Subtetrahedral test for the positive Jacobian of hexahedral elements

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Abstract

Given any eight points in the 3D space, there is a unique trilinear mapping which maps the reference cube to a "hexahedron" having the eight points as its vertices. In the finite element method and many other approximation problems, it requires such a trilinear mapping to be one-to-one and to have a positive Jacobian everywhere. It is a long-time and challenging problem to find a computable test, which is a both necessary and sufficient condition, to ensure the global positivity of the Jacobian of such trilinear mappings. In computation, a sufficient condition may be enough as people would eliminate ill-shaped elements as well as those not invertible elements. In this paper, we will show a subtetrahedral test, used by engineers, is neither necessary nor sufficient. We correct this test by extending the number of subtetrahedra to be checked from 24 to 32. The sufficiency of the new test for a globally positive Jacobian is proven.

Mathematics Subject Classification (2000): 65N30, 65N50
Keywords: Hexahedral finite elements, isoparametric mapping, trilinear mapping, Jacobian, invertibility

1 Introduction

In the finite element computation, each element is inversely mapped to a reference element and all the calculation is done on this reference element. Such a reference mapping must be bijective, and the Jacobian is usually required to be positive everywhere on the reference element (cf [1, 2, 5].) The situation for 2D, quadrilateral elements is relatively simple that a bilinear reference mapping is bijective if and only if the Jacobian is positive at the four corners, i.e., the four corner triangles are "positive" (cf., for example, [3]). But the problem in 3D is much more complicated. Given 8 points in the 3D space, there is a unique trilinear reference mapping. When would this mapping be bijective? When would this mapping have a globally positive Jacobian? Mathematically, is there a necessary and sufficient condition, which can be checked by a computer, for the positivity of the trilinear Jacobian? Computationally, we need a sufficient condition which can be computable and and pass all trilinear mappings for well-shaped hexahedral finite elements. Such a sufficient condition would be called a test by engineers. What is a good test?

Some preliminary studies on the Jacobian of trilinear mappings were done in [7, 8, 9, 6] and the first three questions above were posted explicitly by some authors of, in particular, [7, 8, 6]. The three questions were answered in a sequence of papers nearly thoroughly by the author in [13, 14, 15]. In [13] it is proved that a trilinear reference mapping is bijective if its Jacobian is positive on the boundary. This reduced the conditions for bijectivity in the classic homeomorphism theorem (cf. [12] and references in [2]) in two directions that (1) the requirement of bijectivity on the boundary is removed; and (2) the requirement of the global positivity of the Jacobian is reduced to the boundary positivity. The conjecture of "face-test" in [7] is proved in [14] that if a Jacobian is positive on the boundary, it is positive everywhere. Further, it is shown in the paper that the "edge-test" is valid too provided the reference mapping is bijective on the boundary. The last result provides a computable necessary and sufficient condition for a Jacobian to be globally positive (cf. [15]), answering the third question above.

In this paper, we will try to answer the fourth question above. Independent of the analysis in [13, 14, 15], we will study a test, the subtetrahedral test, presented in a grid-generation bible book [4]. The subtetrahedral test checks the Jacobians of 24 subtetrahedra at the 12 edges of a given hexahedron. The test is a natural extension of the 2D test of checking the Jacobian of 4 subtriangles at 4 vertices of a quadrilateral. The test was claimed and widely accepted that it ensures the global positivity of the Jacobian of the trilinear mapping for any hexahedron (see [4] and references therein). In this paper, we will disprove this claim. We will show that the test is neither a sufficient or a necessary condition, i.e., a hexahedron passes the test may fail to have a globally positive Jacobian, and a hexahedron fails the test may have a globally positive Jacobian. Of course, such a test needs not to be a necessary condition. But this test fails to be a working test as it is not a sufficient condition.

We will modify the subtetrahedral test, by adding 8 subtetrahedra (at 8 vertices) to the list of 24 subtetrahedra (at 12 edges) to be tested. We will prove that the new (32) subtetrahedral test guarantees a positive Jacobian, independent of the analysis and the results of the author's earlier work [13, 14, 15]. We remark that, in [10, 11], two different tests were presented and were shown to be a sufficient condition each for a positive Jacobian. We believe the new subtetrahedral test is simpler, both in mathematics and in computation, than the two tests in [10, 11]. All three tests compute Jacobians of some subtetrahedra. The new test computes only 32 Jacobians while the other two tests needs to compute 64 Jacobians and to check 33 inequalities of the combinations of the Jacobians. Also, we show by an example that the new test might be more powerful than the other two, because the other tests, not the new subtetrahedral test, fail to detect the positivity of the Jacobian for one hexahedron.

The paper is organized as follows. In section 2, trilinear reference mappings are defined and some preliminary lemmas are presented. In section 3, the subtetrahedral test of [4] will be introduced. We will show that the test won't guarantee the positivity of a Jacobian. We will also give an example showing that a hexahedron with a positive Jacobian may fail the test. In the last section, we will extend the subtetrahedral test and we will show that the new subtetrahedral test guarantees the positivity of a Jacobian. We then compare the test with other two existing tests.

2 The 3D Q_1 and P_1 mappings.

In this section, we define the 3D Q_1 mapping, i.e., the trilinear mapping, and the hexahedral element. We will present some simple lemmas concerning Jacobians.

Given 8 points, $v_i = (x_i, y_i, z_i)$, $i = 1, 2, \ldots, 8$, anywhere in the 3D space (see Figure 1), we define an 8-vertex hexahedral finite element by the following 3D Q_1 mapping:

$$F : \hat{Q} \to Q := F(\hat{Q}), \qquad F : (\hat{x}, \hat{y}, \hat{z}) \mapsto (x, y, z),$$

where

$$\begin{pmatrix} x \\ y \\ z \end{pmatrix} = \sum_{i=1}^{8} v_i b_i(\hat{x}, \hat{y}, \hat{z})$$
$$= a_{000} + a_{100}\hat{x} + a_{010}\hat{y} + a_{001}\hat{z} + a_{110}\hat{x}\hat{y} + a_{101}\hat{x}\hat{z} + a_{011}\hat{y}\hat{z} + a_{111}\hat{x}\hat{y}\hat{z}. \qquad (1)$$

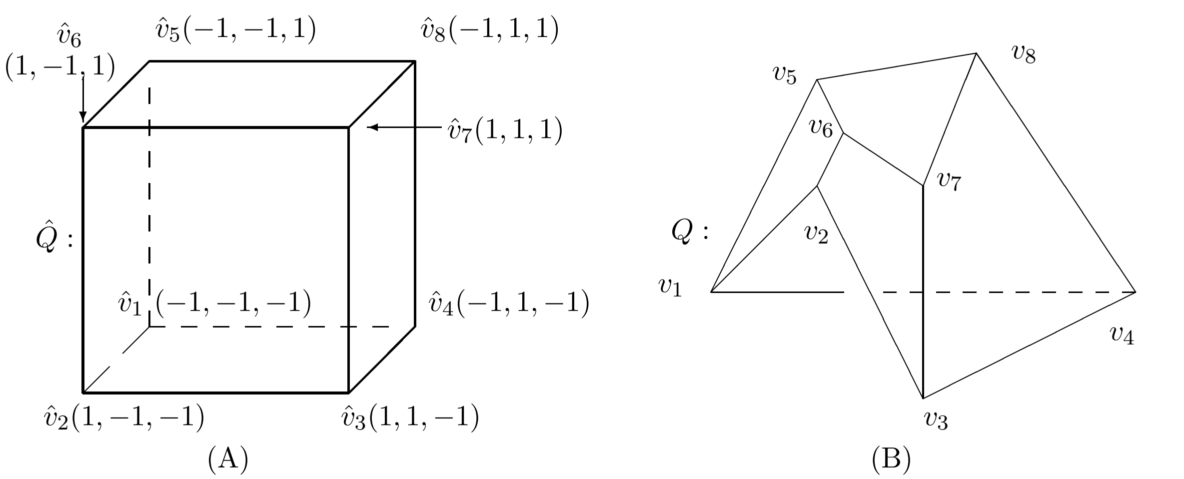
Here the Q_1 nodal basis functions, $b_i(\cdot, \cdot, \cdot)$, defined on the reference element $\hat{Q} = [-1, 1]^3$ in 3D are

$$\begin{cases} b_1 = (1-\hat{x})(1-\hat{y})(1-\hat{z})/8, & b_5 = (1-\hat{x})(1-\hat{y})(1+\hat{z})/8, \\ b_2 = (1+\hat{x})(1-\hat{y})(1-\hat{z})/8, & b_6 = (1+\hat{x})(1-\hat{y})(1+\hat{z})/8, \\ b_3 = (1+\hat{x})(1+\hat{y})(1-\hat{z})/8, & b_7 = (1+\hat{x})(1+\hat{y})(1+\hat{z})/8, \\ b_4 = (1-\hat{x})(1+\hat{y})(1-\hat{z})/8, & b_8 = (1-\hat{x})(1+\hat{y})(1+\hat{z})/8. \end{cases} \tag{2}$$

Therefore we can find the coefficients in (1),

$$\begin{cases} 1: & a_{000} = (v_5+v_6+v_7+v_8)/8 + (v_1+v_2+v_3+v_4)/8, \\ \hat{x}: & a_{100} = (v_2+v_3+v_6+v_7)/8 - (v_1+v_4+v_5+v_8)/8, \\ \hat{y}: & a_{010} = (v_3+v_4+v_7+v_8)/8 - (v_1+v_2+v_5+v_6)/8, \\ \hat{z}: & a_{001} = (v_5+v_6+v_7+v_8)/8 - (v_1+v_2+v_3+v_4)/8, \\ \hat{x}\hat{y}: & a_{110} = (v_5+v_7-v_6-v_8)/8 + (v_1+v_3-v_2-v_4)/8, \\ \hat{x}\hat{z}: & a_{101} = (v_4+v_7-v_3-v_8)/8 + (v_1+v_6-v_2-v_5)/8, \\ \hat{y}\hat{z}: & a_{011} = (v_2+v_7-v_3-v_6)/8 + (v_1+v_8-v_4-v_5)/8, \\ \hat{x}\hat{y}\hat{z}: & a_{111} = (v_5+v_7-v_6-v_8)/8 - (v_1+v_3-v_2-v_4)/8 \\ & \qquad = (v_4+v_7-v_3-v_8)/8 - (v_1+v_6-v_2-v_5)/8 \\ & \qquad = (v_2+v_7-v_3-v_6)/8 - (v_1+v_8-v_4-v_5)/8. \end{cases} \tag{3}$$

Figure 1: The reference cube and a general hexahedron (non-flat surface).



We note that 4 vertices, for example, the top 4 in Figure 1(B), of a face "quadrilateral" of Q may not be on a same plane. Therefore, the "hexahedra" under the study may not have planar faces, as each of the six faces is the image of some nonlinear (Q_1) functions. The Jacobian matrix of the mapping F in (1) is defined by

$$D_F(\hat{x},\hat{y},\hat{z}) = \begin{pmatrix} \frac{\partial x}{\partial \hat{x}} & \frac{\partial x}{\partial \hat{y}} & \frac{\partial x}{\partial \hat{z}} \\ \frac{\partial y}{\partial \hat{x}} & \frac{\partial y}{\partial \hat{y}} & \frac{\partial y}{\partial \hat{z}} \\ \frac{\partial z}{\partial \hat{x}} & \frac{\partial z}{\partial \hat{y}} & \frac{\partial z}{\partial \hat{z}} \end{pmatrix}, \tag{4}$$

and the Jacobian (determinant) of F by

$$J := J_F = \det(D_F)(\hat{x}, \hat{y}, \hat{z}).$$

Remark 2.1 We note that F maps each line on $\hat{Q}$, parallel to either x or y or z axis, to a straight line on Q. For example,

$$F\left(\{(\hat{x}, \hat{y}_0, \hat{z}_0) \ | \ -1 \le \hat{x} \le 1\}\right) = \left\{F(-1, \hat{y}_0, \hat{z}_0) + \frac{1+\hat{x}}{2} F(1, \hat{y}_0, \hat{z}_0) \ | \ -1 \le \hat{x} \le 1\right\}.$$

Therefore each column vector in the Jacobian matrix of F is a constant vector along a line in that direction. For example, the first column vector $\begin{pmatrix} \frac{\partial x}{\partial \hat{x}} & \frac{\partial y}{\partial \hat{x}} & \frac{\partial z}{\partial \hat{x}} \end{pmatrix}$ of D_F is constant on any of the following lines

$$\{(\hat{x}, \hat{y}_0, \hat{z}_0) \ | \ -1 \le \hat{x} \le 1\}.$$

∎

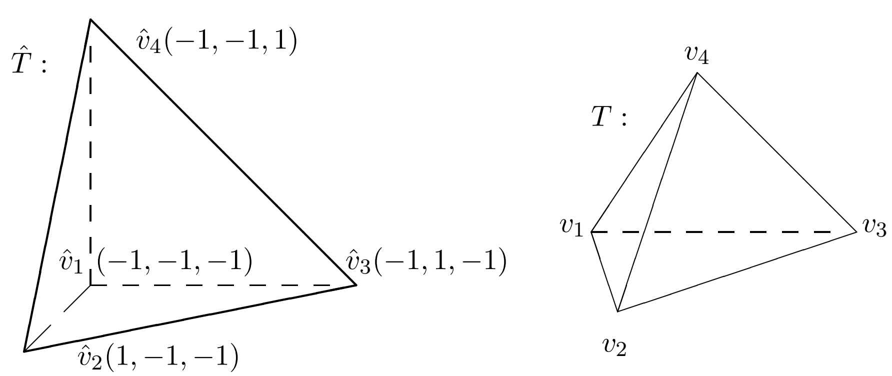
We will relate the Jacobian of a trilinear mapping to that of linear mappings for tetrahedron. For any tetrahedron $T_{v_1 v_2 v_3 v_4}$ shown in Figure 2, we define an affine mapping from the reference tetrahedron $\hat{T}$ to T by

$$F_T(\hat{x}, \hat{y}, \hat{z}) = \sum_{i=1}^{4} v_i \beta_i(\hat{x}, \hat{y}, \hat{z}), \tag{5}$$

where b_i are nodal basis functions on $\hat{T}$:

$$\beta_1 = \frac{1}{2}(-1 - \hat{x} - \hat{y} - \hat{z}), \qquad \beta_2 = \frac{1}{2}(1 + \hat{x}),$$
$$\beta_3 = \frac{1}{2}(1 + \hat{y}), \qquad \beta_4 = \frac{1}{2}(1 + \hat{z}).$$

Figure 2: The reference reference tetrahedron $\hat{T}$ and a general tetrahedron T.



Lemma 2.1 *Let F_T be the reference mapping from $\hat{T}$ to T (Figure 2). The Jacobian matrix of F_T, D_{F_T} is a constant matrix and its determinant, the Jacobian of F_T, is related to a box product:*

$$\det(D_{F_T}) = \frac{1}{8}(\overrightarrow{v_1 v_2} \times \overrightarrow{v_1 v_3}) \cdot \overrightarrow{v_1 v_4}.$$

Proof From (5), by expanding the nodal basis functions, we get

$$F_T(\hat{x},\hat{y},\hat{z}) = \frac{-v_1+v_2+v_3+v_4}{2} + \frac{v_2-v_1}{2}\hat{x} + \frac{v_3-v_1}{2}\hat{y} + \frac{v_4-v_1}{2}\hat{z}. \tag{6}$$

Therefore, the Jacobian matrix is

$$D_{F_T} = \frac{1}{2}\begin{pmatrix} v_2-v_1 & v_3-v_1 & v_4-v_1 \end{pmatrix},$$

a constant matrix. The determinant, i.e., the Jacobian, is a box product

$$\det(D_{F_T}) = \frac{1}{8}(\overrightarrow{v_1v_2}\times\overrightarrow{v_1v_3})\cdot\overrightarrow{v_1v_4}.$$

∎

If the reference mapping for a tetrahedron $T_{v_1v_2v_3v_4}$ has a positive Jacobian, i.e.,

$$J_{v_1v_2v_3v_4} := \frac{1}{8}(\overrightarrow{v_1v_2}\times\overrightarrow{v_1v_3})\cdot\overrightarrow{v_1v_4} > 0. \tag{7}$$

we say the *tetrahedron is positive*, For any nondegenerate triangle $\triangle v_1v_2v_3$ shown in Figure 2, we define its normal vector as

$$\mathbf{n}_{\triangle v_1v_2v_3} = \overrightarrow{v_1v_2}\times\overrightarrow{v_1v_3}. \tag{8}$$

We say a point v_4 is on *the positive side of a triangle* $\triangle v_1v_2v_3$, or the positive side of the plane $v_1v_2v_3$, if the dot product is positive for any one $i=1,2,3$,

$$\mathbf{n}_{\triangle v_1v_2v_3}\cdot\overrightarrow{v_iv_4} > 0. \tag{9}$$

By the new language, we have, by (7) and (9), the following lemma.

Lemma 2.2 *A tetrahedron $T_{v_1v_2v_3v_4}$ is positive if and only if the point v_4 is on the positive side of triangle $\triangle v_1v_2v_3$.*

Lemma 2.3 *When we rotate the base triangle $\triangle v_1v_2v_3$ of a tetrahedron $T_{v_1v_2v_3v_4}$, the resulting tetrahedron is still $T_{v_1v_2v_3v_4}$ physically, but the 3 linear reference mappings F are different. However, the Jacobian of three P_1 mappings remains the same, i.e., (see (7))*

$$J_{v_1v_2v_3v_4} = J_{v_3v_1v_2v_4} = J_{v_2v_3v_1v_4}$$

Proof The normal vector (8) is invariant when we rotate the triangle $\triangle v_1v_2v_3$ to $\triangle v_2v_3v_1$ and $\triangle v_3v_1v_2$. As the point v_i is on the plane of triangle $\triangle v_1v_2v_3$, therefore

$$\mathbf{n}_{\triangle v_1v_2v_3}\cdot\overrightarrow{v_1v_4} = \mathbf{n}_{\triangle v_2v_3v_1}\cdot\overrightarrow{v_1v_4} = \mathbf{n}_{\triangle v_3v_1v_2}\cdot\overrightarrow{v_1v_4}.$$

The lemma follows the formula (7) now. ∎

Lemma 2.4 *Let F_T be the reference mapping from the reference tetrahedron $\hat{T}$ (Figure 2) to the corner tetrahedron $v_1v_2v_4v_5$ of Q in Figure 1. Let F be the reference mapping from the reference cube $Q=[-1,1]^3$ to Q shown in Figure 1. The Jacobian of F at vertex v_1 is equal to the Jacobian of F_T, i.e.,*

$$\det(D_F)(-1,-1,-1) = \det(D_{F_T}). \tag{10}$$

Furthermore the two Jacobian matrices are the same:

$$D_F(-1,-1,-1) = D_{F_T}. \tag{11}$$

Proof When restrict F on the edge $\{[-1,1] \times -1 \times -1\}$, it is a linear function. In fact, $F(\{[-1,1] \times -1 \times -1\}) = v_1 v_2$ and

$$F(\hat{x}, -1, -1) = F_T(\hat{x}, -1, -1) \quad \forall \hat{x} \in [-1,1].$$

Therefore, the first column of the Jacobian matrix $\partial F / \partial \hat{x}$ on the edge is a constant vector:

$$\frac{\partial F}{\partial \hat{x}} = a_{100} - a_{110} - a_{101} + a_{111} = \frac{v_2 - v_1}{2},$$

where (1), (3), (5) and (6) are applied. On the other side, for F_T, which is a linear function everywhere, we have $\partial F_T / \partial \hat{x} = \dfrac{v_2 - v_1}{2}$ as $F_T(-1,-1,-1) = v_1$ and $F_T(1,-1,-1) = v_2$. In the same fashion, we get the identity for the Jacobian matrices:

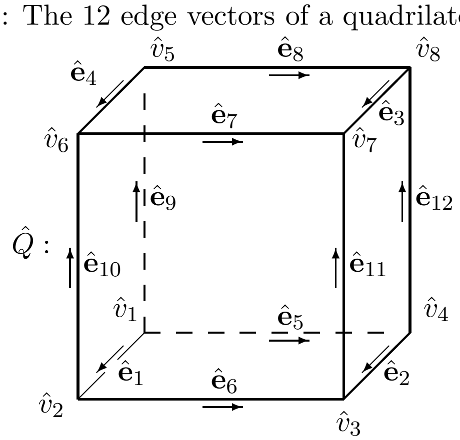
$$D_F(-1,-1,-1) = \frac{1}{2} \begin{pmatrix} v_2 - v_1 & v_4 - v_1 & v_4 - v_1 \end{pmatrix} = D_{F_T}.$$

∎

3 The subtetrahedral test

In this section, we will define a test, used by engineers (cf. [4]), to detect if the Jacobian of a Q_1 reference mapping is globally positive. We will then show by two examples, this test is not a necessary condition for a globally positive Jacobian, neither is a sufficient condition. Therefore, this test fails to be a working test.

Figure 3: The 12 edge vectors of a quadrilateral.

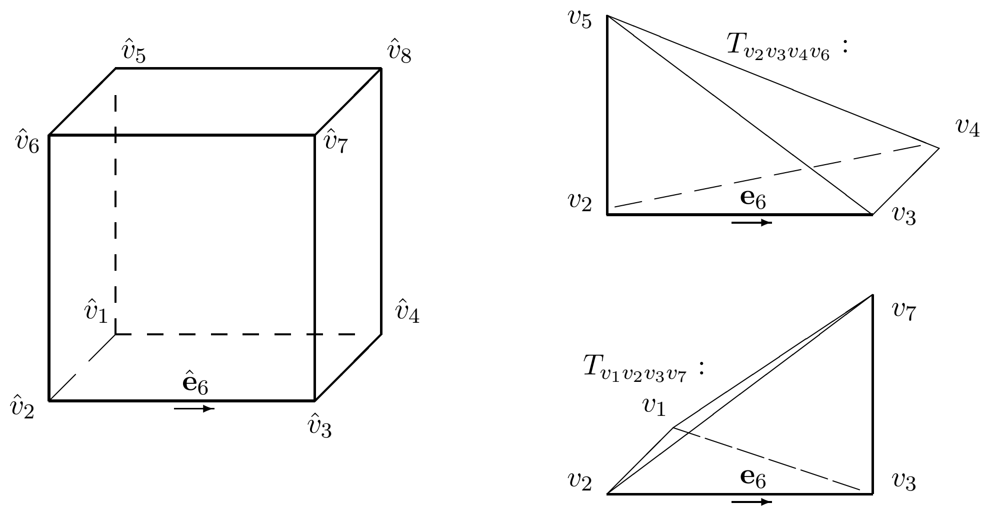


For each hexahedron $Q_{v_1 v_2 v_3 v_4 v_5 v_6 v_7 v_8}$ shown in Figure 1, we number its 12 edge vectors in Figure 3. We note that for each of the 12 edges we can form two subtetrahedra using this edge and two edges, one at each end of this edge. For example, the two such subtetrahedra for edge $\mathbf{e}_6$ are depicted in Figure 4. We list all 24 such subtetrahedra here (see Figure 1 for the vertex orientation). We note that in the list (12), we do not distinguish $T_{v_1 v_2 v_3 v_7}$ and $T_{v_2 v_3 v_1 v_7}$ as their Jacobians are the same, by Lemma 2.3.

$$\begin{aligned}
&T_{v_1 v_2 v_3 v_7}, T_{v_2 v_3 v_4 v_8}, T_{v_3 v_4 v_1 v_5}, T_{v_4 v_1 v_2 v_6}, T_{v_5 v_8 v_7 v_3}, T_{v_8 v_7 v_6 v_2}, \\
&T_{v_7 v_6 v_5 v_1}, T_{v_6 v_5 v_8 v_4}, T_{v_2 v_1 v_5 v_8}, T_{v_4 v_3 v_7 v_6}, T_{v_1 v_4 v_8 v_7}, T_{v_3 v_2 v_6 v_5}, \\
&T_{v_1 v_2 v_3 v_5}, T_{v_2 v_3 v_4 v_6}, T_{v_3 v_4 v_1 v_7}, T_{v_4 v_1 v_2 v_8}, T_{v_5 v_8 v_7 v_1}, T_{v_8 v_7 v_6 v_4}, \\
&T_{v_7 v_6 v_5 v_3}, T_{v_6 v_5 v_8 v_2}, T_{v_5 v_1 v_4 v_6}, T_{v_3 v_7 v_8 v_2}, T_{v_4 v_8 v_5 v_3}, T_{v_2 v_6 v_7 v_1}.
\end{aligned} \tag{12}$$

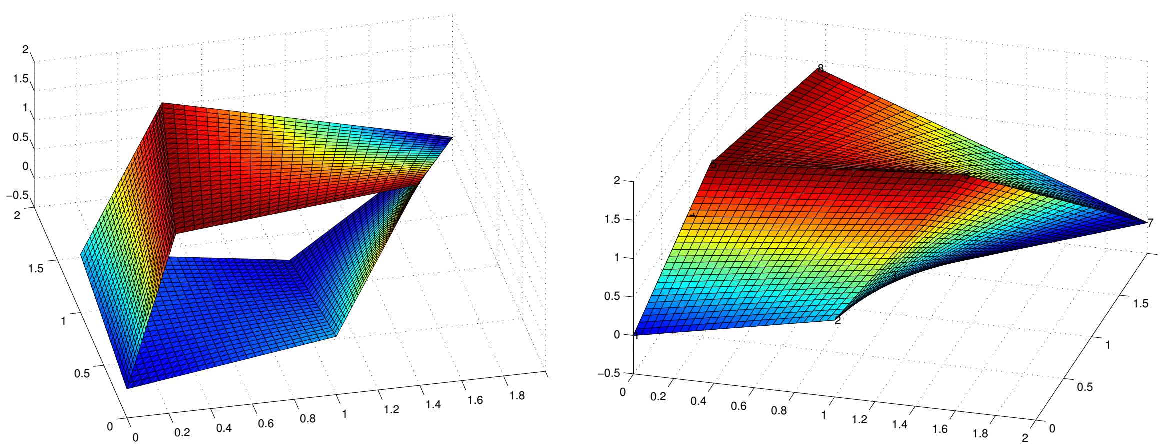
Definition 3.1 The 24-subtetrahedral test is defined as follows [4]. The Jacobian of a trilinear mapping F defined in (1) is positive on $\hat{Q} = [0,1]^3$ if all the 24 Jacobians of P_1 mappings for the edge subtetrahedra in (12) are all positive (see Figures 3 and 4.) ∎

Figure 4: The 2 subtetrahedra at edge $\hat{\mathbf{e}}_6$ (see Figure 3).



Theorem 3.1 *The 24-subtetrahedral test defined in Definition 3.1 is not a necessary condition for the positivity of the Jacobian for the reference Q_1 mapping of the underlying hexahedron. That is, there is a tetrahedron $Q_{v_1v_2v_3v_4v_5v_6v_7v_8}$ having a globally positive Jacobian on $\hat{Q}$ while at least one of the Jacobians for the P_1 mappings for the 24 subtetrahedra listed in (12) is negative.*

Figure 5: A hexahedron having globally positive Jacobian, but negative edge subtetrahedra.



Proof Let Q be the hexahedron defined by the following 8 vertices (see Figure 1).

$$\begin{array}{llll} v_1(0,0,0), & v_2(1,0,0.5), & v_3(1,1,0), & v_4(0,1,0.5) \\ v_5(0.3,0.3,2), & v_6(1.5,0.5,2), & v_7(2,2,-0.1), & v_8(0.5,1.5,2). \end{array} \tag{13}$$

This is a well-shaped hexahedron, obtained by stretching some edges of the unit cube, and twisting. The latter is the reason for producing some negative Jacobians for the 24 subtetrahedra. The 3D pictures of this hexahedron is shown in Figure 5. In the left picture of Figure 5, we did not plot the front and the back faces so that we can view the 8 vertices better. We rotate Q a little further in the right picture of Figure 5. The twist of the hexahedron is shown clearly in this picture.

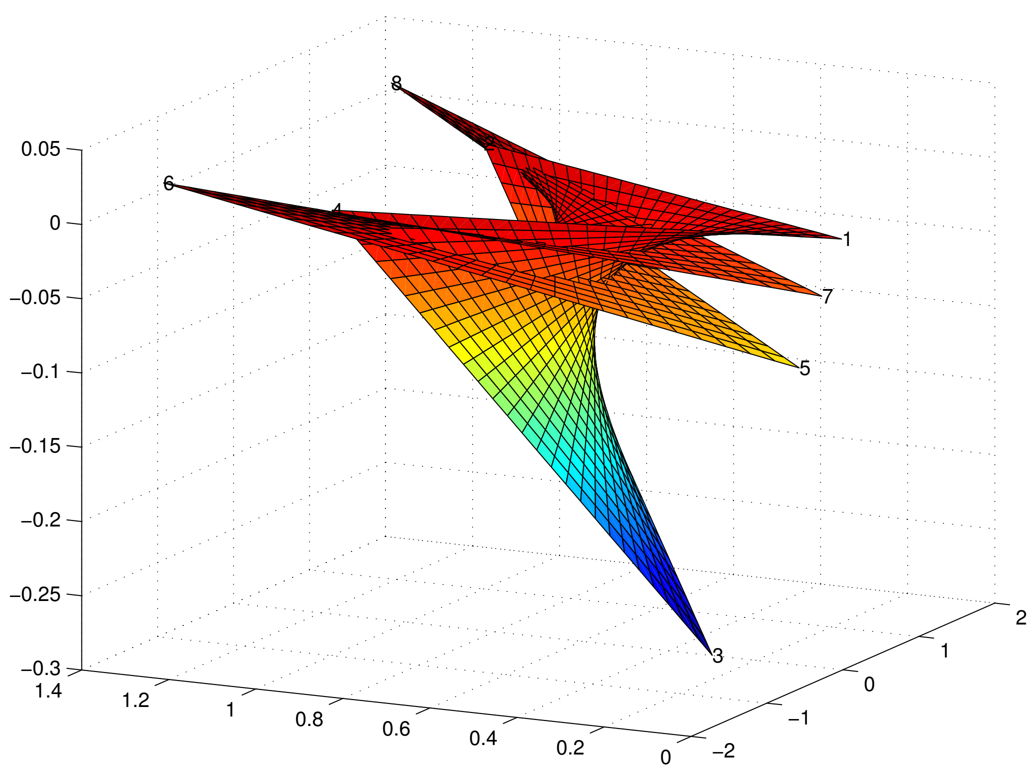
By many means, we can check that the Jacobian J for Q is positive on the whole reference cube $\hat{Q}$. We can compute the Jacobians for the 24 subtetrahedra in (12) and list them below:

$$
\begin{array}{llll}
J_{v_1v_2v_3v_7} = -0.10, & J_{v_2v_3v_4v_8} = 2.00, & J_{v_3v_4v_1v_5} = 2.00, & J_{v_4v_1v_2v_6} = 1.00, \\
J_{v_5v_8v_7v_3} = 1.93, & J_{v_8v_7v_6v_2} = 5.10, & J_{v_7v_6v_5v_1} = 4.03, & J_{v_6v_5v_8v_4} = 2.10, \\
J_{v_2v_1v_5v_8} = 2.25, & J_{v_4v_3v_7v_6} = 2.45, & J_{v_1v_4v_8v_7} = 3.05, & J_{v_3v_2v_6v_5} = 2.05, \\
J_{v_1v_2v_3v_5} = 2.00, & J_{v_2v_3v_4v_6} = 2.00, & J_{v_3v_4v_1v_7} = -0.10, & J_{v_4v_1v_2v_8} = 1.00, \\
J_{v_5v_8v_7v_1} = 4.03, & J_{v_8v_7v_6v_4} = 5.10, & J_{v_7v_6v_5v_3} = 1.93, & J_{v_6v_5v_8v_2} = 2.10, \\
J_{v_5v_1v_4v_6} = 2.25, & J_{v_3v_7v_8v_2} = 2.45, & J_{v_4v_8v_5v_3} = 2.05, & J_{v_2v_6v_7v_1} = 3.05.
\end{array}
$$

The theorem is proven as $J_{v_1v_2v_3v_7}$ and $J_{v_3v_4v_1v_7}$ are negative. ∎

Theorem 3.2 *The 24-subtetrahedral test defined in Definition 3.1 is not a sufficient condition for the positivity of the Jacobian for the reference Q_1 mapping of the underlying hexahedron. That is, there is a tetrahedron $Q_{v_1v_2v_3v_4v_5v_6v_7v_8}$ having a non-positive Jacobian on $\hat{Q}$ while all the 24 Jacobians for the P_1 mappings for the 24 subtetrahedra listed in (12) are positive.*

Figure 6: A negative-Jacobian Q with 24 positive subtetrahedra (top & bottom faces).

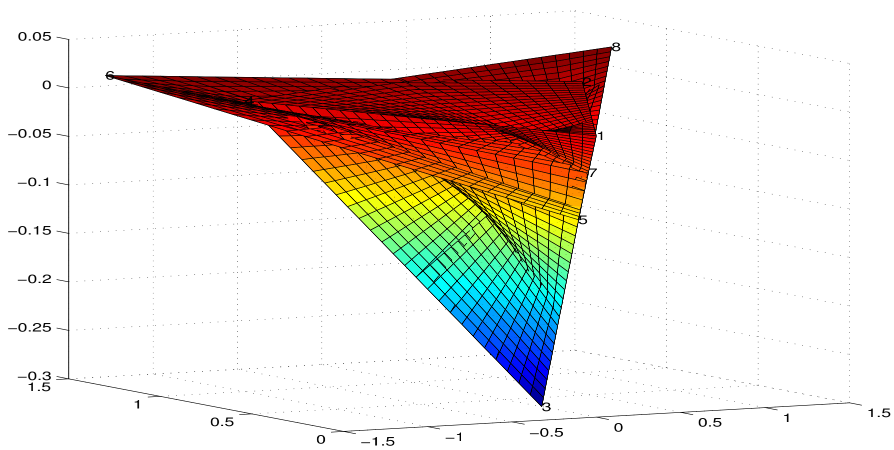


Proof Let Q be the hexahedron defined by the following 8 vertices (see Figure 1 for vertex orientation).

$$\begin{array}{llll} v_1(0,0.002,-0.01), & v_2(1,1,0), & v_3(0,0.3,-0.3), & v_4(-1,1,0), \\ v_5(0,0.1,-0.1), & v_6(-1.5,1.2,0.02), & v_7(0,0.0485,-0.05), & v_8(1.5,1.2,0.02). \end{array} \tag{14}$$

This is a badly-shaped hexahedron. It should not be called a hexahedron probably as its non-flat faces twist and cross each other so much. The 3D pictures of this hexahedron Q is shown in Figures 6 and 7. In Figure 6, we plot only the top and the bottom faces of Q so that we can view the 8 vertices and view the crossing better. From the picture, we can tell that the top face-quadrilateral goes through the bottom face-quadrilateral twice, and that both are of sharp saddle shapes. We rotate Q a little further. and plot it in Figure 7. All 6 faces are plotted. The six faces of the hexahedron cross each other so much and this is shown clearly in Figure 7. We note that the 4 "diagonal" vertices v_1, v_3, v_5 and v_7 are nearly on a same line.

Figure 7: A negative-Jacobian hexahedron with 24 positive edge-subtetrahedra.



The trilinear mapping for the hexahedron Q defined in (14) is not one-to-one, and its Jacobian is negative at most points of $\hat{Q}$. However, all the 24 Jacobians for the 24 subtetrahedra in (12) are all positive for the Q defined in (14) and listed below:

$$\begin{array}{llll} J_{v_1v_2v_3v_7} = .00157, & J_{v_2v_3v_4v_8} = .09200, & J_{v_3v_4v_1v_5} = .00160, & J_{v_4v_1v_2v_6} = .03592, \\ J_{v_5v_8v_7v_3} = .00045, & J_{v_8v_7v_6v_2} = .02709, & J_{v_7v_6v_5v_1} = .00040, & J_{v_6v_5v_8v_4} = .00600, \\ J_{v_2v_1v_5v_8} = .02544, & J_{v_4v_3v_7v_6} = .07019, & J_{v_1v_4v_8v_7} = .10989, & J_{v_3v_2v_6v_5} = .54400, \\ J_{v_1v_2v_3v_5} = .00160, & J_{v_2v_3v_4v_6} = .09200, & J_{v_3v_4v_1v_7} = .00157, & J_{v_4v_1v_2v_8} = .03592, \\ J_{v_5v_8v_7v_1} = .00040, & J_{v_8v_7v_6v_4} = .02709, & J_{v_7v_6v_5v_3} = .00045, & J_{v_6v_5v_8v_2} = .00600, \\ J_{v_5v_1v_4v_6} = .02544, & J_{v_3v_7v_8v_2} = .07019, & J_{v_4v_8v_5v_3} = .54400, & J_{v_2v_6v_7v_1} = .10989. \end{array}$$

As we expected (after seeing Figures 6 and 7), the Jacobian for the hexahedron defined in (14) is not positive on the whole $\hat{Q}$. In fact, it is not even positive at some of the 8 vertices:

$$\begin{array}{llll} J_{v_1v_2v_4v_5} = -0.182, & J_{v_2v_3v_1v_6} = 0.795, & J_{v_3v_4v_2v_7} = -0.501, & J_{v_4v_1v_3v_8} = 0.795, \\ J_{v_5v_8v_6v_1} = 0.332, & J_{v_6v_5v_7v_2} = -0.136, & J_{v_7v_6v_8v_3} = 0.916, & J_{v_8v_7v_5v_4} = -0.136. \end{array}$$

The theorem is proven by y Lemma 2.4, as $J_{v_1v_2v_3v_4}$, for example, is negative. ∎

Remark 3.1 By Theorem 3.2, the subtetrahedral test of [4] fails to ensure a positive Jacobian even after a hexahedron passes the test. This is like many other cases in engineering. For example, the patch test for non-conforming finite elements is not a necessary, nor sufficient condition for a finite element method to provide a convergent solution. But the patch test is used for so long and many years to come. We note that the example of (14) is designed very carefully. It seems such a hexahedron would never be produced by random numbers of computer. It is almost as hard as to get 3 random points in 2D or 3D so that they on a line. Of course, we checked (14) carefully to make sure no wrong result is produced by numerical errors. ∎

4 The improved subtetrahedral test

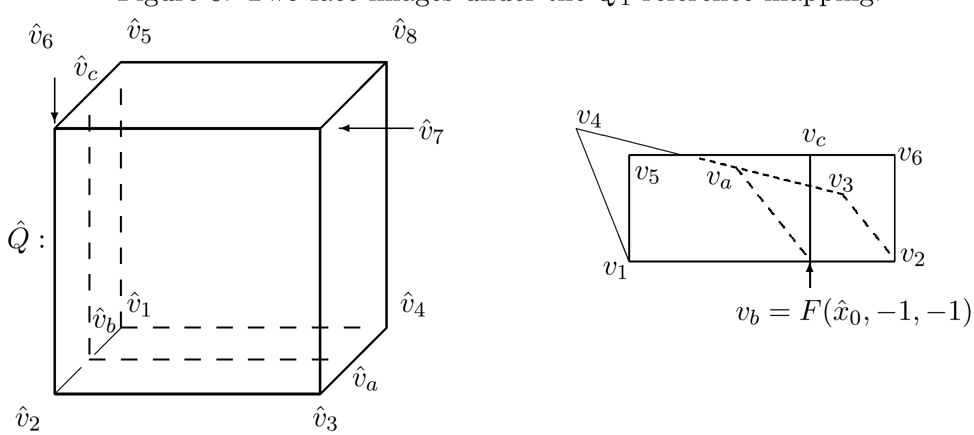
In this section we will modify the subtetrahedral test by extending the list of subtetrahedra for which the Jacobian is to be checked. We then show the new subtetrahedral is a sufficient condition to ensure the global positivity of the Jacobian on hexahedral elements. Therefore, the new subtetrahedral test is truly a working test after the modification. Finally, we will compare the new test with two other existing tests.

Definition 4.1 The 32-subtetrahedral test is defined as follows. The Jacobian of a trilinear mapping F defined in (1) is positive on $\hat{Q} = [0,1]^3$ if all the 32 Jacobians of the P_1 mappings for the 24 subtetrahedra in (12) and for the 8 corner subtetrahedra of Q, i.e.,

$$\begin{aligned} &T_{v_1v_2v_4v_5},\ T_{v_2v_3v_1v_6},\ T_{v_3v_4v_2v_7},\ T_{v_4v_1v_3v_8},\\ &T_{v_5v_8v_6v_1},\ T_{v_6v_5v_7v_2},\ T_{v_7v_6v_8v_3},\ T_{v_8v_7v_5v_4}, \end{aligned} \tag{15}$$

are all positive (see Figures 3 and 4.) ∎

Figure 8: Two face images under the Q_1 reference mapping.



Lemma 4.1 *Let F be the Q_1 reference mapping for a general hexahedron Q shown in Figure 1 such that*

$$F(\hat{v}_i) = v_i, \quad i = 1, 2, ..., 8, a, b, c,$$

where $\hat{v}_a = (\hat{x}_0, 1, -1)$, $\hat{v}_b = (\hat{x}_0, -1, -1)$, and $\hat{v}_c = (\hat{x}_0, -1, 1)$, for some $-1 < \hat{x}_0 < 1$. If (cf. Figure (8) for notations)

$$J_{v_1v_2v_3v_5} > 0, \quad J_{v_1v_2v_4v_5} > 0, \quad J_{v_1v_2v_4v_6} > 0, \quad J_{v_1v_2v_3v_6} > 0$$

then

$$J_{v_1v_bv_av_5} > 0, \quad and \ \ J_{v_1v_bv_av_c} > 0.$$

Proof Because $J_{v_1v_2v_3v_5} > 0$, the point v_5 is on the positive side of triangle $\triangle v_1v_2v_3$, by Lemma 2.2. As $J_{v_1v_2v_3v_6} > 0$, v_6 is on the positive side of $\triangle v_1v_2v_3$ too. See Figure 8. Therefore every point on the line segment v_5v_6 is on the positive side of $\triangle v_1v_2v_3$. In particular, v_c is on the positive side of $\triangle v_1v_2v_3$ and

$$(\overrightarrow{v_1v_2} \times \overrightarrow{v_1v_3}) \cdot \overrightarrow{v_bv_c} > 0. \tag{16}$$

Another way to interpret (16) is that v_3 is on the positive side of $\triangle v_1v_cv_b$. Repeating above steps (symmetrically, in fact), by the two other conditions $J_{v_1v_2v_4v_5} > 0$ and $J_{v_1v_2v_4v_6} > 0$, we conclude that v_4 is also on the positive side of $\triangle v_1v_cv_b$. Therefore, a point, v_a on the line segment v_3v_4 must be also on the positive side of $\triangle v_1v_cv_b$. By Lemma 2.2,

$$(\overrightarrow{v_1v_c} \times \overrightarrow{v_1v_b}) \cdot \overrightarrow{v_1v_a} > 0. \tag{17}$$

(17) is the second inequality to be proved in the theorem, which is also 8 times of the Jacobian $J(\hat{x}_0, -1, -1)$ of the trilinear reference mapping F at point $\hat{v}_b$.

For the first inequality in the theorem, the proof is similar. Because $J_{v_1v_2v_3v_5} > 0$, the point v_3 is on the positive side of the triangle $\triangle v_1v_5v_2$. Because the point v_b is on $\triangle v_1v_5v_2$, v_3 is on the positive side of the triangle $\triangle v_1v_5v_b$ too. Similarly, by $J_{v_1v_2v_4v_5} > 0$, v_4 is on the positive side of $\triangle v_1v_5v_2$ and on the positive side of $\triangle v_1v_5v_b$ consequently. Since v_a is a point on the line segment v_3v_4 and both end points are on the positive side of $\triangle v_1v_5v_b$, we conclude that v_a is on the positive side of $\triangle v_1v_5v_b$ and $J_{v_1v_5v_bv_a} > 0$, which is the first inequality, by Lemma 2.3. ∎

Corollary 4.1 *Let F be the trilinear reference mapping from $\hat{Q}$ to any Q. If Q passes the improved subtetrahedra test defined in Definition 4.1, then the Jacobian for F is positive on all 12 edges of $\hat{Q}$.*

Proof Lemma 4.1 says $J(\hat{x}_0, -1, -1) = \dfrac{1}{8} J_{v_1v_bv_av_c} > 0$ for any $\hat{x}_0 \in [0, 1]$, if Q passes the 32-subtetrahedral test. By rotational symmetry, $J > 0$ on any boundary edge of $\hat{Q}$. ∎

Corollary 4.2 *Let F be the trilinear reference mapping from $\hat{Q}$ to any Q. If Q passes the improved subtetrahedra test defined in Definition 4.1, then the subtetrahedra $Q_{v_1v_bv_cv_4v_5v_cv_dv_8}$ also passes the test, see Figure 8, where, for any $\hat{x}_0 \in [0, 1]$,*

$$v_b = F(\hat{x}_0, -1, -1),\ v_a = F(\hat{x}_0, 1, -1),\ v_d = F(\hat{x}_0, 1, 1),\ v_c = F(\hat{x}_0, -1, 1).$$

Proof By Lemma 4.1, $J_{v_1v_bv_av_5} > 0$, $J_{v_1v_bv_av_c} > 0$, i.e., the Jacobian of one edge-subtetrahedra $T_{v_1v_bv_av_5}$ of (12) and the Jacobian of a corner subtetrahedron $T_{v_1v_bv_av_c}$ are positive. By symmetry, the sub-hexahedron

$$Q_{v_1v_bv_cv_4v_5v_cv_dv_8} = F\left(\{-1 \le \hat{x} \le \hat{x}_0, -1 \le \hat{y} \le 1, -1 \le \hat{z} \le 1\}\right)$$

passes the improved subtetrahedra test as all 32 Jacobians in (12) and (15) are positive. ∎

Corollary 4.3 *Let F be the trilinear reference mapping from $\hat{Q}$ to any Q. If Q passes the improved subtetrahedra test defined in Definition 4.1, then the Jacobian J of F is positive on the boundary $\partial\hat{Q}$.*

Proof To find the sign of the Jacobian at any boundary point, say, without loss of generality, $(\hat{x}_0, \hat{y}_0, -1)$ on the bottom face of $\hat{Q}$, we can apply Lemma 4.1 to the sub-hexahedron

$$Q_1 = F\left(\{-1 \le \hat{x} \le \hat{x}_0, -1 \le \hat{y} \le 1, -1 \le \hat{z} \le 1\}\right)$$

of Q, as Q_1 passes the improved subtetrahedral test too according to Corollary 4.2. Therefore the tetrahedron $v_a v_e v_f v_g$ is positive and consequently the Jacobian of J at $(\hat{x}_0, \hat{y}_0, -1)$ is positive as it is a positive multiple of the Jacobian for the subtetrahedron. Here, see Figure 8, $v_a = F(\hat{x}_0, 1, -1)$, $v_e = F(-1, \hat{y}_0, -1)$,$v_f = F(\hat{x}_0, \hat{y}_0, -1)$, and $v_g = F(\hat{x}_0, \hat{y}_0, 1)$. ∎

Theorem 4.1 *Let F be the trilinear reference mapping from $\hat{Q}$ to a general Q. If Q passes the improved subtetrahedra test defined in Definition 4.1, then the Jacobian J of F is positive everywhere on $\hat{Q}$.*

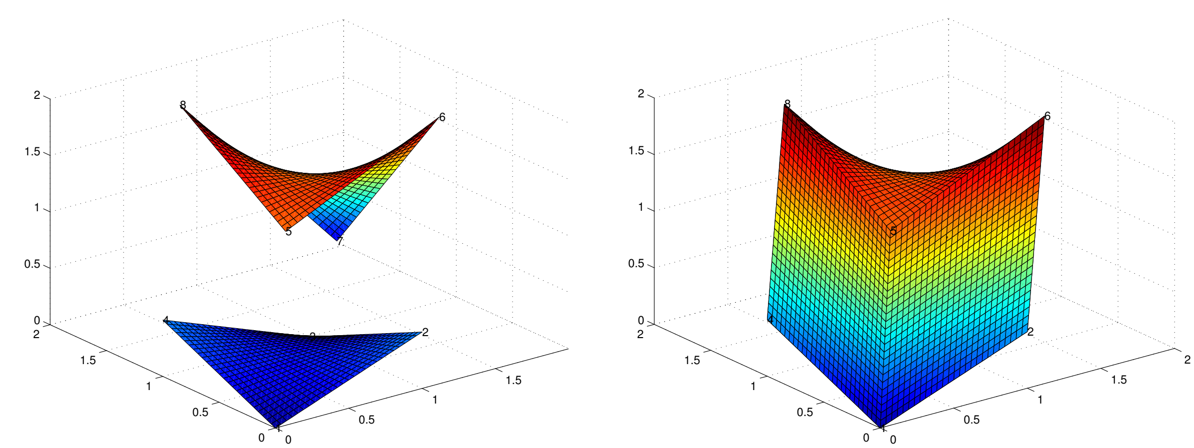
Proof To the Jacobian is positive at any point $(\hat{x}_0, \hat{y}_0, \hat{z}_0)$, we apply Corollary 4.2 to Q, then a sub-hexahedron, and a sub-subhexahedron:

$$\begin{aligned} Q_1 &= F\left(\{-1 \le \hat{x} \le \hat{x}_0, -1 \le \hat{y} \le 1, -1 \le \hat{z} \le 1\}\right), \\ Q_2 &= F\left(\{-1 \le \hat{x} \le \hat{x}_0, -1 \le \hat{y} \le \hat{y}_0, -1 \le \hat{z} \le 1\}\right). \end{aligned}$$

At the end, the point $F(\hat{x}_0, \hat{y}_0, \hat{z}_0)$ is a boundary edge point of Q_2. ∎

Theorem 4.1 ensures that the Jacobian is positive globally if a hexahedron passes the subtetrahedral test, i.e., if 32 Jacobians are positive. Of course, in last section, we have an example showing that the test is not a necessary condition, i.e., if a hexahedron fails the subtetrahedral test, its Jacobian may still be positive everywhere. So one may want to have such a test which works for as more hexahedra as possible, at least, for all well-shaped hexahedra. There are two other tests in literature [10, 11]. These two tests requires the computation of 64 Jacobians of subtetrahedra, while the new test needs only 32. In addition, the other tests need to compute some combinations of the 64 Jacobians and check the positivity of 33 numbers, while our test needs 32 positive Jacobians. To save space, we do not introduce the notations of the other two tests here. Readers can check [10, 11] for details. It is apparent that the new test is much simpler. We will show by an example that the new subtetrahedral test could be powerful than the other tests, i.e., the subtetrahedral test can declare the positivity of the Jacobian for this hexahedron while the other tests fail.

Figure 9: A hexahedron for which the subtetrahedral test works but the [10, 11] tests do not.



We consider the following hexahedron Q (see Figure 1 for vertex orientation).

$$\begin{array}{llll} v_1(0,0,0), & v_2(1,0,0.5), & v_3(1,1,0), & v_4(0,1,0.5), \\ v_5(0.3,0.3,1.5), & v_6(1.5,0.5,2), & v_7(1.8,1.8,0.2), & v_8(0.5,1.5,2). \end{array} \tag{18}$$

The hexahedron Q defined in (18) is a minor perturbation of the Q in (13). So both hexahedra are very well shaped. It would pass nearly any mathematical requirements for shape-regularity of hexahedral elements used in literature. This can be seen from the two pictures in Figure 9. Again, on the left, we plot only the top and the bottom faces, while the whole hexahedron is plotted in the right picture of Figure 9.

We then check the Q in (18) by the subtetrahedral test to conclude its Jacobian is globally positive as all the 32 subtetrahedra in Definition 4.1 are positive:

$$
\begin{array}{llll}
J_{v_1v_2v_3v_7} = 0.200, & J_{v_2v_3v_4v_8} = 2.000, & J_{v_3v_4v_1v_5} = 1.500, & J_{v_4v_1v_2v_6} = 1.000, \\
J_{v_5v_8v_7v_3} = 1.340, & J_{v_8v_7v_6v_2} = 4.200, & J_{v_7v_6v_5v_1} = 2.640, & J_{v_6v_5v_8v_4} = 1.600, \\
J_{v_2v_1v_5v_8} = 1.500, & J_{v_4v_3v_7v_6} = 2.100, & J_{v_1v_4v_8v_7} = 2.600, & J_{v_3v_2v_6v_5} = 1.800, \\
J_{v_1v_2v_3v_5} = 1.500, & J_{v_2v_3v_4v_6} = 2.000, & J_{v_3v_4v_1v_7} = 0.200, & J_{v_4v_1v_2v_8} = 1.000, \\
J_{v_5v_8v_7v_1} = 2.640, & J_{v_8v_7v_6v_4} = 4.200, & J_{v_7v_6v_5v_3} = 1.340, & J_{v_6v_5v_8v_2} = 1.600, \\
J_{v_5v_1v_4v_6} = 1.500, & J_{v_3v_7v_8v_2} = 2.100, & J_{v_4v_8v_5v_3} = 1.800, & J_{v_2v_6v_7v_1} = 2.600, \\
J_{v_1v_2v_4v_5} = 1.200, & J_{v_2v_3v_1v_6} = 1.500, & J_{v_3v_4v_2v_7} = 1.000, & J_{v_4v_1v_3v_8} = 1.500, \\
J_{v_5v_8v_6v_1} = 1.800, & J_{v_6v_5v_7v_2} = 2.900, & J_{v_7v_6v_8v_3} = 3.200, & J_{v_8v_7v_5v_4} = 2.900.
\end{array}
$$

However, when we apply the two tests in [10, 11], we could not draw any conclusion as one of the 31 numbers to be checked there fails to be positive (see [11] for the definitions for the notations):

$$
\begin{aligned}
\alpha_{i_1i_2i_3} =& 1.20,\ 1.50,\ 1.00,\ 1.50,\ 1.80,\ 2.90,\ 3.20,\ 2.90; \\
\sum_{i_k} \beta_{i_li_m}^{ki_k} =& 2.50,\ 4.24,\ 2.20,\ 5.54,\ 2.50,\ 4.24, 2.20,\ 5.54,\ 3.00,\ 4.40,\ 4.40,\ 4.20; \\
2\bar{\kappa}_{000} + 2\bar{\kappa}_{111} =& 12.96; \\
\sum_{i_l,i_m} \gamma_{i_li_m}^{ki_k} =& 2.60,\ 1.54,\ 4.90,\ 5.44,\ 1.54,\ 2.60, 5.44,\ 4.90,\ -1.12,\ 4.40,\ 4.40,\ 5.28.
\end{aligned}
$$

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