Global condition number of trilinear mapping. Application to 3-D grid generation.

©L.V. Branets, V.A. Garanzha
Computing Center RAS, Vavilov Str.40, Moscow, 117967, RUSSIA,
e-mail: garan@ccas.ru

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 nongenerate. However more refined estimates require analysis of the properties of these local mappings. There are exist many methods for 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 Jacobi matrices. The basic requirements for the quality measures can be formulated as follows:

1) The ability to quantify the deviation of finite element cell from "ideal" cell (say cube or unilateral simplex) in terms of shape and size;

2) constructivity, i.e. the possibility of practical creation of finite element grids satisfying the quality criteria;

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 discrete characteristics, and the mapping quality measure, which is continual characteristics.

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

Let us consider a spatial nondegenerate mapping defined by

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

which maps an "ideal" domain D, say the unit hypercube, in the logical coordinates $\{\xi_1, \ldots, \xi_n\}$ onto domain Ω in physical coordinates.

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 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 $H^T H$ has the sense of "accompanying" metrics defined in the logical space and let

$$A = H^{-T} S^T.$$

Let us introduce the following scalar functions of matrices

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

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 $\beta^{\frac{1}{n}}$ is actually the shape distortion measure introduced by Reshetnyak [3] in the context of the theory of mappings with 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 function $E_\theta(A)$ is that it is possible to obtain the following minimax bounds on the eigenvalues of matrix AA^T when the distortion measure E_θ is bounded from above [2]

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

which is crucial property of mappings in grid generation [1].

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

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

Amoung the 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 the criteria 1)-3) formulated above. We will show that it is also complete in the above sense when the low order isoparametric finite elements are considered.

The algebraic properties of the distortion measure

Let us introduce the following definitions:

1) Let us call by the "boolean" partition of unity matrix into k parts the set of matrices $I_1^\nu, \dots, I_k^\nu$ with the following properties: every matrix I_j^ν is a diagonal matrix with only zero and unity elements and the sum of these matrices is equal to unity matrix $\sum_{j=1}^k I_j^\nu = I$. The lower index for matrix I_j^ν shows its position in the set, the upper index shows the partition number. There are k^n different "boolean" partitions of unity $n \times n$ matrix into k parts (number of words with length n from the alphabete with length k), hence $\nu \in \{1, 2, \dots, k^n\}$.

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

$$\tilde{S}_\nu = \sum_{j=1}^k S_j I_j^\nu,$$

which corresponds to some "boolean" partition ν, i.e. $\tilde{S}_\nu$ is the matrix with i-th column being the i-th 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* $\tilde{S}_\nu = \sum_{j=1}^m S_j I_j^\nu$ *of* $n \times n$ *matrices* $S_1, \dots, S_m$ *the following inequality hold*

$$E_\theta(\tilde{S}_\nu) \le C, \ \det \tilde{S}_\nu > 0.$$

Let

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

where Λ_j *are the diagonal matrices, then*

$$E_\theta(S) \le C, \tag{6}$$

moreover, there exist the coefficients $a_\nu \geq 0$, $\sum_{\nu=1}^{m^n} a_\nu = 1$, *such that*

$$E_\theta(S) \leq \sum_{\nu=1}^{m^n} a_\nu E_\theta(\tilde{S}_\nu). \tag{7}$$

The proof of this theorem is rather cumbersome and is omitted here for the sake of brevity.

This theorem has the following important implications. If the Jacobi matrix of a mapping can be presented in the form (5), then the m-ary composition provides the set of "composite basises" 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).

Variational principle for maximum-norm minimization of distortion measure

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

$$\det A > 0, \;\; E_\theta(A) < 1/t \tag{8}$$

Then $\mathcal{F}(0)$ denotes the set of nondegenerate mappings and $\mathcal{F}(1)$ is the isometric mapping. The practical implementation strategy for the minimization of $E_\theta(A)$ is to construct such functional which after discretization has an infinite barrier on the boundary of the feasible set $\partial\mathcal{F}(t)$ 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]

$$\arg\min_{\mathbf{r}(\xi)} \int_{\mathcal{D}} f(A) d\xi, \tag{9}$$

where

$$f(A) = (1-t)\det H \frac{\phi(A)}{\det A - t\phi(A)}, \tag{10}$$

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

Volumetric factor is given by

$$v = \int_{\mathcal{D}} \det S d\xi / \int_{\mathcal{D}} \det H d\xi,$$

when the volume of the domain Ω is known, otherwise v is specified apriori.

The minimization problem (9), (10) makes sense inside the feasible set (provided that this feasible set is not empty) defined by inequality

$$\det A - t\phi(A) > 0. \tag{11}$$

Discretization of the functional in the 3-D case

In order to discretize functional (9) the conventional finite element procedure is applied where local mapping in each cell is assumed to be linear or polylinear one.

We consider only 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 with number c let us denote the vector of all cell vertices by

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

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

If the cell $\mathcal{D}_c$ 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

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

Using the above notations the discrete counterpart of problem (9) can be formulated as follows: find the vector $\mathbf{R}$ as the solution to the following minimization problem

$$\mathbf{R} = \arg\min_{\mathbf{R}} \mathcal{I}^h, \quad \mathcal{I}^h = \sum_{c=1}^{N_c} \sum_{q(c)=1}^{N_q} f(A)|_{q(c)} \sigma_{q(c)}, \tag{12}$$
$$A = (\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3), \quad \mathbf{a}_i|_{q(c)} = H_{q(c)}^{-T} Q_{q(c)} \mathcal{R}_c \mathbf{X}^i.$$

Here subscript $q(c)$ denotes q-th "quadrature node" for the integral over cell $\mathcal{D}_c$, N_q matrices $Q_{q(c)}$ actually describe the discretization of the functional (9) on each element and $\sum_{q(c)=1}^{N_q} \sigma_{q(c)} = 1, \quad \sigma_{q(c)} > 0$.

The feasible set $\mathcal{F}^h(t)$ is defined by $N_c N_q$ nonlinear inequalities

$$\det A - t\phi(A)|_{q(c)} > 0, \tag{13}$$

Volumetric factor v is specified apriori or is defined by

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

when the volume of computational domain is known.

In order to account for boundary conditions we seek $\mathbf{R}$ as follows: $\mathbf{R} = (I - B)\mathbf{R}_b + B\mathbf{R}_{in}$, where $B \in \mathbb{R}^{N_v \times N_v}$ is the diagonal matrix with the entries b_{ij}, such that $b_{ii} = 1$, if the i-th node of the gride is internal one, i.e. its coordinates are unknown, and $b_{ii} = 0$, when i-th gride node lies on the boundary and is fixed. $\mathbf{R}_{in}$, $\mathbf{R}_b$ 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 coordinates onto the tetrahedron with vertices $\mathbf{v}_1, \mathbf{v}_2, \mathbf{v}_3, \mathbf{v}_4$ in physical coordinates is linear and can be written via the natural coordinates [4] resulting in the following equality

$$\begin{pmatrix} 1 \\ x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} 1 & 1 & 1 & 1 \\ \mathbf{v}_1 & \mathbf{v}_2 & \mathbf{v}_3 & \mathbf{v}_4 \end{pmatrix} \begin{pmatrix} 1 & 1 & 1 & 1 \\ \mathbf{l}_1 & \mathbf{l}_2 & \mathbf{l}_3 & \mathbf{l}_4 \end{pmatrix}^{-1} \begin{pmatrix} 1 \\ \xi_1 \\ \xi_2 \\ \xi_3 \end{pmatrix}. \qquad (14)$$

Basis vectors of such a mapping are constant and, consequently, function E_θ is constant. If E_θ satisfies (8) the local estimates on γ, Γ for this mapping are obviously true. However if $1/t$ is uniform upper bound for distortion E_θ of every tetrahedra present in the grid then γ, Γ represent the global condition number of the grid.

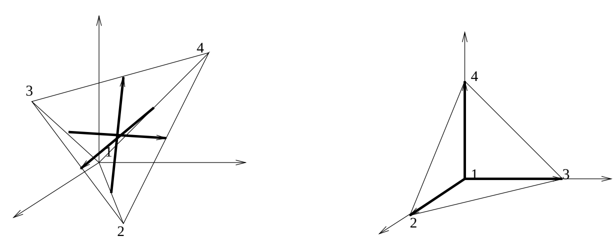

Figure 1: Equilateral tetrahedron and rectangular tetrahedron inscribed in unit cube. Covariant basis vectors are shown in bold

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

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

Quadrature rule in this case looks as follows

$$Q = \frac{1}{2}\begin{pmatrix} -1 & 1 & 1 & -1 \\ -1 & 1 & -1 & 1 \\ -1 & -1 & 1 & 1 \end{pmatrix}, \; N_q = 1, \; \sigma_i = 1. \tag{15}$$

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

$$\mathbf{g}_1 = \mathbf{v}_2 - \mathbf{v}_1, \; \mathbf{g}_2 = \mathbf{v}_3 - \mathbf{v}_1, \; \mathbf{g}_3 = \mathbf{v}_4 - \mathbf{v}_1,$$
$$Q = \begin{pmatrix} -1 & 1 & 0 & 0 \\ -1 & 0 & 1 & 0 \\ -1 & 0 & 0 & 1 \end{pmatrix}, \; N_q = 1, \; \sigma_i = 1. \tag{16}$$

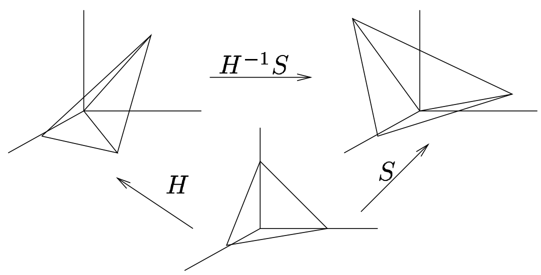

Figure 2: Prescription of target shape for tetrahedra via composition of mappings

If the target shape of the tetrahedron is not one of the above basic ones, then we should introduce the matrix H as the Jacobi matrix for the mapping of the ideal tetrahedron onto target tetrahedron. This mapping is again defined by equality (14) 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 4×4 matrix by eliminating first row and first column. Here $\mathbf{w}_1, \ldots, \mathbf{w}_4$ are the Cartesian coordinates of the vertices of target tetrahedron. When the target shape is specified the discrete functional does not depend on the choice of ideal tetrahedron in logical space and the simplest expressions for the functional are obtained when the rectangular corner tetrahedron is chosen as the ideal one. Then the matrix H is defined simply as

$$H = \begin{pmatrix} \mathbf{w}_2 - \mathbf{w}_1 & \mathbf{w}_3 - \mathbf{w}_1 & \mathbf{w}_4 - \mathbf{w}_1 \end{pmatrix}$$

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

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

4.2 Hexahedral cell

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

$$\mathbf{r}(\xi_1, \xi_2, \xi_3) = \sum_{i,j,k=0}^{1} (1-\xi_1)^{1-i}\xi_1^i (1-\xi_2)^{1-j}\xi_2^j (1-\xi_3)^{1-k}\xi_3^k \mathbf{r}(i,j,k), \quad (17)$$

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

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

$$S = \sum_{\alpha} S_\alpha \Lambda_\alpha, \ \Lambda_\alpha \geq 0, \ \sum_{\alpha} \Lambda_\alpha = 1,$$

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

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

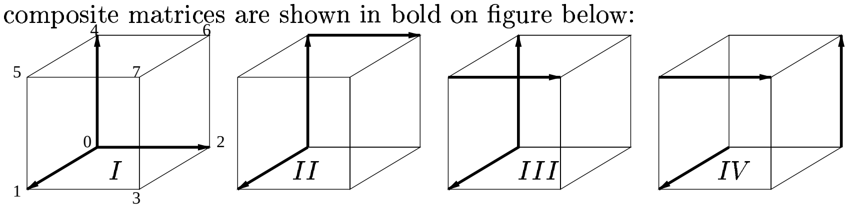

Figure 3: Construction of composite matrices for trilinear mapping

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

The exact expressions for matrices Q for approximation, based upon $N_q = 64$, can be easily obtained from (17). For example the columns of composite matrix $\tilde{S}_0$ are given by (see Figure 3,I)

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

Here it is assumed that the numbering of cell vertices on Figure 3 is related to triple indexing in (17) via

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

Composite matrices shown on figure above constitute the quadrature rule with following weights

$$\sigma_I = \frac{1}{27}, \; \sigma_{II} = \frac{1}{2 \cdot 27}, \; \sigma_{III} = \frac{1}{4 \cdot 27}, \; \sigma_{IV} = \frac{1}{8 \cdot 27},$$

which guarantees the patch test property for resulting approximation.

The target shape specification for hexahedron is more complicated compared to tetrahedra. It can be done as well via composition of mappings and matrix H. However for the sake of compatibility H by itself should be the Jacobi matrix of trilinear mapping so its entries are the functions of $\xi_1, \; \xi_2, \; \xi_3$.

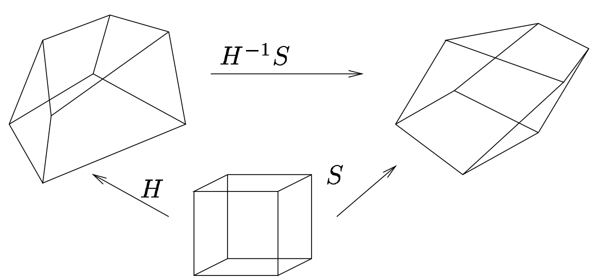

Figure 4: Prescription of target shape for hexahedra via composition of trilinear mappings.

The most natural way for hexahedron shape prescription is to construct the same set of elementary composite matrices $\tilde{H}_\nu$ for H and consider the distortion measures of matrices $\tilde{H}_\nu^{-1}\tilde{S}_\nu$ as the distortion measure of deviation from 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 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 affine cell which severely restricts the class of allowable deformations.

In order to reduce computational costs one should use simplified approximation of cell distortion based on some set of quadrature rule. For example one can use approximation based on 8 quadrature points in the hexahedron vertices and one central node, or even the simplest approximation consisting of 4 tetrahedra per trlinear cell, which is barely enough to fix the target shape of 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. Jacobi matrix for all these mappings can be shown to take a form (5).

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

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

Solution technique

In order to solve the discrete minimization problem (12) we use preconditioned gradient method coupled with a line search technique. The key ingredient of this algorithm is the choice of nonlinear preconditioning and the solution technique for linear systems arising in resulting implicit method. To this end we use an approach suggested in [6], where symmetric positive definite approximation of Hessian matrix of functional (12) was constructed analytically and efficient and robust iterative linear solver from [5] was used.

Let us define the following matrices

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

Since the target functional possesses the strong ellipticity property we get

$P_{ii} = P_{ii}^T > 0$. The reduced Hessian matrix of (12) is assembled as follows

$$\tilde{\mathcal{H}} = \begin{pmatrix} \tilde{\mathcal{H}}_{11} & 0 & 0 \\ 0 & \tilde{\mathcal{H}}_{22} & 0 \\ 0 & 0 & \tilde{\mathcal{H}}_{33} \end{pmatrix}, \tag{18}$$

$$\tilde{\mathcal{H}}_{ii} = I - B + \sum_{c=1}^{N_c} \sum_{q(c)=1}^{N_q} \sigma_{q(c)} B \mathcal{R}_c^T Q_{q(c)}^T P_{ii} Q_{q(c)} \mathcal{R}_c B \tag{19}$$

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

5.1 Procedure for grid untangling

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

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

$$\mathcal{I}_\varepsilon^h = \sum_{c=1}^{N_c} \sum_{q(c)=1}^{N_q} f_\varepsilon(A)|_{q(c)} \sigma_{q(c)},\ \ f_\varepsilon(A) = \det H \left(\frac{\phi(A) + b\,\varepsilon\, \mathrm{tr}(AA^T)}{\chi_\varepsilon(\det A)} \right), \tag{20}$$

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

$$\chi_\varepsilon(q) = \frac{q}{2} + \frac{1}{2}\sqrt{\varepsilon^2 + q^2},\quad q = \det A \tag{21}$$

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 reduced Hessian of the functional $\tilde{\mathcal{H}}$ 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 initial guess $\mathbf{R}^0$,

$$\begin{aligned} \text{for } k\ &= 0, 1, 2, \ldots \\ &\varepsilon_{k+1} = \gamma(\varepsilon_b, \mathbf{R}^k) \\ &\text{find minimization direction } \mathbf{P}^k = -\tilde{\mathcal{H}}_\varepsilon^{-1} \nabla \mathcal{I}_{\varepsilon_k}^h \\ &\text{solve approximately } \tau_k = \arg\min_\tau \mathcal{I}_{\varepsilon_k}^h(\mathbf{R}^k + \tau \mathbf{P}^k), \\ &\mathbf{R}^{k+1} = \mathbf{R}^k + \tau_k \mathbf{P}^k \\ &\text{if } q_{\min}(\mathbf{R}^k) > 0,\ \text{then } \varepsilon_{k+1} = \varepsilon_b,\ \text{stop.} \end{aligned} \tag{22}$$

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 (22) can be solved using the finite choice from the set $\tau \in \{1, 2^{-1}, \dots, 2^{-N_\tau}\}$, where $N_\tau = 32$.

The reduced Hessian matrix $\tilde{\mathcal{H}}_\varepsilon$ is defined by equality (18), where in the expression for $\tilde{\mathcal{H}}_{ii}$ the matrix P_{ii} is replaced by P_{ii}^ε defined below

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

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

5.2 Procedure for contracting the feasible set

Let us consider the solution of the following minimization problem

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

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

$$\mathbf{a}_i|_{q(c)} = H_{q(c)}^{-T} Q_{q(c)} \mathbf{X}_c^i, \;\; \mathbf{X}_c^i = \mathcal{R}_c \mathbf{X}^i, \qquad (23)$$

As an initial guess we choose a nondegenerate grid from $\mathcal{F}(0)$ and we set $t_0 = 0$.

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

$$\begin{aligned}
&\text{for } k = 0, 1, 2, \dots \\
&\quad \text{find minimization direction } \mathbf{P}^k = -\tilde{\mathcal{H}}^{-1} \nabla \mathcal{I}^h(t_k) \\
&\quad \text{solve approximately } \tau_k = \arg\min_\tau \mathcal{I}^h(t_k)(\mathbf{R}^k + \tau \mathbf{P}^k), \qquad (24) \\
&\quad \mathbf{R}^{k+1} = \mathbf{R}^k + \tau_k \mathbf{P}^k, \;\; t_{k+1} = (1 - dt) t_{\min}(\mathbf{R}^k)
\end{aligned}$$

Here

$$t_{\min} = \min_{q(c)} \frac{\det A}{\phi(A)} \bigg|_{q(c)},$$

and delay dt is computed using the norm of the gradient of the functional $\mathcal{I}^h(t_k)$.

Numerical experiments

1. The domain shape recovery for given deformation field. Suppose that the mapping of rectangular domain in logical coordinates onto the target domain is given by equality

$$\mathbf{w}(\xi_1, \xi_2, \xi_3) = \begin{pmatrix} (R + \xi_3)\cos\left(\frac{L-\xi_1}{R}\sin\varphi\right) \\ \xi_2 + (L - \xi_1)\cos\varphi \\ (R + \xi_3)\sin\left(\frac{L-\xi_1}{R}\sin\varphi\right) \end{pmatrix}. \tag{25}$$

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

Suppose that the initial guess is the uniform grid in the rectangular domain $0 \le x_1 \le L,\ 0 \le x_2, x_3 \le 1$, while the target domain described by the above mapping has a spiral shape. We chose $R = 1,\ \varphi = \pi/3,\ L = \frac{4\pi R}{\sin\varphi}$ 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 functional based only on 4 tetrahedra for hexahedral cell and prescribing the target shape for each of this tetrahedra via exact tetrahedra shapes computed from (25) we achieve exact shape recovery.

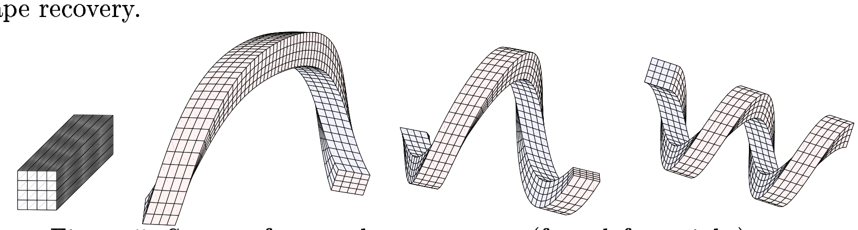

Figure 5: Stages of exact shape recovery (from left to right)

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

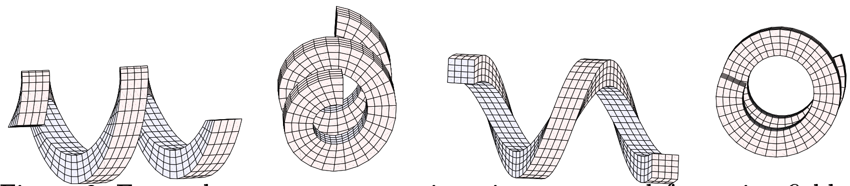

Figure 6: Exact shape recovery vs. piecewise-constant deformation field

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

2. Grid untangling test. We consider a mapping of unit cube with uniform grid in logical coordinates onto the cube of the same size when smaller cube inside is rotated around x_3 axis on the angle α. The points inside smaller cube are fixed hence the computational domain is in fact a cube with a rotated cubic hole inside. All nodes on external and internal cubes are fixed and present the uniform square grids. By "zero initial guess" below we mean the tangled grid with zero values of internal vertices and correct boundary values.

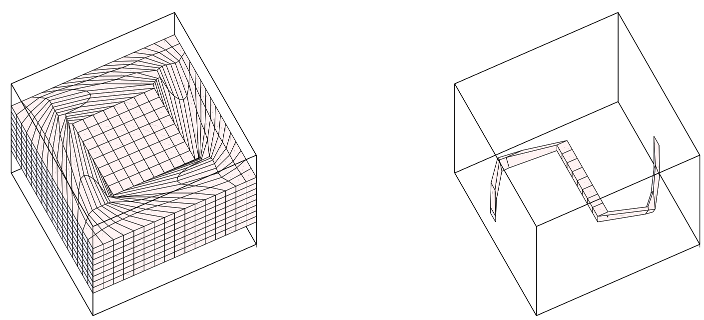

Figure 7: $\alpha = \pi/2$

The untangling works fine for the configuration shown on Figure 7 where $\alpha = \pi/2$. In this figure on the left we show the coordinate surface $\xi_3 = \text{const}$ passing through the cube center and the grid on the cube boundary. On the right it is shown the "beam" made from the chain of the hexahedral cells. The trilinear mapping inside each grid cell is nondegenerate.

In the case $\alpha = \pi$ when started from zero initial guess the untangling procedure was locked in the situation showed on Figure 7. Note that the grid is badly folded. In this example feasible set is the union of disjoint connected subsets. Moreover, with grid refinement 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 (20) outside the feasible set.

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

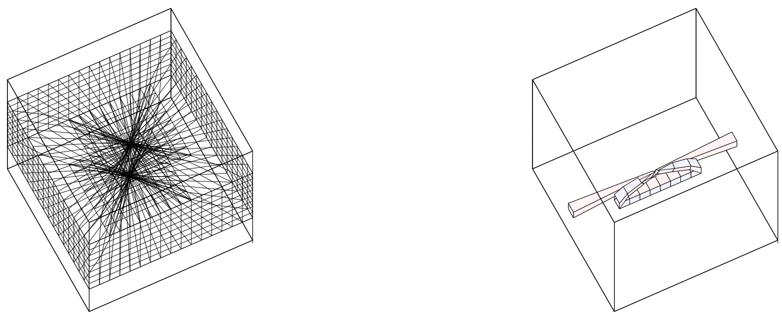

Figure 8: $\alpha = \pi$ with zero initial guess

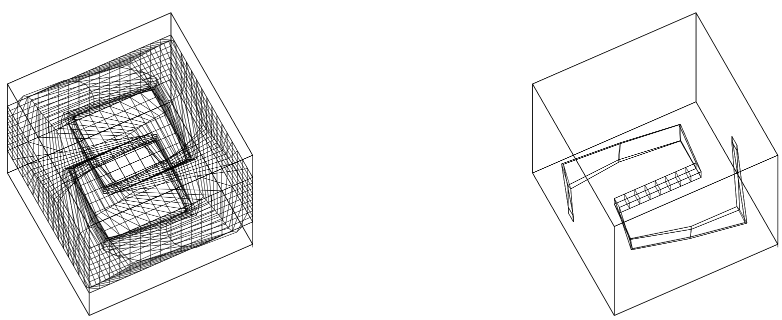

Figure 9: $\alpha = \pi$ with nonzero initial guess

Note the presence of severely distorted hexahedra in the grid shown on Figure 9. The trilinear mapping in all grid cells is nondegenerate, however if one splits some hexahedra into tetrahedra using standard splittings into 5, 6 and other numbers of tetrahedra, then the signed volume of some tetrahedra will be negative. This is true in particular for very thin hexahedra shown on Figure 9, right. This problem looks very simple but it is enough to break down the simplified approximation methods for hexahedral cells based on simplified quadrature rules or splitting into tetrahedra, especially on coarse grids. Only the slowest method based on the approximation based on 64 composite basises was consistently and reliably providing the desired results.

Conclusions

The 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.

Global grid untangling procedure was tested on hard 3-D examples demonstrating ability to work in black box mode and high level of robustness.

References

[1] S.K. Godunov, V.M. Gordienko and G.A. Chumakov. Quasi-isometric parametrization of a curvilinear quadrangle and a metric of constant curvature. //Siberian Advances in Mathematics. 1995, V.5, N.2, P.1-20.

[2] V.A. Garanzha. Barrier variational generation of quasi-isometric grids. //Comp. Math. and Math. Phys. V.40, N.11, 2000, PP.1617-1637.

[3] Reshetnyak Y.G., Mappings with bounded deformation as extremals of Dirichlet type integrals - Siberian Math. J., 9, 1968, 487-498.

[4] G. Strang, J. Fix Analysis of finite element method.// Prentice-Hall, Englewood Cliffs, NJ, 1973.

[5] Kaporin I.E. On preconditioning conjugate gradient method when solving discrete counterparts of differential problems.// Diff. Uravn. 1990. V.26. N.7. PP.1225-1236.

[6] V.A. Garanzha, I.E. Kaporin. Regularization of the barrier variational grid generation method.// Comp. Math. and Math. Phys., 1999. N.9. PP.1489-1503.

[7] V.A. Garanzha, Max-norm optimization of spatial mappings with application to grid generation, construction of surfaces and shape design. 2001, these Proceedings, PP. 61-74.