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THE FINITE ELEMENT METHOD WITH SEMIREGULAR HERMITE CUBIC TETRAHEDRAL ELEMENTS

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Two-dimensional and three-dimensional simplicial *semiregular* finite elements are very interesting from the theoretical viewpoint and useful for applications: their theory is relatively new, many problems open and modelling constructions with their aid is flexible.

We explain first the notions regular, semiregular and irregular element in the case of triangles. We say that a triangle is *regular* iff it satisfies *minimum angle condition*, i. e. its smallest angle is bounded away from zero. We say that a triangle is *semiregular* iff it satisfies *maximum angle condition*, i. e. the maximum angle of the triangle is less or equal to $\gamma_0 < \pi$. It should be noted that the smallest angle of a semiregular triangle can be arbitrary small. We say that a triangle is *irregular* if it does not satisfy the maximum angle condition. Such triangles can have two angles arbitrarily small. (See Figs. 1-3.)

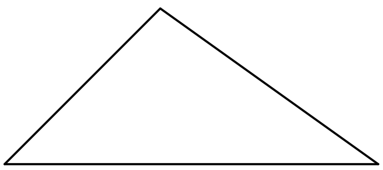

Fig.1. A regular triangle

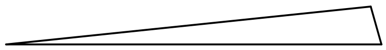

Fig. 2. A semiregular triangle

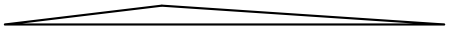

Fig.3. An irregular triangle

In the case of tetrahedra we start with the notion "a semiregular tetrahedron". Its definition is a generalization of the two-dimensional case: A tetrahedron is semiregular iff the maximum angle made by two arbitrary faces is less or equal to $\omega_0 < \pi$. There are three basic types of semiregular tetrahedra (see Figs. 4-6). We say that a tetrahedron is *regular* iff it is semiregular and has regular triangular faces.

A tetrahedron which is not semiregular is called irregular. Such a tetrahedron can have regular triangular faces (see Fig.7, where the tetrahedron has vertices $[0,0,0]$, $[1,0,0]$, $[0,1,0]$ and $[\frac{1}{3},\frac{1}{3},\varepsilon]$; here ε can be arbitrarily small).

Semiregular triangles and tetrahedrons of the Lagrange type (i. e., where function values are considered as parameters only) were studied in many papers (see, for example, [AD], [BA], [BG], [Du], [Gr], [Ja], [Kř1], [Kř2], [Sh], [Sy, pp. 209-213]). This paper is focused on simplexes with cubic polynomials of the Hermite type. Such finite elements have some parameters *standard*: In the case of triangles these parameters are function values and both first partial derivatives prescribed at the vertices – together nine parameters. In the case of tetrahedrons these parameters are function values and three first partial derivatives prescribed at the vertices – together sixteen parameters.

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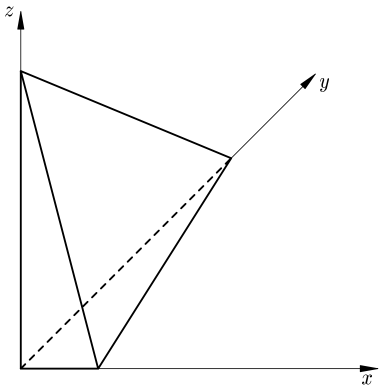

Fig.4. A semiregular tetrahedron of type $K1$

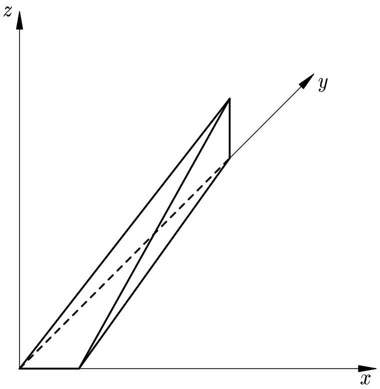

Fig. 5. A semiregular tetrahedron of type $K2$

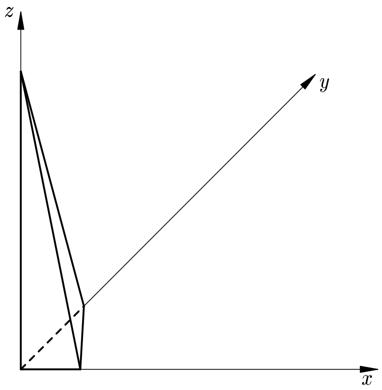

Fig.6. A semiregular tetrahedron of type $K3$

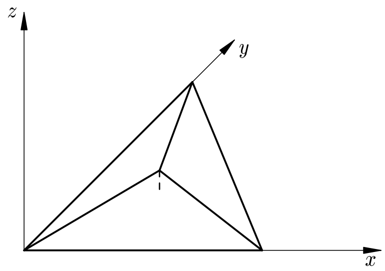

Fig. 7. An Irregular tetrahedron

In the case of cubic Hermite triangles one parameter can be chosen in various ways; the only requirement is its independence on the previous nine parameters. Usually this parameter is the function value at the centre of gravity of the triangle. However, such a choice gives only an estimate for the gradient of the type (see[Zl])

$$\left|\frac{\partial u}{\partial x_k}(P) - \frac{\partial u_I}{\partial x_k}(P)\right| \leq \frac{CM_4}{\sin\alpha_T} h_T^3 \quad \forall P \in \overline{T}, \tag{1}$$

where $u(x_1, x_2)$ is the interpolated function belonging to $C^4(\overline{T})$ and satisfying

$$\left|D^i u(x_1, x_2)\right| \leq M_4\,, \quad |i| = 4, \tag{2}$$

$u_I(x_1, x_2)$ its cubic Hermite interpolant, h_T the length of the greatest side of T and α_T the minimum angle of T; C is a generic constant.

Estimate (1) needs the minimum angle condition. To obtain an estimate suitable for semiregular triangles the choice of the tenth parameter must be more sophisticated. Following [Že] we can choose

$$\frac{\partial u_I}{\partial n_a}(Q) = \frac{\partial u}{\partial n_a}(Q), \tag{3}$$

where Q is the midpoint of the shortest side a of the triangle and n_a the unit normal to this side. In this case we obtain (see [Že])

$$\left|\frac{\partial u}{\partial x_i}(P) - \frac{\partial u_I}{\partial x_k}(P)\right| \leq \frac{CM_4}{\sin\beta} h_T^3 \quad \forall P \in \overline{T}, \tag{4}$$

where β is the second angle of the triangle ($\alpha \leq \beta \leq \gamma$). In [Že] also other possibilities of the choice of the tenth parameter are analyzed.

In the case of tetrahedra the situation is more delicate. We explain why. In the two-dimensional case only nine parameters (prescribed at the vertices) are needed for guaranteeing the C^0-continuity in a triangulation. In the three-dimensional case *all* twenty parameters of the cubic polynomial on a tetrahedron are necessary for guaranteeing the C^0-continuity. This follows from the fact that if two tetrahedra have a common face we need for guaranteeing the C^0-continuity ten parameters on the face – and only nine of them are obtained as linear combinations of the parameters prescribed at the vertices of the common face. Thus the problem how to choose the remaining four parameters on a semiregular tetrahedron is more complicated than in the two-dimensional case. However, it can be shown (see [ŽZ]) that the three-dimensional case is in a certain way a generalization of the two-dimensional case. We present now the main results of [ŽZ].

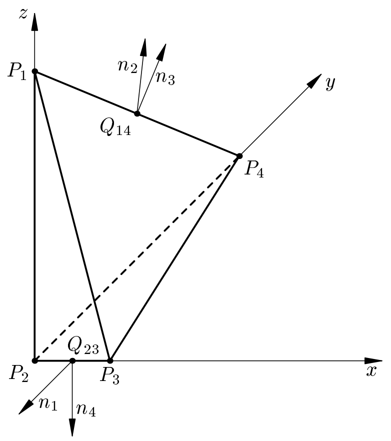

Fig.8 Choosing the normals in the case of $K1$

We shall denote by $P_1, \ldots, P_4$ the vertices of the tetrahedron $\overline{K1}$ (see Fig. 8) and by Q_{ij} the midpoint of the edge P_iP_j. The symbol ϱ_i will denote the plane containing the triangular face $\overline{T}_i$ opposite to the vertex P_i. The symbol n_i denotes the unit normal to the boundary ∂T_i of the triangle $\overline{T}_i$; this normal lies, of course, in the plane ϱ_i.

The symbols α_i ($i = 2, 3, 4$) will denote three angles at the vertex P_1 lying in triangular faces $\overline{T}_2$, $\overline{T}_3$, $\overline{T}_4$. Similarly, β_i ($i = 1, 3, 4$) denote the angles at the vertex P_2, γ_i ($i = 1, 2, 4$) denote the angles at the vertex P_3 and δ_i ($i = 1, 2, 3$) the angles at the vertex P_4. The symbol ω_{ij} will denote the angle made by the planes ϱ_i and ϱ_j.

The main result can be formulated in the following theorem.

THEOREM 0.1. *Let $u \in C^4(\overline{K})$ and let $|D^\alpha u(P)| \leq M_4$ for all $|\alpha| = 4$ and all $P \in K$. Let $p(x, y, z)$ be a polynomial of degree not greater than three which satisfies for $\overline{K} = \overline{K1}$ or $\overline{K} = \overline{K2}$ the relations*

$$D^\alpha p(P_j) = D^\alpha u(P_j) \quad |\alpha| \leq 1 \quad (j = 1, \ldots, 4), \tag{5}$$

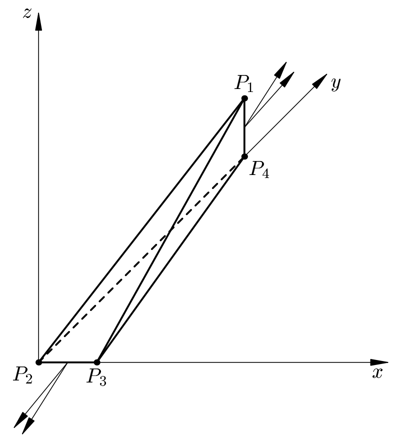

Fig. 9. Choosing the normals in the case of $K2$

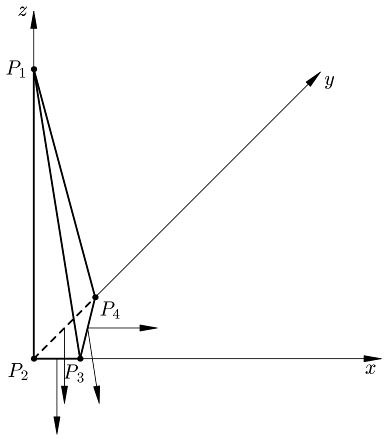

Fig. 10. Choosing the normals in the case of $K3$

$$\begin{aligned}(6)\qquad &\frac{\partial p}{\partial n_1}(Q_{23}) = \frac{\partial u}{\partial n_1}(Q_{23}), \quad \frac{\partial p}{\partial n_2}(Q_{14}) = \frac{\partial u}{\partial n_2}(Q_{14}),\\ &\frac{\partial p}{\partial n_3}(Q_{14}) = \frac{\partial u}{\partial n_3}(Q_{14}), \quad \frac{\partial p}{\partial n_4}(Q_{23}) = \frac{\partial u}{\partial n_4}(Q_{23}).\end{aligned}$$

Then relations (5), (6) determine uniquely the polynomial $p(x,y,z)$ and the function

$$(7)\qquad \varphi(x,y,z) \equiv u(x,y,z) - p(x,y,z)$$

satisfies relations

$$(8)\qquad \left|\frac{\partial\varphi}{\partial x}(A)\right|,\ \left|\frac{\partial\varphi}{\partial y}(A)\right|,\ \left|\frac{\partial\varphi}{\partial z}(A)\right| \le \frac{CM_4h^3}{\sin\omega\sin\sigma} \quad \forall A \in \overline{K1}\,,$$

$$(9)\qquad |\varphi(A)| \le \frac{CM_4h^4}{\sin\omega\sin\sigma} \quad \forall A \in \overline{K1}$$

where in the case of $\overline{K1}$ and $\overline{K2}$ the angles ω and σ are defined by relations

$$(10)\qquad \omega = \min(\omega_{12}, \omega_{24}), \quad \sigma = \min(\alpha_2, \alpha_3, \gamma_1, \gamma_4, \delta_2, \delta_3)\,.$$

The modification of the assumption (6) is in case of $\overline{K3}$ clear and in this case we have

$$(11)\qquad \omega = \min(\omega_{12}, \omega_{23}, \omega_{24}), \quad \sigma = \min(\gamma_1, \gamma_2, \gamma_4, \delta_2, \delta_3)\,.$$

Sketch of the proof

Relations (5)–(7) with $|D^\alpha u(P)| \le M_4$ $(\forall|\alpha| = 4)$ imply

$$(12)\qquad D^\alpha\varphi(P_i) = 0 \quad |\alpha| \le 1 \quad (i = 1,\ldots,4),$$

$$(13)\qquad \frac{\partial\varphi}{\partial n_1}(Q_{23}) = \frac{\partial\varphi}{\partial n_2}(Q_{14}) = \frac{\partial\varphi}{\partial n_3}(Q_{14}) = \frac{\partial\varphi}{\partial n_4}(Q_{23}) = 0\,, l; abel13$$

$$|D^\alpha \varphi(P)| \le M_4 \quad |\alpha| = 4 \quad \forall P \in \overline{K1}\,, \tag{14}$$

At each plane ϱ_i we can choose a Cartesian coordinate system x_i, y_i. The axis z_i belonging to this system is oriented in the direction of the normal to the triangular face $\overline{T}_i$, so that it is not necessary to choose a special symbol for the normals to the triangular faces.

Theorem 0.1 and relations (12) – (14) imply the following estimates:

$$|\varphi(P)| \le CM_4 h^4 \quad \forall P \in \partial K\,, \tag{15}$$

$$\left|\frac{\partial\varphi}{\partial x_i}(P)\right|, \left|\frac{\partial\varphi}{\partial y_i}(P)\right| \le \frac{CM_4h^3}{\sin\sigma} \qquad \forall P \in \overline{T}_i \quad (i = 1, \dots, 4), \tag{16}$$

Relations (12) and (13) imply:

$$\frac{\partial\varphi}{\partial z_j}(P_i) = 0 \quad (i = 1, \dots, 4;\ j = 1, \dots, 4,\ j \ne i)\,, \tag{17}$$

$$\frac{\partial\varphi}{\partial z_1}(Q_{23}) = \frac{\partial\varphi}{\partial z_4}(Q_{23}) = \frac{\partial\varphi}{\partial z_2}(Q_{14}) = \frac{\partial\varphi}{\partial z_3}(Q_{14}) = 0\,. \tag{18}$$

As to the derivatives $\frac{\partial\varphi}{\partial x_i}$ at the midpoints Q_{ij} of edges the preceding results imply after some calculations (see [ŽZ])

$$\left|\frac{\partial\varphi}{\partial z_i}(Q_{jk})\right| \le \frac{CM_4}{\sin\omega\sin\sigma}h^3 \quad (i = 1, \dots, 4; j \ne i, k \ne i, k \ne j). \tag{19}$$

Now we come to the crucial point of our considerations which consists of several applications of the following Lemma 0.2, which was proved in [Zl].

LEMMA 0.2. *Let the function $\psi(x_i, y_i)$ be continuous on a closed triangle $\overline{T}_i$ and have bounded derivatives of third order in its interior T_i by a constant K_3. Further, let $\psi(P_j) = \eta_j$, $\psi(Q_{km}) = \zeta_{km}$, P_j being the vertices of $\overline{T}_i$ and Q_{km} the midpoints of its sides. Then we have on $\overline{T}_i$*

$$|\psi(x_i, y_i)| \le 6\eta + \frac{1}{3}K_3h^3, \quad \eta = \max(|\eta_j|, |\zeta_{km}|). \tag{20}$$

Lemma 0.2 and relations (14), (17), (19) imply the following estimates (we set $\psi = \frac{\partial\varphi}{\partial z_i}$):

$$\left|\frac{\partial\varphi}{\partial z_i}(P)\right| \le \frac{CM_4h^3}{\sin\omega\sin\sigma} \quad \forall P \in \overline{T}_i \quad (i = 1, \dots, 4). \tag{21}$$

As x_i, y_i, z_i are Cartesian coordinate systems, we have in the global Cartesian coordinate system x, y, z, according to (16) and (21):

$$\left|\frac{\partial\varphi}{\partial x}(P)\right|,\ \left|\frac{\partial\varphi}{\partial y}(P)\right|,\ \left|\frac{\partial\varphi}{\partial z}(P)\right| \le \frac{CM_4h^3}{\sin\omega\sin\sigma} \qquad \forall P \in \overline{T}_i \quad (i = 1, \dots, 4). \tag{22}$$

Let $A \in \overline{K1}$ $(A \neq P_1)$ be an arbitrary fixed point and $\varrho(A)$ the plane passing through the point A and parallel with the (x, y)-plane. Let $\overline{T} = \varrho(A) \cap \overline{K1}$. At every point $P \in \partial T$ estimates (22) are satisfied; hence, using again Lemma 0.2, we obtain estimates (8).

In estimating function values we shall use the following lemma which is proved in [Zl, Lemma 5]:

LEMMA 0.3. *Let* $g(0) = \eta_0$, $g(l) = \eta_1$, $g'(0) = k_0$, $g'(l) = k_1$ *and* $|g^{(4)}(s)| \leq K_4$ *in* $(0, l)$. *Then for* $s \in [0, l]$

$$|g(s)| \leq \max |\eta_j| + \frac{4l}{27}(|k_0| + |k_1|) + \frac{K_4}{16 \cdot 24} l^4 .$$

Let $A \in \overline{K1}$ be an arbitrary fixed point for which $A \neq P_1$. Let $B \in \overline{T}_1$ be the point lying on the line passing through P_1, A. Let us set $l = \operatorname{dist}(P_1, B)$ and let us consider the function $g = \varphi\big|_{P_1 B}$. Then, using Lemma 0.3, we obtain estimate (9) from relations (12), (14), (15), (16) (with $i = 1$) and (21) (with $i = 1$).

It remains to prove that relations (5), (6) determine uniquely the polynomial $p(x, y, z)$: If $u(x, y, z)$ is a polynomial of third degree, then $M_4 = 0$ and estimate (4.9) yields $u(x, y, z) = p(x, y, z)$.

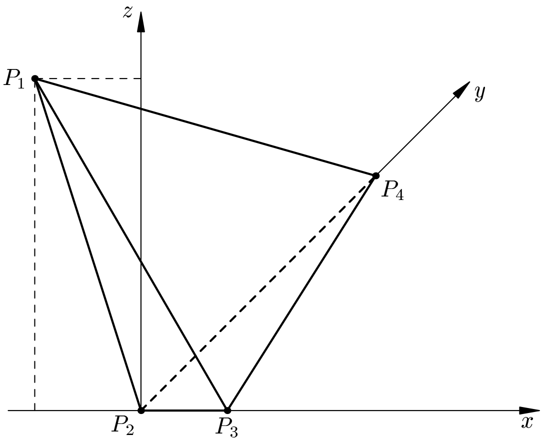

Fig. 11 A general case of type $K1$

Of course Theorem 0.1 holds not only for tetrahedrons $\overline{K1}$, $\overline{K2}$ and $\overline{K3}$ but also for tetrahedrons arising from $\overline{K1}$, $\overline{K2}$ and $\overline{K3}$ by deformation (see, e.g., Fig. 11 where $\operatorname{dist}(P_1, (y, z)) > 0$ and maybe $\operatorname{dist}(P_1, (x, z)) > 0$). The only restriction is that the tetrahedron remains semiregular after this deformation.

The most used tetrahedrons are flat tetrahedrons which arise from $\overline{K1}$ by means of deformation (see Fig. 12). However, in such tetragonalizations the finite element method cannot be used. The explanation is clear from Fig. 13: on a common face of two tetrahedrons the tenth parameters (i.e., normal derivatives) are situated on different sides of the face; thus the continuity of the global function is not guaranteed.

It seems that we have arrived into a closed street. However, there is a remedy which has at least three variants which we shall introduce. The first one is sketched in Fig. 14. Instead of prescribing two normal derivatives at the point Q_{12} in the directions n_{123} and n_{126} we prescribe only one in the normal direction n_{123} which lies in the plane $P_1P_2P_3$. The twentieth parameter in the tetrahedron $P_1P_2P_3P_6$ will be

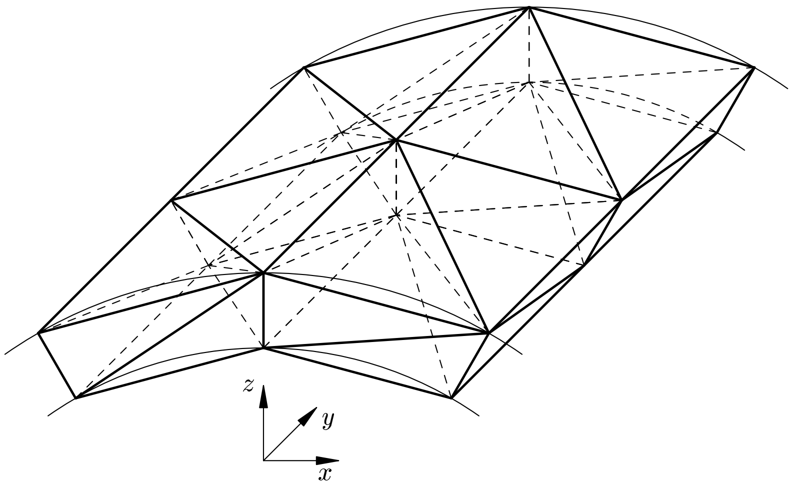

Fig 12 The use of semiregular tetrahedral elements

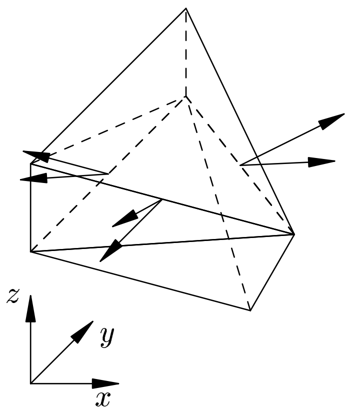

Fig. 13 Disaster

prescribed at the point Q_{26} as the normal derivative in the direction n^*_{126} which lies in the plane $P_1P_2P_6$. This is the only parameter prescribed at the point Q_{26}. Instead of the derivative $\frac{\partial\varphi}{\partial n_{264}}(Q_{26})$ we prescribe the normal derivative $\frac{\partial\varphi}{\partial n^*_{264}}(Q_{46})$. If the tetragonalization has only one layer (see Fig. 12) then we can prescribe at the point Q_{46} the derivative $\frac{\partial\varphi}{\partial n_{456}}(Q_{46})$ (in this case we obtain at this point a better accuracy - see later); however from the symmetry reason we can prescribe the derivative $\frac{\partial\varphi}{\partial n^*_{456}}(Q_{45})$. Doing this we obtain a piecewise polynomial function which is continuous in the polyhedron with six vertices $P_1, \dots, P_6$ which consist of three tetrahedrons $P_1P_2P_3P_6$, $P_1P_2P_6P_4$, $P_2P_6P_4P_5$ with disjoint interiors.

Of course, we must pay something for this change: now a semiregular (flat) tetrahedron cannot have the short edge arbitrarily small; we must assume that (see Fig. 15)

$$\operatorname{dist}(P_2, P_3) = O(h^{1+\varepsilon}), \quad 0 < \varepsilon < 3. \tag{23}$$

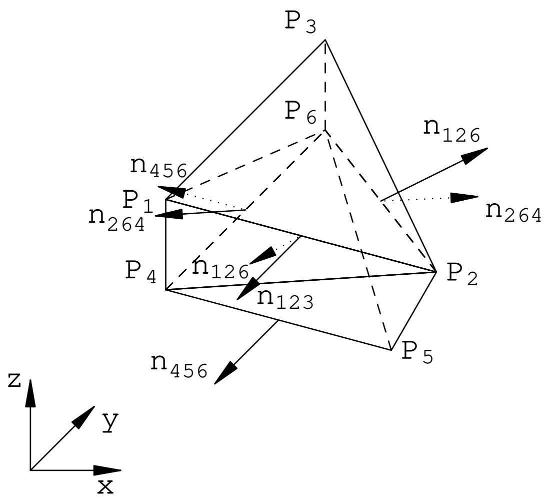

Fig. 14 The remedy

Then

$$\sin \omega_{23} = \frac{O(h^{1+\varepsilon})}{O(h)} \geq Ch^{\varepsilon} \quad (0 < \varepsilon < 3).$$

In applications we usually take (because of error estimates) $\varepsilon = 1$.

Inspecting the proof of Theorem 0.1 we see that at the point Q_{14} (a critical point) we have

$$\left| \frac{\partial \varphi}{\partial z_2}(Q_{14}) \right|, \left| \frac{\partial \varphi}{\partial z_3}(Q_{14}) \right| \leq C^* h^{3-\varepsilon}. \tag{24}$$

Other relations and estimates from (17)–(19) remain without any change. Thus, instead of estimates (8), (9) we derive

$$\left| \frac{\partial \varphi}{\partial x}(A) \right|, \left| \frac{\partial \varphi}{\partial y}(A) \right|, \left| \frac{\partial \varphi}{\partial z}(A) \right| \leq \frac{CM_4 h^{3-\varepsilon}}{\sin \omega \sin \sigma} \quad \forall A \in \overline{K1}, \tag{25}$$

$$|\varphi(A)| \leq \frac{CM_4 h^{4-\varepsilon}}{\sin \omega \sin \sigma} \quad \forall A \in \overline{K1}, \tag{26}$$

where $0 < \varepsilon < 3$.

The second variation: Instead of conditions

$$\frac{\partial \varphi}{\partial n_2}(Q_{14}) = \frac{\partial \varphi}{\partial n_3}(Q_{24}) = 0$$

we prescribe

$$\varphi(S_2) = \varphi(S_3) = 0$$

where S_2 and S_3 are the centers of gravity of the triangular faces T_2 and T_3, respectively. We shall have again one critical point Q_{14} at which (24) hold with a possibly greater constant C^*. Thus we arrive again to estimates (25), (26).

The third variation (the case of the classical parameters for the cubic Hermite tetrahedral finite element): Instead of four normal derivatives (see Fig. 15) we prescribe

$$\varphi(S_i) = 0 \quad (i = 1, \dots, 4)$$

where S_i is the center of gravity of the triangular face T_i $(i = 1, \dots, 4)$. In this case all six midpoints Q_{ij} of edges P_iP_j are critical points; we have instead of (18), (19)

$$\left| \frac{\partial \varphi}{\partial z_i}(Q_{jk}) \right| \le C^* h^{3-\varepsilon} \quad (i = 1, \dots, 4; j \neq i, k \neq i, k \neq j).$$

Estimates (25), (26) again hold; only numerical experiments will show whether the third variation is worse (because of six critical points instead of one).

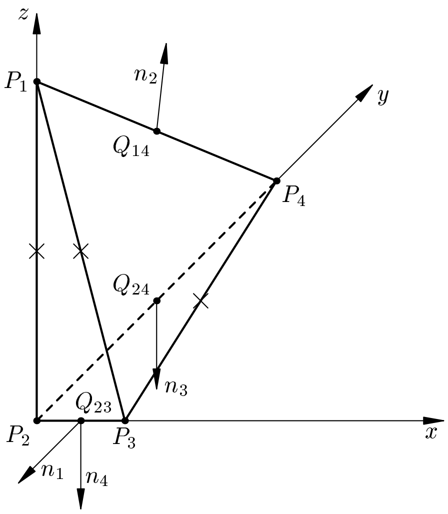

Fig.15 To the estimates (25),(26)

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