

Remarks on the Geometric Properties of Trivariate Maps

VASILIS ZAFIRIS

University of Houston-Downtown
Computer & Mathematical Sciences
Houston, TX 77002, USA
zafirisyv@uhd.edu

Abstract: Trivariate polynomial maps are often used to model volumetric objects in three-space. It is necessary, therefore, to efficiently compute points, vectors, and other geometric properties of such objects. These properties are formulated in terms of the metric and the curvature tensors associated with the map. The simplest trivariate map is the trilinear. This map and its Jacobian are represented in tensor product Bézier form and a pyramid algorithm is utilized to compute points and vectors associated with the map. In addition, sufficient conditions for the positivity of the Jacobian are given and an algorithm for solving the inversion problem is derived.

Key-Words: trivariate map, metric, curvature, Jacobian, Bézier form, pyramid algorithm, inversion

1 Introduction

While in the past, there has been considerable research on the development of techniques for visualizing volume data, more recently, there has been an increasing interest in modeling volume data and trivariate objects, see e.g., [18]. And even though several Computer Aided Geometric Design (CAGD) text and reference books, see e.g. [3, 5, 11, 17, 21] introduce trivariate and multivariate constructs, CAGD has been mostly concerned with univariate and bivariate objects, see e.g., [1, 2, 7, 8, 9, 19, 20]. The CAGD field has positively impacted almost every industry around us, and a historical account of the major developments in CAGD can be found in [8].

On the other hand, the need to optimally design and efficiently represent surface and volume model prototypes that are necessary for the prep and post-processing phases of numerical simulations of complex systems and physical phenomena had a tremendous impact in advancing CAGD. More often than not, this involves the numerical solution of systems of partial differential equations utilizing finite difference, finite element or finite volume methods over realistic three-dimensional geometries. Inherent to any of these solution methods is, in addition to the discrete representation of the differential and/or integral operators in the equations, the discrete representation of the solution domain. This discrete domain over which the discrete equations are solved is called a *grid* or a *mesh*. Bivariate two-dimensional grid cells are usually triangles, quadrilaterals, or the increasingly popular multi-sided Voronoi shapes. The trivariate extensions of these shapes in three-dimensions are tetrahedra, pentahedra, and hexahedra.

Even though structured hexahedral grids are not as flexible to represent complex geometries compared to tetrahedral grids and it is difficult to apply adaptive local grid refinement procedures on them, they are the preferred grid structures for many computational applications. In this work we focus on hexahedral grid cells that are images of tensor product trivariate maps defined on unit cubes.

For a given number of vertices, hexahedral grids provide better approximation properties than corresponding tetrahedral grids. Given n vertices, Edelsbrunner [6] notes that, the number of tetrahedra in a tetrahedral grid is of order n^2 , whereas the number of hexahedra in a hexahedral grid is of order n . For hexahedral elements in three dimensions, Knupp [13] has discussed the invertibility of the isoparametric mapping. Yuan et al. [23] suggested an analytic way of deriving the mapping relations and distortion measures for hexahedral isoparametric elements utilizing the theory of geodesics. Ushakova [22] and Knabner et al. [12] have addressed the non-degeneracy of hexahedral grid cells in terms of the Jacobian of the trilinear map, and Knupp [14] utilized the Jacobian matrix norm as a quality metric for hexahedral cells.

The rest of the paper is organized as follows. In section 2, the reference map is specified and a pyramid algorithm is utilized to efficiently evaluate the map and the derivatives of the map. Also, an iterative solution to the map inversion problem is derived. *We should note that the non-local inversion of the trilinear map, is an open problem in scientific computing.* Having the elements of the tangent plane available, in section 3, we begin with the the Jacobian of the map and represent it in Bézier form. From the well-

known properties of Bézier objects a sufficient condition for positive Jacobian is derived. Clearly, this condition provides sufficient conditions for the local invertability of the trilinear map. Then utilizing the metric and curvature tensors we present additional geometric properties associated with trivariate maps and hexahedral grid cells. In section 4, conclusions and outlook are given.

2 Parametric Polynomial Volumes

In terms of parametric mappings, each three-dimensional hexahedron in an n -dimensional affine space, with $n \geq 3$, can be described as the image or trace $P(\Xi^3)$ of a mapping $P : \Xi^3 \rightarrow \Omega^n$, where Ξ^3 is called the *parameter space* and Ω^n the *object space*. The representation of the map can be specified by first choosing an affine frame for the parametric space Ξ^3 , denoted as $(\xi_0, \{\alpha_1, \alpha_2, \alpha_3\})$, and similarly, an affine frame $(\omega_0, \{\beta_1, \dots, \beta_n\})$ for the object space Ω^n . A three-dimensional *parametric polynomial volume* of tri-degree (d^1, d^2, d^3) can be represented by a mapping

$$\xi = \xi_0 + \sum_{i=1}^3 \xi^i \alpha_i \in \Xi^3 \xrightarrow{P} P(\xi) = \omega_0 + \sum_{k=1}^n P^k \beta_k \in \Omega^n$$

where each coordinate function $P^k = P^k(\xi^1, \xi^2, \xi^3)$ is a real-valued polynomial, and the degree of each $\xi^i \in \mathbb{R}$ in all P^k is at most $d^i \in \mathbb{Z}_+$.

Parametric polynomial volumes are extensions of parametric polynomial curves and surfaces and trivariate instances of multivariate constructs as discussed in [5, 11, 21]. Alternatively, constructions of m -dimensional parametric curvilinear volumes imbedded in n -dimensional spaces, with $m \leq n$, utilizing smooth mappings

$$P : (\Xi^m, g^\Xi) \longrightarrow (\Omega^n, g^\Omega),$$

where (Ξ^m, g^Ξ) and (Ω^n, g^Ω) are Riemannian manifolds with covariant metric tensors g^Ξ and g^Ω , are discussed in [10, 15, 16, 24]. Essentially, the mapping P is assumed to be an imbedding. That is, the mapping has constant rank, i.e., the Jacobian matrix of P at any point ξ is $m = \text{rank } P = \dim \Xi^m$, it is injective, and a homeomorphism onto its image $P(\Xi^m)$, with its topology as a subspace of Ω^n . Such constructions are necessarily local. The coordinates (ξ^1, \dots, ξ^m) of any point on the imbedded submanifold $P(\Xi^m) \subset \Omega^n$ are called *curvilinear coordinates*.

2.1 The Trilinear Map

Consider the simplest form of the trivariate map in the Euclidean three-space \mathbb{R}^3 . Setting $d^1 = d^2 = d^3 = 1$,

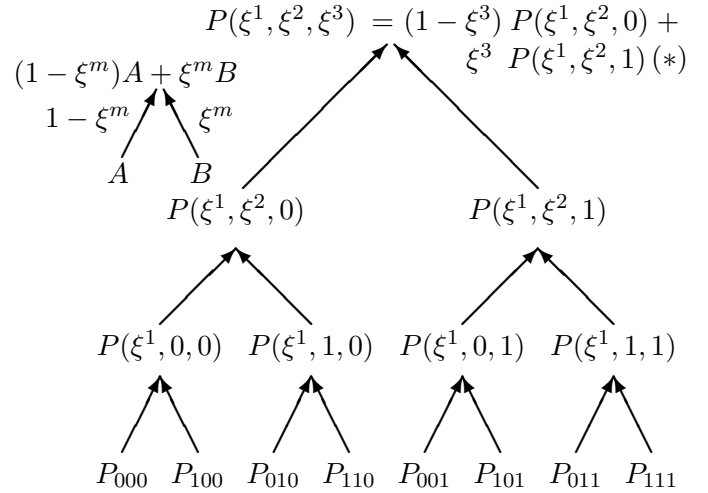


Figure 1: Pyramid algorithm for computing the point P and the vectors $\partial_3 P$, $\partial_{23} P$, and $\partial_{123} P$ at (ξ^1, ξ^2, ξ^3) .

the trilinear map from the unit-cube $[0, 1]^3 \equiv \Xi^3$ onto $\Omega^3 \subset \mathbb{R}^3$ is written

$$\begin{aligned} P(\xi) &= (P^1(\xi), P^2(\xi), P^3(\xi)) \\ &= \sum_{i,j,k=0}^1 P_{ijk} B_i^1(\xi^1) B_j^1(\xi^2) B_k^1(\xi^3), \end{aligned}$$

where the vertices of the hexahedron $P_{ijk} \in \Omega^3$ are the Bézier control points, and $B_0^1(\xi^m) = 1 - \xi^m$, $B_1^1(\xi^m) = \xi^m$, $m = 1, 2, 3$, are the linear Bernstein polynomials. The control points P_{ijk} , $\{i, j, k\} \in \{0, 1\}$ are connected if and only if any two out of the three subscripts are the same.

The partial derivatives of the map are the covariant basis vectors tangent to coordinate lines. Clearly, since the map P is linear in each i -direction, $i = 1, 2, 3$, the tangent vector $\partial_i P(\xi)$ at any point $P(\xi)$ on the hexahedron is obtained by bilinear interpolation of the four edge vectors. We can utilize a pyramid construct [9] to efficiently represent not only point evaluation, but also evaluation of derivatives of the map, see Fig. 1. Given the control points P_{ijk} , $\{i, j, k\} \in \{0, 1\}$ and $\xi = (\xi^1, \xi^2, \xi^3) \in [0, 1]^3$ we first interpolate, as is shown in the key, along the four edges in the ξ^1 direction, then in the ξ^2 and finally, in the ξ^3 direction to obtain the point $P(\xi) = P(\xi^1, \xi^2, \xi^3)$ on the hexahedron. Also, the derivatives of the map can simply be obtained by differencing:

$$\begin{aligned} \partial_3 P(\xi) &= P(\xi^1, \xi^2, 1) - P(\xi^1, \xi^2, 0), \\ \partial_{23} P(\xi) &= \{P(\xi^1, 1, 1) - P(\xi^1, 0, 1)\} - \\ &\quad \{P(\xi^1, 1, 0) - P(\xi^1, 0, 0)\}, \\ \partial_{123} P(\xi) &= \{\Delta_{11}^1 - \Delta_{01}^1\} - \{\Delta_{10}^1 - \Delta_{00}^1\}, \end{aligned}$$

where $\Delta_{ab}^1 = P_{1ab} - P_{0ab}$. The remaining partials, $\partial_1 P$, $\partial_2 P$, $\partial_{12} P$, etc., can be computed similarly.

2.1.1 Inversion of the Trilinear Map

Here we give an iterative solution to the inversion problem:

$$\begin{array}{ll} \text{GIVEN} & P(\xi) \in \Omega^3 \subset \mathbb{R}^3 \\ \text{FIND} & \xi = (\xi^1, \xi^2, \xi^3) \in \Xi^3 \equiv [0, 1]^3 \end{array}$$

without the need of computing the Jacobian of the map. Solving for ξ^3 , from

$$P(\xi^1, \xi^2, \xi^3) = (1 - \xi^3) P(\xi^1, \xi^2, 0) + \xi^3 P(\xi^1, \xi^2, 1),$$

see (*) in Fig. 1, we get

$$\xi^3 = \Delta^3 \cdot \partial_3 P(\xi) / \|\partial_3 P(\xi)\|^2, \quad (1)$$

where $\Delta^3 = P(\xi^1, \xi^2, \xi^3) - P(\xi^1, \xi^2, 0)$, and $\|u\| = \sqrt{u \cdot u}$ is the Euclidean norm of $u \in \mathbb{R}^3$ associated with the Euclidean inner product on \mathbb{R}^3 . Similarly, for ξ^1 and ξ^2 , we write

$$\xi^m = \Delta^m \cdot \partial_m P(\xi) / \|\partial_m P(\xi)\|^2, \quad (2)$$

where $m = 1, 2$ and

$$\begin{aligned} \partial_1 P(\xi) &= P(1, \xi^2, \xi^3) - P(0, \xi^2, \xi^3), \\ \partial_2 P(\xi) &= P(\xi^1, 1, \xi^3) - P(\xi^1, 0, \xi^3), \\ \Delta^1 &= P(\xi^1, \xi^2, \xi^3) - P(0, \xi^2, \xi^3), \\ \Delta^2 &= P(\xi^1, \xi^2, \xi^3) - P(\xi^1, 0, \xi^3). \end{aligned}$$

Once again, *the algebraic inversion of the trilinear map is open problem in scientific computing.*

3 Geometric Properties of the Map

First and second order geometric properties of the map can be formulated in terms of the first and second fundamental forms. The first fundamental form, $g_{ij} d\xi^i d\xi^j$, describes the intrinsic geometry of the map, while the second fundamental form $h_{ij} d\xi^i d\xi^j$, describes the extrinsic geometry. The coefficients of both forms are specified by the inner products:

$$\begin{aligned} g_{ij}(\xi) &= \partial_i P(\xi) \cdot \partial_j P(\xi) \quad \text{and} \\ h_{ij}(\xi) &= \partial_{ij} P(\xi) \cdot n(\xi), \quad i, j = 1, 2, 3, \end{aligned}$$

where $n(\xi)$ is the unit normal to the tangent plane at the point $P(\xi) \in \Omega^3$.

3.1 First Order Properties

First order geometric properties are formulated in terms of the components of the covariant metric tensor associated with the map and can be used to measure angles and lengths of the covariant vectors on the tangent plane. Evidently, the Jacobian of the map is the most important geometric property since a change of the Jacobian sing at a point ξ corresponds to a singular map and a grid cell with zero volume at that point.

3.1.1 Jacobian of the Trilinear Map

At any ξ in $[0, 1]^3$, the Jacobian matrix of the map is the 3×3 matrix of the partial derivatives

$$JP(\xi) = [\partial_j P^i]_{i,j=1,2,3} = \left[\frac{\partial P^i}{\partial \xi^j} \right]_{i,j=1,2,3} \quad (3)$$

and the determinant of this matrix, denoted by J , is the Jacobian of the map

$$\begin{aligned} J(\xi) &= \partial_1 P(\xi) \cdot (\partial_2 P(\xi) \times \partial_3 P(\xi)) \\ &= \det [JP(\xi)] = \begin{vmatrix} \partial_1 P^1 & \partial_2 P^1 & \partial_3 P^1 \\ \partial_1 P^2 & \partial_2 P^2 & \partial_3 P^2 \\ \partial_1 P^3 & \partial_2 P^3 & \partial_3 P^3 \end{vmatrix}, \end{aligned}$$

where $P^i \equiv P^i(\xi)$, $i = 1, 2, 3$, are the coordinate functions of P , that is $P(\xi) = (P^1(\xi), P^2(\xi), P^3(\xi))$. Since the polynomial map $P : \Xi^3 \rightarrow \Omega^3$ is continuously differentiable, its derivative at ξ , $DP(\xi)$, is given by the Jacobian matrix at ξ : $DP(\xi) = JP(\xi)$.

In the practice of finite element methods, we transfer the domain of mappings, derivatives, and integrals in the approximate variational formulation of the problem *from* each grid cell in the object or physical domain *to* the parametric reference domain. This is an essential step for the efficient implementation of finite element methods, especially, in multi-dimensional problems and in higher-order finite element methods. For example, a scalar function $F_{\Omega^3} : \Omega^3 \subset \mathbb{R}^3 \rightarrow \mathbb{R}$ on a grid cell, is transferred to the reference domain Ξ^3 by composing F_{Ω^3} with the geometric mapping $P : \Xi^3 \subset \mathbb{R}^3 \rightarrow \Omega^3$. The transformed function is then written as $F_{\Xi^3} = F_{\Omega^3} \circ P : \Xi^3 \rightarrow \mathbb{R}$.

However, transformations of differential operators, such as gradient, divergence, curl, and others, may not only involve the derivative and the Jacobian of the mapping P , but also, of its inverse P^{-1} , as appropriate [4]. Clearly, the invertibility of P and the invertibility of the derivative of the map, $DP = JP$, are connected. In the first place, if the Jacobian $J(\xi) \neq 0$, then P^{-1} exists and is smooth in some neighborhood of $P(\xi)$. The derivative of P^{-1} at $P(\xi)$, $DP^{-1}(P(\xi))$, is the inverse of the derivative of P at ξ : $DP^{-1}(P(\xi)) = (DP(\xi))^{-1}$. Moreover, if $J(\xi) = 0$, then P does not have a differentiable inverse P^{-1} in some neighborhood of $P(\xi)$, even though a non-differentiable inverse P^{-1} may still exist. Finally, if P is bijective on Ξ^3 , then P^{-1} exists on $\Omega^3 = P(\Xi^3)$ and therefore, for every $\omega \in \Omega^3$, there exists a unique $\xi \in \Xi^3$, such that $P(\xi) = \omega$.

In practice, since it is hard to find such an inverse map P^{-1} defined everywhere in Ω^3 , we often perform local inversion numerically using Newton's method. But even local inversion requires the Jacobian of the

map to be non-singular near the root not for Newton's method to converge. As far as we know, *the inversion of the tri-linear map has been an outstanding open problem in scientific computing.*

3.1.2 Sufficient Conditions for the local inversion of the Trilinear Map

Since the Jacobian is a real-valued function on the unit-cube $\xi = (\xi^1, \xi^2, \xi^3) \in [0, 1]^3 \mapsto J(\xi) \in \mathbb{R}$, and the partials $\partial_{\xi^i} P$ are linear in ξ^j and ξ^k , where $\{i, j, k\}$ is a cyclic permutation of $\{1, 2, 3\}$, the Jacobian is at most quadratic in each ξ^i , and can therefore be written as

$$J(\xi) = \sum_{i,j,k=0}^2 C_{ijk} (\xi^1)^i (\xi^2)^j (\xi^3)^k, \quad (4)$$

where $C_{ijk} \in \mathbb{R}$. The coefficients C_{ijk} , $i, j, k = 0, 1, 2$, can be expressed in terms of the partial derivatives of the Jacobian at $\xi = 0$:

$$C_{ijk} = \frac{1}{i! j! k!} \partial_{\xi^1}^i \partial_{\xi^2}^j \partial_{\xi^3}^k J(\xi) \quad (5)$$

where $\partial_{\xi^m}^n$ denotes the n -th partial with respect to ξ^m for $m = 1, 2, 3$. Next, in terms of the quadratic Bernstein polynomials the Jacobian is written as

$$J(\xi) = \sum_{i,j,k=0}^2 C_{ijk}^B B_i^2(\xi^1) B_j^2(\xi^2) B_k^2(\xi^3), \quad (6)$$

where $B_s^r(u) = \binom{r}{s} (1-u)^{r-s} u^s$, $\binom{r}{s} = \frac{r!}{s!(r-s)!}$, are the Bernstein polynomials of degree r , and $s = 0, 1, \dots, r$. Note also from either(4) or (6), $J(\xi) = 0$ represents *an implicit surface*, a quadric, in \mathbb{R}^3 . The coefficients $C_{ijk}^B \in \mathbb{R}$ can be expressed, see e.g., [19], in terms of the coefficients $C_{lmn} \in \mathbb{R}$ as

$$C_{ijk}^B = \sum_{l=0}^i \sum_{m=0}^j \sum_{n=0}^k \frac{\binom{i}{l} \binom{j}{m} \binom{k}{n}}{\binom{i}{l} \binom{j}{m} \binom{k}{n}} C_{lmn},$$

where the coefficients C_{lmn} are obtained from (5) in terms of the hexahedral vertices $P_{ijk} \in \Omega^3$, $\{i, j, k\} \in \{0, 1\}$.

The representation of the Jacobian in parametric tensor product Bézier form induces the well-known geometric properties of the Bézier objects. This form of the Jacobian and the associated Bézier control polygon can be obtained using the linear precision and the partition of unity properties of the Bernstein basis functions. From the linear precision property, any parameter $\xi^i \in [0, 1]$, can be expressed as

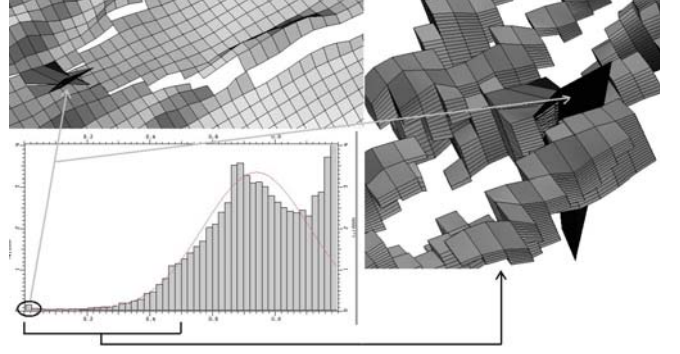


Figure 2: Measuring the Jacobian

$\xi^i = \sum_{m=0}^2 \frac{m}{2} B_m^2(\xi^i)$ where the $\frac{m}{2}$ coefficients are uniformly spaced on $[0, 1]$. Using the partition of unity of the Bernstein basis, $\sum_{m=0}^2 B_m^2(\xi^i) = 1$, we can therefore write

$$\begin{aligned} \xi^i &= \sum_{m=0}^2 \frac{m}{2} B_m^2(\xi^i) \\ &= \sum_{k,l,m=0}^2 \frac{m}{2} B_k^2(\xi^1) B_l^2(\xi^2) B_m^2(\xi^i). \end{aligned}$$

The Jacobian in *parametric tensor product Bézier form* can now be written as:

$$\begin{aligned} J^B(\xi) &= (\xi, J(\xi)) = (\xi^1, \xi^2, \xi^3, J(\xi)) \\ &= \sum_{i,j,k=0}^2 J_{ijk} B_i^2(\xi^1) B_j^2(\xi^2) B_k^2(\xi^3) \end{aligned}$$

where $J_{ijk} = (\frac{i}{2}, \frac{j}{2}, \frac{k}{2}, C_{ijk}^B) \in \mathbb{R}^4$ are the *Bézier points* forming the *Bézier control polygon* in \mathbb{R}^4 . The numbers $C_{ijk}^B \in \mathbb{R}$ are referred to as the *Bézier ordinates* of $J(\xi)$, and $(\frac{i}{2}, \frac{j}{2}, \frac{k}{2}) \in [0, 1]^3$ as the *Bézier abscissae*, see e.g., [11]. The geometric object generated by the points $(\xi, J(\xi))$, $\xi \in [0, 1]^3$, is a *hyper-surface* in \mathbb{R}^4 . We now give *sufficient conditions* for the Jacobian positivity and, as a result, for the local inversion of the trilinear map.

Lemma 3.1 *If $C_{ijk}^B > 0$ for all $i, j, k = 0, 1, 2$, then the Jacobian*

$$J(\xi) \geq C_{MIN} = \min \{C_{ijk}^B\} \quad \text{for all } \xi \in [0, 1]^3,$$

and the trilinear map, P , is locally invertible with a differentiable inverse, P^{-1} , in a neighborhood of $P(\xi) \in \Omega^3 \subset \mathbb{R}^3$.

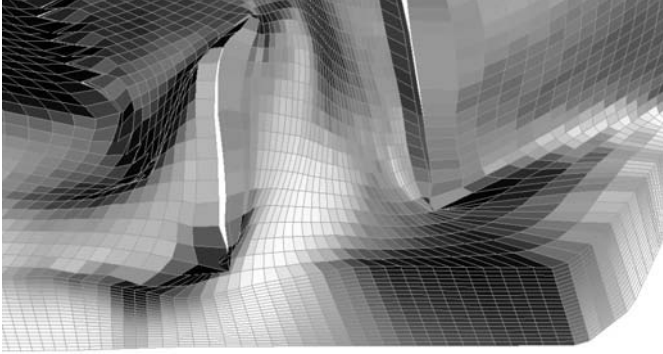


Figure 3: Measuring Orthogonality

3.1.3 The Metric Tensor and Orthogonality

For any point $\xi \in \Xi^3$, the covariant metric tensor, is given by

$$G(\xi) = [g_{ij}(\xi)]_{i,j=1,2,3} = (JP(\xi))^\top JP(\xi),$$

and the determinant of G is

$$\begin{aligned} g(\xi) = \det [g_{ij}(\xi)] &= \det ((JP(\xi))^\top JP(\xi)) \\ &= \det (JP(\xi))^\top \det (JP(\xi)) \\ &= J^2(\xi) \geq 0. \end{aligned} \quad (7)$$

If θ_{ij} denotes the angle between the covariant tangent vectors $\partial_i P(\xi)$ and $\partial_j P(\xi)$, the elements of the metric tensor are

$$\begin{aligned} g_{ij} &= \partial_i P \cdot \partial_j P \\ &= \|\partial_i P\| \|\partial_j P\| \cos \theta_{ij} \\ &= \sqrt{g_{ii}} \sqrt{g_{jj}} \cos \theta_{ij}. \end{aligned} \quad (8)$$

Clearly, the metric tensor is a symmetric second order covariant tensor and it is a diagonal tensor at any point were the tangent vectors are orthogonal. Therefore, $g/(g_{11}g_{22}g_{33}) = 1$ if and only if the tangent vectors are orthogonal.

Also note that, if the Jacobian matrix, JP , is invertible, the metric tensor, G , is positive definite since the quadratic form

$$\begin{aligned} v^\top G v &= v^\top (JP)^\top (JP) v \\ &= ((JP)v)^\top ((JP)v) \\ &= \|(JP)v\|^2 > 0 \end{aligned}$$

for any non-zero vector $v = (v_1, v_2, v_3) \in \mathbb{R}^3$.

3.2 Second-Order Metrics

Second-order quality metrics intend to quantify the grid cell deformation by computing the curvatures of

the cell faces. The curvatures can be computed using the components of the second order covariant tensor

$$h_{ij}(\xi) = \partial_{ij} P(\xi) \cdot n(\xi), \quad i, j = 1, 2, 3,$$

classically known as the coefficients of the second fundamental form. Let us fix one parameter of the map, $\xi^3 = \xi_0$, and compute the curvatures on that face. Then for $\xi = (\xi^1, \xi^2, \xi_0)$, we have $P(\xi) = (P^1(\xi), P^2(\xi), P^3(\xi))$, the normal to the face is

$$n(\xi) = \frac{\partial_1 P \times \partial_2 P}{\|\partial_1 P \times \partial_2 P\|}.$$

The three components of the normal n are

$$n_k = \frac{1}{\sqrt{g}} \left[\partial_1 P^{k+1} \partial_2 P^{k+2} - \partial_1 P^{k+2} \partial_2 P^{k+1} \right],$$

where $k = 1, 2, 3, k + 3 \mapsto k$, and

$$g = (\partial_1 P \times \partial_2 P)^2 = g_{11}g_{22} - g_{12}^2$$

is the determinant of the metric tensor on the face $\xi^3 = \xi_0$. For the trilinear map, the coefficients of the second fundamental form, $h_{ij} = \partial_{ij} P \cdot n$, for $i, j = 1, 2$, simplify to

$$h_{11} = h_{22} = 0, \quad \text{and} \quad h_{12} = \sum_{k=1}^3 \partial_{12} P^k n_k.$$

As a result, the mean curvature, H , and the Gaussian curvature, K , take a simple form:

$$H = \frac{1}{2g} (g_{22}h_{11} - 2g_{12}h_{12} + g_{11}h_{22}) = -\frac{1}{g} g_{12}h_{12},$$

$$K = \frac{1}{g} (h_{11}h_{22} - h_{12}^2) = -\frac{1}{g} h_{12}^2.$$

Thus on the faces of the trilinear hexahedral there are only hyperbolic points, ($K < 0$), or planar points, ($K = 0$). Curve and surface curvatures are frequently used in CAGD for the detection of local imperfections of geometric objects using curvature plots.

4 Conclusions and Outlook

From the metric and curvature tensors of the trilinear map important geometric properties such as, the Jacobian, the angle of covariant tangent vectors, the Gaussian and mean curvatures are derived. Trilinear maps can only generate hexahedral cells having hyperbolic or parabolic faces. In field simulations, computations must be performed on grids cells of positive volume, i.e., all grid cells must have positive Jacobian. Also,

for structured grids, a high degree of orthogonality especially on the field boundary is critical for computational accuracy. Examples of geologic grid models are shown on which the Jacobian and the orthogonality of grid cells are measured. In addition, a sufficient condition for positive lower-bound on the Jacobian is given, and an iterative approach to the inversion problem is derived. Higher order trivariate polynomial maps provide much richer geometric structures for applications and certainly more challenges in their analysis. Third order geometric properties measuring torsion and third order invariants associated with trivariate maps should provide further insight into the geometry of these constructs.

Acknowledgments:

I would like to thank Landmark Graphics Co., Houston, TX., for providing financial support for this work. Also, would like to thank the reviewers for their constructive suggestions in improving this paper.

References:

- [1] Bartels, R. H., J. C. Beatty, and B. A. Barsky, *An Introduction to Splines for Use in Computer Graphics and Geometric Modeling*, Morgan Kaufmann Publishers, San Francisco, CA, 1987.
- [2] Boor de, C., *A Practical guide to Splines*, Springer-Verlag, New York, NY, 1978. Revised Edition, 2001.
- [3] Boor de, C., K. Höllig, and S. Riemenschneider, *Box Splines*, Springer-Verlag, New York, NY, 1993.
- [4] Ciarlet, P. G., *The Finite Element Method for Elliptic Problems*, Classics in Applied Mathematics, SIAM, Philadelphia, PA, 2002.
- [5] Cohen, E., R.F. Riesenfeld, and G. Elber, *Geometric Modeling with Splines: An Introduction*, A K Peters, Ltd., Natick, MA, 2001.
- [6] Edelsbrunner, H., *Geometry and Topology for Mesh Generation*, Cambridge University Press, Cambridge, UK, 2001.
- [7] Farin, G., *Curves and Surfaces for CAGD a Practical Guide*, Fifth Edition, Morgan Kaufmann Publishers, San Francisco, CA, 2002.
- [8] Farin, G., J. Hoschek, and M-S. Kim, Editors, *Handbook of Computer Aided Geometric Design*, Elsevier Science, Boston, MA, 2002.
- [9] Goldman, R. N., *Pyramid Algorithms*, Morgan Kaufmann Publishers, San Francisco, CA, 2003.
- [10] Hansen, G. A., R. W. Douglas, and A. Zardecki, *Mesh Enhancement*, Imperial College Press, London, UK, 2005.
- [11] Hoschek, J., and D. Lasser, *Fundamentals of Computer Aided Geometric Design*, A K Peters, Ltd., Wellesley, MA, 1993.
- [12] Knabner, P., S. Korotov, and G. Summ, Conditions for the Invertibility of the Isoparametric Mapping for Hexahedral Finite Elements, *Finite Elements in Analysis and Design*, **40** (2003), 159–172.
- [13] Knupp, P. M., On the invertibility of the isoparametric map, *Comp. Meth. Appl. Mech & Engr.*, **78** (1990), 313–329.
- [14] Knupp, P. M., Achieving finite element mesh quality via optimization of the Jacobian matrix norm and associated quantities. Part II: a framework for volume mesh optimization, *IJNME* **48** (2000), 1165–1185.
- [15] Liseikin, V. D., *Grid Generation Methods*, Springer-Verlag, New York, NY, 1999.
- [16] Liseikin, V. D., *A Computational Differential Geometry Approach to Grid Generation*, Springer-Verlag, New York, NY, 2004.
- [17] Mortenson, M. E., *Geometric Modeling*, Second Edition, Wiley, New York, NY, 1997.
- [18] Nielson, G. M., Volume Modelling, in *Volume Graphics*, M. Chen et al. (eds.), Springer, 2000, 29–48.
- [19] Patrikalakis, N. M., and T. Maekawa, *Shape Interrogation for Computer Aided Design and Manufacturing*, Springer-Verlag, New York, NY, 2002.
- [20] Piegel L., and W. Tiller, *The NURBS Book*, Springer-Verlag, New York, NY, 1995.
- [21] Prautzsch, H., W. Boehm, and M. Paluszny, *Bézier and B-Spline Techniques*, Springer-Verlag, New York, NY, 2002.
- [22] Ushakova, O. V., Conditions of non degeneracy of three-dimensional cells. A formula of a volume of cells, *SIAM J. Sci. Comput.*, **23** (2001), 1274–1290.
- [23] Yuan, K. Y., Y. S. Huang, H. T. Yang and T. H. H. Pian, The inverse mapping and distortion measures for 8-node hexahedral isoparametric elements, *Computational Mechanics*, **14** (1994), 189–199.
- [24] Zafiris, V. G., *Constructs on Manifolds Applied to Grid Generation*, Ph.D. Dissertation, University of Houston, Houston, TX, 1996.