Conditions for the invertibility of the isoparametric mapping for 3D multilinear finite elements

G. Summ, P. Knabner and S. Korotov
Institute for Applied Mathematics
Martensstraße 3
D-91058 Erlangen

August 27, 2001

Abstract

We consider the isoparametric transformation, which maps a given reference element onto a global element given by its vertices, for multilinear finite elements on pyramids, prisms and hexahedra. In the cases of pyramids and prisms we derive easily computable conditions on the position of the vertices, which ensure that the isoparametric transformation is invertible. In the case of hexahedra we present an algorithm that checks arbitrarily sharp sufficient conditions for the positivity of the Jacobian determinant.

Introduction

It is well known that hexahedral meshes provide better approximation properties than tetrahedral meshes with the same degrees of freedom. On the other hand, the generation of (locally refined) hexahedral meshes for complex 3D domains is very difficult, whereas the generation of tetrahedral meshes is much easier or at least much better understood. A combination of hexahedral and tetrahedral elements in one mesh needs in addition elements that have both triangular and quadrilateral faces: these elements can be pyramidal or prismatic finite elements.

Throughout this paper we use the notion “finite element” for a triple \((K, P, \Sigma)\) in the sense introduced by Ciarlet (cf. [1], p. 93 f.). We restrict ourselves to Lagrange finite elements, i.e., the degrees of freedom \(\sigma_i \in \Sigma, i = 1, \ldots, N = |\Sigma|\), are point evaluations \(\sigma_i(p) := p(a_i)\) for all ansatz functions \(p \in P\) and a vertex \(a_i\) of \(K\). All the finite elements considered here are isoparametrically equivalent to a reference element \((\bar{K}, \bar{P}, \bar{\Sigma})\) via an invertible mapping \(F_K: \bar{K} \rightarrow K\), where \(F_K \in \bar{P}^3\) (see [1], p. 229 f.). Thus the finite element \((K, P, \Sigma)\) is uniquely defined by the geometric set \(K\), which is therefore often called “element”.

In the process of grid generation usually only the vertices of an element \(K\) are available. Then the transformation \(F_K \in \bar{P}^3\) is uniquely defined by the requirement
to map the vertices $\hat{a}_i$ of $\hat{K}$ to the desired vertices $a_i$ of $K$:

$$F_K(\hat{z}) = \sum_{i=1}^{N} \hat{\phi}_i(\hat{x}) a_i,$$

(1)

where $\hat{\phi}_i$, $i = 1, \ldots, N$, are the basis functions of $\hat{P}$ fulfilling $\hat{\phi}_i(\hat{a}_j) = \delta_{ij}$ for $j = 1, \ldots, N$. In this paper we address the question, under which conditions on the position of the vertices $a_i$ the mapping $F_K$ is invertible. More precisely, we derive conditions that ensure $\det D F_K \neq 0$ in $\hat{K}$. We remark that this inequality implies the global invertibility of $F_K$, if the second derivatives of $F_K$ are constant (cf. [1], proof of Thm. 37.2), which is the case for multilinear pyramidal and prismatic finite elements. Furthermore this inequality is necessary for the boundedness of the expression $\|\det D F_K\|_{0,\infty,\hat{K}} \|\det D F_K^{-1}\|_{0,\infty,K}$, which appears, when the interpolation error is estimated via transformation to the reference element and back.

We start with general considerations in Section 1. In Sections 2 and 3 we consider the pyramidal and prismatic cases and derive easily computable relations for the vertices such that the corresponding isoparametric mapping $F_K$ is invertible if these relations hold. Finally, in Section 4 we present an algorithm that checks arbitrarily sharp conditions for the positivity of the Jacobian determinant $\det D F_K$ in $\hat{K}$.

1 General considerations

1.1 Decomposition of the isoparametric mapping

We will use the following decomposition (cf. [2]) of the isoparametric mapping $F_K$ into an affine-linear part $F_T$ and a nonlinear part $\hat{F}_K$: $F_K = F_T \circ \hat{F}_K$.

![Figure 1: Decomposition of isoparametric mapping](image)

Here the affine-linear mapping $F_T$ maps the unit tetrahedron $\hat{T}$ onto the tetrahedron $T = \text{conv}\{a_i \mid i \in I_T\}$ with the vertices $a_i$, $i \in I_T$, where $I_T \subset \{1, \ldots, N\}$. If the vertices $a_i$, $i = 1, \ldots, N$, do not lie in one plane, it is possible to find an index set $I_T$ such that $F_T$ is invertible. Then we can define the nonlinear mapping $F_K \in \hat{P}^n$ by the requirement $F_K(\hat{a}_i) = \hat{a}_i = F_T^{-1}(a_i)$, i.e. (cf. (1)),

$$F_K(\hat{z}) = \sum_{i=1}^{N} \hat{\phi}_i(\hat{x}) a_i.$$
Since \( \det DF_K = \det DF_T \cdot \det DF_R \) and \( \det DF_T \) is a constant, it suffices to check if \( \det DF_K \neq 0 \). As \( \det DF_R \) contains less free parameters than \( \det DF_K \) this decomposition yields a significant simplification.

### 1.2 Positivity of quadratic polynomials

In the prismatic and hexahedral case we have to consider quadratic polynomials over the unit segment \([0,1]\). The following result will be useful:

**Lemma 1.1** A quadratic polynomial \( p \) defined by \( p(\tau) = c_0 + c_1 \tau + c_2 \tau^2 \) is positive on \([0,1]\) if and only if the following conditions are satisfied:

\[
\begin{align*}
  i) & \quad c_0 > 0, \\
  ii) & \quad c_0 + c_1 + c_2 > 0, \\
  iii) & \quad c_0 \geq c_2 \quad \text{or} \quad c_1 > -2\sqrt{|c_0c_2|}.
\end{align*}
\]

### 2 Pyramidal finite elements

#### 2.1 The pyramidal reference element

The pyramidal reference element is defined by \( \hat{K} = \text{conv} \{\hat{a}_i\} \), where the vertices \( \hat{a}_i, i = 1, \ldots, 5 \) are given below, and depicted in Fig. 2.

Vertices of pyramidal reference element \( \hat{K} \):

\[
\begin{align*}
  \hat{a}_1 &= \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}, & \hat{a}_2 &= \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \\
  \hat{a}_3 &= \begin{pmatrix} 1 \\ 1 \\ 0 \end{pmatrix}, & \hat{a}_4 &= \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, & \hat{a}_5 &= \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}.
\end{align*}
\]

Figure 2: Pyramidal reference element

The following basis functions \( \hat{\phi}_i, i = 1, \ldots, 5 \), which fulfill \( \hat{\phi}_i(\hat{a}_j) = \delta_{ij} \) for \( j = 1, \ldots, 5 \), have been suggested in [5]. They are bilinear on the tetrahedron quadrilateral face and linear on the triangular faces:

\[
\begin{align*}
  \hat{\phi}_1(\hat{x}) &= 1 - \xi - \eta - \zeta + \xi\eta + \min(\xi, \eta)\zeta, \\
  \hat{\phi}_2(\hat{x}) &= \xi - \xi\eta - \min(\xi, \eta)\zeta, \\
  \hat{\phi}_3(\hat{x}) &= \xi\eta + \min(\xi, \eta)\zeta, \\
  \hat{\phi}_4(\hat{x}) &= \eta - \xi\eta - \min(\xi, \eta)\zeta, \\
  \hat{\phi}_5(\hat{x}) &= \zeta,
\end{align*}
\]

where \( \hat{x} = (\xi, \eta, \zeta)^T \).

Obviously, the basis functions \( \hat{\phi}_i, i \neq 5 \), are not continuously differentiable. This astonishing fact is necessary to avoid the relation \( \hat{p}(\hat{a}_1) + \hat{p}(\hat{a}_3) = \hat{p}(\hat{a}_2) + \hat{p}(\hat{a}_4) \), which would be necessary for continuously differentiable \( \hat{p} \in \bar{P} \) (cf. [3]).
2.2 Conditions for the invertibility of the isoparametric mapping

Corresponding to (1) the isoparametric mapping \( F_K \) is given by:

\[
F_K(\hat{x}) = a_1 + (a_2 - a_1)\eta + (a_4 - a_1)\xi + (a_5 - a_1)\zeta + (a_1 + a_3 - a_2 - a_4)(\xi\eta + \min(\xi,\eta)\zeta).
\]

After decomposition with \( I_T = \{1, 2, 4, 5\} \) we obtain the simplified nonlinear mapping

\[
F_K(\hat{x}) = \hat{x} + (\tilde{a}_3 - \tilde{a}_3)\xi\eta + \min(\xi,\eta)\zeta.
\]

Note that \( F_K \) consists of the identity mapping plus some nonlinear term that depends on the deviation \( \tilde{a}_3 = \hat{a}_3 \).

As \( F_K \) is not continuously differentiable, we have to split \( \hat{K} \) into \( \hat{K} = \hat{T}_1 \cup \hat{T}_2 \), where \( \hat{T}_1 := \text{conv}\{\tilde{a}_1, \tilde{a}_2, \tilde{a}_3, \tilde{a}_5\} \), \( \hat{T}_2 := \text{conv}\{\tilde{a}_1, \tilde{a}_3, \tilde{a}_4, \tilde{a}_5\} \), to compute the Jacobian determinant:

\[
\det DF_K|_{\hat{T}_1}(\hat{x}) = 1 - \xi - \eta - \zeta + \tilde{y}_3\xi + \tilde{x}_3\eta + \tilde{z}_3\zeta + \tilde{x}_3\zeta + \tilde{z}_3\xi,
\]

\[
\det DF_K|_{\hat{T}_2}(\hat{x}) = 1 - \xi - \eta - \zeta + \tilde{y}_3\xi + \tilde{x}_3\eta + \tilde{x}_3\eta + \tilde{x}_3\zeta + \tilde{z}_3\xi.
\]

As linear functions attain their extrema in the vertices of \( \hat{T}_1 \), \( \det DF_K \) is positive in \( \hat{T}_1 \), if \( \tilde{y}_3 > 0 \) and \( \tilde{x}_3 + \tilde{y}_3 + \tilde{z}_3 > 1 \), and \( \det DF_K \) is positive in \( \hat{T}_2 \) if \( \tilde{x}_3 > 0 \) and \( \tilde{x}_3 + \tilde{y}_3 + \tilde{z}_3 > 1 \). As the second derivatives of \( F_K \) are constant, we can conclude the invertibility of \( F_K \) in \( \hat{T}_1 \) and \( \hat{T}_2 \). A cumbersome, but elementary computation then yields the following result (cf. [3, Thm. 2.1]):

**Theorem 2.1** The simplified isoparametric transformation \( F_K \) for pyramidal finite elements is invertible in \( \hat{K} \) if

\[
\tilde{x}_3 > 0 \quad \text{and} \quad \tilde{y}_3 > 0 \quad \text{and} \quad \tilde{x}_3 + \tilde{y}_3 + \tilde{z}_3 > 1.
\]

2.3 Example of a distorted pyramidal element

An picture of a pyramidal element that violates (3) is given in Fig. 3. We have chosen \( a_i = \tilde{a}_i \) for \( i \in I_T = \{1, 2, 4, 5\} \) such that \( \hat{K} = K \), in particular \( \tilde{a}_3 = a_3 \).

Vertices of pyramidal element \( \hat{K} \):

\[
a_1 = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}, \quad a_2 = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \quad a_3 = \begin{pmatrix} 2 \\ -1 \\ 0 \end{pmatrix}, \quad a_4 = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, \quad a_5 = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}.
\]

Note that \( \tilde{y}_3 = y_3 < 0 \).

Figure 3: Distorted pyramidal element
3 Prismatic finite elements

3.1 The prismatic reference element

The prismatic reference element is defined by $K = \text{conv} \{ \tilde{a}_i \}$, where the vertices $\tilde{a}_i$, $i = 1, \ldots, 6$, are given below, and depicted in Fig. 4.

Vertices of prismatic reference element $K$:

\[
\begin{align*}
\tilde{a}_1 &= \begin{pmatrix} 0 \\ 0 \end{pmatrix}, & \tilde{a}_2 &= \begin{pmatrix} 1 \\ 0 \end{pmatrix}, & \tilde{a}_3 &= \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \\
\tilde{a}_4 &= \begin{pmatrix} 0 \\ 1 \end{pmatrix}, & \tilde{a}_5 &= \begin{pmatrix} 0 \\ 1 \end{pmatrix}, & \tilde{a}_6 &= \begin{pmatrix} 0 \\ 1 \end{pmatrix}.
\end{align*}
\]

Figure 4: Prismatic reference element

The basis functions $\hat{\phi}_i$, $i = 1, \ldots, 6$, for the prismatic reference element, which fulfill $\hat{\phi}_i(\hat{a}_j) = \delta_{ij}$ for $j = 1, \ldots, 6$, are simply products of linear basis functions on the unit triangle and linear basis functions on the unit segment. Thus they are bilinear on the quadrilateral faces and linear on the triangular faces.

\[
\hat{\phi}_1(\hat{x}) = (1 - \xi - \eta)(1 - \zeta), \quad \hat{\phi}_2(\hat{x}) = \xi(1 - \zeta), \quad \hat{\phi}_3(\hat{x}) = \eta(1 - \zeta),
\]
\[
\hat{\phi}_4(\hat{x}) = (1 - \xi - \eta)\zeta, \quad \hat{\phi}_5(\hat{x}) = \xi\zeta, \quad \hat{\phi}_6(\hat{x}) = \eta\zeta,
\]

where we use again $\hat{x} = (\xi, \eta, \zeta)^T$.

3.2 Conditions for the invertibility of the isoparametric mapping

Applying (1) yields the following expression for the isoparametric mapping:

\[
F_K(\bar{x}) = a_1 + (a_2 - a_1)\xi + (a_3 - a_1)\eta + (a_4 - a_1)\zeta + (a_5 - a_4 - a_3)\xi\zeta + (a_1 + a_6 - a_3 - a_4)\eta\zeta.
\]

A decomposition with $I_T = \{1, 2, 3, 4\}$ yields:

\[
F_K(\hat{x}) = \hat{x} + (\hat{a}_5 - \hat{a}_6)\xi \zeta + (\hat{a}_6 - \hat{a}_5)\eta \zeta
\]

such that again $F_K$ consists of the identity mapping plus some nonlinear terms that depend on the deviations $\hat{a}_5 - \hat{a}_6$ and $\hat{a}_6 - \hat{a}_5$. Obviously, the second derivatives of $F_K$ are constant again. Therefore the positivity of the Jacobian determinant of
the mapping \( F_\tilde{K} \) implies its invertibility. Since the Jacobian determinant
\[
\det DF_\tilde{K}(\bar{x}) = 1 + (\tilde{z}_6 - 1)\zeta + (\tilde{y}_6 - 1)\eta + ((\bar{x}_6 - 1) + (\bar{y}_6 - 1))\zeta \\
+ ((\bar{y}_6 - 1)(\tilde{z}_6 - 1) - \bar{y}_6 (\tilde{z}_6 - 1)) \zeta \zeta \\
+ ((\bar{x}_6 - 1)(\tilde{z}_6 - 1) - \bar{x}_6 (\tilde{z}_6 - 1)) \eta \zeta \\
+ ((\bar{x}_6 - 1)(\bar{y}_6 - 1) - \bar{x}_6 \bar{y}_6) \zeta^2
\]

is a linear function in \( \zeta, \eta \) for fixed \( \zeta, \eta \), \( \det DF_\tilde{K}(\bar{x}) \) attains its extremal values at the edges \([\bar{a}_1, \bar{a}_4],[\bar{a}_2, \bar{a}_5]\) and \([\bar{a}_3, \bar{a}_6]\). Thus we can conclude that
\[
\det DF_\tilde{K}(\bar{x}) > 0 \quad \forall \bar{x} \in \tilde{K} \iff \begin{cases} \det DF_\tilde{K}(0,0,\zeta) > 0 \\
\text{and} \quad \det DF_\tilde{K}(1,0,\zeta) > 0 \end{cases} \quad \forall \zeta \in [0,1].
\]

Applying Lemma 1.1 to these three quadratic polynomials finally yields the following result (cf. [3, Thm. 3.1]):

**Theorem 3.1** The simpliﬁed isoparametric transformation \( F_\tilde{K} \) for prismatic elements is invertible in \( \tilde{K} \) if each of the following conditions is satisﬁed:

\[
\begin{align*}
\bar{x}_6 \bar{y}_6 &> \bar{x}_6 \bar{y}_6, \\
\bar{x}_6 + \bar{y}_6 &\geq \bar{x}_6 \bar{y}_6 - \bar{x}_6 \bar{y}_6 \\
\text{or } \bar{x}_6 + \bar{y}_6 - 2 &> -2\sqrt{|(\bar{x}_6 - 1)(\bar{y}_6 - 1) - \bar{x}_6 \bar{y}_6|}
\end{align*}
\]

(4)

\[
\begin{align*}
\tilde{z}_6 &> 0, \\
\bar{y}_6(\bar{x}_6 + \bar{z}_6 - 1) &> \bar{y}_6(\bar{x}_6 + \bar{z}_6 - 1), \\
\tilde{z}_6 &\geq (\bar{x}_6 - 1)(\bar{y}_6 - 1) - \bar{x}_6 \bar{y}_6 \\
\text{or } \bar{x}_6 - 1 + \tilde{z}_6(\bar{y}_6 - 1) - \bar{y}_6(\bar{z}_6 - 1) &> -2\sqrt{\left|\tilde{z}_6((\bar{x}_6 - 1)(\bar{y}_6 - 1) - \bar{x}_6 \bar{y}_6)\right|}
\end{align*}
\]

(5)

\[
\begin{align*}
\tilde{z}_6 &> 0, \\
\bar{y}_6(\bar{x}_6 + \bar{z}_6 - 1) &> \bar{y}_6(\bar{x}_6 + \bar{z}_6 - 1), \\
\tilde{z}_6 &\geq (\bar{x}_6 - 1)(\bar{y}_6 - 1) - \bar{x}_6 \bar{y}_6 \\
\text{or } \bar{y}_6 - 1 + \tilde{z}_6(\bar{x}_6 - 1) - \bar{x}_6(\bar{z}_6 - 1) &> -2\sqrt{\left|\tilde{z}_6((\bar{x}_6 - 1)(\bar{y}_6 - 1) - \bar{x}_6 \bar{y}_6)\right|}
\end{align*}
\]

(6)

Note that for \( \tilde{z}_6 = \tilde{z}_6 = 1 \) the conditions in (4), (5) and (6) coincide.

3.3 Examples of distorted prismatic finite elements

Again, we present some examples of prismatic elements that violate one of the conditions in Theorem 3.1. We restrict our considerations to the case, where \( \alpha_i = \bar{a}_i \) for \( i \in I_T = \{1, 2, 3, 4\} \) such that \( K = \tilde{K} \), in particular \( \bar{a}_5 = a_5 \) and \( \bar{a}_6 = a_6 \).

(a) We obtain an example of a prismatic finite element \( K \), which violates the first condition in (4) and the second condition in (5) and (6), when we choose...
$a_5 = (1,1,1)^T$ and $a_6 = (2,1,1)^T$ (see Fig. 5 (a)). If we switch $a_5$ and $a_6$, all conditions in Theorem 3.1 will be satisfied and $F_K$ will be invertible.

(b) For our second example we choose $a_5 = (-2,1,1)^T$ and $a_6 = (1,-1,1)^T$ (see Fig. 5 (b)). Then the last condition in (4)–(6) is violated and $F_K$ is not invertible. If we switch $a_5$ and $a_6$, the first condition in (4) and the second condition in (5) and (6) will be violated and $F_K$ will not be invertible again. Thus in this case a simple switching of the vertices $a_5$ and $a_6$ will not give an invertible isoparametric mapping.

In this context a natural question arises: Is there always a numbering of the vertices such that the corresponding isoparametric transformation is invertible? We do not dwell on this subject here.

4 Hexahedral finite elements

4.1 The hexahedral reference element

The hexahedral reference element is defined by $\bar{K} = \text{conv} \{\bar{a}_i\}$, where the vertices $\bar{a}_i$, $i = 1, \ldots, 8$ are given below, and depicted in Fig. 6.

The well known basis functions $\hat{\phi}_i$, $i = 1, \ldots, 8$, for the hexahedral reference element, which fulfill $\hat{\phi}_i(\bar{a}_j) = \delta_{ij}$ for $j = 1, \ldots, 8$, can be obtained as products of linear basis functions on the unit segment.

\[
\begin{align*}
\hat{\phi}_1(\hat{x}) &= (1 - \xi)(1 - \eta)(1 - \zeta), & \hat{\phi}_2(\hat{x}) &= \xi(1 - \eta)(1 - \zeta), \\
\hat{\phi}_3(\hat{x}) &= \xi\eta(1 - \zeta), & \hat{\phi}_4(\hat{x}) &= (1 - \xi)\eta(1 - \zeta), \\
\hat{\phi}_5(\hat{x}) &= (1 - \xi)(1 - \eta)\zeta, & \hat{\phi}_6(\hat{x}) &= \xi(1 - \eta)\zeta, \\
\hat{\phi}_7(\hat{x}) &= \xi\eta\zeta, & \hat{\phi}_8(\hat{x}) &= (1 - \xi)\eta\zeta, 
\end{align*}
\]

where we use again $\hat{x} = (\xi, \eta, \zeta)^T$. 

Figure 5: Distorted prismatic elements
4.2 The isoparametric mapping and its Jacobian determinant

According to (1) the isoparametric mapping is given by:

\[ F_K(\hat{x}) = a_1 + (a_2 - a_1)\xi + (a_4 - a_1)\eta + (a_5 - a_1)\zeta \\
+ (a_1 + a_3 - a_2 - a_4)\xi\eta + (a_1 + a_6 - a_2 - a_5)\xi\zeta + (a_1 + a_8 - a_4 - a_5)\eta\zeta \\
+ (a_2 + a_4 + a_5 + a_7 - a_1 - a_3 - a_6 - a_8)\xi\eta\zeta. \]

A decomposition with \( I_F = \{1, 2, 4, 5\} \) yields:

\[ F_K(\hat{x}) = \hat{x} + (\hat{a}_3 - \hat{a}_1)\xi(1-\zeta) + (\hat{a}_6 - \hat{a}_6)\xi(1-\eta) + (\hat{a}_7 - \hat{a}_7)\xi\eta\zeta + (\hat{a}_8 - \hat{a}_8)(1-\zeta)\eta\zeta \]

such that \( F_K \) consists again of the identity mapping plus some nonlinear terms that depend now on the deviations \( \hat{a}_3 - \hat{a}_1, \hat{a}_6 - \hat{a}_6, \hat{a}_7 - \hat{a}_7 \) and \( \hat{a}_8 - \hat{a}_8 \). Unfortunately, the second derivatives of this mapping \( F_K \) are not constant and it is not clear, if the positivity of the Jacobian determinant of the mapping \( F_K \) is sufficient for its global invertibility. A straightforward computation shows that the Jacobian determinant \( \det DF_K \) is quadratic in each variable:

\[ \det DF_K(\hat{x}) = \sum_{i,j,k=0}^{2} c_{ijk}\xi^i\eta^j\zeta^k, \]

where the coefficients \( c_{ijk} \) depend on \( \hat{a}_\nu - \hat{a}_\nu, \nu = \{3, 6, 7, 8\} \). The dependence of the coefficients \( c_{ijk} \) on the deviations \( \hat{a}_\nu - \hat{a}_\nu \) is given explicitly in [4].

4.3 An algorithm to check the positivity of the Jacobian determinant

To our knowledge it is not possible to derive explicit relations, which ensure that the Jacobian determinant \( \det DF_K \) is positive. Instead, we present an algorithm that checks arbitrarily sharp sufficient conditions for the positivity of \( \det DF_K \). This algorithm is based on a recursive application of Lemma 1.1. As the nonlinear
condition $c_1 > -2\sqrt{|c_0 c_2|}$ in (2) is not appropriate for our recursive approach, we replace it by linear ones that are sufficient for the positivity of $\det D F_R$. To obtain these linear conditions, we approximate the quadratic function $p(\tau) = c_0 + c_1 \tau + c_2 \tau^2$ from below by piecewise linear functions $t_M$. The index $M > 0$ corresponds to the number of linear conditions, we obtain. The piecewise linear parts $t_{M,m}$ of $t_M$ are tangents to $p$ at the points $\frac{m}{M}$ for $m = 0, 1, \ldots, M$. Thus they are of the form

$$t_{M,m}(\tau) = p \left( \frac{m}{M} \right) + p' \left( \frac{m}{M} \right) \left( \tau - \frac{m}{M} \right) = \left( 2c_2 \frac{m}{M} + c_1 \right) \tau + c_0 - c_2 \left( \frac{m}{M} \right)^2 .$$

Now we define $t_M$ by

$$t_M(\tau) = \max_{m=0,\ldots,M} t_{M,m}(\tau) .$$

Of course, $t_M \leq p$ holds if and only if $c_2 \geq 0$. But in our algorithm, we have to use this approximation only in the case when the first two conditions in (2) are fulfilled and the first part of the third condition is not. Therefore the inequality $c_2 > c_0 > 0$ holds. As two neighboring tangents $t_{M,m}$ and $t_{M,m+1}$ intersect at $\tau = \frac{2m+1}{2M}$, we get the following description of $t_M$:

$$t_M(\xi) = t_{M,m}(\xi) \quad \text{for} \quad \xi \in \begin{cases} \left[ 0, \frac{1}{2M} \right] , & \text{if } m = 0 , \\ \left[ \frac{2m-1}{2M} , \frac{2m+1}{2M} \right] , & \text{if } m \in \{ 1, \ldots, M - 1 \} , \\ \left[ \frac{2M-1}{2M} , 1 \right] , & \text{if } m = M . \end{cases}$$

Obviously, the minimum of $t_M$ in $(0, 1)$ is attained at one of these intersection points. Hence we obtain

$$t_M(\xi) > 0 \ \forall \ \xi \in (0, 1) \iff c_0 + \frac{2m + 1}{2M} c_1 + \frac{m^2 + m}{M^2} - c_2 > 0 \ \text{for } m = 0, 1, \ldots, M-1 .$$

![Figure 7: Approximation of parabola from below](image_url)

An example for the approximation of a convex parabola by piecewise tangents from below is depicted in Fig. 7. If we choose a series $(M_i)_{i=1,2,\ldots}$ of values for $M$, where $M_{i+1}$ is a multiple of $M_i$, the series of minimal values of $t_M$, will be monotone, i.e. $\min_{\tau \in [0,1]} t_{M_i}(\tau) \leq \min_{\tau \in [0,1]} t_{M_{i+1}}(\tau)$ for $i = 1, 2, \ldots$. 


Now we define a procedure Pos1D that checks these conditions:

\[
\text{Pos1D}(M, (c_i)_i) = 1, \text{ if } \left\{ \begin{array}{l}
c_0 > 0 \quad \text{and} \\
c_0 + c_1 + c_2 > 0 \quad \text{and} \\
c_0 - c_2 \geq 0 \quad \text{or} \\
c_0 + \frac{2m+1}{2M} c_1 + \frac{m^2+m}{M^2} c_2 > 0 \\
\text{for } m = 0, 1, \ldots, M - 1
\end{array} \right. 
\]

\[
\text{Pos1D}(M, (c_i)_i) = 0 \quad \text{elsewhere}.
\]

From the considerations above it follows that \( p(\tau) = c_0 + c_1 \tau + c_2 \tau^2 > 0 \) for each \( \tau \in [0, 1] \), if Pos1D\((M, (c_i)_i) = 1 \) for some \( M \).

In the next step we consider a quadratic polynomial in two variables

\[
P(\xi, \eta) = \sum_{i,j=0}^{2} c_{ij} \xi^i \eta^j = \left( \sum_{i=0}^{2} c_{i0} \xi^i \right) + \left( \sum_{i=0}^{2} c_{i1} \xi^i \right) \eta + \left( \sum_{i=0}^{2} c_{i2} \xi^i \right) \eta^2.
\]

We treat \( P \) as a quadratic polynomial in \( \eta \), where the coefficients depend on \( \xi \). Then we use the ideas that led to the definition of Pos1D and the procedure Pos1D itself to define a procedure Pos2D:

\[
\text{Pos2D}(M, (c_{ij})_{ij}) = 1, \text{ if } \left\{ \begin{array}{l}
\text{Pos1D}(M, (c_{i0})_i) = 1 \quad \text{and} \\
\text{Pos1D}(M, (c_{i0} + c_{i1} + c_{i2})_i) = 1 \quad \text{and} \\
\text{Pos1D}(M, (c_{i0} - c_{i2})_i) = 1 \quad \text{or} \\
\text{Pos1D}(M, (c_{i0} + \frac{2m+1}{2M} c_{i1} + \frac{m^2+m}{M^2} c_{i2})_i) = 1 \\
\text{for } m = 0, 1, \ldots, M - 1
\end{array} \right. 
\]

\[
\text{Pos2D}(M, (c_{ij})_{ij}) = 0 \quad \text{elsewhere}.
\]

Obviously we have \( P(\xi, \eta) > 0 \) for each \( (\xi, \eta) \in [0, 1]^2 \), if Pos2D\((M, (c_{ij})_{ij}) = 1 \) for some \( M \).

Finally we apply these ideas to a quadratic polynomial in three variables

\[
J(\xi, \eta, \zeta) = \sum_{i,j,k=0}^{2} c_{ijk} \xi^i \eta^j \zeta^k = \left( \sum_{i,j=0}^{2} c_{ij0} \xi^i \eta^j \right) + \left( \sum_{i,j=0}^{2} c_{ij1} \xi^i \eta^j \right) \zeta + \left( \sum_{i,j=0}^{2} c_{ij2} \xi^i \eta^j \right) \zeta^2
\]

and treat it as a quadratic polynomial in \( \zeta \), where the coefficients depend on \( \xi \) and \( \eta \). Analogously to the definition of Pos2D we define a procedure Pos3D:

\[
\text{Pos3D}(M, (c_{ijk})_{ijk}) = 1, \text{ if } \left\{ \begin{array}{l}
\text{Pos2D}(M, (c_{ij0})_{ij}) = 1 \quad \text{and} \\
\text{Pos2D}(M, (c_{ij0} + c_{ij1} + c_{ij2})_{ij}) = 1 \quad \text{and} \\
\text{Pos2D}(M, (c_{ij0} - c_{ij2})_{ij}) = 1 \quad \text{or} \\
\text{Pos2D}(M, (c_{ij0} + \frac{2m+1}{2M} c_{ij1} + \frac{m^2+m}{M^2} c_{ij2})_{ij}) = 1 \\
\text{for } m = 0, 1, \ldots, M - 1
\end{array} \right. 
\]

\[
\text{Pos3D}(M, (c_{ijk})_{ijk}) = 0 \quad \text{elsewhere}.
\]
Again, we obtain the implication \( J(\xi, \eta, \zeta) > 0 \) for each \((\xi, \eta, \zeta) \in [0, 1]^3\), if \( Pos3D(M, (c_{ijk})_{ijk}) = 1 \) for some \( M \). Thus we can use the procedure Pos3D to check if the Jacobian determinant \( J(\xi, \eta, \zeta) := \det DF_K(\xi, \eta, \zeta) \) is positive in \( K \).

Our algorithm to check if the Jacobian determinant \( \det DF_K \) vanishes therefore consists of the following four parts:

1) computation of the affine-linear mapping \( F_T \) and test if \( \det DF_T \neq 0 \),
2) calculation of the vertices \( \bar{a}_i = F_T^{-1}(a_i) \) of \( \bar{K} \),
3) computation of the coefficients \( c_{ijk}, i, j, k = 0, 1, \ldots \), of \( \det DF_K \),
4) testing the positivity of \( \det DF_K \) using procedure Pos3D.

### 4.4 Examples of distorted hexahedral finite elements

Like in the prismatic case, we restrict our considerations to the case, where \( a_i = \bar{a}_i \) for \( i \in I_T = \{1, 2, 4, 5\} \) such that \( K = K \) (and \( F_K = \bar{F}_K \)), in particular \( \bar{a}_2 = a_3 \), \( \bar{a}_4 = a_6 \), \( \bar{a}_7 = a_7 \) and \( \bar{a}_8 = a_8 \). Hence we can skip the steps 1) and 2) in the algorithm above and have to consider only the steps 3) and 4).

(a) We begin with a choice of the vertices \( a_i \) for \( i = 3, 6, 7, 8 \) such that the isoparametric mapping \( t_K \) is not invertible in \( K \), since \( \det DF_K \) will be zero. We consider the vertices

\[
a_3 = \begin{pmatrix} 1.5 \\ 1.25 \\ 0 \end{pmatrix}, \quad a_6 = \begin{pmatrix} 1 \\ -0.5 \\ 1 \end{pmatrix}, \quad a_7 = \begin{pmatrix} 1 \\ 0.5 \\ 1 \end{pmatrix}, \quad a_8 = \begin{pmatrix} -0.5 \\ 1 \\ 1 \end{pmatrix}.
\]

The computation of the coefficients \( c_{ijk} \) of \( \det DF_K \) leads to the following expression for \( \det DF_K \):

\[
\det DF_K(\tilde{x}) = \frac{1}{16} \left( 16 + 4\xi + 8\eta - 8\xi\eta - 2\xi^2\eta - 4\xi\eta^2 \\
- 4\xi^2\zeta + 2\eta\zeta - 2\xi^3\eta\zeta - 4\eta^2\zeta - 8\xi\eta\zeta - 4\xi^2\zeta - 2\xi\eta\zeta^2 - 2\xi\eta^2\zeta \right).
\]

Applying Pos3D to those coefficients yields \( Pos3D(M, (c_{ijk})_{ijk}) = 0 \) for every \( M \). Indeed, \( \det DF_K(1, 1, 1) = -\frac{1}{16} \) such that \( F_K \) is not invertible.

The shape of the resulting element \( K \) is depicted in Fig. 8 using views from different angles. While in view (a) the element looks very similar to the unit cube, one might guess from view (b) some sort of distortion in the vicinity of \( a_7 \).

(b) Our next example shows, how the algorithm may fail for too small values of \( M \). We choose the vertices

\[
a_3 = \begin{pmatrix} 1.5 \\ 0.5 \\ 0 \end{pmatrix}, \quad a_6 = \begin{pmatrix} 1.5 \\ 0 \\ 1.5 \end{pmatrix}, \quad a_7 = \begin{pmatrix} 0.5 \\ 1 \\ 0.5 \end{pmatrix}, \quad a_8 = \begin{pmatrix} 0 \\ 0.5 \\ 1.5 \end{pmatrix}.
\]

After computation of the coefficients \( c_{ijk} \) of \( \det DF_K \) we obtain the following expression for \( \det DF_K \):

\[
\det DF_K(\tilde{x}) = \frac{1}{4} \left( 4 - \xi^2 + 4\eta - 6\xi\eta + 3\xi^2\eta + \eta^2 - \xi\eta^2 + 2\xi\zeta + 2\xi^2\zeta - 6\eta\zeta \\
- 2\xi\eta\zeta + \xi^2\eta\zeta - 3\eta^2\zeta + 2\xi\eta^2\zeta - \zeta^2 + 2\xi\zeta^2 + 3\eta\zeta^2 + \xi\eta\zeta^2 \right).
\]
For these coefficients and $M = 1$ we get $\text{Pos3D}(1, (c_{ijk})_{ijk}) = 0$, but for $M \geq 2$ we get $\text{Pos3D}(M, (c_{ijk})_{ijk}) = 1$. Since $\det DF_K(\hat{x}) > \det DF_K(2/5, 1, 1) = 3/10 > 0$ for all $\hat{x} \in \hat{K}$ the Jacobian determinant $\det DF_K$ is positive in $\hat{K}$ and the isoparametric mapping $F_K$ is locally invertible.

As one can see from Fig. 9 (a) the face with the vertices $a_3$, $a_4$, $a_7$ and $a_8$ is strongly distorted. This is caused by the fact that $a_4$ and $a_7$ are very close to each other. From the view in Fig. 9 (b) we can see that this face is well shaped. (c) Finally we present an example, where the algorithm fails for a series of values of $M$. We consider the vertices

$$a_3 \left( \begin{array}{c} 1.5 \\ 0.5 \\ 0 \end{array} \right) , \quad a_6 \left( \begin{array}{c} 0.5 \\ 0.5 \\ 1.25 \end{array} \right) , \quad a_7 \left( \begin{array}{c} 1.0 \\ 0.75 \\ 0.5 \end{array} \right) , \quad a_8 \left( \begin{array}{c} 0.25 \\ 0.5 \\ 1.5 \end{array} \right).$$
The computation of the coefficients \( c_{ijk} \) yields:

\[
\det DF_K(\hat{x}) = \frac{1}{64} \left( 64 - 16\xi - 8\xi^2 + 64\eta - 88\xi\eta + 40\xi^2\eta + 16\eta^2 - 40\xi\eta^2 \\
- 64\zeta - 8\xi\zeta + 44\xi^2\zeta - 44\eta\zeta - 4\xi\eta\zeta + 12\eta^2\zeta + 10\xi\eta^2\zeta \\
+ 8\xi^2 + 4\xi^2 + 11\xi\eta\zeta^2 \right).
\]

When we apply Pos3D for \( M = 2^k, k = 0, 1, 2, 3, 4, 5 \), we get for \( M = 1, 2, 4, 8, 16 \) the results \( \text{Pos3D}(M, (c_{ijk})_{ijk}) = 0 \), but \( \text{Pos3D}(32, (c_{ijk})_{ijk}) = 1 \). Again a consideration of \( \det DF_K \) yields \( \det DF_K(\hat{x}) > 0 \) in \( \hat{K} \) such that \( F_K \) is locally invertible. Therefore a high computational effort is needed to obtain the correct result for this example. On the other hand it may be desirable to reject such strongly distorted elements because they may cause numerical problems during finite element computations.

![Diagram](a) ![Diagram](b)

Figure 10: Strongly distorted hexahedral element with \( \det DF_K > 0 \)

From the view in Fig. 10 (a) this element looks very strangely shaped. One can see that especially the face with the vertices \( a_5, a_6, a_7 \) and \( a_8 \) is strongly distorted due to the closeness of \( a_6 \) and \( a_8 \). From the different view in Fig. 10 (b) we can see the element looks much nicer, but nevertheless also distorted.

## 5 Conclusion

In this paper we considered the isoparametric mapping for multilinear finite elements on pyramids, prisms and hexahedra. We presented a decomposition of this mapping, which reduces the number of free parameters. For pyramidal and prismatic finite elements we derived algebraic inequalities that imply the invertibility of the isoparametric mapping. In the hexahedral case we developed a procedure that can be used to check the positivity of the Jacobian determinant.

Some questions appeared or remained open:

- What is the correct numbering of a given set of vertices, i.e., how should these vertices be ordered to obtain an invertible isoparametric mapping?
• Is it possible to obtain algebraic inequalities for the hexahedral elements, too?
• Does the local invertibility of the isoparametric mapping for hexahedral finite elements imply its global invertibility?

References


