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Control of the Metric Properties of Spatial Mappings

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Abstract—An attempt is made to formulate the general requirements on variational principles used for the construction of mappings in grid generation and geometric modeling. The variational principle proposed earlier by the author for constructing quasi-isometric mappings is shown to satisfy many of these requirements. The important case of mapping construction when the controlling metric is discontinuous is analyzed separately. The technique proposed is used to design a grid generation algorithm that is stable with respect to the errors in the surface description and is suitable for CAD applications.

1. GENERAL REQUIREMENTS ON THE VARIATIONAL PRINCIPLE

Variational grid generation methods [1–7] have become key tools in real-life applications. Despite considerable progress in this area, practical techniques generally lack any theoretical justification. We try to formulate the general requirements that should be satisfied by a variational principle for mapping construction.

Denote by Ω_0 a domain in coordinates $\eta = \{\eta_1, \ldots, \eta_n\}$. A spatial mapping $y(\eta)$: $\mathbb{R}^n \longrightarrow \mathbb{R}^n$ is sought as a minimizer of a functional depending on the gradient of the mapping:

$$\int_{\Omega_0} f(\nabla_\eta y) d\eta, \quad f : \mathbb{R}^{n \times n} \longrightarrow \mathbb{R}, \tag{1.1}$$

where $\nabla_\eta y$ denotes the matrix with entries $\partial y_i / \partial \eta_j$.

A fairly comprehensive survey of statements of variational problems for functionals of this class can be found in [8], where mathematical elasticity with finite deformations is considered, including well-posedness conditions, restrictions on the geometry of domains, boundary conditions, and the regularity of solutions to variational problems.

However, variational principles for grid generation and geometric modeling differ from those used in elasticity, because the basic requirements they should satisfy are different. Below, we formulate these requirements as applied to the construction of mappings with prescribed properties.

1. A variational problem should be well posed, and its solution should exist and should be stable with respect to input data. A well-known standard condition is ellipticity. Unfortunately, it is well known that the ellipticity condition does not guarantee the well-posedness of nonlinear variational problems.

2. A variational principle should not admit singular mappings as solutions; i.e., the natural class of admissible mappings consists of locally invertible quasi-isometric mappings [9]. The quasi-isometry condition means that, for arbitrary sufficiently close points (say α and β in coordinates η), it holds that

$$\frac{L}{C}|\beta - \alpha| \le |y(\beta) - y(\alpha)| \le LC|\beta - \alpha|, \tag{1.2}$$

where $C > 0$ is a constant, $|\cdot|$ denotes the length of a vector, and L is a characteristic length scale.

3. Solutions to a variational problem should be as smooth as possible.

4. The ability to construct quasi-uniform mappings is a key property in grid generation problems. The quasi-uniformity of a mapping means that it does not produce large distortions. This can be written in invariant form as

$$L/C_1 \le \sigma_i(\nabla_\eta y) \le LC_1; \tag{1.3}$$

here, σ_i are the singular values of $\nabla_\eta y$ (i.e., the square roots of the eigenvalues of $\nabla_\eta^T y \nabla_\eta y$) and $C_1 > 0$ is a constant. In fact, this is another definition of a quasi-isometric mapping, provided that the inequalities hold almost everywhere. It follows from (1.2) that $y(\eta)$ is locally Lipschitz and its gradient belongs to $\mathbb{L}_\infty$. On the other hand, any function with its gradient in $\mathbb{L}_\infty$ is locally Lipschitz.

In what follows, (1.3) is used as the definition of a quasi-isometric mapping.

5. The deviations of solutions to variational problems from target solutions should be max-norm bounded, which also naturally leads to the concept of quasi-isometry. It may happen that the properties of the target mapping are known but it is unclear how it can be constructed.

6. The method for mapping construction should apply to a fairly wide class of regions; in particular, the smoothness conditions for the boundary should not be very restrictive.

7. Solutions to variational problems should be orientation-preserving and, under proper boundary conditions, should be a global homeomorphism. From a practical point of view, this means that solutions should satisfy a set of easy-to-check algebraic conditions that lead to the required global topological properties. The most prominent examples of such conditions can be found in [10, 11].

It was shown in [10] that a mapping $y(\eta)$ from a certain Sobolev class that satisfies the bounded distortion (bounded deformation) inequality

$$\det \nabla_\eta y > K\left(\frac{1}{n}\operatorname{tr}(\nabla_\eta y^T \nabla_\eta y)\right)^{n/2}, \quad 0 < K \le 1, \tag{1.4}$$

almost everywhere is open and discrete. This means that the image of any open set under this mapping is also an open set, and any point in the image can have a finite number of preimages.

The following remarkable result was proved in [11]. Suppose that $y(\eta)$ is an orientation-preserving mapping from a certain Sobolev class (i.e., $\det\nabla_\eta y > 0$ almost everywhere) and a functional of form (1.1) is bounded and, on the boundary of the domain of $y(\eta)$, coincides with continuous diffeomorphism. Then, $y(\eta)$ is a global homeomorphism. The restrictions imposed on the geometry of the domain and on the smoothness of its boundary in this theorem are fairly weak, so the theorem applies to practically important cases, for example, when the domain boundary is Lipschitz.

It should be noted that both results are applicable to quasi-isometric mappings. On the other hand, quasi-isometry and the property of the Jacobian to be positive almost everywhere are insufficient for the local invertibility of the mapping.

8. There are several highly developed approaches to the construction of mappings.

The harmonic mappings approach [12] is relatively simple in practice and is based on convex functionals. In many practically important two-dimensional cases, it guarantees the construction of one-to-one mappings. However, if the boundary of the domain is nonsmooth, then the dilatation of the harmonic mapping (i.e., the ratio of the maximum to minimum singular values of the Jacobi matrix) is unbounded near the boundary. This phenomenon is well known in mechanics as stress concentration. In the case of a harmonic mapping with a nonsmooth metric, an unbounded dilatation can appear inside the domain. When the dilatation is unbounded, the harmonic mappings are unstable with respect to input data.

The conformal mapping technique yields a complete solution to the problem in relatively simple cases. It was shown in [9] how one can construct a mapping of a curvilinear quadrangle onto a square such that it is conformal with respect to a special metric and is quasi-isometric. However, the total metric distortion (i.e., the constant C_1) in this approach is far from its minimum, and the approach cannot be applied to domains with nonsmooth (i.e., Lipschitz) boundaries and cannot be generalized to the three-dimensional case.

2. WELL-POSED VARIATIONAL PROBLEM

The basic principles for well-posed variational problems of constructing orientation-preserving mappings have been formulated in the context of elasticity theory with finite deformations. In fact, the idea of using variational principles from mechanics in grid generation has been exploited quite extensively [4]. However, as noted above, the requirements imposed on the variational principles in these areas are overly different. At the same time, mathematical analysis tools developed in mechanics can be applied to grid generation.

Below is a brief review of the properties of variational problems (1.1) that guarantee the existence of a minimizer (see [13]).

1. The function $f(\nabla_\eta y)$ is polyconvex. This means that it can be written as a convex function of minors of $\nabla_\eta y$. In the two-dimensional case, this means that there exists a convex function $g(\cdot, \cdot)$ such that $f(\nabla_\eta y) = g(\det\nabla_\eta y, \nabla_\eta y)$. In the three-dimensional case, this implies the existence of a convex function $g(\cdot, \cdot, \cdot)$ such that $f(\nabla_\eta y) = g(\det\nabla_\eta y, \nabla_\eta y, \operatorname{adj}\nabla_\eta y)$, where $\operatorname{adj} Q = Q^{-1}\det Q$ denotes the adjugate matrix.

2. The function $f(\nabla_\eta y)$ is bounded from below and tends to $+\infty$ as the feasible $y(\eta)$ approaches the boundary of the feasible set, for example, as $\det\nabla_\eta y \longrightarrow +0$.

3. The function $f(\nabla_\eta y)$ satisfies certain growth conditions (see [13]).

4. The set of feasible mappings is defined by a polyconvex inequality [8]. An example of such an inequality is (1.4), which defines a convex set in the $(n^2 + 1)$-dimensional space of entries of the matrix $\nabla_\eta y$ and its determinant. More exactly, the boundary of this set is a paraboloid of the nth degree. Another example is the inequality $\det\nabla_\eta y > 0$, which defines a half-space in the same $(n^2 + 1)$-dimensional space, i.e., defines a convex set.

These conditions, together with the constraints imposed on the domain and the boundary conditions, allow us to prove an existence theorem for the variational problem.

A crucial property is polyconvexity. Any polyconvex functional is rank one convex; i.e.,

$$f(\lambda S_1 + (1-\lambda)S_2) \le \lambda f(S_1) + (1-\lambda)f(S_2)$$

for arbitrary S_1 and S_2 such that $\operatorname{rank}(S_1 - S_2) \le 1$, $0 \le \lambda \le 1$. When $f(\cdot)$ is sufficiently smooth, rank one convexity is equivalent to the Legendre–Hadamard (ellipticity) condition.

3. VARIATIONAL PRINCIPLE FOR QUASI-ISOMETRIC MAPPINGS

In [4], the quasi-isometry condition was written as a polyconvex inequality

$$\det\nabla_\eta y > t\phi_\theta(\det\nabla_\eta y, \nabla_\eta y), \quad 0 < t \le 1,$$
$$\phi_\theta(J, T) = \theta\left[\frac{1}{n}\operatorname{tr}(T^{\mathrm{T}}T)\right]^{n/2} + \frac{1-\theta}{2}\left(v + \frac{J^2}{v}\right), \quad 0 < \theta < 1, \tag{3.1}$$

where $v > 0$ is a constant that defines the average target value of $\det\nabla_\eta y$.

Inequality (3.1) defines a convex bounded domain in the same $(n^2 + 1)$-dimensional space, and the boundary of this domain is a figure resembling an ellipsoid.

It was shown in [14] that the constant C_1 in (1.3) can be evaluated by using (3.1):

$$C_1 < \left(c_2 + \sqrt{c_2^2 - 1}\right)^{1/n}\left(c_1 + \sqrt{c_1^2 - 1}\right)^{(n-1)/n}, \quad c_1 = \frac{1-(1-\theta)t}{\theta t}, \quad c_2 = \frac{1-\theta t}{(1-\theta)t}, \quad L = v^{1/n}.$$

This inequality shows that $1/t$ has the meaning of the total metric distortion.

The variational principle for constructing quasi-isometric mappings is

$$\int_{\Omega_0} f(\nabla_\eta y)d\eta, \quad f = (1-t)\frac{\phi_\theta(\det\nabla_\eta y, \nabla_\eta y)}{\det\nabla_\eta y - t\phi_\theta(\det\nabla_\eta y, \nabla_\eta y)}. \tag{3.2}$$

This functional satisfies most of the conditions above. Its minimization is a well-posed problem in the sense that, if the feasible set (3.1) is nonempty, then a minimizer exists and is a quasi-isometric mapping (see [15]).

By analogy with elasticity problems, it is naturally expected that the uniqueness of a solution and the convergence of finite-element approximations to an exact solution can be proved if the domain boundary and the boundary conditions are very smooth and the solution is close to the identity mapping.

In contrast to elasticity problems, the variational method (3.2) does not admit the Lavrent'ev phenomenon, since minimally regular solutions are locally Lipschitz [15]. The Lavrent'ev phenomenon means different minimizers in different function spaces.

The unsolved theoretical problems include the stability conditions for minimizers and the proof that a minimizer lies strictly inside the feasible set (i.e., at a finite distance from its boundary), if this assertion is valid. The latter problem is related to the existence of a weak variational formulation for the Euler–Lagrange equations (3.2). These problems have also not been completely solved in elasticity [16].

4. CONTROL OF THE PROPERTIES OF THE DESIRED MAPPING VIA COMPOSITION OF MAPPINGS

The variational principle for constructing quasi-uniform mappings has been considered thus far. In practice, however, it is necessary to construct mappings and grids with prescribed distributions of the shape, size, and orientation of elements. We do not discuss the control of orientation (i.e., the angles of a local basis of the mapping with respect to the absolute coordinate axes), which is a very complicated and incompletely solved problem. Nevertheless, a general polyconvex functional allowing the construction of quasi-isometric mappings with orientation control was proposed in [17], where some numerical results were presented as well. Only shape and size control is considered here. The general idea is to apply the same functional and to use a composition of mappings for controlling the local metric properties of the desired mapping. This approach is illustrated in Fig.1.

The mapping $y(\eta)$ is represented as a composition of mappings $\xi(\eta)$, $x(\xi)$, and $y(x)$. Here, ξ and x are assumed to be coordinates in the n-dimensional space and y may be coordinates in an m-dimensional space, $m \geq n$. In particular, $y(x)$ may define a surface parameterization. The mappings $y(x)$ and $\eta(\xi)$ are specified, and $x(\xi)$ is the new desired solution.

The idea of using a composition of mappings for grid control was suggested in [2].

It is assumed that $y(x)$ and $\eta(\xi)$ are quasi-isometric mappings but possibly with large constants C_1.

Using the notations

$$H = \nabla_\xi \eta, \quad S = \nabla_\xi x, \quad Q = \nabla_x y, \quad T = \nabla_\eta y, \quad J = \det T,$$

we obtain

$$T = QSH^{-1}, \quad J = \frac{\det Q \det S}{\det H}, \quad d\eta = \det H d\xi$$

and functional (3.2) is rewritten as

$$\int_\Omega f(Q\nabla_\xi x H^{-1}) \det H d\xi, \tag{4.1}$$

where $\eta(\Omega) = \Omega_0$. Since f depends only on orthogonal invariants of the matrix $T^T T$, we use the equalities

$$T^T T = H^{-T} S^T G S H^{-1}, \quad G(x) = Q^T Q, \quad \tilde{H}(\xi) = H^T H$$

and the fact that $\mathrm{tr}(AB) = \mathrm{tr}(BA)$ to conclude that f can be written as a function of orthogonal invariants of the matrix $S^T G S \tilde{H}^{-1}$ (see [14]).

From a formal point of view, the desired mapping can be treated as a mapping between two manifolds, $(\xi, \tilde{H}(\xi))$ and $(x, G(x))$, each endowed with its own metric [12], which is illustrated in Fig. 1b. In fact, this is a fairly general formulation, since Q and H can now be rectangular matrices, and the metric tensors $\tilde{H}(\xi)$ and $G(x)$ are not assumed to be smooth. The only constraint is that their eigenvalues are positive and have uniform lower and upper bounds. It will be shown below that, when the input control data are two metric tensors, the functional is locally constructed (say on a single finite element) by using the factorized representation (4.1).

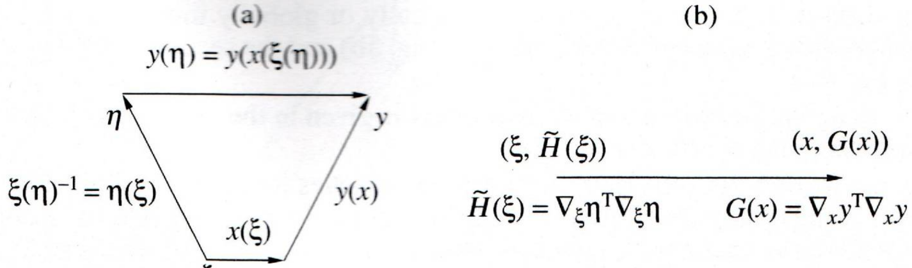

Fig. 1.

5. FUNDAMENTAL DIFFICULTIES IN DISCRETIZATION

In contrast to "standard" variational problems (i.e., those related to finite element solution of linear elliptic equations), discretization problems in mapping theory are mostly unsolved.

1. Surprisingly, the problem of approximating a locally invertible mapping by a converging sequence of locally invertible piecewise affine mappings is not solved even for quasi-isometric mappings, not speaking about more general Sobolev mappings [16].

2. A more complicated problem is as follows. Given a mapping with a metric distortion $1/t$ (1.3) below a certain threshold, is it possible to construct a sequence of converging piecewise affine mappings, each having a metric distortion below the same threshold?

3. The variational principle for surface grid generation must be invariant with respect to the surface parameterization, including the case of nonsmooth parameterizations. How can this property be implemented on the discrete level? What is the counterpart of the finite element patch test condition [18] in the case of spatial mappings?

A reasonable hypothesis is that the difficulties associated with discretization in the two-dimensional case can be overcome by applying A.D. Aleksandrov's theory of metrics with a bounded curvature (a survey of this theory can be found in [19]). Roughly speaking, the main result of Aleksandrov's theory is that every metrically connected space with a bounded curvature is the limit of a properly converging sequence of spaces with polyhedral metrics, each having a bounded curvature. Geodesic triangles in Aleksandrov spaces are well defined, so this concept can be used to construct a discrete approximation to functional (4.1).

6. GEODESIC TRIANGLES AND THE PATCH TEST FOR GRID FUNCTIONALS

Consider a practically important case of surfaces in a three-dimensional space; i.e., $n = 2$ and $m = 3$. We require that the discrete approximation of the functional satisfy the following simple compatibility condition. Consider a mapping between two developable surfaces. Then, under suitable boundary conditions, functional (4.1) should attain an absolute minimum on an isometric mapping. We require that the discrete functional attain an absolute minimum on the same isometric mapping.

Since the problem is considered here from the point of view of the intrinsic surface geometry, the shape of the surface in the three-dimensional space is not important. In particular, different developable surfaces are considered indistinguishable, as shown in Fig. 2.

To construct a discrete approximation of (4.1) with full allowance for all of the controls introduced, we assume that a triangulation is given in coordinates ξ and construct a composition of mappings analogous to that in (4.1), which is shown in Fig. 3. The matrix QSH^{-1} must approximate the gradient of the mapping $\nabla_\eta y$. Symbols mark the unknowns of the variational problem. The unknowns are the images of the nodes of this triangulation in coordinates x. For each triangle, the mapping $y(\eta)$ is assumed to be affine, but $y(x)$ and $\eta(\xi)$ are not affine and must be approximated on each triangle. The idea of the approximation is very simple and also goes back to Aleksandrov. It is illustrated in Fig. 4, which shows the construction of an affine approximation to $y(x)$ and an approximation to $\nabla_x y(x)$.

Consider three points, A, B, and C, in coordinates x and calculate their images under the mapping $y(x)$. Connecting these points by geodesics, we obtain a geodesic triangle on the surface $y(x)$. Replacing this triangle by a flat one, with the side lengths equal to those of the former, we obtain a local affine approximation to $y(x)$ and a natural formula for the matrix Q, which can easily be written and is omitted here. This operation is always well defined, because the distances between the points along the geodesics satisfy the triangle inequality, provided that the three points do not lie on the same geodesic. Note that the spatial orientation of the resulting flat triangle is unimportant, since the functional depends only on Q^TQ.

Suppose that we are given a developable surface in the three-dimensional space of y and two different flattenings of that surface. A flattening is meant as a locally or globally invertible mapping of the surface onto the plane. Let the first flattening be isometric (see Fig. 5b) and the second flattening be quasi-isometric and distorted (see Fig. 5c).

Suppose that a triangulation with fixed connectedness is given in the plane. The coordinates of its nodes are sought by minimizing the functional.

Since $G = I$ in the former case, the discrete functional reaches its absolute minimum, provided that the target shape of each plane triangle is chosen correctly. It can easily be shown that the solution via composition of mappings in the latter case can be reduced to the former case, and the functional also attains its absolute minimum. Thus, irrespective of the surface parameterization, which is defined by a mapping of the plane projection onto the surface, the optimal geodesic mesh is the same (of course, provided that all geodesics are uniquely determined, which is not true in some situations).

7. GLOBAL PARAMETERIZATION OF SURFACES VIA FLATTENING AND UNFOLDING

In the example shown in Fig. 5, the surface parameterization was constructed by means of flattening. This approach has become a major tool in geometric modeling [20], in particular, because it can provide a global parameterization for surfaces consisting of numerous patches with a local parametrization. This is a typical formulation for geometric modeling in computer-aided design (CAD), where the surface of an element may consist of 4000–5000 elementary patches, each defined by a rational B-spline.

Any triangulated surface homeomorphic to a disk with holes can be flattened (see [20]). A more general statement can be formulated in the form of a conjecture.

Conjecture. *Under reasonable constraints, any bounded-curvature manifold homeomorphic to a disk with holes admits a quasi-isometric flattening.*

To construct a surface mesh, one has to construct a global surface parameterization. This can be done, for example, by flattening the surface.

However, it seems that an optimal strategy is to use a finite number of cuts and a quasi-isometric flattening. Finally, we obtain a combination of flattening and unfolding. The resulting plane domain is covered

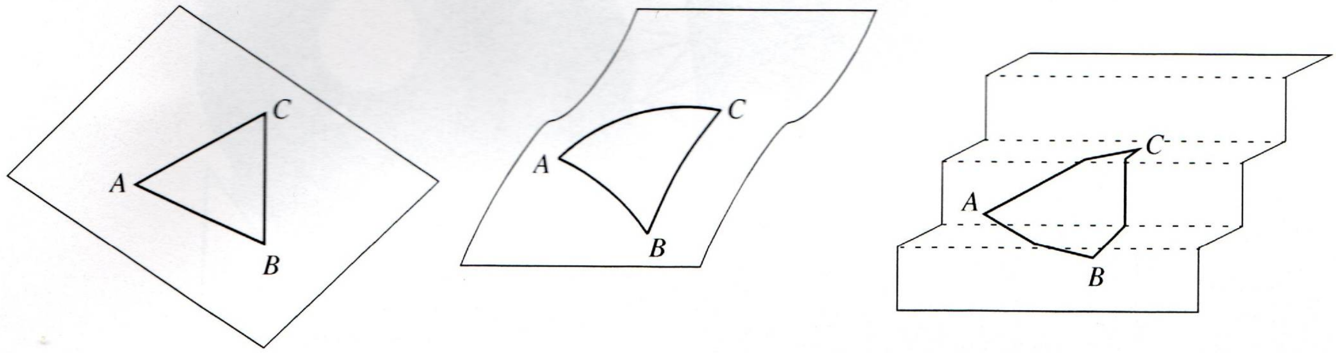

Fig. 2.

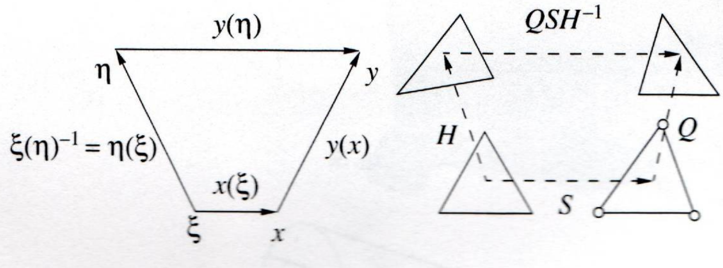

Fig. 3.

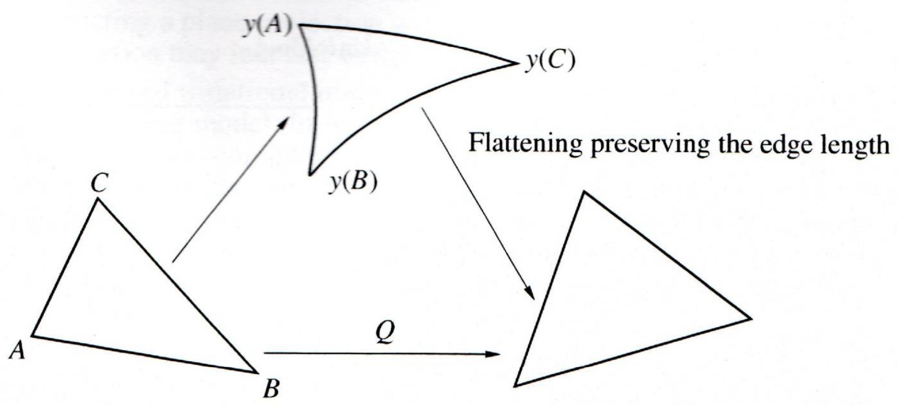

Fig. 4.

with an anisotropic mesh, for example, following the method described in [21]. The mesh is improved by applying the variational method described above, and, next, the plane mesh is mapped back onto the surface and is glued. The determination of an optimal system of cuts is a complicated problem. Apparently, the basic criterion for constructing a system of cuts should be a decrease in the absolute curvature of the surface down to a threshold value. The simplest example is a finite cone, whose curvature is determined by the vertex angle. However, when cut from the vertex to the boundary, the surface becomes developable; i.e., the curvature is equal to zero.

These approaches are illustrated in Fig. 6.

In fact, a perfect mesh on a surface should not depend on the system of cuts, at least locally, i.e., for small variations in the system of cuts. In practice, this is a very restrictive requirement, which means that the nodes of a plane mesh do not necessarily lie on the lines of gluing.

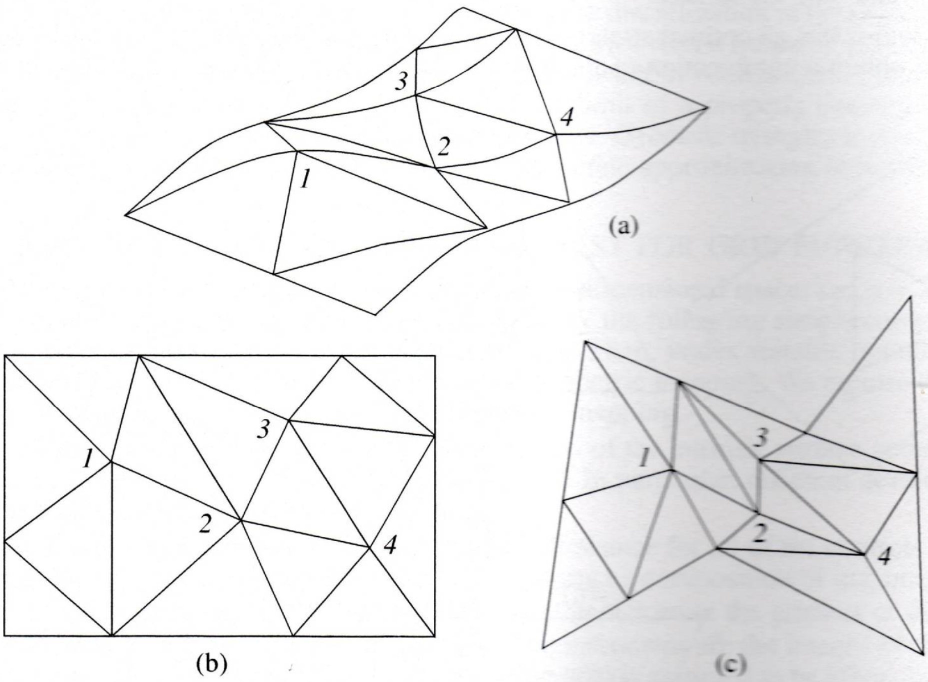

Fig. 5.

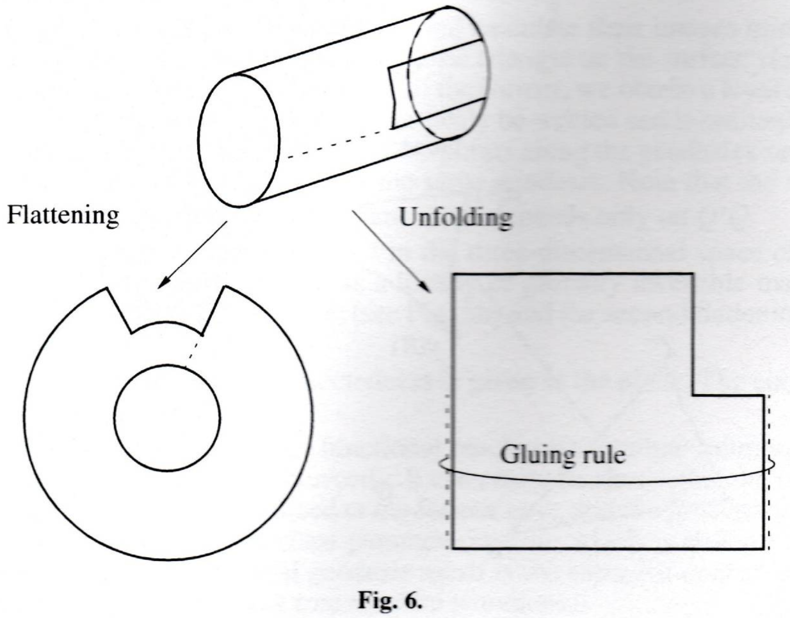

Fig. 6.

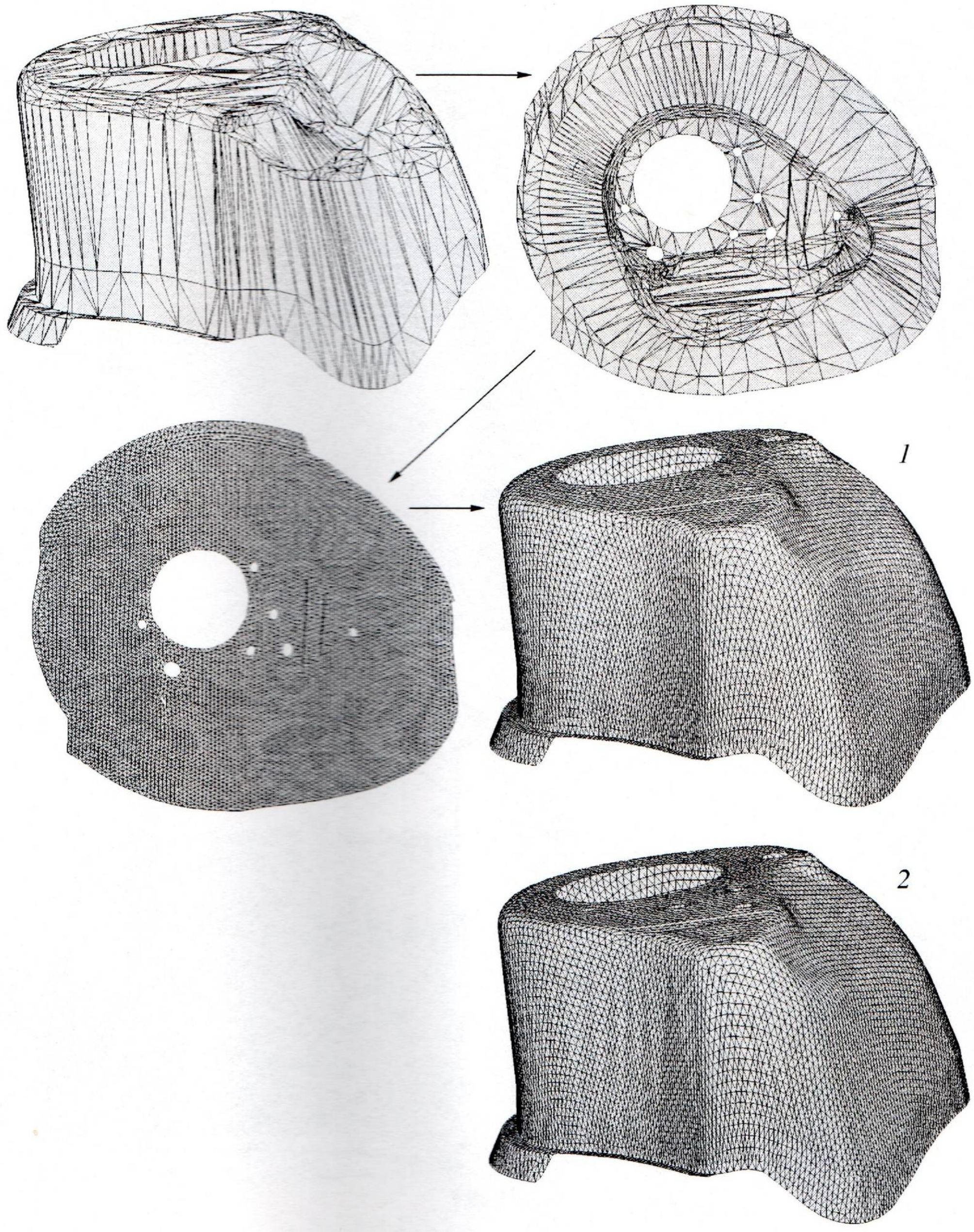

Fig. 7.

Another serious difficulty is that quasi-isometric flattening with least distortion may have self-intersections. The problem of constructing a plane projection with no self-intersections was solved in [17], but it is clear that the total metric distortion may increase in that case.

Both the flattening operation and variational improvement of plane grids can be performed in the framework of the composition-of-mapping model. In the flattening operation, the target shape of each plane triangle is given by the matrix H, which is computed by flattening the geodesic triangle of the surface. In plane mesh improvement, flattening has already defined a global parameterization of $y(x)$, so the matrix Q has to be recomputed for each plane triangle in the course of optimization. If an additional adaptation is required (say adaptation to the curvature of the surface), then it suffices to use another definition of the metric $G(x)$, but the rule for constructing Q remains the same, since the length of geodesics is defined only by the metric.

8. NUMERICAL EXPERIMENTS

A practical method for minimizing the functional suggested is based on the idea of a frozen metric G. Obviously, the matrix H for each triangle is computed only once and "accompanies" each triangle during

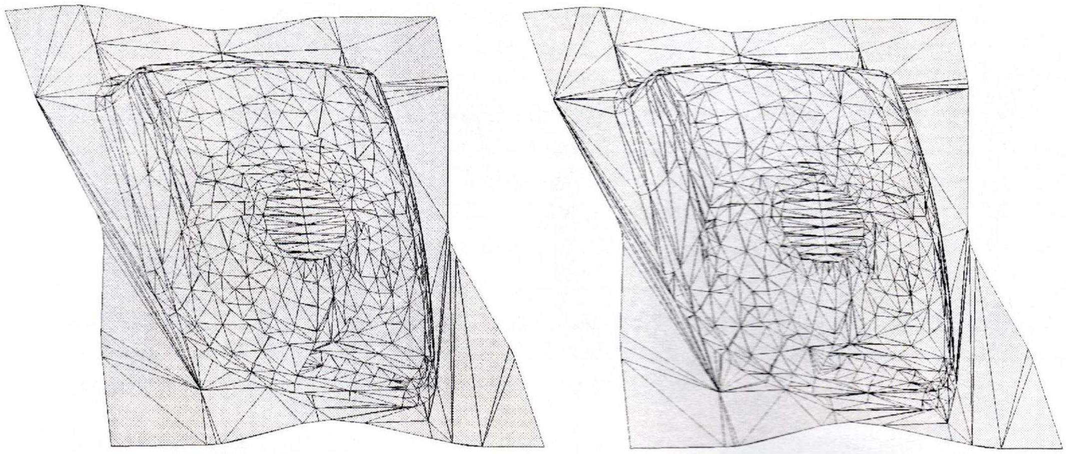

Fig. 8.

(a) (b)

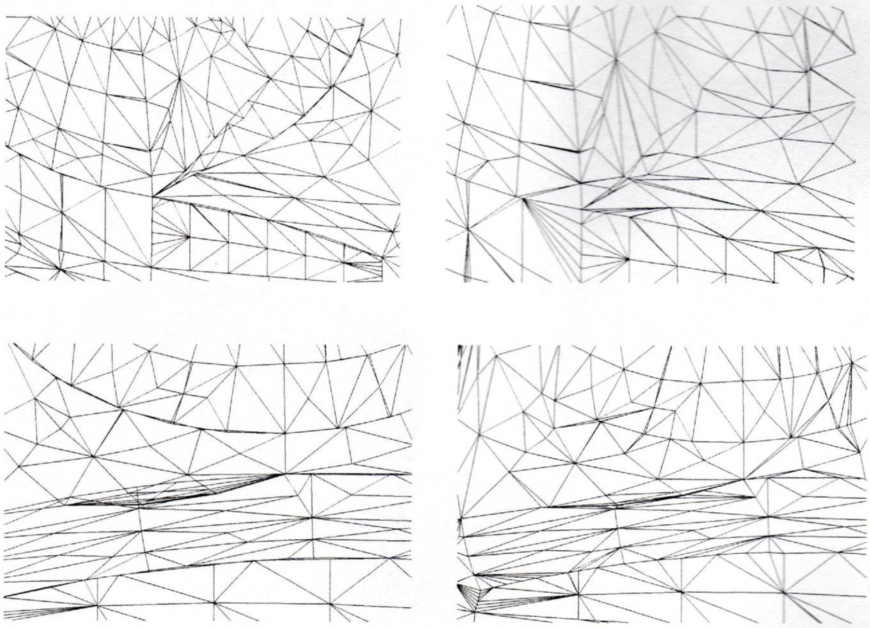

Fig. 9.

the minimization process. This can be interpreted as the shape/size definition in Lagrangian coordinates. On the other hand, the matrix Q changes as soon as the triangle vertices are updated. This behavior resembles the shape/size definition in Eulerian coordinates.

The idea of an iterative method is to solve partial minimization problems for the functional in which $f = f(Q^{k-1}S^kH^{-1})$ for each triangle; here, k is the iteration number. In practice, a partial minimization problem involves one or two inner iterations of the preconditioned gradient method [14]. This approach was found to be very stable and rapidly convergent.

In practice, one can have a surface description different from geodesic triangulations, for example, a tessellation, which approximates the surface with a prescribed chordal error. In that case, one has to construct a quasi-isometric flattening of extremely ill-conditioned triangulations [17].

An example of a meshing procedure based on global flattening is shown in Fig. 7. Note the difference between versions *1* and *2*. In both cases, the mesh quality is quite good, but the patch test is violated for the discrete functional in case *2*. As a result, traces of a nonsmooth surface parametrization can be seen on the final mesh, and difficulties in mesh convergence can be expected.

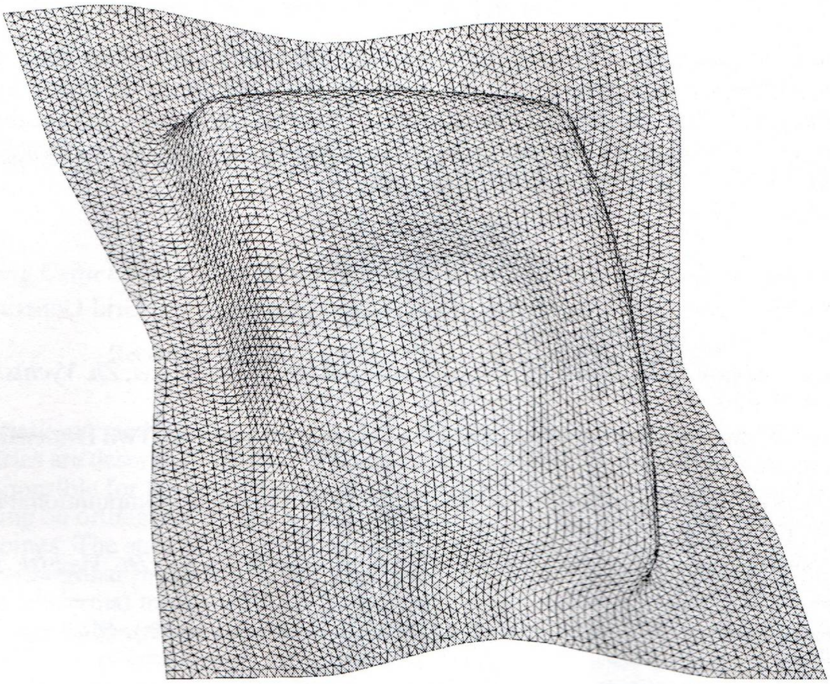

Fig. 10.

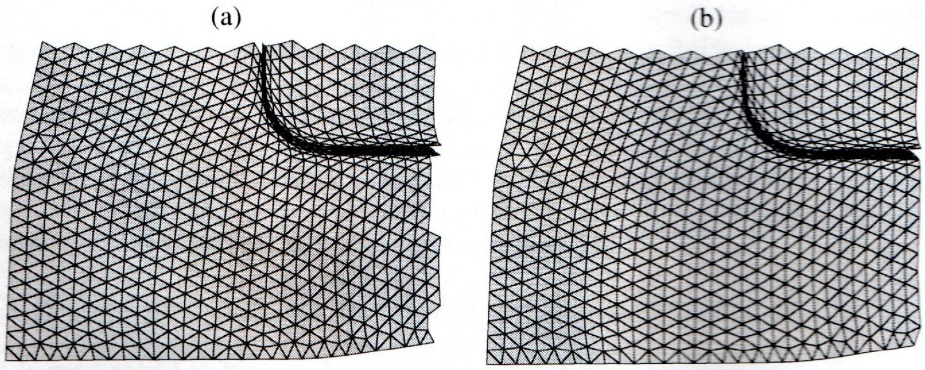

Fig. 11.

Numerical experience suggests that difficulties in the construction of a quasi-isometric flattening are caused not by ill-conditioned triangles in the original surface description but rather by surface wrinkles, especially needle-shaped. In that case, the integral analogue of the Gaussian curvature of the surface (i.e., the curvature in the sense of Aleksandrov) is very large, and flattening with low metric distortion does not exist. That is why a key operation in the repair of geometry is a smoothing of parasitic wrinkles. They frequently appear during the assembly of a surface from CAD patches, in filling holes and slits, and in eliminating topological defects.

An example of a fault-tolerant meshing procedure is shown in Figs. 8–11. Figure 8 displays patch stitching with the repair of the mesh topology and the geometry of the surface. Figure 9 shows fragments of repaired surface triangulations: separate triangulated patches (Fig. 9a) and repaired triangulations (Fig. 9b). An optimized surface mesh is presented in Fig. 10. Figure 11 shows surface mesh fragments in the case when the patch test condition is violated (Fig. 11a) and is satisfied (Fig. 11b). After eliminating the defects, the flattening procedure is very good despite a large number of ill-conditioned facets. Nevertheless, the mapping $y(x)$ is visually nonsmooth because of the very large facets in the original surface description. However, the optimal mesh is not sensitive to this nonsmoothness. The quasi-isometry constant C_1 for local mappings in triangles of the resulting mesh is about 1.3, which seems to be quite close to the unimprovable result.

9. CONCLUSIONS

A number of unsolved problems in grid generation and geometric modeling have been considered. An attempt was made to formulate the general requirements on the variational principle for constructing maps in grid generation and geometric modeling. The important case of mapping construction when the controlling metric is discontinuous was analyzed separately. Based on the theoretical technique suggested, a practical algorithm was developed for surface grid generation.

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