Pyramidal finite elements

Joel Phillips

Doctor of Philosophy

Department of Mathematics and Statistics

McGill University

Montreal, Quebec

2010-11-01

A thesis submitted to McGill University in partial fulfillment of the requirements of the degree of Doctor of Philosophy

ABSTRACT

Pyramidal finite elements can be used as “glue” to combine elements with triangular faces (e.g. tetrahedra) and quadrilateral faces (e.g. hexahedra) in the same mesh. Existing pyramidal finite elements are low order or unsuitable for mixed finite element formulations. In this thesis, two separate families of pyramidal finite elements are constructed. The elements are equipped with unisolvent degrees of freedom and shown to be compatible with existing high order tetrahedral and hexahedral elements. Importantly, the elements are shown to deliver high order approximations and to satisfy a “commuting diagram property”, which ensures their suitability for problems whose mixed formulation lies in the spaces of the de Rham complex. It is shown that all pyramidal elements must use non-polynomial basis functions and that this means that the classical theory of finite elements is unable to determine what quadrature methods should be used to assemble stiffness matrices when using pyramids. This problem is resolved by extending the classical theory and a quadrature scheme appropriate for high order pyramidal elements is recommended. Finally, some numerical experiments using pyramidal elements are presented.

ABRÉGÉ

Les éléments finis pyramidaux peuvent servir comme «colle» pour combiner des éléments avec faces triangulaires (p. ex. tétraèdres) et avec faces quadrilaterales (p. ex. hexaèdres) dans un même maillage. Les éléments finis pyramidaux qui existent présentement sont soit de bas-ordre ou ne sont pas convenables pour les formulations mixtes d'éléments finis. Dans cette thèse, deux familles d'éléments finis pyramidaux sont construites. Les éléments sont équipés de degrés de libertés unisolvents et on démontre qu'ils sont compatibles avec les éléments pré-existantes triangulaires et quadrilaterales d'ordres élevés. On démontre notamment que les éléments produisent des approximations d'ordres élevés et satisfassent une «propriété de diagramme commutatif». Ceci assure que les éléments sont convenables pour des problèmes avec formulation mixte dans les espaces du complexe de Rham. On démontre que tous les éléments pyramidaux doivent utiliser des fonctions de base non-polynômes et que conséquemment la théorie classique des éléments finis ne peut pas déterminer quelles méthodes de quadrature devrait être employées pour assembler des matrices de rigidité lorsque les pyramides sont utilisées. Le problème est résolu en élargissant la théorie classique et une méthode de quadrature appropriée pour les éléments finis pyramidaux est suggérée. Finalement, des simulations numériques avec éléments pyramidaux sont présentées.

TABLE OF CONTENTS

LIST OF TABLES

LIST OF FIGURES

Figure page

ACKNOWLEDGEMENTS

I would not have entered the McGill mathematics programme had not Tony Humphries and Nilima Nigam been willing to take a punt on an unconventional applicant and I am grateful to both of them. However, it is Nilima who has had to live with most of the consequences and she deserves a special thank you. I followed most of her advice eventually, and probably ought to have done so initially. Leszek Demkowicz also provided advice, in addition to inspiration and a generous invitation to visit him and his group in Texas. I was introduced to finite element research during a workshop at the Banff International Research Station and started to think seriously about pyramidal elements whilst attending a summer school organised by the Centro Internazionale Matematico Estivo. A big thank you to Barbara Keyfitz and Alison Conway for facilitating my long-term visit to the Fields Institute, where many of the ideas were developed, and to Timo Betcke for the flexible interpretation of "post-doc" that allowed me to finish things off. I received funding from the Institut des Sciences Mathématiques, McGill University and, in several different forms, from the National Sciences and Engineering Research Council.

Hannah and Amanda both helped mitigate the progressive geographic non-locality that developed throughout my studies and despite my best efforts, I was unable to exhaust either's hospitality. Emilie translated the abstract and Neil, Dave and Simon helped with mathematical discussions, diversions, and friendship. Marilyn and Jonathan will be pleased to know that yes it is, finally, finished, although I expect not as much as Michelle, whose tolerance extends far beyond any reasonable bounds. Finally, thanks to Arthur for providing entertainment over the last year and, for a few months, the most convincing excuse for my tardiness.

Preface

Outline

This thesis consists of an introduction plus four chapters, which are based on three manuscripts. Chapters 2 and 3 contain the text of the paper "High order finite elements on pyramids, approximation spaces, unisolvency and exactness". Although this paper was eventually submitted to IMA Journal of Numerical Analysis as one work, it was originally conceived in two parts, and that division has been maintained across the two chapters. Chapter 4 consists of the paper "Numerical integration for high order pyramidal finite elements", which has been submitted to ESAIM Mathematical Modelling and Numerical Analysis. The content of chapter 5 is unpublished, but it is intended that it will form the basis for a longer paper exploring the numerical behaviour of pyramidal finite elements.

Contributions of authors

Chapters 2, 3 and 4 are based on papers which are co-authored with Nilima Nigam. Nilima Nigam provided guidance and criticism throughout the development of results described in these papers and was significantly involved in later revisions. However, the key ideas in all three chapters, including the constructions of all the families of pyramidal elements; the strategies for all the theorems and the proofs of all the results are due to Joel Phillips. Chapter 5 is the sole work of Joel Phillips.

CHAPTER 1
Introduction

1.1 Background and Motivation

Much of the work detailed in this thesis was motivated by talks given at a workshop at the Banff International Research Station in February 2006 and a C.I.M.E. summer school in Cetraro, Italy in June 2006; in particular, the proposition of Leszek Demkowicz that:

> "A successful three-dimensional Finite Element code for Maxwell equations must include all four kinds of geometrical shapes: tets, hexas, prisms, and pyramids. The theory of the exact sequence and higher order elements for the pyramid element remains to be one of the most urgent research issues."[13]

In this introduction we will provide some background for this statement. We will describe the finite element method and explain the importance of the "exact sequence" and "higher order elements". Most significantly, for what follows in later chapters, we will show how pyramidal elements can be useful, what work has already been done and what problems remain.

Mathematicians and engineers have used finite elements to obtain approximate numerical solutions to systems of partial differential equations for over forty years. Tens of thousands of papers and hundreds of books have been written about their properties. Good introductions to the subject can be found in many of these, including [15, 40, 58, 71, 87, 17, 25].

The finite element method is a technique for constructing a finite dimensional approximation to a space of functions (or distributions) $V(\Omega)$ where the domain, Ω, is an n-dimensional manifold. Typically, $\Omega \subset \mathbb{R}^n$ and n equals 1,2 or 3. A partition, or mesh, $\mathcal{T} = \{K_1, \ldots, K_M\}$, is defined such that $\Omega = \bigcup_{i=1}^{M} K_i$. Associated with each K_i is an approximation space, V_i, and a set of independent linear functionals, $\Sigma_i \subset V(\Omega)'$, which form a basis for the dual space, V_i'. The triple, (K_i, V_i, Σ_i), is known as a *finite element* and the Σ_i are called the *degrees of freedom*.

When $\overline{K}_i \cap \overline{K}_j \neq \emptyset$, it is often the case that the set, $\Sigma_i \cap \Sigma_j$, is also non-empty. Any members of $\Sigma_i \cap \Sigma_j$, are called *external* degrees of freedom (a degree which is not external is a *volume* or *internal* degree). The approximation space, $V_h \subset V(\Omega)$, is defined as the set of all functions, v, such that $v|_{K_i} \in V_i$ and for which all external degrees are well defined. Conventionally, the addition of a subscript, h, is used to indicate that V_h is constructed using a mesh $\mathcal{T} = \mathcal{T}_h$ where $\operatorname{diam} K_i \leq h$ for all $K_i \in \mathcal{T}_h$. The specification of the degrees of freedom is equivalent to the definition of an interpolation operator, $\Pi_h : V(\Omega) \to V_h$, where $\Pi_h u$ is defined to be the unique $u_h \in V(\Omega)$ such that $\sigma(u_h) = \sigma(u)$ for all degrees of freedom, $\sigma \in \bigcup_{i=1}^{M} \Sigma_i$.

On each element, there is a unique basis, (v_j), for V_i such that $\sigma_k(v_j) = \delta_{jk}$ for all $\sigma_k \in \Sigma_i$. The v_j are known as *shape functions*. When Σ_i consists of point evaluations, i.e. each $\sigma_k(v) = v(x_k)$ for some $x_k \in K_i$, then (K_i, V_i, Σ_i) is described as a *nodal* finite element and the v_j are nodal shape functions.

1.2 Example: an elliptic problem

To use these spaces to approximate the solution of a system of partial differential equations, we first cast the problem to be solved into variational form. For a simple example (which loosely follows the presentation in [15]), suppose that $\Omega \subset \mathbb{R}^n$ is a bounded domain and that $u \in C^2(\Omega) \cap C_0(\overline{\Omega})$ is a solution to the second order elliptic problem with homogeneous Dirichlet boundary conditions:

$$-\sum_{i,j=1}^{n} \frac{\partial}{\partial x_i} \mathcal{A}_{ij}(x) \frac{\partial}{\partial x_j} u(x) = f(x) \qquad x \in \Omega, \tag{1.1}$$

$$u(x) = 0 \qquad x \in \partial\Omega, \tag{1.2}$$

for some function $f \in C(\overline{\Omega})$ and symmetric matrices $\mathcal{A}(x)$ which have entries, $\mathcal{A}_{ij} \in C^1(\overline{\Omega})$. By ellipticity we mean that the $\mathcal{A}$ are symmetric and uniformly positive definite, i.e. for all $x \in \Omega$, $e^t \mathcal{A}(x) e \geq \epsilon > 0$ for any unit vector, $e \in \mathbb{R}^n$, $|e| = 1$. If we formally multiply (1.1) by a test function, v, and integrate by parts, it is easy to see that if u is a classical solution of (1.1), it must satisfy the variational problem:

$$a(u, v) = \langle f, v \rangle \qquad \forall v \in C^2(\Omega) \cap C_0(\overline{\Omega}), \tag{1.3}$$

where the symmetric bilinear form, $a(u, v) := \int_\Omega \nabla v^t \mathcal{A} \nabla u dx$ and we have written $\langle f, v \rangle = \int_\Omega f v dx$. Any u which satisfies (1.3) will also be the (unique) minimiser of the functional:

$$J(v) := \frac{1}{2} a(v, v) - \langle f, v \rangle \, dx \tag{1.4}$$

over all functions $v \in C^2(\Omega) \cap C(\overline{\Omega})$. There is, however, no guarantee that such a minimiser exists. We can fix this by expanding our search to a weak solution of (1.3) over all functions, v, in the Sobolev space[1] $H_0^1(\Omega)$.

[1] For a domain, $\Omega \subset \mathbb{R}^n$, define the semi-norm, $|v|_{r,\Omega} = \left(\sum_{|\alpha|=r} \int_\Omega (D^\alpha v)^2 \right)^{1/2}$, where the α are multi-indices. For an order $k \in \mathbb{N}$ the Sobolev spaces, $H^k(\Omega)$ and $H_0^k(\Omega)$ are the respective completions of $C^\infty(\Omega)$ and $C_0^\infty(\Omega)$ in the norm, $\|v\|_{k,\Omega} := \left(\sum_{r=0}^{k} |v|_{r,\Omega}^2 \right)^{1/2}$.

Since each $\mathcal{A}_{ij} \in C^1(\overline{\Omega}) \subset L^1(\Omega)$, the bilinear form, $a : H_0^1(\Omega) \times H_0^1(\Omega) \to \mathbb{R}$ (defined by completion) is continuous, i.e. there exists a constant, C such that:

$$|a(u,v)| \leq C\|u\|_1\|v\|_1 \qquad \forall u,v \in H_0^1(\Omega) \tag{1.5}$$

We also specified that the coefficients, $\mathcal{A}$, should be uniformly positive definite and so, after using the homogeneous Dirichlet boundary conditions to apply the Poincaré-Friedrich's inequality, we obtain a *coercivity* constant, α, such that

$$a(u,u) \geq \alpha\|u\|_1^2, \qquad \forall u \in H_0^1(\Omega). \tag{1.6}$$

By the Lax-Milgram theorem, $J(v)$ has a unique minimiser $u \in H_0^1(\Omega)$ for any $f \in H^{-1}(\Omega)$. The minimiser will be a solution of the weak problem,

$$a(u,v) = \langle f, v\rangle\,, \qquad \forall v \in H_0^1(\Omega) \tag{1.7}$$

and since $\alpha\|u\|_1^2 \leq a(u,u) = \langle f,u\rangle \leq \|f\|_{-1}\|u\|_1$, the solution, u, satisfies the bound:

$$\|u\|_1 \leq \frac{1}{\alpha}\|f\|_{-1}. \tag{1.8}$$

The original space, $C^2(\Omega) \cap C_0(\overline{\Omega})$ is a dense subset of $H_0^1(\Omega)$ and $C(\Omega) \subset H^{-1}(\Omega)$ so any classical solution will also solve (1.7).

Now suppose that by the procedure outlined in section 1.1, we know how to construct finite element approximation spaces, $V_h \subset H_0^1(\Omega)$. The ellipticity condition will still be satisfied

---

Negative and fractional order Sobolev spaces can also be defined, in particular, if Ω is Lipschitz then $H^{-1}(\Omega)$ is the dual space of $H_0^1(\Omega)$. Details can be found in [71].

and so the minimiser of (1.4) in V_h is characterised by

$$a(u_h, v_h) = \langle f, v_h \rangle\,, \qquad \forall v_h \in V_h \tag{1.9}$$

Given a basis $\{e_i\}$ for V_h, we can write $u_h = \sum_i U_i e_i$. The vector of coefficients, U_i can be found by (constructing and) solving the linear algebraic system: $AU = F$ where A is a matrix with components $A_{ij} = a(e_i, e_j)$ and F is a vector with components $F_i = \int_\Omega f e_i$.

The obvious next question is, "how good is u_h as an approximation to u?". By subtracting (1.9) from (1.7) we obtain

$$a(u - u_h, v) = 0 \quad \forall v \in V_h. \tag{1.10}$$

Now, given any $v_h \in V_h$,

$$\alpha \|u - u_h\|_1^2 \le a(u - u_h, u - u_h) \tag{1.11}$$

$$= a(u - u_h, u - v_h) + a(u - u_h, v_h - u_h) \tag{1.12}$$

$$\le C\|u - u_h\|_1 \|u - v_h\|_1. \tag{1.13}$$

The first and third lines involve the constants of continuity and coercivity, C and α, which were defined in (1.5) and (1.6). The term $a(u - u_h, v_h - u_h)$ is zero because $v_h - u_h \in V_h$ and so (1.10) applies. Dividing through by $\|u - u_h\|_1$ on both sides of (1.2) and taking an infimum over all $v_h \in V_h$ gives the result known as Céa's lemma [22]:

$$\|u - u_h\|_1 \le \frac{C}{\alpha} \inf_{v_h \in V_h} \|v_h - u\|_1, \tag{1.14}$$

which bounds the error, $\|u - u_h\|_1$ in terms of the best possible approximation to u in V_h. Some insight is also provided by a slightly weaker result obtained by a duality argument:

Lemma 1. *Suppose that $a(\cdot,\cdot)$ satisfies* (1.5) *and* (1.6) *and let u and u_h be the solutions of* (1.7) *and* (1.9)*, then:*

$$\|u - u_h\|_1 \leq \left(1 + \frac{C}{\alpha}\right) \inf_{v_h \in V_h} \|u - v_h\|_1. \tag{1.15}$$

Proof. Consider the linear functional $f_{v_h} \in V_h'$ defined as

$$\langle f_{v_h}, w_h \rangle := a(u_h - v_h, w_h) \tag{1.16}$$

for all $w_h \in V_h$. Following the same argument as for (1.8), $\|u_h - v_h\|_1 \leq \frac{1}{\alpha}\|f_{v_h}\|_{V_h'}$. Adding (1.10) to (1.16), we see that $\langle f_{v_h}, w_h \rangle = a(u - v_h, w_h)$ and so, by (1.5), $\|f_{v_h}\|_{V_h'} \leq C\|u - v_h\|_1$. Hence $\|u_h - v_h\|_1 \leq \frac{C}{\alpha}\|u - v_h\|_1$ and equation (1.15) follows from the triangle inequality. □

The difference here is that we have not used the ellipticity of $a(\cdot,\cdot)$ directly, merely the continuity of the continuous operator and the existence of an inverse of the discrete operator that is bounded by $\frac{1}{\alpha}$.

In either case, the key to estimating $\|u - u_h\|_1$ is understanding the behaviour of the *best approximation error*, $\inf_{v_h \in V_h} \|v_h - u\|_1$. We will show shortly how it can be controlled in terms of properties of V_h. First, however, lets take a detour and look at some topics that are not illustrated by our simple example problem.

1.3 Mixed formulations and the commuting diagram

The replacement of the continuous space by a discrete approximation in the weak formulation, (1.9), is known as the *Galerkin* method (similarly, property (1.10) is known as *Galerkin orthogonality*); in particular, since the bilinear form, $a(\cdot,\cdot)$ is symmetric and so the problem can be characterised as a minimisation, it is the *Ritz-Galerkin* method. There are many variations and extensions to this framework. The *Rayleigh-Ritz* method discretises the variational form, (1.4), directly; *Petrov-Galerkin* schemes use different spaces for the test and trial functions, v_h and u_h. The condition that $V_h \subset U(\Omega)$ is not necessary: such methods are called *non-conforming*. An important class of non-conforming methods are the *Discontinuous Galerkin* (DG) methods, where rather than using external degrees of freedom to ensure continuity between elements, discontinuities are allowed, but penalised. In our simple example, the discrete problem inherits the ellipticity, and hence unique solvability, property directly from the underlying problem. Non-conformities typically mean that more care must be taken to ensure unique solvability; often this can be handled using a *variational crimes* framework [17]. Another kind of variational crime arises when (inexact) numerical integration is used to construct A and F; we examine a particular instance of this problem in detail in Chapter 4.

It was the specification that the $\mathcal{A}$ are positive definite (and symmetric) which meant that the variational form of our problem involved the search for a minimiser. More general problems have an associated variational form that is a saddle-point problem. This occurs when, for example, a Lagrange multiplier is used to introduce a constraint. Such a situation arises when modelling many different physical phenomena; in chapter 5 we will see a specific example when we ensure that our solution to Stokes' problem is divergence free.

Finite element solution techniques for these problems are known as *mixed methods*. The first general analysis of the convergence and stability properties of mixed methods was given by Brezzi [18] which built on earlier work of Babuska, [7]. In this section we present a summary of some of the results presented in the book by Brezzi and Fortin [40], which should be consulted for proofs and more details.

The prototypical mixed problem has the weak form: Let V and Q be Hilbert spaces; for some $f \in V'$ and $g \in Q'$, find $u \in V, q \in Q$ such that

$$\begin{aligned} a(u, v) + b(v, p) &= \langle f, v \rangle \quad \forall v \in V, \\ b(u, q) &= \langle g, q \rangle \quad \forall q \in Q. \end{aligned} \tag{1.17}$$

If $a(\cdot, \cdot)$ is symmetric, then (1.17) characterises the solution of the saddle point problem

$$\inf_{v \in V} \sup_{q \in Q} \left\{ \frac{1}{2} a(v, v) + b(v, q) - \langle f, v \rangle - \langle g, q \rangle \right\}. \tag{1.18}$$

The bilinear forms, $a(\cdot, \cdot)$ and $b(\cdot, \cdot)$ induce linear operators $A : V \to V'$ and $B : V \to Q'$ defined as

$$\langle Au, v \rangle := a(u, v), \qquad \langle Bv, q \rangle := b(v, q) \qquad \forall u, v \in V, \ \forall q \in Q. \tag{1.19}$$

We will also require the adjoint operators, $A^t : V \to V'$ and $B^t : Q \to V'$, defined as $\left\langle A^t u, v \right\rangle := a(v, u)$ and $\left\langle B^t q, v \right\rangle := b(v, q)$ for all $u, v \in V$ and $q \in Q$.

Problem (1.17) has a solution for all $f \in V'$ and $g \in \operatorname{Im} B \subseteq Q'$ if and only if B has closed range in Q' and the restriction of A to the kernel of B, $\ker B$, is invertible. The closed range condition is equivalent to the "inf-sup" property that there exists some $k_0 > 0$ such that:

$$\sup_{v \in V} \frac{b(v, q)}{\|v\|_V} \geq k_0 \|q\|_{Q / \ker B^t} \quad \forall q \in Q. \tag{1.20}$$

The invertibility of A on $\ker B$ is implied by the existence of some $\alpha_0 > 0$ such that $\|Au\|_{(\ker B)'} \geq \alpha_0 \|u\|_V$ and $\|A^t u\|_{(\ker B)'} \geq \alpha_0 \|u\|_V$ for all $u \in \ker B$. If these properties hold, we can obtain the bounds:

$$\|u\|_V \leq \frac{1}{\alpha_0}\|f\|_{V'} + \frac{1}{k_0}\left(1 + \frac{\|A\|}{\alpha_0}\right)\|g\|_{Q'}, \tag{1.21}$$

$$\|p\|_{Q/\ker B^t} \leq \frac{1}{k_0}\left(1 + \frac{\|A\|}{\alpha_0}\right)\|f\|_{V'} + \frac{\|A\|}{k_0^2}\left(1 + \frac{\|A\|}{\alpha_0}\right)\|g\|_{Q'}. \tag{1.22}$$

Given finite dimensional subspaces, $V_h \subset V$ and $Q_h \subset Q$, we can pose the discrete problem: find $u_h \in V_u$ and $p_h \in Q_h$ such that

$$\begin{aligned} a(u_h, v_h) + b(v_h, p_h) &= \langle f, v_h \rangle \quad \forall v_h \in V_h \\ b(u_h, q_h) &= \langle g, q_h \rangle \quad \forall q_h \in Q_h \end{aligned} \tag{1.23}$$

As with the elliptic problem presented earlier, there are two important questions to answer: "Is there a unique solution (u_h, p_h)?" and "What can we say about $\|u - u_h\|_v$ and $\|p - p_h\|_Q$?".

Unlike the elliptic case, the discrete problem does not automatically inherit the solvability properties of the continuous problem. Define the operators $A_h : V_h \to V_h'$ and $B_h : V_h \to Q_h'$ as

$$\langle A_h u_h, v_h \rangle = a(u_h, v_h) \qquad \langle B_h v_h, q_h \rangle = b(v_h, q_h) \qquad \forall u_h, v_h \in V_h,\ \forall q_h \in Q_h$$

There are two issues. Firstly, since $Q_h \subset Q$, it is not necessarily the case that $\ker B_h \subseteq \ker B$ and so the coercivity, for example, of A on $\ker B$ does not imply the coercivity of A_h on $\ker B_h$. This must be addressed on a case by case basis; for example, sometimes A is coercive on the whole of V which immediately implies the coercivity of A_h on $\ker B_h \subset V$. Secondly, although $\operatorname{Im} B_h$ is always closed (because Q_h is finite dimensional) we must ensure that $g \in \operatorname{Im} B_h \subset Q_h'$. To make sense of this last statement, note that any projection,

$P_{Q_h} : Q \to Q_h$ induces a projection $P_{Q'_h} : Q' \to Q'_h$ via

$$\left\langle P_{Q'_h} g, q \right\rangle = \langle g, P_{Q_h} q\rangle = \left\langle P^t_{Q_h} g, q \right\rangle \quad \forall q \in Q_h$$

and for a solution to exist, what we actually require is that $P_{Q'_h} g \in \operatorname{Im} B_h$. We want this to be true for any $g \in B$ and it was shown in [39] that two equivalent conditions are

- $\ker B^t_h = \ker B^t \cap Q_h \subset \ker B^t$.
- For any $u \in V$, there exists a $u_h = \Pi_h u \in V_h$ such that $b(u - \Pi_h u, q_h) = 0$, $\forall q_h \in Q_h$.

The second of these is known as *Fortin's criterion.* It is nicely illustrated by the commutativity of the diagram,

$$\begin{array}{ccc} V & \xrightarrow{B} & Q' \\ \Pi_h \downarrow & & \downarrow P'_{Q_h} \\ V_h & \xrightarrow{B_h} & Q'_h \end{array} \tag{1.24}$$

Suppose that Fortin's criterion is indeed satisfied and that there exists some $\alpha_h > 0$ such that $\|A_h u\|_{(\ker B_h)'} \geq \alpha_h \|u\|_V$ and $\|A^t_h u\|_{(\ker B_h)'} \geq \alpha_h \|u\|_V$ for all $u \in \ker B_h$. Since B_h is closed, there exists a k_h such that

$$\sup_{v_h \in V_h} \frac{b(v_h, q_h)}{\|v_h\|_V} \geq k_h \|q_h\|_{Q/\ker B^t_h} \quad \forall q_h \in Q_h \tag{1.25}$$

Following the same reasoning used to obtain the weaker form of Cea's lemma (1.15) and using the bounds, (1.21) and (1.22) applied to the discrete problem, (1.23), we can bound the error in the approximate solution in terms of the best approximation error:

$$\begin{aligned} \|u - u_h\|_V + k_h \|p - p_h\|_{Q/\ker B^t} \leq \left(1 + \frac{\|A\|}{\alpha_h}\right)\left(1 + \frac{\|B\|}{k_h}\right)(1 + \|A\|) \inf_{v_h \in V_h} \|u - v_h\|_V + \\ \left(k_h + \|B\| \left(1 + \frac{1 + \|A\|}{\alpha_h}\right)\right) \inf_{q_h \in Q_h} \|p - q_h\|_Q. \end{aligned} \tag{1.26}$$

Individual (and slightly tighter) bounds for each of the terms on the left-hand side are given in [40]. However, (1.26) is sufficient to illustrate that the error depends on the discrete inf-sup parameter, k_h. In particular, to achieve an optimal convergence rate as $h \to 0$, it is important that we can uniformly bound $k_h \geq k_{h0}$ for some $k_{h0} > 0$.

Assume that Fortin's criterion, (1.24), holds and that the Π_h are uniformly continuous (in h) with $\|\Pi_h v\| \leq C_V \|v\|$. Then we obtain, for any $q_h \in Q_h$:

$$\begin{aligned}
\sup_{v_h \in V_h} \frac{b(v_h, q_h)}{\|v_h\|_V} &= \sup_{v \in V} \frac{b(\Pi_h v, q_h)}{\|\Pi_h v\|_V} && \text{(surjectivity of } \Pi_h\text{)} \\
&\geq \frac{1}{C_V} \sup_{v \in V} \frac{b(\Pi_h v, q_h)}{\|v\|_V} && \text{(uniform continuity of } \Pi_h\text{)} \\
&= \frac{1}{C_V} \sup_{v \in V} \frac{b(v, q_h)}{\|v\|_V} && \text{(Fortin's criterion)} \\
&\geq \frac{k_0}{C_V} \|q_h\|_{Q/\ker B^t} && \text{(the continuous inf-sup condition, (1.20)).}
\end{aligned}$$

Now, $q_h = P_{Q_h} q_h$ and by (1.24), $\ker B_h^t = P_{Q_h}(\ker B^t)$, so, provided that there is a constant, C_Q, such that $\|P_{Q_h}\| \leq C_Q$ uniformly, we have

$$\begin{aligned}
\|q_h\|_{Q/\ker B_h^t} &= \inf_{r_h \in \ker B_h^t} \|q_h + r_h\|_Q \\
&= \inf_{r \in \ker B^t} \|P_{Q_h}(q_h + r)\|_Q \\
&\leq C_Q \inf_{r \in \ker B^t} \|q_h + r\|_Q = C_Q \|q_h\|_{Q/\ker B^t},
\end{aligned}$$

which establishes the uniform bound: $k_h \geq \frac{k_0}{C_Q C_V}$.

The lesson here is that the existence of uniformly bounded interpolation operators that make the diagram, (1.24), commute is a sufficient condition for the stability and approximability (indeed, quasi-optimality) of discrete problem, (1.23).

The commuting diagram property is also important in establishing the convergence of eigenvalue approximations. Arnold et al, [6], cast the operator $B : V \to Q$ as a chain map in a Hilbert complex and $B_h : V_h \to Q_h$ in a subcomplex. The commuting interpolation operators, Π_h and P_{Q_h} are therefore cast as co-chain maps. They say:

> "It has long been observed that for mixed finite element approximation of eigenvalue problems, stability and approximability alone, while sufficient for convergence of approximations of the source problem, is not sufficient for convergence of the eigenvalue problem. ... We prove eigenvalue convergence under the same sort of assumptions we use to establish stability and convergence for the source problem, namely subcomplexes, bounded cochain projections, and approximability. ... We believe that subcomplexes with bounded cochain projections provide an appropriate framework for the analysis of the eigenvalue problem, since, as far as we know, these properties hold in all examples where eigenvalue convergence has been obtained by other methods."

Our motivation was the finite element solution of Maxwell's equations and, more generally, any problems that can be expressed in terms of the operators, grad, curl and div. Our Hilbert complex is therefore the de Rham complex and in chapters 2 and 3 we will seek finite element approximation spaces, $\mathcal{U}_h^{(s)}$ and (interpolation) operators, $\Pi_h^{(s)}$, that make the following diagram commute:

$$\begin{array}{ccccccc} H^1(\Omega) & \xrightarrow{\nabla} & \mathbf{H}(\mathrm{curl},\Omega) & \xrightarrow{\nabla\times} & \mathbf{H}(\mathrm{div},\Omega) & \xrightarrow{\nabla\cdot} & L^2(\Omega) \\ \Pi_h^{(0)}\downarrow & & \Pi_h^{(1)}\downarrow & & \Pi_h^{(2)}\downarrow & & \Pi_h^{(3)}\downarrow \\ \mathcal{U}_h^{(0)}(\Omega) & \xrightarrow{\nabla} & \mathcal{U}_h^{(1)}(\Omega) & \xrightarrow{\nabla\times} & \mathcal{U}_h^{(2)}(\Omega) & \xrightarrow{\nabla\cdot} & \mathcal{U}_h^{(3)}(\Omega). \end{array} \tag{1.27}$$

1.4 Best approximation and hp methods

Lets return to the simple example from section 1.2 and consider the best approximation error, $\inf_{v_h \in V_h} \|u - v_h\|_V$ that features in the error estimate, (1.14). We will work with $V = H^1(\Omega)$.

Lemma 2. *Let Ω be a Lipschitz domain and suppose that V_h is an approximation space based on a shape regular*[2] *mesh $\mathcal{T}_h$ for Ω which contains all members of $H^1(\Omega)$ which are element-wise polynomial of degree $k-1$, i.e.*

$$V_h \subset \left\{ v \in H^1(\Omega) : v|_{K_i} \in P^{k-1} \ \forall \ K_i \in \mathcal{T}_h \right\}, \tag{1.28}$$

and that there exists a bounded interpolation operator $\Pi_h : H^k(\Omega) \to V_h$. Then

$$\inf_{v \in V_h} \|v - u\|_1 \leq C h^{k-1} |u|_k \quad \forall u \in H^k(\Omega)$$

for some constant $C = C(\Omega, k) > 0$.

Proofs of approximation results like this typically rely upon the following result from Bramble and Hilbert, [16]:

Lemma 3 (Bramble Hilbert Lemma)**.** *Let Y be a normed space and let $D \subset \mathbb{R}^n$ be a Lipschitz domain. Suppose that an operator, $B : H^k(D) \to Y$ is bounded and that the kernel of B contains P^{k-1}, the space of polynomials of degree at most $k-1$. Then $\|Bv\|_Y \leq C |v|_k$ for some constant, C.*

---

[2] In section 1.5 we will see that the elements, K_i can be related to a reference element, K by a map, $\phi_i : \hat{K} \to K_i$. Shape regularity means that the condition numbers of the Jacobians of these maps, $D\phi_i$, are uniformly bounded for $i = 1..M$. The consequence is that the elements cannot be arbitrarily thin or distorted.

Sketch of proof of Lemma 2. We first build an element-wise estimate. By a Sobolev extension theorem, $P^{k-1} \subset V_i = V_h|_{K_i}$. So, since Π_h is a projection, $P^{k-1} \subset \ker(I - \Pi_h)|_{K_i}$. Hence by Lemma 3, $\|u - \Pi_h u\|_{1,K_i} \le C_1 |u|_{k,K_i}$. We can apply a scaling argument to see that $\|u - \Pi_h u\|_{1,K_i} \le C_2 h^{k-1} |u|_{k,K_i}$ for $h < 1$, where C_2 depends on C_1 and the shape-regularity of K_i. Summing over all elements gives $\|u - \Pi_h u\|_{1,\Omega} \le C_2 h^{k-1} |u|_{k,\Omega}$. □

Full details of the proof can be found in standard text-books, [17, 25]. A particularly simple version is given for $n = 2$ in [15].

The process of producing successively better meshes, $\mathcal{T}_{h_n}$ where $h_{n+1} < h_n$ is known as *h-refinement*. When the degree, p, of the largest complete space of polynomials present in each V_i is fixed, the resulting method is the *h-version* of the finite element method. An alternative way of achieving a better approximation is to keep the mesh fixed, but to increase p. This is the *p-version* of the finite element method (when the mesh contains just one element, it is also called the *spectral method*). Denoting such a family of approximation spaces as V_p, it is possible to obtain estimates of the form:

$$\inf_{v \in V_p} \|v - u\|_1 \le C(k) p^{-k} \|u\|_{k+1}. \tag{1.29}$$

For smooth functions, the estimate has super-polynomial convergence; when u is analytic, it is in fact exponential.

The tools of the h- and p-versions may be combined: increasing polynomial order of elements where the function being approximated is smooth, and reducing h locally in the vicinity of singularities. This is known as the *hp-version* of the finite element method. Babuska and Guo showed that by using such an approach, exponential convergence can still be achieved for functions which are only the solutions of elliptic problems with piecewise analytic data [44]. The analysis required for the p- and hp- versions is similar; a thorough review is given in [8] and more details, including tighter estimates than (1.29), are contained in the book by Schwab [71].

When the regularity of the solution can be determined beforehand, a series of appropriately graded meshes can be constructed *a priori*. In general, however, the approximate solutions themselves must be relied upon to provide information about what kind of refinements to perform. A programme to develop a general method for applying the *hp*-method was outlined in [33, 64, 66]. A summary of the work on *hp*-adapativity is given in [34] and more details are given in [31]. We have already seen that both the stability and approximation properties of a finite element method depend on the existence of interpolation operators with specific properties; the *hp*-adaptivity approaches require concrete implementations. This lead to the idea of *projection-based interpolation*, outlined in [32] and [29]. The projection-based interpolation framework can be used to construct commuting interpolation operators with quasi-optimal p-approximation behaviour on arbitrary finite element domains. In chapter 3, we will make use of projection-based interpolation to construct the volume degrees of freedom for our pyramidal elements.

1.5 Finite element approximation spaces for the de Rham complex

The characterisation of each finite element as a triple, (K_i, V_i, Σ_i), is due to Ciarlet, [25]. With this formalism, each element is constructed in terms of a reference element $(\hat{K}, \hat{V}, \hat{\Sigma})$ and a (very) smooth bijection, $\phi_i : \hat{K} \to K_i$. The reference domain, $\hat{K} \subset \mathbb{R}^n$, is usually a simple shape, for example an n-simplex or n-cube. For the h-version of the finite element method, a single reference element may suffice: all the differences between the elements can be captured by the ϕ_i. For the p-method, or if $\mathcal{T}$ is a *hybrid* mesh, containing shapes of different types (e.g. both rectangles and triangles), multiple reference elements are needed. For a scalar-valued approximation space, $V(\Omega) \subset H^1(\Omega)$ we define the element-wise approximation spaces in terms of the reference element as $V_i = \left\{ \hat{v} \circ \phi_i^{-1} : \hat{v} \in \hat{V} \right\}$. Similarly we define each $\sigma \in \Sigma_i$ in terms of a degree of freedom on the reference element, $\hat{\sigma} \in \hat{\Sigma}$ as $\sigma(v) = \hat{\sigma}(v \circ \phi_i)$ for any $v \in V(\Omega)$.

This is equivalent to saying that the reference degrees of freedom, $\hat{\sigma}$ induce an interpolation operator on the reference element, $\hat{\Pi}$ and that $\Pi_i := \Pi_h|_{K_i} = \hat{\Pi} \circ \phi_i^{-1}$. But we have an additional requirement: we want to construct approximation spaces, $\mathcal{U}_h^{(s)}(\Omega)$ and interpolation operators, $\Pi_h^{(s)}$ for $s \in \{0, 1, 2, 3\}$ which satisfy the commuting diagram property, (1.27). Suppose that we have constructed reference spaces, $\hat{\mathcal{U}}^{(s)}(\hat{K})$ and operators $\hat{\Pi}^{(s)}$ which satisfy the diagram, then, for example, it may not be true that $\nabla \circ \Pi_i^{(0)} = \hat{\Pi}_i^{(1)} \circ \nabla$ (it is, in fact, only true when ϕ_i is a dilatation). There are several ways to conceptualise the resolution of this issue:

1. The differential forms school, popularised in [46, 5, 6] casts the elements of the spaces $H^1(\Omega)$, $\mathbf{H}(\text{curl}, \Omega)$, $\mathbf{H}(\text{div}, \Omega)$ and $L^2(\Omega)$ as proxies to differential s-forms belonging to the spaces[3] $H\Lambda^{(s)}(\Omega)$ for $s = 0, 1, 2, 3$. The exterior derivatives, grad, curl and div are then all instances of the chain map, d and $\phi_i : \hat{K} \to K_i$ is a manifold diffeomorphism which induces a pull-back mapping $\phi_i^* : \Lambda^{(s)}(K_i) \to \Lambda^{(s)}(\hat{K})$. Pull-backs commute with d, so we can define $\mathcal{U}_h^{(s)}(\Omega) = \left\{ v \in H\Lambda^{(s)}(\Omega) | \phi_i^* v \in \hat{\mathcal{U}}^{(s)}(\hat{K})\ i = 1..M \right\}$ and $\Pi_i^{(s)} = (\phi_i^{-1})^* \circ \hat{\Pi}^{(s)} \circ \phi_i^*$.

2. The concrete instantiations of the differential form pull-backs in terms of the vector proxies are easily calculable and their use precedes the more modern differential forms

[3] See [5] for a precise definition of the Sobolev spaces of differential s-forms, $H\Lambda^{(s)}(\Omega)$. In chapter 4, we will use the slightly different notation, $\mathcal{H}^{(s)}(\Omega)$

abstraction. For example, if we define $\phi_i^* v := v \circ \phi_i$ for $v \in H^1(\Omega)$ then an application of the chain rule to the commuting diagram condition that $\nabla \phi^* v = \phi^* \nabla v$ suggests that we take the change of variables formula, $\phi^* E = D\phi^t [E \circ \phi]$ for $E \in \mathbf{H}(\mathrm{curl}, \Omega)$. A slightly more involved calculation reveals that the correct formula for $F \in \mathbf{H}(\mathrm{div}, \Omega)$ is Piola's transform, $\phi^* F = |D\phi|\, D\phi^{-1}[F \circ \phi]$, [68].

In chapters 2 and 3 we follow a hybrid of these two approaches: taking advantage of the notational convenience of the differential forms, but also providing explicit definitions using vector calculus where appropriate.

3. In chapter 4 we take a slightly different view. Rather than thinking of $\hat{K}$ as a separate manifold, we treat it as a chart domain. Each $\phi_i^{-1} : K_i \to \hat{K}$ is now a chart map and the differential forms are covariant tensors. The pull-backs are thus cast as covariant changes of coordinates. This approach is, to the best my knowledge, novel within the mathematical finite element community. It is perhaps closer in spirit to the engineering practice of defining finite elements in terms of (barycentric) coordinate systems.

When $\Omega \subset \mathbb{R}^3$, the most common choices for the reference elements, $\hat{K}$, are tetrahedra (3-simplices) or cubes. It is common to let ϕ_i be an affine map (in which case the cubes map to parallelepipeds). But sometimes more general choices are allowed. In particular, if ϕ_i is trilinear then the cubes will map to general hexahedra. When the components of ϕ_i are allowed to be polynomials of the same degree as the approximation space, the elements are called *isoparametric*.

High order finite elements for each of the spaces in (1.27) on tetrahedral and hexahedral domains were first introduced by Nedelec, [59]. A good description of the elements is given

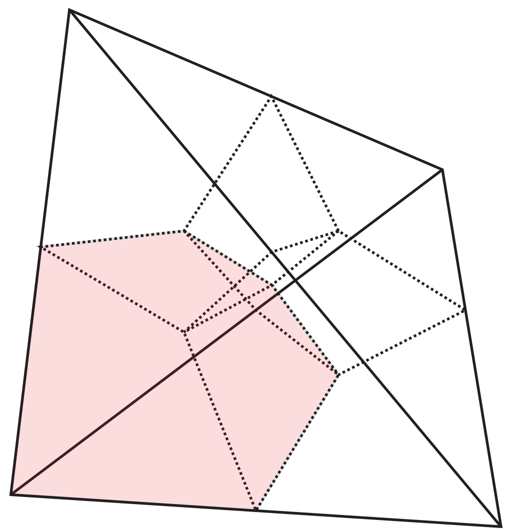

Figure 1–1: Partitioning of one tetrahedron into four hexahedra, one of which is highlighted as an illustration.

in [58]. The elements' degrees of freedom consist of integrals against spaces of test functions on sub-complexes (i.e. vertices, edges, faces and the volumes) of their domains.

1.6 Hybrid meshes

The availability of these tools naturally prompts the question, "Which are best, tetrahedral or hexahedral elements?" After all, Whitney showed that any (reasonable) 3-manifold may be tesselated using tetrahedra [83] and since any tetrahedron may be divided into four hexahedra (see figure 1–1), it is perfectly possible, and most likely simpler, to implement a finite element method based on a mesh that contains just one type of shape. Unfortunately (but fortunately for this work), there is not a clear answer. Each element type has different properties and their suitability depends on the characteristics of the problem being solved.

The product structure of the cube allows the construction of hexahedral shape functions as a tensor product of three univariate functions. This allows for various optimisations. For example, the naive per-element cost of a projection onto the space of shape functions on a tetrahedron or hexahedron is $O(p^6)$: there are $O(p^3)$ shape functions, and evaluation at $O(p^3)$ quadrature points is required for each inner product. For tetrahedra, this is the best that can be done, but on the hexahedron, sum-factorisation can exploit the tensor product structure to reduce this cost to $O(p^4)$ (subject to an $O(p^3)$ increase in storage costs) [72]. When the element is based on a parallelepiped, costs for some operations can be reduced even further [71]. Another consequence of the hexahedral product construct is that we can refine anisotropically, which can be useful for dealing with boundary layers. See, for example, [69, 78, 37].

On the other hand, irregularities in a solution require h-refinement to achieve accurate approximations. These irregularities are often localised (a classic example would be the Fichera corner). Local h-refinement of tetrahedral meshes is straightforward, but for cuboid or parallelepiped meshes, *hanging nodes* are required. A hanging node is a degree of freedom on the boundary of an element for which there is no corresponding degree on the neighbouring element. See figure 1–2 for a simple example for rectangles in 2D. Hanging nodes present particular problems for both the analysis and computation of finite element methods. For example, it is no longer possible to build commuting interpolants element-wise. An analysis of the stability and approximability of finite elements with hanging nodes for the 2D de Rham complex is given in [70] and [2]. The 3D Stokes problem is considered in [78] but I am unaware of a general analysis in 3D. The effect of hanging nodes on an *hp* algorithm which uses interpolation operators to make decisions about adaptivity is discussed in [52].

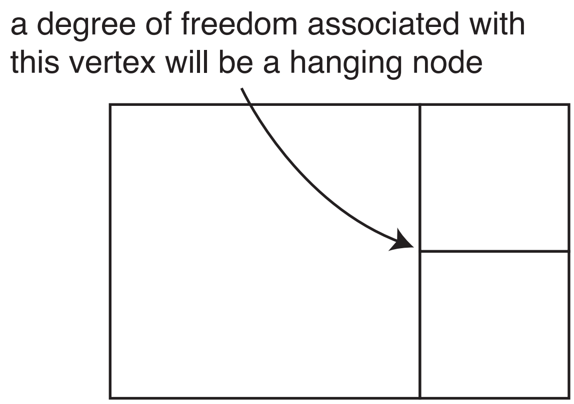

Figure 1–2: A hanging node

In an ideal world then, we might use a hybrid mesh containing tetrahedra to provide localised h-refinement and computationally-efficient cuboids to fill large spaces in which the solution is regular. This is the source of our motivation for considering pyramidal finite elements: if hexahedra and tetrahedra are combined in one mesh (and hanging nodes are to be avoided) then a layer of quadrilateral-based pyramids will be needed to "glue" the triangular and quadrilateral faces of the tets and hexes. This situation is nicely illustrated in [65]. Note that (triangularly) prismatic elements are also required; these turn out to be relatively straightforward to construct and analyse [24].

Pyramidal elements also arise more explicitly when attempting to mesh thin three dimensional structures using prismatic elements [54]. A practical example is mentioned in [41]. The authors build a finite element model of the inner ear, which contains several thin structures: the tympanic membrane, the oval window and the basilar membrane. A naive mesh generator would typically fill these structures with an unfeasibly large number of small elements. So, instead, they instruct the mesh generator to treat each structure as a two dimensional surface that should be covered with triangles. Figure 1–3 shows how these

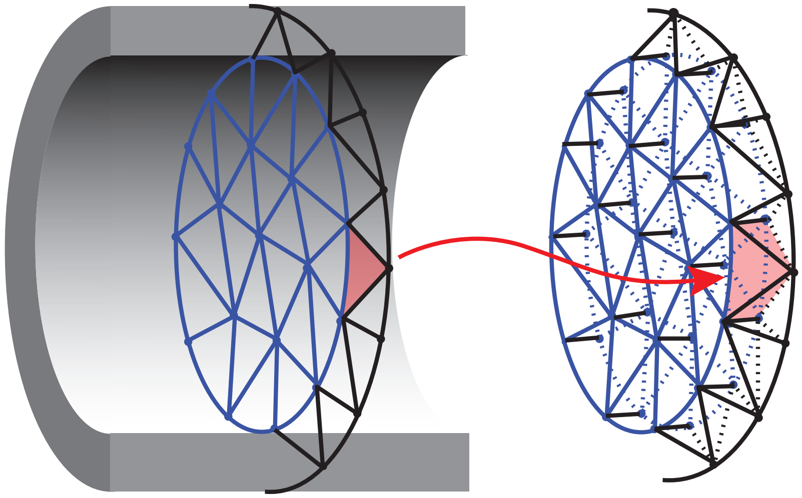

Figure 1–3: When a membrane which is initially meshed as a surface is thickened, pyramids arise in the surrounding transition layer

surfaces are then "thickened" into a cylinder of prismatic elements. The thickening process means that a layer of tetrahedra and pyramids appears around the brim of the cylinder where faces of elements which had touched the surface have been forced apart.

1.7 H^1-conforming pyramidal elements

The first person to publish a construction of a H^1-conforming pyramidal element appears to have been Bedrosian, [11]. He demonstrates first and second order nodal shape functions on the pyramid which will match neighbouring tetrahedra and hexahedra shape functions exactly and makes the important observation that:

> "... no finite polynomial shape functions would satisfy the C^0 continuity requirements ..."

The insufficiency of polynomial basis functions for the construction of pyramidal finite elements has been observed by several different authors independently. Chatzi and Preparata describe the construction of high order pyramidal basis functions [23][4] :

> "The functions are ratios of polynomials, but reduce to polynomials on the boundaries of the shape. We also prove that polynomial basis functions for Lagrangian pyramids do not exist."

Wieners proves the following as a theorem [84]:

> "There exists no continuously differentiable conforming shape functions for the pyramid which is linear resp. bilinear on the faces."

Our own version of this result is Theorem 4 in chapter 2, where we demonstrate the existence of a function whose restriction to each the face of the pyramid is polynomial, yet cannot be interpolated by a polynomial.

The significance of these results is that attempting to construct a pyramidal finite element using purely polynomial shape functions is not just sub-optimal, it is impossible. This may come as something of a surprise! Whilst it is common for finite elements to include rational functions (in fact, any non-affine element, for example, an irregular quadrilateral, does so), these functions are still, in the words of Ciarlet, "almost polynomial". Indeed, he writes that the approximation space for an isoparametric element

[4] It is asserted in [12] that the approximation spaces of Chatzi and Preparata do not include polynomials so unfortunately their method is inconsistent.

> "... generally contains functions which are not polynomials ... However, this complication is ignored in practical computation, inasmuch as all the computations are performed on [the reference element]."[25]

In contrast, the rational functions required for pyramidal elements are very much present on the reference element and are in no sense "almost polynomial": in chapter 4 we will see that the approximation spaces on each element are not even contained in the Sobolev space $H^3(K)$. This will mean that we need to take care over a particular application of Lemma 3 to the estimation of the quadrature error when using pyramidal elements.

Bedrosian refers to his basis functions as "rabbit functions", an expression originally used by Wachspress to describe functions which are "pulled out of a hat" [80]. Wachspress's book provides a construction of high order H^1-conforming shape functions on very general domains: simply connected regions of $\mathbb{R}^2$ and $\mathbb{R}^3$ bounded by a finite set of algebraic curves or surfaces (subject to some additional permissibility constraints) which he describes as *polypols* and *polypoldra* respectively. His shape functions are rational functions.

On shapes which are diffeomorphic to triangles, squares, tetrahedra and cubes, Wachspress's elements appear to be direct descriptions of isoparametric elements in mesh coordinates, rather than the more conventional approach of using a reference element. The effort required to deal with general polpols and polypoldra disguises what is arguably the more important contribution: the construction of high order H^1-conforming finite elements on arbitrary convex polygons and many convex polyhedra. The construction does not cover all polyhedra because he restricts his attention to shapes whose vertices are all order three; this means that his construction is not applicable to pyramids, where the "top" vertex is order four.

The purpose of the restriction to vertices of order three is to keep all the roots of the denominators of the rational shape functions outside the finite element domain. Interestingly, the constraint was unnecessary: twenty years later, Warren determined that the construction still works for arbitrary convex polyhedra [81, 82, 79] and so the first pyramidal elements could arguably be attributed to Wachspress. We shall see in chapter 2 that for the rational functions in our pyramidal elements, the denominator is indeed zero on the boundary of the domain but only at the top vertex and that this singularity is removable. Incidentally, Warren also proved the uniqueness of a generalisation of barycentric coordinates on convex polyhedra [3], which provides yet another proof of the necessity of rational functions on pyramids.

High order H^1-conforming pyramidal approximation spaces were constructed independently by Sherwin, Karniadakis and Warburton [72, 74]. This builds on earlier work to construct orthogonal shape functions [73] and more details are given in their book [51]. Bergot et al provide an excellent summary of continuous pyramidal finite elements [12] in which they point out that Sherwin's pyramids only contain complete spaces of polynomials under affine transformations, not under more general transformations that transform the base quadrilateral bilinearly.

Bergot et al also prove that a family of approximation spaces first suggested by Zaglmayr [85] and described in [31] is in fact "optimal" for pyramids, in that the pth space is the smallest space that contains the complete family of polynomials of degree p under a family of transformations which allow the base to map to a general quadrilateral and that associated external degrees are identical to those on the faces of tetrahedral and hexahedral elements. They recognise that our original spaces, described in chapter 2, also satisfy these conditions, although they are larger than Zaglmayr's. The new families that we present in chapter 4 include the Bergot spaces as the H^1-conforming case.

Bergot et al come to some conclusions about the effect of numerical integration on H^1-conforming pyramidal finite elements. In chapter 4 we shall see that whilst these conclusions are correct, the reasoning is insufficient because it fails to properly address the effect of the non-polynomial shape functions. Our analysis redresses this problem and also extends the result to the pyramidal finite elements for all the spaces of the de Rham complex.

1.8 Pyramidal elements for the de Rham complex

Zganski et al were the first to publish numerical experiments with H^1-conforming pyramidal elements [86]; they follow this up with first order $\mathbf{H}$(curl)-conforming elements [28] that are compatible with first and second order tetrahedral and hexahedral edge elements. Graglia et al [43] provide their own (different) $\mathbf{H}$(curl)-conforming elements along with the first $\mathbf{H}$(div)-conforming family at orders one and two. They also provide numerical evidence for an absence of spurious modes, which suggests that their elements may satisfy a commuting diagram property.

The first explicit treatment of the commutativity property on pyramids is given by Gradinaru and Hiptmair [42], who prove that their first order, "Whitney", elements commute with the de Rham complex. Bossavit shows that this construction is in some sense canonical, in that it can be derived from a unified principle that also delivers the first order tetrahedral, hexahedral and prismatic elements, [14]. An attempt at a canonical construction of high order elements is given in [35], but no consideration is given to the commutativity property.

In parallel with our work for high order elements, Zaglmayr constructed a family of commuting pyramidal elements based on the theory of local exact sequences. She presents the local exact sequence theory in her thesis, [85], but does not discuss the pyramid. A description of the approximation spaces for the elements is given in [31] but no analysis of the commuting diagram property or approximability properties has been published.

Our own elements start on what we describe as the *infinite pyramid*, which is discussed extensively in chapters 2 and 3. More conventionally, Zaglmayr works on cubes, which are mapped to the pyramid using the "Duffy transformation" [36]:

$$F : (x, y, z) \mapsto (x(1 - z), y(1 - z), z)$$

Finally, we observe that Duffy's use of this mapping to tensorialise pyramidal quadratures was predated by Stroud [76]. Stroud appears to have fallen victim to Stigler's law [75], perhaps because of the naming choices in [56].

CHAPTER 2
High order finite elements on pyramids, part I: approximation spaces.

This chapter is part I of the paper "High order finite elements on pyramids", submitted to IMA Journal of Numerical Analysis. The two parts of the paper were eventually combined into one part for submission but the natural division into two chapters is preserved here. This chapter contains an introduction to the problem and constructions of the approximation spaces for the elements.

The references to this paper by two works which are cited elsewhere in this thesis, [12, 31], were based on the draft placed on the arXiv in 2006 and substantially revised in 2007 and 2010 [62].

2.1 Introduction

High order conforming finite elements for $H(\text{curl})$ and $H(\text{div})$ spaces based on meshes composed of tetrahedra and hexahedra were first presented by Nedelec, [59]. The demands of the specific problem geometry (regions with complex features as inclusions) or efficient calculation (design of unstructured hexahedral meshes) may necessitate the use of hybrid meshes which include both tetrahedral and hexahedral elements, see e.g. [12]. If these meshes are to avoid hanging nodes then they will, in general, contain pyramids. A hybrid mesh may contain tetrahedra to provide localised h-refinement and computationally-efficient cuboids to fill large spaces in which the solution is regular, and pyramids to glue these together. This situation is nicely illustrated in [65]. Note that (triangularly) prismatic elements are also required; these turn out to be relatively straightforward to construct and analyse, see e.g. [24]. Pyramidal elements also arise more explicitly when attempting to mesh thin three dimensional structures using prismatic elements, see [54, 41].

Consider a contractible domain $D \in \mathbb{R}^3$ which is triangulated using a mesh containing both tetrahedral and hexahedral elements. If one is to avoid hanging nodes or edges, the triangulation must also, in general, include quadrilateral-based pyramids. In what follows, we assume these pyramids can be mapped in an affine manner to a reference pyramid, Ω, which has a square base and is defined as:

$$\Omega = \{\boldsymbol{\xi} = (\xi, \eta, \zeta) \in \mathbb{R}^3 \mid \xi, \eta, \zeta \geq 0,\ \xi \leq 1 - \zeta,\ \eta \leq 1 - \zeta\}. \tag{2.1}$$

It is our aim to construct high order finite elements on such a pyramid. Concretely, in this paper we present finite element triples, $(\Omega, \mathcal{U}^{(s),k}(\Omega), \Sigma^{(s),k})$, for positive integers k which are unisolvent conforming finite elements for $H^1(\Omega)$, $H(\text{curl}, \Omega)$, $H(\text{div}, \Omega)$ and $L^2(\Omega)$ respectively for $s = 0, 1, 2, 3$. Here $\mathcal{U}^{(s),k}(\Omega)$ are the kth order finite dimensional approximation spaces and the sets $\Sigma^{(s),k}$ are the associated degrees of freedom. We seek finite elements with the following properties **P1-P3**:

P1) *Compatibility:* Not only should the elements be conforming, but the restriction of each element to its triangular and quadrilateral face(s) should match that of the corresponding canonical tetrahedral and hexahedral finite element. This means that both the spaces spanned by the traces and the external degrees of freedom on faces and edges are the same as those of the usual tetrahedral/hexahedral elements. In other words, the elements should satisfy the correct *patching conditions* on inter-element boundaries, [42]. We will use [58] as our reference for the tetrahedral and hexahedral spaces and external degrees of freedom, see Table 2–1.

Table 2–1: Edge and face degrees of freedom for tetrahedral and hexahedral reference elements.

	Edge e	Face f	
	tetrahedra & hexahedra	tetrahedra	hexahedra
$H^1(\Omega)$	$\int_e pq\,ds$ $\forall q \in P^{k-2}(e)$	$\int_f pq\,dA$ $\forall q \in P^{k-3}(f)$	$\int_f pq\,dA$ $\forall q \in Q^{k-2,k-2}(f)$
$\mathbf{H}(\text{curl}, \Omega)$	$\int_e \mathbf{u} \cdot \mathbf{t}q\,ds$ $\forall q \in P^{k-1}(e)$	$\int_f \mathbf{u} \cdot \mathbf{q}\,dA$ $\forall \mathbf{q} \in P^{k-2}(f), \mathbf{q} \cdot \nu = 0$	$\int_f \mathbf{u} \times \nu \cdot \mathbf{q}\,dA$ $\mathbf{q} \in Q^{k-2,k-1} \times Q^{k-1,k-2}(f)$
$\mathbf{H}(\text{div}, \Omega)$	–	$\int_f \mathbf{u} \cdot \nu q\,dA$ $\forall q \in P^{k-1}(f)$	$\int_f \mathbf{u} \cdot \nu q\,dA$ $\forall q \in Q^{k-1,k-1}(f)$

The vertex degrees of freedom for the $H^1(\Omega)$ elements on tetrahedra and hexahedra are the same. There are no exterior degrees of freedom for the $L^2(\Omega)$ approximants. t is the unit tangent along an edge, and ν the unit outer normal to a face.

P2) *Approximation:* The discrete spaces $\mathcal{U}^{(s),k}(\Omega)$ should allow for high-order approximation to the spaces $H^1(\Omega), \mathbf{H}(\text{curl}, \Omega)$, etc. In particular, given a positive integer p, it should be possible to choose k such that all polynomials of degree p (we denote these as P^p) are contained in $\mathcal{U}^{(s),k}(\Omega)$.

P3) *Stability:* The elements satisfy a commuting diagram property:

$$\begin{array}{ccccccc} H^r(\Omega) & \xrightarrow{\nabla} & \mathbf{H}^{r-1}(\text{curl}, \Omega) & \xrightarrow{\nabla\times} & \mathbf{H}^{r-1}(\text{div}, \Omega) & \xrightarrow{\nabla\cdot} & H^{r-1}(\Omega) \\ \Pi^{(0)}\big\downarrow & & \Pi^{(1)}\big\downarrow & & \Pi^{(2)}\big\downarrow & & \Pi^{(3)}\big\downarrow \\ \mathcal{U}^{(0)}(\Omega) & \xrightarrow{\nabla} & \mathcal{U}^{(1)}(\Omega) & \xrightarrow{\nabla\times} & \mathcal{U}^{(2)}(\Omega) & \xrightarrow{\nabla\cdot} & \mathcal{U}^{(3)}(\Omega) \end{array} \tag{2.2}$$

Here $\Pi^{(s)}$, s=0,1,2,3, denote interpolation operators induced by the degrees of freedom, $\Sigma^{(s),k}$, and r is chosen so that the interpolation operators are well defined.

Gradinaru and Hiptmair [42] constructed "Whitney" elements satisfying properties **P1** and **P3** and our family of elements includes these as the lowest order case, see Section 2.5. In the engineering literature, Zgainski et al [28, 86] appear to have discovered the same first order $H(\text{curl})$-conforming element independently and also demonstrated a second order element. In [12] the authors describe high-order finite elements for $H^1(\Omega)$, but not the other spaces. Graglia et al [43] constructed $H(\text{curl})$ and $H(\text{div})$ elements of arbitrarily high order. Similarly, Sherwin [72] demonstrated H^1-conforming elements also satisfying properties (1) and (2). These high order constructions provide an explicit scheme for determining nodal basis functions; none of them address the commuting diagram property, **P3**.

The mimetic finite difference method, originally presented in 1997 [49] and further developed by several authors (e.g., [53, 21, 20, 19]) develops low-order approximations on polyhedral meshes and hence includes pyramids as a special case.

Our starting point is an observation: that it is not always possible to extend polynomial data on the faces of a pyramid using a polynomial within the pyramid. Indeed, it is *impossible* to construct useful $H^1(\Omega)$ pyramidal finite elements using only polynomial basis functions. Specifically, in Theorem 4, we demonstrate an $H^1(\Omega)$ function which has polynomial traces on the faces of the pyramid, but which does not admit a polynomial representation in the pyramid itself.

Theorem 4. *Let Ω be the pyramid defined in* (2.1). *Consider the function $u : \Omega \to \mathbb{R}$ defined by*

$$u(\xi, \eta, \zeta) = \frac{\xi\zeta(\xi + \zeta - 1)(\eta + \zeta - 1)}{1 - \zeta}.$$

Then,

1. *$u \in H^1(\Omega)$,*
2. *u has polynomial traces on the pyramid faces,*
3. *u cannot be represented by any polynomial function on Ω which also satisfies property (**P1**).*

Proof. It is straightforward to verify (1). It is easy to see $u|_{\eta=0} = -\xi\zeta(\xi+\zeta-1)$ and $u = 0$ on the other faces of the pyramid. This establishes (2).

We prove (3) by contradiction. Since Ω has Lipschitz boundary, we can extend u to a function $U \in H^1(\mathbb{R}^3)$ (see, for example, [1]). Suppose that we could represent $u = U|_\Omega$ by a polynomial function p, in a manner consistent with property (**P1**). The traces of U on the faces will then be interpolated exactly by the polynomial finite elements on the adjacent neighbouring tetrahedra and hexahedra. Since an H^1-conforming approximation must be continuous across interelement faces, we must have $p = U$ on each face of the pyramid.

Since $U = u = 0$ on four of the faces of the pyramid, we can factorise:

$$p(\xi, \eta, \zeta) = \xi\zeta(\xi+\zeta-1)(\eta+\zeta-1)\left[r(\xi,\zeta) + \eta s(\xi,\eta,\zeta)\right], \tag{2.3}$$

where r and s are polynomial. Further, $U = -\xi\zeta(\xi+\zeta-1)$ on the face $\eta = 0$ and so:

$$p(\xi, 0, \zeta) = \xi\zeta(\xi+\zeta-1)(\zeta-1)r(\xi,\zeta) = -\xi\zeta(\xi+\zeta-1), \tag{2.4}$$

which implies that $(\zeta-1)r(\xi,\zeta) = -1$. This contradicts the polynomial nature of r. □

A similar result is presented in [84], where it is claimed that, under the assumption that shape functions must be polynomial, there exists no continuously differentiable conforming shape functions for the pyramid which are linear / bilinear on the faces.

The insufficiency of polynomials can be seen in all previous successful attempts to construct pyramidal finite elements. In addition to [42], finite element bases that include rational functions are given by, e.g., [43, 72, 28, 86]. In [38, 65, 84, 55] the authors use piecewise polynomial functions via a macro-element that divides the pyramid into two or four tetrahedra. Interestingly, although [80] only applies his construction to a class of polyhedra that does not include pyramids, this restriction appears to be unnecessary and the "rational finite elements" given therein appear to include the high order H^1 pyramidal elements as a special case.

The major contribution of this paper is a comprehensive development of high-order finite elements on a pyramidal element. We will present candidate approximation spaces $\mathcal{U}^{(s),k}(\Omega)$ for $s = 0, 1, 2, 3$ and $k \in \mathbb{N}$, by first developing these on an infinite reference pyramid. We also show that these spaces admit convenient Helmholtz-like decompositions, and that their traces on faces and edges are consistent with traces from neighbouring elements. Hence property **P1** is satisfied by $\mathcal{U}^{(s),k}(\Omega)$. As a concrete example, we verify that our first order elements agree with those presented in [42].

Next, we provide a description of the degrees of freedom, $\Sigma^{(s),k}$ and demonstrate unisolvency. The exterior degrees of freedom agree precisely with those specified by neighbouring tetrahedral or hexahedral elements. Properties **P2** and **P3** are also established. We will use the projection-based interpolation described in [29, 32] to solve the difficult problem of defining the internal degrees of freedom on a pyramid. It is possible to use projection-based interpolation for the external degrees too, and we believe that the *hp* framework of which it is a part will also accommodate our element. However, this is not our immediate objective and the external degrees described in [58] allow for a more explicit exposition.

In Section 3.2, we show that the discrete spaces $\mathcal{U}^{(s),k}(\Omega)$ form an exact subcomplex. of the de Rham complex. That is, we show that $d\mathcal{U}^{(s),k}(\Omega) \subset \mathcal{U}^{(s+1),k}(\Omega)$ for $s = 0, 1, 2$, and that any discrete $(s+1)$–form which has a vanishing exterior derivative is derivable from a discrete potential which is an s–form. These spaces, along with the interpolants which are induced by the degrees of freedom, satisfy a "commuting diagram property" which is crucial to the stable computation of mixed problems. Finally we show that these finite elements are indeed high-order in the sense that they include high-degree polynomials. While the inclusion of high-degree polynomials is an important step towards approximability, we shall show in a subsequent paper that the usual finite element arguments need modification in our context. In particular, since the spaces $\mathcal{U}^{(s),k}(\Omega)$ contain rational functions, it is not true that high derivatives evaluate to 0, in sharp contrast to the situation for polynomials.

The organization of the rest of this paper is as follows:

Section 2.2: *The infinite reference element: some preliminaries*

Section 2.3: *The approximation spaces* $\mathcal{U}^{(s),k}(K_\infty)$ *on the infinite pyramid*

Section 2.4: *The approximation spaces* $\mathcal{U}^{(s),k}(\Omega)$ *on the finite pyramid*

Section 3.1: *The degrees of freedom* $\Sigma^{(s),k}$ *and unisolvency*

Section 3.2: *Interpolation and exact sequence property*

Section 3.3: *Polynomial approximation property*

Appendix 3.A: *Shape functions*

2.2 The infinite reference element: some preliminaries

To construct the finite elements, we shall make use of two reference elements: the *finite pyramid*, Ω, already introduced in (2.1), and the *infinite pyramid* K_∞. The infinite pyramid is an unusual, but instructive domain; it possesses hexahedral symmetries which will allow us to specify or study important properties for the approximation spaces. We will then map these spaces to the finite pyramid.

We will typically use the symbols (x, y, z) as coordinates on the infinite pyramid and (ξ, η, ζ) on the finite pyramid. The infinite reference pyramid is defined as

$$K_\infty = \{\mathbf{x} = (x, y, z) \in \mathbb{R}^3 \cup \infty \mid x, y, z \geq 0,\ x \leq 1,\ y \leq 1\}. \tag{2.5}$$

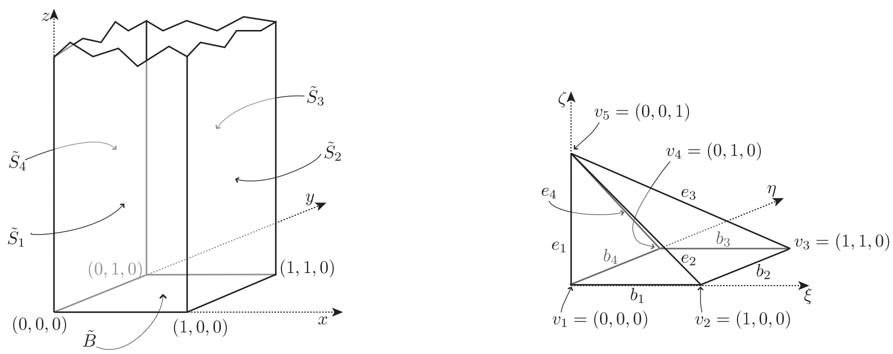

Figure 2–1: Left: The infinite pyramid K_∞. Right: The finite reference pyramid Ω

Figure 2–1 shows the two pyramids. The vertical faces of the infinite pyramid lie in the planes $y = 0$, $x = 1$, $y = 1$, $x = 0$. We denote them as $S_{1,K_\infty}, S_{2,K_\infty}, S_{3,K_\infty}$, and S_{4,K_∞} respectively, and the corresponding faces on the finite pyramid $S_{i,\Omega} = \phi(S_{i,K_\infty})$. Let B_{K_∞} refer to the base face, $z = 0$, of the infinite pyramid and B_Ω the base face of the finite pyramid. The vertices of the finite pyramid are denoted v_i, $i = 1..5$, with v_5 the point $(0,0,1)$.

2.2.1 The infinite reference element: pullbacks

To associate the finite and infinite pyramids, define the bijection $\phi : K_\infty \to \Omega$

$$\phi(x,y,z) = \left(\frac{x}{1+z}, \frac{y}{1+z}, \frac{z}{1+z}\right), \qquad \phi(\infty) = (0,0,1), \tag{2.6}$$

which is a diffeomorphism if we restrict the domain to $K_\infty \backslash \infty$ (and the range to the finite pyramid with its tip removed).

The infinite pyramid will serve as a tool for the construction of the function spaces for the elements. We thus need to understand how to map functions between spaces on the finite pyramid, $\mathcal{U}^{(s),k}(\Omega)$ and the infinite pyramid, $\mathcal{U}^{(s),k}(K_\infty)$. A major consideration is for approximation spaces on the infinite pyramid to satisfy an exact sequence property. To have this exact sequence property preserved on the finite pyramid, it is necessary that the mappings between the spaces on the finite and infinite pyramids commute with the grad, curl and div operators.

In the language of differential geometry, where the elements of each space can be considered to be proxies for 0, 1, 2 and 3-forms, the mappings should be pullbacks. We shall use the same notation for each map - the context will never be ambiguous. We point the reader to [5] for an excellent treatment of the finite element exterior calculus. In this paper, we will switch between referring to objects as forms or functions, depending on the context. Formally (because we have not yet defined the appropriate Sobolev spaces on the infinite pyramid):

$$\forall u \in H^1(\Omega) \qquad \phi^* u = u \circ \phi, \tag{2.7a}$$

$$\forall E \in \mathbf{H}(\text{curl}, \Omega) \qquad \phi^* E = D\phi^T \cdot [E \circ \phi], \tag{2.7b}$$

$$\forall \mathbf{v} \in \mathbf{H}(\text{div}, \Omega) \qquad \phi^* \mathbf{v} = |D\phi| \, D\phi^{-1} \cdot [\mathbf{v} \circ \phi], \tag{2.7c}$$

$$\forall q \in L^2(\Omega) \qquad \phi^* q = |D\phi| \, [q \circ \phi], \tag{2.7d}$$

where $D\phi$ is the Jacobian matrix, $\frac{1}{(z+1)^2}\begin{pmatrix} z+1 & 0 & -x \\ 0 & z+1 & -y \\ 0 & 0 & 1 \end{pmatrix}$.

The pullbacks are bijections and the inverse pullback, $(\phi^*)^{-1}$ is equal to $(\phi^{-1})^*$. Since $z \geq 0$, $D\phi^T D\phi$ is positive definite.

The infinite reference element is a convenient tool, since it possesses both rotational symmetries and the tensorial nature of regular hexahedral elements. This is particularly useful while discussing traces onto the boundaries of the pyramid.

2.2.2 The infinite reference element: Sobolev spaces

The infinite reference pyramid has obvious symmetries, which make it easier to specify and analyze approximation spaces. However, it has semi-infinite extent along the z-direction, and we must therefore take some care when identifying the images of $H^1(\Omega)$, $H(\text{curl}, \Omega)$ etc. under the pullbacks, ϕ^*. Not surprisingly, these Sobolev spaces will have weighted norms.

Definition 5. *Let Ω_∞ be the infinite pyramid defined in* (2.5)*, and $\phi : K_\infty \to \Omega$ be the pullback map. We define the following inner product spaces:*

$H^1_w(\Omega_\infty)$ is the closure of the set of smooth scalar-valued functions $v : K_\infty \to \mathbb{R}$ under the norm induced by the inner product

$$(u, v)_{H^1_w(K_\infty)} := \int_{K_\infty} \frac{uv}{(1+z)^4} + (\nabla u)^T \mathcal{A} \nabla v d\mathbf{x}.$$

Here $\mathcal{A} = |D\phi| D\phi^{-1} D\phi^{-1^T}$ is positive definite. $H_w(\text{curl}, \Omega_\infty)$ is the closure of the set of smooth vector-valued functions (1-forms) $F : K_\infty \to (\mathbb{R})^3$ under the norm induced by inner product

$$(F, G)_{H_w(\text{curl}, K_\infty)} := \int_{K_\infty} (F)^T \mathcal{A}(G) + (\text{curl}\, F)^T \mathcal{B}(\text{curl}\, G) d\mathbf{x}.$$

Here $\mathcal{B} = |D\phi^{-1}| D\phi^T D\phi$, and is positive definite. $H_w(\text{div}, K_\infty)$ is the closure of the set of smooth vector-valued functions (2-forms) $F : K_\infty \to (\mathbb{R})^3$ with inner product

$$(F, G)_{H_w(\text{div}, K_\infty)} := \int_{K_\infty} (F)^T \mathcal{B}(G) + (\text{div}\, F)^T (1+z)^4 (\text{div}\, G) d\mathbf{x}.$$

$L^2_w(K_\infty)$ is the closure of the set of smooth scalar-valued functions (3-forms) with inner product,

$$(u, v)_{L^2_w(K_\infty)} := \int_{K_\infty} (1+z)^4 (uv) d\mathbf{x}.$$

Remark 6. *We observe that the inner products on the infinite pyramid are weighted by powers of* $\frac{1}{(1+z)}$. *The subscript* w *is used to emphasize that these are weighted norms. The weights are entirely specified by the projective mapping,* ϕ, *and the associated pull-backs for the various forms. It is important to note, for example, that* $\|u\|^2_{L^2_w(K_\infty)} = \int_{K_\infty} \frac{u^2}{(1+z)^4} d\mathbf{x}$ *if* u *is a zero form, while* $\|u\|^2_{L^2_w(K_\infty)} = \int_{K_\infty} u^2(1+z)^4 d\mathbf{x}$ *if* u *is a 3-form.*

The following theorem relates these spaces to the more familiar Sobolev spaces on the finite pyramid:

Lemma 7. *It is easy to verify that the inner product spaces* $H^1_w(K_\infty)$, $H_w(\text{curl}, K_\infty)$, $H_w(\text{div}, K_\infty)$ *and* $L^2_w(K_\infty)$ *in Definition 5 are Hilbert spaces. Morever,* $\phi^* : H^1(\Omega) \to H^1_w(K_\infty)$ *is an isometry. The analogous statements are true for* $H_w(\text{curl}, K_\infty)$, $H_w(\text{div}, K_\infty)$ *and* $L^2_w(K_\infty)$.

Proof. The pullbacks, ϕ^* are formally bijections because $\phi : K_\infty \to \Omega$ is a bijection. Suppose $\tilde{u}$ is a 0-form in $H^1(\Omega)$ and let $u = \phi^* \tilde{u}$. Then

$$\|\tilde{u}\|^2_{L^2(\Omega)} = \int_{K_\infty} |D\phi||u(\mathbf{x})|^2 d\mathbf{x} = \int_{K_\infty} \frac{1}{(1+z)^4} |u(\mathbf{x})|^2 d\mathbf{x}.$$

Now, the gradient and pull-back operator commute. We can thus use the appropriate pull-back to obtain

$$\begin{aligned} \|\nabla \tilde{u}\|^2_{L^2(\Omega)} &= \int_\Omega |\nabla \tilde{u}|^2 d\boldsymbol{\xi} = \int_\Omega |D\phi^{-1^T} \nabla u \circ \phi^{-1}|^2 d\boldsymbol{\xi} \\ &= \int_{K_\infty} |D\phi||D\phi^{-1^T} \nabla u|^2 d\mathbf{x} = \int_{K_\infty} \nabla u^T \mathcal{A} \nabla u d\mathbf{x}. \end{aligned}$$

Hence $\|\tilde{u}\|^2_{H^1(\Omega)} = \|\tilde{u}\|^2_{L^2(\Omega)} + \|\nabla \tilde{u}\|^2_{L^2(\Omega)} = \|u\|_{H^1_w(K_\infty)}$. The proofs for $H_w(\text{curl}, K_\infty)$, $H_w(\text{div}, K_\infty)$ and $L^2_w(K_\infty)$ follow analogously. □

We collect here, for convenience, concrete instantiations of the inverse pullback mapping.

$$\forall u \in H^1_w(\Omega_\infty), \qquad (\phi^{-1})^* u = u \circ \phi^{-1}, \tag{2.8a}$$

$$\forall E \in H_w \operatorname{curl}, K_\infty), \qquad (\phi^{-1})^* E = [(1+z) \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ x & y & 1+z \end{pmatrix} \cdot E] \circ \phi^{-1}, \tag{2.8b}$$

$$\forall \mathbf{v} \in H_w(\operatorname{div}, K_\infty), \qquad (\phi^{-1})^* \mathbf{v} = [(1+z)^2 \begin{pmatrix} 1+z & 0 & -x \\ 0 & 1+z & -y \\ 0 & 0 & 1 \end{pmatrix} \cdot \mathbf{v}] \circ \phi^{-1}, \tag{2.8c}$$

$$\forall q \in L^2_w(K_\infty), \qquad (\phi^{-1})^* q = [(1+z)^4 q] \circ \phi^{-1}. \tag{2.8d}$$

2.2.3 Rotations and traces

Define $R_{K_\infty} : K_\infty \to K_\infty$ to be the affine mapping that sends the infinite pyramid to itself and rotates it a quarter turn about the axis $x = y = \frac{1}{2}$, that is, the vertical face S_{1,K_∞} is mapped to S_{2,K_∞}, the face S_{2,K_∞} is mapped to S_{3,K_∞}, etc. Explicitly,

$$R_{K_\infty} : (x, y, z) \mapsto (1 - y, x, z). \tag{2.9}$$

We can also define a mapping that sends the finite pyramid to itself, rotating the faces, $R : \Omega \to \Omega$ by

$$R = \phi \circ R_{K_\infty} \circ \phi^{-1}, \qquad R : (\xi, \eta, \zeta) \mapsto (1 - \eta - \zeta, \xi, \zeta).$$

It is clear that if an approximation space $\mathcal{U}^{(s),k}(K_\infty)$ is invariant under the mapping R_{K_∞}, its (inverse) pullback to the finite pyramid will be invariant under R. This property will prove convenient when we consider exterior shape functions and exterior degrees of freedom.

The trace map from a manifold to a submanifold is the pullback of the inclusion map for differential forms (see, for example, [6], pg 41 ff.) and so we expect that zero trace data will be preserved by the pullback mapping. The following lemma makes this explicit in our concrete vector calculus formulation, where traces for 1-forms consist only of the tangential components and for 2-forms the normal components. We suppose that S_{K_∞} is a surface of the infinite pyramid and let S_Ω be its image under ϕ on the finite pyramid.

Lemma 8.

- *A vector proxy to a 1-form, u, is normal to S_Ω at a point $\xi = \phi(x)$ if and only if the pullback $\phi^* u$ is normal to S_{K_∞} at x.*
- *A vector proxy to a 2-form, u, is tangent to S_Ω at a point $\xi = \phi(x)$ if and only if the pullback $\phi^* u$ is tangent to S_{K_∞} at x.*

Proof. Let S_Ω be described (locally) by $S_\Omega = \{\xi : f(\xi) = 0\}$. Define $g = f \circ \phi$, then $S_{K_\infty} = \{x : g(x) = 0\}$. To establish the first result, let u be a 1-form which is normal to S_Ω at ξ, then

$$u(\xi) = \lambda(\xi)\nabla f(\xi) \tag{2.10}$$

for some scalar function λ. By the chain rule, and substituting (2.10)

$$\nabla g(x) = (D\phi)^T(x) \cdot (\nabla f)(\phi(x)) = (D\phi)^T(x) \cdot \frac{u(\phi(x))}{\lambda(\phi(x))} = \frac{\phi^* u}{\lambda(\phi(x))}$$
$$\Rightarrow \lambda(\phi(x))\nabla g(x) = \phi^* u(x).$$

Hence, $\phi^* u$ is normal to S_{K_∞} at x if u is normal to S_Ω at ξ. The converse statement follows since ϕ is a bijection.

To establish the second result, let u be a 2-form which is tangent to S_Ω, meaning that $u \cdot \nabla f = 0$. The chain rule gives us $\nabla g = (D\phi)^T(\nabla f) \circ \phi$ and by definition of the pullback, $\phi^* u = |D\phi|(D\phi)^{-1} \cdot (u \circ \phi)$, hence:

$$\begin{aligned}\phi^* u \cdot \nabla g &= |D\phi|(u \circ \phi)^T \cdot (D\phi^{-1})^T \cdot (D\phi)^T \cdot [(\nabla f) \circ \phi] \\ &= |D\phi|(u^T \cdot \nabla f) \circ \phi = 0.\end{aligned}$$

Hence $\phi^* u$ is tangent to S_{K_∞}. Again, the proof of the converse follows by noting that ϕ is a bijection. □

Any construction of conforming finite elements must include consideration of the traces of approximants onto inter-element boundaries. To this end, we introduce some notation for the trace maps to the different faces of the reference pyramids. L^2-conforming elements do not require any external degrees of freeom so we need not define traces for $\mathcal{U}^{3,k}(K_\infty)$.

Definition 9. *Let S_{i,K_∞} be a vertical face of K_∞. For $s = 0, 1, 2$, $k \in \mathbb{N}$ and $i = 1..4$ define the trace map Γ^s_{i,K_∞} on $\mathcal{U}^{s,k}(K_\infty)$ as the pullback of the inclusion $S_{i,K_\infty} \hookrightarrow K_\infty$. We denote by $\Gamma^s_{i,\Omega}$ the corresponding trace onto the triangular faces of the finite pyramid Ω. We similarly define the trace maps onto the base faces, that is, Γ^s_{B,K_∞} and $\Gamma^s_{B,\Omega}$ are the trace maps to B_{K_∞} and B_Ω respectively.*

A useful consequence is that trace maps commute with ϕ^*, (e.g. $\Gamma^s_{i,K_\infty} \circ \phi^* = \phi^* \circ \Gamma^s_{i,\Omega}$) so results we establish on faces and edges of K_∞ will carry over to the finite pyramid.

We can now describe the inter-element compatibility conditions to be satisfied by the traces of our approximation spaces. From [58], we can concisely denote trace spaces on each face of the kth order tetrahedral and hexahedral elements by the polynomial spaces $\tau^{(s),k}$ and $\sigma^{(s),k}$ respectively. On the triangular face $S_{1,\Omega}$ and the base face B_Ω, these spaces are defined as

$$\tau^{(0),k}(\xi,\zeta) = P^k(\xi,\zeta) \qquad \sigma^{(0),k}(\xi,\eta) = Q^{k,k}(\xi,\eta) \tag{2.11a}$$

$$\tau^{(1),k}(\xi,\zeta) = (P^{k-1}(\xi,\zeta))^2 \oplus S^{k,2}(\xi,\zeta) \quad \sigma^{(1),k}(\xi,\eta) = Q^{k-1,k}(\xi,\eta) \times Q^{k,k-1}(\xi,\eta) \tag{2.11b}$$

$$\tau^{(2),k}(\xi,\zeta) = P^{k-1}(\xi,\zeta) \qquad \sigma^{(2),k}(\xi,\eta) = Q^{k-1,k-1}(\xi,\eta) \tag{2.11c}$$

where $S^{k,2}(\xi,\zeta) = \{w(\xi,\zeta) \in (\tilde{P}^k)^2 | (\xi-\xi_0, \zeta-\zeta_0)\cdot w = 0\}$ for some fixed (ξ_0,ζ_0). In order to satisfy the compatibility condition **(P1)**, then, our approximation spaces will need to satisfy the constraints

$$\Gamma^s_{1,K_\infty} u \in \tau^{(s),k}(\xi,\zeta) \qquad \forall u \in \mathcal{U}^{(s),k}(\Omega), \forall s = 0,1,2 \tag{2.12}$$

on the face $S_{1,\Omega}$. Analogous constraints will hold on all the other faces of the pyramid Ω.

The discussions above suggest the face-wise constraints which must be satisfied by any approximation spaces $\mathcal{U}^{(s),k}(\Omega)$. However, as was demonstrated by Theorem 4 the difficulty of interpolation on a pyramid stems from the need to find an interpolant that match trace data on *all* the faces simultaneously. This point will be discussed later.

2.3 The approximation spaces $\mathcal{U}^{(s),k}(K_\infty)$ on the infinite pyramid

In this section we present the approximation spaces $\mathcal{U}^{(s),k}(K_\infty)$ on the infinite pyramid. These will be used, via the pullback map, to construct the approximation spaces $\mathcal{U}^{(s),k}(\Omega)$ on the finite pyramid. As a preliminary step, we identify families of "rational polynomials" on K_∞ which will be used extensively. We want the spaces on the finite pyramid Ω to contain all polynomials up to a specified degree. Consider the effect of the pullback mapping ϕ on a polynomial of degree k, $p = \xi^\alpha \eta^\beta \zeta^\gamma \in H^1(\Omega)$, where $\alpha + \beta + \gamma = k$:

$$\phi^* p = \frac{x^\alpha y^\beta z^\gamma}{(1+z)^k}. \tag{2.13}$$

From Lemma 7, the pullback $\phi^* p \in H^1_w(K_\infty)$. This motivates our next definition:

Definition 10. *Let $Q^{l,m,n}(x, y, z)$ be the space of polynomials of maximum degree l, m, n in x, y, z respectively. Define the space of* k-weighted tensor product polynomials*:*

$$Q_k^{l,m,n}(x, y, z) = \left\{ \frac{u}{(1+z)^k} \ : \ u \in Q^{l,m,n}(x, y, z) \right\}.$$

It will be helpful to remember the inclusion:

$$Q_k^{l,m,n} \subset Q_{k+1}^{l,m,n+1}. \tag{2.14}$$

Let $\boldsymbol{P}^n(x, z)$ be polynomials of maximum total degree n in (x, z) and define the space of k-weighted polynomials of degree n

$$\boldsymbol{P}_k^n(x, z) = \left\{ \frac{u(x, z)}{(1+z)^k} \ : \ u(x, z) \in \boldsymbol{P}^n(x, z) \right\}. \tag{2.15}$$

2.3.1 $H^1_w(K_\infty)$-conforming approximation spaces

We recall from [58] that the finite element approximation space for the kth order hexahedral element consists of polynomials of form $p = \xi^\alpha \eta^\beta \zeta^\gamma \in Q^{k,k,k}$ with $0 \le \alpha, \beta, \gamma \le k$. From (2.13), we know that $\phi^* p = \frac{x^\alpha y^\beta z^\gamma}{(1+z)^r} \in H^1_w(K_\infty)$, where $\alpha + \beta + \gamma = r$. We might therefore expect to base an approximation space for $H^1_w(K_\infty)$ on the k-weighted space, $Q_k^{k,k,k}$. However, there are some elements of $Q_k^{k,k,k}$ which, when pulled back to the finite pyramid, become undefined at $\boldsymbol{\xi}_0 = (0, 0, 1)$. The problem arises with elements of the form $\frac{x^a y^b z^k}{(1+z)^k}$ on the infinite pyramid. The following examples are illustrative.

Example 11. *Consider the monomial* $p_1(x,y,z) = x$ *on the infinite pyramid. The inverse pull-back onto the finite pyramid is* $(\phi^{-1})^*p = \frac{\xi}{1-\zeta}$. *The limit* $\lim_{\boldsymbol{\xi}\to\boldsymbol{\xi}_0}(\phi^{-1})^*p$ *depends on the path by which we approach* $\boldsymbol{\xi}_0$. *Specifically, if we take the path* $\alpha_\lambda(t) = (\lambda(1-t), 0, t)$ *then* $\lim_{t\to 1}(\phi^{-1})^*p(\alpha_\lambda(t)) = \lambda$.

Example 12. *Consider the function* $p_2(x,y,z) = \frac{z^k}{(1+z)^k}$ *on the infinite pyramid. Pulled back to the finite pyramid,* $(\phi^{-1})^*p_2 = \zeta^k$. *We must therefore retain* p_2 *in the approximation space on the infinite pyramid.*

Lemma 13. *Let* Ω_∞ *be the infinite pyramid described above, and* $k \geq 1$ *be a fixed integer.*

- *Functions* $p(x,y,z) := \frac{x^a y^b z^c}{(1+z)^k} \in Q_k^{k,k,k-1}$ *satisfy* $p \in H_w^1(K_\infty)$.
- *If* $p(x,y,z) = \frac{r(x,y)z^k}{(1+z)^k}, r(x,y) \in Q^{k,k}(x,y)$, *then* $\lim_{\boldsymbol{\xi}\to\boldsymbol{\xi}_0}(\phi^{-1})^*(p)$ *is only well-defined if* $r(x,y) \equiv 1$.

Proof. We can verify the first statement by using Definition 1. The second statement can be proved by contradiction, as in Example 11. □

This result and the examples suggest the basis functions to include in a finite-dimensional approximation space for $H_w^1(K_\infty)$.

Definition 14. *Let* k *be a positive integer. We define the underlying spaces* $\overline{\mathcal{U}^{(0)}}(K_\infty)$

$$\overline{\mathcal{U}^{(0)}}(K_\infty) = Q_k^{k,k,k-1} \oplus \operatorname{span}\left\{\frac{z^k}{(1+z)^k}\right\}. \tag{2.16}$$

Lemma 15. *The rational polynomials* $\left\{\frac{x^a y^b z^c}{(1+z)^k}, 0 \leq a, b \leq k, 0 \leq c \leq k-1\right\}$ *and* $\frac{z^k}{(1+z)^k}$ *form a basis for* $\overline{\mathcal{U}^{(0)}}(K_\infty)$. *Moreover,* $\overline{\mathcal{U}^{(0)}}(K_\infty)$ *can be represented as*

$$\overline{\mathcal{U}^{(0)}}(K_\infty) = \{u \in Q_k^{k,k,k} : \nabla u \in Q_k^{k-1,k,k-1} \times Q_k^{k,k-1,k-1} \times Q_{k+1}^{k,k,k-1}\}. \tag{2.17}$$

Proof. The basis functions are determined by using the definition of $\overline{\mathcal{U}^{(0)}}(K_\infty)$ and Lemma 13. The gradients of rational functions of the form $\frac{x^a y^b z^c}{(1+z)^k}$ are 1-forms in $Q_k^{k-1,k,k-1} \times Q_k^{k,k-1,k-1} \times Q_{k+1}^{k,k,k-1}$. Moreover, $\nabla \frac{z^k}{(1+z)^k} = (0, 0, \frac{kz^{k-1}}{(1+z)^{k+1}})^T$. The reverse inclusion follows readily by a similar calculation. This establishes the alternative characterization of $\overline{\mathcal{U}^{(0)}}(K_\infty)$. □

We must now constrain these spaces to obtain the approximation spaces which satisfy the compatibility constraints **P1**. This follows the discussion in Section 2.2.3, and specifically (2.12).

Definition 16. *Let k be a positive integer. We define the kth order approximation spaces $\mathcal{U}^{(0)}(K_\infty)$:*

$$\mathcal{U}^{(0)}(K_\infty) = \{u \in \overline{\mathcal{U}^{(0)}}(K_\infty) \mid \Gamma_{1,K_\infty} \in P_k^k[x,z], \text{ similarly on } S_{i,K_\infty}, i = 2,3,4\}. \quad (2.18)$$

Since we will be working in the projection-based interpolation framework while specifying internal degrees of freedom, we define a subspace $\mathcal{U}_0^{(0)}(K_\infty)$, consisting of functions in $\mathcal{U}^{(0)}(K_\infty)$ with zero trace on the boundary of K_∞. Clearly, $\mathcal{U}_0^{(0)}(K_\infty) = \{x(1-x)y(1-y)zu,\ u \in Q_k^{k-2,k-2,k-2}\}$.

In Appendix 3.A, we present the shape functions in $\mathcal{U}^{(0)}(K_\infty)$ associated with the faces, edges and vertices of K_∞. These are linearly independent. Moreover, the number of these functions associated with a given triangular or square face is exactly the same as the dimension of trace spaces $\tau^{(0),k}$ or $\sigma^{(0),k}$ respectively.

2.3.2 $H_w(\text{curl}, K_\infty)$-conforming approximation spaces

We now present the construction of the approximation space, $\mathcal{U}^{(1)}(K_\infty)$, of $H_w(\text{curl}, K_\infty)$. As before, this construction is motivated by the ultimate goal of constructing a finite element approximation space for $H_w(\text{curl}, \Omega)$ which satisfies property (**P1**).

To satisfy the commuting diagram property we will need, at the very least, to have $\nabla\mathcal{U}^{(0)}(K_\infty) \subset \mathcal{U}^{(1)}(K_\infty)$. The alternate characterization of $\overline{\mathcal{U}^{(0)}}(K_\infty)$ in Lemma 15 suggests that we might consider the space $Q_k^{k-1,k,k-1} \times Q_k^{k,k-1,k-1} \times Q_{k+1}^{k,k,k-1}$ as a candidate for an approximation space for $H_w(\text{curl}, K_\infty)$. However, this space includes functions that are undefined at the point $\boldsymbol{\xi}_0 = (0, 0, 1)$ on the finite pyramid. We must be careful here to identify what kind of discontinuities we wish to exclude on the finite pyramid. Firstly, we are not interested in point values of these functions, only their tangential components. Secondly, given a particular tangent direction, $\overline{v}$ on a face of the finite pyramid, it only makes sense to consider limits taken along paths on faces tangent to $\overline{v}$. The following examples illuminate these points.

Example 17. *Consider* $u = \begin{pmatrix} y/(1+z) \\ 0 \\ 0 \end{pmatrix} \in Q_k^{k-1,k,k-1} \times Q_k^{k,k-1,k-1} \times Q_{k+1}^{k,k,k-1}$. *Its (inverse) pullback to the finite pyramid is,* $(\phi^{-1})^* u = \begin{pmatrix} \eta/(1-\zeta) \\ 0 \\ \xi\eta/(1-\zeta)^2 \end{pmatrix}$.

Let $\overline{v} = (0, -1, 1)$ *and consider the path* $\alpha_\lambda(t) = (\lambda(1-t), 1-t, t)$. *This path lies on the face* S_3 *for* $\lambda \in [0, 1]$, *and* S_3 *is tangent to* $\overline{v}$. *The limit of the component of* $(\phi^{-1})^* u$ *tangent to* $\overline{v}$ *at* $\boldsymbol{\xi}_0$ *along the path* α_λ *is* $\lim_{t\to 1} u(\alpha_\lambda(t)) \cdot \overline{v} = \lambda$. *This limit therefore depends on the path taken to approach* $\boldsymbol{\xi}_0$.

Example 18. *Let* $u = \frac{z^{k-1}}{(1+z)^{k+1}} \begin{pmatrix} r_x z \\ r_y z \\ -r \end{pmatrix}, \quad r \in Q^{k,k}[x,y], r_x := \frac{\partial r}{\partial x}, r_y := \frac{\partial r}{\partial y}$, *be a 1-form defined on the infinite pyramid. Note that we can write* $u = \nabla(\frac{rz^k}{(1+z)^{k+1}}) - \begin{pmatrix} 0 \\ 0 \\ \frac{(k+1)rz^{k-1}}{(1+z)^{k+2}} \end{pmatrix}$, *from which it is apparent that* $u \in H_w(\mathrm{curl}, K_\infty)$.

With these examples in hand, we are able to define approximation spaces for $H_w(\mathrm{curl}, K_\infty)$.

Definition 19. *Let* $k \geq 1$ *be an integer. We define the underlying space for* $H_w(\mathrm{curl}, K_\infty)$*:*

$$\overline{\mathcal{U}^{(1)}}(K_\infty) := Q_{k+1}^{k-1,k,k-1} \times Q_{k+1}^{k,k-1,k-1} \times Q_{k+1}^{k,k,k-2} \oplus \left\{ \frac{z^{k-1}}{(1+z)^{k+1}} \begin{pmatrix} r_x z \\ r_y z \\ -r \end{pmatrix}, \quad r \in Q^{k,k}[x,y] \right\}. \quad (2.19)$$

We have again used the notation $r_x := \frac{\partial r}{\partial x}, r_y := \frac{\partial r}{\partial y}$*. An equivalent characterization of the underlying space* $\overline{\mathcal{U}^{(1)}}(K_\infty)$ *is given as*

$$\overline{\mathcal{U}^{(1)}}(K_\infty) = \{u \in Q_{k+1}^{k-1,k,k} \times Q_{k+1}^{k,k-1,k} \times Q_{k+1}^{k,k,k-1} : \nabla \times u \in Q_{k+2}^{k,k-1,k-1} \times Q_{k+2}^{k-1,k,k-1} \times Q_{k+2}^{k-1,k-1,k}\}, \quad (2.20)$$

We now add constraints on the tangential traces, analogous to (2.12), to get the full definition of the approximation space $\mathcal{U}^{(1)}(K_\infty)$. Concretely, let n_i be the (outward) normal to the vertical faces S_{i,K_∞} of K_∞. Then $\Gamma^1_{i,K_\infty} u := u \times n_i|_{S_{i,K_\infty}}$ for $u \in \overline{\mathcal{U}^{(1)}(K_\infty)}$.

Definition 20. *Let $k \geq 1$ be an integer. Define*

$$\mathcal{U}^{(1)}(K_\infty) = \Big\{ u \in \overline{\mathcal{U}^{(1)}(K_\infty)} \;\Big|\; \Gamma^1_{1,K_\infty} u \in (P^{k-1}_{k+1}[x,z])^2 \oplus \tilde{P}^{k-1}_{k+1}[x,1+z] \begin{pmatrix} 1+z \\ -x \end{pmatrix}$$

$$\text{and similarly on } S_{i,K_\infty}, i = 2,3,4, \Big\}, \quad (2.21)$$

where

$$\tilde{P}^{k-1}_{k+1}[x,1+z] = \frac{1}{(1+z)^{(k+1)}} \operatorname{span}\left\{ x^a (1+z)^{k-1-a}, 0 \leq a \leq k-1 \right\}.$$

We can also identify elements in $\mathcal{U}^{(1)}(K_\infty)$ whose (tangential) traces vanish on ∂K_∞. We denote the set of these as $\mathcal{U}^{(1)}_0(K_\infty)$.

In Appendix 3.A we have tabulated the edge and face shape functions for $\mathcal{U}^{(1)}(K_\infty)$. These are linearly independent, and are consistent along shared edges. The same will be true of the pull-backs onto the finite pyramid.

2.3.3 $H_w(\operatorname{div}, K_\infty)$ and $L^2_w(K_\infty)$-conforming approximation spaces

Following a similar strategy to the previous sections, we construct approximation spaces $\mathcal{U}^{(2)}(K_\infty)$ for $\mathbf{H}_w(\operatorname{div}, K_\infty)$, such that their pull-backs to the finite pyramid provide approximation spaces for $\mathbf{H}(\operatorname{div}, \Omega)$. Again, we want $\operatorname{curl} u \in \mathcal{U}^{(2)}(K_\infty)$, $\forall u \in \overline{\mathcal{U}^{(1)}}(K_\infty)$. Now, the curls of functions $u \in \overline{\mathcal{U}^{(1)}}(K_\infty)$ satisfy

$$\nabla \times u \in Q^{k,k-1,k-1}_{k+2} \times Q^{k-1,k,k-1}_{k+2} \times Q^{k-1,k-1,k-1}_{k+1}.$$

Not all of these will have well-defined normal traces, and we must exclude these.

Definition 21. *The underlying space for the* $\mathbf{H}(\text{div})$*-conforming element is defined as:*

$$\overline{\mathcal{U}^{(2)}}(K_\infty) = Q_{k+2}^{k,k-1,k-2} \times Q_{k+2}^{k-1,k,k-2} \times Q_{k+2}^{k-1,k-1,k-1} \oplus \frac{z^{k-1}}{(1+z)^{k+2}} \begin{pmatrix} 0 \\ 2s \\ s_y(1+z) \end{pmatrix} \oplus \frac{z^{k-1}}{(1+z)^{k+2}} \begin{pmatrix} 2t \\ 0 \\ t_x(1+z) \end{pmatrix}. \tag{2.22}$$

Here $s(x,y) \in Q^{k-1,k}[x,y]$, $s_y := \frac{\partial s}{\partial y}$, *and* $t(x,y) \in Q^{k,k-1}[x,y], t_x := \frac{\partial t}{\partial x}$. *An alternate characterization of* $\overline{\mathcal{U}^{(2)}}(K_\infty)$ *is*

$$\overline{\mathcal{U}^{(2)}}(K_\infty) = \{u \in Q_{k+2}^{k,k-1,k-1} \times Q_{k+2}^{k-1,k,k-1} \times Q_{k+2}^{k-1,k-1,k} : \nabla \cdot u \in Q_{k+3}^{k-1,k-1,k-1}\}. \tag{2.23}$$

We equip this space with constraints on normal traces to obtain the full definition of the approximation space $\mathcal{U}^{(2)}(K_\infty)$ on the infinite pyramid:

Definition 22. *The* k*th order approximation space for* $H_w(\text{div}, K_\infty)$ *is*

$$\mathcal{U}^{(2)}(K_\infty) = \{u \in \overline{\mathcal{U}^{(2)}} \mid \Gamma_{1,K_\infty}^{(2)} \in P_{k+2}^{k-1}[x,z], \textit{similarly on } S_{i,K_\infty}, i = 2,3,4\}. \tag{2.24}$$

Again, we can identify the 2-forms in $\mathcal{U}^{(2)}(K_\infty)$ with vanishing normal traces on the faces of K_∞. We denote this set by $\mathcal{U}_0^{(2)}(K_\infty)$. In Appendix 3.A, we have written down a basis for $\mathcal{U}_0^{(2)}(K_\infty)$, and augmented it with shape functions for the faces.

Since we want the divergence operator to be surjective as a map from $\mathcal{U}^{(2)}(K_\infty)$ to the associated approximation space of $L_w^2(K_\infty)$, the approximation space for $L^2(K_\infty)$ (considered as the space of 3-forms) consists precisely of $\text{div}\,\mathcal{U}^{(2)}(K_\infty)$. There is no longer any need to define an underlying space.

Definition 23. *We define the approximation space* $\mathcal{U}^{(3)}(K_\infty)$ *for* $L_w^2(K_\infty)$ *as*

$$\mathcal{U}^{(3)}(K_\infty) = Q_{k+3}^{k-1,k-1,k-1}. \tag{2.25}$$

2.4 The approximation spaces $\mathcal{U}^{(s),k}(\Omega)$ on the finite pyramid

We are now readily able to define the approximation spaces for the de Rham sequence on the finite pyramid, based on the approximation spaces on the infinite pyramid K_∞:

Definition 24. *Let Ω be the finite reference pyramid as defined in* (2.1)*. Then, the kth order conforming subspaces on the finite pyramid Ω are*

$$\mathcal{U}^{(s),k}(\Omega) := \left\{ (\phi^{-1})^* u : u \in \mathcal{U}^{(s),k}(K_\infty) \right\}, \qquad s = 0,1,2,3. \tag{2.26}$$

We also denote by

$$\overline{\mathcal{U}^{(s),k}(\Omega)} := \left\{ (\phi^{-1})^* u : u \in \overline{\mathcal{U}^{(s),k}(K_\infty)} \right\}, \qquad s = 0,1,2,3. \tag{2.27}$$

the underlying spaces.

Theorem 25. *Let k be a positive integer. The finite dimensional spaces defined in* (24) *satisfy:*

$$\mathcal{U}^{(0)}(\Omega) \subset H^1(\Omega), \qquad \mathcal{U}^{(1)}(\Omega) \subset H(\mathrm{curl}, \Omega), \tag{2.28}$$

$$\mathcal{U}^{(2)}(\Omega) \subset H(\mathrm{div}, \Omega), \qquad \mathcal{U}^{(3)}(\Omega) \subset L^2(\Omega). \tag{2.29}$$

Proof. The proof follows from the definitions and properties of $\mathcal{U}^{(s),k}(K_\infty)$, the pull-back map ϕ, and Lemma 7. $\square$

In the following subsections, we shall establish several useful properties of these spaces. The analysis will typically be performed for the approximation spaces on the infinite pyramid, where the basis functions are tensorial in nature, and hexahedral symmetries can be used, which allows for simple calculations in many cases. The properties of the pull-back operator will allow us to demonstrate the results on the finite pyramid.

2.4.1 $H^1(\Omega)$-conforming approximation spaces

In this subsection, we demonstrate that the grad operator is injective on $\mathcal{U}_0^{(0)}(\Omega)$, the set of bubble functions on the pyramid.

Lemma 26. *Let $\mathcal{U}_0^{(0)}(\Omega)$ be the subset of $\mathcal{U}^{(0)}(\Omega)$, consisting of functions whose trace onto the faces and edges of Ω are zero. If some $v \in \mathcal{U}_0^{(0)}(\Omega)$ satsifies $\nabla v = 0$ then $v \equiv 0$ on Ω.*

Proof. This follows from Poincaré's inequality. □

We can easily see that $\mathcal{U}_0^{(0)}(\Omega) = \left\{(\phi^{-1})^* u : u \in \mathcal{U}_0^{(0)}(K_\infty)\right\}$. From the remarks following (2.18), it follows that $\dim \mathcal{U}_0^{(0)}(\Omega) = \dim \mathcal{U}_0^{(0)}(K_\infty) = (k-1)^3$. Note that from the definition of $\mathcal{U}_0^{(0)}(K_\infty)$ and the discussion in Section 2.2.3, the face traces of functions in $\mathcal{U}^{(0)}(\Omega)$ are compatible with those of neighbouring tetrahedral and hexahedral elements. Finally, the shape functions in the Appendix 3.A show that the edge traces are well-defined, and that edge traces can be specified in consistent manner.

2.4.2 $H(\text{curl}, \Omega)$-conforming approximation spaces

We shall establish that the grad operator maps $\overline{\mathcal{U}^{(0)}(\Omega)}$ into $\overline{\mathcal{U}^{(1)}}(\Omega)$. This is an important step towards showing exactness of the diagram in 2.2. We then show that the curl operator is injective on a certain subspace of $\mathcal{U}^{(1)}(\Omega)$, which will be used in establishing unisolvency of the edge elements on the pyramid. We will finally demonstrate a discrete Helmholtz decomposition. Note that from the definition of $\mathcal{U}_0^{(1)}(K_\infty)$ and the discussion in Section 2.2.3, the face traces of functions in $\mathcal{U}^{(1)}(\Omega)$ are compatible with those of neighbouring tetrahedral and hexahedral elements.

Lemma 27. *The gradient operator is well defined as a map from $\overline{\mathcal{U}^{(0)}}(\Omega)$ into $\overline{\mathcal{U}^{(1)}}(\Omega)$.*

Proof. It is easier to work on the infinite pyramid. Recall that a basis for $\overline{\mathcal{U}^{(0)}}(K_\infty)$ is given by functions of the form $u_{a,b,c} = \frac{x^a y^b z^c}{(1+z)^k}$, where a, b and c are integers and $a \in [0, k]$,

$b \in [0,k]$ and $c \in [0,k-1]$ or $u_{a,b,c} = \frac{z^k}{(1+z)^k}$. We will show that the gradients of each of these functions lie in $\overline{\mathcal{U}^{(1)}}(\Omega)$. The result is trivial for $c = 0$. For $c \geq 1$,

$$\nabla u_{a,b,c} = \frac{1}{(1+z)^{k+1}} \begin{pmatrix} ax^{a-1}y^b(z^{c+1}+z^c) \\ bx^a y^{b-1}(z^{c+1}+z^c) \\ x^a y^b((c-k)z^c + cz^{c-1}) \end{pmatrix}.$$

If $c \leq k-2$ then $\nabla u_{a,b,c} \in Q_{k+1}^{k-1,k,k-1} \times Q_{k+1}^{k,k-1,k-1} \times Q_{k+1}^{k,k,k-2}$. In the case $c = k-1$, we can let $r = x^a y^b$ in (2.19) and then the remainder

$$\nabla u_{a,b,c} - \frac{z^{k-1}}{(1+z)^{k+1}} \begin{pmatrix} r_x z \\ r_y z \\ -r \end{pmatrix} = \frac{1}{(1+z)^{k+1}} \begin{pmatrix} ax^{a-1}y^b z^{k-1} \\ bx^a y^{b-1} z^{k-1} \\ cx^a y^b z^{k-2} \end{pmatrix}, \tag{2.30}$$

which is in $Q_{k+1}^{k-1,k,k-1} \times Q_{k+1}^{k,k-1,k-1} \times Q_{k+1}^{k,k,k-2}$. Finally, if $c = k$ then choosing $r = 1$ in (2.19) suffices. Now use the definition of $\overline{\mathcal{U}^{(s),k}}(\Omega)$ in terms of the inverse pull-back of functions in $\overline{\mathcal{U}^{(s),k}}(K_\infty)$, and the commutativity of the grad with the pull-backs, to conclude the result. □

Note that the previous result also follows immediately from the (unproven) equivalent characterisations of the underlying spaces, (2.17) and (2.20). An important subset of $\mathcal{U}^{(1)}(\Omega)$ is the functions with vanishing tangential traces.

Definition 28. *Define $\mathcal{U}_0^{(1)}(\Omega)$ to be the subspace of functions in $\mathcal{U}^{(1)}(\Omega)$ with zero tangential component on the boundary of Ω.*

From Lemma 8, we know that if $u \in \mathcal{U}^{(1)}(\Omega)$ has zero tangential traces on a particular face or edge of Ω, then its pullback to K_∞ will have zero tangential traces on the associated face or edge. This allows us to characterize $\mathcal{U}_0^{(1)}(\Omega)$.

Lemma 29. *Functions in* $\mathcal{U}_0^{(1)}(\Omega)$ *can be represented as* $(\phi^{-1})^*(u)$*, where* $u \in \mathcal{U}_0^{(1)}(K_\infty)$ *have the form*

$$u = \begin{pmatrix} y(1-y)zq_1 \\ x(1-x)zq_2 \\ x(1-x)y(1-y)q_3 \end{pmatrix} + \frac{z^{k-1}}{(1+z)^{k+1}} \begin{pmatrix} r_x z \\ r_y z \\ -r \end{pmatrix}, \tag{2.31}$$

where $q \in Q_{k+1}^{k-1,k-2,k-2} \times Q_{k+1}^{k-2,k-1,k-2} \times Q_{k+1}^{k-2,k-2,k-2}$ *and* $r = x(1-x)y(1-y)\rho$*,* $\rho \in Q^{k-2,k-2}[x,y]$*. We have denoted* $r_x := \frac{\partial r}{\partial x}, r_y := \frac{\partial r}{\partial y}$*.*

Proof. It is easily verified that the functions u in (2.31) have zero tangential traces on the edges and faces of K_∞, and therefore their inverse pullbacks $(\phi^{-1})^*(u)$ belong to $\mathcal{U}_0^{(1)}(\Omega)$. Note also that

$$\dim \mathcal{U}_0^{(1)}(\Omega) = \dim \mathcal{U}_0^{(1)}(K_\infty) = k(k-1)^2 + k(k-1)^2 + (k-1)^3 + (k-1)^2 = 3k(k-1)^2.$$

□

The curl operator has a non-empty null space in $\mathcal{U}_0^{(1)}(\Omega)$, consisting of gradients. We can precisely characterize the complement of the gradients in $\mathcal{U}_0^{(1)}(\Omega)$.

Definition 30. *Define* $\mathcal{U}_{0,\mathrm{curl}}^{(1)}(\Omega) \subset \mathcal{U}_0^{(1)}(\Omega)$ *as*

$$\mathcal{U}_{0,\mathrm{curl}}^{(1)}(\Omega) := \left\{ v | v = (\phi^{-1})^* u, u \in \mathcal{U}_{0,\mathrm{curl}}^{(1)}(K_\infty) \right\},$$

where $\mathcal{U}_{0,\mathrm{curl}}^{(1)}(K_\infty) \subset \mathcal{U}_0^{(1)}(K_\infty)$ *consists of functions* u *of the form*

$$u = \begin{pmatrix} y(1-y)zq_1 \\ x(1-x)zq_2 \\ x(1-x)y(1-y)\rho \end{pmatrix}, \tag{2.32}$$

with $q_1 \in Q_{k+1}^{k-1,k-2,k-2}, q_2 \in Q_{k+1}^{k-2,k-1,k-2}, \rho \in Q_{k+1}^{k-2,k-2}[x,y]$*.*

We now show that $\mathcal{U}^{(1)}_{0,\text{curl}}(\Omega)$ contains no gradients.

Lemma 31. *Let $\mathcal{U}^{(1)}_{0,\text{curl}}(\Omega)$ be defined as above. Then $\mathcal{U}^{(1)}_{0,\text{curl}}(\Omega) \subset \mathcal{U}^{(1)}_{0}(\Omega)$, and the curl operator is injective on $\mathcal{U}^{(1)}_{0,\text{curl}}(\Omega)$. In other words,* $\operatorname{grad}\mathcal{U}^{(0)}_{0}(\Omega) \cap \mathcal{U}^{(1)}_{0,\text{curl}}(\Omega) = \{0\}$.

Proof. The set inclusion $\mathcal{U}^{(1)}_{0,\text{curl}}(\Omega) \subset \mathcal{U}^{(1)}_{0}(\Omega)$ follows by the definitions of $\mathcal{U}^{(1)}_{0,curl}(\Omega)$ and $\mathcal{U}^{(1)}_{0}(\Omega)$. To see that the curl operator is injective on $\mathcal{U}^{(1)}_{0,\text{curl}}(\Omega)$, we first show that the curl operator is injective on $\mathcal{U}^{(1)}_{0,\text{curl}}(K_\infty)$. The argument proceeds by contradiction.

If $k = 1$ then $\mathcal{U}^{(1)}_{0,\text{curl}}(K_\infty)$ is empty. Assume $k \geq 2$ and let $u \in \mathcal{U}^{(1)}_{0,\text{curl}}(K_\infty)$ be as in (2.32). Let either ρ or q_2 not equal to zero and write $\rho = \frac{r(x,y)}{(1+z)^{k+1}}$, $r \in Q^{k-2,k-2}(x,y)$. Suppose that $\nabla \times u = 0$. From the x-component, we obtain

$$\frac{1}{(1+z)^{k+1}} \frac{\partial}{\partial y} (y(1-y)r) - \frac{\partial}{\partial z} (zq_2) = 0.$$

There is no z-dependence in r so we can factorise $q_2 = f(z)g(x,y)$, where $f \in P^{k-2}(z)$ satisfies

$$\frac{d}{dz} \frac{zf(z)}{(1+z)^{k+1}} = \frac{1}{(1+z)^{k+1}}.$$

This is impossible, and so $\rho = q_2 = 0$. A similar consideration of the y-component shows that $q_1 = 0$. We have just established that the curl operator is injective on $\mathcal{U}^{(1)}_{0,\text{curl}}(K_\infty)$. Since the pullback and curl commute, the curl is injective on $\mathcal{U}^{(1)}_{0,\text{curl}}(\Omega)$. □

We can now state a discrete Helmholtz decomposition for $\mathcal{U}^{(1)}_{0}(\Omega)$:

Lemma 32. *The discrete approximation space $\mathcal{U}^{(1)}_{0}(\Omega) \subset \mathbf{H}(\text{curl}, \Omega)$ of functions with vanishing tangential traces on $\partial\Omega$ admits a Helmholtz decomposition. That is, if $v \in \mathcal{U}^{(1)}_{0}(\Omega)$, we can write $v = \nabla q + w$ with $q \in \mathcal{U}^{(0)}_{0}(\Omega)$ and $w \in \mathcal{U}^{(1)}_{0,\text{curl}}(\Omega)$.*

Proof. If $q \in \mathcal{U}_0^{(0)}(\Omega)$, it has zero trace on all the faces and edges of Ω. Therefore, the tangential components of ∇q are also zero on the faces and edges. We already know that grad maps $\overline{\mathcal{U}^{(0)}}(\Omega)$ into $\overline{\mathcal{U}^{(1)}}(\Omega)$ from Lemma 27, and so it is clear that grad maps $\mathcal{U}_0^{(0)}(\Omega)$ into $\mathcal{U}_0^{(1)}(\Omega)$. Injectivity of this map follows from Lemma 26. Now we count dimensions. From Section 2.4.1 we saw that $\dim \mathcal{U}_0^{(0)}(\Omega) = (k-1)^3$, and from Lemma 31,

$$\dim \mathcal{U}_{0,\text{curl}}^{(1)}(\Omega) = \dim \mathcal{U}_{0,\text{curl}}^{(1)}(K_\infty) = k(k-1)^2 + k(k-1)^2 + (k-1)^2 = (2k+1)(k-1)^2.$$

From the same lemma, we know $\text{grad}\, \mathcal{U}_0^{(0)}(\Omega) \cap \mathcal{U}_{0,\text{curl}}^{(1)}(\Omega) = 0$. Both of these are subspaces of $\mathcal{U}_0^{(1)}(\Omega)$. So,

$$\dim \left\{ \text{grad}\, \mathcal{U}_0^{(0)}(\Omega) \cup \mathcal{U}_{0,\text{curl}}^{(1)}(\Omega) \right\} = (2k+1)(k-1)^2 + (k-1)^3 = 3k(k-1)^2$$

which is the dimension of $\mathcal{U}_0^{(1)}(\Omega)$. Hence $\mathcal{U}_0^{(1)}(\Omega) = \text{grad}\, \mathcal{U}_0^{(0)}(\Omega) \oplus \mathcal{U}_{0,\text{curl}}^{(1)}(\Omega)$. □

2.4.3 $H(\text{div}, \Omega)$-conforming approximation spaces

In this subsection we shall establish that $\text{curl}\, \overline{\mathcal{U}^{(1)}}(\Omega) \subset \overline{\mathcal{U}^{(2)}}(\Omega)$. We then show that the divergence operator is injective on a certain subspace of $\mathcal{U}^{(2)}(\Omega)$. We finally demonstrate a decomposition of this discrete space.

Lemma 33. *The curl operator maps elements of* $\overline{\mathcal{U}^{(1)}}(\Omega)$ *into* $\overline{\mathcal{U}^{(2)}}(\Omega)$.

The proof of this lemma is a calculation similar to that for Lemma 27, and is omitted here.

We now need to identify elements of $\mathcal{U}^{(2)}(\Omega)$ which have vanishing normal traces on the faces of the finite pyramid. Denote these by $\mathcal{U}_0^{(2)}(\Omega)$. From Lemma 8, we know that if $\Gamma_{i,\Omega}^2 u = 0$ for some $u \in \mathcal{U}^{(2)}(\Omega)$, then the pull-back $\Gamma_{i,K_\infty}^2 \phi^* u = 0$ on the associated face of K_∞. This allows us to characterize $\mathcal{U}_0^{(2)}(\Omega)$ easily.

Lemma 34. *Functions in* $\mathcal{U}_0^{(2)}(\Omega)$ *can be represented as* $(\phi^{-1})^*(u)$, *where* $u \in \mathcal{U}_0^{(2)}(K_\infty)$ *have the form*

$$\frac{z^{k-1}}{(1+z)^{k+2}} \begin{pmatrix} 2t \\ 2s \\ (1+z)\,(s_y + t_x) \end{pmatrix} + \begin{pmatrix} x(1-x)\chi_1 \\ y(1-y)\chi_2 \\ z\chi_3 \end{pmatrix}, \tag{2.33}$$

where $s = y(1-y)\sigma$, $t = x(1-x)\tau$, *with* $\chi_1 \in Q_{k+2}^{k-2,k-1,k-2}$, $\chi_2 \in Q_{k+2}^{k-1,k-2,k-2}$, $\chi_3 \in Q_{k+2}^{k-1,k-1,k-2}$, $\sigma \in Q^{k-1,k-2}(x,y), s_y := \frac{\partial s}{\partial y}$, *and* $\tau \in Q^{k-2,k-1}(x,y), t_x := \frac{\partial t}{\partial x}$.

Proof. It is easily verified that functions of the form (2.33) have vanishing normal components on the faces S_{i,K_∞} of the infinite pyramid; their (inverse) pullbacks to the finite pyramid will thus have vanishing normal components on the faces $S_{i,\Omega}$ of Ω. □

We note also that

$$\begin{aligned} \dim \mathcal{U}_0^{(2)}(\Omega) &= \dim \mathcal{U}_0^{(2)}(K_\infty) \\ &= k(k-1)^2 + k(k-1)^2 + k^2(k-1) + k(k-1) + k(k-1) \\ &= 3k^3 - 3k^2. \end{aligned}$$

We now present a subspace of $\mathcal{U}_0^{(2)}(\Omega)$ on which the divergence operator will be injective.

Definition 35. *Define* $\mathcal{U}_{0,\mathrm{div}}^{(2)}(\Omega) := \{v | v = (\phi^{-1})^*(u), u \in \mathcal{U}_{0,\mathrm{div}}^{(2)}(K_\infty)\}$ *where*

$$\mathcal{U}_{0,\mathrm{div}}^{(2)}(K_\infty) := \mathrm{span}\{\frac{z^{k-1}}{(1+z)^{k+2}} \begin{pmatrix} r_y + 2t \\ r_x + 2s \\ (1+z)(r_{xy} + s_y + t_x) \end{pmatrix}\} \oplus \mathrm{span}\{\begin{pmatrix} 0 \\ 0 \\ z\chi_3 \end{pmatrix}\} \tag{2.34}$$

and where $r(x,y) = x(1-x)y(1-y)p(x,y), p \in Q^{k-2,k-2}, t = x(1-x)\tilde{t}, \tilde{t} \in P^{k-2}(x)$, $s = y(1-y)\tilde{s}, \tilde{s} \in P^{k-2}(y)$, *and* $\chi_3 \in Q^{k-1,k-1,k-2}_{k+2}$.

Lemma 36. *The divergence operator is injective on* $\mathcal{U}^{(2)}_{0,\mathrm{div}}(\Omega)$.

Proof. We shall first show that the divergence operator is injective on $\mathcal{U}^{(2)}_{0,\mathrm{div}}(K_\infty)$. Let u be as in (2.34). If $\nabla \cdot u = 0$, then

$$0 = \nabla \cdot u = \frac{(k-1)z^{k-2}}{(1+z)^{k+2}}(r_{xy} + t_x + s_y) + \frac{\partial}{\partial z}(z\chi_3).$$

We factorize $\chi_3 = \sum_{i=0}^{k-2} \frac{z^i}{(1+z)^{k+2}} q_i(x,y)$ and compare coefficients of like powers of z. Since r, t and s have no dependence on z, we obtain

$$\begin{aligned} 0 &= \frac{(k-1)z^{k-2}(r_{xy} + t_x + s_y)}{(1+z)^{k+2}} + \frac{d}{dz}\left(\sum_{i=0}^{k-2} \frac{z^{i+1} q_i(x,y)}{(1+z)^{k+2}}\right) \\ &= \frac{(k-1)z^{k-2}(r_{xy} + t_x + s_y)}{(1+z)^{k+2}} + \left(\sum_{i=0}^{k-2} \frac{z^{i+1}(i-k-1) + (1+i)z^i}{(1+z)^{k+3}} q_i(x,y)\right). \end{aligned}$$

This is impossible, unless

$$(r_{xy} + t_x + s_y) = 0, \quad q_i(x,y) = 0.$$

However, t only depends on x, and s only depends on y. From the form of r, it must be that $r \equiv 0 \equiv t \equiv s$. Therefore, $\nabla u \neq 0$ for any non-zero $u \in \mathcal{U}^{(2)}_{0,\mathrm{div}}(K_\infty)$. Using the properties of the pullback operator, $\nabla \cdot v = 0 \Rightarrow v \equiv 0$ for all $v \in \mathcal{U}^{(2)}_{0,\mathrm{div}}(\Omega)$. The desired result on Ω will follow by the properties of the pullback operator ϕ and the commutativity of ϕ with the divergence. $\square$

It is easy to see that

$$\dim \mathcal{U}^{(2)}_{0,\mathrm{div}}(\Omega) = \dim \mathcal{U}^{(2)}_{0,\mathrm{div}}(K_\infty) = (k-1)^2 + 2(k-1) + k^2(k-1) = k^3 - 1.$$

Just as in the previous section, we can use Lemma (36) to exhibit a convenient decomposition of the discrete approximation space.

Lemma 37. *Any* $v \in \mathcal{U}_0^{(2)}(\Omega)$ *can be decomposed as* $v = \nabla \times w_1 + w_2$ *with* $w_1 \in \mathcal{U}_{0,\mathrm{curl}}^{(1)}(\Omega)$*,* $w_2 \in \mathcal{U}_{0,\mathrm{div}}^{(2)}(\Omega)$*.*

Proof. Lemma 33 tells us that the curl operator maps $\overline{\mathcal{U}^{(1)}}(\Omega)$ into $\overline{\mathcal{U}^{(2)}}(\Omega)$. Observe that if the tangential components of v are zero on some surface then the component of $\nabla \times v$ that is normal to the surface will also be zero and so the curl operator maps $\mathcal{U}_{0,\mathrm{curl}}^{(1)}(\Omega)$ into $\mathcal{U}_0^{(2)}(\Omega)$. By Lemma 31 we know that this mapping is injective.

By construction, $\mathcal{U}_{0,\mathrm{div}}^{(2)}(\Omega)$ is a subset of $\mathcal{U}_0^{(2)}(\Omega)$ and by lemma 36, $\nabla \cdot w \neq 0$ for all $w \in \mathcal{U}_{0,\mathrm{div}}^{(2)}(\Omega)$. Hence $\mathcal{U}_{0,\mathrm{div}}^{(2)}(\Omega) \cap \mathcal{U}_{0,\mathrm{curl}}^{(1)}(\Omega)$ is empty. We now count dimensions. We established in the proof of Lemma (36) that $\mathcal{U}_{0,\mathrm{div}}^{(2)}(\Omega)$ has dimension $k^3 - 1$ and from the previous section we know $\mathcal{U}_{0,\mathrm{curl}}^{(1)}(\Omega)$ has dimension $2k^3 - 3k^2 + 1$. Thus,

$$\dim(\mathrm{curl}\,\mathcal{U}_{0,\mathrm{curl}}^{(1)}(\Omega) \cup \mathcal{U}_{0,\mathrm{div}}^{(2)}(\Omega)) = 3k^3 - 3k^2 = \dim \mathcal{U}_0^{(2)}(\Omega),$$

which shows that $\mathcal{U}_0^{(2)}(\Omega) = \mathrm{curl}\,\mathcal{U}_{0,\mathrm{curl}}^{(1)}(\Omega) \oplus \mathcal{U}_{0,\mathrm{div}}^{(2)}(\Omega)$. This establishes the desired decomposition. □

2.4.4 $L^2(\Omega)$-conforming approximation spaces

We note that the dimension of $\mathcal{U}^{(3)}(\Omega) = \dim \mathcal{U}^{(3)}(K_\infty) = \dim(Q_{k+3}^{k-1,k-1,k-1}) = k^3$. It is a straightforward matter to determine that the divergence operator is well defined as a map from $\overline{\mathcal{U}^{(2)}}(\Omega)$ to $\mathcal{U}^{(3)}(\Omega)$. We record the result here in a lemma.

Lemma 38. *The divergence operator maps elements of* $\overline{\mathcal{U}^{(2)}}(\Omega)$ *into* $\mathcal{U}^{(3)}(\Omega)$*.*

Lemma 39. *Any element* $u \in \mathcal{U}^{(3)}(\Omega)$ *can be written uniquely as*

$$u = \nabla \cdot w + \lambda, \qquad w \in \mathcal{U}_{0,\mathrm{div}}^{(2)}(\Omega),\ \lambda \in \mathbb{R}.$$

Proof. From Lemma 38, we know that $\operatorname{div} \mathcal{U}^{(2)}_{0,\mathrm{div}}(\Omega) \subset \mathcal{U}^{(3)}(\Omega)$. We also know that the constants belong to $\mathcal{U}^{(3)}(\Omega)$. Now, $\dim(\operatorname{div} \mathcal{U}^{(2)}_{0,\mathrm{div}}(\Omega)) = k^3 - 1$, which is one less than the dimension of $\mathcal{U}^{(3)}(\Omega)$. Now, suppose we could find $w \in \operatorname{div} \mathcal{U}^{(2)}_{0,\mathrm{div}}(\Omega)$ so that $\nabla w = 1$ on Ω. By definition of $\mathcal{U}^{(2)}_{0,\mathrm{div}}(\Omega)$, we know that w has zero normal components on the faces of Ω. From the divergence theorem, this is impossible. Hence, we have shown that the constants are not contained in $\operatorname{div} \mathcal{U}^{(2)}_{0,\mathrm{div}}(\Omega)$, and therefore $\operatorname{div} \mathcal{U}^{(2)}_{0,\mathrm{div}}(\Omega) \oplus \mathbb{R} = \mathcal{U}^{(3)}(\Omega)$. This completes the proof. □

We finish this subsection with an important component of the proof that our elements satisfy property **P1**.

Lemma 40. *The spaces of traces of the approximation spaces, $\mathcal{U}^{(s),k}(\Omega)$ on the faces of the pyramid are the same as those of the corresponding tetrahedral and hexahedral elements. Specifically $\Gamma^s_{i,\Omega}\mathcal{U}^{(s),k}(\Omega) = \tau^{(s),k}$ and $\Gamma^s_{B,\Omega}\mathcal{U}^{(s),k}(\Omega) = \sigma^{(s),k}$.*

Proof. In Appendix 3.A, we collect shape functions in Tables 3–1, 3–2 and 3–3 of the approximation spaces $\mathcal{U}^{(s),k}(\Omega)$ for $s = 0, 1$ and 2 respectively. It can also be easily (though tediously) verified that the traces of these shape functions on each face span the corresponding trace space from the tetrahedral and hexahedral elements. This demonstrates that $\Gamma^s_{i,\Omega}\mathcal{U}^{(s),k}(\Omega) \supseteq \tau^{(s),k}(S_{i,\Omega})$ for $i = 1, 2, 3, 4$ and $\Gamma^s_{B,\Omega}\mathcal{U}^{(s),k}(\Omega) \supseteq \sigma^{(s),k}(B)$.

Set equality is seen by examining the infinite pyramid case. By construction, if $u \in \mathcal{U}^{s,k}(K_\infty)$, then its trace $\Gamma^{(s)}_{1,K_\infty} u$ on the vertical face S_{1,K_∞} lies in the space

$$P^k_k, \quad (P^{k-1}_{k+1}[x,z])^2 \oplus \tilde{P}^{k-1}_{k+1}[x, 1+z] \begin{pmatrix} 1+z \\ -x \end{pmatrix}, \quad P^{k-1}_{k+2}$$

for $s = 0, 1, 2$ respectively. This means that $\dim(\Gamma^{(s)}_{1,\Omega}\mathcal{U}^{(s),k}(\Omega) \leq \dim \tau^{(s),k}(S_{i,\Omega})$, which establishes that $\Gamma^{(s)}_{1,\Omega}\mathcal{U}^{(s),k}(\Omega) = \tau^{(s),k}(S_{1,\Omega})$. Also, elements of $\Gamma^{(s)}_{i,\Omega}\mathcal{U}^{s,k}(\Omega)$ consist of the pullbacks of functions in $\Gamma^{s}_{i,K_\infty}\mathcal{U}^{(s),k}(K_\infty)$. Therefore, rotational symmetry means similar statements hold for the other faces as well. Finally, the dimension of $\Gamma^{s}_{B,\Omega}\mathcal{U}^{(s),k}(\Omega)$ is equal to that of $\sigma^{(s),k}(B)$ and so $\Gamma^{s}_{B,\Omega}\mathcal{U}^{(s),k}(\Omega) = \sigma^{(s),k}(B)$ □

The implication of Lemma 40 is important: the spaces $\mathcal{U}^{(s),k}(\Omega)$ allow for full compatibility well-known tetrahedral and hexahedral finite elements across interelement boundaries. This should allow for the seamless integration of pyramidal elements into a hybrid mesh consisting of tetrahedra and hexahedra.

2.5 First order elements on the pyramid

The approximation spaces $\mathcal{U}^{(s),k}(\Omega)$ constructed above include the elements presented by Gradinaru and Hiptmair [42] as the special case $k = 1$. To demonstrate this, we will map the basis functions presented in that paper onto the infinite pyramid, and demonstrate that these (pulled-back) elements belong to $\mathcal{U}^{(s),k}(K_\infty)$. The properties of the pullback then allow us to conclude the set inclusions on the finite pyramid. The reason for this indirect approach is the tensorial nature of the approximation spaces on K_∞, which makes it easier to examine basis functions.

- **The lowest-order $H^1(\Omega)$ element**: The basis functions for the $H^1(\Omega)$ element given in equation 3.2 of [42] are denoted $\pi_i,\ i = 1..5$. Set $\tilde{\pi}_i = \phi^*\pi_i$.

$$\tilde{\pi}_1 = \frac{(x-1)(y-1)}{1+z}, \quad \tilde{\pi}_2 = \frac{x(y-1)}{1+z}, \quad \tilde{\pi}_3 = \frac{(x-1)y}{1+z}, \quad \tilde{\pi}_4 = \frac{xy}{1+z},$$
$$\tilde{\pi}_5 = \frac{z}{1+z}.$$

  It is clear that $\tilde{\pi}_i \in \mathcal{U}^{(0),1}(K_\infty)$.

- **The lowest-order $\mathbf{H}(\mathrm{curl}, \Omega)$ element:** We proceed as in the $H^1(\Omega)$ case. Set $\tilde{\gamma}_i = \phi^* \gamma_i$ where the γ_i, $i = 1..8$ are the basis functions for the curl-conforming element in [42][1] :

$$\tilde{\gamma}_1 = \frac{1}{(1+z)^2}\begin{pmatrix} 1-y \\ 0 \\ 0 \end{pmatrix}, \quad \tilde{\gamma}_2 = \frac{1}{(1+z)^2}\begin{pmatrix} 0 \\ x \\ 0 \end{pmatrix}, \quad \tilde{\gamma}_3 = \frac{1}{(1+z)^2}\begin{pmatrix} y \\ 0 \\ 0 \end{pmatrix},$$
$$\tilde{\gamma}_4 = \frac{1}{(1+z)^2}\begin{pmatrix} 0 \\ 1-x \\ 0 \end{pmatrix}, \quad \tilde{\gamma}_5 = \frac{1}{(1+z)^2}\begin{pmatrix} z(1-y) \\ z(1-x) \\ (1-y)(1-x) \end{pmatrix}, \quad \tilde{\gamma}_6 = \frac{1}{(1+z)^2}\begin{pmatrix} z(y-1) \\ zx \\ x(1-y) \end{pmatrix},$$
$$\tilde{\gamma}_7 = \frac{1}{(1+z)^2}\begin{pmatrix} zy \\ z(x-1) \\ y(1-x) \end{pmatrix}, \quad \tilde{\gamma}_8 = \frac{1}{(1+z)^2}\begin{pmatrix} -zy \\ -zx \\ xy \end{pmatrix} \tag{2.35}$$

These are also the pullbacks of the basis functions for the first order curl conforming element given by Graglia et al. [43]. Note that these are all edge shape functions. It is easy to see that $\tilde{\gamma}_i$ are shape functions specified in the previous section for $H_w(\mathrm{curl}, K_\infty)$ with $k = 1$.

[1] There are minor typographical errors in [42] for two of the one-forms. Based on the preceding calculations in that paper, the correct expressions are

$$\gamma_6 = \begin{pmatrix} -z + \frac{yz}{1-z} \\ \frac{xz}{1-z} \\ x - \frac{xy}{1-z} + \frac{xyz}{(1-z)^2} \end{pmatrix}, \quad \gamma_7 = \begin{pmatrix} \frac{yz}{1-z} \\ -z + \frac{xz}{1-z} \\ y - \frac{xy}{1-z} + \frac{xyz}{(1-z)^2} \end{pmatrix}$$

- **The lowest-order $\mathbf{H}(\mathrm{div},\Omega)$ element:** Set $\tilde{\zeta}_i = \phi^*\zeta_i$, where $\zeta_i,\ i = 1..5$ are the divergence-conforming basis functions

$$\begin{aligned}\tilde{\zeta}_1 &= \frac{1}{(1+z)^3}\begin{pmatrix}0\\2(y-1)\\z\end{pmatrix}, \quad \tilde{\zeta}_2 = \frac{1}{(1+z)^3}\begin{pmatrix}2(x-1)\\0\\z\end{pmatrix},\\ \tilde{\zeta}_3 &= \frac{1}{(1+z)^3}\begin{pmatrix}2x\\0\\z\end{pmatrix}, \quad \tilde{\zeta}_4 = \frac{1}{(1+z)^3}\begin{pmatrix}0\\2y\\z\end{pmatrix}, \tilde{\zeta}_5 = \frac{1}{(1+z)^3}\begin{pmatrix}0\\0\\-1\end{pmatrix}.\end{aligned} \tag{2.36}$$

For completeness, we note that $\mathcal{U}^{(3),1}(\Omega)$ consists of the constants, which map to multiples of $\frac{1}{(1+z)^4}$ on the infinite pyramid. The above collections of functions are consistent with the definitions (2.16), (2.19), (2.22) and (2.25).

CHAPTER 3

High order finite elements on pyramids, part II: unisolvency and exactness

This chapter is part II of the paper "High order finite elements on pyramids", submitted to IMA Journal of Numerical Analysis. It contains a specification of the degrees of freedom for the pyramidal elements and demonstrates that the degrees are unisolvent and induce interpolation operators that satisfy a commuting diagram property.

3.1 The degrees of freedom $\Sigma^{(s),k}$ and unisolvency

We now define degrees of freedom $\Sigma^{(s),k}$ which are linearly independent and unisolvent for the finite element approximation spaces $\mathcal{U}^{(s),k}(\Omega)$. Our construction is based on the premise of "patching" as discussed in [42]: "the traces of discrete differential forms onto any interelement boundary (a (n-1)-face) have to be unique and they have to be fixed by the degrees of freedom associated with that face". This means the exterior degrees of freedom for Ω must be identical with those of neighbouring tetrahedra or hexahedra. Thus, to satisfy property **P1**, we insist that the degrees of freedom on interelement boundaries (vertices, edges and faces) are the same as those from neighboring tetrahedra and hexahedra. Another important consideration is locality. The authors in [42] correctly identify that: "expressions for integrals on edges contained on a face $S_{i,\Omega}$ should only depend on the degrees of freedom on that face"; addressing this challenge reveals the difficulty of treating a pyramid as a degenerate finite hexahedral element. In our case, the degrees are chosen to be local *ab initio*, but the challenge is to prove unisolvency.

In this section we use the same exterior degrees of freedom as specified in [58]. We show that these are indeed dual to the exterior shape functions specified in Appendix 3.A. We then have to specify degrees of freedom for the remaining objects in the approximation space; for these we use the projection-based degrees of freedom as in Demkowicz [32]. We finally show that the set of degrees of freedom are unisolvent. Throughout this and the subsequent sections, if P is some finite-dimensional vector space, we will use the notation $\mathcal{B}\left[P\right]$ to denote an arbitrary basis.

3.1.1 H^1-conforming element

In order to fully describe the H^1-conforming finite element on a pyramid, we need to specify 4 classes of functionals which form a dual set to the approximating basis functions: vertex, edge, face and volume degrees of freedom. We call the set of these functionals $\Sigma^{(0),k}$, and then show that $(\Omega, \mathcal{U}^{(0)}(\Omega), \Sigma^{(0),k})$ is a conforming and unisolvent element for $H^1(\Omega)$. We shall follow the presentation in Chapter 5 of [58].

Depending on k not all of the degrees of freedom will be needed. We explicitly design the vertex, edge and face classes of these degrees of freedom to match those of tetrahedral or hexahedral elements. In order that the function evaluations be well-defined, let $p \in H^{3/2+\epsilon}(\Omega)$ for some $\epsilon > 0$.

1. *Vertex degrees of freedom:* let v_i, $i = 1..5$ be the vertices of the finite pyramid. Then M_V is the set of vertex degrees of freedom m_{v_i} where

$$m_{v_i}(p) := p(v_i), i = 1..5.$$

   These are identical to the vertex degrees of freedom on tetrahedral or hexahedral elements.

2. *Edge degrees of freedom:* these are given by the set M_E of functionals of the form

$$m_{e,q}(p) := \int_e pq\, ds, \quad q \in \mathcal{B}\left[P^{k-2}(e)\right], \qquad \text{for each edge, } e. \tag{3.1a}$$

There are $k-1$ linearly independent functionals $m_{e,q}$ for each of the eight edges $e \in E$. The form of these degrees of freedom is the same for "vertical" edges, e_i, and base edges, b_i. Again, these are identical to the edge degrees of freedom on tetrahedral or hexahedral elements. If $k < 2$ these degrees of freedom are not used.

3. *Face degrees of freedom:* the degrees of freedom on the triangular faces, M_S correspond to those on the faces of tetrahedral elements. They have the form:

$$m_{S_i,q}(p) = \int_{\Gamma_i} pq\, dA, \quad q \in \mathcal{B}\left[P^{k-3}(S_{i,\Omega})\right], \quad i = 1..4. \tag{3.1b}$$

   There are $(k-1)(k-2)/2$ such degrees for each face.

   The degrees of freedom on the base face, M_B correspond to those for hexahedral elements:

$$m_{B,l}(p) = \int_{B} pq\, dA, \quad q \in \mathcal{B}\left[Q^{k-2,k-2}(B)\right]. \tag{3.1c}$$

   There are $(k-1)^2$ such degrees. The face degrees of freedom are $M_F = M_S \cup M_B$. If $k < 2$ these degrees of freedom are not used.

4. *Volume degrees of freedom:* denote by $\mathcal{U}_0^{(0)}(\Omega)$ the subset of $\mathcal{U}^{(0)}(\Omega)$ with zero boundary traces. Then the volume degrees of freedom are given by

$$M_\Omega := \left\{p \mapsto \int_\Omega \nabla p \cdot \nabla q\, dV, \quad q \in \mathcal{B}\left[\mathcal{U}_0^{(0)}(\Omega)\right]\right\}. \tag{3.1d}$$

   The dimension of $\mathcal{U}_0^{(0)}(\Omega)$ is $(k-1)^3$. If $k < 2$ these degrees of freedom are not used.

The set of all degrees of freedom for $s = 0$ is $\Sigma^{(0),k} := M_V \cup M_E \cup M_F \cup M_\Omega$. We can now state the major conformance and unisolvency result:

Theorem 41. *The element* $(\Omega, \mathcal{U}^{(0)}(\Omega), \Sigma^{(0),k})$ *is* H^1*-conforming and unisolvent.*

Proof. To show that this element is conforming, we need to establish that the vanishing of the vertex, edge and face degrees of freedom on a face of the pyramid for some $p \in \mathcal{U}^{(0)}(\Omega)$ implies that $p \equiv 0$ on that face. By Lemma 40 the trace $\Gamma^0_{i,\Omega} p$ to the triangular face $S_{i,\Omega}$ lies in $\tau^{(0),k}$. The trace $\Gamma^0_{B,\Omega} p$ lies in $\sigma^{(0),k}$. Now, we have chosen the degrees of freedom so that on each each face they are also identical to to those of the corresponding (conforming) tetrahedral or hexahedral element. The vanishing of the external degrees of freedom associated with a face therefore implies that $p \equiv 0$ on that face, see Lemmas 5.47 and 6.9 of [58]

For unisolvency we need to show that for any vector $(u_i) \in \mathbb{R}^{\dim \Sigma^{(0),k}}$, there exists a unique element $u \in \mathcal{U}^{(0)}(\Omega)$ with $m_i(u) = u_i \ \forall m_i \in \Sigma^{(0),k}$. We first observe that $\dim \Sigma^{(0),k} = k^3 + 3k + 1 = \dim \mathcal{U}^{(0)}(\Omega)$ and so uniqueness implies existence, i.e. we need to show that if *all* the degrees of freedom of $p \in \mathcal{U}^{(0)}(\Omega)$ vanish, then $p \equiv 0$ on Ω. We have just seen that the vanishing of the external degrees of freedom implies $p = 0$ on $\partial\Omega$ and hence $p \in \mathcal{U}^{(0)}_0(\Omega)$. The vanishing of the volume degrees of freedom implies that

$$\int_\Omega \nabla p \cdot \nabla q \, dV = 0, \quad \forall q \in \mathcal{U}^{(0)}_0(\Omega).$$

Hence $\int_\Omega |\nabla p|^2 \, dV = 0$, from which we easily see that $p \equiv 0$. □

3.1.2 $H(\text{curl})$-conforming element

A curl-conforming pyramidal element is defined by the triple $(\Omega, \mathcal{U}^{(1)}(\Omega), \Sigma^{(1),k})$ where the degrees of freedom $\Sigma^{(1),k}$ are associated with the edges, faces, and volume of the pyramid. Again, we follow the presentation of [58]: let t be a unit tangent vector along the edge e, ν be the normal to a given face, and let $u \in H^r(\text{curl}, \Omega)$ be smooth enough that the following functionals are well-defined:

1. *Edge degrees of freedom*:

$$M_E := \left\{ u \mapsto \int_e u \cdot tq\, ds, \quad \forall q \in \mathcal{B}\left[P^{k-1}(e_i)\right] \quad \forall e \in E \right\} \tag{3.2a}$$

2. *Face degrees of freedom*: here we must differentiate between the triangular and square faces of the pyramid. On the triangular faces, we specify face degrees of freedom which are identical to those for tetrahedral elements:

$$M_S := \left\{ u \mapsto \int_{S_{i,\Omega}} u \cdot q\, dA, \quad \forall q \in \mathcal{B}\left[T_i\right] \quad i = 1..4 \right\} \tag{3.2b}$$

where $T_i = \left\{ q \in (P^{k-2}(S_{i,\Omega}))^3 \mid q \cdot \nu = 0 \right\}$

On the base face, B, the degrees of freedom are identical to those for hexahedral elements:

$$M_B := \left\{ u \mapsto \int_B u \cdot q\, dA, \quad \forall q \in \mathcal{B}\left[Q^{k-2,k-1}(B) \times Q^{k-1,k-2}(B)\right] \right\}. \tag{3.2c}$$

The class of face degrees of freedom is then $M_F = M_S \cup M_B$.

3. *Volume degrees of freedom*: here we must specify the degrees of freedom associated with "gradient bubbles" $\nabla \mathcal{U}_0^{(0)}(\Omega)$ and "curl bubbles" $\mathcal{U}_{0,\text{curl}}^{(1)}(\Omega)$.

$$M_\Omega^{\text{grad}} := \left\{ u \mapsto \int_\Omega u \cdot \nabla q\, dV, \quad \forall q \in \mathcal{B}\left[\mathcal{U}_0^{(0)}(\Omega)\right] \right\}, \tag{3.2d}$$

$$M_\Omega^{\text{curl}} := \left\{ u \mapsto \int_\Omega \nabla \times u \cdot \nabla \times v\, dV, \quad \forall v \in \mathcal{B}\left[\mathcal{U}_{0,\text{curl}}^{(1)}(\Omega)\right] \right\} \tag{3.2e}$$

The volume degrees are then $M_\Omega := M_\Omega^{\text{grad}} \cup M_\Omega^{\text{curl}}$

We must demonstrate that the finite element $(\Omega, \mathcal{U}^{(1)}(\Omega), \Sigma^{(1),k})$ is indeed curl-conforming and that specifying the degrees of freedom for a $u \in \mathcal{U}^{(1)}(\Omega)$ uniquely specifies u. This is the content of the next theorem:

Theorem 42. *The element* $(\Omega, \mathcal{U}^{(1)}(\Omega), \Sigma^{(1),k})$ *is curl-conforming and unisolvent.*

Proof. By an analogous argument to that given for the $s = 0$ case in Theorem 41 we see that the vanishing of the external degrees for any $u \in \mathcal{U}^{(1)}(\Omega)$ implies that $u \in \mathcal{U}_0^{(1)}(\Omega)$ and thus that the element is conforming. All that remains is to show that if $u \in \mathcal{U}_0^{(1)}(\Omega)$ and all the volume degrees also vanish, then $u \equiv 0$. From Lemma 32 we can write

$$u = \nabla q' + v', \qquad q' \in \mathcal{U}_0^{(0)}(\Omega), v' \in \mathcal{U}_{0,\mathrm{curl}}^{(1)}(\Omega).$$

Since the gradient-bubble degrees of freedom, $M_\Omega^{\mathrm{grad}}(u)$ vanish, we have

$$\int_\Omega (v' + \nabla q') \cdot \nabla q \, dV = 0, \quad \forall q \in \mathcal{U}_0^{(0)}(\Omega), \Rightarrow \int_\Omega |\nabla q'|^2 = 0.$$

This allows us to conclude $\nabla q' = 0$. Moreover, since the curl-bubble degrees of freedom $M_\Omega^{\mathrm{curl}}(u)$ also vanish, we have

$$\int_\Omega \nabla \times (v' + \nabla q') \cdot \nabla \times v \, dV = 0, \quad \forall v \in \mathcal{U}_{0,\mathrm{curl}}^{(1)}(\Omega) \Rightarrow \int_\Omega |\nabla \times v'|^2 \, dV = 0.$$

Since the curl map was injective on $\mathcal{U}_{0,\mathrm{curl}}^{(1)}(\Omega)$, we know that $v' = 0$. This establishes unisolvency. □

3.1.3 $H(\mathrm{div})$-conforming element

By now the strategy of defining a conforming element using the space $\mathcal{U}^{(s),k}$ is familiar: we define exterior degrees of freedom to ensure conformancy, and use a Helmholtz-like decomposition of the approximation space to ensure unisolvency. For the triple $(\Omega, \mathcal{U}^{(2)}(\Omega), \Sigma^{(2),k})$, we define the degrees of freedom by specifying the face and volume degrees:

1. *Face degrees of freedom*: we have to specify separate degrees of freedom on the triangular and square faces. On the triangular faces $S_{i,\Omega}, i = 1..4$, we specify degrees of freedom M_S in terms of the basis functions q of $(P^{k-1}(S_{i,\Omega})$. On the base face B, we specify the face degrees of freedom M_B in terms of the basis function q of

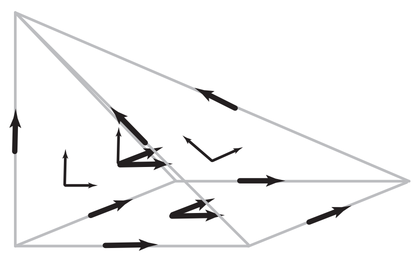

Figure 3–1: A representation of the curl degrees of freedom for $k = 2$. The degrees solely associated with the two rear triangular faces have been omitted. Bold arrows indicate two degrees of freedom. $\mathcal{U}_0^{(0),2}$ contributes one volume degree and $\mathcal{U}_{0,\mathrm{curl}}^{(1)}$ contributes four (two pairs).

$Q^{k-1,k-1}(B)$.

$$M_S := \left\{ u \mapsto \int_{S_{i,\Omega}} u \cdot \nu q \, dA, \quad \forall q \in \mathcal{B}\left[(P^{k-1}(S_{i,\Omega})\right], \quad i = 1..4 \right\} \tag{3.3a}$$

$$M_B := \left\{ u \mapsto \int_B u \cdot \nu q \, dA, \quad \forall q \in \mathcal{B}\left[Q^{k-1,k-1}(B)\right] \right\}. \tag{3.3b}$$

The set of face degrees of freedom are then $M_F = M_S \cup M_B$.

2. *Volume degrees of freedom*: $M_\Omega := M_\Omega^{\mathrm{curl}} \cup M_\Omega^{\mathrm{div}}$ where

$$M_\Omega^{\mathrm{curl}} := \left\{ u \mapsto \int_\Omega u \cdot \nabla \times v \, dV, \quad \forall v \in \mathcal{B}\left[\mathcal{U}_{0,\mathrm{curl}}^{(1)}(\Omega)\right] \right\}, \tag{3.3c}$$

$$M_\Omega^{\mathrm{div}} := \left\{ u \mapsto \int_\Omega \nabla \cdot u \, \nabla \cdot v \, dV, \quad \forall v \in \mathcal{B}\left[\mathcal{U}_{0,\mathrm{div}}^{(2)}(\Omega)\right] \right\}. \tag{3.3d}$$

Again, $\Sigma^{(2),k} := M_F \cup M_\Omega$.

Theorem 43. *The finite element triple* $(\Omega, \mathcal{U}^{(2)}(\Omega), \Sigma^{(2),k})$ *is divergence-conforming and unisolvent.*

Proof. Conformance follows by an argument similar to that for Theorems 41 and 42. For unisolvency, if all the degrees of freedom for a given $u \in \mathcal{U}^{(2)}(\Omega)$ vanish, then we must show that $u \equiv 0$. Now, since the element is conforming, we know that vanishing face degrees of freedom means $u \in \mathcal{U}_0^{(2)}(\Omega)$.

From Lemma 37, $u \in \mathcal{U}_0^{(2)}(\Omega)$ can be written as $u = \nabla \times w_1 + w_2$ with $w_1 \in \mathcal{U}_{0,\mathrm{curl}}^{(1)}(\Omega)$, $w_2 \in \mathcal{U}_{0,\mathrm{div}}^{(2)}(\Omega)$. The vanishing of the $M_\Omega^{\mathrm{curl}}(u)$ and $M_\Omega^{\mathrm{div}}(u)$ degrees of freedom implies that $\nabla \times w_1 = 0, \operatorname{div} w_2 = 0$. Now, the curl operator is injective on $\mathcal{U}_{0,\mathrm{curl}}^{(1)}(\Omega)$ from Lemma 31, and so $w_1 = 0$. The divergence operator is injective on $\mathcal{U}_{0,\mathrm{div}}^{(2)}(\Omega)$ from Lemma 36, and so $w_2 = 0$. This establishes the result. $\square$

3.1.4 L^2-conforming element

Functions in $L^2(\Omega)$ do not have well-defined traces on $\partial\Omega$, so we only need to specify volume degrees of freedom to completely define the finite element triple $(\Omega, \mathcal{U}^{(3)}(\Omega), \Sigma^{(3),k})$. The volume degrees specify the contribution from the "divergence bubble" and the constants

$$M_\Omega := \left\{ p \mapsto \int_\Omega p \nabla \cdot v \, dV, \quad \forall v \in \mathcal{B}\left[\mathcal{U}_{0,\mathrm{div}}^{(2)}(\Omega)\right] \right\}, \tag{3.4a}$$

$$M_1(p) = \left\{ p \mapsto \int_\Omega p \, dV \right\}. \tag{3.4b}$$

This specifies $\Sigma^{(3),k} := M_\Omega \cup M_1$. Unisolvency follows immediately by using Lemma 39.

3.2 Interpolation and exact sequence property

During the process of construction of the approximation subspaces $\mathcal{U}^{(s),k}$ for $H^1(\Omega)$, $H(\mathrm{curl}, \Omega)$, $H(\mathrm{div}, \Omega)$ and $L^2(\Omega)$ we saw that $d\overline{\mathcal{U}}^{(s),k}(\Omega) \subset \overline{\mathcal{U}}^{(s+1),k}(\Omega)$ for $s = 0, 1, 2$. The degrees of freedom presented in the previous section induce interpolation operators, $\Pi^{(s)}$. In this section we show that these interpolation operators make the diagram, (2.2), commute. An immediate corollary will be that the approximation spaces $\mathcal{U}^{(s),k}(\Omega)$ satisfy an exact sequence property. The degrees of freedom induce an interpolation operator on each element. We have to be careful about choosing the spaces that we are able to interpolate; for example, the vertex degrees for the H^1-conforming element require us to take point values, which are not defined for a general $H^1(\Omega)$ function. Details of the regularity required for the external degrees can be found in [58]. The problem is discussed for projection-based interpolation in [29]. For our purposes it is enough to know that it is possible to choose $r > 1$ such that all the degrees of freedom are well defined on the spaces $H^r(\Omega)$, $\mathbf{H}^{r-1}(\text{curl}, \Omega)$, and $\mathbf{H}^{r-1}(\text{div}, \Omega)$. The sets of degrees of freedom then induce interpolation operators in the expected way.

Definition 44. *Let $k \in \mathbb{N}$ be given and $s \in \{0, 1, 2, 3\}$. Let u be an $s-$form which is smooth enough for $m(u)$ to be well defined for every degree of freedom, $m \in \Sigma^{(s),k}(u)$. We define the local interpolation operator $\Pi^{(s)}$ by requiring that $\Pi^{(s)}(u) \in \mathcal{U}^{(s),k}(\Omega)$ and*

$$m(u) = m(\Pi^{(s)}u) \quad \forall m \in \Sigma^{(s),k}. \tag{3.5}$$

The interpolation operator is well-defined, since the degrees of freedom, $\Sigma^{(s),k}$, are unisolvent for the approximation space, $\mathcal{U}^{(s),k}(\Omega)$. It is local on the faces, edges and vertices of Ω, and agrees with the choice for high-degree elements presented in [58]. Therefore, the construction of a global interpolant on a mesh which includes pyramidal elements will be simple. The volume degrees of freedom are reminiscent of, and inspired by, the projection-based interpolation framework of [29]. Providing optimal *hp* estimates of the interpolation error in this framework is technical, and relies on the use of a basis-preserving extension operator. We leave this for future work.

Equipped with these interpolation operators, the finite elements satisfy a commuting diagram property:

Theorem 45. *Let $r > 0$ be chosen so that the interpolation operators $\Pi^{(s)}$ are well-defined. Then the diagram*

$$\begin{array}{ccccccc} H^r(\Omega) & \xrightarrow{d} & \mathbf{H}^{r-1}(\mathrm{curl},\Omega) & \xrightarrow{d} & \mathbf{H}^{r-1}(\mathrm{div},\Omega) & \xrightarrow{d} & H^{r-1}(\Omega) \\ \Pi^{(0)}\Big\downarrow & & \Pi^{(1)}\Big\downarrow & & \Pi^{(2)}\Big\downarrow & & \Pi^{(3)}\Big\downarrow \\ \mathcal{U}^{(0)}(\Omega) & \xrightarrow{d} & \mathcal{U}^{(1)}(\Omega) & \xrightarrow{d} & \mathcal{U}^{(2)}(\Omega) & \xrightarrow{d} & \mathcal{U}^{(3)}(\Omega) \end{array} \tag{3.6}$$

commutes.

Proof. For each $s = 0, 1, 2$, we have to show that $d\Pi^s p = \Pi^{s+1} dp$ for any $s-$form, p. This is equivalent to showing that $\Pi^{(s+1)} d(p - \Pi^{(s)} p) = 0$, which, in turn is equivalent to showing that

$$\forall m \in \Sigma^{(s+1),k}, \quad m(d(p - \Pi^{(s)} p) = 0, . \tag{3.7}$$

We split the proof by considering the exterior degrees of freedom separately. For each $s = 0, 1$, the external degrees of freedom are identical to those stated in [58]. Therefore we can adopt components of the proofs of commutativity from [59, 58] to see that the $m(d(p - \Pi^{(s)} p) = 0$ for each exterior degree of freedom, $m \in \Sigma^{(s+1),k}$, $s = 0, 1$. There are no external degrees of freedom in $\Sigma^{(3),k}$.

We still need to demonstrate (3.7) for the volume degrees of freedom in $\Sigma^{(s+1),k}$. The argument follows that of [29].

Let's start with $s = 0$. There are two classes of volume degrees of freedom in $\Sigma^{(1),k}$. The first is given in (3.2d). Let $m_v \in M_\Omega^{\mathrm{curl}}$ be a degree of freedom associated with the test function $v \in \mathcal{U}^{(1)}_{0,\mathrm{curl}}(\Omega)$

$$m_v(d(p - \Pi^{(0)}p)) = \int_\Omega \nabla \times \nabla(p - \Pi^{(0)}\nabla p) \cdot \nabla \times v \, dV = 0.$$

The second type of volume degree is given in (3.2e). Let $m_q \in M^{\mathrm{grad}}_\Omega$ be the degree of freedom associated with some $q \in \mathcal{U}^{(0)}_0(\Omega)$. Then

$$m_q(d(p - \Pi^{(0)}p)) = \int_\Omega \nabla(p - \Pi^{(0)}p) \cdot \nabla q \, dV = 0 \tag{3.8}$$

because of the definition of the interpolation operator, (3.5) and the H^1 volume degrees of freedom, (3.1d). Here the important point is that the same space of test functions is used in each of these sets of degrees of freedom.

The proof for $s = 1$ follows from a similar argument, this time using the equivalence of (3.3c) and (3.2e) to deal with the homogenous divergence-free part.

For $s = 2$, the degrees, M_Ω given in (3.4a) can be dealt with in the same fashion as (3.8). For the final degree of freeom, M_1, given in (3.4b), we note that

$$\int_\Omega \nabla \cdot (p - \Pi^{(2)}p) = \int_{\partial\Omega} (p - \Pi^{(2)}p) \cdot \nu dS = 0$$

because we have already established the commutativity of the external degrees and the test functions used for the external degrees include constants on each face. □

Theorem 46. *The following sequence is exact*

$$\mathbb{R} \longrightarrow \mathcal{U}^{(0)}(\Omega) \xrightarrow{\nabla} \mathcal{U}^{(1)}(\Omega) \xrightarrow{\nabla\times} \mathcal{U}^{(2)}(\Omega) \xrightarrow{\nabla\cdot} \mathcal{U}^{(3)}(\Omega) \longrightarrow 0. \tag{3.9}$$

Proof. We need to show the inclusions $d\mathcal{U}^{(s),k}(\Omega) \subset \mathcal{U}^{(s+1),k}(\Omega)$ for $s = 0, 1, 2$ and the property if u is an $s+1$ form with $du = 0$, then $u = dv$ for some $v \in \mathcal{U}^{(s),k}(\Omega)$.

By the definitions, (2.16), (2.19), (2.22) and (2.25), we see that $d\overline{\mathcal{U}^{(s),k}}(\Omega) \subset \overline{\mathcal{U}^{(s+1),k}}(\Omega)$ for $s = 0, 1, 2$. By Theorem 40 it follows that the face restrictions inherit the exact sequence property for tetrahedral and hexahedral elements, so that $d\mathcal{U}^{(s),k}(\Omega) \subset \mathcal{U}^{(s+1),k}(\Omega)$.

To show the second property, which is equivalent to demonstrating the existence of discrete potentials, we shall use Theorem 45. First let $s = 0$, and suppose $u \in \mathcal{U}^{(1),k}(\Omega)$ satisfies $\nabla \times u = 0$. Then there is a continuous $v \in H^1(\Omega)$ such that $u = \nabla v$. Using the commuting diagram property, $u = \Pi^{(1)} u = \Pi^{(1)} \nabla v = \nabla \Pi^{(0)} v$, and thus u is derivable from a discrete potential. The argument for $s = 1$ and $s = 2$ is identical. □

3.3 Polynomial approximation property

We now need to show that our approximation spaces $\mathcal{U}^{(s),k}(\Omega)$ allow for high-degree approximation. Concretely, given any desired degree $q \in \mathbb{N}$, we need to demonstrate that we can choose k so that polynomials of degree q are contained in $\mathcal{U}^{(s),k}(\Omega)$. We start with the L^2-conforming element.

Lemma 47. *The L^2-conforming element exactly interpolates all polynomials up to degree $k-1$. That is, $P^{k-1}(\Omega) \subset \mathcal{U}^{(3)}(\Omega)$.*

Proof. A basis for $P^{k-1}(\Omega)$ is given by functions of the form

$$u = \xi^a \eta^b (1-\zeta)^c$$

where a, b, c are non-negative integers and $a + b + c \leq k - 1$. Using the pullback formula, we see that

$$\phi^* u = \frac{x^a y^b (1+z)^{k-1-(c+a+b)}}{(1+z)^{k+3}},$$

which is in $Q_{k+3}^{k-1,k-1,k-1} = \mathcal{U}^{(3)}(\Omega)$. □

Lemma 48. *The* $H(\mathrm{div})$*-conforming element exactly interpolates all polynomials up to degree* $k-1$*. That is,* $\boldsymbol{P}^{k-1} \subset \mathcal{U}^{(2)}(\Omega)$*.*

Proof. A basis for $\boldsymbol{P}^{k-1}$ is given by functions of the form:

$$\begin{pmatrix} \xi^{a_1}\eta^{b_1}(1-\zeta)^{c_1} \\ 0 \\ 0 \end{pmatrix}, \quad \begin{pmatrix} 0 \\ \xi^{a_2}\eta^{b_2}(1-\zeta)^{c_2} \\ 0 \end{pmatrix}, \quad \begin{pmatrix} 0 \\ 0 \\ \xi^{a_3}\eta^{b_3}.(1-\zeta)^{c_3} \end{pmatrix} \tag{3.10}$$

where the a_i, b_i, c_i are non-negative integers and $a_i+b_i+c_i \leq k-1$. Pullback these functions to the infinite pyramid to get:

$$\begin{pmatrix} \frac{x^{a_1}y^{b_1}(1+z)^{\overline{c_1}}}{(1+z)^{k+2}} \\ 0 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ \frac{x^{a_2}y^{b_2}(1+z)^{\overline{c_2}}}{(1+z)^{k+2}} \\ 0 \end{pmatrix}, \frac{x^{a_3}y^{b_3}(1+z)^{\overline{c_3}}}{(1+z)^{k+2}} \begin{pmatrix} x \\ y \\ 1+z \end{pmatrix}. \tag{3.11}$$

Here we have written $\overline{c_i} = k-1-(c_i+a_i+b_i)$. The constraint $a_i+b_i+c_i \leq k-1$ ensures that if $\mathbf{u}$ is as in (3.10), then $\phi^*\mathbf{u} \in Q_{k+2}^{k,k-1,k-1} \times Q_{k+2}^{k-1,k,k-1} \times Q_{k+2}^{k-1,k-1,k}$. Moreover, divergence commutes with pullback, so $\nabla \cdot \phi^*\mathbf{u} = \phi^*\nabla \cdot \mathbf{u}$. Now $\mathbf{u} \in \boldsymbol{P}^{k-1} \Rightarrow \nabla \cdot \mathbf{u} \in \boldsymbol{P}^{k-2}$ and so by Lemma 47, $\phi^*\nabla \cdot \mathbf{u} \in Q_{k+3}^{k-1,k-1,k-1}$. We have thus established that $\phi^*(u) \in \overline{\mathcal{U}^{(2)}}(K_\infty)$, where we used the characterization of the underlying space (2.19).

Now, since u is a polynomial 2-form, its normal trace onto a triangular face of Ω will be a polynomial of the same or less degree, and hence the surface constraints in (2.24) will be satisfied automatically. Hence $\phi^*\mathbf{u} \in \mathcal{U}^{(2)}(K_\infty)$, which means that $u \in \mathcal{U}^{(2)}(\Omega)$. □

The existence of polynomials in the $\mathbf{H}(\mathrm{curl})$-conforming element may be proved in a similar manner:

Lemma 49. *The* $\mathbf{H}(\mathrm{curl})$*-conforming element exactly interpolates all polynomials up to degree* $k-1$*. That is,* $\boldsymbol{P}^{k-1} \subset \mathcal{U}^{(1)}(\Omega)$

Proof. Take basis functions for $\boldsymbol{P}^{k-1}$ as in (3.10). The pullbacks of these 1-forms to the infinite pyramid are:

$$\frac{x^{a_1}y^{b_1}(1+z)^{\overline{c_1}}}{(1+z)^{k+1}}\begin{pmatrix} z+1 \\ 0 \\ -x \end{pmatrix}, \frac{x^{a_2}y^{b_2}(1+z)^{\overline{c_2}}}{(1+z)^{k+1}}\begin{pmatrix} 0 \\ z+1 \\ -y \end{pmatrix}, \begin{pmatrix} 0 \\ 0 \\ \frac{x^{a_3}y^{b_3}(1+z)^{\overline{c_3}}}{(1+z)^{k+1}} \end{pmatrix}. \tag{3.12}$$

The constraint on the a_i, b_i, c_i ensures that these functions are all members of $Q_{k+1}^{k-1,k,k} \times Q_{k+1}^{k,k-1,k} \times Q_{k+1}^{k,k,k-1}$. We then use the commutativity of the curl operator with the pull-back, the previous lemma, and the fact that the tangential traces $\Gamma_{i,\Omega}^{(1)}u$ for polynomial 1-forms u satisfy the surface constraints of (20), shows that the functions in (3.12) are in fact in $\mathcal{U}^{(1)}(K_\infty)$. □

For the H^1-conforming element, we gain an extra polynomial degree (in fact, there are some polynomials of degree k present in $\mathcal{U}^{(1)}(\Omega)$ and $\mathcal{U}^{(2)}(\Omega)$, but not all of them).

Lemma 50. *The H^1-conforming element exactly interpolates all polynomials up to degree k. That is, $P^k \subset \mathcal{U}^{(0)}(\Omega)$*

Proof. Let $p = \xi^a \eta^b \zeta^c$, a, b, c be non-negative integers and $a + b + c \leq k$.

$$\phi^* p = \frac{x^a y^b z^c (1+z)^{k-(a+b+c)}}{(1+z)^k}, \tag{3.13}$$

If $a + b \neq 0$ it is clear that $\phi^* p \in Q_k^{k,k,k-1}$. On the other hand, if $a + b = 0$, we obtain $\phi^* p \in \{\frac{z^k}{(1+z)^k}\}$. Therefore, polynomial zero-forms p of the form (50) satisfy $\phi^* p \in Q_k^{k,k,k-1} \oplus \frac{z^k}{(1+z)^k} = \overline{\mathcal{U}^{(0)}}(\Omega)$, as required. Arguments similar to the previous cases demonstrate the inclusion $\phi^* p \in \mathcal{U}^{(0)}(K_\infty)$, and hence $p \in \mathcal{U}^{(0)}(\Omega)$. □

3.4 Conclusion

We have shown that the finite element approximation spaces $\mathcal{U}_k^s(\Omega)$ equipped with the external degrees of freedom from [58] and projection-based interpolation for the internal degrees of freedom are unisolvent and satisfy a commuting diagram property. All the kth order spaces include the complete family of polynomials of degree $k-1$ and the H^1-conforming space includes all the degree k polynomials too.

These finite element spaces are based on rational basis functions. It is not surprising that arguments which rely on the polynomial or highly differentiable nature of regular finite element spaces will fail in the current situation. In upcoming work we present a careful analysis of quadrature errors for these approximation spaces.

3.A Appendix: Shape functions

In Tables 3–1, 3–2 and 3–3, we present shape functions for $\mathcal{U}^{(s),k}(\Omega)$ for each $s = 0, 1, 2$. This is not a hierarchical construction, and no attention has been paid to the conditioning of any resulting stiffness matrices. We make use of the auxiliary coordinates, $\alpha_\xi := (1-\zeta-\xi)$ and $\alpha_\eta := (1-\zeta-\eta)$.

Representative shape functions for 0-forms on a pyramid.

Infinite Pyramid	Finite Pyramid	Comments
$\frac{(1-x)(1-y)}{(1+z)^k}$	$\frac{\alpha_\xi\alpha_\eta}{(1-\zeta)^{2-k}}$	Vertex function associated with vertex v_1.
$\frac{z^k}{(1+z)^k}$	ζ^k	Vertex function associated with vertex v_5.
$\frac{(1-x)(1-y)z^a}{(1+z)^k}$	$\frac{\alpha_\xi\alpha_\eta\zeta^a}{(1-\zeta)^{2+a-k}}$	Edge functions associated with edge e_1, $1 \le a \le k-1$.
$\frac{(1-y)(1-x)x^a}{(1+z)^k}$	$\frac{\alpha_\xi\alpha_\eta\xi^a}{(1-\zeta)^{2+a-k}}$	Edge functions associated with base edge b_1, $1 \le a \le k-1$.
$\frac{(1-x)(1-y)x^a z^b}{(1+z)^k}$	$\frac{\alpha_\xi\alpha_\eta\xi^a\zeta^b}{(1-\zeta)^{2+a+b-k}}$	Face shape functions associated with triangular face $S_{1,\Omega}$, $1 \le a, b, a+b \le k-1$.
$\frac{(1-x)(1-y)x^a y^b}{(1+z)^k}$	$\frac{\alpha_\xi\alpha_\eta\xi^a\eta^b}{(1-\zeta)^{2+a+b-k}}$	Face shape functions associated with base face B, $1 \le a, b \le k-1$.
$\frac{x(1-x)y(1-y)zx^a y^b z^c}{(1+z)^k}$	$\frac{\xi^{a+1}\eta^{b+1}\zeta^{c+1}\alpha_\xi\alpha_\eta}{(1-\zeta)^{5+a+b+c-k}}$	Volume shape functions, $0 \le a, b, c \le k-2$.

Table 3–1: Shape functions on a pyramid. Since the approximation space $\mathcal{U}^{(0),k}(K_\infty)$ is invariant under the rotation, $R_\infty : K_\infty \to K_\infty$, it is only necessary to demonstrate shape functions for a representative base vertex, vertical edge, base edge and vertical face. Then, using (2.9) and the subsequent remarks, the inverse pullback of these to the finite pyramid will also be invariant under the rotation R. Note that $\alpha_\xi := (1-\zeta-\xi)$ and $\alpha_\eta := (1-\zeta-\eta)$.

Representative shape functions for 1-forms on a pyramid.

Infinite Pyramid	Finite Pyramid	Comments
$\begin{pmatrix} 0 \\ 0 \\ \frac{(x-1)(y-1)(1+z)^c}{(1+z)^{k+1}} \end{pmatrix}$	$\begin{pmatrix} 0 \\ 0 \\ \frac{\alpha_\eta \alpha_\xi}{(1-\zeta)^{3+c-k}} \end{pmatrix}$	Edge functions associated with e_1, $0 \leq c \leq k-1$.
$\frac{1}{(1+z)^{k+1}} \begin{pmatrix} x^c(1-y) \\ 0 \\ 0 \end{pmatrix}$	$\frac{\xi^c \alpha_\eta}{(1-\zeta)^{1+c-k}} \begin{pmatrix} 1 \\ 0 \\ \frac{\xi}{1-\zeta} \end{pmatrix}$	Edge functions associated with base edge b_1, $0 \leq c \leq k-1$.
$\frac{z(1-y)}{(1+z)^{k+1}} \begin{pmatrix} x^a(1+z)^c \\ 0 \\ 0 \end{pmatrix}$	$\frac{\zeta \alpha_\eta \xi^a}{(1-\zeta)^{2+c+a-k}} \begin{pmatrix} 1 \\ 0 \\ \frac{\xi}{1-\zeta} \end{pmatrix}$	Face functions associated with triangular face $S_{1,\Omega}$, $0 \leq a, c, \quad c+a \leq k-2$.
$\frac{x(1-x)(1-y)}{(1+z)^{k+1}} \begin{pmatrix} 0 \\ 0 \\ x^a z^c \end{pmatrix}$	$\begin{pmatrix} 0 \\ 0 \\ \frac{\xi^{1+a}\alpha_\xi \alpha_\eta \zeta^c}{(1-\zeta)^{4+a+c-k}} \end{pmatrix}$	Face functions for $S_{1,\Omega}$, $0 \leq c, a, \quad c+a \leq k-3$.
$\frac{(1-y)(1-x)x^a(1+z)^{k-a-2}}{(1+z)^{k+1}} \begin{pmatrix} z \\ 0 \\ -x \end{pmatrix}$	$\begin{pmatrix} \alpha_\eta \alpha_\xi \xi^a \zeta \\ 0 \\ -\alpha_\eta \alpha_\xi \xi^{a+1} \end{pmatrix}$	Face functions for $S_{1,\Omega}$, $0 \leq a \leq k-2$.
$\frac{1}{(1+z)^{k+1}} \begin{pmatrix} y(1-y)x^a y^b \\ 0 \\ 0 \end{pmatrix}$	$\frac{\alpha_\eta \xi^a \eta^{b+1}}{(1-\zeta)^{2+a+b-k}} \begin{pmatrix} \eta \\ 0 \\ \frac{\xi}{1-\zeta} \end{pmatrix}$	Face shape functions for base face B_Ω, $a \leq k-1, b_1 \leq k-2$.
$\frac{1}{(1+z)^{k+1}} \begin{pmatrix} 0 \\ x(1-x)x^a y^b \\ 0 \end{pmatrix}$	$\frac{\alpha_\zeta \xi^{a+1} \eta^b}{(1-\zeta)^{2+a+b-k}} \begin{pmatrix} 0 \\ \xi \\ \frac{\eta}{1-\zeta} \end{pmatrix}$	Face shape functions for B_Ω, $a \leq k-2, b \leq k-1$.
$\frac{y(1-y)z\,x^a y^b z^c}{(1+z)^{k+1}} \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}$	$\frac{\alpha_\eta \xi^a \eta^{b+1} \zeta^{1+c}}{(1-\zeta)^{3+a+b+c-k}} \begin{pmatrix} 1 \\ 0 \\ \frac{\xi}{1-\zeta} \end{pmatrix}$	Volume shape functions, $0 \leq a \leq k-1$, $0 \leq b, c \leq k-2$.
$\frac{x(1-x)zx^a y^b z^c}{(1+z)^{k+1}} \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}$	$\frac{\xi^{a+1}\eta^b \zeta^{1+c} \alpha_\xi}{(1-\zeta)^{3+a+b+c-k}} \begin{pmatrix} 0 \\ 1 \\ \frac{\eta}{1-\zeta} \end{pmatrix}$	Volume shape functions, $0 \leq b \leq k-1$, $0 \leq a, c \leq k-2$.
$\frac{x(1-x)y(1-y)x^a y^b z^c}{(1+z)^{k+1}} \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$	$\frac{\xi^{1+a}\eta^{1+b}\zeta^c \alpha_\xi \alpha_\eta \tilde{q}}{(1-\zeta)^{3+a+b+c-k}} \begin{pmatrix} 0 \\ 0 \\ \frac{1}{(1-\zeta)^2} \end{pmatrix}$	Volume shape functions, $0 \leq a, b, c \leq k-2$.
$\frac{z^{k-1}}{(1+z)^{k+1}} \begin{pmatrix} \frac{\partial r}{\partial x} z \\ \frac{\partial r}{\partial y} z \\ -r \end{pmatrix}$	$\zeta^{k-1} \begin{pmatrix} \zeta \frac{\partial \tilde{r}}{\partial \xi}(1-\zeta) \\ \zeta \frac{\partial \tilde{r}}{\partial \eta}(1-\zeta) \\ -\tilde{r} + \zeta(\xi \frac{\partial \tilde{r}}{\partial \xi} + \eta \frac{\partial \tilde{r}}{\partial \eta}) \end{pmatrix}$	Volume shape functions, $0 \leq a, b \leq k-2$.
$r = x(1-x)y(1-y)x^a y^b,$	$\tilde{r} = \frac{\xi^{1+a}\alpha_\xi \eta^{1+b}\alpha_\eta}{(1-\zeta)^{a+b+4}}$	

Table 3–2: H(curl)-conforming shape functions on a pyramid. Since the approximation space $\mathcal{U}^{(1),k}(K_\infty)$ is invariant under the rotation, $R_\infty : K_\infty \to K_\infty$, it is only necessary to demonstrate shape functions for a representative base vertex, vertical edge, base edge and vertical face. Then, using (2.9) and the subsequent remarks, the inverse pullback of these to the finite pyramid will also be invariant under the rotation R. There are three distinct types of shape functions for the vertical faces, two for the base face, and four for the volume. Note that $\alpha_\xi := (1-\zeta-\xi), \alpha_\eta := (1-\zeta-\eta)$.

Representative shape functions for 2-forms on a pyramid.

Infinite Pyramid	Finite Pyramid	Comments
$\frac{1}{(1+z)^{k+2}}\begin{pmatrix}0\\2(1-y)x^az^b\\-z^k\end{pmatrix}$	$\zeta^k\begin{pmatrix}\frac{\xi}{1-\zeta}\\\frac{\eta}{(1-\zeta)}\\-1\end{pmatrix}+\begin{pmatrix}0\\\frac{2\alpha_\eta\xi^a\eta^b}{(1-\zeta)^{2+a+b-k}}\\0\end{pmatrix}$	Face shape functions associated with $S_{1,\Omega}$, $a,b\geq 0$, $a+b\leq k-1$.
$\frac{1}{(1+z)^{k+2}}\begin{pmatrix}0\\0\\x^ay^b\end{pmatrix}$	$(1-\zeta)^{k-a-b-1}\begin{pmatrix}\xi^{1+a}\eta^b\\\xi^a\eta^{b+1}\\\xi^a\eta^b\end{pmatrix}$	Base face shape functions, $0\leq a,b\leq k-1$.
$\frac{z^{k-1}}{(1+z)^{k+2}}\begin{pmatrix}2t\\0\\(1+z)(t_x)\end{pmatrix}$ $t=x(1-x)x^ay^b$	$\zeta^{k-1}\begin{pmatrix}2\tilde{t}\\0\\0\end{pmatrix}+\zeta^{k-1}\tilde{t}_x\begin{pmatrix}-\frac{\xi}{1-\zeta}\\\frac{-\eta}{1-\zeta}\\1\end{pmatrix}$ $\tilde{t}=\xi^{1+a}\alpha_\xi\eta^b(1-\zeta)^{-a-b-2}$	Volume shape functions, $0\leq a\leq k-2, 0\leq b\leq k-1$.
$\frac{z^{k-1}}{(1+z)^{k+2}}\begin{pmatrix}0\\2s\\(1+z)(s_y)\end{pmatrix}$ $s=y(1-y)x^ay^b$	$\zeta^{k-1}\begin{pmatrix}0\\2\tilde{s}\\0\end{pmatrix}+\zeta^{k-1}\tilde{s}_y\begin{pmatrix}-\frac{\xi}{1-\zeta}\\\frac{-\eta}{1-\zeta}\\1\end{pmatrix}$ $\tilde{s}=\xi^a\alpha_\eta\eta^{b+1}(1-\zeta)^{-a-b-2}$	Volume shape functions, $0\leq a\leq k-1, 0\leq b\leq k-2$.
$\dfrac{x^ay^bz^c}{(1+z)^{k+2}}\begin{pmatrix}x(1-x)\\0\\0\end{pmatrix}$	$\frac{\xi^a\eta^b\zeta^c}{(1-\zeta)^{2+a+b+c-k}}\begin{pmatrix}\xi\alpha_\xi\\0\\0\end{pmatrix}$	Volume shape functions, $0\leq a,c\leq k-2, 0\leq b\leq k-1$.
$\dfrac{x^ay^bz^c}{(1+z)^{k+2}}\begin{pmatrix}0\\y(1-y)\\0\end{pmatrix}$	$\frac{\xi^a\eta^b\zeta^c}{(1-\zeta)^{2+a+b+c-k}}\begin{pmatrix}0\\\eta\alpha_\eta\\0\end{pmatrix}$	Volume shape functions, $0\leq b,c\leq k-2, 0\leq a\leq k-1$.
$\dfrac{x^ay^bz^c}{(1+z)^{k+2}}\begin{pmatrix}0\\0\\z\end{pmatrix}$	$\frac{\xi^a\eta^b\zeta^{c+1}}{(1-\zeta)^{2+a+b+c-k}}\begin{pmatrix}-\xi\\-\eta\\1-\zeta\end{pmatrix}$	Volume shape functions, $0\leq a,b,c\leq k-2$.

Table 3–3: $H(\text{div})$-conforming shape functions on a pyramid. Since the approximation space $\mathcal{U}^{(2)}(K_\infty)$ is invariant under the rotation, $R_\infty : K_\infty \to K_\infty$, it is only necessary to demonstrate shape functions for a representative base vertex, vertical edge, base edge and vertical face. Then, using (2.9) and the subsequent remarks, the inverse pullback of these to the finite pyramid will also be invariant under the rotation R. Note that $\alpha_\xi := (1-\zeta-\xi), \alpha_\eta := (1-\zeta-\eta)$.

CHAPTER 4
Numerical integration for high order pyramidal finite elements

This chapter consists of the paper "Numerical integration for high order pyramidal finite elements", submitted to ESAIM: Mathematical Modelling and Numerical Analysis. It presents research that was a direct continuation of that presented in the previous chapters. The difficulties of using numerical integration on pyramidal elements are described and a resolution is found. In the process, a new family of pyramidal finite elements is presented and extensive use is made of the language of differential forms to unify arguments across all the spaces of the de Rham complex.

Throughout this chapter, we make reference to prior work, [63], which is the paper whose contents were presented in chapters 2 and 3.

4.1 Introduction

In prior work, [63], we presented a family of high-order finite element approximation spaces on a pyramidal element. Pyramidal finite elements are used in applications as "glue" in heterogeneous meshes containing hexahedra, tetrahedra and prisms. Various constructions of high order pyramidal elements have been proposed [28, 86, 43, 42, 85, 63]. A useful summary of the approaches taken for H^1-conforming elements is given by Bergot et al. [12], who also provide some motivating numerical results for the performance of methods based on meshes containing pyramidal elements. If they are to be used to implement stable mixed methods, such elements should also satisfy a commuting diagram property. In addition to our work, elements satisfying this property were constructed by Zaglmayr based on the theory of local exact sequences, [85], and are summarised in [31].

Our aim here is to study the errors due to numerical integration on arbitrarily high order pyramidal finite elements that approximate each of the spaces of the de Rham complex. Numerical quadrature is an important component of matrix assembly, and work on the use of quadrature schemes for finite element methods has been recently focussed on issues of efficiency and fast implementation, see e.g. [57]. The classical analysis of the effect of quadrature, see, e.g. [25, 17], has the lesser objective, nicely summed up in [25], of

> "[giving] sufficient conditions on the quadrature scheme which insure that the effect of the numerical integration does not decrease [the] order of convergence."

The approximation spaces we presented in [63] were shown to include complete sets of polynomials and so, at first glance, one might expect the classical arguments should hold in the case of the pyramidal finite elements as well. Somewhat to our surprise, this was not the case: see Example 58. Our exclusive focus in this paper, therefore, is a careful analysis of the errors introduced by quadrature when pyramidal finite elements are used.

A prototypical (linear) problem associated with the weak form of a PDE is of the form:

$$\text{For } a : V \times V \to \mathbb{R} \text{ and } f \in V', \text{ find } u \in V \text{ such that:} \quad a(u,v) = f(v) \quad \forall\, v \in V, \tag{4.1}$$

where V is a normed space of functions on a domain, $\Omega \subset \mathbb{R}^n$, $a(\cdot,\cdot)$ is a bilinear form, and $f(\cdot)$ is linear functional on V. One approximation strategy is then to partition Ω using a triangulation, and replace V by a (finite dimensional) finite element approximation subspace, V_h, where h is a parameter associated with the size of the mesh. One then obtains a numerical approximation $u_h \in V_h$ to the true solution $u \in V$. A typical result is that the approximate solution converges to the true solution at some rate, $O(h^k)$ where the order of convergence, k, depends on the degree of largest complete space of polynomials used in the finite element approximation space.

In general, the bilinear form, $a(\cdot, \cdot)$ and the right hand side $f(\cdot)$ are evaluated using numerical integration rules. These are additional sources of errors in the approximate solution.

In this paper we will show that the quadratures described as conical product formulae by Stroud [76] are an appropriate choice for our pyramidal elements, in particular, that the nth order quadrature rule can be used for the integration of bilinear forms involving nth order elements without decreasing the order of covergence. The main challenge arises from the fact that the classical theory is only applicable to finite elements with approximation spaces consisting purely of polynomials, yet pyramidal elements necessarily include functions other than polynomials, specifically rational functions with denominators which have roots on the boundary of the pyramid [63, 84, 3]. In contrast to the claim in [12], we show that the importance of these rational functions in constructing interpolants means that it is not possible to achieve global estimates of the consistency error by summing element-wise estimates that only deal with polynomials.

Section 4.2 introduces a framework that will allow us to unify our analysis for discrete approximations to each of the spaces of the de Rham complex. We also recall the definitions of the approximation spaces for the elements in [63] and the quadrature rules given in [76]. In section 4.3 we show that the conical product formulae are exact for products of all pairs of functions from the approximation spaces, including the non-polynomials. The intuition from the classical theory would be that this is all that is required. However, as discussed, in section 4.4 we show that the reasoning behind this intuition is insufficient when functions other than polynomials are present. To overcome this, we derive a generalisation of the standard Bramble-Hilbert argument. In section 4.5 we present new families of approximation spaces that allow us to take advantage of this generalisation (and which can be used to construct new pyramidal finite elements in their own right). Finally, we pull everything together in section 4.6 and show that Stroud's quadrature rules satisfy the desired property for both the new and original families of elements.

4.2 Definitions

4.2.1 Differential forms

We will want to make general statements that apply to approximations to each of the spaces of the de Rham complex. It is natural and increasingly popular to use differential forms and the exterior calculus in such a discussion [5, 6]. However, we will be dealing with pyramids, which are set firmly in three dimensions, and so will endeavour to keep things as concrete as possible. Consequently, at the expense of a few extra preliminaries, we will be able to keep much of the notation familiar to users of vector calculus.

Let $\Omega \subset \mathbb{R}^n$ and define $\Lambda^{(s)}(\Omega)$ as the space of differential s-forms on Ω. A point, $x \in \Omega$, has coordinates $(x^i)_{i=0...n}$ and a given $u \in \Lambda^{(s)}(\Omega)$ can be expressed in terms of its components, $u = \sum_\alpha u_\alpha dx^{\alpha_1} \wedge \cdots \wedge dx^{\alpha_s}$ where each $u_\alpha \in C^\infty(\Omega)$ and the multi-indices, $\alpha = \alpha_1 \cdots \alpha_s$ run over the set, Υ_s, of all increasing sequences, $\{1...s\} \to \{1...n\}$.

Define $\Theta^{(s)}(\Omega)$ to be the space of all (covariant) tensors, $A : \Lambda^{(s)}(\Omega) \times \Lambda^{(s)}(\Omega) \to C^\infty(\Omega)$ that can be defined in terms of the pointwise representation,

$$A(u, v)(x) := A^{\alpha\beta}(x) u_\alpha(x) v_\beta(x) \quad \forall u, v \in \Lambda^{(s)}(\Omega), \tag{4.2}$$

where we are using the Einstein summation convention, $A^{\alpha\beta} u_\alpha v_\beta := \sum_{\alpha,\beta\in\Upsilon_s} A^{\alpha\beta} u_\alpha v_\beta$. We will insist that $A^{\alpha\beta}$ is anti-symmetric in the first s and second s components, which makes the representation unique.

A tensor, $A \in \Theta^{(s)}(\Omega)$ induces a bilinear form on $\Lambda^{(s)}(\Omega)$:

$$(u, v)_{A,\Omega} := \int_\Omega A^{\alpha\beta}(x) u_\alpha(x) v_\beta(x) dx.$$

Let $\mathcal{T}$ be a partition of Ω where every $K \in \mathcal{T}$ is the image of a simple reference domain, $\hat{K} \subset \mathbb{R}^n$, under a diffeomorphism $\phi_K : \hat{K} \to K$. On each K, the *reference coordinates*, $\hat{x} = (x^{\hat{i}})_{\hat{i}=0\ldots n}$ of any point $x \in K$, are given by $\hat{x} = \phi_K^{-1}(x)$. Given $u \in \Lambda^{(s)}(K)$, the reference coordinate system induces a new set of components $u_{\hat{\alpha}}$. Differential forms are contravariant, so the components transform as:

$$u_{\hat{\alpha}} = \sum_{\alpha \in \Upsilon_s} \frac{\partial x^{\alpha_1}}{\partial x^{\hat{\alpha}_1}} \cdots \frac{\partial x^{\alpha_s}}{\partial x^{\hat{\alpha}_s}} u_\alpha. \tag{4.3}$$

The components of a covariant tensor, $A \in \Theta^{(s)}(\Omega)$ transform as:

$$A^{\hat{\alpha}\hat{\beta}} = \sum_{\alpha,\beta \in \Upsilon_s} \frac{\partial x^{\hat{\alpha}_1}}{\partial x^{\alpha_1}} \cdots \frac{\partial x^{\hat{\alpha}_s}}{\partial x^{\alpha_s}} \frac{\partial x^{\hat{\beta}_1}}{\partial x^{\beta_1}} \cdots \frac{\partial x^{\hat{\beta}_s}}{\partial x^{\beta_s}} A^{\alpha\beta}. \tag{4.4}$$

Note that $A^{\alpha\beta}(x) u_\alpha(x) v_\beta(x) = A^{\hat{\alpha}\hat{\beta}}(\hat{x}) u_{\hat{\alpha}}(\hat{x}) v_{\hat{\beta}}(\hat{x})$ is just a 0-form and that we have the change of variables formula on each element, K:

$$(u, v)_{A,K} = \int_K A^{\alpha\beta} u_\alpha v_\beta d\mathbf{x} = \int_{\hat{K}} A^{\hat{\alpha}\hat{\beta}} u_{\hat{\alpha}} v_{\hat{\beta}} \det(D\phi_K) d\hat{x}, \tag{4.5}$$

where $D\phi_K$ is the Jacobian of ϕ_K and $\det(D\phi_K)$ is the determinant of the Jacobian.

When $n = 2$ and $n = 3$, it is conventional to think of differential forms in terms of proxy fields. The spaces $\Lambda^{(0)}(\Omega)$ and $\Lambda^{(n)}(\Omega)$ are always isomorphic to the scalar field, $C^\infty(\Omega)$. When $n = 3$, the spaces $\Lambda^{(1)}(\Omega)$ and $\Lambda^{(2)}(\Omega)$ are isomorphic to the vector field, $(C^\infty(\Omega))^3$. For $u \in \Lambda^{(s)}(\Omega)$, we denote the components of the proxy field as u_i for $i \in \mathcal{I}_s = \left\{1, \ldots, \binom{3}{s}\right\}$.

The isomorphisms for the vector fields are given by

$$u \in \Lambda^{(1)}(\Omega) \mapsto \begin{pmatrix} u_1 \\ u_2 \\ u_3 \end{pmatrix}, \quad u \in \Lambda^{(2)}(\Omega) \mapsto \begin{pmatrix} u_{23} \\ -u_{13} \\ u_{12} \end{pmatrix}.$$

With these identifications, the exterior derivatives, $d : \Lambda^{(s)}(\Omega) \to \Lambda^{(s+1)}(\Omega)$ for $s = 0, 1, 2$ become the familiar grad, curl and div.

As with the differential forms, we will decorate the subscripts (and superscripts) of proxies with symbols to indicate the coordinate system that is being used to determine the components of the proxy fields. Given some $u \in \Lambda^{(s)}(\Omega)$, $u_{i'}$ is the ith component of its proxy in the coordinate system $x' = \left(x^{1'}, x^{2'}, x^{3'}\right)$. We will also write $u' = (u_{i'})_{i \in \mathcal{I}_s}$ to indicate all the components of the vector (or scalar) field.

For a coordinate change, $x = \phi(x')$, the weights appearing in the contravariant and covariant transformation rules, (4.3) and (4.4), can be written in terms of the entries of a $\binom{3}{s} \times \binom{3}{s}$ matrix, $w_\phi^{(s)}$. We choose to let $w_\phi^{(s)}$ to be the weight in the covariant transformation so that, for $u \in \Lambda^{(s)}(\Omega)$

$$\sum_{i' \in \mathcal{I}_s} \left(w_\phi^{(s)}\right)_{i,i'} u_{i'} = u_i \quad \forall i \in \mathcal{I}_s. \tag{4.6}$$

The weights can be calculated in terms of the Jacobian, $D\phi$:

$$w_\phi^{(0)} = 1, \qquad w_\phi^{(1)} = D\phi^{-1^t}, \qquad w_\phi^{(2)} = \det(D\phi^{-1}) D\phi, \qquad w_\phi^{(3)} = \det(D\phi^{-1}). \tag{4.7}$$

The exterior derivative is an intrinsic property of any manifold. This means that it is independent of coordinates; equivalently, the exterior derivative commutes with coordinate transformation.

The use of a reference coordinate system is a familiar concept. In the engineering literature, shape functions for finite elements on simplices are often defined in terms of barycentric coordinates. After thinking of a scalar or vector field as a proxy to a differential form, the use of the reference coordinate system to study a shape function is analogous to mapping the differential form to a reference element using a pullback.

4.2.2 Sobolev spaces

Let the Sobolev semi-norms $|\cdot|_{W^{k,p}(\Omega)}$ and $|\cdot|_{H^k(\Omega)} = |\cdot|_{W^{k,2}(\Omega)}$ have their standard meanings. Define semi-norms and norms for any $u \in \Lambda^{(s)}(\overline{\Omega})$ as

$$|u|_{k,\Omega}^2 := \sum_{i \in \mathcal{I}_s} |u_i|_{H^k(\Omega)}^2 , \qquad \|u\|_{k,\Omega}^2 := \sum_{r=0}^{k} |u|_{r,\Omega}^2 .$$

The Sobolev spaces, $H^r\Lambda^{(s)}(\Omega)$ and $\mathcal{H}^{(s),r}(\Omega)$ are then defined as the completion of $\Lambda^{(s)}(\overline{\Omega})$ in the norms $\|u\|_{r,\Omega}$ and $\|u\|_{\mathcal{H}^{(s),r}(\Omega)} := \|u\|_{r,\Omega}^2 + \|du\|_{r,\Omega}^2$ respectively.

As a short-hand, we will write $\mathcal{H}^{(s)}(\Omega) = \mathcal{H}^{(s),0}(\Omega)$. The spaces of proxy fields corresponding to $\mathcal{H}^{(0)}(\Omega)$, $\mathcal{H}^{(1)}(\Omega)$, $\mathcal{H}^{(2)}(\Omega)$ and $\mathcal{H}^{(3)}(\Omega)$ are the familiar $H^1(\Omega)$, $H(\mathrm{curl}, \Omega)$, $H(\mathrm{div}, \Omega)$ and $L^2(\Omega)$.

Note[1] that $H^{r+1}\Lambda^{(s)}(\Omega) \subseteq \mathcal{H}^{(s),r}(\Omega)$ and in particular $\mathcal{H}^{(0),r}(\Omega) = H^{r+1}\Lambda^{(0)}(\Omega) \cong H^{r+1}(\Omega)$, and $\mathcal{H}^{(n),r}(\Omega) = H^r\Lambda^{(n)}(\Omega) \cong H^r(\Omega)$.

For $A \in \Theta^{(s)}(\overline{\Omega})$, we similarly define

$$|A|_{k,\infty,\Omega}^2 := \sum_{i,j \in \mathcal{I}_s} \left|A^{ij}\right|_{W^{k,\infty}(\Omega)}^2 , \qquad \|A\|_{k,\infty,\Omega}^2 := \sum_{r=0}^{k} |A|_{r,\infty,\Omega}^2$$

and define $W^{r,\infty}\Theta^{(s)}(\Omega)$ to be the completion of $\Theta^{(s)}(\overline{\Omega})$ in $\|\cdot\|_{r,\infty,\Omega}$.

[1] When $r = 0$, this is the observation that $H^1(\Omega)^3 \subset H(\mathrm{curl}, \Omega)$ and $H^1(\Omega)^3 \subset H(\mathrm{div}, \Omega)$.

For a given K and $u \in \Lambda^{(s)}(\overline{K})$ and $A \in \Theta^{(s)}(\overline{K})$, define the *reference semi-norms*.[2]

$$|u|_{k,\hat{K}} := \sum_{\hat{i}\in\mathcal{I}_s} \left|u_{\hat{i}}\right|_{H^k(\hat{K})}, \qquad |A|_{k,\infty,\hat{K}} := \sum_{\hat{i},\hat{j}\in\mathcal{I}_s} \left|A^{\hat{i}\hat{j}}\right|_{W^{k,\infty}(\hat{K})}.$$

Suppose that $(\mathcal{T}_h)_{h>0}$ is a family of shape-regular partitions of Ω, where every $K \in \mathcal{T}_h$ is affine equivalent to $\hat{K}$ and each ϕ_K satisfies

$$\|D\phi_K\| \leq h \quad \text{and} \quad \|D\phi_K^{-1}\| \leq \frac{\rho}{h} \tag{4.8}$$

for some $\rho \geq 1$. For any $u \in \mathcal{H}^{(s),k}(K)$ and $A \in W^{k,\infty}\Theta^{(s)}(K)$, we have the inequalities

$$\frac{1}{C\rho^{k+s}} \frac{h^{k+s}}{\det(D\phi_K)^{1/2}} |u|_{k,K} \leq |u|_{k,\hat{K}} \leq C \frac{h^{k+s}}{\det(D\phi_K)^{1/2}} |u|_{k,K} \tag{4.9}$$

$$\frac{1}{C\rho^k} h^{k-2s} |A|_{k,\infty,K} \leq |A|_{k,\infty,\hat{K}} \leq C\rho^{2s} h^{k-2s} |A|_{k,\infty,K} \tag{4.10}$$

for some constant $C = C(k,n)$ which is independent of h. These can be deduced from the standard scaling argument for Sobolev semi-norms of functions (see, for example, [25]) combined with the transformation rules, (4.3) and (4.4) and the observation that (4.8) implies that $\frac{\partial x^{\alpha_i}}{\partial \hat{x}^{\hat{\alpha}_j}} \leq h$ and $\frac{\partial \hat{x}^{\hat{\alpha}_j}}{\partial x^{\alpha_i}} \leq \frac{\rho}{h}$ for all i, j.

4.2.3 Pyramidal elements

From now on we will assume $\Omega \subset \mathbb{R}^3$. To contain the proliferation of indices, we will use the notation (ξ, η, ζ) for the reference coordinates $(x^{\hat{1}}, x^{\hat{2}}, x^{\hat{3}})$. The reference domain is defined

[2] These are the norms induced by the metric in which the reference coordinates are orthonormal. They are used in the scaling argument in section 4.6.

as the pyramid:

$$\hat{K} = \{(\xi, \eta, \zeta) \mid 0 \leq \zeta \leq 1, 0 \leq \xi, \eta \leq \zeta\}.$$

We have chosen to restrict our analysis to affine maps ϕ_K so each element of the mesh, $K \in \mathcal{T}_h$, will be a parallelogram-based pyramid. We will refer to a general such K, as an *affine pyramid*. Note that this restriction is for the sake of exposition - in practice, the necessity and utility of pyramidal elements is evident in meshes comprised of tetrahedral, prismatic and hexahedral elements as well. In this case, a given element of the mesh is obtained via a mapping from one of three different reference elements. Our accounting of quadrature errors is based on local estimates, and the elements on the pyramid are conforming. Therefore, the extension of the present arguments to mixed meshes is straightforward.

As in [63] we will also use the *infinite pyramid*,

$$K_\infty = \{(x, y, z) \mid 0 \leq x, y \leq 1, 0 \leq z \leq \infty\},$$

as a tool to help analyse and define the pyramidal elements. The finite and infinite pyramids may be identified using the projective mapping,

$$\phi : K_\infty \to \hat{K} \tag{4.11}$$

$$\phi : (x, y, z) \mapsto \left(\frac{x}{1+z}, \frac{y}{1+z}, \frac{z}{1+z}\right), \tag{4.12}$$

which can be thought of as a change of coordinates and so, for any element, K, induces the *infinite pyramid coordinate system*[3] defined as $\tilde{x} = \phi^{-1}\hat{x}$. We shall usually write $\tilde{x} = (x, y, z)$.

[3] so-called because $z \to \infty$ as $(\xi, \eta, \zeta) \to (0, 0, 1)$ at the top of the pyramid.

The corresponding weights in the change of coordinates transformation rule can be calculated explicitly:

$$w_\phi^{(0)} = 1, \tag{4.13a}$$

$$w_\phi^{(1)} = D\phi^{-1^t} = (1+z)\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ x & y & 1+z \end{pmatrix}, \tag{4.13b}$$

$$w_\phi^{(2)} = \det(D\phi^{-1})D\phi = (1+z)^2\begin{pmatrix} 1+z & 0 & -x \\ 0 & 1+z & -y \\ 0 & 0 & 1 \end{pmatrix}, \tag{4.13c}$$

$$w_\phi^{(3)} = \det(D\phi^{-1}) = (1+z)^4. \tag{4.13d}$$

The approximation spaces for the finite elements presented in [63] are defined on the infinite pyramid using *k-weighted* tensor product polynomials, $Q_k^{l,m,n}[x,y,z]$, which are tensor product spaces of polynomials, $Q^{l,m,n}[x,y,z]$, multiplied by a weight $\frac{1}{(1+z)^k}$. That is, $Q_k^{l,m,n}$ is spanned by the set[4]

$$\left\{ \frac{x^a y^b z^c}{(1+z)^k},\ 0 \le a \le l, 0 \le b \le m, 0 \le c \le n \right\}.$$

For each family of elements on the infinite pyramid, an *underlying* approximation space is defined for each order, $k \ge 1$.

- H^1-conforming element underlying space:

$$\overline{\mathcal{U}}_k^{(0)} = Q_k^{k,k,k-1} \oplus \text{span}\left\{ \frac{z^k}{(1+z)^k} \right\}. \tag{4.14a}$$

[4] If l, m or n is negative then $Q^{l,m,n} = \{0\}$

- $\mathbf{H}$(curl)-conforming element underlying space:

$$\overline{\mathcal{U}}_k^{(1)} = Q_{k+1}^{k-1,k,k-1} \times Q_{k+1}^{k,k-1,k-1} \times Q_{k+1}^{k,k,k-2}$$
$$\oplus \left\{ \frac{z^{k-1}}{(1+z)^{k+1}} \begin{pmatrix} z\frac{\partial r}{\partial x} \\ z\frac{\partial r}{\partial y} \\ -r \end{pmatrix}, \quad r \in Q^{k,k}[x,y] \right\}. \tag{4.14b}$$

- $\mathbf{H}$(div)-conforming element space:

$$\overline{\mathcal{U}}_k^{(2)} = Q_{k+2}^{k,k-1,k-2} \times Q_{k+2}^{k-1,k,k-2} \times Q_{k+2}^{k-1,k-1,k-1}$$
$$\oplus \frac{z^{k-1}}{(1+z)^{k+2}} \begin{pmatrix} 0 \\ 2s \\ s_y(1+z) \end{pmatrix} \oplus \frac{z^{k-1}}{(1+z)^{k+2}} \begin{pmatrix} 2t \\ 0 \\ t_x(1+z) \end{pmatrix}, \tag{4.14c}$$

where $s(x,y) \in Q^{k-1,k}[x,y], \quad t(x,y) \in Q^{k,k-1}[x,y]$.

- L^2-conforming element underlying space:

$$\mathcal{U}_k^{(3)} = Q_{k+3}^{k-1,k-1,k-1}. \tag{4.14d}$$

For an element defined on a pyramid, K, the underlying approximation space, $\overline{\mathcal{U}}_k^{(s)}(K)$ is defined as the space containing all the s-forms whose components induced by the infinite pyramid coordinate system lie in $\overline{\mathcal{U}}_k^{(s)}$:[5]

$$\overline{\mathcal{U}}_k^{(s)}(K) = \left\{ u \in \Lambda^{(s)}(K) : \left(u_{\tilde{i}}\right)_{\tilde{i} \in \mathcal{I}_s} \in \overline{\mathcal{U}}_k^{(s)} \right\}. \tag{4.15}$$

[5] We are using coordinate transformations here, but in [63], we used the equivalent approach of defining the underlying spaces as the pullbacks, $\overline{\mathcal{U}}_k^{(s)}(\hat{K}) = \left\{ (\phi^{-1})^* v : v \in \overline{\mathcal{U}}_k^{(s)} \right\}$ and $\overline{\mathcal{U}}_k^{(s)}(K) = \{\phi_K^* v : v \in \overline{\mathcal{U}}_k^{(s)}(\hat{K})\}$.

By inspection, it can be seen that the exterior derivative $d : \overline{\mathcal{U}}_k^{(s)} \to \overline{\mathcal{U}}_k^{(s+1)}$ is well defined, and so, since d is independent of coordinates, the exterior derivative on the spaces on each element,

$$d : \overline{\mathcal{U}}_k^{(s)}(K) \to \overline{\mathcal{U}}_k^{(s+1)}(K) \tag{4.16}$$

is also well defined.

A full explanation of these spaces is provided in [63]. Some motivation may be seen from the following lemma.

Lemma 51. *For a given K and $s \in \{0, 1, 2, 3\}$ let $u \in \overline{\mathcal{U}}_k^{(s)}(K)$. Each component $u_{\hat{i}}$ (where $\hat{i} \in \mathcal{I}_s$) of u in the reference coordinate system satisfies*

$$u_{\hat{i}} \circ \phi \in Q_k^{k,k,k}. \tag{4.17}$$

This means that

$$\overline{\mathcal{U}}_k^{(s)}(K) \subset \mathcal{H}^{(s)}(K). \tag{4.18}$$

Proof. The relationship between the representations of u in the reference and infinite pyramid coordinate systems is given by equation (4.6): $\hat{u} \circ \phi = w_\phi^{(s)} \tilde{u}$, where the weights, $w_\phi^{(s)}$, are given by (4.13). To establish (4.17), each $s \in \{0, 1, 2, 3\}$ needs to be dealt with as a separate case.

When $s = 0$, the weight, $w_\phi^{(0)} = 1$ and it is clear from (4.14a) that $\overline{\mathcal{U}}_k^{(0)} \subset Q_k^{k,k,k}$. When $s = 1$, inspection of (4.14b) reveals that $\overline{\mathcal{U}}_k^{(1)} \subset Q_{k+1}^{k-1,k,k} \times Q_{k+1}^{k,k-1,k} \times Q_{k+1}^{k,k,k-1}$. The weight, $w_\phi^{(1)} = (1+z)\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ x & y & 1+z \end{pmatrix}$, so $w_\phi^{(1)} \tilde{u} \in Q_k^{k,k,k} \times Q_k^{k,k,k} \times Q_k^{k,k,k}$. The cases $s = 2$ and $s = 3$ follow similarly.

Since $Q_k^{k,k,k} \subset L^\infty(K_\infty)$ each $u_{\hat{i}} \circ \phi$ is bounded on K_∞, which means that $u_{\hat{i}}$ is bounded on $\hat{K}$ and therefore u_i is bounded on K. Hence $\|u\|_{0,K}$ is finite. By (4.16), $du \in \overline{\mathcal{U}}_k^{(s+1)}(K)$, so $\|du\|_{0,K}$ is finite too and $u \in \mathcal{H}^{(s)}(K)$. □

In order to construct pyramidal elements that are compatible with neighbouring tetrahedral (and hence polynomial) elements, subspaces of the underlying approximation spaces, $\overline{\mathcal{U}}_k^{(s)}(K)$ are identified that contain only those functions whose traces on the triangular faces of the pyramid are contained in the trace space of the corresponding tetrahedral element[6] . These approximation spaces are denoted $\mathcal{U}_k^{(s)}(K)$. We shall denote by $\mathcal{U}_{k,0}^{(s)}(K)$ the subspaces of $\mathcal{U}_k^{(s)}(K)$ with zero boundary traces. We also recall a key result allowing a Helmholtz decomposition of these spaces, which were proved in [63].

Theorem 52. *Let $\mathcal{U}_{k,0}^{(s)}(K)$ be as defined above. Then the following decompositions hold:*

1. $\mathcal{U}_0^{(1)}(K) = \operatorname{grad} \mathcal{U}_0^{(0)}(K) \oplus \mathcal{U}_{0,\mathrm{curl}}^{(1)}(K)$,
   where $\mathcal{U}_{0,\mathrm{curl}}^{(1)}(K) := \left\{ v | v = (\phi^{-1})^* u, u \in \mathcal{U}_{0,\mathrm{curl}}^{(1)}(K_\infty) \right\}$, *and where* $\mathcal{U}_{0,\mathrm{curl}}^{(1)}(K_\infty) \subset \mathcal{U}_0^{(1)}(K_\infty)$ *consists of functions u of the form*

$$u = \begin{pmatrix} y(1-y)zq_1 \\ x(1-x)zq_2 \\ x(1-x)y(1-y)\rho \end{pmatrix}, \tag{4.19}$$

   where $q_1 \in Q_{k+1}^{k-1,k-2,k-2}, q_2 \in Q_{k+1}^{k-2,k-1,k-2}, \rho \in Q_{k+1}^{k-2,k-2}[x,y]$.

[6] The trace spaces for the tetrahedral Lagrange, Nedelec edge and Nedelec face elements are given in [58]. By construction, the traces of the underlying spaces on the quadrilateral face of the pyramid already match those of the corresponding hexahedral elements

2. $\mathcal{U}_0^{(2)}(K) = \text{curl}\,\mathcal{U}_{0,\text{curl}}^{(1)}(K) \oplus \mathcal{U}_{0,\text{div}}^{(2)}(K)$,
where $\mathcal{U}_{0,\text{div}}^{(2)}(K) := \{v | v = (\phi^{-1})^*(u), u \in \mathcal{U}_{0,\text{div}}^{(2)}(K_\infty)\}$ *and where*

$$\mathcal{U}_{0,\text{div}}^{(2)}(K_\infty) := \text{span}\{\frac{z^{k-1}}{(1+z)^{k+2}} \begin{pmatrix} r_y + 2t \\ r_x + 2s \\ (1+z)(r_{xy} + s_y + t_x) \end{pmatrix}\} \oplus \text{span}\{\begin{pmatrix} 0 \\ 0 \\ z\chi_3 \end{pmatrix}\} \quad (4.20)$$

and where $r(x,y) = x(1-x)y(1-y)p(x,y), p \in Q^{k-2,k-2}, t = x(1-x)\tilde{t}, \tilde{t} \in P^{k-2}(x)$, $s = y(1-y)\tilde{s}, \tilde{s} \in P^{k-2}(y)$, *and* $\chi_3 \in Q_{k+2}^{k-1,k-1,k-2}$.

3. $\text{div}\,\mathcal{U}_{0,\text{div}}^{(2)}(K) \oplus \mathbb{R} = \mathcal{U}^{(3)}(K)$.

Each approximation space $\mathcal{U}_k^{(s)}(K)$ is equipped with a set of degrees of freedom, $\Sigma^{(s)}(K)$, that induce a linear interpolation operator,

$$\Pi_{k,K}^{(s)} : \mathcal{H}^{(s),1/2+\epsilon}(K) \to \mathcal{U}_k^{(s)}(K), \quad \epsilon > 0, \qquad \text{so that } m(u) = m(\Pi_{k,K}^{(s)} u) \qquad \forall m \in \Sigma^{(s)}(K), \tag{4.21}$$

which completes the definition of the finite elements. The necessity of the extra $1/2 + \epsilon$ regularity can be seen as a consequence of taking point evaluations at the vertices of the pyramid for the $s = 0$ elements. It is necessary for both the projection-based interpolants of [29] and the more explicit construction given in [63].

We now need to define a global interpolant. Given a mesh comprised of pyramidal elements, $\mathcal{T}_h$, for Ω, we can assemble a global approximation space for $\mathcal{H}^{(s)}(\Omega)$,

$$\mathcal{V}_h^{(s)} = \{v \in \mathcal{H}^{(s)}(\Omega) : v|_K \in \mathcal{U}_k^{(s)}(K)\ \forall K \in \mathcal{T}_h\}. \tag{4.22}$$

Again, we stress that the restriction that all $K \in \mathcal{T}_h$ be mapped from a reference pyramid is for purposes of exposition. Indeed, the approximation spaces $\mathcal{U}_k^{(s)}(K)$ and the degrees of freedom $\Sigma_k^{(s)}(K)$ were designed to ensure these elements are conforming in a mesh consisting of tetrahedral and hexahedral elements. The element-wise interpolation operators respect traces on the boundary of the pyramid, i.e.

$$\operatorname{tr} u|_{\partial K} = 0 \Rightarrow \operatorname{tr} \Pi^{(s)}_{k,K} u|_{\partial K} = 0,$$

so we define a bounded global interpolation operator $\Pi_h^{(s)} : \mathcal{H}^{(s),1/2+\epsilon}(\Omega) \rightarrow \mathcal{V}_h^{(s)}$ by $(\Pi_h^{(s)} u)|_K := \Pi^{(s)}_{k,K}(u|_K)$ for all $K \in \mathcal{T}_h$.

4.2.4 Conical product rule

Quadrature rules on the pyramid can be deduced as special cases of the conical product rule presented by Stroud [76, 45]. Stroud defines the quadrature scheme for any continuous function, $f \in C(\hat{K})$,

$$S(f) := \sum_{i,j,l} f(\xi_i(1-\zeta_l), \xi_j(1-\zeta_l), z_l)\lambda_i\lambda_j\mu_l. \tag{4.23}$$

He shows that given $n \geq 0$, a sufficient condition for $S(p) = \int_{\hat{K}} p \; d\hat{x}$ for any polynomial, $p \in \mathbb{P}^n(\hat{x})$, is that the two one-dimensional quadrature schemes given by the points ξ_i and ζ_l with respective weights λ_i and μ_l satisfy

$$\sum_i \lambda_i g(\xi_i) = \int_0^1 g(x)dx \quad \forall g \in \mathbb{P}^n, \tag{4.24}$$

$$\sum_i \mu_i h(\zeta_i) = \int_0^1 (1-z)^2 h(z)dz \quad \forall h \in \mathbb{P}^n. \tag{4.25}$$

The $k+1$ point Gauss-Legendre quadrature rule can be used to generate ξ_i and λ_i that make (4.24) exact for polynomials of degree $2k+1$. The $k+1$ point Gauss-Jacobi scheme based on the shifted Jacobi polynomial[7] , $P_{k+1}^{(2,0)}$, generates ζ_i and μ_i that make (4.25) exact for polynomials of degree $2k+1$. We denote the quadrature scheme for $\hat{K}$ based on (4.23) that uses these points and weights as $S_{k,\hat{K}}$. The error,

$$E_{k,\hat{K}}(f) := S_{k,\hat{K}}(f) - \int_{\hat{K}} f(\hat{x})d\hat{x}.$$

will be zero when $f \in \mathbb{P}^{2k+1}$.

The one dimensional quadratures, (4.24) and (4.25) are based on Jacobi polynomials, so their Lebesgue constants grow like $O(n^{1/2})$ and $O(n^{5/2})$ respectively [77, p. 336]. The Lebesgue constant is based on a sup norm, so the mapping to the pyramid is irrelevant; (4.23) behaves like a tensor product, so its Lebesgue constant grows like $O(n^{7/2})$.

When $f \in C(K)$, where K is a pyramid equipped with a change of coordinates $\phi_K : \hat{K} \to K$, we can define the quadrature and error functionals:

$$S_{k,K}(f) := S_{k,\hat{K}}\left(|D\phi_K|\,\hat{f}\right) \sim \int_K f(x)dx, \tag{4.26}$$

$$E_{k,K}(f) := E_{k,\hat{K}}\left(|D\phi_K|\,\hat{f}\right) = S_{k,K}(f) - \int_K f(x)dx, \tag{4.27}$$

where $\hat{f} = f \circ \phi_K$, i.e. the expression of f in the reference coordinate system, $\hat{x}$.

4.3 Pyramidal approximation spaces and quadrature

Now lets look at the effect of the conical product rules on our approximation spaces. If u and v are polynomials of degree k then their product, $uv \in \mathbb{P}^{2k}$ so from Stroud's work, we know that $S_{k,\hat{K}}(uv) = \int_{\hat{K}} uv$. In this section, we shall prove the stronger result:

[7] The Jacobi polynomials, $P_n^{(a,b)}(s)$, $n \geq 0$, are typically defined on the interval $[-1,1]$. Under the change of variables, $s = 2t-1$, they orthogonal with respect to the weight $(1-t)^a t^b$ on the interval $[0,1]$.

Theorem 53. *Let K be an affine pyramid; fix $k \geq 1$; let $s \in \{0,1,2,3\}$ and let $A \in \Theta^s(K)$ be a constant tensor field. Then for any $u, v \in \mathcal{U}_k^{(s)}(K)$, the quadrature scheme $S_{k,K}$ exactly evaluates the product, $(u,v)_{A,K}$, i.e.*

$$S_{k,K}(A^{ij}u_iv_j) = (u,v)_{A,K}.$$

To do this, we first need to understand exactly which functions our quadrature scheme integrates exactly.

Lemma 54. *Suppose that f is a function defined on a pyramid, K, and that the representation of f in the infinite pyramid coordinate system, $\tilde{f} = f \circ \phi_K \circ \phi$, lies in the space $Q_{2k+1}^{2k+1,2k+1,2k+1}$. Then the quadrature scheme, $S_{k,K}$ is exact for f:*

$$S_{k,K}(f) = \int_K f dx$$

Proof. It suffices to consider functions p with a representation in the infinite pyramid coordinate system:

$$\tilde{p}(x,y,z) = \frac{x^a y^b}{(1+z)^c} \qquad 0 \leq a,b,c \leq 2k+1,$$

since these monomials span the space $Q_{2k+1}^{2k+1,2k+1,2k+1}$. In finite reference coordinates, p has the form $\hat{p}(\xi,\eta,\zeta) = \xi^a\eta^b(1-\zeta)^{c-a-b}$, and so, using (4.23):

$$\begin{aligned}
S_{k,K}(p) &= S_k(\det(D\phi_K)\hat{p}) \\
&= \det(D\phi_K)\sum_{i,j,l}\xi_i^a(1-\zeta_l)^a\xi_j^b(1-\zeta_l)^b(1-\zeta_l)^{c-a-b}\lambda_i\lambda_j\mu_l \\
&= \det(D\phi_K)\sum_i \lambda_i\xi_i^a\sum_j\lambda_j\xi_i^b\sum_l\mu_l(1-\zeta_l)^c \\
&= \det(D\phi_K)\int_0^1 s^a ds\int_0^1 t^b dt\int_0^1(1-\zeta)^{c+2}d\zeta.
\end{aligned}$$

The last step is justified because each of the sums is a quadrature rule applied to a polynomial of degree $\leq 2k+1$ and so we can apply (4.24) and (4.25). Apply the change of variables $\xi = (1-\zeta)s$ and $\eta = (1-\zeta)t$ to obtain:

$$\begin{aligned} S_{k,K}(p) &= \det(D\phi_K) \int_0^1 \int_0^{1-\zeta} \int_0^{1-\zeta} (1-\zeta)^{c-a-b} \xi^a \eta^b \, d\xi d\eta d\zeta \\ &= \det(D\phi_K) \int_{\hat{K}} \hat{p}(\xi, \eta, \zeta) d\hat{x} \\ &= \int_K p dx. \end{aligned}$$

□

We can now prove Theorem 53 where, in fact, we will only need Lemma 54 to be true for $\tilde{f} \in Q_{2k}^{2k,2k,2k}$, which is a subspace of $Q_{2k+1}^{2k+1,2k+1,2k+1}$.

Proof of Theorem 53. Let $u, v \in \mathcal{U}_k^{(s)}(K)$. $A \in \Theta^{(s)}(K)$ is a constant and so, by the first part of Lemma 51, in infinite reference coordinates, the function $A(u,v)$ satisfies:

$$A^{\tilde{i}\tilde{j}} u_{\tilde{j}} v_{\tilde{i}} \in Q_{2k}^{2k,2k,2k}.$$

Hence by Lemma 54,

$$S_{k,K}\left(A^{ij} u_j v_i\right) = \int_K A^{ij} u_j v_i = (u,v)_{A,K}.$$

□

Observe that for the spaces $\mathcal{U}_k^{(3)}(K)$, the integrand, $A^{\tilde{i}\tilde{j}} u_{\tilde{j}} v_{\tilde{i}} \in Q_{2k-2}^{2k-2,2k-2,2k-2}$, so we could in fact use the scheme S_{k-1}.

4.4 Numerical integration and convergence

In this section, we will demonstrate that the classical theory of the effect of quadrature breaks down for pyramid elements and derive a generalisation of the Bramble Hilbert Lemma that we will use to resolve the problem.

Let $a : \mathcal{H}^{(s)}(\Omega) \times \mathcal{H}^{(s)}(\Omega) \to \mathbb{R}$ be an elliptic bilinear form and let $V \subset \mathcal{H}^{(s)}(\Omega)$ be chosen so that the problem of finding $u \in V$ such that

$$a(u, v) = f(v) \quad \forall v \in V \tag{4.28}$$

has a unique solution for any linear functional, $f \in V'$. A discrete version of this problem is to find $u_h \in V_h$ such that

$$a_h(u_h, v) = f(v) \quad \forall v \in V_h, \tag{4.29}$$

where V_h is an approximating subspace of V and a_h approximates a using numerical integration.[8] When V_h is assembled using polynomial elements of degree k, the analysis of the effect of the numerical integration is classical; good expositions may be found in [25, 17].

For an example, take an elliptic bilinear form $a : H^1_0(\Omega) \times H^1_0(\Omega) \to \mathbb{R}$, defined as

$$a(u, v) = \int_\Omega A(du, dv)\, dx \tag{4.30}$$

where $A \in W^{k,\infty}\Theta^{(1)}(\Omega)$ and is uniformly positive definite.

Assume that $V_h \subset H^1_0(\Omega)$ is some approximation space assembled using kth order polynomial finite elements and that there exists a numerical integration rule, $S_{h,k,\Omega}(\cdot)$, which satisfies $S_{h,k,\Omega}(\partial_i u \partial_j v) = \int_\Omega (\partial_i u \partial_j v)$ for any i and j and all pairs of functions $u, v \in V_h$. Let $a_h(u, v) = S_{h,k,\Omega}(A(du, dv))$. It is shown in [25, page 179] that the solution of (4.29)

[8] We choose not to consider the effect of approximating $f(\cdot)$ by some $f_h(\cdot)$ using numerical integration because it is no different on the pyramid than for other elements. Error estimates may be obtained by applying the standard argument and using Theorem 53.

will satisfy the error estimate:

$$\|u - u_h\|_1 \leq Ch^k(|u|_{k+1} + \|A\|_{k,\infty}\|u\|_{k+1}).$$

This result is contingent on an estimate of the consistency error:

$$\sup_{w_h \in V_h} \frac{|a(\Pi_h u, w_h) - a_h(\Pi_h u, w_h)|}{\|w_h\|_1} \leq Ch^k \|A\|_{k,\infty}\|u\|_{k+1}, \tag{4.31}$$

where $\Pi_h : H_0^1(\Omega) \to V_h$ is an interpolation operator. The constant $C = C(\Omega, k)$ is independent of h.

More generally, an analysis for mixed problems can be found in [40]. The conclusion is the same: in order to preserve an $O(h^k)$ approximation error, each bilinear form must satisfy an $O(h^k)$ consistency error estimate.

The key ingredient in the proof of the consistency error estimate, (4.31) is a local estimate:

Theorem 55 (See [25], Theorem 4.1.2)**.** *Given a simplex, $K \in \mathcal{T}_h$, assume that the quadrature rule is exact for P^{2k-2}. That is, for any polynomial $\psi \in \mathbb{P}^{2k-2}(K)$, the quadrature error, $E_K(\psi) = 0$. Then there exists a constant C independent of K and h such that*

$$\forall A \in W^{k,\infty}(K), \quad \forall p, q \in \mathbb{P}^k(K)$$
$$|E_K(A(dp, dq))| \leq Ch^k \|A\|_{k,\infty,K}\|dp\|_{k-1,K}\,|dq|_{0,K}$$

□

This theorem is proved by combining a scaling argument with the following famous result from [16].

Theorem 56 (Bramble-Hilbert Lemma)**.** *Let $\Omega \subset \mathbb{R}^n$ be open with Lipschitz-continuous boundary. For some integer $k \geq 0$ and $p \in [0, \infty]$ let the linear functional, $f : W^{k+1,p}(\Omega) \to$*

$\mathbb{R}$ *have the property that* $\forall \psi \in \mathbb{P}^k(\Omega)$, $f(\psi) = 0$. *Then there exists a constant* $C(\Omega)$ *such that*

$$\forall v \in W^{k+1,p}(\Omega), \quad |f(v)| \leq C(\Omega) \|f\|_{W^{k+1,p}(\Omega)'} |v|_{k+1,p,\Omega}$$

where $\|\cdot\|_{W^{k+1,p}(\Omega)'}$ *is the operator norm.* □

In our more general framework, we may conjecture that an analogous statement to Theorem 55 is

Conjecture 57. *Let* $K \in \mathcal{T}_h$ *be a pyramid. Let* $s \in \{0, 1, 2, 3\}$ *and* $A \in W^{k,\infty}\Theta^{(s)}(K)$. *Then*

$$\forall v, w \in \mathcal{U}_k^{(s)}(K) \tag{4.32}$$

$$|E_{K,k}(A(v, w))| \leq Ch^k \|A\|_{k,\infty,K} \|v\|_{k-1,K} \|w\|_{0,K} \tag{4.33}$$

This conjecture is true, but useless. The problem is that, unlike the situation for purely polynomial spaces, we cannot differentiate basis functions arbitrarily. We do not have the inclusion, $\mathcal{U}_k^{(s)}(K) \subset \mathcal{H}^{(s),k-1}(K)$ for $k \geq 3$. The following example is illustrative:

Example 58. *Take the* $\mathcal{U}_k^{(0)}(\hat{K})$ *shape function associated with the base vertex,* $(1, 1, 0)$*:*

$$v(\xi, \eta, \zeta) = \frac{\xi\eta}{1 - \zeta}. \tag{4.34}$$

The L^2 *norm of its third partial* ζ*-derivative,*

$$\int_{\hat{K}} \left(\frac{\partial^3 v}{\partial \zeta^3}\right)^2 d\hat{x} = \int_0^1 \int_0^{1-\zeta} \int_0^{1-\zeta} \left(\frac{-6\xi\eta}{(1-\zeta)^4}\right)^2 d\xi d\eta d\zeta \tag{4.35}$$

$$= \int_0^1 \frac{9}{(1-\zeta)^2} d\zeta, \tag{4.36}$$

is infinite.

This means that a direct application of the argument in [25, section 4.1] would fail when we attempt to use the Bramble-Hilbert lemma (Theorem 56) to obtain the estimate

$$\left|\Pi^{(s)}_{k,\hat{K}} u\right|_{r,\hat{K}} \leq C \left|u\right|_{r,\hat{K}} \qquad \forall r \in \{0, \ldots, k\}. \tag{4.37}$$

An attempt is made to avoid this problem in [12] by using the additional projector $\pi_r : H^{r+1}(K) \to \mathbb{P}^r$ satisfying

$$\forall p \in \mathbb{P}^r(K) \quad \pi_r p = p$$

on each element, K. This allows element-wise estimates to be established. Unfortunately, there is no conforming interpolant onto element-wise polynomials for pyramidal elements (see [63] or [84]). In particular, there will be discontinuities at the element boundaries, which means that $\|u - \pi_r u\|_{1,\Omega}$ cannot be bounded. The alternative interpretation of π_r as a global projection onto polynomials would not allow the element-wise estimates to be obtained.

Our solution starts with the observation that not all of the members of each $\mathcal{U}^{(s)}_k(K)$ behave as badly as the function v defined in (4.34). There are subspaces of polynomials and of rational functions that can be differentiated more times before blowing up. For example, we will see in the proof of Lemma 67 that $v(\xi, \eta, \zeta)\xi^r \in H^{r+2}(\hat{K})$. So, we start by developing an analogue of (4.37) that, loosely speaking, allows us to retain as much regularity as possible.

Theorem 59. *Let $\Omega \subset \mathbb{R}^n$ be an open set with Lipschitz boundary. Fix $\alpha \geq 0$ and let $k \geq \alpha$ be an integer. Suppose that:*

- *$R^k \subset H^\alpha(\Omega)$ is a finite dimensional space which includes all polynomials of degree k;*
- *$\Pi : H^\alpha(\Omega) \to R^k$ is a bounded linear projection;*

- *There exist* $V_r \subset H^r(\Omega)$ *for each* $r \in \{0, \ldots, k\}$ *such that we can decompose*

$$R^k = V_0 \oplus \cdots \oplus V_k.$$

Meaning that for a given $u \in H^k(\Omega)$*, the interpolant,* $\Pi u \in R^k$*, may be decomposed into unique functions,* $v_r \in V_r$*,*

$$\Pi u = v_0 + \cdots + v_k.$$

Then we have the following estimates for some of the functions, v_r*:*

- *For each* r *satisfying* $\alpha \leq r \leq k$*:*

$$|v_r|_r \leq C\,|u|_r\,. \tag{4.38}$$

- *If, additionally,* $\tilde{\mathbb{P}}^r \subset V_r$*, where the space* $\tilde{\mathbb{P}}^r$ *consists of polynomials of homogeneous degree,* r*, then for each* r *satisfying* $\alpha \leq r+1 \leq k$*:*

$$|v_r|_r \leq C\,|u|_{r+1} + |u|_r\,. \tag{4.39}$$

Proof. For a given $r \geq \alpha$, write $W_r = V_r \cup \mathbb{P}^{r-1}$. It follows from the definitions that $W_r \subset R^k$ so we can let $\Psi_r : R^k \to W_r$ be any surjective linear projection. Ψ_r is a linear map between finite spaces, so the operator $(I - \Psi_r \circ \Pi) : H^r(\Omega) \to W_r \subset H^r(\Omega)$ is bounded. Also, since both Ψ_r and Π are projections, and $\mathbb{P}^{r-1} \subset \mathbb{P}^k \subset R^k$ we see that $\mathbb{P}^{r-1} \subset \ker(I - \Psi_r \circ \Pi)$. The Bramble-Hilbert lemma gives

$$\|(I - \Psi_r \circ \Pi)u\|_r \leq C\,|u|_r\,.$$

By the definition of W_r, we have $(\Psi_r \circ \Pi)u = v_r + p$ for some $p \in \mathbb{P}^{r-1}$. So $|u - v_r - p|_r \leq C|u|_r$, which implies

$$|v_r|_r \leq C|u|_r + |u|_r + |p|_r = (C+1)|u|_r .$$

The proof of (4.39) follows a similar argument. The operator $(I - \Psi_r \circ \Pi) : H^{r+1}(\Omega) \to W_r \subset H^r(\Omega)$ is bounded because $r+1 \leq k$. The additional condition, $\tilde{\mathbb{P}}^r \subset V_r$, means that $\mathbb{P}^r \subset W_r$ and so $\mathbb{P}^r \subset \ker(I - \Psi_r \circ \Pi)$. □

4.5 A new family of pyramidal approximation spaces

As identified in [12], the space $\mathcal{U}_k^{(0)}$ is sub-optimal in that there exist smaller spaces which contain the same complete space of polynomials and which are compatible with neighbouring tetrahedral and hexahedral elements. Here we will identify subspaces, $\mathcal{R}_k^{(s)}(K)$, of each of the original approximation spaces, $\mathcal{U}_k^{(s)}(K)$ that can be used to construct finite elements with the same approximation and compatibility properties and that still satisfy a commuting diagram property. This would be an interesting exercise in its own right but within the context of this paper we shall see that the importance of these spaces is that they support a decomposition in the manner of Theorem 59 into subspaces that still have enough "room" for us to apply a Bramble-Hilbert type argument in Lemma 69.

We start the construction of these spaces in the infinite pyramid coordinate system using spaces of k-weighted polynomials, $Q_k^{[l,m]}$, which we define in terms of basis functions $\frac{x^a y^b}{(1+z)^c}$ where a,b and c are non-negative integers.

$$Q_k^{[l,m]} = \text{span}\left\{ \frac{x^a y^b}{(1+z)^c} \;:\quad c \leq k,\; a \leq c+l-k,\; b \leq c+m-k \right\}. \qquad (4.40)$$

These spaces can be characterised via a decomposition into spaces of exactly r-weighted polynomials,

$$Q_k^{[l,m]} = \bigoplus_{r=0}^{k} Q_r^{r+l-k,r+m-k,0}. \tag{4.41}$$

It is also helpful to observe that $\frac{x^a y^b}{(1+z)^c} \mapsto \xi^a \eta^b (1-\zeta)^{c-a-b}$ under the coordinate transformation, $(\eta, \xi, \zeta) = \phi(x, y, z)$ given by (4.11). So if the representation in the infinite pyramid coordinate system of some polynomial $f(\hat{x})$ is $\tilde{f} \in Q_k^{[l,m]}$ then f is at most degree k in (ξ, η, ζ) and at most degree l and m in (ξ, ζ) and (η, ζ) respectively.

Now define the spaces $\mathcal{R}_k^{(s)}$ as

$$\mathcal{R}_k^{(0)} = Q_k^{[k,k]}, \tag{4.42a}$$

$$\mathcal{R}_k^{(1)} = \left(Q_{k+1}^{[k-1,k]} \times Q_{k+1}^{[k,k-1]} \times \{0\}\right) \oplus \{\nabla u : u \in Q_k^{[k,k]}\}, \tag{4.42b}$$

$$\mathcal{R}_k^{(2)} = \left(\{0\} \times \{0\} \times Q_{k+2}^{[k-1,k-1]}\right) \oplus \left\{\nabla \times u : u \in \left(Q_{k+1}^{[k-1,k]} \times Q_{k+1}^{[k,k-1]} \times \{0\}\right)\right\}, \tag{4.42c}$$

$$\mathcal{R}_k^{(3)} = Q_{k+3}^{[k-1,k-1]}. \tag{4.42d}$$

The decomposition in the definitions means that with the identification made as in Section 4.2.1, the exterior derivatives, $d : \mathcal{R}_k^{(s)} \to \mathcal{R}_k^{(s+1)}$ (precisely, the grad, curl and div operators) are well defined. The gradient is injective on $Q^{[k,k]}/\mathbb{R}$; the curl is injective on $\left(Q_{k+1}^{[k-1,k]} \times Q_{k+1}^{[k,k-1]} \times \{0\}\right)$ and the divergence is a bijection from $\left(\{0\} \times \{0\} \times Q_{k+2}^{[k-1,k-1]}\right)$ to $Q_{k+3}^{[k-1,k-1]}$, so the sequence,

$$\mathbb{R} \longrightarrow \mathcal{R}_k^{(0)} \xrightarrow{\nabla} \mathcal{R}_k^{(1)} \xrightarrow{\nabla\times} \mathcal{R}_k^{(2)} \xrightarrow{\nabla\cdot} \mathcal{R}_k^{(3)} \longrightarrow 0$$

is exact. The following three lemmas relate these spaces to the $\mathcal{U}_k^{(s)}$ spaces. To avoid the proofs distracting from our main argument we have postponed them to Appendix 4.A.

Lemma 60. *The spaces* $\mathcal{R}_k^{(s)}$ *are subspaces of the* $\overline{\mathcal{U}}_k^{(s)}$*:*

$$\mathcal{R}_k^{(s)} \subseteq \overline{\mathcal{U}}_k^{(s)} \quad \forall s \in \{0, 1, 2, 3\}.$$

□

In fact, for $k \geq 2$ the $\mathcal{R}_k^{(s)}$ are strict subsets of the $\overline{\mathcal{U}}_k^{(s)}$.

Definition 61. *For a given* $s \in \{0, 1, 2, 3\}$ *and* $k \geq 0$*, we define the approximation space*[9] *on a pyramid,* K*, as those differential forms whose infinite coordinate representation lie in* $\mathcal{R}_k^{(s)}$*:*

$$\mathcal{R}_k^{(s)}(K) = \left\{ u \in \Lambda^{(s)}(K) : \left(u_{\tilde{i}}\right) \in \mathcal{R}_k^{(s)} \right\}. \tag{4.43}$$

These spaces still contain all the polynomials that were shown to be present in the spaces $\mathcal{U}_k^{(s)}(K)$ in [63]. Specifically:

Lemma 62. *If* K *is an affine (i.e. parallelogram-based) pyramid then, for* $k \geq 1$*,*

$$\mathbb{P}^k \subset \mathcal{R}_k^{(0)}(K)$$
$$\left(\mathbb{P}^{k-1}\right)^{\binom{3}{s}} \subset \mathcal{R}_k^{(s)}(K) \qquad s \in \{1, 2, 3\}$$

□

Just as with the original spaces, $\mathcal{U}_k^{(s)}(K)$, the new spaces are compatible with Nedelec's elements, which were first outlined in [59]:

Lemma 63. *Let* K *be a pyramid. For each* $s \in \{0, 1, 2\}$ *there is a trace operator that takes elements of* $\mathcal{H}^{(s)}(K)$ *to some distribution on the boundary,* ∂K*. The image of* $\mathcal{R}_k^{(s)}(K)$

[9] c.f. the original approximation spaces, (4.15)

under this operator consists of all traces of elements of $\mathcal{H}^{(s)}(K)$ whose restriction to each triangular or quadrilateral face of K is the trace of a corresponding kth order Lagrange, edge and face approximation function on a neighbouring tetrahedron or hexahedron. □

Note that the original approximation spaces, $\mathcal{U}_k^{(s)}(K)$ were defined by explicitly identifying the subsets of underlying spaces, $\overline{\mathcal{U}}_k^{(s)}(K)$ which had such polynomial trace spaces. For the $\mathcal{R}_k^{(s)}(K)$, the polynomial trace property is inherent and this additional step is not required.

It is the demand that we can match polynomial traces on all faces simultanously in Lemma 63 which creates the need for rational functions in our spaces. For example, there is no polynomial whose trace is the lowest order bubble on one triangular face and zero on all other faces.

From Lemmas 60 and 63 we see that:

Corollary 64. *The new approximation spaces are subspaces of the original approximation spaces.*

$$\mathcal{R}_k^{(s)} \subseteq \mathcal{U}_k^{(s)}. \qquad s \in \{0, 1, 2, 3\}$$

□

We can reuse the interpolation operators from the old spaces, (4.21), to create interpolation operators for the new spaces. Since the trace spaces of $\mathcal{R}_k^{(s)}$ are the same as $\mathcal{U}_k^{(s)}$, we just need to define projections $\Xi_{k,K}^{(s)} : \mathcal{U}_k^{(s)}(K) \to \mathcal{R}_k^{(s)}(K)$ that do not change the trace data. We denote the subspace of all shape-functions in $\mathcal{R}_k^{(s)}(K)$ with zero trace as $\mathcal{R}_{k,0}^{(s)}(K)$.

Definition 65. *For $u \in \mathcal{U}_k^{(s)}(K)$, define $\Xi_{k,K}^{(s)} : \mathcal{U}_k^{(s)}(K) \to \mathcal{R}_k^{(s)}(K)$ as*

$$\Xi_{k,K}^{(s)} u := v_u + w_u$$

where $v_u \in \mathcal{R}_k^{(s)}(K)$ *is some function satisfying* $v_u|_{\partial K} = u|_{\partial K}$ *and* $w_u \in \mathcal{R}_{k,0}^{(s)}(K)$ *is the minimizer of the functional* $v \to \|d(u - v_u - v)\|_0$ *over the admissible set* $\mathcal{A}_{k,K}^{(s)}$*, defined as:*

$$\mathcal{A}_{k,K}^{(0)} := \mathcal{R}_{k,0}^{(0)}(K) \tag{4.44}$$

$$\mathcal{A}_{k,K}^{(s)} := \left\{ v \in \mathcal{R}_{k,0}^{(s)}(K) : (v, dw) = 0 \ \ \forall w \in \mathcal{R}_{k,0}^{(s-1)}(K) \right\}, s = 1, 2, 3. \tag{4.45}$$

Lemma 63 means that the trace spaces of $\mathcal{R}_k^{(s)}(K)$ and $\mathcal{U}_k^{(s)}(K)$ are identical, so it is always possible to find an extension, v_u. The spaces $\mathcal{A}_{k,K}^{(s)}$ are non-empty because they always contain the zero-element so there always exists a minimiser, w_u. The uniqueness of w_u (for a given choice of v_u) can be established using a Friedrichs-type inequality and it is then clear that $\Xi_{k,K}^{(s)} u$ is independent of the choice of v_u.

In fact, the operators $\Xi_{k,K}^{(s)} u$ are just the projection-based interpolants of $\mathcal{U}_k^{(s)}(K)$ onto $\mathcal{R}_k^{(s)}(K)$. More details of projection-based interpolation can be found in [29], which also establishes the important commutativity property: $\Xi_{k,K}^{(s+1)} \circ d = d \circ \Xi_{k,K}^{(s)}$.

Now define the maps $\Phi_{k,K}^{(s)} : \mathcal{H}^{(s),1/2+\epsilon}(K) \to \mathcal{R}_k^{(s)}(K)$ as

$$\Phi_{k,K}^{(s)} = \Xi_{k,K}^{(s)} \circ \Pi_{k,K}^{(s)}. \tag{4.46}$$

Since both $\Xi_{k,K}^{(s)}$ and $\Pi_{k,K}^{(s)}$ commute with d, so does $\Phi_{k,K}^{(s)}$. Note that if $\Pi_{k,K}^{(s)}$ were a projection based interpolant, then $\Phi_{k,K}^{(s)}$ would be too.

Of course, defining an interpolation operator is equivalent to defining degrees of freedom. The above construction implies that the internal degrees for the new elements, $\mathcal{R}_k^{(s)}$ are analogous to those defined for $\mathcal{U}_k^{(s)}$ in [63]. Whereas the old elements used bases for Helmholtz decompositions of $\mathcal{U}_{k,0}^{(s)}(K)$ as test functions for the degrees; the new elements require Helmholtz decompositions of $\mathcal{R}_{k,0}^{(s)}(K)$ which can be readily determined from the full-space Helmholtz decomposition implied in the definitions, (4.42). The external degrees of freedom for both sets of elements are identical.

As with (4.22), for a given k, we can assemble a global approximation space,

$$\mathcal{S}_h^{(s)} = \{v \in \mathcal{H}^s(\Omega) : v|K \in \mathcal{R}_k^{(s)}(K)\ \forall K \in \mathcal{T}_h\} \tag{4.47}$$

and define a global bounded interpolation operator $\Phi_h^{(s)} : \mathcal{H}^{(s),1/2+\epsilon}(\Omega) \to \mathcal{S}_h^{(s)}$ by $(\Phi_h^{(s)}u)|_K = \Phi_{k,K}^{(s)}(u|_K)$ for all $K \in \mathcal{T}_h$.

Now that we have defined the new elements, we shall present a decomposition that is compatible with Theorem 59.

Definition 66. *Given a pyramid, K and $s \in \{0,1,2,3\}$ define, for each $r \geq 0$, the subspace of all the s-forms in $\mathcal{R}_k^{(s)}(K)$ whose components are exactly r-weighted when composed with $\phi : K_\infty \to \hat{K}$.*

$$\mathcal{X}_{r,k}^{(s)}(K) = \left\{ v \in \mathcal{R}_k^{(s)}(K)\ :\ v_{\hat{i}} \circ \phi \in Q_r^{r+1,r+1,0} \right\}.$$

Note that although the domain of $v_{\hat{i}} \circ \phi$ is K_∞, the condition is on the components in the reference coordinate system, $v_{\hat{i}}$, rather than the infinite pyramid coordinate system $v_{\tilde{i}}$. In effect, what we are saying is that each $\mathcal{X}_{r,k}^{(s)}(K)$ is spanned by s-forms whose components have the form

$$e(\xi,\eta,\zeta) = \xi^a \eta^b (1-\zeta)^{r-a-b} \tag{4.48}$$

where $a, b \leq r+1$.

Lemma 67. *For an affine pyramid, K and for each $s \in \{0,1,2,3\}$ and $k \geq 1$, each of the spaces $\mathcal{X}_{r,k}^{(s)}(K)$ satisfy the criterion for V_r from Theorem 59. In fact,*

$$\mathcal{X}_{r,k}^{(s)}(K) \subset H^{r+1}\Lambda^{(s)}(K).$$

Additionally, the semi-norm $|\cdot|_{r,K}$ *is actually a norm on each space* $\mathcal{X}^{(s)}_{r,k}(K)$.

Proof. Let $u \in \mathcal{X}^{(s)}_{r,k}(K)$. Each $u_{\hat{\imath}}$ can be written in terms of functions, $e(\xi,\eta,\zeta) = \xi^a\eta^b(1-\zeta)^{r-a-b}$. When $a+b>r$, these will be rational functions with a singularity at $\zeta = 1$. We need to understand their differentiability on the finite pyramid. Let $\gamma = (\gamma_1,\gamma_2,\gamma_3)$ be a multi-index. The partial derivative,

$$\frac{\partial^\gamma e}{\partial \hat{x}^\gamma} = C\xi^{a-\gamma_1}\eta^{b-\gamma_2}(1-\zeta)^{r-b-a-\gamma_3}$$

where $C = C(\gamma,a,b,r)$ is a (possibly zero) constant dependent only on γ, a, b and r. Hence

$$\int_{\hat{K}}\left(\frac{\partial^\gamma e}{\partial \hat{x}^\gamma}\right)^2 = C\int_0^1\int_0^{1-\zeta}\int_0^{1-\zeta}\xi^{2a-2\gamma_1}\eta^{2b-2\gamma_2}(1-\zeta)^{2r-2b-2a-2\gamma_3}d\xi d\eta d\zeta \tag{4.49}$$

$$= C\int_0^1(1-\zeta)^{2(r+1-\gamma_1-\gamma_2-\gamma_3)}d\zeta \tag{4.50}$$

This integral is finite if $r+1-|\gamma| > -1/2$, so $e \in H^{\lfloor r+3/2-\epsilon\rfloor}(\hat{K})$. By affine equivalence of K and $\hat{K}$, $u \in H^{\lfloor r+3/2-\epsilon\rfloor}(K) \subset H^{r+1}(K)$.

Finally, (4.48) shows that each $e(\xi,\eta,\zeta)$ is either a rational function, or a polynomial of degree exactly r, so $|e|_{r,\hat{K}} \neq 0$. Hence $|u|_{r,K} \neq 0$ and $|\cdot|_{r,K}$ is a semi-norm on $\mathcal{X}^{(s)}_{r,k}(K)$. □

Lemma 68. *For an affine pyramid, K and for each $s \in \{0,1,2,3\}$ and $k \geq 1$, each of the spaces $\mathcal{R}^{(s)}_k(K)$ may be decomposed:*

$$\mathcal{R}^{(s)}_k(K) = \mathcal{X}^{(s)}_{0,k}(K) \oplus \cdots \oplus \mathcal{X}^{(s)}_{k,k}(K)$$

Proof. The decomposition (4.41) makes the claim look plausible. The details are left to Appendix 4.A. □

4.6 The effect of numerical integration on the pyramid

We are now ready to assemble all this machinery to prove a version of Theorem 55 for pyramidal finite elements. The first step is to establish an error estimate for each of the spaces in the decompositions in terms of the reference norms. Recall that in (4.26) we defined $S_{k,K}(\cdot)$ as the quadrature scheme which is exact for functions in P^{2k+1} on the pyramid, K, and that we call the error functional for this scheme $E_{k,K}(\cdot)$. We will also use the pointwise representation, $A(u,v) = A^{ij}u_i v_j$ given in (4.2).

Lemma 69. *For any $s \in \{0,1,2,3\}$ and an affine pyramid, K, let $v \in \mathcal{X}_{r,k}^{(s)}(K)$, $w \in \mathcal{R}_k^{(s)}(K)$ and $A \in W^{k+1,\infty}\Theta^{(s)}(K)$. Then the error in the evaluation of the bilinear form, $(v,w)_{A,K}$ using the scheme $S_{k,K}(\cdot)$ can be bounded in terms of the reference (semi-)norms*

$$|E_{k,K}(A(v,w))| \leq C \det(D\phi_K)\, |A|_{k-r+1,\infty,\hat{K}}\, |\hat{v}|_{r,\hat{K}}\, \|\hat{w}\|_{0,\hat{K}} \tag{4.51}$$

where $C = C(k)$ is a constant that depends only on k.

Proof. We can transform the error functional onto the reference pyramid using (4.27).

$$E_{k,K}(A(v,w)) = E_{k,K}\left(A^{ij}v_i w_j\right) = E_{k,\hat{K}}\left(\det(D\phi_K)A^{\hat{i}\hat{j}}v_{\hat{i}}w_{\hat{j}}\right) = \det(D\phi_K)E_{k,\hat{K}}\left(A^{\hat{i}\hat{j}}v_{\hat{i}}w_{\hat{j}}\right). \tag{4.52}$$

We are able to take $\det(D\phi_K)$ outside the integral because ϕ_K is affine. Define the linear functional $G \in W^{k-r+1,\infty}\Theta^{(s)}(\hat{K})'$ as

$$G(B) = E_{k,\hat{K}}\left(B^{\hat{i}\hat{j}}v_{\hat{i}}w_{\hat{j}}\right) \quad \forall B \in W^{k-r+1,\infty}\Theta^{(s)}(\hat{K}). \tag{4.53}$$

Since $S_k(\cdot)$ takes point values of its argument,

$$|G(B)| \leq C\|B^{\hat{i}\hat{j}}v_{\hat{i}}w_{\hat{j}}\|_{\infty,\hat{K}} \leq C\|B\|_{k-r+1,\infty,\hat{K}}\|\hat{v}\|_{\infty,\hat{K}}\|\hat{w}\|_{\infty,\hat{K}}.$$

Furthermore, all norms are equivalent on the finite dimensional spaces, $\mathcal{X}_{r,k}^{(s)}(\hat{K})$ and $\mathcal{R}_k^{(s)}(\hat{K})$, and, by the last part of Lemma 67, $|\cdot|_{r,\hat{K}}$ is a norm for $\mathcal{X}_{r,k}^{(s)}$. So G is continuous and $\|G\| \leq C\,|\hat{v}|_{r,\hat{K}}\,\|\hat{w}\|_{0,\hat{K}}$. All of the equivalences of norms are done on the reference pyramid, so the constant, C depends only on k (in particular, it does not depend on K).

From the definition of $\mathcal{X}_{r,k}^{(s)}$, we know that each $v_{\hat{i}} \circ \phi \in Q_r^{r+1,r+1,0}$ and by Lemma 51 and Corollary 64, $w_{\hat{j}} \circ \phi \in Q_k^{k,k,k}$ for each $\hat{j} \in \mathcal{I}_s$. Now suppose that B is polynomial of degree $k-r$, i.e. each component, $B^{\hat{i}\hat{j}} \in \mathbb{P}^{k-r}$ for each $\hat{i}, \hat{j} \in \mathcal{I}_s$. Then $B^{\hat{i}\hat{j}} \circ \phi \in Q_{k-r}^{[k-r,k-r]}$. We can assemble these facts to see that

$$\left(B^{\hat{i}\hat{j}} v_{\hat{i}} w_{\hat{j}}\right) \circ \phi = \left(B^{\hat{i}\hat{j}} \circ \phi\right)\left(v_{\hat{i}} \circ \phi\right)\left(w_{\hat{j}} \circ \phi\right) \in Q_{2k+1}^{2k+1,2k+1,2k+1}.$$

So, by Lemma 54, the quadrature error, $E_{k,\hat{K}}\left(B^{\hat{i}\hat{j}} v_{\hat{i}} w_{\hat{j}}\right) = 0$. Therefore, $\mathbb{P}^{k-r} \subset \ker G$ and we can apply Theorem 56 (the Bramble-Hilbert Lemma) to obtain

$$|G(A)| \leq C\,|A|_{k-r+1,\infty,\hat{K}}\,|v|_{r,\hat{K}}\,\|w\|_{0,\hat{K}} \quad \forall A \in W^{k-r+1,\infty}\Theta^{(s)}(\hat{K})$$

For some constant $C = C(k)$. Substituting (4.53) and (4.52) gives the desired result. □

We can now apply a scaling argument to get an element-wise estimate on the quadrature error. Recall that we defined the interpolation operator, $\Phi_K^{(s)} : \mathcal{H}^{(s),1/2+\epsilon}(K) \to \mathcal{R}_k^{(s)}(K)$ in (4.46).

Lemma 70. *Let K be an affine pyramid satisfying the shape-regularity condition,* (4.8)*, for some $\rho \geq 1$. Fix $s \in \{0,1,2,3\}$ and take $k \geq 2$. Then*

$$\forall u \in H^k\Lambda^{(s)}(K), w \in \mathcal{R}_k^{(s)}(K) \text{ and } A \in W^{k+1,\infty}\Theta^{(s)}(K) \tag{4.54}$$

$$\left|E_{k,K}(A(\Phi_{k,K}^{(s)}u, w))\right| \leq \left(Ch^{k+1}\right)\|A\|_{k+1,\infty,K}\|u\|_{k,K}\|w\|_{0,K} \tag{4.55}$$

where $C = C(k)$ a constant dependent only on k, and $0 < h < C$.

Proof. Use the decomposition given in Lemma 68 to write

$$\Phi^{(s)}_{k,K} u = v_0 + \cdots + v_k \text{ where } v_r \in \mathcal{X}^{(s)}_{r,k}(K).$$

By Lemma 69, we know that for each $r \in \{0 \ldots k\}$,

$$|E_{k,K}(A(v_r, w))| \le C\,|D\phi_K|\,|A|_{k-r+1,\infty,\hat{K}}\,|v_r|_{r,\hat{K}}\,\|w\|_{0,\hat{K}}. \tag{4.56}$$

The interpolation operator is bounded on $\mathcal{H}^{(s),1/2+\epsilon}(K)$ which is a subset of $H^{3/2+\epsilon}\Lambda^{(s)}(K)$ so Theorem 59 is applicable with $\alpha > 3/2$. Pick some $\alpha \in (3/2, 2]$ so that when $r \ge 2$ we can use the first estimate, (4.38), to obtain:

$$|E_{k,K}(A(v_r, w))| \le C\,|D\phi_K|\,|A|_{k-r+1,\infty,\hat{K}}\,|u|_{r,\hat{K}}\,\|\hat{w}\|_{0,\hat{K}}. \tag{4.57}$$

Now apply the inequalities (4.9) and (4.10) to the semi-norms (and norm) on the right-hand side to obtain

$$\begin{aligned}
|E_{k,K}(A(v_r, w))| &\le C\,|D\phi_K|\,h^{k-r+1-2s}\rho^{2s}\,|A|_{k-r+1,\infty,K}\,\frac{h^{r+s}}{|D\phi_K|^{1/2}}\,|u|_{r,K}\,\frac{h^s}{|D\phi_K|^{1/2}}\|\hat{w}\|_{0,K} \\
&= Ch^{k+1}\,|A|_{k-r+1,\infty,K}\,|u|_{r,K}\,\|w\|_{0,K},
\end{aligned}$$

where the generic constant, C still depends only on k.

When $r = 1$, we can similarly apply the second estimate from Theorem 59 given in (4.39) to obtain:

$$|E_{k,K}(A(v_1, w))| \le Ch^{k+1}\,|A|_{k,\infty,K}\left(|u|_{1,K} + h\,|u|_{2,K}\right)\|w\|_{0,K}. \tag{4.58}$$

For $r = 0$, note that $\|v_0\|_{0,\hat{K}} \le C\|u\|_{3/2+\epsilon,\hat{K}} \le C\left(|u|_{0,\hat{K}} + |u|_{1,K} + |u|_{2,\hat{K}}\right)$, so

$$|E_{k,K}(A(v_0, w))| \le Ch^{k+1}\,|A|_{k+1,\infty,K}\left(|u|_{0,K} + h\,|u|_{1,K} + h^2\,|u|_{2,K}\right)\|w\|_{0,K} \tag{4.59}$$

Summing over the v_r, we obtain (4.55). $\square$

Summing these errors over each element gives an estimate for the global consistency error due to the numerical integration (we shall ignore the $O(h^{k+2})$ terms). Recall that in (4.47) we defined the global approximation space, $\mathcal{S}_h^{(s)} \subset \mathcal{H}^{(s)}(\Omega)$.

Theorem 71. *Let $s \in \{0,1,2,3\}$, $k \geq 2$ and assume that $\mathcal{S}_h^{(s)}$ is constructed using a shape regular mesh, $\mathcal{T}_h$ and finite elements, $\mathcal{R}_k^{(s)}(K)$ for each $K \in \mathcal{T}_h$. Let $A \in W^{k+1,\infty}\Theta^{(s)}(\Omega)$ and $u \in H^{(s),k}(\Omega)$. Then the interpolant $\Phi_h^{(s)} u \in \mathcal{S}_h^{(s)}$ satisifies*

$$\sup_{w_h \in \mathcal{S}_h^{(s)}} \frac{\left|(\Phi_h^{(s)} u, w_h)_{A,\Omega} - (\Phi_h^{(s)} u, w_h)_{A,h,k,\Omega}\right|}{\|w_h\|_0} \leq Ch^{k+1}\|A\|_{k+1,\infty,\Omega}\|u\|_{k,\Omega}$$

where we define $(v,w)_{A,h,k,\Omega} := \sum_{K \in \mathcal{T}_h} S_{K,k}\left(A(v,w)\right)$. Here $C > 0$ is a constant which only depends on k, and $0 < h < C$.

Proof. Let $w_h \in \mathcal{S}_h^{(s)}$.

$$\begin{aligned}
\left|(\Phi_h^{(s)} u, w_h)_{A,\Omega} - (\Phi_h^{(s)} u, w_h)_{A,h,k,\Omega}\right| &\leq C \sum_{K \in \mathcal{T}_h} E_{k,K}(A(\Phi_{k,K}^{(s)} u, w_h)) \\
&\leq Ch^{k+1} \sum_{K \in \mathcal{T}_h} \|A\|_{k+1,\infty,K}\|u\|_{k,K}\|w_h\|_{0,K} \\
&\leq Ch^{k+1}\|A\|_{k+1,\infty,\Omega} \left(\sum_{K \in \mathcal{T}_h} \|u\|_{k,K}^2\right)^{1/2} \left(\sum_{K \in \mathcal{T}_h} \|w_h\|_{0,K}^2\right)^{1/2} \\
&\leq Ch^{k+1}\|A\|_{k+1,\infty,\Omega}\|u\|_{k,\Omega}\|w_h\|_{0,\Omega}
\end{aligned}$$

Dividing through by $\|w_h\|_{0,\Omega}$ gives the result. $\square$

In the proof of Lemma 69, the important condition for w was that $w_{\hat{\jmath}} \circ \phi \in Q_k^{k,k,k}$. So, by Lemma 51, we could equally well have taken $w \in \mathcal{U}_k^{(s)}(K)$. Furthermore, $\mathcal{S}_h^{(s)} \subset \mathcal{V}_h^{(s)}$ means that $\Phi_h^{(s)} u \in \mathcal{V}_h^{(s)}$. Hence we have a consistency error estimate for the global approximation spaces $\mathcal{V}_h^{(s)}$ based on the original elements:

Corollary 72. *Under the same assumptions as Theorem 71, let $\mathcal{V}_h^{(s)}$ be constructed using finite elements based on the approximation spaces, $\mathcal{U}_k^{(s)}(K)$. Then the interpolant $\Phi_h^{(s)} u$ satisifies*

$$\sup_{w_h \in \mathcal{V}_h^{(s)}} \frac{\left|(\Phi_h^{(s)} u, w_h)_{A,\Omega} - (\Phi_h^{(s)} u, w_h)_{A,h,k,\Omega}\right|}{\|w_h\|_0} \leq Ch^{k+1} \|A\|_{k+1,\infty,\Omega} \|u\|_{k,\Omega}.$$

□

The error estimate may be applied to more general bilinear forms because of the commutativity $d \circ \Pi_h^{(s)} = \Pi_h^{(s+1)} \circ d$. For example, the consistency error for the elliptic bilinear form, (4.28), is

$$\begin{aligned}
\sup_{v \in \mathcal{S}_h^{(0)}} \frac{\left|a(\Phi_h^{(0)} u, v) - a_h(\Phi_h^{(0)} u, v)\right|}{\|v\|_1} &\leq \sup_{v \in \mathcal{S}_h^{(0)}} \frac{(d\Phi_h^{(0)} u, dv)_{A,\Omega} - (d\Phi_h^{(0)} u, dv)_{A,h,k,\Omega}}{\|dv\|_0} \\
&\leq \sup_{w \in \mathcal{S}_h^{(1)}} \frac{(\Phi_h^{(1)} du, w)_{A,\Omega} - (\Phi_h^{(1)} du, w)_{A,h,k,\Omega}}{\|w\|_0} \\
&\leq Ch^{k+1} \|A\|_{k+1,\infty,\Omega} \|du\|_{k,\Omega} \\
&< Ch^{k+1} \|A\|_{k+1,\infty,\Omega} \|u\|_{k+1,\Omega}.
\end{aligned}$$

A final note: as with the classical theory, the error estimates decay like $O(h^{k+1})$ but these are emphatically not *hp*-estimates. The degree, k enters into the constants in several places, which is to be expected from arguments that rely on the Bramble-Hilbert Lemma.

4.7 Conclusion

The conventional finite element wisdom is that a kth order method requires a kth order quadrature scheme. We have shown that this is still true for some high order pyramidal finite elements, but that the non-polynomial nature of pyramidal elements requires some unconventional reasoning to justify the wisdom.

In the process, we have demonstrated new descriptions of families of high order finite elements for the de Rham complex that satisfy an exact sequence property. We will examine these elements in more detail in future work, but a couple of notes are worth recording here.

- The approximation spaces for the first family in the sequence, $\mathcal{R}_k^{(0)}(K)$ are the same as Zaglmayr's elements, as described in [31], and which [12] describes as optimal with respect to their dimension and compatibility with neighbouring elements.

- Lemma 62 shows that the $\mathcal{R}_k^{(s)}(K)$ spaces contain polynomials corresponding to the tetrahedron of the first type. Zaglmayr has constructed pyramidal elements containing polynomials corresponding to both types of tetrahedron, but only those corresponding to the second type are presented in [31]. It would, clearly, be interesting to compare our $\mathcal{R}_k^{(s)}(K)$ spaces with the construction for the first type.

4.A Properties of the new approximation spaces, $\mathcal{R}_k^{(s)}$

In this appendix, we have collected proofs of various Lemmas in section 4.5.

Proof of Lemma 60. The inclusions

$$Q_n^{[l,m]} \subseteq \left(Q_n^{l,m,\min\{l,m\}-1} + Q_n^{0,0,\min\{l,m\}}\right) \subseteq Q_n^{l,m,\min\{l,m\}}. \tag{4.60}$$

can be verified from the definition, (4.40). By the first inclusion, $Q_k^{[k,k]} \subseteq Q_k^{k,k,k-1} + Q_k^{0,0,k}$, which gives the $s = 0$ case: $\mathcal{R}_k^{(0)} \subseteq \overline{\mathcal{U}}_k^{(0)}$.

The $s = 0$ result implies $\nabla\mathcal{R}_k^{(0)} \subseteq \nabla\overline{\mathcal{U}}_k^{(0)}$. Thus, since $\nabla\overline{\mathcal{U}}_k^{(0)} \subset \overline{\mathcal{U}}_k^{(1)}$, we have $\nabla Q_k^{[k,k]} \subset \overline{\mathcal{U}}_k^{(1)}$, which establishes the result for the second space in the decomposition for $\mathcal{R}_k^{(1)}$, given in (4.42b). To deal with the first space in this decomposition, apply (4.60) and the definition of $\overline{\mathcal{U}}_k^{(1)}$ given in (2.19), to obtain

$$\left(Q_{k+1}^{[k-1,k]} \times Q_{k+1}^{[k,k-1]} \times \{0\}\right) \subseteq \left(Q_{k+1}^{k-1,k,k-1} \times Q_{k+1}^{k,k-1,k-1} \times \{0\}\right) \subset \overline{\mathcal{U}}_k^{(1)}.$$

The $s = 2$ case may be established similarly. The space $\mathcal{R}_k^{(2)}$ is defined via a decomposition into two spaces, (4.42c). The second space in this decomposition can be seen to be a subset of $\overline{\mathcal{U}}_k^{(2)}$ by taking curls of the $s = 1$ result. The first space is dealt with by applying (4.60) directly to the definitions.

Another application of (4.60) gives $\mathcal{R}_k^{(3)} = Q_{k+3}^{[k-1,k-1]} \subseteq Q_{k+3}^{k-1,k-1,k-1} = \overline{\mathcal{U}}_k^{(3)}$. □

Proof of Lemma 62. Since $\mathbb{P}^k$ is preserved by affine transformation, we can work in the reference coordinate system, $\hat{x}$. Recall the components of the proxy representation of some $u \in \Lambda^{(s)}(K)$ in this coordinate system are denoted $u_{\hat{\imath}}$, where $\hat{\imath} \in \mathcal{I}_s$. We will need to show that if all the components, $u_{\hat{\imath}} \in \mathbb{P}^k$ (or, for $s = 1, 2, 3$, $\mathbb{P}^{k-1}$) then $u \in \mathcal{R}_k^{(s)}(K)$. This is equivalent to showing $\tilde{u} \in \mathcal{R}_k^{(s)}$, which we will do using the transformation rule, (4.6), along with the explicit weights associated with the coordinate change $\phi : K_\infty \to \hat{K}$ given in (4.13a)-(4.13d).

We start with the case $s = 0$. Let $\hat{u} \in \Lambda^{(0)}(K)$ be any polynomial, $\hat{u}(\xi, \eta, \zeta) = \xi^a \eta^b (1-\zeta)^c$ where $a + b + c \leq k$. Then

$$\tilde{u} = \left(w_\phi^{(0)}\right)^{-1} \hat{u} \circ \phi = \frac{x^a y^b}{(1+z)^{a+b+c}} \in Q_k^{[k,k]} = \mathcal{R}_k^{(0)}.$$

Similarly, for $s = 3$, take $\hat{u} \in \Lambda^{(3)}(K)$ as $\hat{u}(\xi, \eta, \zeta) = \xi^a \eta^b (1-\zeta)^c$ for $a + b + c \leq k - 1$. Then

$$\tilde{u} = \frac{x^a y^b}{(1+z)^{a+b+c+4}} \in Q_{k+3}^{[k-1,k-1]} = \mathcal{R}_k^{(3)}.$$

The $s = 1$ case involves a little more work. Let $u \in \Lambda^{(1)}(K)$ have polynomial components, $u_{\hat{i}} \in \mathbb{P}^{k-1}$. We can find $q \in \Lambda^{(0)}(K)$ with representation $\hat{q} \in \mathbb{P}^k$ such that $v = u - \nabla q$ has third component (in reference coordinates), $v_{\hat{3}} = 0$. By the result for $s = 0$, $q \in \mathcal{R}_k^{(0)}(K)$, and so (by (4.42b)) $\nabla q \in \mathcal{R}_k^{(1)}(K)$. We need to show that $v \in \mathcal{R}_k^{(1)}(\hat{K})$. Both $v_{\hat{1}}$ and $v_{\hat{2}}$ are in P^{k-1}. Suppose first that $v_{\hat{1}} = \xi^a \eta^b (1-\zeta)^c$ where $m := a + b + c \leq k - 1$ and $v_{\hat{2}} = 0$.

$$\tilde{v} = \left(w_\phi^{(1)}\right)^{-1} \hat{v} \circ \phi = \frac{1}{(1+z)^2} \begin{pmatrix} 1+z & 0 & 0 \\ 0 & 1+z & 0 \\ -x & -y & 1 \end{pmatrix} \begin{pmatrix} \frac{x^a y^b}{(1+z)^m} \\ 0 \\ 0 \end{pmatrix}$$

$$= \begin{pmatrix} \frac{x^a y^b}{(1+z)^{m+1}} \\ 0 \\ -\frac{x^{a+1} y^b}{(1+z)^{m+2}} \end{pmatrix} = \frac{1}{(1+z)^{m+1}} \begin{pmatrix} \left(1 - \frac{a+1}{m+1}\right) x^a y^b \\ -\frac{b}{m+1} x^{a+1} y^{b-1} \\ 0 \end{pmatrix} + \frac{1}{m+1} \nabla \frac{x^{a+1} y^b}{(1+z)^{m+1}}.$$

Compare this last expression with the definition, (4.42b), to determine that $\tilde{v} \in \mathcal{R}_k^{(1)}$. Note that when $a = m$ (which includes the case $a = k-1$), the first term vanishes, because $b = 0$

and $1-\frac{a+1}{m+1}=0$.[10] An identical calculation establishes the same result when $v_{\hat{1}}=0$ and $v_{\hat{2}}=\xi^a\eta^b(1-\zeta)^c$.

For $s=2$, the change of coordinates formula for $u\in\Lambda^{(2)}(K)$ is

$$\tilde{u}=\left(w_\phi^{(2)}\right)^{-1}\hat{u}\circ\phi=\frac{1}{(1+z)^3}\begin{pmatrix}1&0&x\\0&1&y\\0&0&1+z\end{pmatrix}\begin{pmatrix}u_{\hat{1}}\\u_{\hat{2}}\\u_{\hat{3}}\end{pmatrix}\circ\phi \tag{4.61}$$

Suppose that $u_{\hat{1}}=\xi^a\eta^b(1-\zeta)^c$ with $m:=a+b+c\le k-1$. Apply (4.61) to see that the contribution to $\tilde{u}$ is $\left(\frac{x^ay^b}{(1+z)^{m+3}},0,0\right)^t$. Let $p=\frac{1}{m+2}\frac{x^ay^b}{(1+z)^{m+2}}\in Q_{k+1}^{[k-1,k-1]}$ and observe that $\frac{x^ay^b}{(1+z)^{m+3}}=-\frac{\partial p}{\partial z}$ and $\frac{\partial p}{\partial x}=\frac{a}{m+2}\frac{x^{a-1}y^b}{(1+z)^{m+2}}\in Q_{k+2}^{[k-1,k-1]}$ (the case $b=m$ implies that $a=0$ and therefore $\frac{\partial p}{\partial x}=0$, so the final inequality in (4.40) is not violated). Hence

$$\left(w_\phi^{(2)}\right)^{-1}\begin{pmatrix}\xi^a\eta^b(1-\zeta)^c\\0\\0\end{pmatrix}\circ\phi=\nabla\times\begin{pmatrix}0\\p\\0\end{pmatrix}-\begin{pmatrix}0\\0\\\frac{\partial p}{\partial x}\end{pmatrix}\in\mathcal{R}_k^{(2)}$$

Polynomials in the second component can be dealt with similarly. When $u_{\hat{3}}=\xi^a\eta^b(1-\zeta)^c$, the contribution to $\tilde{u}$ is $\left(\frac{x^{a+1}y^b}{(1+z)^{m+3}},\frac{x^ay^{b+1}}{(1+z)^{m+3}},\frac{x^ay^b}{(1+z)^{m+2}}\right)^t$. Hence

$$\left(w_\phi^{(2)}\right)^{-1}\begin{pmatrix}0\\0\\\xi^a\eta^b(1-\zeta)^c\end{pmatrix}\circ\phi=\nabla\times\frac{1}{m+2}\begin{pmatrix}-\frac{x^ay^{b+1}}{(1+z)^{m+2}}\\\frac{x^{a+1}y^b}{(1+z)^{m+2}}\\0\end{pmatrix}+\begin{pmatrix}0\\0\\\left(1-\frac{a+b+2}{m+2}\right)\frac{x^ay^b}{(1+z)^{m+2}}\end{pmatrix}\in\mathcal{R}_k^{(2)}.$$

[10] In other words, $(\xi^a,0,0)^t$ is an exact 1-form.

Note that $\frac{x^a y^b}{(1+z)^{m+2}} \in Q_k^{[k-1,k-1]}$ unless $a = m$ or $b = m$, but in these cases, $\left(1 - \frac{a+b+2}{m+2}\right) = 0$.[11] □

Proof of Lemma 63. An alternative, but less self-contained, way of stating this Lemma would be to claim that the trace spaces of the $\mathcal{R}_k^{(s)}(K)$ elements are identical to those of the original $\mathcal{U}_k^{(s)}(K)$ elements, which satisfy exactly the same compatibility property. Consequently, the strategy and tools of Lemma 40 may be reapplied in an identical fashion. We will therefore just provide a sketch of how this may be done.

First we need to show that the restrictions of the traces of the $\mathcal{R}_k^{(s)}(K)$ functions to each face lie in the trace spaces of the corresponding tetrahedral or hexahedal approximation spaces. Secondly we need to show that any valid trace can be achieved by some member of $\mathcal{R}_k^{(s)}(K)$.

For the first step, convenient definitions of the tetrahedral and hexahedral spaces may be found in [58] and the traces of these spaces are identified explicitly in (2.11). It is just a matter of exhaustive checking to determine that the inclusion holds. As an illustration, observe that members of the $\mathcal{R}_k^{(0)}$ which are non-zero on the face $y = 0$ of the infinite pyramid can be expressed in terms of monomials $\frac{x^a}{(1+z)^c}$, where $a + c \leq k$, which map to $\xi^a \zeta^{k-a-c}$, which will span all polynomials of degree k on the face $\eta = 0$ of the finite pyramid, which is precisely the trace space of the kth order Lagrange tetrahedron.

The second step is equivalent to requiring that the combined external degrees of freedom inherited from the tetrahedra and hexahedra across all the vertices, edges and faces of the pyramid be dual to the trace spaces on the pyramid. So it can be proved by demonstrating a

[11] Just as earth-shattering, this is the observation that $(0, 0, \xi^a)^t$ and $(0, 0, \eta^b)^t$ are exact 2-forms.

linearly independent set of pyramidal shape functions with non-zero traces that is the same size as the set of external degrees of freedom. This task can be made more manageable by instead showing that it is possible to achieve the lowest order bubble on each face, edge and vertex of the pyramid that is zero on every other face, edge or vertex, respectively. (N.B. For completeness, in appendix 3.A, we actually presented an example of all the bubbles, not just the lowest order). Happily, the shape functions associated with the external degrees of freedom presented for the $\mathcal{U}_k^{(s)}(K)$ in tables 3–1, 3–2 and 3–3 also suffice for the $\mathcal{R}_k^{(s)}(K)$.

□

Proof of Lemma 68. Each $\mathcal{X}_{r,k}^{(s)}$ is a subset of $\mathcal{R}_k^{(s)}$, so

$$\mathcal{X}_{0,k}^{(s)}(K) \oplus \cdots \oplus \mathcal{X}_{k,k}^{(s)}(K) \subset \mathcal{R}_k^{(s)}(K)$$

For the reverse inclusion, we will deal with each $s \in \{0,1,2,3\}$, in turn. For every $s \in \{0,1,2,3\}$, the transformation rule, (4.6), gives $\hat{u} \circ \phi = w_\phi^{(s)} \tilde{u}$.

For 0-forms, the weight in the change of coordinates formula $w_\phi^{(0)}$ is equal to 1 so any $u \in \mathcal{R}_k^{(s)}(K)$ satisfies $\hat{u} \circ \phi = \tilde{u} \in \mathcal{R}_k^{(0)} = Q_k^{[k,k]}$. The decomposition, (4.41) gives

$$Q_k^{[k,k]} = Q_0^{0,0,0} \oplus \cdots \oplus Q_k^{k,k,0}$$

which is a subset of $Q_0^{1,1,0} \oplus \cdots Q_0^{k+1,k+1,0}$ so $u \in \mathcal{X}_{0,k}^{(0)}(K) \oplus \cdots \oplus \mathcal{X}_{k,k}^{(s)}(K)$.

For the cases $s = 1$ and $s = 2$, we will consider a basis for $\mathcal{R}_k^{(1)}(K)$ and show that each element, u, of the basis is a member of $\mathcal{X}_{r,k}^{(1)}(K)$ for some $r \in \{0 \ldots k\}$, which amounts to showing that each $u_{\hat{\imath}} \circ \phi \in Q_r^{r+1,r+1,0}$.

From the definition given in (4.42c) it's natural to consider three cases for an element of a basis for $\mathcal{R}_k^{(1)}(K)$. First suppose that $\tilde{u} \in \left(Q_{k+1}^{[k-1,k]} \times 0 \times 0\right)$ with $u_{\tilde{1}} = \frac{x^a y^b}{(1+z)^c}$. From the definition of $Q_{k+1}^{[k-1,k]}$ we see that $0 \leq a \leq c-2$ and $0 \leq b \leq c-1$ and so $2 \leq c \leq k+1$. Then $w_\phi^{(1)}\tilde{u} = \left(\frac{x^a y^b}{(1+z)^{c-1}}, 0, \frac{x^{a+1}y^b}{(1+z)^{c-1}}\right)^t$ and so each $u_{\hat{i}} \in Q_{c-1}^{a+1,b,0} \subset Q_r^{r,r,0}$ where $r = c-1 \in \{1 \dots k\}$. The second case is when $\tilde{u} \in \left(0 \times Q_{k+1}^{[k,k-1]} \times 0\right)$ and the reasoning is identical to the first. Finally suppose that $\tilde{u} = \nabla p$ where $p = \frac{x^a y^b}{(1+z)^c} \in Q_k^{[k,k]}$. When $c = 0$, $p = 1$ and $\nabla p = 0$. So we can take $c \geq 1$ and see that each entry of

$$w_\phi^{(1)}\tilde{u} = \begin{pmatrix} a\frac{x^{a-1}y^b}{(1+z)^{c-1}} \\ b\frac{x^a y^{b-1}}{(1+z)^{c-1}} \\ (a+b-c)\frac{x^a y^b}{(1+z)^{c-1}} \end{pmatrix}$$

is in $Q_r^{r+1,r+1,0}$ for some $r \in \{0 \dots k\}$.

When $u \in \mathcal{R}_k^{(2)}(K)$, lets start with the case $\tilde{u} \in \left(0 \times 0 \times Q_{k+2}^{[k-1,k-1]}\right)$ and write $u_{\tilde{3}} = \frac{x^a y^b}{(1+z)^c}$. Again, it is simple to check that each of the entries in the vector $w_\phi^{(2)}\tilde{u} = \left(-\frac{x^{a+1}y^b}{(1+z)^{c-2}}, -\frac{x^a y^{b+1}}{(1+z)^{c-2}}, \frac{x^a y^b}{(1+z)^{c-2}}\right)^t$ is in $Q_r^{r+1,r+1,0}$ for some $r \in \{0 \dots k\}$. Now suppose that $\tilde{u} = \nabla \times \tilde{v}$ where $\tilde{v} \in \left(Q_{k+1}^{[k-1,k]} \times 0 \times 0\right)$ with $v_{\tilde{1}} = \frac{x^a y^b}{(1+z)^c}$. From the $s = 1$ case, we know that $c \geq 2$ and so its straightforward to verify that each of the entries in

$$w_\phi^{(2)}\tilde{u} = (1+z)^2 \begin{pmatrix} 1+z & 0 & -x \\ 0 & 1+z & -y \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 0 \\ \frac{-cx^a y^b}{(1+z)^{c+1}} \\ \frac{bx^a y^{b-1}}{(1+z)^c} \end{pmatrix} = \begin{pmatrix} \frac{-bx^{a+1}y^b}{(1+z)^{c-2}} \\ \frac{-cx^a y^b}{(1+z)^{c-2}} + \frac{-bx^a y^b}{(1+z)^{c-2}} \\ \frac{bx^a y^{b-1}}{(1+z)^{c-2}} \end{pmatrix}$$

are in $Q_r^{r+1,r+1,0}$ for some $r \in \{0 \dots k\}$. The argument for $\tilde{u} = \nabla \times \tilde{v}$ with $\tilde{v} \in \left(0 \times Q_{k+1}^{[k,k-1]} \times 0\right)$ is the same.

Finally, $u \in \mathcal{R}_k^{(3)}(K)$ means that $\tilde{u} \in Q_{k+3}^{[k-1,k-1]}$. The weight $w_\phi^{(3)} = \frac{1}{(1+z)^4}$ so $\hat{u} \circ \phi = \frac{1}{(1+z)^4}\tilde{u} \in Q_{k-1}^{[k-1,k-1]}$ and the reasoning is the same as the 0-form case. $\square$

CHAPTER 5
Some numerical experiments using pyramidal elements

5.1 Introduction

Several previous works have reported the results of numerical experiments using pyramidal elements. High order H^1-conforming elements were used to compute solutions of the Helmholtz equation in [12, 74]; low order $H(\text{curl})$-conforming elements were used to compute solutions to magnetostatics and Maxwell eigenvalue problems in [43, 28].

In this chapter we will compute a solution to Stokes problem using high order $H(\text{curl})$-, $H(\text{div})$- and L^2-conforming pyramidal elements. The calculations will use PyPyramid, a software library that implements the pyramidal elements based on the approximation spaces $\mathcal{R}_k^{(s)}$ described in chapter 4. The software is not being submitted for consideration as part of this thesis, but it is available from a public repository located at `http://github.com/joelphillips/pypyramid`. The README at the top level of the repository explains how to reproduce all the results that we will present below.

The library is written in Python and makes extensive use of the NumPy and SciPy toolkits [50]. Matplotlib and MayaVi are used for visualisation [48, 67]. Python is already available on many desktop computers and all the libraries are freely downloadable. Alternatively, Enthought, the makers of MayaVi, provide a convenient Python install with all these libraries (and many more) already installed, which is freely available to academic users, `http://www.enthought.com/products/edudownload.php`.

At the time of writing, PyPyramid is capable of calculating approximations to mixed problems on arbitrary unstructured pyramidal meshes using uniform p-refinement, although the meshes that we will use here will be structured. Enhancing the code to support variable p and hp-refinement would not be difficult, nor would including tetrahedral, hexahedral or prismatic elements. However, since there are several good quality open source finite element software libraries that already support all of these (and many more) features (e.g. deal.II, FEniCS and DUNE, [9, 47, 10]) a more sensible approach to the dissemination of the pyramidal elements would be to implement them within one of these existing projects; hopefully PyPyramid will be a useful reference implementation for this process.

The previous paragraph begs the question: why bother to write PyPyramid from scratch, rather than work within one of these existing frameworks? There was some value in the experience gained by writing all of the components of a 3D finite element code, but the main reason is that while adding a new element type for an existing shape (tetrahedron, hexahedron, etc.) to any of the libraries is relatively straightforward, adding a new shape appears to be significantly more difficult.

5.2 Stokes flow

In this section we will compute the solution to Stokes problem using $H(\text{curl})$-, $H(\text{div})$- and L^2-conforming pyramidal elements. We seek a velocity field, u, and pressure, p, in a simply-connected Lipschitz domain, Ω, with boundary, $\Gamma = \partial\Omega$, satisfying:

$$-\triangle u + \nabla p = f \qquad \text{in } \Omega, \tag{5.1a}$$

$$\nabla \cdot u = 0 \qquad \text{in } \Omega, \tag{5.1b}$$

$$u_T = g_T \qquad \text{on } \Gamma, \tag{5.1c}$$

$$u_N = g_N \qquad \text{on } \Gamma_N, \tag{5.1d}$$

$$p = \phi \qquad \text{on } \Gamma_P, \tag{5.1e}$$

where $\Gamma = \Gamma_N \cup \Gamma_P$, $u_N = u \cdot n$ and $u_T = u - nu \cdot n$.

Stokes problem describes the flow of a highly viscous incompressible fluid subject to a forcing, f. We specify the tangential components of the velocity, u_T, everywhere on the boundary, but, as we shall see, we must choose to specify either the normal component of the velocity, u_N, or the pressure. We label the (disjoint) subsets of the boundary on which we specify u_N as Γ_N and the pressure as Γ_P.

To solve problem (5.1) using finite elements, we first need to write down a weak formulation. We will broadly follow the approach in [26], which is similar in spirit to that used to demonstrate the high order hexahedral and tetrahedral edge and face elements in [60, 61].

We can use the identity, $-\triangle u = \nabla \times \nabla \times u - \nabla\nabla \cdot u$, and introduce the vorticity,

$$w = \nabla \times u \tag{5.2}$$

to rewrite (5.1a) as

$$\nabla \times w + \nabla p = f \tag{5.3}$$

Now we multiply (5.2), (5.3) and (5.1b) by test functions to obtain

$$(w, \tau)_\Omega - (\nabla \times u, \tau)_\Omega = 0 \tag{5.4a}$$

$$(\nabla \times w, v)_\Omega + (\nabla p, v)_\Omega = (f, v)_\Omega \tag{5.4b}$$

$$(\nabla \cdot u, q)_\Omega = 0 \tag{5.4c}$$

After a couple of formal integrations-by-parts, we obtain:

$$(w, \tau)_\Omega - (u, \nabla \times \tau)_\Omega = (u_T, n \times \tau)_\Gamma \tag{5.5a}$$

$$(\nabla \times w, v)_\Omega - (p, \nabla \cdot v)_\Omega = (f, v)_\Omega - (p, v \cdot n)_\Gamma \tag{5.5b}$$

$$(\nabla \cdot u, q)_\Omega = 0 \tag{5.5c}$$

Using the notation of section 4.2.2, it is now clear that we should take $w, \tau \in \mathcal{H}^{(1)}(\Omega) = H(\mathrm{curl}, \Omega)$; $u, v \in \mathcal{H}^{(2)}(\Omega) = H(\mathrm{div}, \Omega)$ and $p, q \in \mathcal{H}^{(3)}(\Omega) = L^2(\Omega)$. In this formulation, the pressure boundary condition, (5.1e), is natural, but the normal velocity boundary condition, (5.1d), must be built into to the function spaces. Write

$$\mathcal{H}^{(2)}(\Omega; b) = \left\{ v \in \mathcal{H}^{(2)}(\Omega) : v \cdot n|_{\Gamma_N} = b \right\} \tag{5.6}$$

Our full problem is now to find $w \in \mathcal{H}^{(1)}(\Omega)$, $u \in \mathcal{H}^{(2)}(\Omega; g_N)$ and $p \in \mathcal{H}^{(3)}(\Omega)$ such that:

$$(w, \tau)_\Omega - (u, \nabla \times \tau)_\Omega = (g_T, n \times \tau)_\Gamma \qquad \forall w \in \mathcal{H}^{(1)}(\Omega) \tag{5.7a}$$

$$-(\nabla \times w, v)_\Omega + (p, \nabla \cdot v)_\Omega = (\phi, v \cdot n)_{\Gamma_P} - (f, v)_\Omega \qquad \forall v \in \mathcal{H}^{(2)}(\Omega; 0) \tag{5.7b}$$

$$(\nabla \cdot u, q)_\Omega = 0 \qquad \forall q \in \mathcal{H}^{(3)}(\Omega) \tag{5.7c}$$

This is a mixed problem of the form

$$\begin{bmatrix} A & B^t & 0 \\ B & 0 & C^t \\ 0 & C & 0 \end{bmatrix} \begin{bmatrix} w \\ u \\ p \end{bmatrix} = \begin{bmatrix} G \\ \Phi - F \\ 0 \end{bmatrix} \tag{5.8}$$

where $A = I$, $B = \text{curl}$ and $C = \text{div}$. The theory of mixed problems from section 1.3 can be applied in two steps: first we must show that the operator, $\overline{C} = \begin{bmatrix} 0 & C \end{bmatrix}$, has closed range and that the operator, $\overline{A} = \begin{bmatrix} A & B^t \\ B & 0 \end{bmatrix}$, is invertible on $\ker \overline{C}$. To show that $\overline{A}$ is invertible, we require that B has closed range and that A is invertible on $\ker B$. All these conditions follow immediately from the exactness of the de Rham complex, which enables us to construct a Helmholtz decomposition for each space. We should expect, therefore, that an approximate solution based on a discretisation of these spaces using finite elements that satisfy a commuting diagram property should exist and be stable and should satisfy a quasi-optimal error estimate.

For our model problem, we will consider a fluid travelling through a square pipe under the influence of a pressure gradient. The relevant parameters for problem (5.1) are illustrated in Figure 5–1.

Specifically, let $\Omega = [0, 1]^3$, the unit cube. The "open" boundary, Γ_P, consists of the faces, $\Gamma_{P_\alpha} = \{(x, y, z) \in \Gamma : x = \alpha\}$, for $\alpha = 0, 1$, over which we will prescribe the external pressures, $p = \alpha$ on Γ_{P_α}. $\Gamma_N = \Gamma \setminus \Gamma_P$ consists of the "closed" faces, $y = 0, y = 1, z = 0, z = 1$, on which we prescribe $g_N = 0$. We will assume no-slip boundary conditions on the pipe and no externally imposed velocity at the entrance and exit to the pipe, so $g_T = 0$ everywhere. We also take the forcing, $f = 0$.

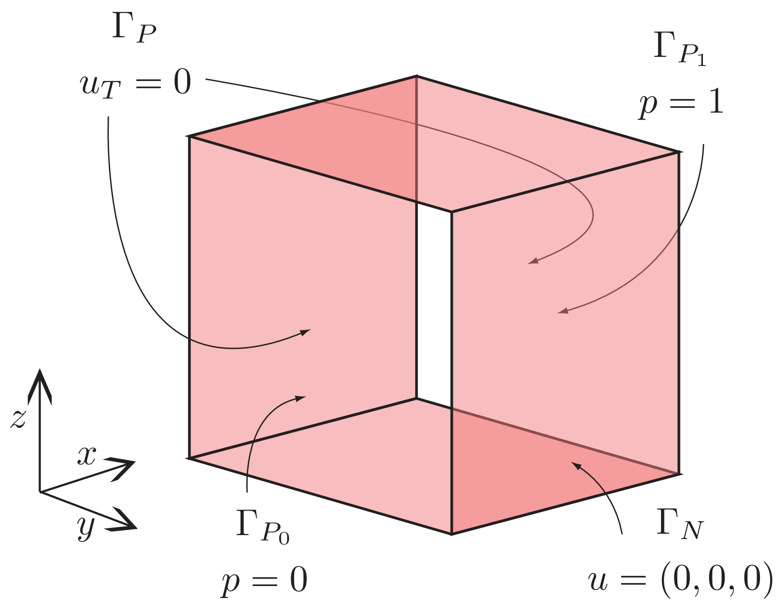

Figure 5–1: Domain for stokes flow experiment

5.3 Reference solution

It is easy to verify that a (and hence the unique) solution to the model problem is the flow

$$u(x, y, z) = (w(y, z), 0, 0) \tag{5.9}$$

$$p(x, y, z) = x \tag{5.10}$$

where w solves Poisson's equation on the unit square:

$$\triangle w = 1 \text{ in } S = [0, 1]^2 \tag{5.11a}$$

$$w = 0 \text{ on } \partial S \tag{5.11b}$$

There are many ways to calculate w accurately. We will use a spectral element method, where $H^1_0(S)$ is approximated using the tensor product space,

$$V_p = \{x(1-x)y(1-y)v(x,y) : v \in Q^{p,p}\}. \tag{5.12}$$

A natural choice for a basis for V_p is the set, $\{v_{ij}(x,y) = \phi_i(x)\phi_j(y) : 0 \leq i,j \leq p\}$, where $\phi_n(t) = t(1-t)J^{1,1}_n(2t-1)$ and $J^{1,1}_n$ is the nth (1,1)-Jacobi polynomial. The functions, ϕ_n, are known as (shifted) *integrated Legendre polynomials* because their derivatives, $\frac{d}{dt}\phi_n(t) = \frac{-1}{(n+1)}L_{n+1}(2t-1)$, where L_n is the nth Legendre polynomial. With this choice, the entries of the stiffness matrix associated with (5.11) are

$$M_{ij,i'j'} := \int_S \nabla v_{ij} \cdot \nabla v_{i'j'} = \frac{1}{(i+1)(i'+1)}\Lambda_{i+1,i'+1}\Phi_{j,j'} + \frac{1}{(j+1)(j'+1)}\Lambda_{j+1,j'+1}\Phi_{i,i'}$$

where $\Lambda_{m,n} = \int_0^1 L_m(t)L_n(t)dt$ and $\Phi_{m,n} = \int_0^1 \phi_m(t)\phi_n(t)dt$. The orthogonality of the Legendre polynomials means that $\Lambda_{m,n} = \frac{1}{2n+1}\delta_{mn}$ and the orthogonality of the Jacobi polynomials, $J^{1,1}_n$, with respect to the weight, $(1-t^2)$ means that $\Phi_{m,n} = 0$ if $|m-n| > 2$. Consequently, $M_{ij,i'j'}$ is highly sparse.

From figure 5–2, we can see that this method appears to converge fast. We will use a calculation with $p > 100$ as the reference solution with which we will compare our pyramidal finite element approximations. Note that the convergence is not exponential; this is because the higher derivatives of the solution, w, are not bounded near the corners of the square. Exponential convergence could be achieved using an hp-method [44], but we have no need of that additional complication here. As a consequence of this lack of regularity, we should also expect limits on the p-convergence of any sequence of approximations to the model problem.

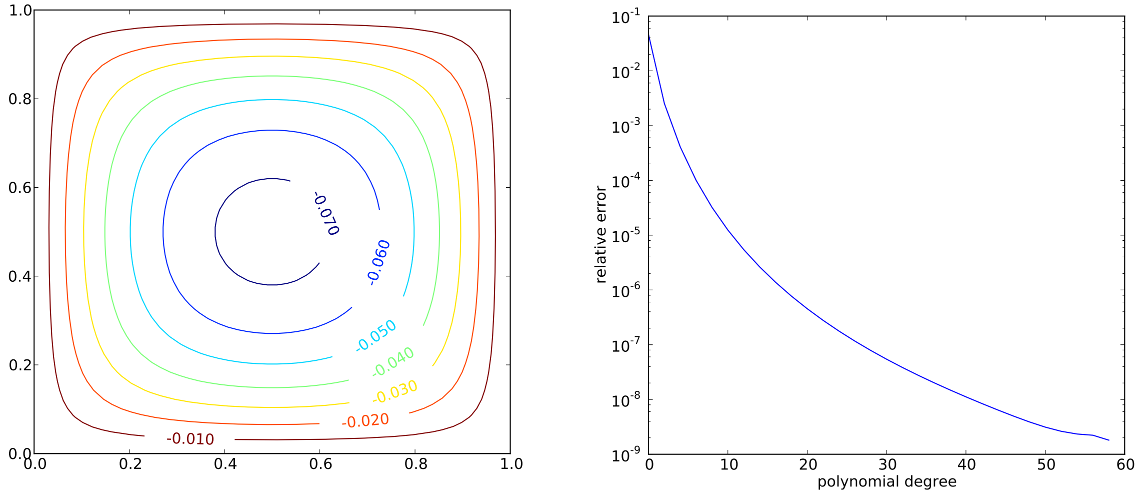

Figure 5–2: Left: approximate solution of problem (5.11) using $V_{40} \subset H_0^1(S)$. Right: relative L^2 error of the approximate solution, using V_{120} as the true solution.

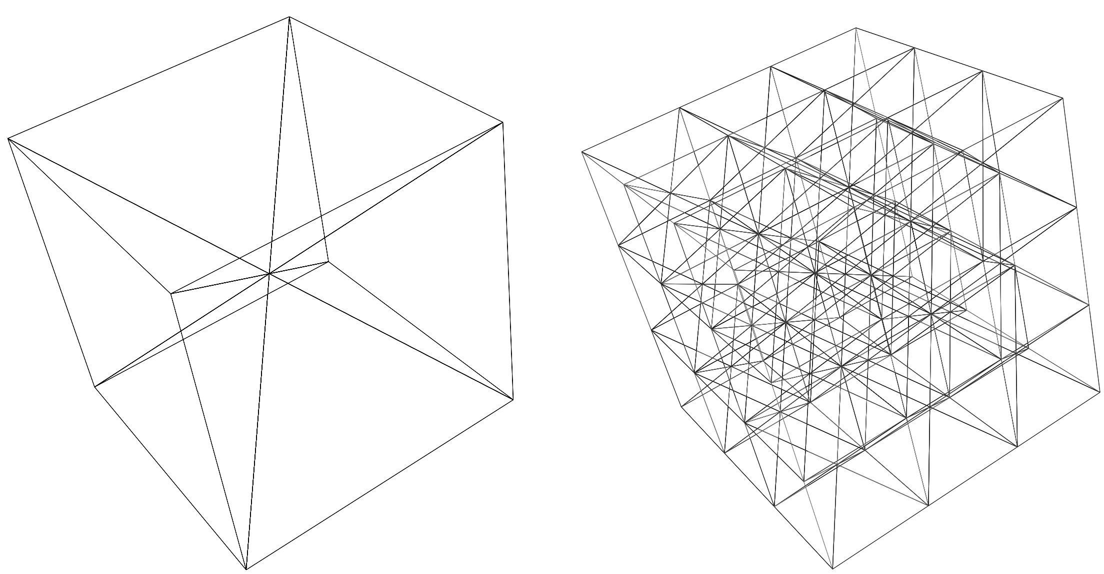

Figure 5–3: Pyramidal-cubic meshes for $N = 1$ and $N = 3$

5.4 Pyramidal finite element formulation

We generate a structured pyramidal mesh, $\mathcal{T}_M$, for the cube, $[0,1]^3$ by first dividing it into M^3 sub-cubes of side $1/M$ and then dividing each of these cubes into 6 pyramids. Figure 5–3 illustrates this process for $M = 1$ and $M = 3$. Clearly, $\dim(\mathcal{T}_M) = 6M^3$. To approximate the spaces, $\mathcal{H}^{(s)}(\Omega)$, $s = 1, 2, 3$, from problem (5.7) we fix some $k \geq 1$ and use the approximation spaces, $\mathcal{R}_k^{(s)}(K)$, from (4.43), on each element, $K \in \mathcal{T}_M$. Following, (4.47), we will call the resulting global approximation spaces,

$$\mathcal{S}_M^{(s)} = \{v \in \mathcal{H}^s(\Omega) : v|K \in \mathcal{R}_k^{(s)}(K)\ \forall K \in \mathcal{T}_M\}. \tag{5.13}$$

To build a discrete approximation to (5.6) it is tempting to write $\mathcal{S}_M^{(2)}(b) = \mathcal{S}_M^{(2)} \cap \mathcal{H}^{(2)}(\Omega; b)$, but this definition would mean that $\mathcal{S}_M^{(2)}(b)$ would be empty if b were not in $\mathrm{tr}^{(2)}(\mathcal{S}_M^{(2)})$, where $\mathrm{tr}^{(2)} : \mathcal{H}^{(2)}(\Omega) \to \mathcal{H}^{(2)}(\Gamma_N)$ is the trace operator. To resolve this, we will take

$$\mathcal{S}_M^{(2)}(b) = \mathcal{S}_M^{(2)} \cap \mathcal{H}^{(2)}(\Omega; \mathrm{tr}^{(2)}\, \Phi_h^{(2)}\, \mathrm{Ext}^{(2)}\, b),$$

where $\Phi_h^{(2)} : \mathcal{H}^2(\Omega) \to \mathcal{S}_M^{(2)}$ is the interpolation operator associated with the finite element approximation and $\mathrm{Ext}^{(2)} : \mathcal{H}^{(2)}(\Gamma_N) \to \mathcal{H}^{(2)}(\Omega)$ is an extension operator (i.e. a right inverse to the trace).

To approximate the solution to problem (5.7), we will find $w_h \in \mathcal{S}_M^{(1)}$, $u_h \in \mathcal{S}_M^{(2)}(g_M)$ and $p_h \in \mathcal{S}_M^{(3)}$ such that:

$$(w_h, \tau_h)_\Omega - (u_h, \nabla \times \tau_h)_\Omega = (g_T, n \times \tau_h)_\Gamma \qquad \forall w_h \in \mathcal{S}_M^{(1)} \tag{5.14a}$$

$$-(\nabla \times w_h, v_h)_\Omega + (p_h, \nabla \cdot v_h)_\Omega = (\phi, v_h \cdot n)_{\Gamma_P} - (f, v_h)_\Omega \qquad \forall v_h \in \mathcal{S}_M^{(2)}(0) \tag{5.14b}$$

$$(\nabla \cdot u_h, q_h)_\Omega = 0 \qquad \forall q_h \in \mathcal{S}_M^{(3)} \tag{5.14c}$$

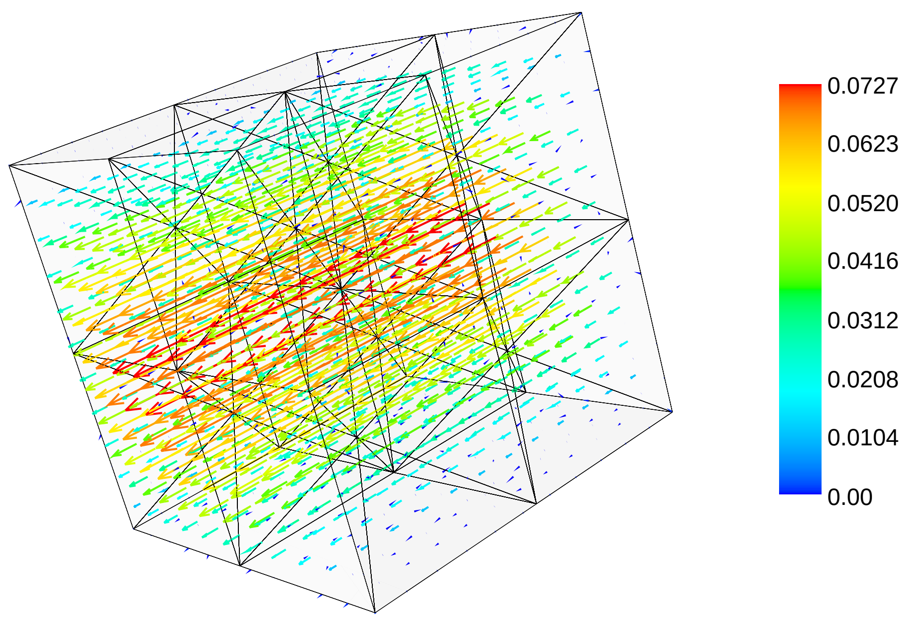

Figure 5–4: Solution to problem (5.14) using 4th-order elements

Figure 5–4 shows the velocity, u_h, of the solution of problem (5.14) with the model boundary conditions given in figure 5–1. For this image, we chose $k = 4$ and $M = 2$ to generate the finite element spaces. In figure 5–5 we take a cross-section at $x = 0.3$ and show the x-component of u_h; the error in the x-component of u_h (compared to the reference solution, u, computed using the spectral element method given in section 5.3) and the pressure p_h. Note that by (5.10), the exact solution for the pressure at $x = 0.3$ is $p = 0.3$ uniformly in y and z.

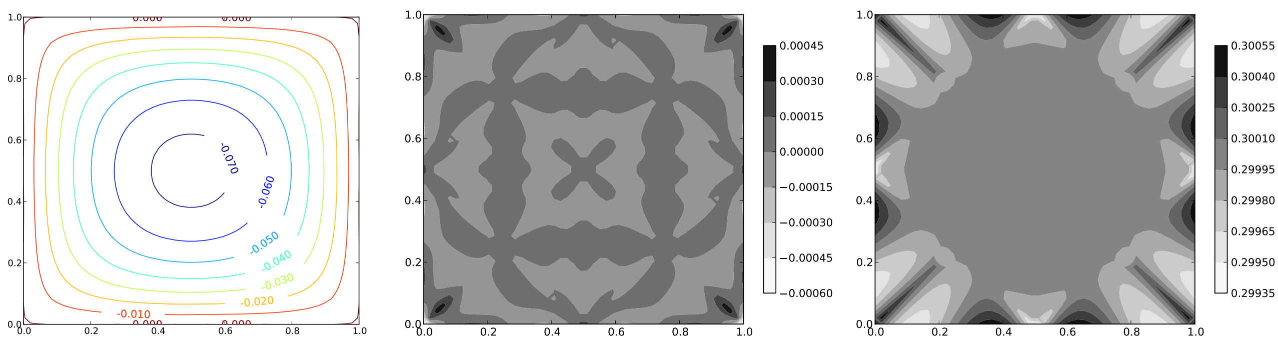

Figure 5–5: The solution of the discrete problem (5.14) on the slice $x = 0.3$ using a mesh composed of forty-eight 4th-order elements ($M = 2$, $k = 4$). Left: x-component of the velocity, u_h; Centre: pointwise error of the velocity, $u - u_h$; Right: pressure, p_h.

5.5 Convergence

Finally, we will analyse the performance of the method as we vary k and M. In each case, we solve the linear system arising from the discrete problem, (5.14), using the sparse direct solver provided by UMFPACK. This places a practical limit on the size of the system of around 30000 degrees of freedom. An iterative method (e.g. BiCGStab) applied to the Schur complement would allow us to solve much bigger problems. Table 5–1 shows the size of the linear system, (5.8), for various choices of k and M.

Table 5–1: Number of degrees of freedom for the approximation of the model Stokes problem, using kth order elements on a mesh of $M \times M \times M$ cubes, each containing 6 pyramids

M \ k	1	2	3	4	5	6
2	282	1468	4230	9240	17170	28692
3	918	4842	14040	30780		
4	2140	11352	33012			
5	4140	22030				
6	7110	37908				
7	11242	60018				
8	16728					
9	23760					
10	32530					
11	43230					

Table 5–2: Error in the velocity of the solution to the model Stokes problem, $\|u - u_h\|_{L^2(\Omega)}$, using kth order elements on a mesh of $M \times M \times M$ cubes, each containing 6 pyramids

M \ k	1	2	3	4	5	6
2	0.4856	0.1160	0.01215	0.001769	3.933×10^{-4}	1.331×10^{-4}
3	0.3490	0.05561	0.004352	5.476×10^{-4}		
4	0.2635	0.03092	0.001866			
5	0.2154	0.01989				
6	0.1790	0.01395				
7	0.1600	0.01149				
8	0.1411					
9	0.1180					
10	0.09727					
11	0.1037					

In table 5–2 we record the error in the approximate velocity u_h. The reference solution, u, is calculated using V_{200}, the spectral approximation space with polynomials of degree 200 in each direction.

Figure 5–6: h- and p-convergence for problem (5.14). The error on each chart is $\|u - u_h\|_{L^2(\Omega)}$, where u_h is the solution computed with the k-order elements on the mesh $\mathcal{T}_M$ and u is the reference solution computed using V_{200}

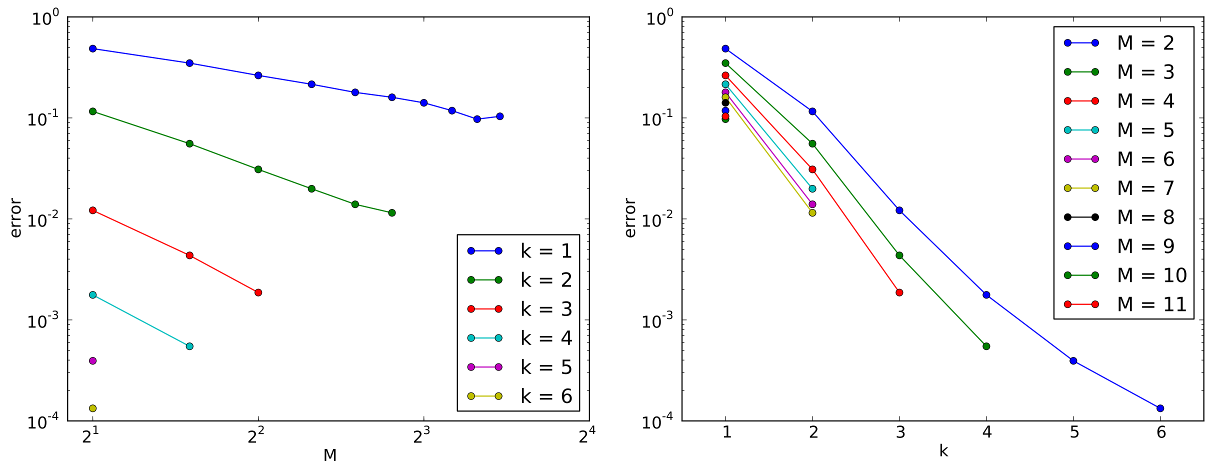

Table 5–3: Implied order of convergence, $m = \frac{\log(e_M/e_{M+1})}{\log((M+1)/M)}$ for $e_M = \|u - u_h\|_{L^2(\Omega)}$, where u_h is calculated using kth order elements on a mesh of $M \times M \times M$ cubes

k \ M	2	3	4	5	6	7	8	9	10
1	0.815	0.976	0.904	1.013	0.727	0.941	1.517	1.837	-0.672
2	1.813	2.040	1.978	1.945	1.258				
3	2.533	2.944							

The charts in figure 5–6 show behaviour of the error as we vary $h = 1/M$ and k. For $k = 1, 2, 3$, table 5–3 collects the implied orders of convergence, m, assuming that $\|u - u_h\|_0 = Ch^m$. We have not measured the error of $\nabla \times u_h$, so we cannot make a direct comparison with any analogy of Lemma 2. However, by Lemma 62, the kth order elements contain only the complete spaces of polynomials of degree $k-1$, so Lemma 2 would not lead us to expect anything better than:

$$\|u-u_h\|_0 = C(k)h^k. \tag{5.15}$$

There is some suggestion from the data in table 5–3 that it may be the case that $\|u-u_h\|_0 = O(h^k)$. Note that $\frac{\log(e_7/e_{11})}{\log(11/7)} = 0.960$, so the growth for $k=1$ at $M=10$ does not necessarily reflect a lack of convergence. The departure from the trend at $k=2$, $M=6$ is less easy to explain and needs further investigation.

The p-convergence is, again, at least consistent with the exponential convergence predicted by (1.29); although, as noted above, we have no reason to expect that $\|u\|_k$ is bounded for all k so we should not expect asymptotic exponential convergence. A final advert for p- and hp-methods is the observation that whilst the combination $M=3$, $k=4$ has 30780 degrees of freedom, the error is 25 times smaller than the error for $M=6$, $k=2$, with 37908 degrees of freedom.

CHAPTER 6
Summary and outlook

Pyramidal finite elements have been a topic of active research for nearly twenty years. The main contributions to the subject presented in this thesis are:

- the construction of high order pyramidal approximation spaces that are compatible with existing high order tetrahedral and hexahedral approximation spaces for each of the spaces of the de Rham complex (Definitions 24 and 61).
- the equipping of these approximation spaces with degrees of freedom that induce interpolation operators that satisfy a *commuting diagram property*, ensuring that the resulting finite elements can be used to build stable approximations to mixed problems (Section 3.1, equation (4.46) and Theorem 45);
- a proof that Stroud's conical product rules can be used to construct numerical integration formulae for pyramidal finite elements which do not decrease the order of convergence (Theorem 71);
- the use of these pyramidal finite elements to construct high order approximations to the solution of a mixed PDE and some preliminary numerical convergence results (Chapter 5).

Many of the ancillary results and techniques that we have used are interesting in their own right. Some of the highlights are:

- a proof of the necessity of non-polynomial basis functions on pyramids (Theorem 4);

- the introduction of the *infinite pyramid* as a tool for analysing pyramidal approximation spaces (Section 2.2);
- explicit constructions of shape functions for pyramidal elements (Tables 3–1, 3–2 and 3–3);
- a concise definition of a family of pyramidal approximation spaces (equations (4.42));
- the idea of constructing finite elements based on a reference coordinate system, rather than a reference element (Section 4.2.3);
- a generalisation of the Bramble Hilbert Lemma (Theorem 59);

The main contributions listed above, along with the unpublished work of Zaglmayr, have enabled authors of generic mixed *hp*-finite element libraries to begin to offer pyramidal elements as part of their standard toolkits [31]. However, there are still some outstanding questions and some un-investigated implications of our work. We detail some of these below.

The infinite pyramid

The pyramidal quadrature rule introduced in section 4.2.4 is commonly interpreted as the consequence of using a Duffy transformation to map the pyramid to a cube and then constructing a tensor product quadrature rule that incorporates the weight $(1-\zeta)^2$ that comes from the determinant of the Jacobian of the transformation. It is natural to ask: shouldn't we also construct the pyramidal approximation spaces on a cube, rather than the infinite pyramid? The naive approach of taking the Nedelec hexahedral elements and pulling them back to the pyramid is shown to fail in [42], so let us go in the other direction and see what our approximation spaces look like when pulled back to the cube. It is easy to see what these spaces look like for the second family of elements. Let $C = [0,1]^3 \subset \mathbb{R}^3$

be the cube. We will parametrise the cube using the coordinates (x, y, ζ) and define the map $\phi_C : K_\infty \to C$ as $\phi_C : (x, y, z) \mapsto (x, y, z/1+z)$. This means that $\phi_C \circ \phi^{-1}$ is the Duffy transformation. Using ϕ_C to pull-back (or change coordinates) for the expressions in (4.42), we obtain:

$$
\begin{aligned}
\mathcal{R}_k^{(0)}(C) &= P_k^{[k,k]}, \\
\mathcal{R}_k^{(1)}(C) &= \left(P_{k+1}^{[k-1,k]} \times P_{k+1}^{[k,k-1]} \times \{0\}\right) \oplus \{\nabla u : u \in P_k^{[k,k]}\}, \\
\mathcal{R}_k^{(2)}(C) &= \left(\{0\} \times \{0\} \times P_{k+2}^{[k-1,k-1]}\right) \oplus \left\{\nabla \times u : u \in \left(P_{k+1}^{[k-1,k]} \times P_{k+1}^{[k,k-1]} \times \{0\}\right)\right\}, \\
\mathcal{R}_k^{(3)}(C) &= \frac{1}{(1-\zeta)^2} P_{k+3}^{[k-1,k-1]} = P_{k+1}^{[k-1,k-1]},
\end{aligned}
$$

where

$$
P_k^{[l,m]} := \operatorname{span}\left\{x^a y^b (1-\zeta)^c \ : c \le k;\ a \le c + l - k;\ b \le c + m - k;\ a, b, c \ge 0\right\}.
$$

Our reason for using the infinite pyramid is partly historical: it is the tool that we started with and it works. A more aesthetically pleasing justification arises from the observation that we can view the infinite pyramid, combined with its point at infinite, as a submanifold of projective 3-space; it is then topologically the same as the as the finite reference pyramid, Ω. In this framework, the projective map, ϕ, is a diffeomorphism, whereas the Duffy transformation is not a bijection: the entire top face of the cube maps to the tip of the pyramid. It is not clear, however, whether that has any significant consequences. It would be interesting to examine what happens to our arguments, for example Lemma 51 and Definition 66 under Duffy coordinates.

In fact, the spaces could be defined directly on the finite reference pyramid and, in some sense, the presentation of the shape functions in section 3.A does exactly that. However, the pullback introduces dependencies between components of the vector-valued spaces, which makes the indirect definitions given via the cube or the infinite pyramid much easier to work with.

Non-affine transformations

The pyramidal approximation spaces contain the complete space of polynomials of a given degree and so any pyramid that can be mapped to the reference pyramid using an affine transformation will also contain this polynomial space However, it is common in finite element implementations to use more general transformations, in particular, quadrilaterals and hexahedra may be transformed bi- and tri-linearly. Bedrosian introduced a pyramidal transformation that is bilinear in the ξ, η coordinates, but is affine in any plane that passes through the top of the pyramid, [11]. It is shown in [12] that the tensor product structure of the H^1-conforming element means that pyramidal elements that are related to the reference domain by a Bedrosian transformation ought not to lose approximability. Based on the work in [4], we might expect that the situation is less straightforward for $H(\text{curl})$- and $H(\text{div})$-conforming elements.

Orthogonal bases

An L^2-orthogonal basis for $\mathcal{R}_k^{(0)}(K)$ is constructed in [12] using Jacobi polynomials (the technique is very similar to that given in [72]). We did not use this basis for PyPyramid because the generalisation to the spaces $\mathcal{R}_k^{(s)}(K)$, $s = 1, 2$ is not obvious. However, it ought to be possible and would likely have benefits for either the conditioning of the resulting stiffness matrix or the inversion of the local Vandermonde matrix used in the stiffness matrix assembly.

Anisotropy

One of the advantages of hexahedral elements is that they allow anisotropic p-refinement. The tensor product structure of the pyramidal approximation spaces suggests that this should be also possible for pyramids in the ξ, η plane. In particular, the definition of the $\mathcal{R}_k^{(s)}$ family in terms of the k-weighted polynomials given in (4.40) looks like it would allow this to be implemented easily.

Non-conformity

Underlying this work has been the assumption that conforming methods are desirable. Non-conforming methods, for example Discontinuous Galerkin or Mortar methods, provide another technique for patching tetrahedra to hexahedra. In some circumstances, non-conforming methods are inappropriate: it is likely to be easier to insert a conforming pyramid element into a code that currently uses conforming tetrahedral or hexahedral elements than to introduce an entirely new paradigm. However, in other situations, non-conforming methods may be a valid alternative. It would be interesting to compare the different approaches. Is it simpler to use non-conforming elements to support hanging nodes, or does the extra flexibility provided by pyramids make conforming elements on hybrid meshes more competitive? Which approach performs better?

More numerics

The numerical example in chapter 5 is rudimentary and leaves many questions unanswered. I hope soon to be able to include pyramidal elements in a more robust finite element package, which supports tetrahedra and hexahedra. It will then be possible to properly examine the effect of hybrid meshes, including the conditioning of the resulting global stiffness matrices.

Extension operators

To fit fully within the *projection-based interpolation* framework (in particular, to obtain quasi-optimal bounds on the interpolation error), it is necessary to postulate the existence of bounded commuting *polynomial-preserving extension operators* [29]. In this context, an extension operator is a right inverse of the trace; "polynomial preserving" means that the extension of the trace of a function belonging to a particular finite element approximation space should also belong to that space; and commuting means that the extensions should commute with the exterior derivative.

These operators have been constructed for tetrahedral and hexahedral elements [27, 30] but the approaches used for each type are quite different, which makes it difficult to just treat the pyramid as a hybrid of the two. Nevertheless, some promising, but inconclusive, investigation leads me to believe that this will be possible. Note that by Theorem 4, it is clear that if we seek analogues for pyramidal elements, we must stretch the meaning of "polynomial-preserving" to allow our rational approximation functions to appear in the volume.

Conjecture 73. *For a pyramid, K and $s \in \{0, 1, 2\}$, denote the trace space of $\mathcal{H}^{(s)}(K)$ as $X^{(s)}(\partial K)$ and the trace operator $\mathrm{tr}^{(s)} : \mathcal{H}^{(s)}(K) \to X^{(s)}(\partial K)$.*

There exist continuous operators, $\mathcal{E}_k^{(s)} : X^{(s)}(\partial K) \to \mathcal{H}^{(s)}(K)$ for $k \geq 1$ such that:

- Extension property: $\mathrm{tr}^{(s)}\, \mathcal{E}_k^{(s)} v = v$ *for all* $v \in X^{(s)}(\partial K)$*;*
- Commutativity: $d\mathcal{E}_k^{(s)} v = \mathcal{E}_k^{(s+1)} dv$ *for all* $v \in X^{(s)}(\partial K)$*;*
- "Polynomial" preservation: *If* $v \in \mathcal{R}_k^{(s)}(K)$ *then* $\mathcal{E}_k^{(s)}\, \mathrm{tr}^{(s)}\, v \in \mathcal{R}_k^{(s)}(K)$.

References

[1] R. A. Adams. *Sobolev spaces*. Academic Press [A subsidiary of Harcourt Brace Jovanovich, Publishers], New York-London, 1975. Pure and Applied Mathematics, Vol. 65.

[2] M. Ainsworth and K. Pinchedez. hp-approximation theory for BDFM and RT finite elements on quadrilaterals. *SIAM Journal on Numerical Analysis*, 40(6):2047–2068, 2003.

[3] American Mathematical Society. *On the uniqueness of barycentric coordinates*, volume 334, 2002.

[4] D. Arnold, D. Boffi, and R. Falk. Approximation by quadrilateral finite elements. *Mathematics of Computation*, 71(239):909–922, 2002.

[5] D. Arnold, R. Falk, and R. Winther. Finite element exterior calculus, homological techniques, and applications. *Acta Numerica*, 15:1–155, 2006.

[6] D. Arnold, R. Falk, and R. Winther. Finite element exterior calculus: from Hodge theory to numerical stability. *Bulletin of the AMS*, 47(2):281–354, 2010.

[7] I. Babuška. Error-bounds for finite element method. *Numerische Mathematik*, 16(4):322–333, 1971.

[8] I. Babuška and M. Suri. The p and hp versions of the finite element method, basic principles and properties. *SIAM Review*, 36(4):578–632, 1994.

[9] W. Bangerth, R. Hartmann, and G. Kanschat. deal.II—a general-purpose object-oriented finite element library. *ACM Transactions on Mathematical Software (TOMS)*, 33(4):24, 2007.

[10] P. Bastian, M. Blatt, A. Dedner, C. Engwer, R. Klofkorn, R. Kornhuber, M. Ohlberger, and O. Sander. A generic grid interface for parallel and adaptive scientific computing. Part II: Implementation and tests in DUNE. *Computing*, 82(2):121–138, 2008.

[11] G. Bedrosian. Shape functions and integration formulas for three-dimensional finite element analysis. *International Journal for Numerical Methods in Engineering*, 35(1):95–108, 1992.

[12] M. Bergot, G. Cohen, and M. Duruflé. Higher-order finite elements for hybrid meshes using new nodal pyramidal elements. *Journal of Scientific Computing*, 42(3):345–381, March 2010.

[13] D. Boffi, F. Brezzi, L. Demkowicz, R. Durán, R. Falk, and M. Fortin. *Mixed finite elements, compatibility conditions, and applications.* Springer, 2008.

[14] A. Bossavit. A uniform rationale for Whitney forms on various supporting shapes. *Mathematics and Computers in Simulation*, 2008.

[15] D. Braess. *Finite Elements: Theory, Fast Solvers, and Applications in Solid Mechanics.* Cambridge University Press, 3 edition, April 2007.

[16] J. H. Bramble and S. R. Hilbert. Estimation of Linear Functionals on Sobolev Spaces with Application to Fourier Transforms and Spline Interpolation. *SIAM Journal on Numerical Analysis*, 7(1):112–124, 1970.

[17] S. Brenner and L. Scott. *The mathematical theory of finite element methods.* Springer Verlag, 2008.

[18] F. Brezzi. On the existence, uniqueness and approximation of saddle-point problems arising from Lagrangian multipliers. *RAIRO Anal. Numer*, 8(2):129–151, 1974.

[19] F. Brezzi, K. Lipnikov, and M. Shashkov. Convergence of the mimetic finite difference method for diffusion problems on polyhedral meshes. *SIAM Journal on Numerical Analysis*, 43(5):1872–1896 (electronic), 2005.

[20] F. Brezzi, K. Lipnikov, and V. Simoncini. A family of mimetic finite difference methods on polygonal and polyhedral meshes. *Mathematical Models and Methods in Applied Sciences*, 15(10):1533–1551, 2005.

[21] J. C. Campbell and M. J. Shashkov. A tensor artificial viscosity using a mimetic finite difference algorithm. *Journal of Computational Physics*, 172(2):739–765, 2001.

[22] J. Cea. Approximation variationnelle des problèmes aux limites. *Annales de L'Institut Fourier*, 14(2):345–444, 1964.

[23] V. Chatzi and F. Preparata. Using pyramids in mixed meshes - point placement and basis functions. Technical report, Brown University Providence, RI, USA, 2000.

[24] Z. Chen and J. Douglas. Prismatic mixed finite elements for second order elliptic problems. *Calcolo*, 26(2):135–148, 1989.

[25] P. G. Ciarlet. *The Finite Element Method for Elliptic Problems.* Society for Industrial Mathematics, April 2002.

[26] B. Cockburn and J. Gopalakrishnan. Incompressible finite elements via hybridization. Part II: The Stokes system in three space dimensions. *SIAM Journal on Numerical Analysis*, 43:1651–1672, 2005.

[27] M. Costabel, M. Dauge, and L. Demkowicz. Polynomial extension operators. *Mathematics of Computation*, 77(264):1967–1999, 2008.

[28] J. Coulomb, F. Zgainski, and Y. Maréchal. A pyramidal element to link hexahedral, prismatic and tetrahedraledge finite elements. *IEEE Transactions on Magnetics*, 33(2 Part 2):1362–1365, 1997.

[29] L. Demkowicz and A. Buffa. H^1, $H(\text{curl})$ and $H(\text{div})$-conforming projection-based interpolation in three dimensions. Quasi-optimal p-interpolation estimates. *Computer Methods in Applied Mechanics and Engineering*, 194(2-5):267–296, 2005.

[30] L. Demkowicz, J. Gopalakrishnan, and J. Schöberl. Polynomial extension operators. Part I. *SIAM Journal on Numerical Analysis*, 46:3006–3031, 2007.

[31] L. Demkowicz, J. Kurtz, D. Pardo, M. Paszenski, and W. Rachowicz. *Computing with hp-Adaptive Finite Elements: Volume 2: Frontiers: Three Dimensional Elliptic and Maxwell Problems with Applications.* Chapman & Hall, 2007.

[32] L. Demkowicz, P. Monk, L. Vardapetyan, and W. Rachowicz. De Rham diagram for *hp* finite element spaces. *Computers & Mathematics with Applications*, 39(7-8):29–38, 2000.

[33] L. Demkowicz, J. Oden, W. Rachowicz, and O. Hardy. Toward a universal *hp* adaptive finite element strategy, Part 1. Constrained approximation and data structure. *Computer Methods in Applied Mechanics and Engineering*, 77(1-2):79–112, 1989.

[34] L. Demkowicz, W. Rachowicz, and P. Devloo. A fully automatic *hp*-adaptivity. *Journal of Scientific Computing*, 17(1):117–142, 2002.

[35] C. Doucet, I. Charpentier, J. Coulomb, and C. Guérin. Extraction of finite element basis functions from the cellular topology of meshes. *IEEE Transactions on Magnetics*, 44(6):726–729, 2008.

[36] M. Duffy. Quadrature over a pyramid or cube of integrands with a singularity at a vertex. *SIAM Journal on Numerical Analysis*, 19(6):1260–1262, 1982.

[37] A. Düster, H. Bröker, and E. Rank. The p-version of the finite element method for three-dimensional curved thin walled structures. *International Journal for Numerical Methods in Engineering*, 52(7):673–703, 2001.

[38] C. Felippa. A compendium of FEM integration formulas for symbolic work. *Engineering Computations*, 21(8):867–890, 2004.

[39] M. Fortin. An analysis of the convergence of mixed finite element methods. *RAIRO Anal. Numer*, 11(R3):341–353, 1977.

[40] M. Fortin and F. Brezzi. *Mixed and Hybrid Finite Element Methods (Springer Series in Computational Mathematics)*. Springer-Verlag Berlin and Heidelberg GmbH & Co. K, December 1991.

[41] P. Gatto and L. Demkowicz. Construction of H^1-conforming hierarchical shape functions for elements of all shapes and transfinite interpolation. *Finite Elements in Analysis and Design*, 46(6):474–486, 2010.

[42] V. Gradinaru and R. Hiptmair. Whitney elements on pyramids. *Electronic Transactions on Numerical Analysis*, 8:154–168, 1999.

[43] R. Graglia and I. Gheorma. Higher order interpolatory vector bases on pyramidal elements. *IEEE transactions on antennas and propagation*, 47(5):775, 1999.

[44] B. Guo and I. Babuška. The hp version of the finite element method. *Computational mechanics*, 1(1):21–41, 1986.

[45] P. C. Hammer, O. J. Marlowe, and A. H. Stroud. Numerical integration over simplexes and cones. *Mathematical Tables and Other Aids to Computation*, 10(55):130–137, 1956.

[46] R. Hiptmair. Canonical construction of finite elements. *Mathematics of Computation*, 68(228):1325–1346, 1999.

[47] J. Hoffman, J. Jansson, C. Johnson, M. Knepley, R. Kirby, A. Logg, L. Scott, and G. Wells. FEniCS, 2006. *URL: http://www.fenics.org.*

[48] J. Hunter. Matplotlib: A 2D graphics environment. *Computing in Science & Engineering*, pages 90–95, 2007.

[49] J. M. Hyman and M. Shashkov. Natural discretizations for the divergence, gradient, and curl on logically rectangular grids. *Computers & Mathematics with Applications*, 33(4):81–104, 1997.

[50] E. Jones, T. Oliphant, P. Peterson, et al. SciPy: Open source scientific tools for Python, 2001–2010.

[51] G. E. Karniadakis and S. J. Sherwin. *Spectral hp element methods for computational fluid dynamics*. Numerical Mathematics and Scientific Computation. Oxford University Press, New York, second edition, 2005.

[52] J. Kurtz and L. Demkowicz. A fully automatic hp-adaptivity for elliptic PDEs in three dimensions. *Computer Methods in Applied Mechanics and Engineering*, 196(37-40):3534–3545, 2007.

[53] Y. Kuznetsov, K. Lipnikov, and M. Shashkov. The mimetic finite difference method on polygonal meshes for diffusion-type problems. *Computational Geosciences*, 8(4):301–324 (2005), 2004.

[54] C. Lee and Q. Xu. A new automatic adaptive 3D solid mesh generation scheme for thin-walled structures. *International Journal for Numerical Methods in Engineering*, 62(11):1519–1558, 2005.

[55] L. Liu, K. B. Davies, K. Yuan, and M. Křížek. On symmetric pyramidal finite elements. *Dynamics of Continuous, Discrete & Impulsive Systems. Series B: Applications & Algorithms*, 11(1-2):213–227, 2004. First Industrial Mathematics Session.

[56] J. Lyness and R. Cools. A survey of numerical cubature over triangles. In *Mathematics of computation, 1943-1993: a half-century of computational mathematics: Mathematics of Computation 50th Anniversary Symposium, August 9-13, 1993, Vancouver, British Columbia*, volume 48, page 127. American Mathematical Society, 1994.

[57] J. Melenk, K. Gerdes, and C. Schwab. Fully discrete *hp*-finite elements: Fast quadrature. *Computer Methods in Applied Mechanics and Engineering*, 190(32-33):4339–4364, 2001.

[58] P. Monk. *Finite element methods for Maxwell's equations*. Numerical Mathematics and Scientific Computation. Oxford University Press, New York, 2003.

[59] J. Nedéléc. Mixed finite elements in $\mathbb{R}^3$. *Numerische Mathematik*, 35(3):315–341, 1980.

[60] J. Nedéléc. Éléments finis mixtes incompressibles pour l'équation de Stokes dans $\mathbb{R}^3$. *Numerische Mathematik*, 39(1):97–112, 1982.

[61] J. Nedéléc. A new family of mixed finite elements in $\mathbb{R}^3$. *Numerische Mathematik*, 50(1):57–81, 1986.

[62] N. Nigam and J. Phillips. Higher-order finite elements on pyramids. *arXiv preprint math/0610206*, 2006.

[63] N. Nigam and J. Phillips. High-order finite elements on pyramids: approximation spaces, unisolvency and exactness. *IMA Journal of Numerical Analysis*, 2010 (submitted).

[64] J. Oden, L. Demkowicz, W. Rachowicz, and T. Westermann. Toward a universal *hp* adaptive finite element strategy, Part 2. A posteriori error estimation. *Computer Methods in Applied Mechanics and Engineering*, 77(1-2):113–180, 1989.

[65] S. Owen and S. Saigal. Formation of pyramid elements for hexahedra to tetrahedra transitions. *Computer Methods in Applied Mechanics and Engineering*, 190(34):4505–4518, 2001.

[66] W. Rachowicz, J. Oden, and L. Demkowicz. Toward a universal *hp* adaptive finite element strategy part 3. design of *hp* meshes. *Computer Methods in Applied Mechanics and Engineering*, 77(1-2):181–212, 1989.

[67] P. Ramachandran and G. Varoquaux. MayaVi: Making 3D data visualization reusable. In *Proceedings of the 7th Python in Science conference (SciPy 2008) http://code.enthought.com/projects/mayavi.*

[68] P. Raviart and J. Thomas. A mixed finite element method for 2-nd order elliptic problems. *Mathematical aspects of finite element methods*, pages 292–315, 1977.

[69] D. Schötzau and C. Schwab. Mixed *hp*-FEM on anisotropic meshes. *Mathematical Models and Methods in Applied Sciences*, 8(5):787–820, 1998.

[70] D. Schötzau, C. Schwab, and R. Stenberg. Mixed hp-FEM on anisotropic meshes II: Hanging nodes and tensor products of boundary layer meshes. *Numerische Mathematik*, 83(4):667–697, 1999.

[71] C. Schwab. *p-and hp-finite element methods: Theory and applications in solid and fluid mechanics.* Oxford University Press, USA, 1998.

[72] S. Sherwin. Hierarchical *hp* finite elements in hybrid domains. *Finite Elements in Analysis and Design*, 27(1):109–119, 1997.

[73] S. Sherwin and G. Karniadakis. A new triangular and tetrahedral basis for high-order (*hp*) finite element methods. *International Journal for Numerical Methods in Engineering*, 38(22):3775–3802, 1995.

[74] S. Sherwin, T. Warburton, and G. Karniadakis. Spectral/*hp* methods for elliptic problems on hybrid grids. *Contemporary Mathematics*, 218:191–216, 1998.

[75] S. Stigler. Stigler's law of eponymy. *Transactions of the New York Academy of Sciences*, 39:147–158, 1980.

[76] A. H. Stroud. *Approximate calculation of multiple integrals.* Prentice-Hall Inc., Englewood Cliffs, N.J., 1971.

[77] G. Szegö. *Orthogonal polynomials. Revised ed.* American Mathematical Society (AMS), 1959.

[78] A. Toselli and C. Schwab. Mixed hp-finite element approximations on geometric edge and boundary layer meshes in three dimensions. *Numerische Mathematik*, 94(4):771–801, 2003.

[79] E. Wachspress. Rational bases for convex polyhedra. *Computers & Mathematics with Applications*, 2009.

[80] E. L. Wachspress. *A rational finite element basis.* Academic Press, Inc. [A subsidiary of Harcourt Brace Jovanovich, Publishers], New York, 1975. Mathematics in Science and Engineering, Vol. 114.

[81] J. Warren. Barycentric coordinates for convex polytopes. *Advances in Computational Mathematics*, 6(1):97–108, 1996.

[82] J. Warren, S. Schaefer, A. Hirani, and M. Desbrun. Barycentric coordinates for convex sets. *Advances in Computational Mathematics*, 27(3):319–338, 2007.

[83] H. Whitney. Geometric integration theory. *Bulletin of the AMS*, 2(9904):10143–3, 1958.

[84] C. Wieners. Conforming discretizations on tetrahedrons, pyramids, prisms and hexahedrons. Technical report, University of Stuttgart.

[85] S. Zaglmayr. *High Order Finite Element methods for Electromagnetic Field Computation.* PhD thesis, Johannes Kepler University, Linz, July 2006.

[86] F.-X. Zgainski, J.-L. Coulomb, Y. Marechal, F. Claeyssen, and X. Brunotte. A new family of finite elements: the pyramidal elements. *IEEE Transactions on Magnetics*, 32(3):1393–1396, May 1996.

[87] O. Zienkiewicz and R. Taylor. *The finite element method for solid and structural mechanics.* Butterworth-Heinemann, 2005.