Geometrical Validity of Curvilinear Pyramidal Finite Elements

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1. Introduction

A method to efficiently determine the geometrical validity of curvilinear finite elements of any order was recently proposed in [1]. The method is based on the adaptive expansion of the Jacobian determinant in a polynomial basis built using Bézier functions, that has both properties of boundedness and positivity. While this technique can be applied to all usual finite elements (triangles, quadrangles, tetrahedra, hexahedra and prisms), it cannot readily be applied to pyramids, due to non-polynomial nature of pyramidal finite element spaces.

In this short paper, we extend the results from [1] to pyramidal elements, by making use of the high-order nodal pyramidal finite element proposed by Bergot et al. [10], which exhibits optimal convergence properties in H^1-norm.

The paper is organized as follows. We begin by briefly recalling the pyramidal finite element space in Section 2, before constructing the function space of the Jacobian determinant in Section 3. Section 4 then introduces a generalized Bézier function basis, which can be used to obtain adaptive bounds on the pyramidal Jacobian determinant. Numerical results showing the sharpness of the estimates are given in Section 5.

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2. Pyramidal Finite Element Space

Let (ξ, η, ζ) denote the coordinates of the reference space and let $\mathcal{P}^r$ denote the pyramidal finite element space at order $r > 0$ defined in [10]. The space $\mathcal{P}^r$ can be expressed as the union of the classical tetrahedral finite space and the product of the triangular finite element space with powers of the non-affine term $\frac{\xi\eta}{1-\zeta}$:

$$\mathcal{P}^r := \left\{ \xi^i \eta^j \zeta^k \,\middle|\, i+j+k \leq r \right\} \bigcup \left\{ \xi^i \eta^j \left(\frac{\xi\eta}{1-\zeta} \right)^{r-l} \,\middle|\, i+j \leq l,\ l \leq r-1 \right\}. \tag{1}$$

In the previous expression all the indices $(i,\ j,\ k,\ l)$ are assumed to be integers greater than or equal to 0. (The same convention is used for all indices throughout the paper.) The previous definition can be rewritten in a more convenient form:

$$\mathcal{P}'^r := \left\{ \left(\frac{\xi}{1-\zeta} \right)^i \left(\frac{\eta}{1-\zeta} \right)^j (1-\zeta)^k \,\middle|\, i,j \leq k,\ \ k \leq r \right\} = \mathcal{P}^r. \tag{2}$$

Proof. We can seperate the space $\mathcal{P}'^r$ into two subspaces, one for which $k \geq i+j$ and the other for which $k < i+j$. We have

$$\mathcal{P}'^r \Big|_{k \geq i+j} = \left\{ \xi^i \eta^j (1-\zeta)^K \,\middle|\, i+j+K \leq r \right\},$$

which is the tetrahedral space. Let us rewrite the second contribution in terms of $\xi^I \eta^J \left(\frac{\xi\eta}{1-\zeta} \right)^K$. We then have $i = I+K$, $j = J+K$ and $k-i-j = -K$, which implies:

$$\mathcal{P}'^r \Big|_{k < i+j} = \left\{ \xi^I \eta^J \left(\frac{\xi\eta}{1-\zeta} \right)^K \,\middle|\, I+J+K \leq r,\ \ 1 \leq K \right\}.$$

By substituting $r-l$ for K, we obtain the non-affine part of Bergot's pyramidal space. And thus eventually $\mathcal{P}'^r = \mathcal{P}^r$. □

In addition to being more convenient for the developments of Section 3, the form (2) offers the advantage of showing that functions of the pyramidal space are generated by the product of integer powers of three elementary subfunctions: $\frac{\xi}{1-\zeta}$, $\frac{\eta}{1-\zeta}$ and $1-\zeta$ (see Figure 1). The first, $\frac{\xi}{1-\zeta}$, is equal to one on face $\xi = 1-\zeta$ and equal to zero on face $\xi = 0$. The second, $\frac{\eta}{1-\zeta}$, is equal to one on face $\eta = 1-\zeta$ and zero on face $\eta = 0$. The third, $1-\zeta$, is

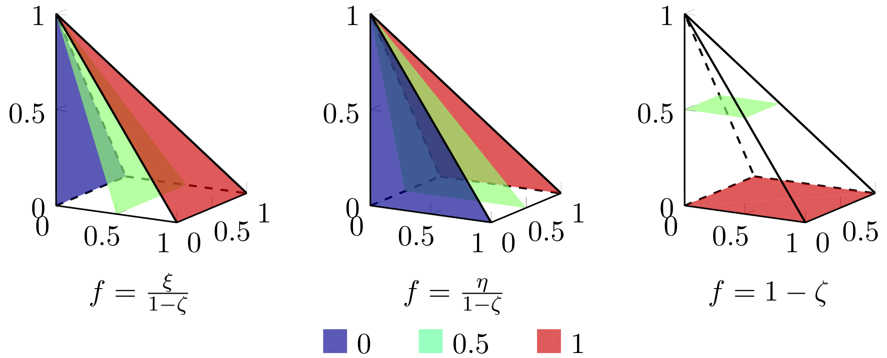

Figure 1: Visualization of the three subfonctions that generate the pyramidal nodal space.

equal to 1 on face $\zeta = 0$ and equal to 0 on the top corner. It is thus similar to what we have for tetrahedra or hexahedra, whose finite element spaces are spanned by the product of integer powers of the subfunctions ξ, η and ζ.

It is easy to see in form (1) that the basis functions are continuous since $\frac{\xi\eta}{1-\zeta}$ is well-defined at the top corner $(0, 0, 1)$. In the second form (2), the functions $\left(\frac{\xi}{1-\zeta}\right)^i$ and $\left(\frac{\eta}{1-\zeta}\right)^j$ are not well-defined but their product with $(1-\zeta)^k$ is well-defined since $k \geq \max(i, j)$.

The pyramidal finite element is characterized by the mapping between a reference pyramid and the actual pyramid in the mesh. To be valid, this mapping should be bijective, which implies that the Jacobian determinant should be positive everywhere inside the domain of definition [1]. This is why, in the two following sections, we first construct the function space of the Jacobian determinant and then present its Bézier expansion.

3. Pyramidal Jacobian Determinant Space

Let $\mathcal{J}^r$ denote the Jacobian determinant space. We have by definition $\mathcal{J}^r = \mathcal{P}^r_{,\xi} \times \mathcal{P}^r_{,\eta} \times \mathcal{P}^r_{,\zeta}$, where $\mathcal{P}^r_{,\bullet}$ is the space obtained by differentiating all the elements of space $\mathcal{P}^r$ with respect to $\bullet$. From (2), we obtain:

$$\mathcal{P}^r_{,\xi} = \left\{ \left(\frac{\xi}{1-\zeta}\right)^{i_1} \left(\frac{\eta}{1-\zeta}\right)^{j_1} (1-\zeta)^{k_1} \;\middle|\; i_1 \le k_1,\;\; j_1 \le k_1+1,\;\; k_1 \le r-1 \right\}$$
$$\mathcal{P}^r_{,\eta} = \left\{ \left(\frac{\xi}{1-\zeta}\right)^{i_2} \left(\frac{\eta}{1-\zeta}\right)^{j_2} (1-\zeta)^{k_2} \;\middle|\; i_2 \le k_2+1,\;\; j_2 \le k_2,\;\; k_2 \le r-1 \right\}$$
$$\mathcal{P}^r_{,\zeta} \subset \left\{ \left(\frac{\xi}{1-\zeta}\right)^{i_3} \left(\frac{\eta}{1-\zeta}\right)^{j_3} (1-\zeta)^{k_3} \;\middle|\; i_3, j_3 \le k_3+1,\;\; k_3 \le r-1 \right\}.$$

The inclusion in the last expression arises from a simplification: we do not discard the case in (2) corresponding to $k - i - j = 0$, which should be discarded when differentiating with respect to ζ. Considering the real space of $\mathcal{P}^r_{,\zeta}$ would only complicate further developments, and not provide any other advantages.

The product of the three spaces leads to the following expression for the Jacobian determinant space:

$$\mathcal{J}^r \subset \left\{ \left(\frac{\xi}{1-\zeta}\right)^{I} \left(\frac{\eta}{1-\zeta}\right)^{J} (1-\zeta)^{K} \;\middle|\; I, J \le K+2,\;\; K \le 3r-3 \right\}, \quad (3)$$

which implies that $\mathcal{J}^r$ is a subset of $\mathcal{P}^{3r-3} \times \left\{ \left(\frac{\xi}{1-\zeta}\right)^{i} \left(\frac{\eta}{1-\zeta}\right)^{j} \middle| i, j \le 2 \right\}$, whose dimension is $\sum_{k=0}^{3r-3} (k+3)^2 = r/2\,(3r+1)(6r+1) - 5$. We see that, while for other element types the Jacobian determinant space is contained in their finite element space of a higher order [1], for pyramids, this is not the case.

The pyramidal Jacobian determinant is not well-defined at the top corner: K can be smaller than the maximum of I and J in which case the term $(1-\zeta)^K$ can not fully compensate the two other terms. As a consequence, one should never sample the Jacobian determinant at the top corner of the pyramid.

4. Bézier Basis for the Pyramidal Jacobian Determinant

While the use of Bézier interpolation to parametrize curves and surfaces is very common in computer graphics, it is less so to expand general functions. One property of Bézier expansion that is useful for our problem is that the interpolant is located inside the convex hull of the control values. This property allows to provide bounds on the interpolant. All positive basis functions that sum up to 1 have this property but, intuitively, the Bézier basis is the one for which the size of the convex hull is the smallest (thus, for which the bounds are the sharpest). Another desired property of Bézier expansion is that it can be recursively "subdivided" [1] which allows to sharpen the bounds.

Polynomial Bézier bases are based on the Bernstein polynomials. At order n, the $n+1$ Bernstein polynomials are defined as

$$B_k^{(n)}(\lambda) := \binom{n}{k} \lambda^k (1-\lambda)^{n-k} \qquad (k = 0, ..., n),$$

where $\binom{n}{k} = \frac{n!}{n!(n-k)!}$ is the binomial coefficient. They sum up to 1 and they are positive on the domain $[0,1]$. In order to compute bounds in the non-polynomial pyramidal Jacobian determinant space, we will search for a basis that can be written as product of a generalization of Bernstein polynomials.

4.1. Generalized Bézier Basis for Pyramids

Let $\Omega_{\text{ref}} \subset \mathbb{R}$ denote the uncentered pyramid, for which $(\frac{\xi}{1-\zeta}, \frac{\eta}{1-\zeta}, 1-\zeta) \in [0,1]^3$. (As usual for Bézier interpolation we will define the Jacobian determinant basis functions on this uncentered pyramid Ω_{ref} instead of the centered pyramid that is often used in Finite Element methods.) From (3), we easily identify the Jacobian determinant basis written with generalized Bernstein functions:

$$J^r_{i,j,k}(\xi,\eta,\zeta) := B_i^{(k+2)}\left(\frac{\xi}{1-\zeta}\right) \; B_j^{(k+2)}\left(\frac{\eta}{1-\zeta}\right) \; B_k^{(3r-3)}(1-\zeta)\,, \qquad (\xi,\eta,\zeta) \in \Omega_{\text{ref}}. \tag{4}$$

Like for hexahedra and prisms, the Jacobian determinant of the first order pyramid is not constant. However it is a function of only $\frac{\xi}{1-\zeta}$ and $\frac{\eta}{1-\zeta}$. This means that sampling of the Jacobian determinant can be done on the $\zeta = 0$ plane, and that recursive subdivision works in the same way as for the quadrangle element [1].

For high-order pyramids, definition (4) is relevant if subdivision is not required (e.g. for optimization). But as explained in the following subsection, recursive subdivision with respect to the ζ-axis does not hold, which motivates the definition of an enriched basis.

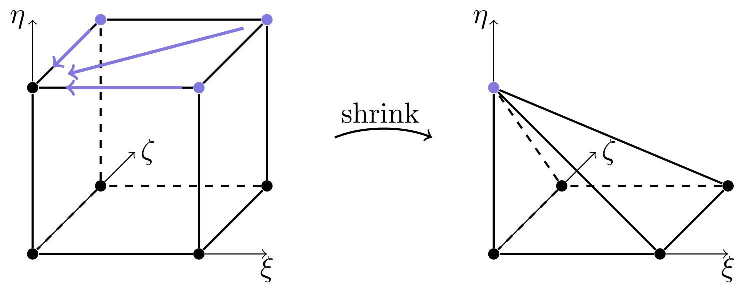

Figure 2: The pyramid can be see as a shrinked cube with the transformation $\xi \mapsto \frac{\xi}{1-\zeta}$ and $\eta \mapsto \frac{\eta}{1-\zeta}$.

4.2. Enriched Generalized Bézier Basis for Pyramids

Let Ω_{bot} denotes the bottom subdomain obtained when cutting the reference pyramid by the plane $\zeta = 1/2$. We note $\boldsymbol{M}_{\text{bot}} : \Omega_{\text{bot}} \to \Omega_{\text{ref}}$ the mapping between the bottom subdomain and the reference pyramid. We have:

$$\boldsymbol{M}_{\text{bot}} : \begin{cases} \xi' \mapsto \xi = \xi' \frac{1-2\zeta'}{1-\zeta'} \\ \eta' \mapsto \eta = \eta' \frac{1-2\zeta'}{1-\zeta'} \\ \zeta' \mapsto \zeta = 2\zeta' \end{cases} .$$

Recursive subdivision is possible for the bottom if the Jacobian determinant can be expanded into the basis whose functions are $S^r_{i,j,k} := J^r_{i,j,k} \circ \boldsymbol{M}_{\text{bot}}$. Those functions are defined on Ω_{bot} and have properties of positivity and partition of unity. Their expression is:

$$S^r_{i,j,k}(\xi,\eta,\zeta) = B_i^{(k+2)}\left(\frac{\xi}{1-\zeta}\right)\ B_j^{(k+2)}\left(\frac{\eta}{1-\zeta}\right)\ B_k^{(3r-3)}\left(1-2\zeta\right), \qquad (\xi,\eta,\zeta) \in \Omega_{\text{bot}}, \tag{5}$$

but it can be shown that they do not span the Jacobian determinant space due to the dependence on k of the two first Bernstein functions. We therefore define the enriched Jacobian determinant basis functions by removing this dependence:

$$E^r_{i,j,k}(\xi,\eta,\zeta) := B_i^{(3r-1)}\left(\frac{\xi}{1-\zeta}\right)\ B_j^{(3r-1)}\left(\frac{\eta}{1-\zeta}\right)\ B_k^{(3r-3)}\left(1-\zeta\right), \qquad (\xi,\eta,\zeta) \in \Omega_{\text{ref}}. \tag{6}$$

These functions correspond to the ones one would obtain by considering a “shrinked” cube (Figure 2). The corresponding basis can be recursively and adaptively subdivided.

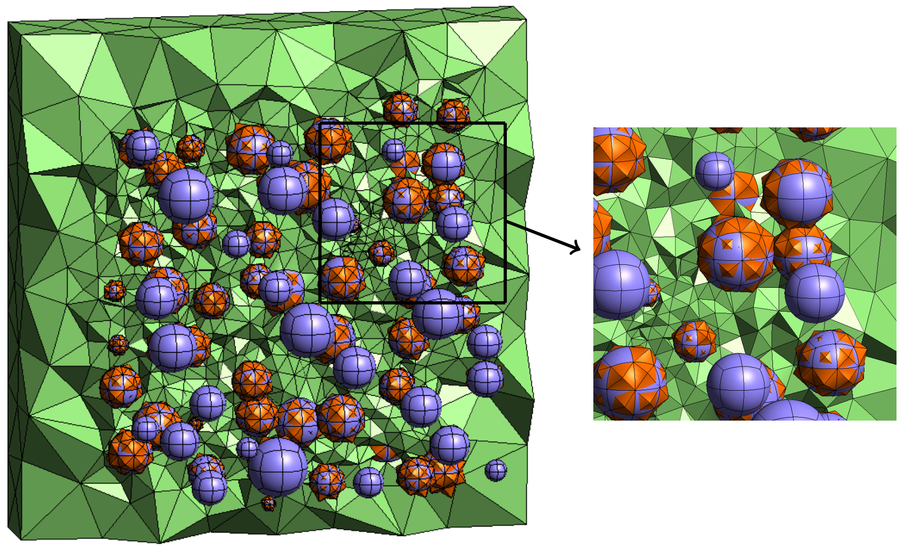

Figure 3: Three-dimensional mesh with second order elements. The geometry consists of a cube with spherical holes. Pyramids (in orange) make the transition from the hexahedra (in blue) that fill the holes to the tetrahedra (in green) that fill the rest of the volume.

As described in [1], fast computation of Bézier coefficients can be achieved by using a transformation matrix that computes control values from nodal values. The Jacobian determinant is sampled at the location of the nodes of a pyramid of order $3r-1$, excepted the node at the top and the four nodes directly below the top. Subdivision works in exactly the same was as for other element types, provided that for the first order pyramid, subdivision is only necessary along the base of the pyramid.

5. Results

We present the results of our algorithm applied to a three-dimensional microstructure. The structure contains spherical holes that are meshed with second order hexahedra. In order to make the transition with the second order tetrahedra that are used for the rest of the geometry, second order pyramids have been generated, around those holes (see Fig. 3). We measure the minimum of distortion $\delta_{\min}$, *i.e.* the minimum of the determinant of the mapping between the straight-sided element and the curved element, as defined in [1]. The analyzed mesh is composed of 180,356 tetrahedra for which 31,696 are curved and 5,809 curved pyramids.

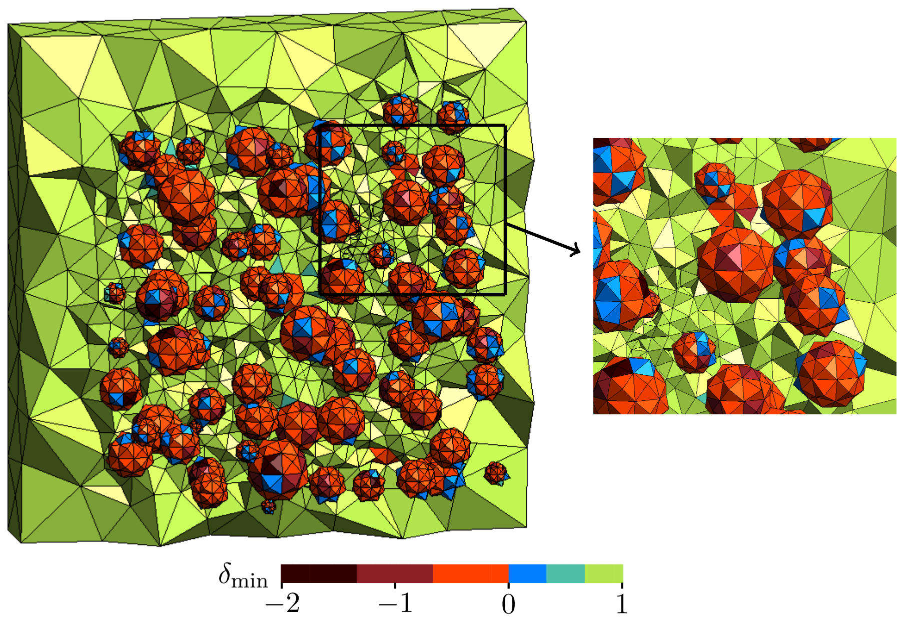

Figure 4: Validity of the mesh. Valid elements are between green and blue and invalid elements are between red and black.

We improved the algorithm presented in [1] in order to compute $\delta_{\min}$ with a given input tolerance ε and detect the invalid elements at the same time. First, we compute the Bézier coefficients of the whole element. Then we enter in a loop:

1. Compute $\delta_{\min}^{\sup}$ and $\delta_{\min}^{\inf}$ (upper and lower bound on $\delta_{\min}$) as in [1]
2. If $\delta_{\min}^{\sup} - \delta_{\min}^{\inf} \leq \varepsilon$ and $\delta_{\min}^{\sup}\, \delta_{\min}^{\inf} \geq 0$, then go to 4
3. Subdivide the (sub)domain that contains the smaller Bézier coefficient and go to 1
4. Return $\delta_{\min}^{\inf}$ (NB: the element is invalid if $\delta_{\min}^{\inf} \leq 0$, else it is valid)

Figure 4 presents the results on the mesh. Our algorithm successfully detects the 4,989 invalid pyramids and the 82 invalid tetrahedra (elements in red to black).

Figure 5 compares the computation time versus the maximal error of our algorithm and the brute-force sampling of the Jacobian determinant. For our algorithm, we measure the time taken to compute bounds with an input tolerance of $\varepsilon = 10^{-e}, e = \{1, \ldots, 7\}$. For the brute-force sampling, the Jacobian determinant is sampled at an increasing number of points. Tetra-

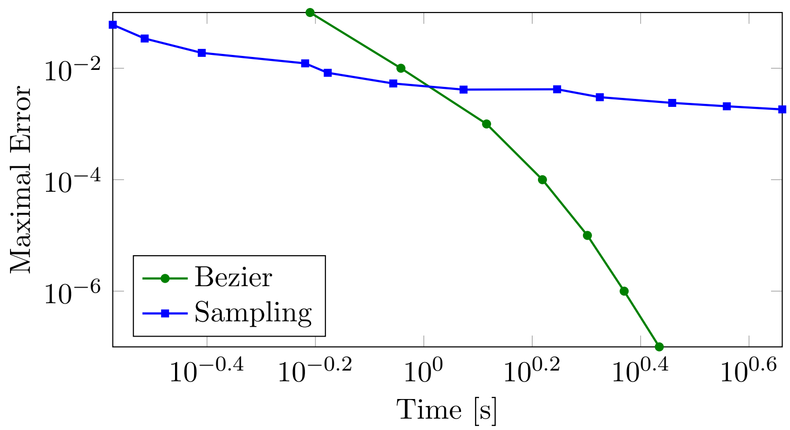

Figure 5: Analyzis of 186,165 second order elements.

hedra points are the nodes of a tetrahedron of order k. For the pyramids, the points are taken as the nodes of a pyramid of order $k+1$ for which we remove the five top nodes, *i.e.*, the same way we sample the Jacobian determinant for our method. We ranged k from 1 to 12 which means that the number of sampling points is comprised between 4 and 455 for tetrahedra and between 9 and 2352 for pyramids. We measured the computation time and the maximal (elementary) error between $\min_{\text{sampling}}(\delta)$ and the best approximation of $\delta_{\min}$ taken as the value computed by our algorithm at tolerance 10^{-7}. Tests have been performed on a Macbook Pro Retina, Mid 2012 @ 2.3GHz.

The brute-force sampling needs more time than our algorithm to reach a maximal error smaller than 4×10^{-3}. But worst, similarly to the results reported in [1] for other element types, the brute-force algorithm is not able to find all invalid pyramids for $k = \{1, \ldots, 12\}$, the maximum number of invalid pyramids found being $4,971$ (instead of $4,989$) at $k = 12$.

6. Conclusion

In this paper we adapted the computation of accurate bounds on Jacobian determinants of curvilinear finite elements to the pyramidal case. The proposed algorithm can either be used to determine the validity or invalidity of curved pyramids, or to provide an efficient way to measure their distortion. The complete implementation of the algorithm is available in the open source mesh generator Gmsh [11] as the `AnalyseCurvedMesh` plugin. Ongoing research includes adaptation of the algorithm to the computation of accurate bounds on a quality measure of the elements based on the metric.

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