\hat{x} = 0, \quad \forall \hat{p} \in \hat{Q} \setminus \mathcal{P}_1.$$

Thus we need only consider the above integral for $\hat{p} \in \mathcal{P}_1$. Integrating by parts, we obtain

$$\int_{\hat{K}} \hat{\nabla} \cdot \hat{\boldsymbol{w}} \, p \, d\hat{x} = - \int_{\hat{K}} \hat{\boldsymbol{w}} \cdot \hat{\nabla} \hat{p} \, d\hat{x} + \int_{\partial \hat{K}} \hat{\boldsymbol{w}} \cdot \hat{\boldsymbol{n}} \, \hat{p} \, d\hat{s}.$$

The first integral vanishes for $\hat{p} \in \mathcal{P}_1$ using the volume degrees of freedom (5.3) since $\hat{\nabla} \hat{p} \in \boldsymbol{\mathcal{P}}_0$. The second term vanishes using the face degrees of freedom (5.2). □

Combining the three lemmas above shows that the discrete de Rham diagram commutes.

8. Approximation estimates

We have shown in the previous sections that necessary conditions for the space $\boldsymbol{V}_h$ to have optimal $O(h)$ approximation in both $\boldsymbol{L}^2$ and $\boldsymbol{H}(\mathrm{div}; \Omega)$ are that the space $\hat{\boldsymbol{V}}$ on the reference element from which $\boldsymbol{V}_h$ is constructed satisfies

$$\hat{\boldsymbol{V}} \supseteq \boldsymbol{S}_0^- \text{ and } \hat{\mathrm{div}} \hat{\boldsymbol{V}} \supseteq R_0.$$

We have further established that the choice $\hat{\boldsymbol{V}} = \hat{\boldsymbol{V}}_0$ satisfies these conditions. We show in this section that the space $\boldsymbol{V}_h$ constructed from $\hat{\boldsymbol{V}}_0$ does have these optimal approximation properties. Throughout, we assume, as usual, that the mesh family $\{\mathcal{T}_h\}_{h>0}$ satisfies (SR-ND1) and (SR-ND2).

Theorem 8.1. *Let $\hat{\boldsymbol{V}} = \hat{\boldsymbol{V}}_0$. Given a hexahedral mesh $\mathcal{T}_h$ of a domain Ω, there exists a constant C depending only on the bound for $\hat{\boldsymbol{\pi}}^{\hat{\boldsymbol{V}}}$ (defined above) and on the shape-regularity/non-degeneracy constants of the mesh $\mathcal{T}_h$, such that*

$$\|\boldsymbol{v} - \boldsymbol{\pi}_h^{\boldsymbol{V}} \boldsymbol{v}\|_{\boldsymbol{L}^2(\Omega)} \le Ch \|\boldsymbol{v}\|_{\boldsymbol{H}^1(\Omega)}, \quad \forall \boldsymbol{v} \in \boldsymbol{H}^1(\Omega), \tag{8.1}$$

$$\|\operatorname{div} \boldsymbol{v} - \operatorname{div} \boldsymbol{\pi}_h^{\boldsymbol{V}} \boldsymbol{v}\|_{L^2(\Omega)} \le Ch \|\operatorname{div} \boldsymbol{v}\|_{H^1(\Omega)}, \quad \forall \boldsymbol{v} \in \boldsymbol{H}^1(\Omega) \text{ with } \operatorname{div} \boldsymbol{v} \in H^1(\Omega). \tag{8.2}$$

We have also shown in the previous sections that necessary conditions for the space $\boldsymbol{U}_h$ to have optimal $O(h)$ approximation in both $\boldsymbol{L}^2$ and $\boldsymbol{H}(\mathbf{curl}\,; \Omega)$ are that the space $\hat{\boldsymbol{U}}$ on the reference element from which $\boldsymbol{U}_h$ is constructed satisfies

$$\hat{\boldsymbol{U}} \supseteq \hat{\nabla} \mathcal{P}_{1,1,1} \text{ and } \hat{\mathbf{curl}}\, \hat{\boldsymbol{U}} \supseteq \boldsymbol{S}_0^-.$$

We have further established that the choice $\hat{\boldsymbol{U}} = \hat{\boldsymbol{U}}_0$ satisfies these conditions. We also show in this section that the space $\boldsymbol{U}_h$ constructed from $\hat{\boldsymbol{U}}_0$ does have these optimal approximation properties.

Theorem 8.2. *Let $\hat{\boldsymbol{U}} = \hat{\boldsymbol{U}}_0$. Given a hexahedral mesh $\mathcal{T}_h$ of a domain Ω, there exists a constant C depending only on the bound for $\hat{\boldsymbol{\pi}}^{\hat{\boldsymbol{U}}}$ (defined above) and on the shape-regularity/non-degeneracy constants of the mesh $\mathcal{T}_h$, such that for all $\boldsymbol{v} \in \boldsymbol{H}^1(\Omega)$ with $\mathbf{curl}\, \boldsymbol{v} \in \boldsymbol{H}^1(\Omega)$,*

$$\|\boldsymbol{v} - \boldsymbol{\pi}_h^{\boldsymbol{U}} \boldsymbol{v}\|_{\boldsymbol{L}^2(\Omega)} \le Ch \left(\|\boldsymbol{v}\|_{\boldsymbol{H}^1(\Omega)} + h \|\mathbf{curl}\ \boldsymbol{v}\|_{\boldsymbol{H}^1(\Omega)} \right), \tag{8.3}$$

$$\|\mathbf{curl}\ \boldsymbol{v} - \mathbf{curl}\ \boldsymbol{\pi}_h^{\boldsymbol{U}} \boldsymbol{v}\|_{\boldsymbol{L}^2(\Omega)} \le Ch \|\mathbf{curl}\ \boldsymbol{v}\|_{\boldsymbol{H}^1(\Omega)}. \tag{8.4}$$

The proof of these estimates makes use of two applications of the Bramble-Hilbert lemma. The first gives a result that provides the correct scaling for all, but the lowest order term. The second uses the fact that the interpolation operators reproduce constants on the physical element to improve the estimate in the lowest order term. We begin by stating some preliminary estimates. Since

$$\hat{D}\boldsymbol{F}(\hat{\boldsymbol{x}}) = \begin{pmatrix} F_1(1,\hat{y},\hat{z}) - F_1(0,\hat{y},\hat{z}) & F_1(\hat{x},1,\hat{z}) - F_1(\hat{x},0,\hat{z}) & F_1(\hat{x},\hat{y},1) - F_1(\hat{x},\hat{y},0) \\ F_2(1,\hat{y},\hat{z}) - F_2(0,\hat{y},\hat{z}) & F_2(\hat{x},1,\hat{z}) - F_2(\hat{x},0,\hat{z}) & F_2(\hat{x},\hat{y},1) - F_2(\hat{x},\hat{y},0) \\ F_3(1,\hat{y},\hat{z}) - F_3(0,\hat{y},\hat{z}) & F_3(\hat{x},1,\hat{z}) - F_3(\hat{x},0,\hat{z}) & F_3(\hat{x},\hat{y},1) - F_3(\hat{x},\hat{y},0) \end{pmatrix},$$

we have for some constant C independent of K,

$$\|\hat{D}\boldsymbol{F}\|_{L^\infty(\hat{K})} \le Ch_K, \qquad \|\hat{J}\boldsymbol{F}\|_{L^\infty(\hat{K})} \le Ch_K^3, \qquad \|\hat{\nabla}(J\boldsymbol{F})\|_{L^\infty(\hat{K})} \le Ch_K^3.$$

Using the cofactor formula for $[\hat{D}\boldsymbol{F}(\hat{\boldsymbol{x}})]^{-1}$, we get for some constant C independent of K,

$$\|J\boldsymbol{F}[\hat{D}\boldsymbol{F}]^{-1}\|_{L^\infty(\hat{K})} \le Ch_K^2, \qquad \|(\partial/\partial \hat{x}_j)(\hat{J}\boldsymbol{F}[\hat{D}\boldsymbol{F}]^{-1})_{ik}\|_{L^\infty(\hat{K})} \le Ch_K^2.$$

Proof. (of Theorem 8.1). Since $\boldsymbol{u} - \boldsymbol{\pi}_K^{\boldsymbol{V}} \boldsymbol{u} = \boldsymbol{P}_F[\hat{\boldsymbol{u}} - \hat{\boldsymbol{\pi}}^{\hat{\boldsymbol{V}}} \hat{\boldsymbol{u}}]$, we get using the usual change of variables, the above estimates, and the assumption that the mesh is shape-regular and non-degenerate that

$$\|\boldsymbol{u} - \boldsymbol{\pi}_K^{\boldsymbol{V}} \boldsymbol{u}\|_{\boldsymbol{L}^2(K)} \le Ch_K^{-1/2} \|\hat{D}\hat{\boldsymbol{u}}\|_{\boldsymbol{L}^2(\hat{K})}.$$

Then, since $\hat{\boldsymbol{u}}(\hat{\boldsymbol{x}}) = \boldsymbol{P}_F^{-1} \boldsymbol{u}(\boldsymbol{x}) = \hat{J}\boldsymbol{F}(\hat{\boldsymbol{x}})[\hat{D}\boldsymbol{F}(\hat{\boldsymbol{x}})]^{-1} \boldsymbol{u}(\boldsymbol{x})$, one finds
(8.5)

$$\hat{D}\hat{\boldsymbol{u}} = \hat{J}\boldsymbol{F}(\hat{\boldsymbol{x}})[\hat{D}\boldsymbol{F}(\hat{\boldsymbol{x}})]^{-1} D\boldsymbol{u}(\boldsymbol{x}) \hat{D}\boldsymbol{F} + \boldsymbol{G}, \text{ where } \boldsymbol{G}_{ij} = \sum_{k=1}^{3} \boldsymbol{u}_k \frac{\partial}{\partial \hat{x}_j} (\hat{J}\boldsymbol{F}(\hat{\boldsymbol{x}})[\hat{D}\boldsymbol{F}(\hat{\boldsymbol{x}})]^{-1})_{ik}.$$

Again changing variables and estimating as above, we find

$$\|\hat{D}\hat{\boldsymbol{u}}\|_{\boldsymbol{L}^2(\hat{K})} \le C[h_K^{3/2}\|D\boldsymbol{u}\|_{\boldsymbol{L}^2(K)} + h_K^{1/2}\|\boldsymbol{u}\|_{\boldsymbol{L}^2(K)}].$$

In both these estimates, the constant C will depend on the shape-regularity/non-degeneracy constants γ and σ defined in (SR-ND1) and (SR-ND2) through the bound on $\|(J\boldsymbol{F})^{-1}\|_{L^\infty(\hat{K})}$ and the constant in the Bramble-Hilbert lemma. Combining these results, we obtain

$$\|\boldsymbol{u} - \boldsymbol{\pi}_K^{\boldsymbol{V}}\boldsymbol{u}\|_{\boldsymbol{L}^2(K)} \le C[h_K\|D\boldsymbol{u}\|_{\boldsymbol{L}^2(K)} + \|\boldsymbol{u}\|_{\boldsymbol{L}^2(K)}]. \tag{8.6}$$

Although this is not the estimate we want, since the lower order term does not scale in the same way as the first derivative terms, we can improve this result by using the fact that for $\boldsymbol{u} \in \boldsymbol{P}_0(K)$, $\hat{\boldsymbol{u}} = \boldsymbol{P}_F^{-1}\boldsymbol{u} \in \boldsymbol{S}_0^- \subseteq \hat{\boldsymbol{V}}$. Then, since $\hat{\boldsymbol{\pi}}^{\hat{\boldsymbol{V}}}$ is exact for $\hat{\boldsymbol{u}} \in \hat{\boldsymbol{V}}$, $\boldsymbol{u} - \boldsymbol{\pi}_K^{\boldsymbol{V}}\boldsymbol{u} = \boldsymbol{P}_F[\hat{\boldsymbol{u}} - \hat{\boldsymbol{\pi}}^{\hat{\boldsymbol{V}}}\hat{\boldsymbol{u}}] = 0$. Hence, we have for all $\boldsymbol{c} \in \boldsymbol{P}_0(K)$, that

$$\|\boldsymbol{u} - \boldsymbol{\pi}_K^{\boldsymbol{V}}\boldsymbol{u}\|_{\boldsymbol{L}^2(K)} \le C[h_K\|D\boldsymbol{u}\|_{\boldsymbol{L}^2(K)} + \|\boldsymbol{u} - \boldsymbol{c}\|_{\boldsymbol{L}^2(K)}].$$

We can now again apply the Bramble-Hilbert lemma (see Lemma 4.3.8 of [6]) to conclude that $\|\boldsymbol{u} - \boldsymbol{c}\|_{\boldsymbol{L}^2(K)} \le Ch_K\|D\boldsymbol{u}\|_{\boldsymbol{L}^2(K)}$, where C will again depend only on the constant γ. This establishes (8.1).

We next consider the proof of (8.2). Letting $p = \operatorname{div}\boldsymbol{u}$, we wish to show that

$$\|\operatorname{div}\boldsymbol{u} - \operatorname{div}\boldsymbol{\pi}_h^{\boldsymbol{V}}\boldsymbol{u}\|_{L^2(\Omega)} = \|(I - \pi_h^W)p\|_{L^2(\Omega)} \le Ch\|p\|_{H^1(\Omega)}.$$

Again applying the standard scaling argument using the Bramble-Hilbert lemma, we obtain the estimates

$$\|p - \pi_K^W p\|_{L^2(K)} \le Ch_K^{-3/2}\|\hat{\nabla}\hat{p}\|_{L^2(\hat{K})}, \qquad \|\hat{\nabla}\hat{p}\|_{L^2(\hat{K})} \le C[h_K^{5/2}\|\nabla p\|_{L^2(K)} + h_K^{3/2}\|p\|_{L^2(K)}],$$

where we have used the facts that since $\hat{\operatorname{div}}\,\hat{\boldsymbol{u}} = \hat{J}\boldsymbol{F}(\hat{\boldsymbol{x}})\operatorname{div}\boldsymbol{u}$, $\hat{p} = J\boldsymbol{F}(\hat{\boldsymbol{x}})p$, and

$$\hat{\nabla}\hat{p} = J\boldsymbol{F}(\hat{\boldsymbol{x}})(D\boldsymbol{F}(\hat{\boldsymbol{x}}))^T\nabla p + p\hat{\nabla}J\boldsymbol{F}.$$

Combining these results, we get

$$\|p - \pi_K^W p\|_{L^2(K)} \le C(h_K\|\nabla p\|_{L^2(K)} + \|p\|_{L^2(K)}). \tag{8.7}$$

Again, this procedure does not give the desired estimate, since the lower order term does not have the necessary scaling. However, since $\pi_K^W p$ is exact for constants, we proceed as above, obtaining (8.2). □

Proof. (of Theorem 8.2) Since $\hat{\boldsymbol{u}}(\hat{\boldsymbol{x}}) = \boldsymbol{R}_F^{-1}\boldsymbol{u} = (D\boldsymbol{F})^T(\hat{\boldsymbol{x}})\boldsymbol{u}(\boldsymbol{x})$, one finds

$$\hat{D}\hat{\boldsymbol{u}} = (D\boldsymbol{F})^T D\boldsymbol{u}(D\boldsymbol{F}) + \boldsymbol{H}, \qquad \text{where} \qquad \boldsymbol{H}_{ij} = \sum_{k=1}^3 \boldsymbol{u}_k \frac{\partial^2 \boldsymbol{F}_k}{\partial\hat{\boldsymbol{x}}_i\partial\hat{\boldsymbol{x}}_j}.$$

Since $\hat{\mathbf{curl}}\,\hat{\boldsymbol{u}}(\hat{\boldsymbol{x}}) = J\boldsymbol{F}(\hat{\boldsymbol{x}})(D\boldsymbol{F}^{-1})(\hat{\boldsymbol{x}})\mathbf{curl}\,\boldsymbol{u}(\boldsymbol{x})$, we can use formula (8.5) of the previous section with $\boldsymbol{u}$ replaced by $\mathbf{curl}\,\boldsymbol{u}$ to get

$$\hat{D}[\hat{\mathbf{curl}}\,\hat{\boldsymbol{u}}] = \hat{J}\boldsymbol{F}(\hat{\boldsymbol{x}})[\hat{D}\boldsymbol{F}(\hat{\boldsymbol{x}})]^{-1}D[\mathbf{curl}\,\boldsymbol{u}(\boldsymbol{x})]\hat{D}\boldsymbol{F} + \boldsymbol{M},$$

where

$$\boldsymbol{M}_{ij} = \sum_{k=1}^3 (\mathbf{curl}\,\boldsymbol{u})_k \frac{\partial}{\partial\hat{x}_j}(\hat{J}\boldsymbol{F}(\hat{\boldsymbol{x}})[\hat{D}\boldsymbol{F}(\hat{\boldsymbol{x}})]^{-1})_{ik}.$$

Then the standard change of variable and scaling argument gives

$$\|\boldsymbol{u} - \boldsymbol{\pi}_K^{\boldsymbol{U}}\boldsymbol{u}\|_{\boldsymbol{L}^2(K)} \le C h_K^{1/2}[\|\hat{D}\hat{\boldsymbol{u}}\|_{\boldsymbol{L}^2(K)} + \|\hat{D}\hat{\mathbf{curl}}\,\hat{\boldsymbol{u}}\|_{\boldsymbol{L}^2(K)}],$$
$$\|\hat{D}\hat{\boldsymbol{u}}\|_{\boldsymbol{L}^2(\hat{K})} \le C[h_K^{1/2}\|D\boldsymbol{u}\|_{\boldsymbol{L}^2(K)} + h_K^{-1/2}\|\boldsymbol{u}\|_{\boldsymbol{L}^2(K)}],$$
$$\|\hat{D}[\hat{\mathbf{curl}}\,\hat{\boldsymbol{u}}]\|_{\boldsymbol{L}^2(\hat{K})} \le C[h_K^{3/2}\|D[\mathbf{curl}\,\boldsymbol{u}]\|_{\boldsymbol{L}^2(K)} + h_K^{1/2}\|\mathbf{curl}\,\boldsymbol{u}\|_{\boldsymbol{L}^2(K)}].$$

Combining all these results, we obtain

$$\|\boldsymbol{u} - \boldsymbol{\pi}_K^{\boldsymbol{U}}\boldsymbol{u}\|_{\boldsymbol{L}^2(K)} \le C[\|\boldsymbol{u}\|_{\boldsymbol{L}^2(K)} + h_K\|D\boldsymbol{u}\|_{\boldsymbol{L}^2(K)} + h_K^2\|D[\mathbf{curl}\,\boldsymbol{u}]\|_{\boldsymbol{L}^2(K)}]. \tag{8.8}$$

As above, we have that $\boldsymbol{\pi}_K^{\boldsymbol{U}}\boldsymbol{u}$ is exact for constants, and so an additional application of the Bramble-Hilbert lemma to the first term gives (8.3). Finally, since $\mathbf{curl}\,\boldsymbol{\pi}_K^{\boldsymbol{U}}\boldsymbol{u} = \boldsymbol{\pi}_K^{\boldsymbol{V}}\mathbf{curl}\,\boldsymbol{u}$, (8.4) follows immediately from (8.1). □

9. Application to mixed finite element methods

We consider in this section the application of the results on $\boldsymbol{H}(\mathrm{div};\Omega)$ and $\boldsymbol{H}(\mathbf{curl}\,;\Omega)$ finite elements to the approximation of a boundary value problem for the vector Poisson's equation in three-dimensions. More specifically, we consider the problem

$$\mathbf{curl}\,\mathbf{curl}\,\boldsymbol{u} - \mathbf{grad}\,\mathrm{div}\,\boldsymbol{u} = \boldsymbol{f}, \quad \text{in } \Omega, \qquad \boldsymbol{u}\times\boldsymbol{n} = 0, \quad \mathrm{div}\,\boldsymbol{u} = 0, \quad \text{on } \partial\Omega,$$

where Ω is a convex polyhedral domain in $\mathbb{R}^3$. Introducing the additional variable $\boldsymbol{\sigma} = \mathbf{curl}\,\boldsymbol{u}$, the mixed formulation is:

Problem (P): Find $\boldsymbol{\sigma} \in \boldsymbol{H}(\mathbf{curl}\,;\Omega)$, $\boldsymbol{u} \in \boldsymbol{H}(\mathrm{div};\Omega)$ such that

$$(\boldsymbol{\sigma},\boldsymbol{\tau}) - (\boldsymbol{u},\mathbf{curl}\,\boldsymbol{\tau}) = 0, \quad \forall\boldsymbol{\tau} \in \boldsymbol{H}(\mathbf{curl}\,;\Omega),$$
$$(\mathbf{curl}\,\boldsymbol{\sigma},\boldsymbol{v}) + (\mathrm{div}\,\boldsymbol{u},\mathrm{div}\,\boldsymbol{v}) = (\boldsymbol{f},\boldsymbol{v}), \quad \forall\boldsymbol{v} \in \boldsymbol{H}(\mathrm{div};\Omega),$$

where $(\cdot,\cdot)$ denotes the $L^2(\Omega)$ inner product. For $\boldsymbol{U}_h \subset \boldsymbol{H}(\mathbf{curl}\,;\Omega)$ and $\boldsymbol{V}_h \subset \boldsymbol{H}(\mathrm{div};\Omega)$, the mixed finite element approximation is:

Problem P_h: Find $\boldsymbol{\sigma}_h \in \boldsymbol{U}_h$ and $\boldsymbol{u}_h \in \boldsymbol{V}_h$ such that

$$(\boldsymbol{\sigma}_h,\boldsymbol{\tau}) - (\boldsymbol{u}_h,\mathbf{curl}\,\boldsymbol{\tau}) = 0, \quad \forall\boldsymbol{\tau} \in \boldsymbol{U}_h$$
$$(\mathbf{curl}\,\boldsymbol{\sigma}_h,\boldsymbol{v}) + (\mathrm{div}\,\boldsymbol{u}_h,\mathrm{div}\,\boldsymbol{v}) = (\boldsymbol{f},\boldsymbol{v}), \quad \forall\boldsymbol{v} \in \boldsymbol{V}_h.$$

To establish stability and quasi-optimal error estimates of this saddle point system, we let $B : [\boldsymbol{H}(\mathbf{curl}\,,\Omega) \times \boldsymbol{H}(\mathrm{div},\Omega)] \times [\boldsymbol{H}(\mathbf{curl}\,,\Omega) \times \boldsymbol{H}(\mathrm{div},\Omega)] \to \mathbb{R}$ denote the bilinear form

$$B(\boldsymbol{\sigma},\boldsymbol{u};\boldsymbol{\tau},\boldsymbol{v}) = (\boldsymbol{\sigma},\boldsymbol{\tau}) - (\boldsymbol{u},\mathbf{curl}\,\boldsymbol{\tau}) + (\boldsymbol{v},\mathbf{curl}\,\boldsymbol{\sigma}) + (\mathrm{div}\,\boldsymbol{u},\mathrm{div}\,\boldsymbol{v}).$$

Following [4], stability and quasi-optimal error estimates are ensured by the existence of positive constants γ and C, independent of h, such that for any $(\boldsymbol{\sigma},\boldsymbol{u}) \in \boldsymbol{U}_h \times \boldsymbol{V}_h$, there exists $(\boldsymbol{\tau},\boldsymbol{v}) \in \boldsymbol{U}_h \times \boldsymbol{V}_h$ satisfying the following conditions.

$$B(\boldsymbol{\sigma},\boldsymbol{u};\boldsymbol{\tau},\boldsymbol{v}) \ge \gamma(\|\boldsymbol{\sigma}\|^2_{\boldsymbol{H}(\mathbf{curl}\,,\Omega)} + \|\boldsymbol{u}\|^2_{\boldsymbol{H}(\mathrm{div},\Omega)}), \tag{9.1}$$

$$\|\boldsymbol{\tau}\|_{\boldsymbol{H}(\mathbf{curl}\,,\Omega)} + \|\boldsymbol{v}\|_{\boldsymbol{H}(\mathrm{div},\Omega)} \le C(\|\boldsymbol{\sigma}\|_{\boldsymbol{H}(\mathbf{curl}\,,\Omega)} + \|\boldsymbol{u}\|_{\boldsymbol{H}(\mathrm{div},\Omega)}). \tag{9.2}$$

In order to verify that these conditions are satisfied, the key step is to first establish appropriate discrete Poincaré inequalities.

Lemma 9.1. *Let*

$$\boldsymbol{Z}_h(\boldsymbol{V}_h) = \{\boldsymbol{w}_h \in \boldsymbol{V}_h : (\boldsymbol{w}_h, \mathbf{curl}\,\boldsymbol{\psi}) = 0, \quad \forall \boldsymbol{\psi} \in \boldsymbol{U}_h\}.$$
$$\boldsymbol{Z}_h(\boldsymbol{U}_h) = \{\boldsymbol{\rho}_h \in \boldsymbol{U}_h : (\boldsymbol{\rho}_h, \mathbf{grad}\, s) = 0, \quad \forall s \in S_h\},$$

Then there exist constants K_1 and K_2 independent of h, such that

$$\|\boldsymbol{w}_h\|_{\boldsymbol{L}^2(\Omega)} \leq K_1 \|\operatorname{div} \boldsymbol{w}_h\|_{L^2(\Omega)}, \quad \boldsymbol{w}_h \in \boldsymbol{Z}_h(\boldsymbol{V}_h),$$
$$\|\boldsymbol{\rho}_h\|_{\boldsymbol{L}^2(\Omega)} \leq K_2 \|\mathbf{curl}\,\boldsymbol{\rho}_h\|_{\boldsymbol{L}^2(\Omega)}, \quad \boldsymbol{\rho}_h \in \boldsymbol{Z}_h(\boldsymbol{U}_h).$$

Proof. Following a standard approach, we first find $\boldsymbol{w} \in \boldsymbol{H}^1(\Omega)$ and $\boldsymbol{\rho} \in \boldsymbol{H}^1(\Omega)$ satisfying $\operatorname{div} \boldsymbol{w} = \operatorname{div} \boldsymbol{w}_h$, $\|\boldsymbol{w}\|_{\boldsymbol{H}^1(\Omega)} \leq C \|\operatorname{div} \boldsymbol{w}_h\|$ and $\mathbf{curl}\,\boldsymbol{\rho} = \mathbf{curl}\,\boldsymbol{\rho}_h$ and $\|\boldsymbol{\rho}\|_{\boldsymbol{H}^1(\Omega)} \leq C \|\mathbf{curl}\,\boldsymbol{\rho}_h\|$. Using the commuting diagram, we then have $\operatorname{div}(\boldsymbol{w}_h - \boldsymbol{\pi}_h^{\boldsymbol{V}} \boldsymbol{w}) = 0$ and $\mathbf{curl}\,(\boldsymbol{\rho}_h - \boldsymbol{\pi}_h^{\boldsymbol{U}} \boldsymbol{\rho}) = 0$ and so $\boldsymbol{w}_h - \boldsymbol{\pi}_h^{\boldsymbol{V}} \boldsymbol{w} = \mathbf{curl}\,\boldsymbol{\psi}$ for some $\boldsymbol{\psi} \in \boldsymbol{U}_h$ and $\boldsymbol{\rho}_h - \boldsymbol{\pi}_h^{\boldsymbol{U}} \boldsymbol{\rho} = \mathbf{grad}\, s$ for some $s \in S_h$. Hence,

$$\|\boldsymbol{w}_h\|^2 = (\boldsymbol{w}_h, \boldsymbol{w}_h - \boldsymbol{\pi}_h^{\boldsymbol{V}} \boldsymbol{w}) + (\boldsymbol{w}_h, \boldsymbol{\pi}_h^{\boldsymbol{V}} \boldsymbol{w}) = (\boldsymbol{w}_h, \boldsymbol{\pi}_h^{\boldsymbol{V}} \boldsymbol{w}) \leq \|\boldsymbol{w}_h\| (\|\boldsymbol{\pi}_h^{\boldsymbol{V}} \boldsymbol{w} - \boldsymbol{w}\| + \|\boldsymbol{w}\|).$$

The result follows directly by applying (8.1). The proof of the second inequality is essentially the same as the first with one additional technicality. Namely, we cannot simply use (8.3) to replace (8.1), since the right hand side also involves the norm $\|\mathbf{curl}\,\boldsymbol{\rho}\|_{\boldsymbol{H}^1(\Omega)}$. However, since $\mathbf{curl}\,\boldsymbol{\rho} = \mathbf{curl}\,\boldsymbol{\rho}_h \in \boldsymbol{V}_h$, we can use inverse assumptions to replace the term $h\|\mathbf{curl}\,\boldsymbol{\rho}_h\|_{\boldsymbol{H}^1(\Omega)}$ by $\|\mathbf{curl}\,\boldsymbol{\rho}_h\|_{\boldsymbol{L}^2(\Omega)}$. Then $\|\boldsymbol{\rho} - \boldsymbol{\pi}_h^{\boldsymbol{U}} \boldsymbol{\rho}\|_{\boldsymbol{L}^2(\Omega)} \leq C \|\boldsymbol{\rho}\|_{\boldsymbol{H}^1(\Omega)}$, and the proof proceeds as above. □

We now establish stability of the approximation scheme.

Theorem 9.2. *For the finite element spaces $\boldsymbol{U}_h$ and $\boldsymbol{V}_h$ defined in the previous sections, the approximation scheme Problem P_h gives a stable approximation to Problem P, i.e., conditions* (9.1) *and* (9.2) *are satisfied.*

Proof. Using the discrete de Rham sequence, we can write $\boldsymbol{u} = \mathbf{curl}\,\boldsymbol{\rho}_h + \boldsymbol{w}_h$ for some $\boldsymbol{\rho}_h \in \boldsymbol{U}_h$ satisfying $(\boldsymbol{\rho}_h, \mathbf{grad}\, s) = 0, \forall s \in S_h$, and some $\boldsymbol{w}_h \in \boldsymbol{V}_h$ satisfying $(\boldsymbol{w}_h, \mathbf{curl}\,\boldsymbol{\psi}) = 0, \forall \boldsymbol{\psi} \in \boldsymbol{U}_h$. Choosing $\boldsymbol{\tau} = \boldsymbol{\sigma} - t\boldsymbol{\rho}_h$, and $\boldsymbol{v} = \boldsymbol{u} + \mathbf{curl}\,\boldsymbol{\sigma}$, with t is to be determined, we obtain

$$\begin{aligned} B(\boldsymbol{\sigma}, \boldsymbol{u}; \boldsymbol{\tau}, \boldsymbol{v}) &= \|\boldsymbol{\sigma}\|^2_{\boldsymbol{H}(\mathbf{curl},\Omega)} - t(\boldsymbol{\sigma}, \boldsymbol{\rho}_h) + \|\operatorname{div} \boldsymbol{u}\|^2_{L^2(\Omega)} + t(\boldsymbol{u}, \mathbf{curl}\,\boldsymbol{\rho}_h). \\ &\geq (1/2)\|\boldsymbol{\sigma}\|^2_{\boldsymbol{H}(\mathbf{curl},\Omega)} - (t^2/2)\|\boldsymbol{\rho}_h\|^2_{\boldsymbol{L}^2(\Omega)} + \|\operatorname{div} \boldsymbol{u}\|^2_{L^2(\Omega)} + t\|\mathbf{curl}\,\boldsymbol{\rho}_h\|^2_{\boldsymbol{L}^2(\Omega)}. \end{aligned}$$

Next note that from the first Poincaré inequality, we get

$$\|\boldsymbol{u}\|^2_{\boldsymbol{L}^2(\Omega)} = \|\mathbf{curl}\,\boldsymbol{\rho}_h\|^2_{\boldsymbol{L}^2(\Omega)} + \|\boldsymbol{w}_h\|^2_{\boldsymbol{L}^2(\Omega)} \leq \|\mathbf{curl}\,\boldsymbol{\rho}_h\|^2_{\boldsymbol{L}^2(\Omega)} + K_1^2 \|\operatorname{div} \boldsymbol{u}\|^2_{L^2(\Omega)},$$

and so

$$\min[1/K_1^2, 1/K_2^2] \|\boldsymbol{u}\|^2_{\boldsymbol{L}^2(\Omega)} \leq (1/K_2^2) \|\mathbf{curl}\,\boldsymbol{\rho}_h\|^2_{\boldsymbol{L}^2(\Omega)} + \|\operatorname{div} \boldsymbol{u}\|^2_{L^2(\Omega)}.$$

Then, choosing $t = 1/K_2^2$ and using the second Poincaré inequality, we get

$$\begin{aligned} B(\boldsymbol{\sigma}, \boldsymbol{u}; \boldsymbol{\tau}, \boldsymbol{v}) &\geq (1/2)\|\boldsymbol{\sigma}\|^2_{\boldsymbol{H}(\mathbf{curl},\Omega)} + \|\operatorname{div} \boldsymbol{u}\|^2_{L^2(\Omega)} + (1/(2K_2^2))\|\mathbf{curl}\,\boldsymbol{\rho}_h\|^2_{\boldsymbol{L}^2(\Omega)}. \\ &\geq (1/2)[\|\boldsymbol{\sigma}\|^2_{\boldsymbol{H}(\mathbf{curl},\Omega)} + \|\operatorname{div} \boldsymbol{u}\|^2_{L^2(\Omega)} + \min[1/K_1^2, 1/K_2^2]\|\boldsymbol{u}\|^2_{\boldsymbol{L}^2(\Omega)}]. \end{aligned}$$

The upper bound (9.2) follows directly from the decomposition of $\boldsymbol{u}$ and the discrete Poincaré inequalities. □

10. $\boldsymbol{H}(\mathrm{div};\Omega)$ ELEMENTS ON RESTRICTED CLASSES OF HEXAHEDRONS

Since the spaces we have constructed for general hexahedrons are quite complicated, we now consider the question of whether there are simpler spaces that give optimal order approximation for special classes of hexahedrons.

10.1. The case $\boldsymbol{h} = 0$. We first consider the case when the map $\boldsymbol{F}$ has no cubic terms. This means that the image of the point $(1,1,1)$ on the reference cube is no longer independent of the choices of the images of the remaining seven vertices.

In this case, we find that the coefficients $E_1, E_2, E_3, H_1, H_2, H_3$ all vanish, so that the 21 dimensional subspace $\hat{\boldsymbol{S}}_0$ of $\boldsymbol{RT}_1$ reduces to a 15 dimensional space. However, in order to form a finite element space of $\boldsymbol{H}(\mathrm{div};\Omega)$, we must retain continuity of $\boldsymbol{u}\cdot\boldsymbol{n}$ across faces, and thus need three degrees of freedom per face (since $\boldsymbol{u}\cdot\boldsymbol{n}$ is a linear on each face). Thus, we consider the 18 dimensional space, in which only the H_i are taken to be zero. Then we can use the same face degrees of freedom as for the 21 dimensional space, i.e., $\int_F (\boldsymbol{u}\cdot\boldsymbol{n}) p\, ds$, $p \in \mathcal{P}_1(F)$.

In addition, in the expression for $J\boldsymbol{F}(\hat{\boldsymbol{x}})$, all the cubic and quartic terms (with the exception of the xyz term) vanish, i.e.,

$$
\begin{aligned}
&\det(\boldsymbol{b}|\boldsymbol{e}|\boldsymbol{h})x^2y = 0, \qquad &&\det(\boldsymbol{b}|\boldsymbol{g}|\boldsymbol{h})x^2z = 0, \qquad &&\det(\boldsymbol{c}|\boldsymbol{e}|\boldsymbol{h})y^2x = 0,\\
&\det(\boldsymbol{c}|\boldsymbol{f}|\boldsymbol{h})y^2z = 0, &&\det(\boldsymbol{d}|\boldsymbol{g}|\boldsymbol{h})z^2x = 0, &&\det(\boldsymbol{d}|\boldsymbol{f}|\boldsymbol{h})z^2y = 0,\\
&\det(\boldsymbol{e}|\boldsymbol{g}|\boldsymbol{h})x^2yz = 0, &&\det(\boldsymbol{e}|\boldsymbol{f}|\boldsymbol{h})xy^2z = 0, &&\det(\boldsymbol{f}|\boldsymbol{g}|\boldsymbol{h})xyz^2 = 0.
\end{aligned}
$$

Thus, we can reduce the 40 dimensional space found earlier to a 28 dimensional space of the form:

$$
\begin{aligned}
\hat{\boldsymbol{u}}_1 &= A_1 + B_1\hat{x} + C_1\hat{y} + D_1\hat{z} + E_1\hat{x}\hat{y} + F_1\hat{x}\hat{z}\\
&\qquad + x(1-x)(G_1 + H_1x + I_1y + J_1z + Kyz)\\
\hat{\boldsymbol{u}}_2 &= A_2 + B_2\hat{x} + C_2\hat{y} + D_2\hat{z} + E_2\hat{y}\hat{x} + F_2\hat{y}\hat{z}\\
&\qquad + y(1-y)(G_2 + I_1x + I_2y + J_2z + Kxz)\\
\hat{\boldsymbol{u}}_3 &= A_3 + B_3\hat{x} + C_3\hat{y} + D_3\hat{z} + E_3\hat{z}\hat{x} + F_3\hat{z}\hat{y}\\
&\qquad + z(1-z)(G_3 + J_1x + J_2y + J_3z + Kxy).
\end{aligned}
$$

If we denote by $\hat{Q}_1$, the span of the monomials

$$\hat{x}, \hat{y}, \hat{z}, \hat{x}\hat{y}, \hat{x}\hat{z}, \hat{y}\hat{z}, \hat{x}^2, \hat{y}^2, \hat{z}^2, \hat{x}\hat{y}\hat{z},$$

then we may choose as degrees of freedom for this space

$$\int_{\hat{F}} (\hat{\boldsymbol{q}}\cdot\hat{\boldsymbol{n}})\hat{p}\, ds, \quad \hat{p} \in \mathcal{P}_1(F), \qquad \int_{\hat{K}} \hat{\boldsymbol{q}}\cdot\hat{\boldsymbol{r}}\, dx, \quad \hat{\boldsymbol{r}} \in \boldsymbol{\mathcal{P}}_0, \qquad \int_{\hat{K}} \hat{\mathrm{div}}\, \hat{\boldsymbol{q}}\, \hat{p}\, dx, \quad \hat{p} \in \hat{Q}_1 \setminus \mathcal{P}_1.$$

10.2. **Truncated pyramids with flat faces.** To simplify the presentation (and without loss of generality), we consider in this section the class of mappings for which the top and bottom faces are parallel to the $x-y$ plane. Thus, $\boldsymbol{F}_3 = a_3 + d_3 z$, i.e., $b_3 = c_3 = e_3 = f_3 = g_3 = h_3 = 0$ (and $d_3 \neq 0$). We then add conditions that constrain the remaining faces to be flat.

Since the plane $\hat{x} = x_0$ maps to:

$$x = a_1 + b_1 x_0 + (c_1 + x_0 e_1)\hat{y} + (d_1 + x_0 g_1)\hat{z} + (f_1 + x_0 h_1)\hat{y}\hat{z},$$
$$y = a_2 + b_2 x_0 + (c_2 + x_0 e_2)\hat{y} + (d_2 + x_0 g_2)\hat{z} + (f_2 + x_0 h_2)\hat{y}\hat{z},$$
$$z = a_3 + b_3 x_0 + (c_3 + x_0 e_3)\hat{y} + (d_3 + x_0 g_3)\hat{z} + (f_3 + x_0 h_3)\hat{y}\hat{z},$$

these points will lie in a plane if there exists constants α, β, and γ, not all zero, such that $\alpha x + \beta y + \gamma z = \delta$, where δ is a constant. For this to occur, we require:

$$(c_1 + x_0 e_1)\alpha + (c_2 + x_0 e_2)\beta + (c_3 + x_0 e_3)\gamma = 0,$$
$$(d_1 + x_0 g_1)\alpha + (d_2 + x_0 g_2)\beta + (d_3 + x_0 g_3)\gamma = 0,$$
$$(f_1 + x_0 h_1)\alpha + (f_2 + x_0 h_2)\beta + (f_3 + x_0 h_3)\gamma = 0.$$

The above system will have a non-trivial solution if $\det(\boldsymbol{c} + x_0\boldsymbol{e}, \boldsymbol{d} + x_0\boldsymbol{g}, \boldsymbol{f} + x_0\boldsymbol{h}) = 0$. Applying similar arguments, we find that $\hat{y} = y_0$ will map to a plane if $\det(\boldsymbol{b} + y_0\boldsymbol{e}, \boldsymbol{d} + y_0\boldsymbol{f}, \boldsymbol{g} + y_0\boldsymbol{h}) = 0$.

We assume that $J\boldsymbol{F}(\hat{\boldsymbol{x}}) \neq 0$ for all $0 \leq \hat{x}, \hat{y}, \hat{z} \leq 1$. In particular, applying this condition at the points $(x_0, 0, 0)$, $(0, y_0, 0)$, and $(0, 0, z_0)$ we get using (3.2) that for $0 \leq x_0, y_0, z_0 \leq 1$,

$$\det(\boldsymbol{b}, \boldsymbol{c} + x_0\boldsymbol{e}, \boldsymbol{d} + x_0\boldsymbol{g}) \neq 0, \quad \det(\boldsymbol{b} + y_0\boldsymbol{e}, \boldsymbol{c}, \boldsymbol{d} + y_0\boldsymbol{f}) \neq 0, \quad \det(\boldsymbol{b} + z_0\boldsymbol{g}, \boldsymbol{c} + z_0\boldsymbol{f}, \boldsymbol{d}) \neq 0.$$

Thus, we conclude that for $x_0 = 0$ and 1, the vectors $\boldsymbol{c} + x_0\boldsymbol{e}$, $\boldsymbol{d} + x_0\boldsymbol{g}$, and $\boldsymbol{f} + x_0\boldsymbol{h}$ are linearly dependent, while the vectors $\boldsymbol{c}+x_0\boldsymbol{e}$, $\boldsymbol{d}+x_0\boldsymbol{g}$, and $\boldsymbol{b}$ are linearly independent. Hence, $\boldsymbol{f} + x_0\boldsymbol{h}$ can be written as a linear combination of $\boldsymbol{c} + x_0\boldsymbol{e}$ and $\boldsymbol{d} + x_0\boldsymbol{g}$. However, since $c_3 = e_3 = f_3 = g_3 = h_3 = 0$, we must have for some constants α_0 and α_2 that

$$\boldsymbol{f} = \alpha_0\boldsymbol{c}, \qquad \boldsymbol{f} + \boldsymbol{h} = \alpha_2(\boldsymbol{c} + \boldsymbol{e}).$$

Analogously, we get for constants γ_0 and γ_2 that

$$\boldsymbol{g} = \gamma_0\boldsymbol{b}, \qquad \boldsymbol{g} + \boldsymbol{h} = \gamma_2(\boldsymbol{b} + \boldsymbol{e}).$$

Hence,

$$\boldsymbol{h} = (\alpha_2 - \alpha_0)\boldsymbol{c} + \alpha_2\boldsymbol{e} = (\gamma_2 - \gamma_0)\boldsymbol{b} + \gamma_2\boldsymbol{e}. \tag{10.1}$$

If we insert (10.1) and the formulas

$$\boldsymbol{f} = \alpha_0\boldsymbol{c}, \qquad \boldsymbol{g} = \gamma_0\boldsymbol{b}, \tag{10.2}$$

in the original definition of the constants A_i^j, B_i^j, etc., and simplify, we obtain for $j = 1, 2, 3$,

$$B_2^j = 0, \quad C_1^j = 0, \quad E_1^j = -\gamma_2 B_3^j, \quad E_2^j = \alpha_2 C_3^j, \quad G_1^j = -\gamma_0 B_3^j, \quad G_2^j = -\alpha_0 C_3^j,$$
$$H_3^j = (\alpha_2 - \alpha_0)C_3^j = -(\gamma_2 - \gamma_0)B_3^j.$$

Hence, we have the general relationship

$$H_3 = E_1 - G_1 = E_2 + G_2.$$

Thus, the original 21 dimensional space for $\hat{\boldsymbol{u}}$ may be reduced to the 17 dimensional space consisting of vectors of the form

$$\begin{aligned}
\hat{\boldsymbol{u}}_1 &= A_1 + B_1\hat{x} + D_1\hat{z} - H_3\hat{x}\hat{y}(1-x) + (E_3 - G_3)\hat{x}\hat{z} + G_1\hat{x}^2 - H_2\hat{x}^2\hat{z},\\
\hat{\boldsymbol{u}}_2 &= A_2 + C_2\hat{y} + D_2\hat{z} + H_3\hat{y}\hat{x}(1-y) - (E_3 + G_3)\hat{y}\hat{z} + G_2\hat{y}^2 + H_1\hat{y}^2\hat{z},\\
\hat{\boldsymbol{u}}_3 &= A_3 + B_3\hat{x} + C_3\hat{y} + D_3\hat{z} - (2G_1 + H_3)\hat{z}\hat{x} + (H_3 - 2G_2)\hat{z}\hat{y} + G_3\hat{z}^2 + H_2\hat{x}\hat{z}^2 - H_1\hat{y}\hat{z}^2,
\end{aligned}$$

which we can further rewrite in the form

$$\begin{aligned}
\hat{\boldsymbol{u}}_1 &= A_1 + (B_1 + G_1)\hat{x} + D_1\hat{z} + I_1\hat{x}\hat{z} + \hat{x}(1-\hat{x})(-G_1 - H_3\hat{y} + H_2\hat{z}),\\
\hat{\boldsymbol{u}}_2 &= A_2 + (C_2 + G_2)\hat{y} + D_2\hat{z} + I_2\hat{y}\hat{z} + \hat{y}(1-\hat{y})(-G_2 + H_3x - H_1z),\\
\hat{\boldsymbol{u}}_3 &= A_3 + B_3\hat{x} + C_3\hat{y} + (D_3 + G_3)\hat{z} + J_1\hat{z}\hat{x} + J_2\hat{z}\hat{y}\\
&\qquad + \hat{z}(1-\hat{z})(-G_3 - H_2\hat{x} + H_1\hat{y}),
\end{aligned}$$

where

$$I_1 = E_3 - G_3 - H_2, \qquad I_2 = H_1 - E_3 - G_3, \qquad J_1 = H_2 - 2G_1 - H_3, \qquad J_2 = H_3 - 2G_2 - H_1.$$

We shall think of these equations as determining E_3, G_3, G_1, G_2 in terms of I_1, I_2, J_1, J_2, H_1, H_2 and H_3.

Since $\hat{\boldsymbol{u}} \cdot \hat{\boldsymbol{n}}$ is of the form $a + bz$ on the faces $\hat{x} = 0, 1$ and $\hat{y} = 0, 1$, we can take as degrees of freedom,

$$\int_F (\hat{\boldsymbol{u}} \cdot \hat{\boldsymbol{n}})p\,ds,$$

where $p = a + bz$ on the four faces $\hat{x} = 0, 1$ and $\hat{y} = 0, 1$ and $p \in \mathcal{P}_1(F)$ on the faces $\hat{z} = 0, 1$. Setting these degrees of freedom equal to zero, $\hat{\boldsymbol{u}}$ will again have the form of (3.7). Hence, the final three degrees of freedom can again be taken as in (3.6).

From (10.1) and (10.2), we also find that some of the terms in the expression for $J\boldsymbol{F}(\hat{\boldsymbol{x}})$ vanish, i.e.,

$$\begin{gathered}
\det(\boldsymbol{b}, \boldsymbol{e}, \boldsymbol{g})x^2 = 0, \qquad \det(\boldsymbol{c}|\boldsymbol{e}|\boldsymbol{f})y^2 = 0, \qquad \det(\boldsymbol{b}|\boldsymbol{e}|\boldsymbol{h})x^2y = 0,\\
\det(\boldsymbol{b}|\boldsymbol{g}|\boldsymbol{h})x^2z = 0, \qquad \det(\boldsymbol{c}|\boldsymbol{e}|\boldsymbol{h})y^2x = 0, \qquad \det(\boldsymbol{c}|\boldsymbol{f}|\boldsymbol{h})y^2z = 0,\\
\det(\boldsymbol{e}|\boldsymbol{g}|\boldsymbol{h})x^2yz = 0, \qquad \det(\boldsymbol{e}|\boldsymbol{f}|\boldsymbol{h})xy^2z = 0.
\end{gathered}$$

Manipulating the equations for $\boldsymbol{h}$, it easily follows that

$$(\gamma_2 - \alpha_2)\boldsymbol{e} = (\gamma_0 - \gamma_2)\boldsymbol{b} + (\alpha_2 - \alpha_0)\boldsymbol{c}, \qquad (\gamma_2 - \alpha_2)\boldsymbol{h} = \alpha_2(\gamma_0 - \gamma_2)\boldsymbol{b} + \gamma_2(\alpha_2 - \alpha_0)\boldsymbol{c}.$$

If $\gamma_2 \neq \alpha_2$, we see that both $\boldsymbol{e}$ and $\boldsymbol{h}$ may be written as linear combinations of $\boldsymbol{b}$ and $\boldsymbol{c}$. Hence,

$$\begin{gathered}
\det(\boldsymbol{e}|\boldsymbol{f}|\boldsymbol{g})xyz = 0, \qquad \det(\boldsymbol{f}|\boldsymbol{g}|\boldsymbol{h})xyz^2 = 0,\\
[-\det(\boldsymbol{c}|\boldsymbol{e}|\boldsymbol{g}) + \det(\boldsymbol{b}|\boldsymbol{c}|\boldsymbol{h}) + \det(\boldsymbol{b}|\boldsymbol{e}|\boldsymbol{f})]xy = 0.
\end{gathered}$$

If $\gamma_2 = \alpha_2 = 0$, then $\boldsymbol{f} = \boldsymbol{g} = -\boldsymbol{h}$ and again the above three terms vanish.

However, since $\boldsymbol{b}$ and $\boldsymbol{c}$ are linearly independent, if $\gamma_2 = \alpha_2 \neq 0$, then $\gamma_0 = \gamma_2$ and $\alpha_0 = \alpha_2$ and so $\alpha_2 = \alpha_0 = \gamma_2 = \gamma_0 \equiv \alpha$. Hence,

$$\boldsymbol{f} = \alpha\boldsymbol{c}, \qquad \boldsymbol{g} = \alpha\boldsymbol{b}, \qquad \boldsymbol{h} = \alpha\boldsymbol{e}.$$

In this case, we would not have the vanishing of the three additional terms, since

$$\det(\boldsymbol{e}|\boldsymbol{f}|\boldsymbol{g})xyz = -\alpha^2 \det(\boldsymbol{b}|\boldsymbol{c}|\boldsymbol{e})xyz, \qquad \det(\boldsymbol{f}|\boldsymbol{g}|\boldsymbol{h})xyz^2 = -\alpha^3 \det(\boldsymbol{b}|\boldsymbol{c}|\boldsymbol{e})xyz^2,$$
$$[-\det(\boldsymbol{c}|\boldsymbol{e}|\boldsymbol{g}) + \det(\boldsymbol{b}|\boldsymbol{c}|\boldsymbol{h}) + \det(\boldsymbol{b}|\boldsymbol{e}|\boldsymbol{f})]xy = -\alpha \det(\boldsymbol{b}|\boldsymbol{c}|\boldsymbol{e})xy,$$

and in general, the vectors $\boldsymbol{b}, \boldsymbol{c}, \boldsymbol{e}$, will be linearly independent. Thus, in the general case, we can only eliminate the 8 basis functions that correspond to the terms in $J\boldsymbol{F}(\hat{\boldsymbol{x}})$ that are zero. Eliminating the appropriate functions from (5.1), we then need to add to our space an 11 dimensional space consisting of functions of the form

$$\begin{aligned}
\hat{\boldsymbol{u}}_1 &= \hat{x}(1-\hat{x})(\tilde{A}_1 + \tilde{B}_2\hat{y} + \tilde{B}_3\hat{z} + \tilde{H}\hat{y}\hat{z}),\\
\hat{\boldsymbol{u}}_2 &= \hat{y}(1-\hat{y})(\tilde{A}_2 + \tilde{B}_2\hat{x} + \tilde{C}_3\hat{z} + \tilde{H}\hat{x}\hat{z}),\\
\hat{\boldsymbol{u}}_3 &= \hat{z}(1-\hat{z})(\tilde{A}_3 + \tilde{B}_3\hat{x} + \tilde{C}_3\hat{y} + \tilde{D}_3\hat{z} + E_3\hat{y}\hat{z} + \tilde{F}_3\hat{x}\hat{z} + \tilde{H}\hat{x}\hat{y} + \tilde{I}_3\hat{x}\hat{y}\hat{z}).
\end{aligned}$$

Combining these spaces, we thus can replace our original 40 dimensional space by a 28 dimensional space of the form

$$\begin{aligned}
\hat{\boldsymbol{u}}_1 &= A_1 + \bar{B}_1\hat{x} + D_1\hat{z} + I_1\hat{x}\hat{z} + \hat{x}(1-\hat{x})(P_1 + Q_1\hat{y} + R_1\hat{z} + K\hat{y}\hat{z}),\\
\hat{\boldsymbol{u}}_2 &= A_2 + \bar{C}_2\hat{y} + D_2\hat{z} + I_2\hat{y}\hat{z} + \hat{y}(1-\hat{y})(P_2 + Q_2x + S_1z + K\hat{x}\hat{z}),\\
\hat{\boldsymbol{u}}_3 &= A_3 + B_3\hat{x} + C_3\hat{y} + \bar{D}_3\hat{z} + J_1\hat{z}\hat{x} + J_2\hat{z}\hat{y}\\
&\quad + \hat{z}(1-\hat{z})(P_3 + R_2\hat{x} + S_2\hat{y} + R_3\hat{z} + K\hat{x}\hat{y} + L_3\hat{y}\hat{z} + M_3\hat{x}\hat{z} + N_3\hat{x}\hat{y}\hat{z}),
\end{aligned}$$

where we have replaced the independent variables B_1, C_2, D_3, $\tilde{A}_1$, $\tilde{A}_2$, $\tilde{A}_3$, and B_2, B_3, C_3, H_1, H_2, H_3 by an equivalent set of independent variables given below.

$$\begin{aligned}
\bar{B}_1 &= B_1 + G_1, & \bar{C}_2 &= C_2 + G_2, & \bar{D}_3 &= D_3 + G_3,\\
P_1 &= -G_1 + \tilde{A}_1, & P_2 &= -G_2 + \tilde{A}_2, & P_3 &= -G_3 + \tilde{A}_3,\\
Q_1 &= -H_3 + B_2, & R_1 &= H_2 + B_3, & S_1 &= -H_1 + C_3,\\
Q_2 &= H_3 + B_2, & R_2 &= -H_2 + B_3, & S_2 &= H_1 + C_3.
\end{aligned}$$

10.3. **General hexahedrons with flat faces.** In the previous section, we have seen that we can construct a simpler linear space in the case of a truncated pyramid, i.e., when all faces are flat and two are parallel. A natural question to ask is whether we can construct a simpler linear space, if we only assume that all faces are flat. However, based on simple symmetry arguments and the results of the previous section, we see that no simpler linear space is possible. If we perform computations for truncated pyramids when two faces of the truncated pyramid are parallel to either the $x-z$ plane or the $y-z$ plane, it is clear that in general, we can not remove any of the coefficients in the 21 dimensional space for $\hat{\boldsymbol{u}}$, based only on the assumption that all the faces are flat. For example, although we found that $B_2 = 0$ if we consider the case of two faces parallel to the $x-y$ plane, B_2 will not be zero if we take faces parallel to the $x-z$ plane. We can also use symmetry arguments to see that none of the eight basis functions corresponding to the eight vanishing terms in $J(\hat{\boldsymbol{x}})$, can be removed, since they will not be zero for one of the other truncated pyramids.

10.4. **Hexahedrons with flat boundary and midplane faces.** We next consider a more restrictive situation, in which we require both the boundary faces and the midplane faces (corresponding to mappings of the planes $\hat{x} = 1/2$, $\hat{y} = 1/2$, and $\hat{z} = 1/2$) to be flat. This case has previously been studied, using a different approach, in [12] and [13].

As we have seen previously, the plane $\hat{x} = x_0$ maps to a plane if $\det[\boldsymbol{c} + x_0\boldsymbol{e}, \boldsymbol{d} + x_0\boldsymbol{g}, \boldsymbol{f} + x_0\boldsymbol{h}] = 0$, the plane $\hat{y} = y_0$ will map to a plane if $\det[\boldsymbol{b} + y_0\boldsymbol{e}, \boldsymbol{d} + y_0\boldsymbol{f}, \boldsymbol{g} + y_0\boldsymbol{h}] = 0$, and $\hat{z} = z_0$ will map to a plane if $\det[\boldsymbol{b}+z_0\boldsymbol{g}, \boldsymbol{c}+z_0\boldsymbol{f}, \boldsymbol{e}+z_0\boldsymbol{h}] = 0$. We then need to seek solutions of the 9 non-linear equations corresponding to the choices $x_0 = 0, 1/2, 1$, $y_0 = 0, 1/2, 1$, and $z_0 = 0, 1/2, 1$. A family of solutions is obtained by letting $\boldsymbol{b}$, $\boldsymbol{c}$, and $\boldsymbol{d}$ be arbitrary linearly independent vectors and choosing $\boldsymbol{e}$, $\boldsymbol{f}$, $\boldsymbol{g}$, and $\boldsymbol{h}$ to satisfy

$$\boldsymbol{e} = \phi\boldsymbol{b} + \psi\boldsymbol{c}, \qquad \boldsymbol{f} = \alpha\boldsymbol{c} + \beta\boldsymbol{d}, \qquad \boldsymbol{g} = \gamma\boldsymbol{b} + \delta\boldsymbol{d}, \qquad \boldsymbol{h} = \gamma\phi\boldsymbol{b} + \alpha\psi\boldsymbol{c} + \beta\delta\boldsymbol{d},$$

where the constants $\alpha, \beta, \gamma, \delta, \phi, \psi$ satisfy the following three equations.

$$\gamma\phi - \alpha\phi - \beta\gamma = 0, \qquad \gamma\psi + \delta\alpha - \alpha\psi = 0, \qquad \delta\beta - \phi\delta - \psi\beta = 0.$$

Then,

$$\boldsymbol{h} = \gamma\boldsymbol{e} + \delta\boldsymbol{f} = \alpha\boldsymbol{e} + \beta\boldsymbol{g} = \psi\boldsymbol{f} + \phi\boldsymbol{g}, \tag{10.3}$$

and it easy to see that with this choice, the three determinant conditions are satisfied for all values of the parameters x_0, y_0, and z_0.

We would like to show that even with these restrictions, we will not obtain a simplification in the linear space for the vector $\hat{\boldsymbol{u}}$. Although we will not establish precisely this result, we will show that in the general form of the 20 dimensional space we obtained in (3.4), none of the constants can be zero for all choices of the variables satisfying the above constraints. By symmetry, we need only check a few of the 21 entries in (3.3). Clearly, A_i^1 will not be zero. By symmetry arguments, we need only check one of the next 9 entries. We see that

$$B_1^1 = f_2b_3 - f_3b_2 = [\alpha c_2 + \beta d_2]b_3 - [\alpha c_3 + \beta d_3]b_2 = -\alpha A_3^1 + \beta A_2^1 \neq 0$$

for all permitted values of α and β. Checking one of the next three entries, we find

$$E_1^1 = h_2b_3 - h_3b_2 = [\gamma\phi b_2 + \alpha\psi c_2 + \beta\delta d_2]b_3 - [\gamma\phi b_3 + \alpha\psi c_3 + \beta\delta d_3]b_2 = -\alpha\psi A_3^1 + \beta\delta A_2^1 \neq 0$$

for all permitted values of α, β, ψ, and δ. Again, checking one of the next three entries,

$$G_1^1 = e_2g_3 - g_2e_3 = [\phi b_2 + \psi c_2][\gamma b_3 + \delta d_3] - [\phi b_3 + \psi c_3][\gamma b_2 + \delta d_2] = \phi\delta A_1^1 - \psi\gamma A_3^1 + \psi\delta A_1^1 \neq 0$$

for all permitted entries of the constants. Finally, we check one of the entries in the last row.

$$\begin{aligned} H_1^1 = f_2h_3 - h_2f_3 = [\alpha c_2 + \beta d_2][\gamma\phi b_3 + \alpha\psi c_3 + \beta\delta d_3] - [\alpha c_3 + \beta d_3][\gamma\phi b_2 + \alpha\psi c_2 + \beta\delta d_2] \\ = -\alpha\gamma A_3^1 + \beta\gamma A_2^1 \neq 0 \end{aligned}$$

for all permitted entries of α, β, γ.

However, for mappings of this type, there will be a simplification in $J\boldsymbol{F}(\hat{\boldsymbol{x}})$. In particular, it easily follows from (10.3) that $\det(\boldsymbol{e}|\boldsymbol{f}|\boldsymbol{h})$, $\det(\boldsymbol{e}|\boldsymbol{g}|\boldsymbol{h})$, $\det(\boldsymbol{f}|\boldsymbol{g}|\boldsymbol{h})$, and $\det(\boldsymbol{e}|\boldsymbol{f}|\boldsymbol{g})$ are all zero. Thus, in this case, $J\boldsymbol{F}(\hat{\boldsymbol{x}})$ no longer contains the four terms x^2yz, y^2xz, z^2xy, and xyz.

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