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The inverse mapping and distortion measures for 8-node hexahedral isoparametric elements

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Abstract The inverse relations of the isoparametric mapping for the 8-node hexahedra are derived by using the theory of geodesics in differential geometry. Such inverse relations assume the form of infinite power series in the element geodesic coordinates, which are shown to be the skew Cartesian coordinates determined by the Jacobian of the mapping evaluated at the origin. By expressing the geodesic coordinates in turn in terms of the isoparametric coordinates, the coefficients in the resulted polynomials are suggested to be the distortion parameters of the element. These distortion parameters can be used to completely describe the inverse relations and the determinant of the Jacobian of the mapping. The meanings of them can also be explained geometrically and mathematically. These methods of defining the distortion measures and deriving the inverse relations of the mapping are completely general, and can be applied to any other two- or three-dimensional isoparametric elements.

1 Introduction

The inverse mapping and distortion measures of the isoparametric elements recently have attracted the attentions of several researchers. For quadrilateral elements in two dimensions, Hua (1990) has developed a complete set of solutions to the inverse transformation based on a case-by-case consideration of the element geometry. For hexahedral elements in three dimensions, Knupp (1990) has discussed the invertibility of the isoparametric mapping. For the needs in remeshing and in stress and nodal quantity contouring, Murti and Valliappan (1986) and Murti et al. (1988) have also discussed the numerical techniques to obtain inverse isoparametric mapping. For the purpose of quantifying the sensitivity of the element to shape distortions, on the other hand, Robinson (1987, 1988) has addressed on the need of formulating the element distortion measures. For the 4-node and 8-node quadrilateral elements, respectively, he has also proposed, based on geometric considerations of the element shape, certain shape parameters as the element distortion measures.

The inverse mapping and distortion measures of the isoparametric elements are certainly important in the theory and practice of finite elements. However, general analytic expressions of the inverse relations of the mapping applicable to any type of isoparametric elements has never been derived previously. What precisely should the definitions of the element distortion measures be also has not been generally agreed. Recently, Yuan and Pian (1993) and Yuan et al. (1993) suggest an analytic way of deriving the inverse relations of the mapping, in which a consistent and general way of defining the element distortion measures has also been proposed. The method they suggest uses the theory of geodesics (Eisenhart 1949; Veblen 1962) in deriving the inverse relation of the mapping. By introducing the geodesic coordinates, or rather the Riemannian normal coordinates, defined at the local origin, they have shown that the inverse relations of the mapping can be derived in the form of power series in these geodesic coordinates.

In Yuan and Pian (1993) and Yuan et al. (1993), the introduced geodesic coordinate system at the origin has been proved to be a skew Cartesian coordinate system, which is linearly related to the local Cartesian coordinate system through the Jacobian of the mapping evaluated at the origin. When these geodesic coordinates are expressed in turn in terms of the isoparametric coordinates, the coefficients in the

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resulted polynomials in isoparametric coordinates have been suggested to be the distortion measures of the element. The meanings of these coefficients have also been shown to be the function values of the Christoffel symbols of the isoparametric coordinate system and their derivatives at the origin. These distortion-measuring parameters thus reflect the rates of change of the basis vectors of the isoparametric coordinate system at the origin.

For the 4-node and the 8-node plane elements, respectively, Yuan and Pian (1993) and Yuan et al. (1993) have shown that the coefficients in the power series of the inverse isoparametric mapping can be completely expressed in terms of these distortion parameters. Similarly, the coefficients in the polynomial of the Jacobian determinant of the mapping can also be expressed entirely in terms of them. Furthermore, when the equations which define the mapping are written into a polynomial in isoparametric coordinates with vector coefficients, a simple geometric interpretation of such distortion parameters can be constructed by using these coefficient vectors and their vector cross products.

Using the theory of geodesics in defining the element distortion measures and deriving the inverse relations of the mapping therefore has many advantages. Since the theory is completely general, its usefulness in the three dimensional case is explored in this paper. For the 8-node hexahedra element considered, it will be shown that the expressions of the geodesic coordinates at the origin lead to the definition of twelve distortion parameters which completely determine all the coefficients in the inverse relations of the mapping. It will also be shown that these twelve parameters completely describe all the coefficients that appear in the polynomial of the determinant of the Jacobian of the mapping.

In this three-dimensional case, a more general geometric interpretation of the twelve distortion parameters can be given by using the coefficient vectors that appear in the isoparametric coordinate transformation and their triple scalar products. For reason of completeness, the aspect ratios and skew angles of the basic parallelepiped determined by the axes of the geodesic coordinate system defined at the local origin can also be suggested as the additional distortion measures. The investigations in this paper are demonstrated by using several example 8-node hexahedra. The inverse mapping and distortion parameters of any other three-dimensional isoparametric element can be similarly obtained by using this approach.

2
Theory

The theory invoked in this paper has its root in tensor analysis on manifolds (Eisenhart 1949; Veblen 1962; Bishop and Goldberg 1968), the technique part of which can be briefly described as follows. In an n-dimensional Riemannian manifold, the geodesics, which is the fundamental geometric figure of such a space, is the integral curves of the following system of differential equations.

$$\frac{d^2\xi^i}{ds^2}+\Gamma^i_{jk}\frac{d\xi^j}{ds}\frac{d\xi^k}{ds}=0 \quad i=1\sim n \tag{1}$$

where ξ^i denote any admissible set of coordinates, s the arc parameters, and $\Gamma^i_{jk}=\Gamma^i_{kj}$ the Christoffel symbols of the ξ^i coordinate system.

Any integral curve of Eq. (1) can be uniquely determined by a point q and a direction specified at q, i.e., by the initial conditions:

$$\xi^i=(\xi^i)_q \quad \text{and} \quad \left(\frac{d\xi^i}{ds}\right)_q=t^i \quad \text{at} \quad s=0. \tag{2}$$

About point q, the integral curve can be expanded into Taylor series in the following form.

$$\xi^i=(\xi^i)_q+t^is+\frac{1}{2}\left(\frac{d^2\xi}{ds^2}\right)_q s^2+\frac{1}{3!}\left(\frac{d^3\xi}{ds^3}\right)_q s^3+\cdots \tag{3}$$

where the subscript q denotes the value of the quantity within the parentheses calculated at the point q.

In Eq. (3), the coefficient of s^2 can be obtained by replacing the second derivative of ξ^i by means of Eq. (1). The coefficients of the higher powers in s can be similarly determined by first differentiating Eq. (1) successively to obtain the following sequence of equations, which must be satisfied by any integral curve of Eq. (1).

$$\frac{d^3\xi^i}{ds^3}+\Gamma^i_{jkl}\frac{d\xi^j}{ds}\frac{d\xi^k}{ds}\frac{d\xi^l}{ds}=0, \quad \frac{d^4\xi^i}{ds^4}+\Gamma^i_{jklm}\frac{d\xi^j}{ds}\frac{d\xi^k}{ds}\frac{d\xi^l}{ds}\frac{d\xi^m}{ds}=0,\ldots \tag{4}$$

in which the functions

$$\Gamma^i_{jkl} = \frac{1}{3} P \left\langle \frac{\partial \Gamma^i_{jk}}{\partial \xi^l} - \Gamma^i_{\alpha k} \Gamma^\alpha_{jl} - \Gamma^i_{j\alpha} \Gamma^\alpha_{kl} \right\rangle \tag{5}$$

and, in general,

$$\Gamma^i_{jkl\cdots mn} = \frac{1}{N} P \left\langle \frac{\partial \Gamma^i_{jkl\cdots m}}{\partial \xi^n} - \Gamma^i_{\alpha kl\cdots m} \Gamma^\alpha_{jn} - \cdots - \Gamma^i_{jkl\cdots \alpha} \Gamma^\alpha_{mn} \right\rangle \tag{6}$$

where $P\langle\,\rangle$ denotes the sum of terms obtainable from the ones inside the bracket by permuting the free subscripts cyclically and N denotes the number of subscripts. The Γ functions so defined are therefore completely symmetric in its subscripts. By means of these differential equations, the higher derivatives of ξ^i can be determined and the series in Eq. (3) can be written into

$$\xi^i = (\xi^i)_q + t^i s - \frac{1}{2} (\Gamma^i_{jk})_q t^j t^k s^2 - \frac{1}{3!} (\Gamma^i_{jkl})_q t^j t^k t^l s^3 - \cdots \tag{7}$$

which can be proved to be convergent (Eisenhart 1949; Veblen 1962).

For all geodesics through point q, it is the Riemann's famous proposition that one puts

$$\bar{\xi}^i = t^i s \tag{8}$$

and substitute it into Eq. (7), with the result

$$\xi^i - (\xi^i)_q = \bar{\xi}^i - \frac{1}{2} (\Gamma^i_{jk})_q \bar{\xi}^j \bar{\xi}^k - \frac{1}{3!} (\Gamma^i_{jkl})_q \bar{\xi}^j \bar{\xi}^k \bar{\xi}^l - \cdots. \tag{9}$$

Since Eq. (9) do not involve the direction t^i, they hold for all geodesics through q and therefore constitute the equations for a transformation of coordinates. In the $\bar{\xi}^i$ coordinates, the equations of the geodesics through the origin assume the form in Eq. (8).

The $\bar{\xi}^i$ coordinates defined at a point q are a type of geodesic coordinates and are known as the Riemannian coordinates (Eisenhart 1949) or the normal coordinates (Veblen 1962; Bishop and Goldberg 1968). In the special case of flat Euclidean space, the geodesics through any point are known to be straight lines. The equations of them must be linear in the Cartesian coordinates used to describe that space. Based on that, one may use the above-described theory to derive the inverse relations of the isoparametric mapping.

3 Inverse mapping of the 8-node hexahedra

Consider a general 8-node hexahedron, as shown in Fig. 1. The equations which define the isoparametric mapping are as follows.

$$\begin{Bmatrix} x \\ y \\ z \end{Bmatrix} = \sum_{i=1}^{8} N_i(\xi, \eta, \zeta) \begin{Bmatrix} x_i \\ y_i \\ z_i \end{Bmatrix} = \begin{Bmatrix} a_0 + a_1\xi + a_2\eta + a_3\zeta + a_4\eta\zeta + a_5\xi\zeta + a_6\xi\eta + a_7\xi\eta\zeta \\ b_0 + b_1\xi + b_2\eta + b_3\zeta + b_4\eta\zeta + b_5\xi\zeta + b_6\xi\eta + b_7\xi\eta\zeta \\ c_0 + c_1\xi + c_2\eta + c_3\zeta + c_4\eta\zeta + c_5\xi\zeta + c_6\xi\eta + c_7\xi\eta\zeta \end{Bmatrix} \tag{10}$$

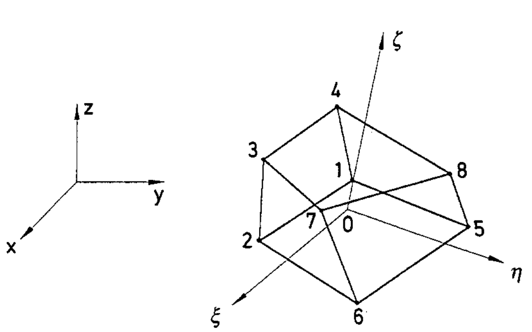
where (x, y, z) denote the global Cartesian coordinates; (ξ, η, ζ) the element natural coordinates; (x_i, y_i, z_i) the nodal coordinates; $N_i(\xi, \eta, \zeta)$ the shape functions,

$$N_i = \tfrac{1}{8}(1 + \xi^i \xi)(1 + \eta^i \eta)(1 + \zeta^i \zeta) \quad i = 1 \sim 8; \tag{11}$$

the coefficients

$$a_0 = \frac{1}{8}\sum_{i=1}^{8} x_i, \quad a_1 = \frac{1}{8}\sum_{i=1}^{8} x_i\xi_i, \quad a_2 = \frac{1}{8}\sum_{i=1}^{8} x_i\eta_i, \quad a_3 = \frac{1}{8}\sum_{i=1}^{8} x_i\zeta_i,$$

$$a_4 = \frac{1}{8}\sum_{i=1}^{8} x_i\eta_i\zeta_i, \quad a_5 = \frac{1}{8}\sum_{i=1}^{8} x_i\xi_i\zeta_i, \quad a_6 = \frac{1}{8}\sum_{i=1}^{8} x_i\xi_i\eta_i, \quad a_7 = \frac{1}{8}\sum_{i=1}^{8} x_i\xi_i\eta_i\zeta_i; \tag{12}$$



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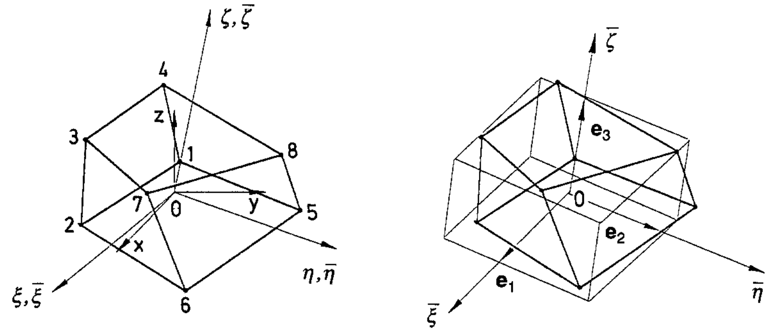


2 a b

Figs. 1, 2. 1 8-node hexahedral element; isoparametric coordinates (ξ, η, ζ). 2 a Local Cartesian coordinates (x, y, z) and geodesic coordinates $(\bar{\xi}, \bar{\eta}, \bar{\zeta})$ at the origin; b basic parallelepiped determined by coefficient vectors e_1, e_2 and e_3

the coefficients b_i and c_i, $i = 0 \sim 7$, can be similarly calculated by using the nodal coordinates y_i and z_i, $i = 1 \sim 8$, respectively.

By denoting the coefficient vectors

$$e_i = \begin{Bmatrix} a_i \\ b_i \\ y_i \end{Bmatrix}, \quad i = 0 \sim 7, \tag{13}$$

Eq. (10) can be written into

$$\begin{Bmatrix} x \\ y \\ z \end{Bmatrix} = e_0 + \xi e_1 + \eta e_2 + \zeta e_3 + \eta\zeta e_4 + \xi\zeta e_5 + \xi\zeta e_6 + \xi\eta\zeta e_7. \tag{14}$$

The Jacobian and its inverse of the coordinate transformation defined by the above equation are, respectively,

$$J = \begin{bmatrix} x_{,\xi} & y_{,\xi} & z_{,\xi} \\ x_{,\eta} & y_{,\eta} & z_{,\eta} \\ x_{,\zeta} & y_{,\zeta} & z_{,\zeta} \end{bmatrix} = \begin{bmatrix} J_{11} & J_{12} & J_{13} \\ J_{21} & J_{22} & J_{23} \\ J_{31} & J_{32} & J_{33} \end{bmatrix}$$

$$= \begin{bmatrix} a_1 + a_5\zeta + a_6\eta + a_7\eta\zeta & b_1 + b_5\zeta + b_6\eta + b_7\eta\zeta & c_1 + c_5\zeta + c_6\eta + c_7\eta\zeta \\ a_2 + a_4\zeta + a_6\xi + a_7\xi\zeta & b_2 + b_4\zeta + b_6\xi + b_7\xi\zeta & c_2 + c_4\zeta + c_6\xi + c_7\xi\zeta \\ a_3 + a_4\eta + a_5\xi + a_7\xi\eta & b_3 + b_4\eta + b_5\xi + b_7\xi\eta & c_3 + c_4\eta + c_5\xi + c_7\xi\eta \end{bmatrix} \tag{15}$$

and

$$J^{-1} = \begin{bmatrix} \xi_{,x} & \eta_{,x} & \zeta_{,x} \\ \xi_{,y} & \eta_{,y} & \zeta_{,y} \\ \xi_{,z} & \eta_{,z} & \zeta_{,z} \end{bmatrix} = \frac{1}{J} \begin{bmatrix} J_{22}J_{33} - J_{23}J_{32} & J_{13}J_{32} - J_{12}J_{33} & J_{12}J_{23} - J_{13}J_{22} \\ J_{23}J_{31} - J_{21}J_{33} & J_{11}J_{33} - J_{13}J_{31} & J_{13}J_{21} - J_{11}J_{23} \\ J_{21}J_{32} - J_{31}J_{22} & J_{12}J_{31} - J_{11}J_{32} & J_{11}J_{22} - J_{12}J_{21} \end{bmatrix} \tag{16}$$

where J is the determinant of the Jacobian. Introducing the notation

$$p_{ijk} = \frac{[e_i e_j e_k]}{[e_1 e_2 e_3]}, \quad i \neq j \neq k, \quad i, j, k = 1 \sim 7 \tag{17}$$

where the triple scalar product $[e_i e_j e_k] = e_i \cdot e_j \times e_k$, one may write J into

$$\begin{aligned} J &= \mathrm{Det}(J) \\ &= J_0(1 + f_1\xi + f_2\eta + f_3\zeta + f_4\eta\zeta + f_5\xi\zeta + f_6\xi\eta + f_7\xi^2 + f_8\eta^2 + f_9\zeta^2 \\ &\quad + f_{10}\eta^2\zeta + f_{11}\eta\zeta^2 + f_{12}\zeta^2\xi + f_{13}\xi^2\zeta + f_{14}\xi^2\eta + f_{15}\xi\eta^2 \\ &\quad + f_{16}\xi\eta\zeta + f_{17}\xi^2\eta\zeta + f_{18}\xi\eta^2\zeta + f_{19}\xi\eta\zeta^2) \end{aligned} \tag{18}$$

in which

$$\begin{array}{llll} J_0 = [e_1 e_2 e_3], & f_1 = p_{125} + p_{163}, & f_2 = p_{124} + p_{623}, & f_3 = p_{523} + p_{143}, \\ f_4 = p_{723} + p_{452} + p_{436}, & f_5 = p_{173} + p_{451} + p_{356}, & f_6 = p_{127} + p_{416} + p_{256}, & f_7 = -p_{156}, \\ f_8 = -p_{426}, & f_9 = -p_{453}, & f_{10} = p_{247}, & f_{11} = -p_{347}, \\ f_{12} = p_{357}, & f_{13} = -p_{157}, & f_{14} = p_{167}, & f_{15} = -p_{267}, \\ f_{16} = 2p_{456}, & f_{17} = p_{756}, & f_{18} = p_{476}, & f_{19} = p_{457}. \end{array} \tag{19}$$

In Eq. (14), the coefficient vector e_0 clearly determines the origin O of isoparametric coordinates. For convenience, introduce at O a local Cartesian coordinate system, as shown in Fig. 2, which can be obtained via rigid body translation of the global Cartesian coordinate system. Then, in this local Cartesian system, all the coefficients and relations in Eqs. (10) to (19) remain unchanged, except that $a_0 = b_0 = c_0 = 0$. For convenience, these local Cartesian coordinates will also be denoted by (x, y, z) in all the following, when no confusion can be caused.

Employ the index notation and put the local Cartesian coordinates $x = x^1$, $y = x^2$, and $z = x^3$, and the element natural coordinates $\xi = \xi^1$, $\eta = \xi^2$, and $\zeta = \xi^3$. The nine Christoffel symbols of the isoparametric coordinate system can be calculated from

$$\Gamma^i_{jk} = \Gamma^i_{kj} = \frac{\partial^2 x^\alpha}{\partial\xi^j \partial\xi^k}\frac{\partial\xi^i}{\partial x^\alpha}. \tag{20}$$

At the origin O, their values are calculated to be

$$\begin{aligned} &(\Gamma^1_{12})_0 = p_{623}, \quad (\Gamma^1_{13})_0 = p_{523}, \quad (\Gamma^1_{23})_0 = p_{423} \\ &(\Gamma^2_{12})_0 = p_{163}, \quad (\Gamma^2_{13})_0 = p_{153}, \quad (\Gamma^2_{23})_0 = p_{143} \\ &(\Gamma^3_{12})_0 = p_{126}, \quad (\Gamma^3_{13})_0 = p_{125}, \quad (\Gamma^3_{23})_0 = p_{124}. \end{aligned} \tag{21}$$

The element geodesic coordinates $(\bar\xi, \bar\eta, \bar\zeta)$ at O can be determined as follows. Since any direction at O can be specified by a straight line passing through O, along which $\frac{dx}{ds} = \frac{x}{s}$, $\frac{dy}{ds} = \frac{y}{s}$ and $\frac{dz}{ds} = \frac{z}{s}$, from Eq. (8),

$$\begin{aligned} \bar\xi &= \left(\frac{d\xi}{ds}\right)_0 s = \left(\frac{\partial\xi}{\partial x}\frac{x}{s} + \frac{\partial\xi}{\partial y}\frac{y}{s} + \frac{\partial\xi}{\partial z}\frac{z}{s}\right)_0 s \\ \bar\eta &= \left(\frac{d\eta}{ds}\right)_0 s = \left(\frac{\partial\eta}{\partial x}\frac{x}{s} + \frac{\partial\eta}{\partial y}\frac{y}{s} + \frac{\partial\eta}{\partial z}\frac{z}{s}\right)_0 s \\ \bar\zeta &= \left(\frac{d\zeta}{ds}\right)_0 s = \left(\frac{\partial\zeta}{\partial x}\frac{x}{s} + \frac{\partial\zeta}{\partial y}\frac{y}{s} + \frac{\partial\zeta}{\partial z}\frac{z}{s}\right)_0 s. \end{aligned} \tag{22}$$

that is,

$$\begin{Bmatrix} \bar\xi \\ \bar\eta \\ \bar\zeta \end{Bmatrix} = (J_0^{-1})^T \begin{Bmatrix} x \\ y \\ z \end{Bmatrix} = \frac{1}{J_0}\begin{bmatrix} b_2c_3 - b_3c_2 & a_3c_2 - a_2c_3 & a_2b_3 - a_3b_2 \\ b_3c_1 - b_1c_3 & a_1c_3 - a_3c_1 & a_3b_1 - a_1b_3 \\ b_1c_2 - b_2c_1 & a_2c_1 - a_1c_2 & a_1b_2 - a_2b_1 \end{bmatrix} \begin{Bmatrix} x \\ y \\ z \end{Bmatrix} \tag{23}$$

and, inversely,

$$\begin{Bmatrix} x \\ y \\ z \end{Bmatrix} = (J_0)^T \begin{Bmatrix} \bar{\xi} \\ \bar{\eta} \\ \bar{\zeta} \end{Bmatrix} = \begin{bmatrix} a_1 & a_2 & a_3 \\ b_1 & b_2 & b_3 \\ c_1 & c_2 & c_3 \end{bmatrix} \begin{Bmatrix} \bar{\xi} \\ \bar{\eta} \\ \bar{\zeta} \end{Bmatrix}. \tag{24}$$

After substituting Eq. (10) into Eq. (23), one obtains

$$\begin{Bmatrix} \bar{\xi} \\ \bar{\eta} \\ \bar{\zeta} \end{Bmatrix} = \begin{Bmatrix} 1 \\ 0 \\ 0 \end{Bmatrix} \xi + \begin{Bmatrix} 0 \\ 1 \\ 0 \end{Bmatrix} \eta + \begin{Bmatrix} 0 \\ 0 \\ 1 \end{Bmatrix} \zeta + \begin{Bmatrix} p_{423} \\ p_{143} \\ p_{124} \end{Bmatrix} \eta\zeta + \begin{Bmatrix} p_{523} \\ p_{153} \\ p_{125} \end{Bmatrix} \xi\zeta + \begin{Bmatrix} p_{623} \\ p_{163} \\ p_{126} \end{Bmatrix} \xi\eta + \begin{Bmatrix} p_{723} \\ p_{173} \\ p_{127} \end{Bmatrix} \xi\eta\zeta. \tag{25}$$

The values $(\Gamma^i_{jk})_0$ in Eq. (21) are seen to be directly given by the nine coefficients of the bilinear terms in ξ, η and ζ in the above equation.

To express the inverse relations of the mapping in terms of these geodesic coordinates, one must calculate the values of the higher order Γ functions at the origin. For the 21 thrid-order functions Γ^i_{jkl} defined in Eq. (5), their values at the origin have been calculated to be

$$\begin{aligned}
(\Gamma^1_{123})_0 &= p_{723} - [(p_{623}p_{143} + p_{523}p_{124}) + (p_{623}p_{523} + p_{423}p_{125}) + (p_{523}p_{623} + p_{423}p_{163})] \\
(\Gamma^2_{123})_0 &= p_{173} - [(p_{163}p_{143} + p_{153}p_{124}) + (p_{163}p_{523} + p_{143}p_{125}) + (p_{153}p_{623} + p_{143}p_{163})] \\
(\Gamma^3_{123})_0 &= p_{127} - [(p_{126}p_{143} + p_{125}p_{124}) + (p_{126}p_{523} + p_{124}p_{125}) + (p_{125}p_{623} + p_{124}p_{163})]
\end{aligned}$$

and

$$\begin{aligned}
(\Gamma^1_{112})_0 &= -2(p_{623}p_{163} + p_{523}p_{126}), & (\Gamma^1_{113})_0 &= -2(p_{623}p_{153} + p_{523}p_{125}) \\
(\Gamma^1_{221})_0 &= -2(p_{623}p_{623} + p_{423}p_{126}), & (\Gamma^1_{223})_0 &= -2(p_{623}p_{423} + p_{423}p_{124}) \\
(\Gamma^1_{331})_0 &= -2(p_{523}p_{523} + p_{423}p_{153}), & (\Gamma^1_{332})_0 &= -2(p_{523}p_{423} + p_{423}p_{143}) \\
(\Gamma^2_{112})_0 &= -2(p_{163}p_{163} + p_{153}p_{126}), & (\Gamma^2_{113})_0 &= -2(p_{163}p_{153} + p_{153}p_{125}). \\
(\Gamma^2_{221})_0 &= -2(p_{163}p_{623} + p_{143}p_{126}), & (\Gamma^2_{113})_0 &= -2(p_{163}p_{423} + p_{143}p_{143}) \\
(\Gamma^2_{331})_0 &= -2(p_{153}p_{523} + p_{143}p_{153}), & (\Gamma^2_{332})_0 &= -2(p_{153}p_{423} + p_{143}p_{143}) \\
(\Gamma^3_{112})_0 &= -2(p_{125}p_{126} + p_{126}p_{163}), & (\Gamma^3_{113})_0 &= -2(p_{126}p_{153} + p_{125}p_{125}) \\
(\Gamma^3_{221})_0 &= -2(p_{124}p_{126} + p_{126}p_{623}), & (\Gamma^3_{223})_0 &= -2(p_{126}p_{423} + p_{124}p_{124}) \\
(\Gamma^3_{331})_0 &= -2(p_{125}p_{523} + p_{124}p_{153}), & (\Gamma^3_{332})_0 &= -2(p_{125}p_{423} + p_{124}p_{143}).
\end{aligned} \tag{26}$$

Notice that the expressions of the first three $(\Gamma^i_{jkl})_0$ values in Eq. (26) involve the three coefficient, p_{723}, p_{173} and p_{127}, of the trilinear terms in Eq. (25). All the other $(\Gamma^i_{jkl})_0$ values, on the other hand, can be expressed in terms of the nine $(\Gamma^i_{jk})_0$ values given in Eq. (21). The values of all the other higher order Γ functions, defined generally in Eq. (6), at the origin can be similarly calculated. It will be shown in the next section that all these values can be expressed in terms of the twelve p_{ijk} parameters that appears in Eq. (25). By substituting these values into Eq. (9) and using the linear relations between $(\bar{\xi}, \bar{\eta}, \bar{\zeta})$ and (x, y, z) given in Eq. (23), one obtains the inverse relations of the mapping defined by Eq. (10).

4
Distortion measures and their meanings

The geodesic coordinates at the origin, $(\bar{\xi}, \bar{\eta}, \bar{\zeta})$ derived, are linearly related to the local Cartesian coordinates (x, y, z) in Eq. (23). They therefore define a skew Cartesian coordinate system, as shown in Fig. 2. The skew system of axes of which are seen determined by the three coefficient vectors e_1, e_2 and e_3. The volume of the parallelepiped spanned by these three vectors is the value of the Jacobian determinant at the origin $J_0 = [e_1\, e_2\, e_3]$, given in Eq. (19).

Equations (25) express the geodesic coordinates in terms of the natural coordinates ξ, η and ζ. They are therefore the expressions of the straight lines passing through the origin in the isoparametric coordinate system. The twelve parameters p_{ijk} in Eq. (25) can be taken as the distortion measures of the element. Geometrically, these twelve parameters can be explained simply as the ratios of the volumes of the parallelepipeds spanned by e_i, e_j and e_k to that spanned by e_1, e_2 and e_3.

In Eq. (14), in which x, y and z now denote local Cartesian coordinates, there are seven coefficient vectors e_i, $i = 1 \sim 7$. Since the p_{ijk}'s defined in Eq. (17) are completely antisymmetric in the subscripts, the number of the nontrivial p_{ijk}'s determined by these seven e_i vectors is

$$\binom{7}{3} = \frac{7!}{3!(7-3)!} = 35.$$

All the $7^3(=343)$ p_{ijk}'s can be written into a three dimensional array. The non-trivial ones of them can be collected and written into

$$\left[\begin{array}{ccccc|cccc|ccc|cc|c}
p_{123} & & & & & & & & & & & & & & \\
p_{124} & p_{134} & & & & p_{234} & & & & & & & & & \\
p_{125} & p_{135} & p_{145} & & & p_{235} & p_{245} & & & p_{345} & & & & & \\
p_{126} & p_{136} & p_{146} & p_{156} & & p_{236} & p_{246} & p_{256} & & p_{346} & p_{356} & & p_{456} & & \\
p_{127} & p_{137} & p_{147} & p_{157} & p_{167} & p_{237} & p_{247} & p_{257} & p_{267} & p_{347} & p_{357} & p_{367} & p_{457} & p_{467} & p_{567}
\end{array}\right] \tag{27}$$

in which $p_{123} = 1$. The twelve p_{ijk} parameters in Eq. (25) appear in the first, second and sixth columns in the above table.

In deriving the inverse relations of the mapping, all the non-trivial p_{ijk}'s may appear in the expressions of the values of the higher order Γ functions at the origin. All of them, besides p_{126}, p_{135}, p_{147}, p_{234}, p_{257} and p_{367}, also appear in the expression of the Jacobian determinant in equation (18). However, it can be readily shown that only the twelve p_{ijk} parameters that have been taken as the distortion measures are truly independent. By using the vector identity

$$[e_i e_j e_k][e_l e_m e_n] = [e_i e_j e_l][e_k e_m e_n] + [e_i e_j e_m][e_l e_k e_n] + [e_i e_j e_n][e_l e_m e_k], \tag{28}$$

one can easily derive the following relations.

$$\begin{aligned}
p_{345} &= p_{134}p_{235} - p_{135}p_{234} \\
p_{346} &= p_{134}p_{236} - p_{136}p_{234} \\
p_{356} &= p_{135}p_{236} - p_{136}p_{235} \\
p_{456} &= p_{124}p_{356} - p_{125}p_{346} - p_{126}p_{345} \\
&\;\;\vdots \\
&\text{etc.}
\end{aligned} \tag{29}$$

All the other p_{ijk}'s therefore can be expressed in terms of these twelve distortion parameters. They are therefore capable of completely describing the Jacobian determinant and the inverse relations of the mapping.

In Eq. (21), nine of the twelve distortion parameters have been shown to be the values of the Christoffel symbols at the origin. In tensor analysis (Bishop and Goldberg 1968), the Chrisoffel symbols completely describe the derivatives of the basis vectors b_j of their associated coordinate system.

$$\begin{aligned}
&\frac{\partial}{\partial \xi^k} b_j = \Gamma^i_{jk} b_i \\
&\frac{\partial}{\partial \xi^k} (\Gamma^i_{jk} b_j) = \left(\frac{\partial \Gamma^i_{jk}}{\partial \xi^l} + \Gamma^m_{jk} \Gamma^i_{ml} \right) b_i \\
&\;\;\vdots
\end{aligned} \tag{30}$$

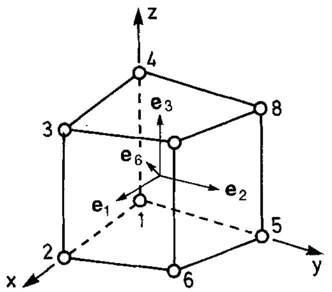
The twelve distortion parameters therefore reflect the rates, and higher-order rates, of changes of the basis vectors b_j of the isoparametric coordinate system at the origin. This interpretation of the distortion measures is the same as that in Yuan and Pian (1993) and in Yuan et al. (1993) for the two-dimensional isoparametric elements.

When the coefficient vectors e_4 to e_7 are zero, all the twelve distortion parameters p_{ijk} vanish. The element may then be regarded as undistorted. However, it can still be stretched and skewed into either a rectangular prism or a parallelepiped, as determined by the three vectors e_1, e_2 and e_3. Following the conventional usage of the term, one may therefore include also the aspect ratios and skew angles of the basic parallelepiped, determined by e_1, e_2 and e_3, as the additional distortion parameters of the element.

5
Examples

In the following, four example 8-node hexahedra are used to illustrate the method described. It should be mentioned that when the determinant of the Jacobian is positive everywhere within the element, the series in Eq. (9) give the exact inverse map throughout the element. The convergence of the series depends on the values of the twelve distortion parameters and the $\bar{\xi}^i$ values. Evidently, the convergence is faster for points closer to the origin.

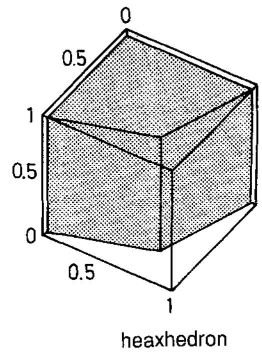
The terms in the series in Eq. (9) are seen grouped into homogeneous polynomials in $\bar{\xi}, \bar{\eta}$, and $\bar{\zeta}$ with increasing degrees. When Eq. (25) is substituted into Eq. (9), the first n groups of polynomials in ξ, η and ζ resulted will be summed to agree with ξ, η and ζ, respectively, to the n-th degree. Therefore, in order to illustrate the convergence of the series, one may plot the approximated shapes of the element resulted by keeping successively the first n groups of polynomials in that series. For $n = 0$, the result is the basic parallelepiped determined by the three coefficient vectors e_1, e_2 and e_3. In each of the examples, the approximations obtained by $n = 0$ to 3 are plotted and presented. The actual value of



$l_1: l_2: l_3 = 0.442: 0.442: 0.5$

$\theta_{12}: \theta_{23}: \theta_{31} = 106.39°: 90°: 90°$

i	0	1	2	3	4	5	6	7	8
x_i	—	0.0	1.0	1.0	0.0	0.0	0.75	0.75	0.0
y_i	—	0.0	0.0	0.0	0.0	1.0	0.75	0.75	1.0
z_i	—	0.0	0.0	1.0	1.0	0.0	0.0	1.0	1.0
a_i	0.4375	0.4375	-0.063	0.0	0.0	0.0	-0.063	0.0	—
b_i	0.4375	-0.063	0.4375	0.0	0.0	0.0	-0.063	0.0	—
c_i	0.5	0.0	0.0	0.5	0.0	0.0	0.0	0.0	—
p_{i23}	—	1.0	—	—	0.0	0.0	-0.167	0.0	—
p_{1i3}	—	—	1.0	—	0.0	0.0	-0.167	0.0	—
p_{12i}	—	—	—	1.0	0.0	0.0	0.0	0.0	—



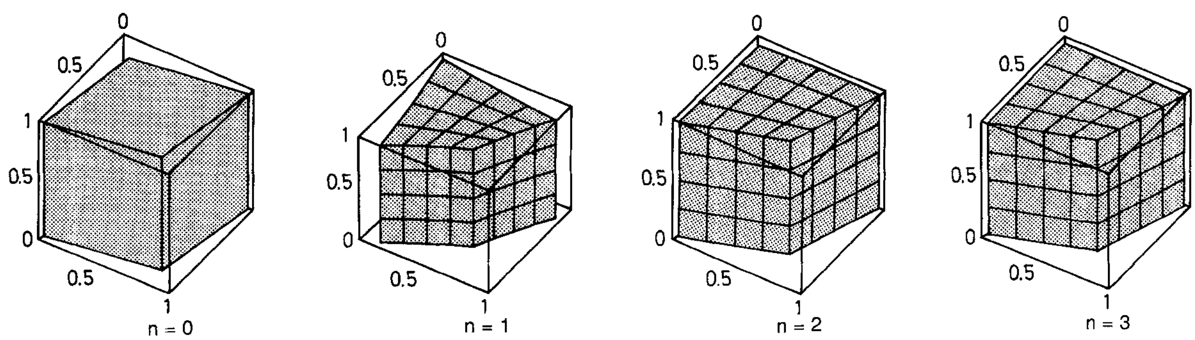


Fig. 3. Example number 1

n that should be used in truncating the series should be determined by the accuracy required. Usually, when the absolute values of the distortion parameters are not overly large, $n = 3$ to 4 will be sufficient.

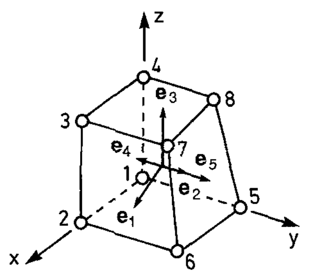
In this paper, the aspect ratios of the element are defined to be the ratios of the side lengths of the basic parallelepiped, i.e., the ratios of the vector lengths of e_1, e_2 and e_3. They are denoted by $l_1 : l_2 : l_3$ in the examples. The skew angles of the element are taken to be the three angles spanned respectively by e_1, and e_2, e_2 and e_3 and e_3 and e_1. They are denoted by θ_{12}, θ_{23}, and θ_{31}, respectively. When $l_1 : l_2 : l_3 =$ 1 : 1 : 1, the basic parallelepiped is unstretched. When $\theta_{12} = \theta_{23} = \theta_{31} = 90°$, the parellelepiped is unskewed.

In the first example, shown in Fig. 3, the hexahedron is distorted from a regular cube by moving nodes 6 and 7 in planes parallel to the x-y plane. The distortion is two-dimensional since the x- and y-coordinates of both the nodes are the same. A non-zero coefficient vector e_6 appears in this example and two distortion parameters, p_{623} and p_{123}, become non-vanishing. The plots of the approximated element shapes show that the 3-rd degree approximation of the series in Eq. (9) is very accurate.

In Fig. 4, a regular cube is again distorted by moving two nodes, 7 and 8, in planes parallel to the x-y coordinate plane. However, distortion produced is such that the nodes 5, 6, 7 and 8 no longer define a plane but a ruled surface. All the seven coefficient vectors become non-zero in this case but there are only four non-zero distortion parameters. The plots of the approximated shapes show that $n = 3$ is accurate enough for use in truncating the series.

The third hexahedron is a frustum of a pyramid, as shown in Fig. 5, which has two planes of symmetry. Two coefficient vectors, e_4 and e_5, become non-zero and there are two non-vanishing distortion parameters. The plots of the approximated element shapes again show that the 3-rd degree approximation is sufficiently accurate.

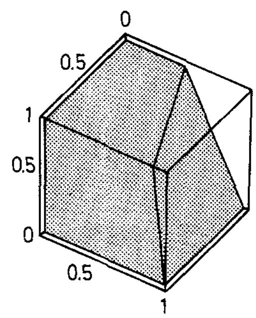
Figure 6 shows the last hexahedron, which is more severly distorted in a general way. All the seven coefficient vectors appear and all the twelve distortion parameters non-vanishing. From the plots



$l_1 : l_2 : l_3 = 0.5025 : 0.425 : 0.5056$

$\theta_{12} : \theta_{23} : \theta_{31} = 84.29° : 98.53° : 90.84°$

i	0	1	2	3	4	5	6	7	8
x_i	—	0.0	1.0	1.0	0.0	0.0	1.0	1.0	0.0
y_i	—	0.0	0.0	0.0	0.0	1.0	1.0	0.9	0.5
z_i	—	0.0	0.0	1.0	1.0	0.0	0.0	1.0	1.0
a_i	0.5	0.5	0.0	0.0	0.0	0.0	0.0	0.0	—
b_i	0.425	0.05	0.425	-0.075	-0.075	0.05	0.05	0.05	—
c_i	0.5	0.0	0.0	0.5	0.0	0.0	0.0	0.0	—
p_{i23}	—	1.0	—	—	0.0	0.0	0.0	0.0	—
p_{1i3}	—	—	1.0	—	-0.177	0.117	0.117	0.117	—
p_{12i}	—	—	—	1.0	0.0	0.0	0.0	0.0	—



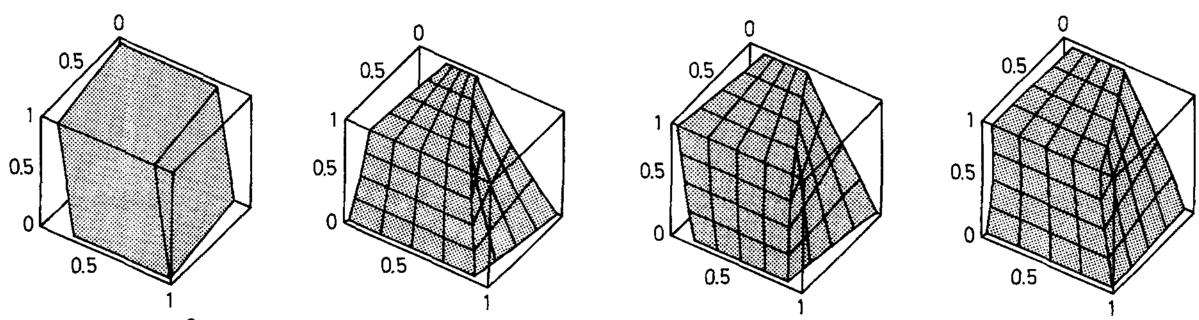
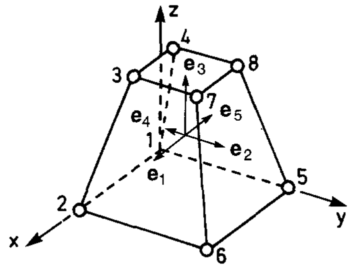
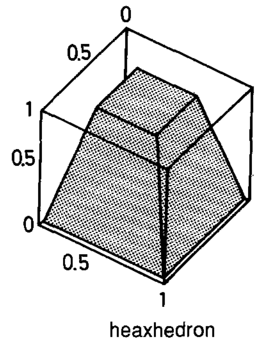


Fig. 4. Example number 2



$l_1 : l_2 : l_3 = 0.375 : 0.375 : 0.4677$
$\theta_{12} : \theta_{23} : \theta_{31} = 90° : 90° : 90°$

i	0	1	2	3	4	5	6	7	8
x_i	—	0.0	1.0	0.75	0.25	0.0	1.0	0.75	0.25
y_i	—	0.0	0.0	0.25	0.25	1.0	1.0	0.75	0.75
z_i	—	0.0	0.0	0.9354	0.9354	0.0	0.0	0.9354	0.9354
a_i	0.5	0.375	0.0	0.0	0.0	-0.125	0.0	0.0	—
b_i	0.5	0.0	0.375	0.0	-0.125	0.0	0.0	0.0	—
c_i	0.4677	0.0	0.0	0.4677	0.0	0.0	0.0	0.0	—
p_{i23}	—	1.0	—	—	0.0	-0.333	0.0	0.0	—
p_{1i3}	—	—	1.0	—	-0.333	0.0	0.0	0.0	—
p_{12i}	—	—	—	1.0	0.0	0.0	0.0	0.0	—



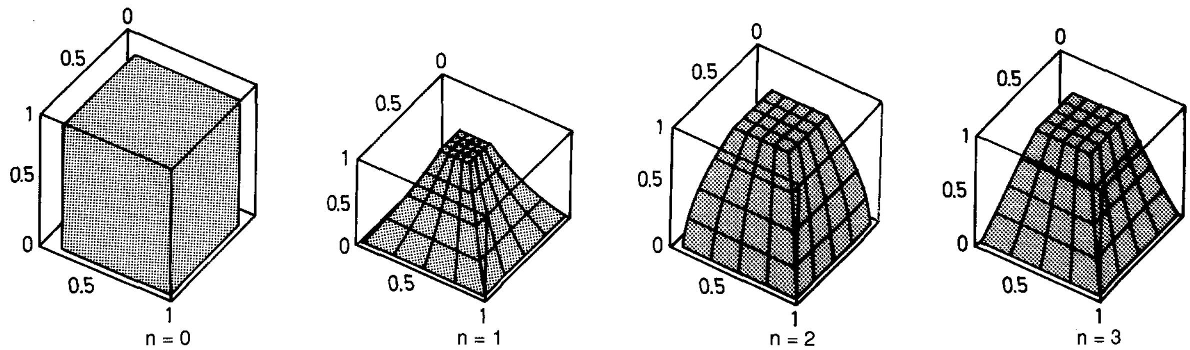


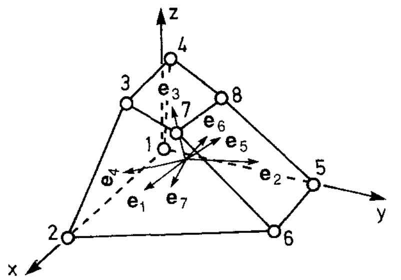
Fig. 5. Example number 3

of the approximated element shapes, it can be seen that the accuracy of the 3rd-degree approximation is less satisfactory. If higher precision is required in truncating the series, one may go to the 4th- or 5th-degree approximations by calculating the required values of the corresponding higher order Γ functions at the origin.

6
Concluding remarks

The usefulness and generality of the theory of geodesics in deriving the inverse mapping and the distrotion measures for the three dimensional isoparametric elements have been demonstrated by using the 8-node hexahedra. Compared to the iterative numerical methods that currently used for inverse mapping, the present method reveals more the structure of the mathematics of the isoparametric system. Such informations can be useful for the development of efficient hybrid/mixed finite element. In Yuan and Pian (1993), it has been demonstrated that use of the geodesic coordinate system for assumed stresses can lead to the development of robust quadrilateral hybrid stress element which is invariant, free of locking, and insensitive to geometric distortion.

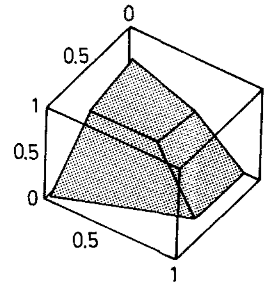
As to the 8-node hexahedra element, it is noted that the uniqueness and invertibility of the isoparametric map is guaranteed by the positivity of the Jacobian determinant everywhere within the element. For the quadrilateral element in two dimensions, the positivity of the Jacobians at four corner nodes is sufficient to guarantee this condition. For the hexahedral element in three dimensions, Knupp (1990) has shown that it is not sufficient by checking only the Jacobians at the eight corner nodes, nor is it sufficient by checking only the Jacobian on the twelve edges. Since the invertibility of the map implies the convergence of the series in Eq. (9), this problem can also be investigated by considering the maximum allowable values of the twelve distortion parameters which guarantee the convergence of the series. For



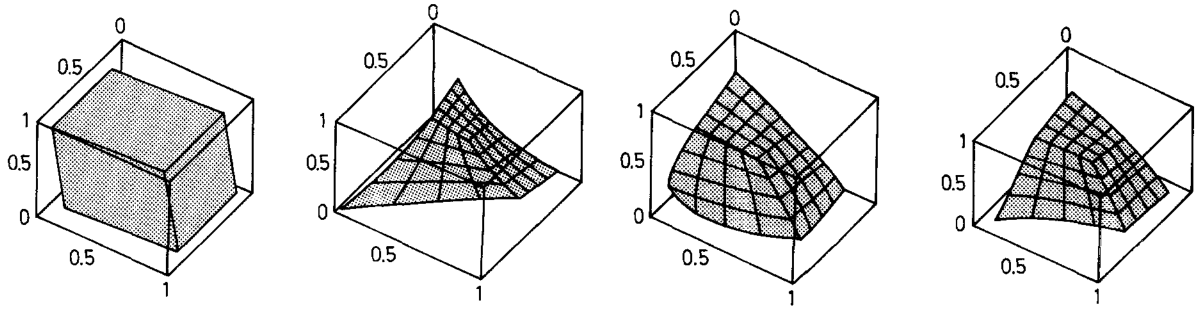
$l_1 : l_2 : l_3 = 0.3991 : 0.4384 : 0.0608$

$\theta_{12} : \theta_{23} : \theta_{31} = 90.79° : 127.77° : 54.07°$

i	0	1	2	3	4	5	6	7	8
x_i	—	0.0	1.1	0.95	0.15	0.	0.85	0.78	0.35
y_i	—	0.0	0.0	0.25	0.12	1.08	1.18	0.77	0.84
z_i	—	0.0	0.0	0.85	0.75	0.0	0.18	0.68	0.73
a_i	0.5225	0.3975	-0.028	0.035	0.035	-0.09	-0.078	-0.015	—
b_i	0.53	0.02	0.4375	-0.035	-0.128	-0.005	-0.013	-0.038	—
c_i	0.399	0.029	-0.001	0.0354	-0.046	-0.016	0.0038	-0.041	—
p_{i23}	—	1.0	—	—	0.0791	-0.0224	-0.199	-0.034	—
p_{1i3}	—	—	1.0	—	-0.306	-0.003	-0.017	-0.093	—
p_{12i}	—	—	—	1.0	-0.138	-0.028	0.0267	-0.114	—



heaxhedron



n = 0 n = 1 n = 2 n = 3

Fig. 6. Example number 4

the series to be convergent everywhere within the element, it is obviously necessary that the absolute values of all p_{ijk}'s be less than one. However, this is not likely to be also a sufficient condition. Further studies can be conducted in this direction to define the maximum degree of geometric distortion that ensures the invertibility of the mapping.

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