Using Pyramids in Mixed Meshes - Point Placement and Basis Functions

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Abstract

For mixed 3D finite element meshes (meshes that contain cubes *and* tetrahedra) pyramids are very convenient because they have both square and triangular faces and can therefore be used in implementing conformal transitions between regions that contain cubes and regions that contain tetrahedra. However, pyramids are rarely used, because the specification of basis functions for them is known to be problematic. Of specific importance it the development of Lagrangian basis functions for pyramids, since Lagrangian standard elements are the most commonly used type of elements today.

In this paper, we present basis functions for pyramidal finite elements that can be used in Lagrangian meshes. 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, and therefore the basis functions shown here are the simplest ones possible. We describe in detail a convenient and elegant method to obtain the basis functions for the order-k pyramid (for any $k > 0$), which uses the functions for the order-$(k-1)$ pyramid. A valid set of basis functions for the order-1 pyramid (which can be used as the basis of the construction) are also presented.

1 Introduction

Problems in physics and engineering defined on a given physical domain are often modeled by a system of partial differential equations, together with appropriate boundary conditions. This data completely describes the physical phenomenon and solving the partial differential equations results in the values of the physical quantities of interest in the defined

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region. However, obtaining a closed-form solution for the equation is often impossible. In these cases we have to settle for using a numerical method to obtain approximate results.

The finite element method is one of the tools commonly used today for these types of problems. During the first step, we discretize the domain by partitioning it into a set of simpler shapes, called *elements*. The resulting collection of elements is called the *finite element mesh* and the process of creating the mesh from the domain is called *mesh generation*. Once the mesh has been created, nodal points are defined on the elements, a basis function is associated with each nodal point and a system of linear equations is constructed and solved. The type of an element depends both on the placement of nodal points on it and the basis functions associated with each nodal point. Lagrangian elements that have the same number of nodal points placed on each edge and internal points placed on a grid are commonly used today.

In a previous paper [4] we have justified in detail, on the basis of simplicity and computational efficiency the adoption of a flexible, highly structured, conformal new type of meshes called "crystalline meshes". One problem not discussed in [4] was the form of the basis functions associated with the nodal points placed on the elements of crystalline meshes. The definition of such functions is particularly significant because (see below) 3D crystalline meshes have pyramidal elements, for which the specification of basis functions is known to be problematic. In this paper we exhibit an efficient and, in our opinion, elegant answer to this important question which provides added incentive to the adoption of crystalline meshes. Specifically, we present a method for constructing basis functions for the Lagrangian pyramids of order $k > 0$.

A set of basis functions for the first-order and second-order pyramids have been previously developed and are used [9, 8, 10]. Our work subsumes that, since we can generate basis functions for the kth order pyramid, where k is any positive integer.

The rest of this paper is organized as follows. Section 2 reviews the definition of crystalline meshes. Section 3 focuses on basis functions, and it explains how they are used and what properties they should exhibit. It also describes standard Lagrangian elements (both in 2D and 3D) and the basis functions associated with them. Section 4 gives the node placement on Lagrangian pyramids and describes the template pyramid we will use. Section 5 is the heart of this paper. It contains a description of the method that we propose to obtain basis functions for the kth order pyramid. Finally, Section 6 gives the conclusions and some future work.

2 Crystalline Meshes

Crystalline meshes are a new type of finite element meshes that combine the advantages of both structured and unstructured meshes, by offering the flexibility of different element densities in different regions of the domain and the ability to generate the system of linear equations quickly and accurately.

We now review the basic properties of 3D crystalline meshes.

1. The basic element type in 3D crystalline meshes is the cube, and in this respect, crystalline meshes are related to octree meshes [14, 7, 11, 13] and Cartesian meshes (see for example [6]). It is well known that cubes outperform tetrahedra for many types of problems [1, 5].
2. Crystalline meshes allow different element densities in different regions of the domain. In general, if we use smaller elements in the mesh, we obtain a more accurate solution,but also increase the size of the mesh (and of the corresponding system of equations). Ideally, we would like to cover "regions of interest", where the value of the solution changes rapidly, either statically or dynamically, with smaller elements.
3. Crystalline meshes are conformal. An element is said to be *conformal* if its intersection with any other element in the mesh is empty, or a vertex, or an edge or a face. A mesh is conformal if all its elements are conformal [3, 12]. Non-conformal points create numerical problems which can only be solved by using complicated specialized techniques, and therefore should be avoided whenever possible.
4. Crystalline meshes consist of elements that have only few distinct shapes. This allows us to precompute the matrices associated with the elements [15] and generate the system of linear equations by assembling them, thereby simplifying the generation of the system of equations and improving the accuracy of the solution.

Notice that since the mesh is conformal, cubes of different size cannot share a face or an edge. Therefore, if the mesh contains two regions with different element density, there will be a (possibly very shallow) transition layer of non-cubical elements between them. Pyramids are ideal shapes to be used as transitional elements, because they have a square face, which can be conformally attached to a cube, and four triangular faces that can be attached to tetrahedra (for an illustration, see Figure 1).

Although pyramids are very powerful as transitional elements, computational scientists avoid using them, due to the difficulty of finding basis functions. In particular, to our knowledge, there is no previous

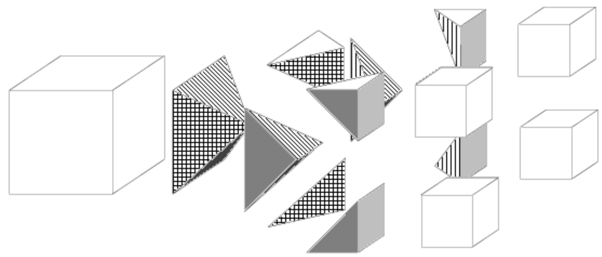


Figure 1: Realizing a conformal transition between cubes of two different sizes. Five pyramids and four tetrahedra can be conformally attached to the larger cube. The resulting surface is partitioned into four square faces, that can be shared with smaller cubes.

work describing how to construct basis functions for pyramids, so that they can be used in a mixed mesh, together with Lagrangian cubes and tetrahedra.

Before describing the structure of our basis functions for the pyramids however, we briefly review their required properties, and the basis functions associated with standard Lagrangian elements.

3 Basis Functions and Lagrangian Elements

Given a partial differential equation defined on a domain, the finite element method computes an approximate solution which is of the form:

$$f(x,y,z) = \sum_{i=1}^{n} x_i \phi_i(x,y,z)$$

The ϕ_i's are functions associated with the nodal points, that have been previously defined (called basis functions) and the x_i's are values computed by solving the system of linear equations.

The process starts by defining nodal points on each of the elements in the mesh and associating a basis function with each of them. As is well known (eg. [15]) basis functions should have the following properties:

- **Property 1.** *Each basis function ϕ_i associated with a nodal point p_i evaluates to 0 on all the points in the physical domain lying outside the elements containing p_i.* This requirement is easy to achieve, by constructing ϕ_i as a piecewise defined function which is identically 0 outside the relevant elements.

- **Property 2.** *The function ϕ_i evaluates to* 1 *on p_i and to* 0 *on all other nodal points.* Notice that nodal points outside the elements containing p_i do not pose a problem, since the function has been defined to evaluate to 0 outside these elements. Thus, the function has to be carefully constructed so that it also evaluates to 0 on nodal points that belong to the elements containing p_i.
- **Property 3.** *The function ϕ_i is continuous.* Since solutions of the PDE are typically continuous it is reasonable to require that they be approximated by continuous functions. The derivatives of the basis functions, however, are not required to be continuous (C_0-continuity).

Let basis function ϕ_i be associated with point p_i. Property 3 requires that ϕ_i be C_0-continuous. This, in conjunction with Property 1 requiring that ϕ_i evaluate to 0 outside of elements containing p_i, yields the following (nonindependent) property:

Property 4. *For each element containing p_i, ϕ_i must be* 0 *on the portions of the element's boundary not containing p_i.*

Moreover, Property 1 and Property 2 yield:

Property 5 *For each element's face containing p_i, ϕ_i must reduce to a correct 2D basis function for that face.*

A common practice when designing basis functions for the nodal points defined on a mesh is to restrict our attention to one element at a time. Every time an element e_i is processed, appropriate basis functions for all nodal points in the element are defined. These basis functions are valid only within the element e_i. When using this policy, however, we have to be careful so that the resulting basis functions exhibit C_0-continuity. Nodal points placed on shared vertices, edges or faces will have several partial functions associated with them, one for each element they belong to. These functions should have the same value on every point on the shared edges and faces.

Mesh elements are characterized by both the placement of nodal points on them and the basis functions associated with the nodal points. The elements most commonly used today are elements of the Lagrange family, named so because the associated basis functions can be expressed as the product of 2 (3 for 3D elements) Lagrange interpolation polynomials.

2D Lagrangian elements of order k have $k+1$ nodal points placed on each of their edges at regular intervals. These points define a grid in a natural way, and additional nodal points are placed on the ver-

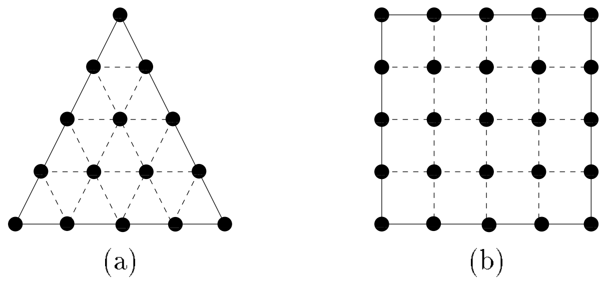


Figure 2: Standard 2D Lagrangian elements of order 4. (a) Triangle. (b) Square. Dashed lines denote the grid used for the placement of the internal nodal points.

tices of this grid. The basis functions associated with each one of the nodal points can be constructed by using the product of Lagrangian polynomials, or any of the standard methods found in literature [15, 2]. Each of the resulting basis functions correctly reduces to a k-th degree polynomial on each of the edges of the element (since it must evaluate to 0 in k points of the edge). Figure 2 shows the node placement on a Lagrangian triangle and a Lagrangian square of order 4.

Standard 3D Lagrangian elements have faces that are valid 2D Lagrangian elements. Nodal points on the faces define a grid in the interior of the elements in a natural way, and internal points are placed on the vertices of this grid. Basis functions for each of the nodal points can be constructed by using generalizations of the methods used for 2D elements. An important property of the resulting basis functions is that the reduction of the function ϕ_i on one of the faces of the 3D element is identically 0 if p_i is not located on that face and, otherwise, it coincides with the valid 2D Lagrangian basis function for p_i on the face. This automatically ensures C_0-continuity on the element boundaries.

Another important characteristic of standard Lagrangian elements is that the basis function ϕ_i associated with the nodal point p_i can also be expressed as a product of functions describing lines (for 2D elements) or planes (for 3D elements) when equated to 0. With a slight abuse of language we shall say that ϕ_i is respectively "a product of lines" or "a product of planes". These geometric primitives cover all nodal points in the element besides p_i, thereby ensuring that the function evaluates to 0 on every nodal point p_j with $i \neq j$, in the element. A normalizing factor ensures that the function evaluates to 1 on p_i.

Lagrangian elements are widely used today because of computational simplicity, guaranteed C_0-continuity and good numerical perfor-

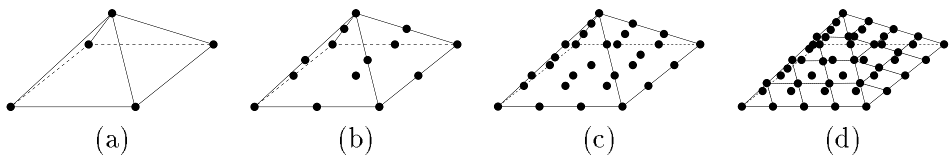


Figure 3: Low order Lagrangian pyramids : (a) first order (b) second order (c) third order (d) fourth order.

mance. For this reason we consider obtaining a pyramid that can be used in mixed (i.e. not necessarily crystalline) meshes together with standard Lagrangian elements of particular importance. In the next section we describe the node placement on such a pyramid.

4 Lagrangian Pyramid

The pyramids that we consider in this paper are polyhedra one face of which is a parallelogram and the other four faces are triangular. Since they are conceived as conformal transition elements in meshes whose standard elements are Lagrangian, we shall refer to them as *Lagrangian pyramids*. The node placement on the faces is the same as on Lagrangian parallelograms and triangles. Since internal nodes are not required for C_0-continuity, we chose not to use any internal points. This simplifies both the actual basis functions and the procedure used in constructing them. Figure 3 shows the node placement on Lagrangian pyramids of order 1, 2, 3 and 4. It is easily established that an order k pyramid has $3k^2 + 2$ nodes (all on its surface).

A common practice in constructing basis functions is to use a standard element (*template*), in a standard frame of reference, ξ, η, ζ and bijectively projected to an element of the same shape in the frame of the mesh. The reverse transformation maps any basis function for a nodal point of the template to a valid basis function for the corresponding nodal point on any mesh element. This bijection allows us to concentrate on finding basis functions for the template whose vertices have conventionally the coordinates shown in Figure 4.

The template and a generic mesh pyramid are shown in Figure 5. Since the base of the mesh pyramid is constrained to be a parallelogram, four points uniquely define it (homologous to template points p_0, p_1, p_3 and p_4), so that the bijection is uniquely specified as:

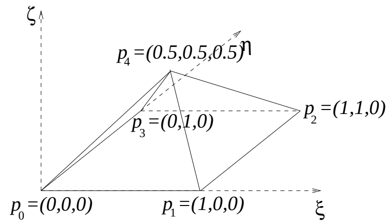
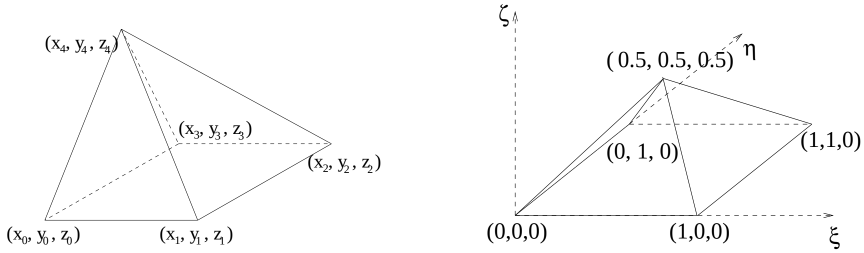


Figure 4: The pyramid chosen as a template. Next to each vertex we denote its number and its coordinates.



(a) (b)

Figure 5: (a) An arbitrary pyramid in the coordinate system (x, y, z). (b) The template pyramid in the coordinate system (ξ, η, ζ)

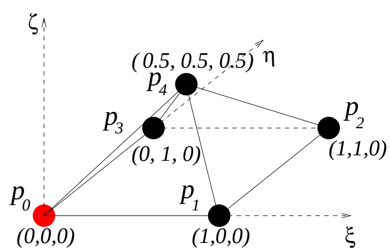


Figure 6: First order template pyramid.

$$
\begin{aligned}
x &= x_0 + (x_1 - x_0)\xi + (x_3 - x_0)\eta + (-x_1 - x_3 + 2x_4)\zeta \\
y &= y_0 + (y_1 - y_0)\xi + (y_3 - y_0)\eta + (-y_1 - y_3 + 2y_4)\zeta \\
z &= z_0 + (z_1 - z_0)\xi + (z_3 - z_0)\eta + (-z_1 - z_3 + 2z_4)\zeta
\end{aligned}
$$

For crystalline meshes the bijection is a composition of a (restricted) homothety and a (restricted) rigid motion.

Differently from standard Lagrangian elements (cubes and tetrahedra), which have polynomial basis functions, we now show that basis functions for Lagrangian pyramids *cannot* be polynomials. In fact, without loss of generality, consider point p_0 on the first order pyramid shown in Figure 6. Function ϕ_0 must:

1. reduce to 0 on the two triangular faces that do not contain p_0.
2. reduce to a linear function on the two triangular faces containing p_0 (since the basis functions for the nodal points of first-order triangles are linear).
3. reduce to a bilinear function on the square face (since the basis functions for nodal points on first-order squares are bilinear).

By Requirement 1 a polynomial basis function must contain *both* factors $(\xi + \zeta - 1)$ and $(\eta + \zeta - 1)$ (which, equated to 0 describe the planes of the two faces). But on face (p_0, p_1, p_4) this product becomes

$$(\xi + \eta - 1)(2\eta - 1)$$

and remains quadratic. Thus we have proved:

Theorem 4.1 *It is impossible to construct* polynomial *basis functions for the first order Lagrangian pyramid.*

5 Basis Functions for Lagrangian Pyramids

In the previous section we proved that we cannot construct polynomial basis functions for the order-1 pyramid. However, there is no reason to restrict the basis functions to polynomials, since to enforce C_0-continuity we only have to ensure that the basis functions reduce to 0 on the faces not containing the corresponding nodal point, and to the correct 2D basis function on the faces containing it. Indeed, we will show that by allowing the basis functions to be ratios of polynomials, we can construct basis functions for a template pyramid of order k, for any integer $k > 0$.

5.1 Basis Functions for the order-1 Pyramid

We begin by constructing the basis functions for the order-1 template pyramid, and later generalize the construction to arbitrary order k.

Referring to Figure 8, the order-1 pyramid has five nodal points, each one of which coincides with one of its vertices. Function $\phi_i(\xi, \eta, \zeta)$ associated with the point $p_i = (\xi_i, \eta_i, \zeta_i)$ must satisfy the general requirements for 3D Lagrangian basis. Since functions ϕ_0, ϕ_1, ϕ_2, and ϕ_3 are equivalent, it suffices to consider in detail ϕ_0 and ϕ_4. Function $\phi_0(\xi, \eta, \zeta)$ must:

1. evaluate to 0 on faces $p_1p_2p_4$ and $p_2p_3p_4$,
2. reduce to a line passing through p_1 and p_4 on face $p_0p_1p_4$ and to a line passing through p_3 and p_4 on face $p_0p_4p_3$,
3. on the base of the pyramid, reduce to the product of two lines, one passing through p_1 and p_2 and the other passing through p_2 and p_3.

By 1.) the expression of ϕ_0 must contain the factors $\xi + \zeta - 1$ and $\eta + \zeta - 1$ (corresponding respectively to the planes containing faces $p_1p_2p_4$ and $p_2p_3p_4$). On faces $p_0p_1p_4$ (of equation $\eta - \zeta = 0$) and $p_0p_4p_3$ (of equation $\xi - \zeta = 0$) this product becomes $(\xi + \zeta - 1)(2\zeta - 1)$ and $(2\zeta - 1)(\eta + \zeta - 1)$, respectively, so that Requirement 2.) is satisfied if we divide the product by the factor $2\zeta - 1$. The expression

$$\frac{(\xi + \zeta - 1)(\eta + \zeta - 1)}{2\zeta - 1} \tag{1}$$

on the base plane $\zeta = 0$ becomes $(\xi - 1)(\eta - 1)$, i.e., it assume value 0 on edges p_1p_2 and p_2p_3, thus satisfying Requirement 3. Therefore, after normalization by a constant factor to ensure the value of 1 on the associated nodal point, the above is a valid expression of ϕ_0. We observe that, although the denominator $2\zeta - 1$ becomes 0 at $p_4 = (\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$, the value of (1) is 0, as can be verified by applying the rule of L'Hospital. It is now a simple exercise to verify that

$$\phi_i(\xi, \eta, \zeta) = (-1)^{i+1} \frac{((-1)^{\xi_i}\xi + \zeta - 1 + \xi_i)((-1)^{\eta_i}\eta + \zeta - 1 + \eta_i)}{2\zeta - 1}, \quad i = 0..3$$

since it is obtained from ϕ_0 by displacing the origin by (ξ_i, η_i) and appropriately reversing the signs of the variables involved in the displacement.

We now consider function ϕ_4, which must reduce to 0 on the base of the pyramid, and to a line passing through the two vertices on the base on each of the triangular faces (e.g., to line $(\xi - 1) = 0$ on face $\xi + \zeta - 1 = 0$). It is immediate that (normalized)

$$\phi_4(\xi, \eta, \zeta) = 2\zeta$$

is the desired function. We conclude

Lemma 5.1 *There exist basis functions for the order-*1 *Lagrangian pyramid, which are* ratios of polynomials*.*

5.2 Generalization to Arbitrary Order k

We now describe an inductive construction process, which, taking as basis the order-1 basis functions, and assuming as a premise the order-$(k - 1)$ fuctions, produces the desired order-k basis functions. We

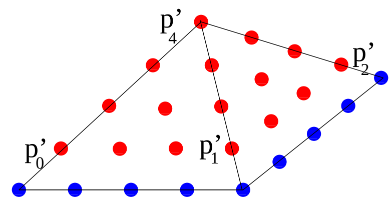


Figure 7: A kth order pyramid for $k = 4$.The nodal points not on the base form a order- $(k-1)$ pyramid. The nodes that are vertices of the order-$(k-1)$ pyramid are shown marked.

begin by classifying the nodal points of the order-k pyramid according to their common requirements. Specifically, we shall distinguish and treat separately:

1. points not on the base (the simpler case);
2. points on the base.

We begin with the points not on the base.

Lemma 5.2 *Given basis functions for the $(k-1)$-st order pyramid which are ratios of polynomials, we can construct basis functions, also ratios of polynomials, for nodal point not on the base of the order-k pyramid.*

Proof: The nodal points not lying on the base (that is, the points for which $\zeta \neq 0$) form a (non-template) order-$(k-1)$ pyramid (see Figure 7). We can map to the present spatial configuration, as indicated in Section 4, the basis functions for the order-$(k-1)$ template pyramid (inductively assumed to be available).

The mapping consists of a translation by $(\frac{1}{2k}, \frac{1}{2k}, \frac{1}{2k})$ followed by a homothety along the three axes by a factor $(k-1)/k$. It follows that the mapping consists in replacing coordinates (ξ, η, ζ) with (ξ', η', ζ') given by:

$$\xi' = \frac{2k\xi - 1}{2k-2}, \eta' = \frac{2k\eta - 1}{2k-2}, \zeta' = \frac{2k\zeta - 1}{2k-2}$$

The functions so obtained have most of the required properties: they reduce to 0 on the triangular faces not containing the associated nodal point, evaluate to 1 on the latter, and to 0 on all the other nodal points lying above the base. However, they have two shortcomings: they don't reduce to 0 on the base of the pyramid, and, on the triangular faces containing the associated point they reduce to a polynomial that is the product of $k-1$ (instead of k) lines. Fortunately, this inadequacy can be remedied by multiplying the functions by ζ. Since

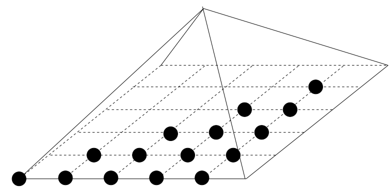


Figure 8: Set of nonequivalent points on the base of a 5th order pyramid.

this multiplication causes the basis function ϕ_i to evaluate to ζ_i on its associated point p_i, the function must be normalized by the factor $\frac{1}{\zeta_i}$. $\square$

We now turn our attention to the more complex case of nodal points on the pyramid's base.

It is convenient to use two indices to denote the points, so that for $0 \leq i, j \leq k$, $p_{i,j} = (\frac{i}{k}, \frac{j}{k}, 0)$. The corresponding basis function $\phi_{i,j}(\xi, \eta, \zeta)$, when set equal to 0, defines a surface in three-dimensional space, which we shall specify by means of its intersections with the pyramid faces that contains the given point (either in their interior or on their boundary). Due to the symmetries of the square, we shall limit our considerations to nonequivalent points, as illustrated in Figure 8.

Our objective is to design functions $\phi_{i,j}(\xi, \eta, \zeta)$ that are ratios of polynomials. Their numerators, therefore, will contain as factors polynomials (called *primitives*), each of which, equated to 0, defines a three-dimensional surface (referred to as a *primitive construct*). By Property 5 of basis functions and the specific properties of Lagrangian elements, the intersection of any such primitive construct with a surface of the pyramid must be a line where the reduction of $\phi_{i,j}$ has value 0. We shall first describe the various primitive constructs to be used.

Definition 5.1 *For each i, $i = 0, 1, \ldots, k$,let*

$$\xi_i^L = \xi + \zeta - \frac{i}{k} \quad \text{and} \quad \xi_i^R = \xi - \zeta - \frac{i}{k}.$$

Both $\xi_i^L = 0$ and $\xi_i^R = 0$ describe planes and reduce on the base to the line $\xi - \frac{i}{k} = 0$ passing by $p_{i,0}$ and $p_{i,k}$. On face $p_0p_1p_4$ of the pyramid (in the plane $\eta - \zeta = 0$) they reduce to the lines $\xi + \eta - \frac{i}{k} = 0$ and $\xi - \eta - \frac{i}{k} = 0$, respectively. We conclude that ξ_i^L and ξ_i^R are valid primitives, since the latter lines, each of which is parallel to one of the edges of the triangular face, are primitives for 2D Lagrangian basis functions.

By the symmetry of the ξ and η directions, we analogously define:

Definition 5.2 *For each j, $j = 0, 1, \ldots, k$, let*

$$\eta_j^L = \eta + \zeta - \frac{j}{k} \quad \text{and} \quad \eta_j^R = \eta - \zeta - \frac{j}{k}.$$

Adapting the preceding discussion to this situation, both η_j^L and η_j^R are verified to be valid primitives.

Convenient additional constructs (corresponding to sheaves of contiguous parallel planes) are given in the following definition:

Definition 5.3 *Let*

$$\Xi^L = \prod_{i=1}^{k-1} \xi_i^L, \qquad \Xi^R = \prod_{i=1}^{k-1} \xi_i^R, \qquad H^L = \prod_{j=1}^{k-1} \eta_j^L, \quad \text{and} \quad H^R = \prod_{j=1}^{k-1} \eta_j^R.$$

Our catalog of primitive constructs is completed by a set of quadric surfaces:

Definition 5.4 *For each i, $0 \le i \le k$ let*

$$\begin{aligned} q_i &= 2\zeta(\xi + \eta - \frac{i}{k}) - (\xi + \zeta - \frac{i}{k})(\eta + \zeta - \frac{i}{k}) \\ &= -\zeta^2 - \xi\eta + \xi\zeta + \eta\zeta + \xi\frac{i}{k} + \eta\frac{i}{k} - \frac{i^2}{k^2} \end{aligned}$$

Notice that $q_i = 0$ belongs to the pencil of quadrics sharing four lines in 3D space, specifically the lines containing $p_{i,0}p_{i,k}$ and $p_{0,i}p_{k,i}$ in the base plane, the line by p_{i0} parallel to edge p_1p_4 on face $p_0p_1p_4$, and the line by $p_{0,i}$ parallel to edge p_3p_4 on face $p_0p_4p_3$. All four lines are primitives in the corresponding Lagrangian squares and triangles, so that the quadric is a valid primitive construct. Whereas the generators of the pencil are degenerate quadrics (pairs of planes), $q_i = 0$ is a hyperbolic paraboloid.

Using the defined primitives we can now tackle the construction of the functions $\phi_{i,j}(\xi, \eta, \zeta)$.

Lemma 5.3 *There exist basis functions that are ratios of polynomials for nodal point lying on the base of the order-k pyramid.*

Proof: We shall restrict the analysis to nonequivalent points, since from the basis function for each of the chosen representatives, by standard linear transformation of coordinates, we can generate the basis function for any point on the pyramid's base.

We distinguish three cases:

1. *Points in the interior of the base*($p_{i,j}$, $0 < j \le i < k$). Such points belong to a single face (the base) of the pyramid. By Property 4 the basis function $\phi_{i,j}$ must reduce to 0 on all triangular faces of the

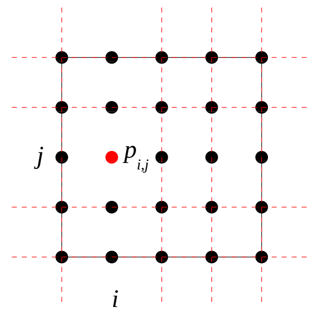


Figure 9: The lines resulting in from factoring the reduction of $\phi_{i,j}$ on the plane $\zeta = 0$.

pyramid and, therefore, it must contain the four factors $\xi_0^R, \xi_k^L, \eta_0^R, \eta_k^L$ corresponding to the four planes of the lateral faces. By Property 5, on the base it must reduce to the appropriate two-dimensional basis function for the corresponding nodal point on the Lagrangian square. As discussed in Section 3 the latter is a product of $2k$ lines, covering all the columns and rows defined by the nodal points different from $p_{i,j}$, i.e., to the product

$$\left(\prod_{\substack{l=0 \\ l \neq i}}^{k} \xi_l^R \prod_{\substack{m=0 \\ m \neq j}}^{k} \eta_m^R \right)_{\zeta=0}$$

It follows that a valid expression for ϕ_{ij} is

$$\boxed{\phi_{i,j} = c_{i,j} \xi_0^R \xi_k^L \eta_0^R \eta_k^L \frac{\Xi^R}{\xi_i^R} \frac{H^R}{\eta_j^R}}$$

where $c_{i,j}$ is a normalizing factor enforcing the value 1 at $p_{i,j}$. The exact value of the factor can be easily computed as being:

$$\boxed{c_{i,j} = (-1)^{i+j} \frac{k^{2k}}{i!(k-i)!j!(k-j)!}}$$

2. *Points in the interior of an edge* (p_{i0}, $i > 0$). Such points belong to two faces, the base and the face on plane $\xi - \zeta = 0$. By Property 4, $\phi_{i,0}$, $i > 0$, must reduce to 0 on each of the three triangular faces not containing the edge, i.e, it must contain the factors $\xi_0^R = \xi - \zeta$,

$\xi_k^L = \xi+\zeta-1$, and $\eta_k = \eta+\zeta-1$. By Property 5, on the triangular face containing the point, the function reduces to the product of k lines, adequately represented by the expression

$$\left(\prod_{j=0}^{i-1} \xi_j^R \prod_{j=i+1}^{k} \xi_j^L\right)_{\eta=\zeta}$$

and, on the base, to the product of $2k$ lines, adequately represented by the expression

$$\left(\prod_{j=0}^{i-1} \xi_j^R \prod_{j=i+1}^{k} \xi_j^L \eta_k^L \prod_{j=1}^{k} \eta_j^R\right)_{\zeta=0}$$

The union of these two sets of factors satisfy the requirements of both faces. However in the reduction to face $p_0 p_1 p_4$ ($\eta = \zeta$), factor η_k^L yields an unwanted $(2\eta - 1)$ factor. This term, however, can be cancelled by a divisor $(2\zeta - 1)$, which does not affect the reduction to the base. We conclude that the following expression satisfies all requirements:

$$\boxed{\phi_{i,0}(\xi,\eta,\zeta) \quad = \quad c_{i,0} \tfrac{\xi_0^R \xi_k^L \eta_k^L}{2\zeta-1} H^R \textstyle\prod_{j=1}^{i-1} \xi_j^R \prod_{j=i+1}^{k-1} \xi_j^L}$$

where, again, $c_{i,0}$ is a normalizing constant with value:

$$\boxed{c_{i,0} = (-1)^{i+1} \frac{k^{2k-1}}{((k-1)!)^2}}$$

3. *Point on the vertex*($p_{0,0}$). Such points belongs to three faces, the base and the two lateral faces on planes $\xi - \zeta = 0$ and $\eta - \zeta = 0$. By Property 4 ϕ_{00} must reduce to 0 on each of the two triangular faces not containing the point, i.e, it must contain the factors ξ_k^L and η_k^L. By Property 5, it must also reduce to a product of $2k$ lines on the base of the pyramid and to a product of k lines on each of the triangular faces containing the point. The defined quadrics can be used to jointly satisfy these requirements, due to their straight-line intersections with the surface of the pyramid. The union of the enumerated factors is the product

$$\xi_k^L \eta_k^L \prod_{j=1}^{k-1} q_j$$

which, for exactly the same reason as in case 2. above, is to be divided by the factor $(2\zeta - 1)$. We conclude that the following expression satisfies all requirements:

$$\boxed{\phi_{0,0}(\xi,\eta,\zeta) = c_{0,0}\frac{\xi_k^L \eta_k^L}{2\zeta-1}\prod_{j=1}^{k-1} q_j}$$

$c_{0,0}$ being the normalizing factor with value:.

$$\boxed{c_{0,0} = (-1)^k \frac{k^{2k-1}}{i!(k-i)!(k-1)!}}$$

□

From Lemmas 2 and 3 we draw the following conclusion:

Theorem 5.4 *For any $k > 0$ there exist basis functions for the order-k Lagrangian pyramid, which are* ratios of polynomials.

6 Conclusions

In this paper we have proven that polynomial basis functions for Lagrangian pyramids do not exist. However, if we allow ratios of polynomials, it is possible to construct basis functions for the kth order Lagrangian pyramid, for any positive integer k. The procedure can be readily automated.

The element matrices constructed from these basis functions have reasonably good numerical behavior. We have used meshes consisting only of Lagrangian pyramids to solve several benchmark problems and we noticed that, although the system of equations resulting from them is not as well conditioned as the one resulting from meshes containing only cubes, the time needed to obtain the solution is comparable.

Finally, having these basis functions allows us to use pyramids as transitional elements, and it must be noted that transitional elements of crystalline meshes represent a small fraction of the total element set.

7 Acknowledgments

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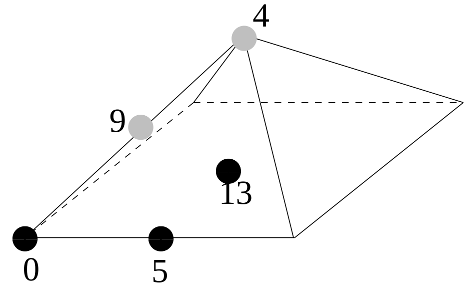

Figure 10: Node placement on the second order Lagrangian pyramid. The standard numbering of the nodes is also shown. Only the set of nonequivalent nodes is shown. The nodes whose basis functions can be obtained from the basis functions of the order-1 pyramid are shown in gray.

A Appendix

In this appendix, we calculate, as an illustration of the method, the basis functions for order-2 and order-3 pyramids.

A.1 Order-2 Pyramid

The order-2 pyramid is shown in Figure 11, where we have highlighted the nonequivalent nodal points whose basis functions are to be computed (the functions for all other points can be obtained by standard coordinate transformations).

Let $\phi_i(\xi, \eta, \zeta)$ denote the basis function for point p_i ($i = 0, 4, 5, 9, 13$). Functions ϕ_4 and ϕ_9 are obtained by scaling the corresponding basis functions ϕ'_4 and ϕ'_0, respectively, of the order-1 pyramid.Since $k = 2$ the coordinate transformations are:

$$\xi' = \frac{4\xi - 1}{2}, \quad \eta' = \frac{4\eta - 1}{2}, \quad \zeta' = \frac{4\zeta - 1}{2}$$

$$\begin{aligned} \phi_4(\xi, \eta, \zeta) &= \frac{1}{1/2}\zeta\phi'_4(\xi', \eta', \zeta') \\ &= 2\zeta(4\zeta - 1) \end{aligned}$$

$$\begin{aligned} \phi_9(\xi, \eta, \zeta) &= \frac{1}{1/4}\zeta\phi'_0(\xi', \eta', \zeta') \\ &= -8\zeta\frac{(\xi + \zeta - 1)(\eta + \zeta - 1)}{2\zeta - 1} \end{aligned}$$

Next we consider the basis functions of points $p_0 = p_{0,0}, p_5 = p_{1,0}$ and $p_13 = p_{1,1}$ on the base. Specializing the general formula and noting that:

$$\Xi^L = (\xi + \zeta - \frac{1}{2}), \Xi^R = (\xi - \zeta - \frac{1}{2}), H^L = (\eta + \zeta - \frac{1}{2}), H^R = (\eta - \zeta - \frac{1}{2})$$

we obtain:

$$\begin{aligned}
\phi_{0,0}(\xi, \eta, \zeta) &= c_{0,0}\frac{\xi_2^L \eta_2^L}{2\zeta - 1}\prod_{j=1}^{1} q_j \\
&= 4\frac{(\xi + \zeta - 1)(\eta + \zeta - 1)}{2\zeta - 1} \\
&\quad \left(-\zeta^2 + \xi\zeta + \eta\zeta - \xi\eta + \frac{1}{2}\xi + \frac{1}{2}\eta - \frac{1}{4}\right) \\
\phi_{1,0}(\xi, \eta, \zeta) &= c_{1,0}\frac{\xi_0^R \xi_2^L \eta_2^L}{2\zeta - 1} H^R \prod_{j=1}^{0} \xi_j^R \prod_{j=2}^{i} \eta_j^L \\
&= 8\frac{(\xi - \zeta)(\xi + \zeta - 1)(\eta - \zeta)}{2\zeta - 1}(\eta - \zeta - \frac{1}{2})
\end{aligned}$$

$$\begin{aligned}
\phi_{1,1}(\xi, \eta, \zeta) = \quad & c_{1,1}\xi_0^R \xi_2^L \eta_0^R \eta_2^L \frac{\Xi^R}{\xi_1^R}\frac{H^R}{\eta_1^R} \\
&= 16(\xi - \zeta)(\xi + \zeta - 1)(\eta - \zeta)(\eta + \zeta - 1)
\end{aligned}$$

since

$$c_{0,0} = (-1)^2\frac{2^2}{(1!)^2} = 4, c_{1,0} = (-1)^2\frac{2^3}{1!1!1!} = 8, c_{1,1} = (-1)^2\frac{2^4}{1!1!1!1!} = 16$$

A.2 Order-3 Pyramid

We now turn our attention to the order-3 pyramid, illustrated in Figure **??**, with the nonequivalent points appropriately highlighted (points on the base, whose basis functions are not obtained by scaling are shown solid).

Functions $\phi_4, phi_{14}, \phi_{13}$ and ϕ_{25} are obtained by scaling the corresponding functions $\phi'_4, \phi'_9, \phi'_0$ and ϕ'_5 of the order-2 pyramid. With the coordinate transformation ($k = 3$) we obtain:

$$\xi' = \frac{6\xi - 1}{4}, \quad \eta' = \frac{6\eta - 1}{4}, \quad \zeta' = \frac{6\zeta - 1}{4}$$

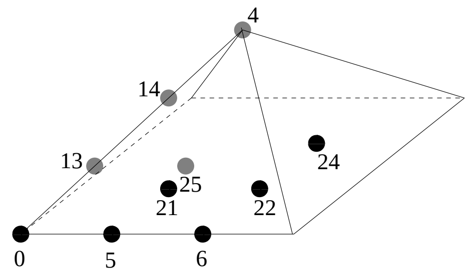

Figure 11: Node placement on the third order Lagrangian pyramid. The standard numbering of the nodes is also shown. Only the set of nonequivalent nodes is shown. The nodes whose basis functions can be obtained from the basis functions of the order-2 pyramid are shown in gray.

$$\begin{aligned}
\phi_4(\xi,\eta,\zeta) &= \frac{1}{1/2}\zeta\phi'_4(\xi',\eta',\zeta') \\
&= 2\zeta(4\zeta-1)(2\zeta-1)
\end{aligned}$$

$$\begin{aligned}
\phi_{14}(\xi,\eta,\zeta) &= \frac{1}{1/3}\zeta\phi'(\xi',\eta',\zeta') \\
&= -9\zeta(6\zeta-1)\frac{(\xi+\zeta-1)(\eta+\zeta-1)}{2\zeta-1}
\end{aligned}$$

$$\begin{aligned}
\phi_{13}(\xi,\eta,\zeta) &= \frac{1}{1/6}\zeta\phi'_0(\xi',\eta',\zeta') \\
&= 9\zeta\frac{(\xi+\zeta-1)(\eta+\zeta-1)}{2\zeta-1} \\
&\quad (-9\zeta^2+9\xi\zeta-9\xi\eta+9\eta\zeta+3\xi+3\eta-2) \\
\phi_{25}(\xi,\eta,\zeta) &= \frac{1}{1/6}\zeta\phi'_5(\xi',\eta',\zeta') \\
&= 54\zeta\frac{(\xi-\zeta)(\xi+\zeta-1)(\eta+\zeta-1)}{2\zeta-1}(3\eta-3\zeta-1)
\end{aligned}$$

Finally, we consider points $p_0 = p_{0,0}, p_5 = p_{1,0}, p_6 = p_{2,0}, p_{21} = p_{2,1}, p_{24} = p_{2,2}$.

Nothing that:

$$\Xi^L = \left(\xi+\zeta-\frac{1}{3}\right)\left(\xi+\zeta-\frac{2}{3}\right) \quad , \quad \Xi^R = \left(\xi-\zeta-\frac{1}{3}\right)\left(\xi-\zeta-\frac{2}{3}\right)$$
$$H^L = \left(\eta+\zeta-\frac{1}{3}\right)\left(\eta+\zeta-\frac{2}{3}\right) \quad , \quad H^R = \left(\eta-\zeta-\frac{1}{3}\right)\left(\eta-\zeta-\frac{2}{3}\right)$$

we have:

$$
\begin{aligned}
\phi_{0,0}(\xi,\eta,\zeta) &= c_{0,0}\frac{\xi_3^L\eta_3^L}{2\zeta-1}\prod_{j=1}^{2}q_j \\
&= -\frac{81}{4}\frac{(\xi+\zeta-1)(\eta+\zeta-1)}{2\zeta-1} \\
&\quad (-\zeta^2+\xi\zeta+\eta\zeta-\xi\eta+\frac{1}{3}\xi+\frac{1}{3}\eta-\frac{1}{9}) \\
&\quad (-\zeta^2+\xi\zeta+\eta\zeta-\xi\eta+\frac{2}{3}\xi+\frac{2}{3}\eta-\frac{4}{9})
\end{aligned}
$$

$$
\begin{aligned}
\phi_{1,0}(\xi,\eta,\zeta) &= c_{1,0}\frac{\xi_0^R\xi_3^L\eta_3^L}{2\zeta-1}H^R\prod_{j=1}^{0}\xi_j^R\prod_{j=2}^{2}\xi_j^L \\
&= \frac{243}{4}\frac{(\xi-\zeta)(\xi+\zeta-1)(\eta+\zeta-1)}{2\zeta-1}(\eta-\zeta-\frac{1}{3}) \\
&\quad (\eta-\zeta-\frac{2}{3})(\xi+\zeta-\frac{2}{3})
\end{aligned}
$$

$$
\begin{aligned}
\phi_{1,1}(\xi,\eta,\zeta) &= c_{1,1}\xi_0^R\xi_3^L\eta_0^R\eta_3^L\frac{\Xi^R}{\xi_1^R}\frac{H^R}{\eta_1^R} \\
&= \frac{729}{4}(\xi-\zeta)(\xi+\zeta-1)(\eta-\zeta)(\eta+\zeta-1) \\
&\quad (\xi-\zeta-\frac{2}{3})(\eta-\zeta-\frac{2}{3})
\end{aligned}
$$

$$
\begin{aligned}
\phi_{2,0}(\xi,\eta,\zeta) &= c_{2,0}\frac{\xi_0^R\xi_k^L\eta_k^L}{2\zeta-1}H^R\prod_{j=1}^{1}\xi_j^R\prod_{j=3}^{2}\xi_j^L \\
&= -\frac{243}{4}\frac{(\xi-\zeta)(\xi+\zeta-1)(\eta+\zeta-1)}{2\zeta-1}(\eta-\zeta-\frac{1}{3}) \\
&\quad (\eta-\zeta-\frac{2}{3})(\xi-\zeta-\frac{1}{3})
\end{aligned}
$$

$$
\begin{aligned}
\phi_{2,2}(\xi,\eta,\zeta) &= c_{2,2}\xi_0^R\xi_3^L\eta_0^R\eta_3^L\frac{\Xi^R}{\xi_2^R}\frac{H^R}{\eta_2^R} \\
&= \frac{729}{4}(\xi-\zeta)(\xi+\zeta-1)(\eta-\zeta)(\eta+\zeta-1) \\
&\quad (\xi-\zeta-\frac{1}{3})(\eta-\zeta-\frac{1}{3})
\end{aligned}
$$

since

$c_{0,0} = (-1)^3\frac{3^4}{(2!)^2} = -\frac{81}{4}$ $\qquad$ $c_{1,0} = (-1)^2\frac{3^5}{1!2!2!} = \frac{243}{4}$

$c_{1,1} = (-1)^2\frac{3^6}{1!2!1!2!} = \frac{729}{4}$ $\qquad$ $c_{2,0} = (-1)^3\frac{3^5}{2!1!2!} = -\frac{243}{4}$

$c_{2,2} = (-1)^4\frac{3^6}{2!1!2!1!} = \frac{729}{4}$