Nondegeneracy Criteria for 3-D Grid Cells. Formulas for a Cell Volume. [1]

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Abstract

Nondegeneracy criteria for three-dimensional grid cells are found for hexahedral cells which are given by eight corner points and generated by the trilinear map from a unit cube to a region defined by these points. The criteria include both nondegeneracy conditions and a special numerical algorithm for testing the Jacobian of a trilinear map on its positivity when sufficient nondegeneracy conditions are not satisfied. Formulas of the Jacobian of the trilinear map and a cell volume are obtained.

Introduction

Numerical solutions of partial differential equations in three dimensions often use hexahedral cells composing a computational grid. The most popular choice [1] for constructing hexahedral cells for given eight corner points is based on a trilinear map from a unit cube to a region defined by these points. After the grid is constructed, it is first of all verified whether the grid is unfolded or not. The nondegeneracy is a common requirement to a computational grid and, hence, a major objective of grid generation algorithms, so both a mathematician developing a grid generation method and a practicing engineer must care about this. Such test is very important, especially, in three dimensions when a visualization of a grid is complicated.
In a number of works (see, for example [2, 3, 4]) attempts to find nondegeneracy criteria for trilinear cells have been undertaken. In [5] conditions of nondegeneracy were found. They were briefly presented in [6]. In this paper, the criteria of nondegeneracy are suggested.
In Section 1 of this work, the criterion of nondegeneracy of cells is formulated in terms of positivity of the Jacobian of the transformation used for generation of cells. Formulas of the Jacobian of trilinear map are obtained

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in Section 2. In Section 3, nondegeneracy criteria are given for trilinear cells: both necessary and sufficient nondegeneracy conditions found in [5] are given, new necessary nondegeneracy conditions are also suggested, and a special numerical algorithm for testing the Jacobian of a trilinear map on its positivity for the cases of nonfulfilment of sufficient nondegeneracy conditions is described. The results of testing hexahedrons randomly selected by the computer are presented.

In Section 4, a new formula of a volume of a cell is derived. Formulas of a volume of a cell published in [1, 7] are rather complex and demand a large amount of computations. Efficient volume computation and another formula of a cell volume were suggested in [8]. The formula given in this work is similar to [8], but requires computation of volumes of ten tetrahedrons.

1. Generation of ruled hexahedral cells

Let eight points $\mathbf{z}_{i_1 i_2 i_3} = (z^1_{i_1 i_2 i_3},\ z^2_{i_1 \text{``} i_2 i_3},\ z^3_{i_1 i_2 i_3}),\ i_1, i_2, i_3 = 0, 1$ be given. The trilinear map

$$\begin{aligned}\mathbf{z}(\mathbf{y}) &= \mathbf{a}_{000} + \mathbf{a}_{100} y^1 + \mathbf{a}_{010} y^2 + \mathbf{a}_{001} y^3 + \\ &+ \mathbf{a}_{110} y^1 y^2 + \mathbf{a}_{101} y^1 y^3 + \mathbf{a}_{011} y^2 y^3 + \mathbf{a}_{111} y^1 y^2 y^3 \qquad (1)\end{aligned}$$

of the unit cube $P = \{\mathbf{y} = (y^1, y^2, y^3) : 0 \le y^l \le 1,\ l = 1, 2, 3\}$ defines the ruled cell with the corners $\mathbf{z}_{i_1 i_2 i_3} = \mathbf{z}(i_1, i_2, i_3),\ i_1, i_2, i_3 = 0, 1$. The vectors $\mathbf{a}_{i_1 i_2 i_3}$ are found from the following relations

$$\begin{aligned}\mathbf{a}_{000} = \mathbf{z}_{000},\ \mathbf{a}_{111} &= \mathbf{z}_{111} - \mathbf{z}_{110} - \mathbf{z}_{101} - \mathbf{z}_{011} + \mathbf{z}_{100} + \mathbf{z}_{010} + \mathbf{z}_{001} - \mathbf{z}_{000}, \\ \mathbf{a}_{001} &= \mathbf{z}_{001} - \mathbf{z}_{000},\ \ \mathbf{a}_{011} = \mathbf{z}_{011} - \mathbf{z}_{010} - \mathbf{z}_{001} + \mathbf{z}_{000}, \\ \mathbf{a}_{010} &= \mathbf{z}_{010} - \mathbf{z}_{000},\ \ \mathbf{a}_{101} = \mathbf{z}_{101} - \mathbf{z}_{100} - \mathbf{z}_{001} + \mathbf{z}_{000}, \\ \mathbf{a}_{100} &= \mathbf{z}_{100} - \mathbf{z}_{000},\ \ \mathbf{a}_{110} = \mathbf{z}_{110} - \mathbf{z}_{100} - \mathbf{z}_{010} + \mathbf{z}_{000}.\end{aligned}$$

The concept of the ruled cell and techniques of generation of grids by such cells can be found, for example, in [1, 7]. In two dimensions, the ruled cell is a quadrilateral. If all eight corners of the cell are different, the edges of the cube are transformed by the trilinear map to straight line edges of the hexahedron, and the faces of the cube to ruled surfaces of the second order or planes (Figures 2, 3, and 4).

The criterion of nondegeneracy of a cell is usually formulated in terms of positivity of the Jacobian (the determinant of the Jacobian matrix) of the map used for generating a grid or a cell [3, 4, 9, 10]. A grid element or a cell is said to be nondegenerate (non-inverted, valid, unfolded, nonsingular) if the Jacobian is positive. In the general case, nonzero Jacobian does not globally guarantee a one-to-one correspondence of the map (example 1.3.4, [10, p.9]). It guarantees only locally. In the case of a trilinear map (smooth map) from a cube (a domain), nonzero Jacobian in the whole cube (including boundary) globally guarantees a one-to-one correspondence of the map (theorem 1, [4, p.**8**-4]). Positivity of the Jacobian provides the same orientation of edges of a cell that a unit cube has. Nondegeneracy of the joint grid is attained by the nondegeneracy of all its cells [4].

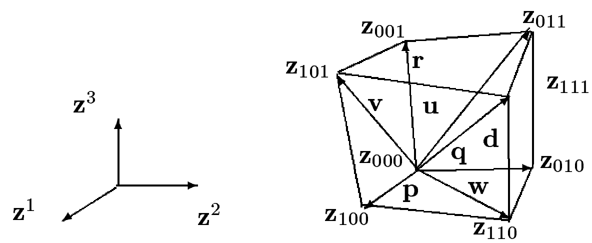

Figure 1. Hexahedral cell.

The Jacobian of the map (1) is equal to the triple scalar product

$$J(y^1, y^2, y^3) = \frac{\partial(z^1, z^2, z^3)}{\partial(y^1, y^2, y^3)} = det\left(\frac{\partial z^i}{\partial y^j}\right) = \left[\frac{\partial \mathbf{z}}{\partial y^1}, \frac{\partial \mathbf{z}}{\partial y^2}, \frac{\partial \mathbf{z}}{\partial y^3}\right]. \qquad (2)$$

The properties of the Jacobian are studied in [2, 3, 4, 9]. In two dimensions, a bilinear map of a unit square is considered. Its Jacobian is a linear function. If the Jacobian is positive at the corners of the square, then due to linearity the Jacobian will be positive everywhere in the square. The converse is also true. In two dimensions, if the Jacobian is positive, then the cell is convex, and the condition of nondegeneracy of cells is equivalent to the condition of convexity of cells [4, 9, 10].

A three-dimensional case is much more complicated. Since the faces of the cell can be nonplanar, the cell can be nonconvex. In [2] it is implied that the Jacobian in three dimensions is positive everywhere if and only if the Jacobian is positive at the corners of a cube. In [3] this statement is shown to be false. It is also demonstrated that for the positivity of the Jacobian in the interior of the cube the positivity of the Jacobian on the edges of the cube is not sufficient. The Jacobian in [3] is written in terms of polynomials the coefficients of which are the values of the Jacobian on the edges.

2. The Jacobian of the trilinear map

For each point $\mathbf{z}_{i_1 i_2 i_3}$, $i_1, i_2, i_3 = 0, 1$, consider the vectors (Fig. 1)

$$\mathbf{p}_{i_1 i_2 i_3} = \mathbf{z}_{\bar{i}_1 i_2 i_3} - \mathbf{z}_{i_1 i_2 i_3}, \quad \mathbf{q}_{i_1 i_2 i_3} = \mathbf{z}_{i_1 \bar{i}_2 i_3} - \mathbf{z}_{i_1 i_2 i_3},$$

$$\begin{aligned}
\mathbf{r}_{i_1 i_2 i_3} &= \mathbf{z}_{i_1 i_2 \bar{i}_3} - \mathbf{z}_{i_1 i_2 i_3}, \quad \mathbf{u}_{i_1 i_2 i_3} = \mathbf{z}_{i_1 \bar{i}_2 \bar{i}_3} - \mathbf{z}_{i_1 i_2 i_3}, \\
\mathbf{v}_{i_1 i_2 i_3} &= \mathbf{z}_{\bar{i}_1 i_2 \bar{i}_3} - \mathbf{z}_{i_1 i_2 i_3}, \quad \mathbf{w}_{i_1 i_2 i_3} = \mathbf{z}_{\bar{i}_1 \bar{i}_2 i_3} - \mathbf{z}_{i_1 i_2 i_3}, \\
\mathbf{d}_{i_1 i_2 i_3} &= \mathbf{z}_{\bar{i}_1 \bar{i}_2 \bar{i}_3} - \mathbf{z}_{i_1 i_2 i_3}.
\end{aligned} \tag{3}$$

Here and hereafter, $\bar{0} = 1,\ \bar{1} = 0$. The partial derivatives $\partial \mathbf{z}/\partial y^k,\ k = 1, 2, 3$ are expressed in terms of vectors (3). Substitution of them into (2) yields

$$J = \left[\sum_{i_2, i_3 = 0}^{1} \mathbf{p}_{0 i_2 i_3} Y_{i_2} Y_{i_3}, \sum_{i_1, i_3 = 0}^{1} \mathbf{q}_{i_1 0 i_3} Y_{i_1} Y_{i_3}, \sum_{i_1, i_2 = 0}^{1} \mathbf{r}_{i_1 i_2 0} Y_{i_1} Y_{i_2} \right]$$

where $Y_{i_l} = i_l + (-1)^{i_l} \left(1 - y^l\right),\ l = 1, 2, 3,\quad i_l = 0, 1,\ (Y_{i_l} = 1 - y^l,\ \text{if } i_l = 0,\ Y_{i_l} = y^l,\ \text{if } i_l = 1)$. Decomposing the triple scalar product of sums of vectors into a sum of triple scalar products and taking common factors of the vectors out of the sign of triple scalar product, we get

$$\begin{aligned}
J &= \sum_{i_1, i_2, i_3 = 0}^{1} \alpha_{i_1 i_2 i_3} {Y_{i_1}}^2 {Y_{i_2}}^2 {Y_{i_3}}^2 + \\
&+ \sum_{k=1}^{3} \sum_{\substack{i_l, i_m = 0, \\ (klm) = (123)}}^{1} \left(\sum_{i_k = 0}^{1} \beta^{k i_k}_{i_l i_m} \right) y^k (1 - y^k) {Y_{i_l}}^2 {Y_{i_m}}^2 + \\
&+ \sum_{k=1}^{3} \sum_{i_k = 0}^{1} \left(\sum_{\substack{i_l, i_m = 0, \\ (klm) = (123)}}^{1} \gamma^{k i_k}_{i_l i_m} \right) {Y_{i_k}}^2 y^l (1 - y^l) y^m (1 - y^m) + \\
&+ \sum_{i_1, i_2, i_3 = 0}^{1} \kappa_{i_1 i_2 i_3} y^1 (1 - y^1) y^2 (1 - y^2) y^3 (1 - y^3)
\end{aligned} \tag{4}$$

where $Y_{i_l} = i_l + (-1)^{i_l} \left(1 - y^l\right),\ l = 1, 2, 3,\quad i_l = 0, 1,\ (Y_{i_l} = 1 - y^l,\ \text{if } i_l = 0,\ Y_{i_l} = y^l,\ \text{if } i_l = 1)$, $\beta^{1 i_1}_{i_2 i_3} = \beta^1_{i_1 i_2 i_3}$, $\beta^{2 i_2}_{i_3 i_1} = \beta^2_{i_1 i_2 i_3}$, $\beta^{3 i_3}_{i_1 i_2} = \beta^3_{i_1 i_2 i_3}$, $\gamma^{1 i_1}_{i_2 i_3} = \gamma^1_{i_1 i_2 i_3}$, $\gamma^{2 i_2}_{i_3 i_1} = \gamma^2_{i_1 i_2 i_3}$, $\gamma^{3 i_3}_{i_1 i_2} = \gamma^3_{i_1 i_2 i_3}$,

$$\begin{aligned}
\alpha_{i_1 i_2 i_3} &= \left[\mathbf{p}_{0 i_2 i_3}, \mathbf{q}_{i_1 0 i_3}, \mathbf{r}_{i_1 i_2 0}\right], \quad \kappa_{i_1 i_2 i_3} = \left[\mathbf{p}_{0 i_2 i_3}, \mathbf{q}_{i_1 0 \bar{i}_3}, \mathbf{r}_{\bar{i}_1 \bar{i}_2 0}\right], \\
\beta^1_{i_1 i_2 i_3} &= \left[\mathbf{p}_{0 i_2 i_3}, \mathbf{q}_{i_1 0 i_3}, \mathbf{r}_{\bar{i}_1 i_2 0}\right], \quad \gamma^1_{i_1 i_2 i_3} = \left[\mathbf{p}_{0 i_2 i_3}, \mathbf{q}_{i_1 0 \bar{i}_3}, \mathbf{r}_{i_1 \bar{i}_2 0}\right], \\
\beta^2_{i_1 i_2 i_3} &= \left[\mathbf{p}_{0 i_2 i_3}, \mathbf{q}_{i_1 0 i_3}, \mathbf{r}_{i_1 \bar{i}_2 0}\right], \quad \gamma^2_{i_1 i_2 i_3} = \left[\mathbf{p}_{0 i_2 i_3}, \mathbf{q}_{i_1 0 \bar{i}_3}, \mathbf{r}_{\bar{i}_1 i_2 0}\right], \\
\beta^3_{i_1 i_2 i_3} &= \left[\mathbf{p}_{0 i_2 i_3}, \mathbf{q}_{i_1 0 \bar{i}_3}, \mathbf{r}_{i_1 i_2 0}\right], \quad \gamma^3_{i_1 i_2 i_3} = \left[\mathbf{p}_{0 i_2 i_3}, \mathbf{q}_{i_1 0 i_3}, \mathbf{r}_{\bar{i}_1 \bar{i}_2 0}\right],
\end{aligned} \tag{5}$$

and indices k, l, m form the permutation of the cycle (123), i.e. k, l, m are equal to the values $1, 2, 3;\ 2, 3, 1;\ 3, 1, 2$, respectively. (The last one is denoted by $(klm) = (123)$).

Let us introduce the notations $\alpha^{1i_1}_{i_2 i_3} = \alpha^{2i_2}_{i_3 i_1} = \alpha^{3i_3}_{i_1 i_2} = \alpha_{i_1 i_2 i_3}$.
The following relations are valid for coefficients (5).

$$\alpha_{i_1 i_2 i_3} = [\mathbf{p}_{0 i_2 i_3}, \mathbf{q}_{i_1 0 i_3}, \mathbf{r}_{i_1 i_2 0}] = \delta_{i_1 i_2 i_3} [\mathbf{p}, \mathbf{q}, \mathbf{r}]_{i_1 i_2 i_3} = J_{i_1 i_2 i_3} = 6V^{pqr}_{i_1 i_2 i_3}, \quad (6)$$

$$\beta^1_{i_1 i_2 i_3} = \left[\mathbf{p}_{0 i_2 i_3}, \mathbf{q}_{i_1 0 i_3}, \mathbf{r}_{\bar{i}_1 i_2 1}\right] = \delta_{i_1 i_2 i_3} [\mathbf{p}, \mathbf{q}, \mathbf{v}]_{i_1 i_2 i_3} = 6V^{pqv}_{i_1 i_2 i_3},$$
$$\beta^2_{i_1 i_2 i_3} = \left[\mathbf{p}_{0 i_2 i_3}, \mathbf{q}_{i_1 0 i_3}, \mathbf{r}_{i_1 \bar{i}_2 0}\right] = \delta_{i_1 i_2 i_3} [\mathbf{p}, \mathbf{q}, \mathbf{u}]_{i_1 i_2 i_3} = 6V^{pqu}_{i_1 i_2 i_3}, \quad (7)$$
$$\beta^3_{i_1 i_2 i_3} = \left[\mathbf{p}_{0 i_2 i_3}, \mathbf{q}_{i_1 0 \bar{i}_3}, \mathbf{r}_{i_1 i_2 0}\right] = \delta_{i_1 i_2 i_3} [\mathbf{p}, \mathbf{u}, \mathbf{r}]_{i_1 i_2 i_3} = 6V^{pur}_{i_1 i_2 i_3},$$

$$\sum_{\substack{i_l, i_m = 0 \\ (klm)=(123)}}^{1} \gamma^{ki_k}_{i_l i_m} = \sum_{\substack{i_l, i_m = 0 \\ (klm)=(123)}}^{1} \bar{\gamma}^{ki_k}_{i_l i_m} =$$
$$= \sum_{\substack{i_l, i_m = 0 \\ (klm)=(123)}}^{1} \left(-\alpha^{ki_k}_{i_l i_m} + \beta^{li_l}_{i_m i_k} + \beta^{mi_m}_{i_k i_l}\right), \quad (8)$$

$$\bar{\gamma}^{1i_1}_{i_2 i_3} = \bar{\gamma}^1_{i_1 i_2 i_3} = \delta_{i_1 i_2 i_3} [\mathbf{d}, \mathbf{q}, \mathbf{r}]_{i_1 i_2 i_3} = 6V^{dqr}_{i_1 i_2 i_3},$$
$$\bar{\gamma}^{2i_2}_{i_3 i_1} = \bar{\gamma}^2_{i_1 i_2 i_3} = \delta_{i_1 i_2 i_3} [\mathbf{p}, \mathbf{d}, \mathbf{r}]_{i_1 i_2 i_3} = 6V^{pdr}_{i_1 i_2 i_3},$$
$$\bar{\gamma}^{3i_3}_{i_1 i_2} = \bar{\gamma}^3_{i_1 i_2 i_3} = \delta_{i_1 i_2 i_3} [\mathbf{p}, \mathbf{q}, \mathbf{d}]_{i_1 i_2 i_3} = 6V^{pqd}_{i_1 i_2 i_3}, \quad (9)$$

$$\sum_{i_1, i_2, i_3 = 0}^{1} \kappa_{i_1 i_2 i_3} = \sum_{i_1, i_2, i_3 = 0}^{1} \sum_{k=1}^{3} \beta^k_{i_1 i_2 i_3} - 2 \sum_{i_1, i_2, i_3 = 0}^{1} \alpha_{i_1 i_2 i_3} =$$
$$= 2\bar{\kappa}_{000} + 2\bar{\kappa}_{111}, \quad (10)$$

$$\bar{\kappa}_{lll} = \delta_{lll} [\mathbf{u}, \mathbf{v}, \mathbf{w}]_{lll} = 6V^{uvw}_{lll}, \quad l = 0, 1, \quad (11)$$

$$\sum_{i_1, i_2, i_3 = 0}^{1} \sum_{k=1}^{3} \gamma^k_{i_1 i_2 i_3} = \sum_{i_1, i_2, i_3 = 0}^{1} \alpha_{i_1 i_2 i_3} + 4\left(\bar{\kappa}_{000} + \bar{\kappa}_{111}\right), \quad (12)$$

$$\sum_{i_1, i_2, i_3 = 0}^{1} \sum_{k=1}^{3} \beta^k_{i_1 i_2 i_3} = 2 \sum_{i_1, i_2, i_3 = 0}^{1} \alpha_{i_1 i_2 i_3} + 2\left(\bar{\kappa}_{000} + \bar{\kappa}_{111}\right). \quad (13)$$

Here and hereafter, $\delta_{i_1 i_2 i_3} = (-1)^{i_1 + i_2 + i_3}$, and lower indices related to brackets refer to each element inside brackets.

So, the Jacobian of the map can be represented by the sum of polynomials of the sixth degree (second degree in each of variables). The coefficients of the polynomial are expressed in terms of the volumes of tetrahedrons of four types (6), (7), (9) ($\bar{\gamma}^k_{i_1 i_2 i_3}$), (11). Tetrahedrons (6) are formed by three edges (with the common corner), tetrahedrons (7) by two edges and "diagonal" of one of adjacent faces, tetrahedrons (9) ($\bar{\gamma}^k_{i_1 i_2 i_3}$) by two edges

and "inner diagonal" of the cell, tetrahedrons (11) by "diagonals" of faces. The total number of tetrahedrons is $8 + 24 + 24 + 2 = 58$.
Finally, substituting (8), (10) into (4) we obtain the Jacobian (4) in the form of a polynomial of the degree not higher than fourth (second in each of variables)

$$\begin{aligned} J &= \sum_{i_1,i_2,i_3=0}^{1} \alpha_{i_1 i_2 i_3} Y_{i_1} Y_{i_2} Y_{i_3} (Y_{i_1} + Y_{i_2} + Y_{i_3} - 2) + \\ &+ \sum_{k=1}^{3} \sum_{\substack{i_l, i_m=0 \\ (klm)=(123)}}^{1} \left(\sum_{i_k=0}^{1} \beta_{i_l i_m}^{k i_k} \right) y^k (1-y^k) Y_{i_l} Y_{i_m}. \end{aligned} \tag{14}$$

Formula (14) can be reduced to the following one

$$\begin{aligned} J &= \sum_{i_1,i_2,i_3=0}^{1} \alpha_{i_1 i_2 i_3} Y_{i_1} Y_{i_2} Y_{i_3} + \qquad (15) \\ &+ \sum_{k=1}^{3} \sum_{\substack{i_l, i_m=0 \\ (klm)=(123)}}^{1} \left(\sum_{i_k=0}^{1} \left(\beta_{i_l i_m}^{k i_k} - \alpha_{i_l i_m}^{k i_k} \right) \right) y^k (1-y^k) Y_{i_l} Y_{i_m}. \end{aligned}$$

Formula (15) requires computations of 8 volumes of tetrahedrons (6) and 12 triple scalar products

$$\begin{aligned} \phi_{i_2 i_3}^1 &= \delta_{i_1 i_2 i_3} \left[\mathbf{p}_{i_1 i_2 i_3}, \mathbf{p}_{\bar{i}_1 \bar{i}_2 i_3}, \mathbf{p}_{i_1 i_2 \bar{i}_3} \right] = \sum_{i_1=0}^{1} \left(\beta_{i_1 i_2 i_3}^1 - \alpha_{i_1 i_2 i_3} \right), \\ \phi_{i_1 i_3}^2 &= \delta_{i_1 i_2 i_3} \left[\mathbf{q}_{\bar{i}_1 \bar{i}_2 i_3}, \mathbf{q}_{i_1 i_2 i_3}, \mathbf{q}_{i_1 i_2 \bar{i}_3} \right] = \sum_{i_2=0}^{1} \left(\beta_{i_1 i_2 i_3}^2 - \alpha_{i_1 i_2 i_3} \right), \qquad (16) \\ \phi_{i_1 i_2}^3 &= \delta_{i_1 i_2 i_3} \left[\mathbf{r}_{\bar{i}_1 i_2 \bar{i}_3}, \mathbf{r}_{i_1 \bar{i}_2 i_3}, \mathbf{r}_{i_1 i_2 i_3} \right] = \sum_{i_3=0}^{1} \left(\beta_{i_1 i_2 i_3}^3 - \alpha_{i_1 i_2 i_3} \right). \end{aligned}$$

The Jacobian J on lines $y^l = \text{const}$, $y^m = \text{const}$, $l \neq m$, $l, m = 1, 2, 3$ is a quadratic trinomial. In particular, on the edges the Jacobian is of the form

$$J \Big|_{\substack{y^l = i_l \\ y^m = i_m}} = \alpha_{i_l i_m}^{k0} \left(1 - y^k\right)^2 + \alpha_{i_l i_m}^{k1} {y^k}^2 + \left(\beta_{i_l i_m}^{k0} + \beta_{i_l i_m}^{k1}\right) y^k \left(1 - y^k\right),$$
$$(klm) = (123), \quad i_l, i_m = 0, 1. \tag{17}$$

Using (17), the formula (15) can be rewritten in terms of values of J on the edges as in [3].

If a hexahedral cell is a parallelepiped, then $\alpha_{i_1 i_2 i_3} = \alpha_{000} = \beta^k_{i_1 i_2 i_3}$, $k = 1, 2, 3$, $i_k = 0, 1$, and the formula for the Jacobian (15) is simplified

$J = \alpha_{000}(1 - y^1 - y^2 - y^3) + \alpha_{100} y^1 + \alpha_{010} y^2 + \alpha_{001} y^3 = \alpha_{000} = \text{const.}$

3. Positivity of the Jacobian of a trilinear map

Necessary conditions 1. The condition $J > 0$ implies the inequalities

$$J\left(i_1, i_2, i_3\right) = \alpha_{i_1 i_2 i_3} > 0, \quad i_1, i_2, i_3 = 0, 1;$$

$$J\left(y^1, y^2, y^3\right)\Bigg|_{\substack{y^k = \frac{1}{2} \\ y^l, y^m = i_l, i_m}} = \frac{1}{4} \sum_{\substack{i_k = 0 \\ (klm) = (123)}}^{1} \left(\alpha^{k i_k}_{i_l i_m} + \beta^{k i_k}_{i_l i_m}\right) > 0, i_l, i_m = 0, 1; \quad (18)$$

$$J\left(y^1, y^2, y^3\right)\Bigg|_{\substack{y^k = i_k \\ y^l, y^m = \frac{1}{2}}} = \frac{1}{8} \sum_{\substack{i_l, i_m = 0 \\ (klm) = (123)}}^{1} \left(\beta^{l i_l}_{i_m i_k} + \beta^{m i_m}_{i_k i_l}\right) > 0, \ i_k = 0, 1;$$

$$J\left(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right) = \frac{1}{16}\left(\sum_{i_1, i_2, i_3 = 0}^{1} \sum_{k=1}^{3} \beta^k_{i_1 i_2 i_3} - \sum_{i_1, i_2, i_3 = 0}^{1} \alpha_{i_1 i_2 i_3}\right) > 0$$

which compose the necessary conditions 1 of nondegeneracy of a cell.

Sufficient conditions 1. The polynomials corresponding to the coefficients from (4) in the interior of the cube P are positive. Hence, if coefficients $\alpha_{i_1 i_2 i_3}$ are positive, and the rest of the coefficients are greater than or equal to zero, then the Jacobian is positive in the interior. It is easy to see that J is positive on the boundary.

Since the coefficients $\gamma^k_{i_1 i_2 i_3}$, $\sum\limits_{i_1, i_2, i_3 = 0}^{1} \kappa_{i_1 i_2 i_3}$ can be expressed in terms of $\alpha_{i_1 i_2 i_3}$, $\beta^k_{i_1 i_2 i_3}$, the conditions of the positivity of the Jacobian (sufficient conditions 1) have the form:

$$\alpha_{i_1 i_2 i_3} > 0, \ i_1, i_2, i_3 = 0, 1;$$

$$\sum_{\substack{i_k = 0 \\ (klm) = (123)}}^{1} \beta^{k i_k}_{i_l i_m} \geq \mathrm{B}^k_{i_l i_m}, i_l, i_m = 0, 1; \quad (19)$$

$$\sum_{\substack{i_l, i_m=0\\(klm)=(123)}}^{1} \gamma^{ki_k}_{i_l i_m} = \sum_{\substack{i_l, i_m=0\\(klm)=(123)}}^{1} \left(\beta^{li_l}_{i_m i_k} + \beta^{mi_m}_{i_k i_l} - \alpha^{ki_k}_{i_l i_m}\right) \geq \Gamma^k_{i_k},\ i_k = 0,1;$$

$$2\bar{\kappa}_{000} + 2\bar{\kappa}_{111} = \sum_{i_1,i_2,i_3=0}^{1} \sum_{k=1}^{3} \beta^k_{i_1 i_2 i_3} - 2 \sum_{i_1,i_2,i_3=0}^{1} \alpha_{i_1 i_2 i_3} \geq \mathrm{K}$$

where $\alpha_{i_1 i_2 i_3}$, $\beta^k_{i_1 i_2 i_3}$ are calculated according to formulas (6), (7), and

$$\mathrm{B}^k_{i_l i_m} = \Gamma^k_{i_k} = \mathrm{K} = 0. \tag{20}$$

The conditions (19) and (20) are satisfied, in particular, for hexahedral cells with the same orientation of vectors of 58 tetrahedrons (6), (7), (9), (11) corresponding to coefficients $\alpha_{i_1 i_2 i_3}$, $\beta^k_{i_1 i_2 i_3}$, $\bar{\gamma}^k_{i_1 i_2 i_3}$, $\bar{\kappa}_{000}$, $\bar{\kappa}_{111}$, that a cube has (right-handed orientation). Note also that necessary conditions 1 coincide with (19) where equality signs are excluded (strict inequality form of (19)) and the following expressions are used

$$\mathrm{B}^k_{i_l i_m} = -\sum_{i_k=0}^{1} \alpha^{ki_k}_{i_l i_m},\ \Gamma^k_{i_k} = -\sum_{i_l, i_m=0}^{1} \alpha^{ki_k}_{i_l i_m},\ \mathrm{K} = -\sum_{i_1,i_2,i_3=0}^{1} \alpha_{i_1 i_2 i_3}.$$

It is clear that necessary conditions 1 assume a wider range of values for $\alpha_{i_1 i_2 i_3}$, $\beta^k_{i_1 i_2 i_3}$ than sufficient conditions 1. Both conditions include 27 inequalities (for 8 corners, 12 edges, 6 faces, and the interior part of a cell). The expression for J is also positive, if (16) and (6) are positive. However these conditions restrict (in comparison with (19)) the set of values of $\alpha_{i_1 i_2 i_3}$, $\beta^k_{i_1 i_2 i_3}$ for which J is positive. So, sufficient conditions 1 are more general conditions.

Necessary and sufficient conditions of positivity of the Jacobian on the edges. The Jacobian on edges is either a linear function or a quadratic trinomial, so it is easy to find necessary and sufficient conditions of its positivity on the edges

$$\alpha_{i_1 i_2 i_3} > 0,\ i_1, i_2, i_3 = 0,1;$$

$$\sum_{i_k=0}^{1} \beta^{ki_k}_{i_l i_m} > -2\sqrt{\alpha^{k0}_{i_l i_m} \alpha^{k1}_{i_l i_m}},\ (klm) = (123),\ i_l, i_m = 0,1. \tag{21}$$

The Jacobian J on the faces $y^l = 0,1$, $l = 1,2,3$ and general formula (15) can be written (see [5],[6]) as quadratic trinomial in one variable with fixed other variables (one or two, respectively). An attempt to find necessary and sufficient conditions of positivity of the Jacobian using its representation in the form of quadratic trinomial fails since even in the case of faces the discriminant of quadratic trinomial is a fourth-degree polynomial in one variable; in the general case, the discriminant will be the polynomial in two variables. Because of above reasons an analysis of the discriminant on the property of having fixed sign fails. However, it is possible to find sufficient conditions more general than (19) and necessary conditions more particular than (18).

Sufficient conditions 2. Sufficient conditions 2 [5],[6] coincide with strick inequality form of (19) (conditions (19) where equality signs are excluded) with the parameters

$$\begin{aligned}
\mathrm{B}^k_{i_l i_m} &= -2\min(\alpha^{k0}_{i_l i_m}, \alpha^{k1}_{i_l i_m}),\ (klm) = (123),\ i_l, i_m = 0,1; \\
\Gamma^k_{i_k} &= -2 \min_{j_l, j_m = 0,1} \left(2\alpha^{k i_k}_{j_l j_m} + \sum_{i_l=0}^{1} \beta^{l i_l}_{j_m i_k} + \sum_{i_m=0}^{1} \beta^{m i_m}_{i_k j_l} \right), \\
& \qquad (klm) = (123),\ i_k = 0,1; \\
\mathrm{K} = -2 \min_{j_1, j_2, j_3 = 0,1} & (3\alpha_{j_1 j_2 j_3} + 2(\sum_{i_2, i_3 = 0}^{1} \gamma^1_{j_1 i_2 i_3} + \sum_{i_1, i_3 = 0}^{1} \gamma^2_{i_1 j_2 i_3} + \\
& + \sum_{i_1, i_2 = 0}^{1} \gamma^3_{i_1 i_2 j_3}) + \sum_{i_1=0}^{1} \beta^1_{i_1 j_2 j_3} + \sum_{i_2=0}^{1} \beta^2_{j_1 i_2 j_3} + \sum_{i_3=0}^{1} \beta^3_{j_1 j_2 i_3}).
\end{aligned}$$

Obviously, that cells satisfying sufficient conditions 1 satisfy sufficient condition 2. Sufficient conditions 2 are more general than sufficient conditions 1 but demand more computations. It is possible to show that when sufficient conditions 1 are satisfied necessary conditions 1 also hold. (But not vice versa).

Necessary conditions 2. Since on lines $y^l, y^m = \mathrm{const},\ \ l, m = 1,2,3,$ $l \neq m$ the Jacobian is either a linear function or a quadratic trinomial, we can get necessary and sufficient conditions of positivity of the Jacobian on these lines, and, thus, restrict general necessary conditions. To get necessary conditions 2 we shall write down necessary and sufficient conditions of Jacobian's positivity on the edges and so called "middle" lines. So, necessary conditions 2 will be composed of conditions (21) and the following conditions

$$\phi^2_{i_1 0} + \phi^2_{i_1 1} \quad > \quad -2(\alpha_0 + \alpha_1 + 2\sqrt{\alpha_0 \alpha_1}),\ \alpha_j = J(i_1, j, 0.5),$$

$$\phi^3_{i_1 0} + \phi^3_{i_1 1} > -2(\alpha_0 + \alpha_1 + 2\sqrt{\alpha_0\alpha_1}),\ \alpha_j = J\left(i_1, 0.5, j\right), j = 0, 1,$$

$$\begin{aligned}
\phi^1_{i_2 0} + \phi^1_{i_2 1} &> -2(\alpha_0 + \alpha_1 + 2\sqrt{\alpha_0\alpha_1}),\ \alpha_j = J\left(j, i_2, 0.5, \right), \\
\phi^3_{0 i_2} + \phi^3_{1 i_2} &> -2(\alpha_0 + \alpha_1 + 2\sqrt{\alpha_0\alpha_1}),\ \alpha_j = J\left(0.5, i_2, j\right), j = 0, 1,
\end{aligned}$$

$$\begin{aligned}
\phi^1_{0 i_3} + \phi^1_{1 i_3} &> -2(\alpha_0 + \alpha_1 + 2\sqrt{\alpha_0\alpha_1}),\ \alpha_j = J\left(j, 0.5, i_3\right), \\
\phi^2_{0 i_3} + \phi^2_{1 i_3} &> -2(\alpha_0 + \alpha_1 + 2\sqrt{\alpha_0\alpha_1}),\ \alpha_j = J\left(0.5, j, i_3\right), j = 0, 1
\end{aligned}$$

on "middle" lines for the planes $y^1 = i_1,\ y^2 = i_2,\ y^3 = i_3,\ \ i_k = 0, 1,\ \ k = = 1, 2, 3$, respectively, and

$$\sum_{i_1, i_2 = 0}^{1} \phi^k_{i_1 i_2} > -4(\alpha_0 + \alpha_1 + 2\sqrt{\alpha_0\alpha_1}),$$

$$\alpha_{i_k} = J\left(y^1, y^2, y^3\right)\Big|_{\substack{y^k = i_k \\ y^l, y^m = 0.5}},\ i_k = 0, 1,\ (klm) = (123)$$

on "middle" lines passing through the center point $(0.5, 0.5, 0.5)$. Here values of J are given in (18), and ϕ^k_{lm} are given in (16).

Numerical results. To see how general the obtained conditions are, a numerical experiment was carried out. The corners of hexahedron were selected randomly. Of 10^7 hexahedrons randomly generated by the computer only 36251 were found to have positive Jacobians at the corners of a cell. From them only 14622 cases satisfied necessary conditions 1 for edges, 14010 cases satisfied necessary conditions 1 for faces, and 14004 cases satisfied necessary conditions 1 for the whole cell. Necessary conditions 2 allowed us to exclude some more degenerate cells. The number of cases when necessary conditions 2 were satisfied, was equal to 11533.

The Jacobian was positive in 11481 cases. Sufficient conditions 1 were satisfied in 33.93% of the cases (from the number 11481), sufficient conditions 2 were satisfied in 65.08% of the cases. In 11660 cases the Jacobian was positive on the edges (conditions (21)), 98.46% of them had positive Jacobian everywhere in the whole cell. The success rate of necessary conditions 2 was 99.54%.

In Figures 2 and 3 there are hexahedrons nondegeneracy of which was checked by means of sufficient conditions 1 and 2, respectively. Figure 4 gives hexahedral cell nondegeneracy of which was established by a special numerical algorithm of testing the Jacobian on its positivity. Figures 2 a, 3 , and 4 a show the edges of cells, Figures 2 b, 3 b, and 4 b show the faces of cells (hidden lines are removed).

a *b*

Figure 2. Hexahedral cell satisfying sufficient conditions 1: a — edges, b — faces.

a *b*

Figure 3. Hexahedral cell satisfying sufficient conditions 2: a — edges, b — faces.

a *b*

Figure 4. Hexahedral cell nondegeneracy of which was established by a special numerical algorithm: a — edges, b — faces.

All computations were performed on a personal computer. A computer code generated for each case, first, a hexahedron and, then, checked different types of conditions. For all cases, necessary conditions 2 were checked. For some cases, sufficient conditions 1 and sufficient conditions 2 were checked.

Besides checking all these conditions in some cases a special numerical algorithm of testing the Jacobian on its positivity in the whole cube was applied. On the personal computer Pentium 3 (800 MHz), such a test of 10^7 cases demanded about 1 minute of computation (58 seconds). The test of sufficient conditions 2 (as the most expensive) for 10^7 nondegenerate cells required about one and half minute of computation (95 seconds).
Numerical results showed the following.
1. Necessary conditions allowed to exclude a great number of cells which were degenerate.
2. Less than in one third of cases when the Jacobian was positive at the corners of a cell the Jacobian was positive everywhere in the cell. So, it would be unreliable to draw a conclusion about the invertibility of the Jacobian on the base of positive Jacobians at the corners of a cell.
3. Necessary and sufficient conditions of positivity of the Jacobian on the edges (provided that necessary conditions 1 were satisfied) in a large percentage of cases gave positive Jacobian everywhere in the cell. The success rate of necessary conditions 2 was higher. However, both of these conditions also did not guarantee the invertibility of the trilinear map.
4. Sufficient conditions 2 permitted to recognize the nondegeneracy of cells in most of the cases.
5. In other cases, nondegeneracy was established by a special numerical algorithm.

A special numerical algorithm of testing the Jacobian on its positivity. Initially in [5], to estimate the success rate of nondegeneracy conditions, computation of the Jacobian was carried out in the unit cube on the uniform grid with the number of nodes $10 \times 10 \times 10$. The number of cases with positive Jacobians on such a grid was 11582 provided that necessary conditions 1 were satisfied.
To recognize nondegenerate cells for the cases when necessary conditions 2 were satisfied but sufficient conditions 2 were not satisfied a special algorithm of testing the Jacobian on its positivity was developed. It is an algorithm of minimizing the Jacobian in unit cube. It consists of two stages. First stage is a preliminary minimizing. On this stage we minimize the Jacobian on lines $y^1 = (i_1 - 1)/(L - 1),\ y^2 = (i_2 - 1)/(L - 1),\ L = 10,\ i_k = 1, ..., L,\ k = 1, 2$. Since on these lines the Jacobian is a guadratic trinomial, we can do this exactly. As a result of such minimizing, we have initial approximation J^0_{min} of a minimal value of J and a corresponding global minimizer as starting point for the next stage. On the next stage (correction of the minimal value) minimizing is carried out on each iteration along coordinate directions $y^1,\ y^2,\ y^3$, sequentially. On the line corresponding

to each direction we also solve the optimization problem for the Jacobian precisely as for quadratic trinomial. We utilize such minimizing on each iteration until the condition $|J^n_{min} - J^{n-1}_{min}| < \epsilon$ will be satisfied. Here, J^n_{min} is a minimal value of the Jacobian on n iteration, ϵ is a small parameter. If on one of the stages nonpositive value of the Jacobian appears, the process is also terminated. In this case the cell is considered degenerate. Otherwise, the cell is considered nondegenerate. Such an algorithm of minimizing the Jacobian in the unit cube allowed us to exclude about 100 degenerate cases. The number of nodes of the grid for the preliminary minimizing was chosen by the experiment. The small parameter ϵ was equal to 10^{-7}.

4. A formula of a cell volume

Integrate the Jacobian J. Let us use, for example, (15) and (13)

$$\begin{aligned} V &= \iiint\limits_{0\le y^l\le 1} J dy^1 dy^2 dy^3 = \frac{1}{24} \sum_{i_1,i_2,i_3=0}^{1} \sum_{k=1}^{3} \beta^k_{i_1 i_2 i_3} = \\ &= \frac{1}{12} \left(\sum_{i_1,i_2,i_3=0}^{1} \alpha_{i_1 i_2 i_3} + \bar{\kappa}_{000} + \bar{\kappa}_{111} \right). \end{aligned}$$

Conclusions

The criteria obtained allow to establish nondegenaracy of trilinear cells.

If sufficient conditions 1 or 2 hold, the cell is nondegenerate. Sufficient conditions 1 demand less computations than sufficient conditions 2. If necessary conditions 2 are not satisfied, the cell is degenerate.

In the case of cells satisfying necessary conditions 2 but not satisfying sufficient conditions 2, a special numerical algorithm of testing the Jacobian on its positivity allows to recognize nondegenerate cells. If this algorithm gives nonpositive minimal value of the Jacobian, then the cell is degenerate. Otherwise, the cell is nondegenerate.

The formula of a volume of a cell is simple and does not demand verification of numerous conditions and computations as in [1, 7].

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