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2 authors:

Larisa V. Branets
ExxonMobil

Vladimir A. Garanzha
Russian Academy of Sciences

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Distortion measure of trilinear mapping. Application to 3-D grid generation

L. V. Branets and V. A. Garanzha*,†

Computing Center of Russian Academy of Sciences, Vavilova 40, Moscow 117967, Russia

SUMMARY

Distortion measures for polylinear mappings are investigated. It is shown that certain distortion measures satisfy the maximum principle which allows us to obtain upper bounds on the distortion measures for hexahedral cells and other types of elements widely used in the finite element method. These estimates allow to apply a maximum-norm optimization technique for spatial mappings in the case of finite element grids consisting of hexahedra. A global hexahedral grid untangling procedure suggested earlier was tested on hard 3-D examples demonstrating its ability to work in a black box mode and its high level of robustness. Copyright © 2002 John Wiley & Sons, Ltd.

KEY WORDS: trilinear mapping; distortion measures; hexahedral grid generation; grid untangling; shape recovery

1. DISTORTION MEASURES AND GLOBAL CONDITION NUMBER

It is generally agreed that a grid cell in the finite element method can be described as an image of the mapping of some 'ideal' domain. It is generally agreed as well that this mapping should be non-degenerate. However, more refined estimates require analysis of the properties of these local mappings. There exist many methods for the evaluation of the mapping quality based on the so-called geometric quality measures, the best known one being the minimal angle criteria for triangular finite elements in 2-D.

In the present work, we consider the characterization of the local mappings based on the analysis of algebraic properties of the corresponding Jacobi matrices.

The basic requirements for the quality measures can be formulated as follows:

(1) ability to quantify the deviation of a finite element cell from some 'ideal' cell (say cube or equilateral simplex) in terms of shape and size;
(2) constructivity, i.e. the possibility of practical creation of finite element grids satisfying the quality criteria;

* Correspondence to: V. A. Garanzha, Computing Center of Russian Academy of Sciences, Vavilova 40, Moscow 117967, Russia.
† E-mail: garan@ccas.ru

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(3) simplicity;
(4) maximum principle.

The last property means that satisfying the quality criteria in a finite set of 'measurement points' or 'quadrature nodes' for special classes of mappings common in finite element analysis should be enough to obtain uniform quality estimates of the mapping. In fact property (4) provides the relationship between the cell quality measure, which is a discrete characteristics, and the mapping quality measure, which is a continuous characteristic.

It is convenient to define the quality measure as a dimensionless function in the sense that it is equal to 0 for a degenerate cell and is equal to 1 for a cell with a given volume and shape. In what follows, the inverse of this measure, obviously belonging to the range $[1;\infty)$ will be called the distortion measure.

Let us consider a spatial non-degenerate mapping defined by

$$\mathbf{r}=\mathbf{r}(\xi_1,\ldots,\xi_n), \quad \mathbf{r}=(x_1,\ldots,x_n)^{\mathrm{T}} \tag{1}$$

which maps an 'ideal' domain D, say the unit hypercube, in logical co-ordinates $\{\xi_1,\ldots,\xi_n\}$ onto a domain Ω in physical co-ordinates.

In order to describe the above mapping, we will use the following notations:

$$S=(\mathbf{g}_1,\ldots,\mathbf{g}_n), \quad \mathbf{g}_i=\frac{\partial\mathbf{r}}{\partial\xi_i}$$

where S is the Jacobi matrix of mapping (1) and $\mathbf{g}_i$ are the covariant basis vectors. Let us introduce the matrix $H=H(\xi)$, $\det H>0$, quite arbitrary at this point, such that $H^{\mathrm{T}}H$ has the meaning of an 'accompanying' metrics defined in the logical space and let

$$A=H^{-\mathrm{T}}S^{\mathrm{T}}$$

Let us introduce the following scalar functions of matrices

$$\mu(A)=\frac{1}{2}\left(\frac{\det A}{v}+\frac{v}{\det A}\right), \quad \beta(A)=\frac{(1/n\,\mathrm{tr}(AA^{\mathrm{T}}))^{n/2}}{\det A} \tag{2}$$

where $\mu(A)$ is the volumetric distortion measure of mapping (1), $\beta(A)$ is the shape distortion measure of mapping (1) and v is the constant volumetric factor. The function $\beta^{1/n}$ is actually the shape distortion measure introduced by Reshetnyak [1] in the context of the theory of mappings with a bounded distortion.

Using the above functions it is possible to define the overall distortion measure as follows [2]:

$$E_\theta(A)=\theta\mu(A)+(1-\theta)\beta(A) \tag{3}$$

where θ is a parameter, $0<\theta<1$. An important property of the function $E_\theta(A)$ is that it is possible to obtain the following minimax bounds on the eigenvalues of the matrix AA^{T} when the distortion measure E_θ is bounded from above [2]:

$$\gamma^2 v^{2/n} I<AA^{\mathrm{T}}<\Gamma^2 v^{2/n} I, \quad \Gamma=\frac{1}{\gamma}, \quad \gamma>0 \tag{4}$$

which is a crucial property of mappings in grid generation [3].

And vice versa, uniform eigenvalue bounds for the matrix AA^{T} allow to obtain a uniform upper bound of the distortion measure E_θ. It is also important that in the limit case of an ideal mapping when $E_\theta(A)=1$ we get $\gamma=1,\ \Gamma=1$.

We will refer to the value Γ/γ as the isometric condition number or the global condition number which underlines the fact that bounds (4) are valid for all admissible values of ξ_i.

Among all mappings (1) the most interesting are those which minimize the ratio Γ/γ, while satisfying specified boundary conditions or other constraints.

The distortion measure E_θ satisfies criteria (1)–(3) formulated above. We will show that it also satisfies the maximum principle in the above sense when low-order isoparametric finite elements are considered.

2. THE ALGEBRAIC PROPERTIES OF THE DISTORTION MEASURE

Let us introduce the following definitions:

(1) Let us define the so-called 'boolean' partition of the unity matrix into k parts the set of matrices $I_1^v,\dots,I_k^v$ with the following properties: every matrix I_j^v is a diagonal matrix with only zero and unit elements and the sum of these matrices is equal to the unity matrix $\sum_{j=1}^k I_j^v = I$. The subindex for the matrix I_j^v shows its position in the set, the superindex shows the partition number. There are k^n different 'boolean' partitions of the unity $n\times n$ matrix into k parts (number of words with length n from the alphabet with length k), hence $v\in\{1,2,\dots,k^n\}$.

(2) Let us denote by the k-ary composition of matrices $S_1,\dots,S_k$ the matrix

$$\tilde{S}_v=\sum_{j=1}^{k} S_j I_j^v$$

which corresponds to some 'boolean' partition v, i.e. $\tilde{S}_v$ is the matrix with ith column being the ith column of any matrix from the set $S_1,\dots,S_k$. The number of such 'composite' matrices is equal to k^n as well.

Using these definitions we can formulate the following theorem.

Theorem 1

Let for any m-ary composition $\tilde{S}_v=\sum_{j=1}^m S_j I_j^v$ of $n\times n$ matrices $S_1,\dots,S_m$ the following inequalities hold:

$$E_\theta(\tilde{S}_v)\leqslant C,\quad \det\tilde{S}_v>0$$

Let

$$S=\sum_{j=1}^{m} S_j\Lambda_j,\qquad \sum_{j=1}^{k}\Lambda_j=I,\quad \Lambda_j\geqslant 0 \tag{5}$$

where Λ_j are the diagonal matrices, then

$$\det S>0\quad\text{and}\quad E_\theta(S)\leqslant C \tag{6}$$

Moreover, there exist coefficients $a_v \geqslant 0$, $\sum_{v=1}^{m^n} a_v = 1$, such that

$$E_\theta(S) \leqslant \sum_{v=1}^{m^n} a_v E_\theta(\tilde{S}_v) \tag{7}$$

Proof
The positiveness of the determinant of S follows directly from the formula of the determinant decomposition with respect to column sums.

For any feasible S the distortion measure $E_\theta(S)$ satisfies the following Legendre–Hadamard (strong ellipticity) condition [4]

$$\sum_{i,j,k,m=1}^{n} \frac{\partial^2 E_\theta(S)}{\partial s_{ik}\, \partial s_{jm}}\, t_i t_j\, p_k\, p_m > 0$$

where s_{ij} are entries of the matrix S and t_i, p_i are non-zero real numbers. Since E_θ is a smooth function of S, the ellipticity condition is equivalent to the following rank one convexity condition

$$E_\theta(\lambda_1 S_1 + \lambda_2 S_2) < \lambda_1 E_\theta(S_1) + \lambda_2 E_\theta(S_2), \qquad \lambda_i > 0, \quad \lambda_1 + \lambda_2 = 1, \quad \operatorname{rank}(S_1 - S_2) = 1 \tag{8}$$

Obviously, this convexity condition is valid in the case of a matrix sum with multiple terms provided that the difference between any two matrices has rank less or equal to 1, say

$$E_\theta\left(\sum_{i=1}^{P} \lambda_i S_i\right) \leqslant \sum_{i=1}^{P} \lambda_i E_\theta(S_i), \quad \lambda_i \geqslant 0, \qquad \sum_{i=1}^{P} \lambda_i = 1, \quad S_i = (U, \mathbf{s}_i, V) \tag{9}$$

where $U \in \mathbb{R}^{n\times(p-1)}$, $V \in \mathbb{R}^{n\times(n-p)}$ and $\mathbf{s}_i \in \mathbb{R}^n$. The matrix $S = \sum_{j=1}^{m} S_j \Lambda_j$ can be written as follows:

$$S = \sum_{j=1}^{m} S_j \Lambda_j = \sum_{j=1}^{m} \mu_j^p \Xi_j^p, \quad \mu_j^p = (\Lambda_j)_{pp}, \qquad \sum_{j=1}^{m} \mu_j^p = 1, \quad \mu_j^p \geqslant 0$$

$$\Xi_j^p = (\text{first } p-1 \text{ columns of } S, (S_j)_p, \text{ last } n-p \text{ columns of } S)$$

where $(S_j)_p$ denotes pth column of the matrix S_j.

Applying the above expansion to the matrix S with $p = 1$ we obtain a convex sum, where for each term $E_\theta(\Xi_j^1)$ the second column can be used in order to generate a representation (9) which in turn allows to represent $E_\theta(\Xi_j^1)$ via the convex sum of simpler terms. Repeating this procedure $n-1$ times we arrive at elementary terms which do not allow further decomposition and these terms are precisely those defined in the k-ary composition of the matrix S. Since a composition of convex sums with the sum of coefficients equal to 1 is again a convex sum with unit sum of coefficients, the theorem is proved. □

This theorem has the following important implications. If the Jacobi matrix of a mapping can be presented in form (5), then the m-ary composition provides the set of 'composite bases' or 'quadrature points' where the distortion measure should be bounded from above to guarantee uniform mapping distortion bounds which is essentially the maximum principle (4).

3. VARIATIONAL PRINCIPLE FOR MAXIMUM-NORM MINIMIZATION OF DISTORTION MEASURE

In Reference [2] it was suggested to introduce the parametrized feasible set $\mathscr{F}(t)$, consisting of mappings with a quality above a threshold value t via inequalities

$$\det A > 0, \quad E_\theta(A) < 1/t \tag{10}$$

Then $\mathscr{F}(0)$ denotes the set of non-degenerate mappings and $\mathscr{F}(1)$ is the isometric mapping. The practical implementation strategy for the minimization of $E_\theta(A)$ is to construct such a functional which after discretization has an infinite barrier on the boundary of the feasible set $\partial\mathscr{F}(t)$ and then to 'contract' this set which means to find the grid with maximum possible quality measure $t = t_{\max}$.

Let us consider the following minimization problem [2]

$$\arg \min_{\mathbf{r}(\xi)} \int_{\mathscr{D}} f(A)\, \mathrm{d}\xi \tag{11}$$

where

$$f(A) = (1-t) \det H \, \frac{\phi(A)}{\det A - t\phi(A)} \tag{12}$$

$$\phi(A) = (1-\theta)\left(\frac{1}{n}\operatorname{tr}(AA^{\mathrm{T}})\right)^{n/2} + \frac{\theta}{2}\left(v + \frac{(\det A)^2}{v}\right), \quad 0<\theta<1$$

Volumetric factor is given by

$$v = \int_{\mathscr{D}} \det S \, \mathrm{d}\xi \Big/ \int_{\mathscr{D}} \det H \, \mathrm{d}\xi$$

when the volume of the domain Ω is known, otherwise v is specified *a priori*.

The minimization problem (11), (12) makes sense inside the feasible set (provided that this feasible set is not empty) defined by the inequality

$$\det A - t\phi(A) > 0 \tag{13}$$

4. DISCRETIZATION OF THE FUNCTIONAL IN THE 3-D CASE

In order to discretize functional (11) a conventional finite element procedure is applied where the local mapping in each cell is assumed to be linear or polylinear.

We consider only the 3-D case when $n=3$. Suppose that the valid connectivity structure of the grid is defined by N_c grid cells. In the cell number c, let us denote the vector of all cell vertices by

$$\mathbf{R}_c^{\mathrm{T}} = ({\mathbf{X}_c^1}^{\mathrm{T}}, {\mathbf{X}_c^2}^{\mathrm{T}}, {\mathbf{X}_c^3}^{\mathrm{T}}), \quad \mathbf{X}_c^i \in \mathbb{R}^{N_{cv}}$$

where N_{cv} is the number of vertices in the single grid cell.

If the cell $\mathscr{D}_c$ is defined by the ordered set of N_{cv} integer numbers $v_1(c), \ldots, v_{N_{cv}}(c)$, which are the pointers to the cell vertices in the total list of the grid nodes, then the following equality holds

$$\mathbf{X}_c^i = \mathscr{R}_c \mathbf{X}^i, \quad \mathscr{R}_c = \{r_{ij}\}, \quad r_{ij} = \begin{cases} 1, & j = v_i(c) \\ 0, & j \neq v_i(c) \end{cases} \quad \mathscr{R}_c \in \mathbb{R}^{N_{cv} \times N_v}$$

Using the above notations the discrete counterpart of problem (11) can be formulated as follows: find the vector $\mathbf{R}$ as the solution to the following minimization problem:

$$\mathbf{R} = \arg\min_{\mathbf{R}} \mathscr{I}^h, \quad \mathscr{I}^h = \sum_{c=1}^{N_c} \sum_{q(c)=1}^{N_q} f(A)|_{q(c)} \sigma_{q(c)} \tag{14}$$

$$A = (\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3), \;\; \mathbf{a}_i|_{q(c)} = H_{q(c)}^{-\mathrm{T}} Q_{q(c)} \mathscr{R}_c \mathbf{X}^i.$$

Here subscript $q(c)$ denotes qth 'quadrature node' for the integral over the cell $\mathscr{D}_c$, N_q matrices $Q_{q(c)}$ actually describe the discretization of functional (11) on each element and $\sum_{q(c)=1}^{N_q} \sigma_{q(c)} = 1, \;\; \sigma_{q(c)} > 0$.

The feasible set $\mathscr{F}^h(t)$ is defined by $N_c N_q$ non-linear inequalities

$$\det A - t\phi(A)|_{q(c)} > 0 \tag{15}$$

The volumetric factor v is specified *a priori or* is defined by

$$v = \sum_{c=1}^{N_c} \int_{\mathscr{D}_c} \det S \, \mathrm{d}\xi \Bigg/ \sum_{c=1}^{N_c} \int_{\mathscr{D}_c} \det H \, \mathrm{d}\xi$$

when the volume of computational domain is known.

In order to take into account the boundary conditions we seek $\mathbf{R}$ as follows: $\mathbf{R} = (I - B)\mathbf{R}_{\mathrm{b}} + B\mathbf{R}_{\mathrm{in}}$, where $B \in \mathbb{R}^{N_v \times N_v}$ is a diagonal matrix with entries b_{ij}, such that $b_{ii} = 1$, if the ith node of the grid is the internal one, i.e. its co-ordinates are unknown, and $b_{ii} = 0$, when ith grid node lies on the boundary and is fixed. $\mathbf{R}_{\mathrm{in}}$, $\mathbf{R}_b$ are the unknown vector and the given vector satisfying the boundary conditions, respectively.

4.1. Tetrahedral cells

The mapping of the 'ideal' tetrahedron with vertices $\mathbf{l}_1, \mathbf{l}_2, \mathbf{l}_3, \mathbf{l}_4$ in logical co-ordinates onto the tetrahedron with vertices $\mathbf{v}_1, \mathbf{v}_2, \mathbf{v}_3, \mathbf{v}_4$ in physical co-ordinates is linear and can be written via the natural co-ordinates [5] resulting in the following equality:

$$\begin{pmatrix} 1 \\ x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} 1 & 1 & 1 & 1 \\ \mathbf{v}_1 & \mathbf{v}_2 & \mathbf{v}_3 & \mathbf{v}_4 \end{pmatrix} \begin{pmatrix} 1 & 1 & 1 & 1 \\ \mathbf{l}_1 & \mathbf{l}_2 & \mathbf{l}_3 & \mathbf{l}_4 \end{pmatrix}^{-1} \begin{pmatrix} 1 \\ \xi_1 \\ \xi_2 \\ \xi_3 \end{pmatrix} \tag{16}$$

The basis vectors of such a mapping are constant and, consequently, the function E_θ is constant. If E_θ satisfies (10), the local estimates on γ, Γ for this mapping are obviously true. However, if $1/t$ is a uniform upper bound for the distortion E_θ of every tetrahedra present in the grid then γ, Γ represent the global condition number of the grid.

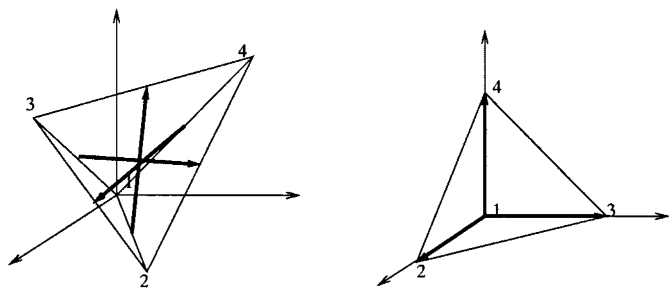

Figure 1. Equilateral tetrahedron and rectangular tetrahedron inscribed in unit cube. Covariant basis vectors are shown in bold.

For example, if we consider equilateral tetrahedron in a logical space as the ideal one (see Figure 1(left)), then the covariant basis vectors of mapping (1) are written as

$$\mathbf{g}_1 = \tfrac{1}{2}(\mathbf{v}_2 + \mathbf{v}_3 - \mathbf{v}_1 - \mathbf{v}_4), \quad \mathbf{g}_2 = \tfrac{1}{2}(\mathbf{v}_2 + \mathbf{v}_4 - \mathbf{v}_1 - \mathbf{v}_3), \quad \mathbf{g}_3 = \tfrac{1}{2}(\mathbf{v}_3 + \mathbf{v}_4 - \mathbf{v}_1 - \mathbf{v}_2)$$

The quadrature rule in this case looks as follows:

$$Q = \frac{1}{2}\begin{pmatrix} -1 & 1 & 1 & -1 \\ -1 & 1 & -1 & 1 \\ -1 & -1 & 1 & 1 \end{pmatrix}, \quad N_q = 1, \quad \sigma_i = 1 \tag{17}$$

For a rectangular corner tetrahedron (see Figure 1(right)) we get

$$\mathbf{g}_1 = \mathbf{v}_2 - \mathbf{v}_1, \quad \mathbf{g}_2 = \mathbf{v}_3 - \mathbf{v}_1, \quad \mathbf{g}_3 = \mathbf{v}_4 - \mathbf{v}_1$$

$$Q = \begin{pmatrix} -1 & 1 & 0 & 0 \\ -1 & 0 & 1 & 0 \\ -1 & 0 & 0 & 1 \end{pmatrix}, \quad N_q = 1, \quad \sigma_i = 1 \tag{18}$$

If the target shape of the tetrahedron is not one of the above basic types, then we should introduce the matrix H as the Jacobi matrix for the mapping of the ideal tetrahedron onto a target tetrahedron (Figure 2). This mapping is again defined by equality (16) so H is written as follows:

$$H = \left(\begin{pmatrix} 1 & 1 & 1 & 1 \\ \mathbf{w}_1 & \mathbf{w}_2 & \mathbf{w}_3 & \mathbf{w}_4 \end{pmatrix} \begin{pmatrix} 1 & 1 & 1 & 1 \\ \mathbf{l}_1 & \mathbf{l}_2 & \mathbf{l}_3 & \mathbf{l}_4 \end{pmatrix}^{-1} \right)_{2:4}$$

i.e., H is obtained from a 4×4 matrix by eliminating its first row and first column. Here $\mathbf{w}_1, \ldots, \mathbf{w}_4$ are the Cartesian co-ordinates of the vertices of the target tetrahedron. When the target shape is specified, the discrete functional does not depend on the choice of the ideal tetrahedron in logical space and the simplest expressions for the functional are obtained when

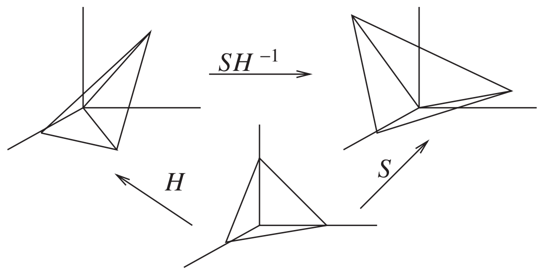

Figure 2. Prescription of target shape for tetrahedra via composition of mappings.

the rectangular corner tetrahedron is chosen as the ideal one. Then the matrix H is defined simply as

$$H = (\mathbf{w}_2 - \mathbf{w}_1 \quad \mathbf{w}_3 - \mathbf{w}_1 \quad \mathbf{w}_4 - \mathbf{w}_1)$$

So, when, for example, the equilateral tetrahedron is the target shape we get

$$H = \begin{pmatrix} 1 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 1 \end{pmatrix}, \quad H^{-\mathrm{T}} = \frac{1}{2} \begin{pmatrix} 1 & 1 & -1 \\ -1 & 1 & 1 \\ 1 & -1 & 1 \end{pmatrix}$$

4.2. Hexahedral cell

The trilinear mapping of a unit cube on the hexahedral cell with straight edges can be written as follows:

$$\mathbf{r}(\xi_1, \xi_2, \xi_3) = \sum_{i,j,k=0}^{1} (1-\xi_1)^{1-i} \xi_1^i (1-\xi_2)^{1-j} \xi_2^j (1-\xi_3)^{1-k} \xi_3^k \mathbf{r}(i,j,k) \tag{19}$$

where $\mathbf{r}(i,j,k)$ denotes the vectors of the co-ordinates of the cell vertices in the lexicographic numbering and $0 \leqslant \xi_i \leqslant 1$.

It can be shown that the Jacobi matrix of the trilinear mapping can be written as follows:

$$S = \sum_\alpha S_\alpha \Lambda_\alpha, \quad \Lambda_\alpha \geqslant 0, \quad \sum_\alpha \Lambda_\alpha = 1$$

where every Λ_α is a diagonal matrix and the sum contains 4 different terms. The above equality is simply the matrix formulation of the well-known fact that each basis vector $\mathbf{g}_i$ of the trilinear mapping is constant on the edges $\xi_i = 0$ or $\xi_i = 1$ and is a linear convex combination of the edge basis vectors of the same family in any point inside the trilinear cell.

In order to apply Theorem 1 and thus to evaluate the distortion measure of the trilinear mapping it is sufficient to evaluate the $E_\theta(S)$ on 64 different composite matrices $\tilde{S}_v = \sum_\alpha S_\alpha I_\alpha^v$. The vectors constituting the columns of the composite matrices are shown in bold in Figure 3.

The remaining 60 triples can be obtained from the above ones by rotation and reflection in logical co-ordinates (when reflecting the orientation should be changed to retain right basis).

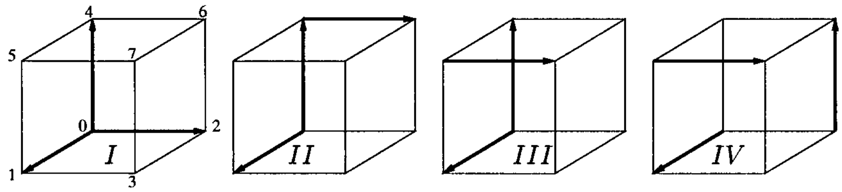

Figure 3. Construction of composite matrices for trilinear mapping.

The exact expressions for matrices Q for approximation, based upon $N_q = 64$, can be easily obtained from (19). For example the columns of the composite matrix $\tilde{S}_0$ are given by (see Figure 3,I)

$$\begin{aligned} \tilde{\mathbf{g}}_1 &= \mathbf{r}_1 - \mathbf{r}_0 \\ \tilde{\mathbf{g}}_2 &= \mathbf{r}_2 - \mathbf{r}_0, \\ \tilde{\mathbf{g}}_3 &= \mathbf{r}_4 - \mathbf{r}_0 \end{aligned} \qquad Q = \frac{1}{27}\begin{pmatrix} -1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ -1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ -1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \end{pmatrix}$$

Here it is assumed that the numbering of the cell vertices in Figure 3 is related to triple indexing in (19) via

$$\mathbf{r}_{4i+2j+k} = \mathbf{r}(i, j, k)$$

The composite matrices shown in the figure above constitute a quadrature rule with the following weights:

$$\sigma_{\mathrm{I}} = \frac{1}{27}, \quad \sigma_{\mathrm{II}} = \frac{1}{2 \cdot 27}, \quad \sigma_{\mathrm{III}} = \frac{1}{4 \cdot 27}, \quad \sigma_{\mathrm{IV}} = \frac{1}{8 \cdot 27}$$

which guarantees the patch test property for the resulting approximation.

The target shape specification for a hexahedron is more complicated compared to tetrahedra. It can be done as well via composition of mappings and matrix H (Figure 4). However, for the sake of compatibility H by itself should be the Jacobi matrix of a trilinear mapping so its entries are the functions of ξ_1, ξ_2, ξ_3.

The most natural way for a hexahedron shape prescription is to construct the same set of elementary composite matrices $\tilde{H}_v$ for H and to consider the distortion measures of the matrices $\tilde{H}_v^{-1}\tilde{S}_v$ as the distortion measure of deviation from the target shape given by $E_\theta(H(\xi)^{-1}S(\xi))$. There is a hypothesis which is not proved yet, this research is under way, that Theorem 1 can be generalized to cover the presence of the matrix $H(\xi)$. Obviously, Theorem 1 is true when H is constant on the cell; however, in this case the target cell shape is just an affine cell which severely restricts the class of allowable deformations.

In order to reduce computational costs one should use a simplified approximation of a cell distortion based on some set of quadrature rules. For example, one can use an approximation based on 8 quadrature points in the hexahedron vertices and one central node, or even the simplest approximation consisting of 4 tetrahedra per trilinear cell, which is barely enough to fix the target shape of the hexahedral cell.

The same reasoning can be directly applied to the general case of polylinear mappings covering quadrilateral cells, prisms and various low-order finite elements in higher dimensions. The Jacobi matrix for all these mappings can be shown to take form (5).

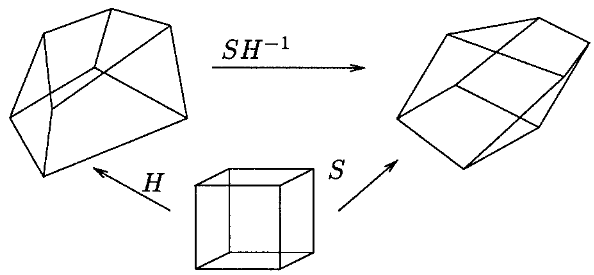

Figure 4. Prescription of target shape for hexahedra via composition of trilinear mappings.

The important consequence of Theorem 1 for the distortion measure E_θ is that the recursive subdivision of the hexahedron into smaller ones, induced by uniform subdivision of a cube into smaller cubes, cannot increase the upper bound on the distortion provided that coefficient v is changed in a consistent manner.

Thus with uniform cell refinement the global upper bound for distortion measures of all grid cells cannot increase, which in turn means that the global condition number remains bounded.

5. SOLUTION TECHNIQUE

In order to solve the discrete minimization problem (14) we use a preconditioned gradient method coupled with a line search technique. The key ingredient of this algorithm is the choice of a non-linear preconditioning and the solution technique for the linear systems arising in the resulting implicit method. To this end we use an approach suggested in Reference [6], where a symmetric positive definite approximation of the Hessian matrix of functional (14) was constructed analytically and an efficient and robust iterative linear solver from Kaporin [8] was used.

Let us define the following matrices:

$$P_{ii} = \frac{\partial^2 f}{\partial \mathbf{a}_i^{\mathrm{T}} \partial \mathbf{a}_i}$$

Since the target functional possesses the strong ellipticity property, we get $P_{ii} = P_{ii}^{\mathrm{T}} > 0$. The reduced Hessian matrix of (14) is assembled as follows:

$$\tilde{\mathscr{H}} = \begin{pmatrix} \tilde{\mathscr{H}}_{11} & 0 & 0 \\ 0 & \tilde{\mathscr{H}}_{22} & 0 \\ 0 & 0 & \tilde{\mathscr{H}}_{33} \end{pmatrix} \tag{20}$$

$$\tilde{\mathscr{H}}_{ii} = I - B + \sum_{c=1}^{N_c} \sum_{q(c)=1}^{N_q} \sigma_{q(c)} B \mathscr{R}_c^{\mathrm{T}} Q_{q(c)}^{\mathrm{T}} P_{ii} Q_{q(c)} \mathscr{R}_c B \tag{21}$$

It is obvious that $\tilde{\mathscr{H}} = \tilde{\mathscr{H}}^{\mathrm{T}} \geqslant 0$ is inside the feasible set. If at least one vertex is fixed (i.e. there exist $b_{ii} = 0$) then $\tilde{\mathscr{H}} > 0$ on any feasible grid.

5.1. Procedure for grid untangling

In order to construct a feasible solution we suggest to use a penalty formulation, which is based on the technique [6], and can be written as follows:
Find the solution of the following minimization problem

$$\mathbf{R} = \lim_{\varepsilon \to \varepsilon_l,\ \varepsilon \geqslant \varepsilon_l} \arg \min_{\mathbf{R}} \mathscr{I}_\varepsilon^h$$

$$\mathscr{I}_\varepsilon^h = \sum_{c=1}^{N_c} \sum_{q(c)=1}^{N_q} f_\varepsilon(A)|_{q(c)}, \sigma_{q(c)}, \quad f_\varepsilon(A) = \det H \left(\frac{\phi(A) + b\,\varepsilon\,\mathrm{tr}\,(AA^{\mathrm{T}})}{\chi_\varepsilon(\det A)} \right) \tag{22}$$

$$\mathbf{a}_i|_{q(c)} = H_{q(c)}^{-\mathrm{T}} Q_{q(c)} \mathbf{X}_c^i, \quad \mathbf{X}_c^i = \mathscr{R}_c \mathbf{X}^i$$

$$\chi_\varepsilon(q) = \frac{q}{2} + \frac{1}{2}\sqrt{\varepsilon^2 + q^2}, \quad q = \det A \tag{23}$$

and $\varepsilon_l > 0$ is sufficiently small.

Here $b > 0$ is the constant. The additional term is introduced in order to avoid the situation when the reduced Hessian of the functional $\tilde{\mathscr{H}}$ has zero rows and columns. This term was not necessary in the plane case.

The iterative solution scheme for this problem looks as follows:

Choose an initial guess $\mathbf{R}^0$,

$$\begin{aligned}
&\text{for } k = 0, 1, 2, \ldots \\
&\qquad \varepsilon_{k+1} = \gamma(\varepsilon_b, \mathbf{R}^k) \\
&\qquad \text{find minimization direction } \mathbf{P}^k = -\tilde{\mathscr{H}}_\varepsilon^{-1} \nabla \mathscr{I}_{\varepsilon_k}^h \\
&\qquad \text{solve approximately } \tau_k = \arg \min_\tau \mathscr{I}_{\varepsilon_k}^h(\mathbf{R}^k + \tau \mathbf{P}^k) \\
&\qquad \mathbf{R}^{k+1} = \mathbf{R}^k + \tau_k \mathbf{P}^k \\
&\qquad \text{if } q_{\min}(\mathbf{R}^k) > 0, \text{ then } \varepsilon_{k+1} = \varepsilon_b, \text{ stop}
\end{aligned} \tag{24}$$

Here $q_{\min}(\mathbf{R})$ is the minimal value of $q = \det A$ over all quadrature nodes of all grid cells $\mathbf{R}$, $\varepsilon_b = 10^{-9}$, function γ is defined as follows:

$$\gamma(\varepsilon, \mathbf{R}) = \sqrt{\varepsilon_b^2 + 0.04(\min(q_{\min}(\mathbf{R}), 0))^2}$$

The minimization problem for the function of single variable (24) can be solved using the finite choice from the set $\tau \in \{1, 2^{-1}, \ldots, 2^{-N_\tau}\}$, where $N_\tau = 32$.

The reduced Hessian matrix $\tilde{\mathscr{H}}_\varepsilon^{-1}$ is defined by equality (20), where in the expression for $\tilde{\mathscr{H}}_{ii}$ the matrix P_{ii} is replaced by P_{ii}^ε defined below:

$$P_{ii}^\varepsilon = \frac{\partial^2 f_\varepsilon}{\partial \mathbf{a}_i^{\mathrm{T}} \partial \mathbf{a}_i} + \frac{\chi_\varepsilon''}{\chi_\varepsilon^2} \det H \phi \mathbf{a}^i \mathbf{a}^{i\mathrm{T}}$$

The matrix $\tilde{\mathscr{H}}_\varepsilon$ has the same properties as $\tilde{\mathscr{H}}$ but still is positive definite (or semidefinite) for any infeasible, i.e. 'tangled' grid. The validations of this untangling procedure are considered in References [6, 7].

5.2. Procedure for contracting the feasible set

Let us consider the solution of the following minimization problem

$$\mathbf{R} = \arg\min_{\mathbf{R}} \mathscr{I}^h(t)$$

$$\mathscr{I}^h(t) = \sum_{c=1}^{N_c} \sum_{q(c)=1}^{N_q} f(A)|_{q(c)} \sigma_{q(c)}, \quad f(A) = f_2 = (1-t)\det H \frac{\phi(A)}{\det A - t\phi(A)} \tag{25}$$

$$\mathbf{a}_i|_{q(c)} = H_{q(c)}^{-\mathrm{T}} Q_{q(c)} \mathbf{X}_c^i, \quad \mathbf{X}_c^i = \mathscr{R}_c \mathbf{X}^i$$

As an initial guess we choose a non-degenerate grid from $\mathscr{F}(0)$ and we set $t_0 = 0$.

In order to contract the feasible set $\mathscr{F}(t)$ the following iterative solution scheme is suggested:

$$\begin{aligned}
&\text{for } k = 0, 1, 2, \ldots \\
&\qquad \text{find minimization direction } \mathbf{P}^k = -\tilde{\mathscr{H}}^{-1} \nabla \mathscr{I}^h(t_k) \\
&\qquad \text{solve approximately } \tau_k = \arg\min_{\tau} \mathscr{I}^h(t_k)(\mathbf{R}^k + \tau \mathbf{P}^k), \\
&\qquad \mathbf{R}^{k+1} = \mathbf{R}^k + \tau_k \mathbf{P}^k, \;\; t_{k+1} = (1-dt) t_{\min}(\mathbf{R}^k)
\end{aligned} \tag{26}$$

Here

$$t_{\min} = \min_{q(c)} \left. \frac{\det A}{\phi(A)} \right|_{q(c)}$$

The value of dt is defined using the norm of the gradient of the functional $\mathscr{I}^h(t_k)$.

6. NUMERICAL EXPERIMENTS

6.1. The domain shape recovery for given deformation field

Suppose that the mapping of a rectangular domain in logical co-ordinates onto the target domain is given by the equality

$$\mathbf{w}(\xi_1, \xi_2, \xi_3) = \begin{pmatrix} (R+\xi_3)\cos\left(\dfrac{L-\xi_1}{R}\sin\varphi\right) \\ \xi_2 + (L-\xi_1)\cos\varphi \\ (R+\xi_3)\sin\left(\dfrac{L-\xi_1}{R}\sin\varphi\right) \end{pmatrix} \tag{27}$$

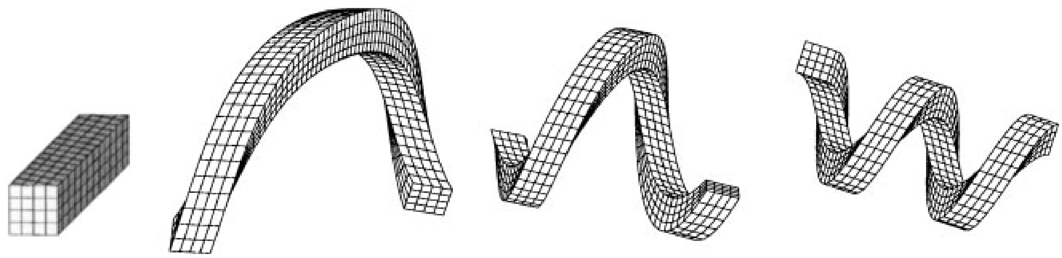

Figure 5. Stages of exact shape recovery (from left to right).

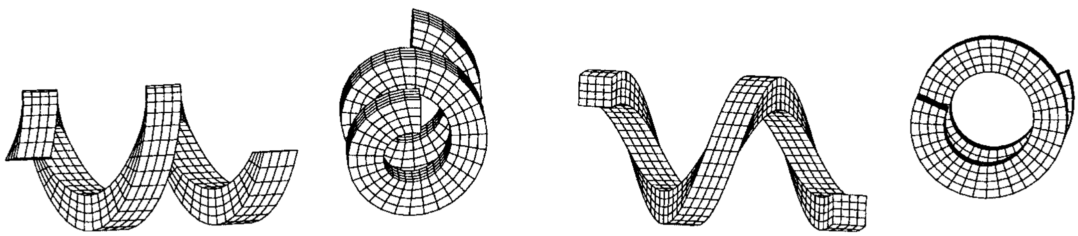

Figure 6. Exact shape recovery vs piecewise-constant deformation field.

Then the pointwise deformation is given by the shape control matrix $H=(\partial\mathbf{w}/\partial\xi_1, \partial\mathbf{w}/\partial\xi_2, \partial\mathbf{w}/\partial\xi_3)$.

Suppose that the initial guess is the uniform grid in the rectangular domain $0\leqslant x_1\leqslant L,\ 0\leqslant x_2, x_3\leqslant 1$, while the target domain described by the above mapping has a spiral shape. We chose $R=1,\ \varphi=\pi/3,\ L=4\pi R/\sin\varphi$ for the spiral with two turns. The idea of this test is to reproduce the shape of the domain using distributed deformation field.

Using the simplest approximation of the functional based only on 4 tetrahedra for a hexahedral cell and prescribing the target shape for each of these tetrahedra via the exact tetrahedra shapes computed from (27) we achieve the exact shape recovery (Figure 5).

However, when the deformation is defined by a constant matrix H on each hexahedral cell the final domain had a shape of a spiral with only one and a half turns (Figure 6).

Here relatively small local errors in description of cell shapes lead to the numerical solution with final error comparable to the solution norm.

This simple example illustrates the importance of a proper target shape definition for hexahedra which also plays a key role in the solution of such problems of mechanics as shape recovery from stressed state and springback.

6.2. Grid untangling test

We consider a construction of a non-degenerate grid in a domain with a cubic cavity inside.

The structured hexahedral grid in this example is the mapping of the unit cube with a uniform grid in logical co-ordinates onto the cube of the same size when a smaller cubic cavity inside is rotated around x_3 axis with an angle of rotation α. The points inside the smaller cube are fixed. All nodes on the external and internal cubes are fixed and represent

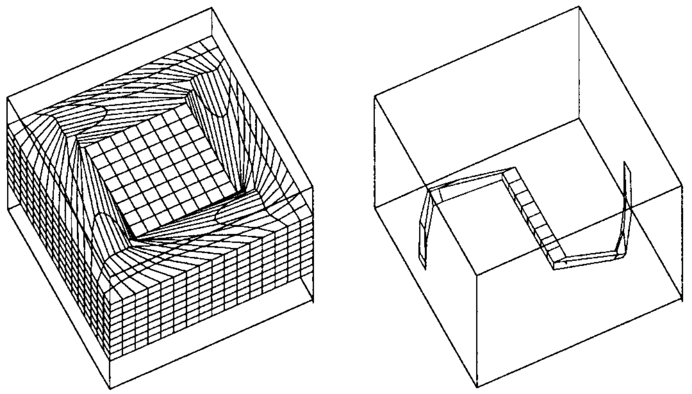

Figure 7. $\alpha = \pi/2$.

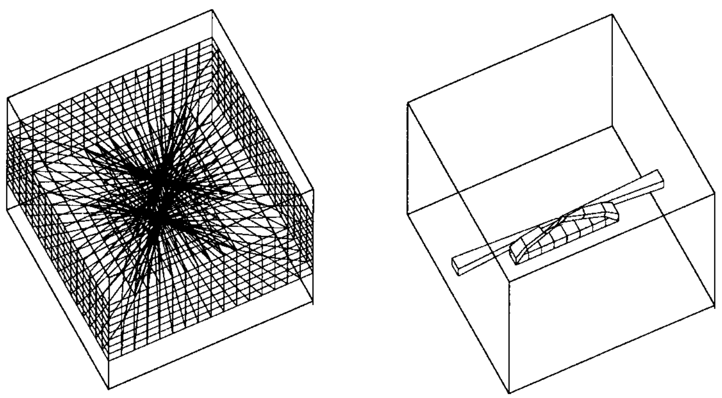

Figure 8. $\alpha = \pi$ with zero initial guess.

the surface grids with square cells. By "zero initial guess" below we mean the badly folded grid with zero values of the internal vertices and correct boundary values.

The untangling procedure works fine for the configuration shown in Figure 7 where $\alpha = \pi/2$. In the left figure we show the co-ordinate surface $\xi_3 = \text{const}$ passing through the cube centre and the grid on the cube boundary. The right figure shows the "beam" made from the chain of the hexahedral cells. The trilinear mapping inside each grid cell is non-degenerate.

In the case $\alpha = \pi$ when started from zero initial guess the untangling procedure was locked in the situation showed in Figure 8. Note that the grid is badly folded. In this example the feasible set is the union of disjoint connected subsets. Moreover, if the grid is refined, the number of such disjoint subsets increases. In this case the untangling procedure was not able to "choose" between clockwise- and counterclockwise rotated solutions. This example requires further investigation but it seems to indicate that we have the stationary point of discrete functional (22) outside the feasible set.

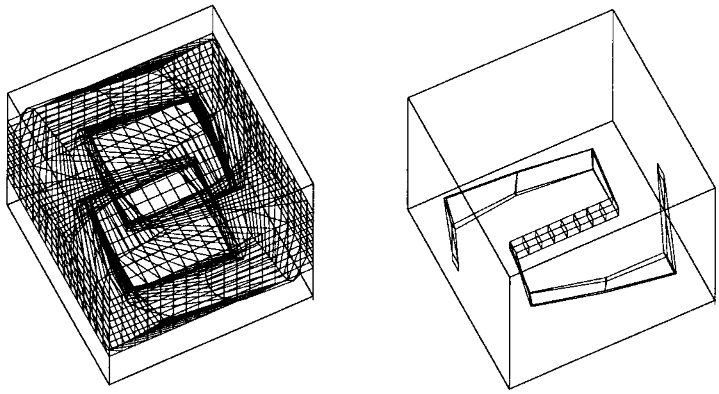

Figure 9. $\alpha = \pi$ with non-zero initial guess.

However, if we take as an initial guess the feasible solution of the same problem with $\pi/2 < \alpha < \pi$, which is still infeasible for $\alpha = \pi$ then the untangling procedure successfully builds a non-degenerate grid.

Note the presence of severely distorted hexahedra in the grid shown in Figure 9. The trilinear mapping in all grid cells is non-degenerate; however, if one splits some cells into tetrahedra using standard splittings into 5 or 6 tetrahedra, then the signed volume of some tetrahedra will be negative. This is true in particular for very thin hexahedra shown in Figure 9 (right). Using quadrature rules may lead to another pathology when the grid spills out beyond the domain boundaries while the Jacobian of the local mapping in each cell is strictly positive in the quadrature nodes.

The suggested test case is very simple but it can be made extremely stiff and present a negative example where the simplified approximation methods for hexahedral cells based on simplified quadrature rules or splitting into tetrahedra fail, especially on coarse grids. Only the slowest method based on 64 composite bases was consistent and reliable.

7. CONCLUSIONS

A maximum-norm optimization technique for spatial mappings was used to control the properties of the local mappings in the finite element method, in particular in the case of hexahedral cells.

The global grid untangling procedure was tested on difficult 3-D examples demonstrating its ability to work in a black box mode and its high level of robustness.

Further research is necessary in order to develop approximation methods for hexahedral cells which are simple enough while still allowing to obtain guaranteed bounds on the trilinear mapping distortion measures.

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