Metric control of spatial mappings

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1. General requirements for variational principle

Variational grid generation methods [1]-[5] have become important tools in many real-life applications. Despite considerable progress in this area, lots of unsolved problems still exist. Some of them are the subject of this paper.

Let us denote by Ω_0 domain in coordinates $\eta = \{\eta_1, \dots, \eta_n\}$. The spatial mapping of interest $y(\eta) : \mathbb{R}^n \to \mathbb{R}^n$ is constructed as a minimizer of the functional depending on the gradient of the mapping:

$$\int_{\Omega_0} f(\nabla_\eta y) d\eta, \quad f : \mathbb{R}^{n\times n} \to \mathbb{R}, \tag{1}$$

where $\nabla_\eta y$ denotes matrix with entries $\frac{\partial y_i}{\partial \eta_j}$.

Comprehensive review of mathematical formulation of minimization problems for such class of functionals, including analysis of conditions of wellposedness, regularity of solutions, restrictions on domains and boundary conditions can be found in [15].

The variational principle used for grid generation and geometric modelling obviously differs from those in mechanics and other areas and should satisfy the following basic requirements:

1.1 Variational problem should be well posed, its solution should exist and should be stable with respect to input data. So the minimal requirement is the ellipticity condition. However it is well known that for highly nonlinear functionals of interest here, ellipticity conditions do not guarantee well posedness of variational problem.

1.2 Variational principle should not admit singular mappings as minimizers, hence the class of admissible mappings consists of locally invertible quasi-isometric mappings [7]. The quasi-isometry means that for any two sufficiently close points in η coordinates, say α and β, the following inequality holds:

$$\frac{L}{C}|\beta - \alpha| \le |y(\beta) - y(\alpha)| \le LC|\beta - \alpha|, \tag{2}$$

where $C > 0$ is the constant, $|\cdot|$ is the Euclidean length and L is the length scale.

1.2 Solutions of variational problem should be as smooth as possible.

1.4 Ability to construct quasi-uniform mappings is a key property in grid generation. Invariant definition of a quasi-uniform mapping reads as follows:

$$\frac{L}{C_1} \le \sigma_i(\nabla_\eta y) \le LC_1, \qquad (3)$$

where σ_i are singular values of $\nabla_\eta y$ and $C_1 > 0$ is a constant. In fact this is equivalent definition of quasi-isometric mapping, provided that inequalities are valid almost everywhere. From (2) it follows that $y(\eta)$ is locally Lipschitz, so its gradient belongs to $\mathbb{L}_\infty$ and inequality (3) holds. On the other hand, any function with gradient belonging to $\mathbb{L}_\infty$ is locally Lipschitz. In what follows we will use (3) as the definition of quasi-isometric mapping.

1.5 Deviation of optimal solutions from the target ones should be bounded in maximum norm, which also naturally leads to quasi-isometry concept.

1.6 Solutions of variational problem should be locally invertible and with proper boundary conditions should be globally one-to-one. From the practical point of view this means that relatively easily checked and/or guaranteed algebraic properties of solutions should lead to required global topological properties. Important examples of such relations are due to Reshetnyak [8] and Ball [11]. In [8] it was shown that a mapping $y(\eta)$ from a certain Sobolev class satisfying bounded distortion inequality

$$\det \nabla_\eta y > K \left(\frac{1}{n} \operatorname{tr}(\nabla_\eta y^{\mathrm{T}} \nabla_\eta y) \right)^{\frac{n}{2}}, \ 0 < K \le 1 \qquad (4)$$

almost everywhere is open and discrete. Namely image of any open set under this mapping is open set, and any point can have only finite number of preimages. In [11] it was proved that a mapping $y(\eta)$ from a certain Sobolev class such that

$$\det \nabla_\eta y > 0$$

almost everywhere and certain functional similar to (1) is bounded, then $y(\eta)$ is globally one-to-one. So if it is possible to prove that solution of variational problem does satisfy suitable algebraic constraints, the global invertibility condition is guaranteed. Quasi-isometric mappings satisfy both Reshetnyak and Ball conditions.

1.7 There are several well established approaches to construction of mappings. Harmonic mappings approach is relatively simple and based on convex functionals [16]. In many practically important 2-D cases it guarantees construction of one-to-one mappings. However in the presence of nonsmooth boundaries the dilatation of harmonic mapping (i.e. the ratio of maximal to minimal singular values of Jacobi matrix) near boundaries can be unbounded. This phenomenon is very well known in mechanics as stress concentration. In the case of harmonic map with nonsmooth metrics the unbounded dilatation can be present far from boundaries. When singularities are present the harmonic maps are not stable with respect to input data.

The conformal mappings technique provides complete solution to the problem in the simple cases. In [7] it was shown how to construct mapping of curvilinear quadrangle onto square which is both conformal and quasi-isometric. However in this approach total metric distortion, i.e. constant C_1 is far from minimal, this approach cannot be applied for domains with nonsmooth boundaries and cannot be generalized to 3-D case.

2. How to obtain well posed variational problem

The basic principles of well-posed variational problems for construction of locally invertible mappings are formulated in the context of mathematical theory of elasticity with finite deformations. In fact the idea of using variational principles from mechanics in grid generation was exploited quite extensively [3]. However variational principles in mechanics generally violate the above requirements and should not be applied as it is. But mathematical tools developed in mechanics are quite universal and should be applied. Let us briefly review basic mathematical principles for well posed variation problem (1) formulated by Ball [9]:

1. Function $f(\nabla_\eta y)$ should be polyconvex, i.e. it can be written as a convex function of minors of $\nabla_\eta y$. In 2-D case it means that there exists convex function $g(\cdot,\cdot)$, such that $f(\nabla_\eta y) = g(\det \nabla_\eta y, \nabla_\eta y)$. In 3-D case the existence of convex function $g(\cdot,\cdot,\cdot)$ is assumed, such that $f(\nabla_\eta y) = g(\det \nabla_\eta y, \nabla_\eta y, \mathrm{adj}\nabla_\eta)$, where $\mathrm{adj}Q = Q^{-\mathrm{T}} \det Q$ denotes the adjugate matrix.

2. $f(\nabla_\eta y)$ should be bounded from below and should tend to $+\infty$ when feasible $y(\eta)$ tends to the boundary of the feasible set, for example when $\det \nabla_\eta y \to +0$.

3. $f(\nabla_\eta y)$ should satisfy certain growth conditions [9].

4. The set of addmissible mappings should be defined by polyconvex inequality [13]. An example of such inequality is (4), which defines a convex set in the $n^2 + 1$-dimensional space of matrix $\nabla_\eta y$ entries plus its determinant. Another example is inequality $\det \nabla_\eta y > 0$ which defines in the same $n^2 + 1$-dimensional space the half-space which is convex as well.

The above conditions allow to prove existence theorem for functional of interest. The most fundamental property is the polyconvexity. Any polyconvex functional is also rank one convex, namely.

$$f(\lambda S_1 + (1-\lambda) S_2) \leq \lambda f(S_1) + (1-\lambda) f(S_2), \text{ where } \mathrm{rank}(S_1 - S_2) = 1.$$

When $f(\cdot)$ is smooth enough the rank one convexity is equivalent to Legendre-

Hadamard (ellipticity) condition. Functionals violating the polyconvexity condition should be rejected.

3 Variational principle for quasi-isometric mappings

In [6] it was suggested a quasi-isometric mapping definition which is polyconvex in the above sense

$$\det \nabla_\eta y > t\phi_\theta(\det \nabla_\eta y, \nabla_\eta y),\ 0 < t \leq 1, \tag{5}$$

$$\phi_\theta(J,T) = \theta(\frac{1}{n}\operatorname{tr}(T^{\mathrm{T}}T))^{\frac{n}{2}} + \frac{(1-\theta)}{2}(v + \frac{J^2}{v}), 0 < \theta < 1,$$

and $v > 0$ is a constant which defines the target average value of $\det \nabla_\eta y$. As was shown in [6], (5) allows direct evaluation of constant C_1 from (3), namely

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

We see that value $1/t$ has the meaning of total metric distortion.

Now the variational principle for construction of quasi-isometric mappings looks as follows

$$\int_{\Omega_0} f(\nabla_\eta y)d\eta,\ \ f = (1-t)\frac{\phi_\theta(\det \nabla_\eta y, \nabla_\eta y)}{\det \nabla_\eta y - t\phi_\theta(\det \nabla_\eta y, \nabla_\eta y)}. \tag{6}$$

This variational principle satisfies all requirements formulated in previous section. It is well posed [13]. If feasible set (5) is not empty then minimizer exists and is a quasi-isometric mapping [13]. Due to similarity with elasticity problems it is natural to expect that global uniqueness of solution and convergence of finite element approximations is provable for problems with very smooth boundary conditions and solution close to identity mapping. However numerical experiments suggest that convergence of finite element approximations is observed in quite general cases so further theoretical analysis is necessary. Unlike elasticity problems, no Lavrentiev phenomenon is possible for (6) since minimally regular solutions are still locally Lipschitz [13]. The Lavrientev phenomenon generally means different minimizers in different functional spaces. The unsolved theoretical problems include the stability conditions for minimizers, the proof (if any) that the minimizer lies strictly inside the feasible set, and somewhat related problem of existence of weak variational formulation of Euler-Lagrange equations of the functional. These problems are not fully solved in elasticity as well [10].

4. Control of the mappings properties via composition of mappings

Up to this point we have considered the variational principle for construction of quasi-uniform mappings. However in practice it is necessary to construct mappings and grids with controlled variations of local shape, size and orientation of elements. We do not consider here orientation/alignment control which is very complicated and essentially unsolved problem. More general functional allowing for construction of quasi-isometric mappings with orientation control was suggested in [18]. Here only shape and size control is considered. General idea is to use composition of mappings in order to modify the properties of solutions. It is illustrated on Fig.1.

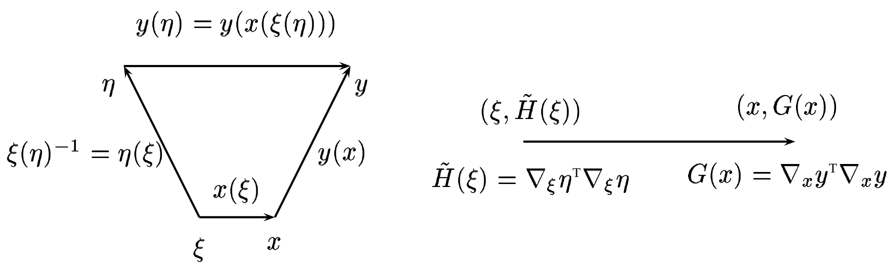

Fig. 1. Composition of mappings. $y(x)$ and $\eta(\xi)$ are prescribed mappings, $^{-1}$ means inverse mapping.

The mapping $y(\eta)$ is represented as a composition of mappings $\xi(\eta)$, $x(\xi)$ and $y(x)$. It is assumed that ξ and x are coordinates in n-dimensional space, while more general case of y coordinates in m-dimensional space, $m \geq n$ is considered as well. In particular $y(x)$ may define a parameterization of surface. The mappings $y(x)$ and $\eta(\xi)$ are specified while the function is $x(\xi)$ is the new unknown solution. We assume again that $y(x)$ and $\eta(\xi)$ are quasi-isometric mappings, but possibly with large constants C_1. Using the notations

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

we get

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

and functional (6) is simply rewritten as

$$\int_\Omega f(Q \nabla_\xi x H^{-1}) \det H d\xi, \qquad (7)$$

where $\eta(\Omega) = \Omega_0$. Note that function f depends only on orthogonal invariants of matrix $T^{\mathrm{T}}T$, and using equalities

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

and the fact that $\operatorname{tr}(AB) = \operatorname{tr}(BA)$ we get that f can be written via orthogonal invariants of the matrix [6]

$$S^{\mathrm{T}} G S \tilde{H}^{-1},$$

and from the formal point of view we have a familiar formulation of a mapping between two Riemannian manifolds $(\xi, \tilde{H}(\xi))$, $(x, G(x))$ [16], which is illustrated on Fig.1(right). This formulation is quite general since matrices Q and H now can be non-square ones and metric tensors $\tilde{H}(\xi), G(x)$ are not assumed to be smooth. The only restriction is that their eigenvalues are positive and should have uniform lower and upper bounds. We will show later that even when input control data are just two metric tensors, discrete approximation to functional on each simplex element naturally employs factorized representation (7).

5. Fundamental discretization problems

Unlike other "standard" problems, say related to finite element solution of linear elliptic problems, the discretization problems in the mappings theory are fundamental and mostly unsolved.

5.1 Surprisingly the problem of approximation of locally invertible mapping by a converging sequence of locally invertible piecewise affine mappings is not solved even for quasi-isometric mappings, not saying about general Sobolev mappings [10].

5.2 Composition of mappings is not closed with respect to Sobolev norms. Hence we do not know general solution for very simple problem: how to approximate by locally invertible piecewise affine mapping a composition of a general quasi-isometric mapping and a locally invertible piecewise affine mapping (which is quasi-isometric by default).

5.3 More difficult problem: given a mapping with metric distortion below certain threshold $1/t$ (5). Is it possible to construct a sequence of converging piecewise affine mappings, each being below the same threshold $1/t$? If it is possible, how to do it in practice?

5.4 Variational principle for surface grid generation should be invariant with respect to surface parameterization, including the case of nonsmooth parameterizations. How this property can be implemented on the discrete level? What is the counterpart of the finite element patch test condition [14] in the case of spatial mappings?

Our hypothesis is that the solutions to above discretization problems should be based on Alexandrov theory of metrics with bounded curvature (see comprehensive review of Alexandrov theory in [19]. Roughly speaking, every metrically connected space with bounded curvature is the limit of converging sequence of spaces with polyhedral metrics, each having bounded curvature. The geodesic triangles in Alexandrov spaces are well defined so we can use this concept for construction of discrete approximation to functional (7).

6. Geodesic triangles and patch test for grid functionals

Let us consider now the case of surfaces in 3-D, so $n = 2,\ m = 3$. We require that discrete approximation to functional should satisfy simple compatibility condition. Let us consider a mapping between two developable surface. Then with proper boundary conditions functional (7) should attain absolute minimum on the isometric mapping. We require that discrete functional attains absolute minimum on the same isometric mapping.

Since we consider here the intrinsic geometry problem, the particular shape of surface is not relevant.

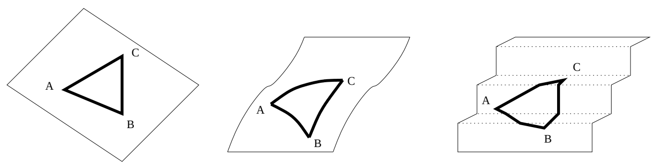

Fig. 2. Undistinguishable geodesic triangles on developable surfaces.

In particular different developable surfaces are undistinguishable which is illustrated on the Fig. 2.

In order to build discrete approximation to (7) fully employing all introduced controls we assume that certain triangulation is available in coordinates ξ and construct a composition of mappings, similar to those in (7).

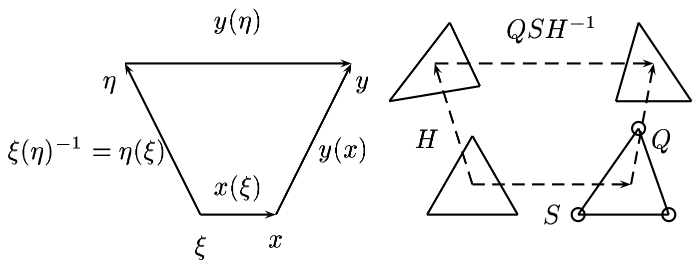

Fig. 3. Composition of mappings and their approximation by composition of affine mappings. Matrix QSH^{-1} is supposed to approximate gradient $\nabla_\eta y$. $\circ$ symbols mark the unknowns of the variational problem.

Our unknowns are images of the nodes of this triangulation in coordinates

x. For each triangle mapping $y(\eta)$ is already assumed to be affine. However mappings $y(x)$ and $\eta(\xi)$ are not affine ones and should be somehow approximated on each triangle. The idea of approximation is very simple and is attributed to Alexandrov as well:

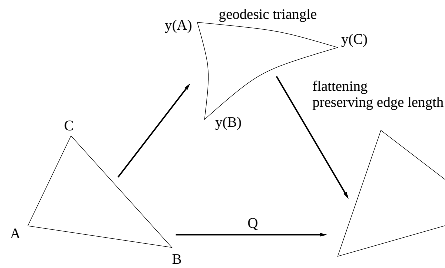

Fig. 4. Construction of affine approximation to $\nabla_x y(x)$.

Let us take three points A, B, C in x-coordinates and compute their images under mapping $y(x)$. Connecting these three points via geodesics we obtain geodesic triangle on the surface $y(x)$. And finally replacing this triangle by a flat one with edge lengths coinciding with those of geodesic triangle, we obtain local affine approximation to $y(x)$ and natural formula for matrix Q which can be easily derived and is omitted here. This operation is always well defined since distance along geodesics satisfies triangle rule. Note that the spatial orientation of last flat triangle is irrelevant since functional depends only on matrix $Q^{\mathrm{T}}Q$.

Suppose that we have a certain developable surface in 3-D space y and two different flattening of this surface. The first one is isometric (see Fig. 5 (left)) and the second one is distorted and is quasi-isometric (see Fig. 5 (right)).

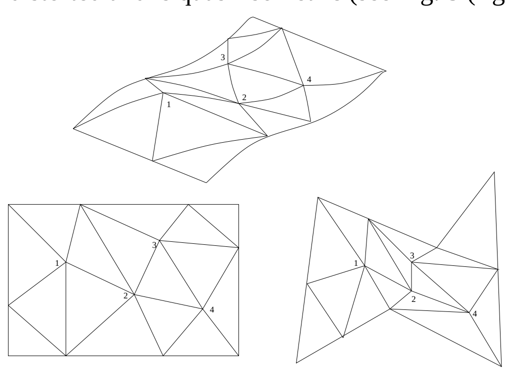

Fig. 5. Patch test: different flattenings and parameterizations of the developable surface and the same optimal mesh on surface.

Since in the first case $G = I$, discrete functional will attain its absolute minimum provided that target shapes for each plane triangle are correctly chosen. It can be easily shown that in the second case the solution via composition of mappings can be reduced to the first one and functional also attains absolute minimum, so independently of surface parameterization, optimal geodesic grid on the surface is the same (of course provided that all geodesics are unique, which is not always the case).

7. Global parameterization of surfaces via unfolding and flattening

In example shown on Fig. 5 the surface parameterization was constructed via flattening operation. This is very powerful tool in geometric modelling [12]. In particular it can provide global parameterization for surfaces defined by mutiple patches (in real life up to 4-5 thousands). Any triangulated surface homeomorphic to disk with holes can be flattened [12]. More general statement can be formulated as a hypothesis: *every manifold with bounded curvature homeomorphic to disk with holes admits quasi-isometric flattening*.

In order to build surface mesh single global parameterization is necessary. Two basic approaches are possible here:

A. Surface unfolding based on construction of geodesic triangulation, flattening of each triangle via edge straightening, connected unfolding of triangles on the plane, meshing of polygon with consistent meshes along cuts and backward folding and mapping onto the surface. This is in fact famous cut and paste operation due to Alexandrov.

B. Surface flattening based on construction of geodesic triangulation, flattening of each triangle via edge straightening, global quasi-isometric flattening, anisotropic meshing of plane domains [17], mesh improvement using variational method described above, mapping of plane mesh back to the surface. Robust method for quasi-isometric flattening was suggested in [18].

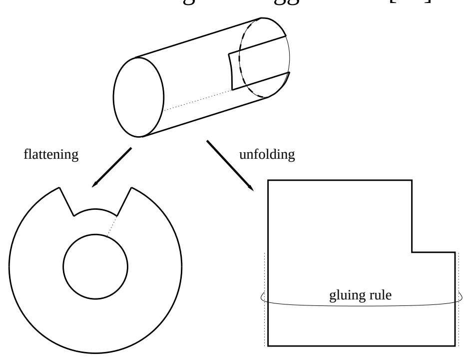

Fig. 6. Flattening vs. unfolding for surface parameterization.

A: Advantages: minimal metric distortion in unfolding operation. Drawbacks: lots of internal cuts, complicated coupling conditions along cuts, not practical for large number of geodesic triangles.
B: Advantages: no cuts, single global plane mesh. Drawbacks: global flattening is not simple, in some cases large metric distortions are inevitable.

It seems that the optimal strategy is to use a finite number of cuts and perform global quasi-isometric flattening combined with unfolding, to construct plane mesh and to do backward folding and mapping. Finding optimal cuts is very hard and unsolved problem.

Both flattening operation and variational improvement of plane grids can be done using the composition of mapping framework. In flattening operation the target shape for each plane triangle is given via matrix H which in turn is computed via flattening of geodesic triangle of the surface. In plane mesh improvement operation flattening have already defined global parameterization of surface $y(x)$, so it is necessary to recompute matrix Q for each plane triangle during optimization procedure. If additional adaptation is necessary, say adaptation to curvature of surface, then we just have different definition of metrics $G(x)$, but the same rules for construction of matrix Q, since length of geodesics is defined only by $G(x)$.

8. Numerical experiments

The practical minimization method for suggested functional is based on the idea of frozen metrics G. Similar idea was successfully used in [**?**]. Obviously matrix H for each triangle is computed only once and “accompany” each triangle during the minimization process. We can interpret it as shape/size definition in “Lagrangian” coordinates. On the other hand matrix Q changes each time triangle vertices are updated, it behaves more like shape/size definition in “Eulerian” coordinates. So the idea of iterative solution is to solve partial minimization problem for functional where for each triangle $f = f(Q^{k-1}S^kH^{-1})$, k being the iteration number. Generally this partial minimization problem involves just 1-2 iterations of preconditioned gradient method [6]. This approach was found very stable and converged quite fast.

In practice one can have surface description different from geodesic triangulation, say tesselation which approximates geometry with prescribed chordal error. Then the basic problem is to compute quasi-isometric flattening of extremely ill-conditioned triangulation [18].

An example of meshing procedure based on global flattening is shown on Fig. 7. Note the difference between meshes on subfigures A and B. In both cases mesh quality is quite good, but in the case B discrete functional violated the patch test and the problems with mesh convergence are expected.

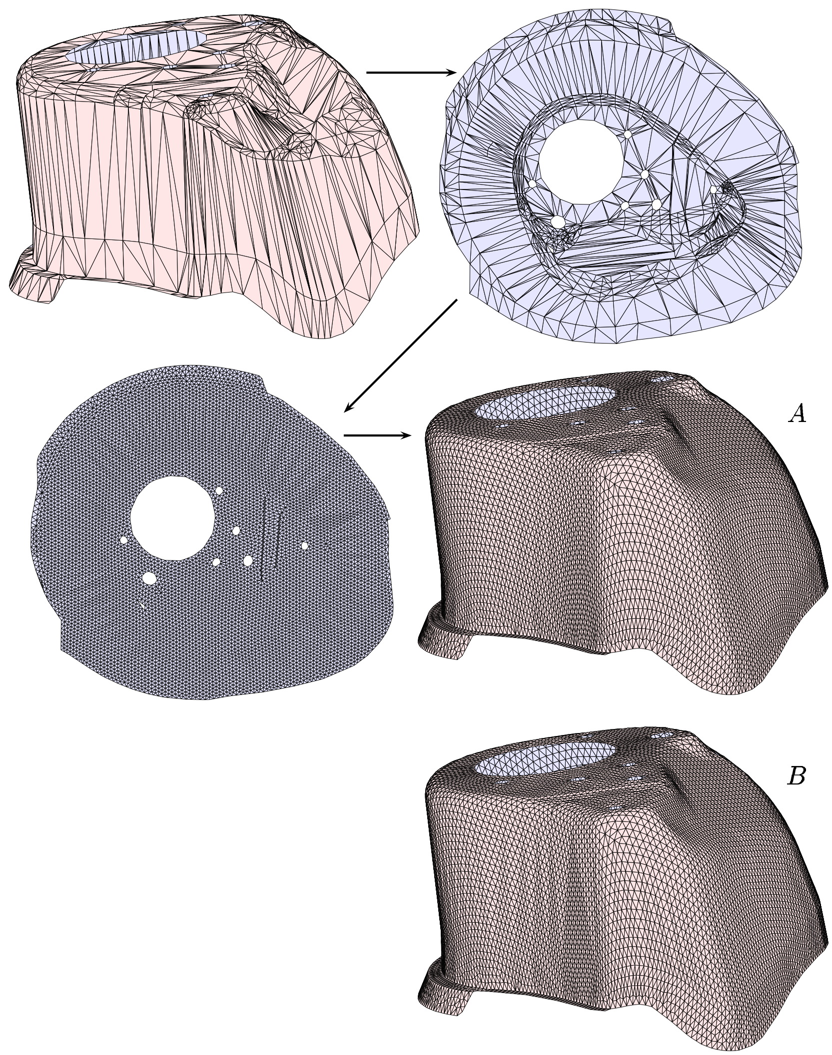

Fig. 7. Surface meshing via quasi-isometric flattening, plane grid generation and variational improvement. **A** - mesh constructed using discrete functional satifying patch test; **B** - patch test is violated.

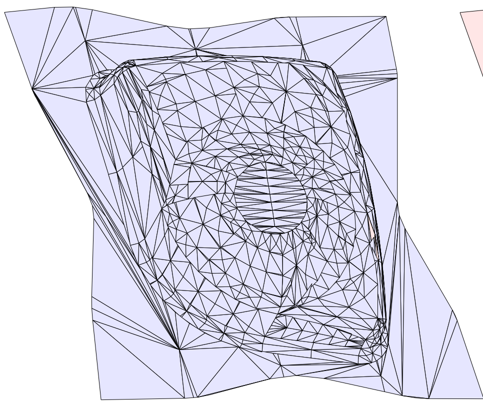

Fig. 8. Patch stitching with repair of topology and geometry of the surface.

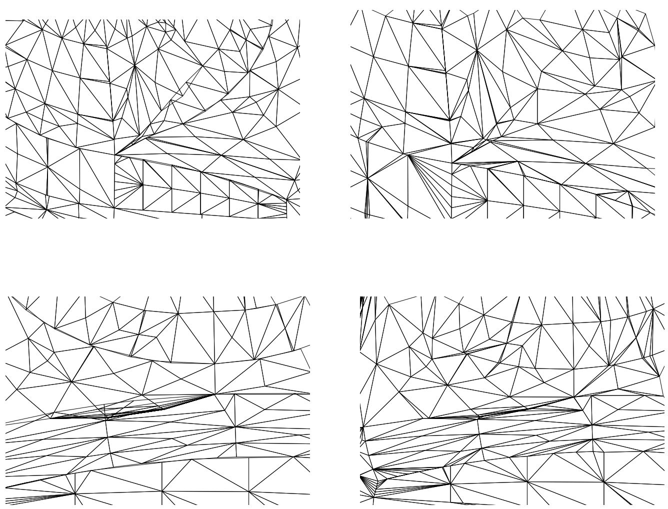

Fig. 9. Fragments of repaired surface tesselations. Left - separate tesselated patches, right - repaired triangulations.

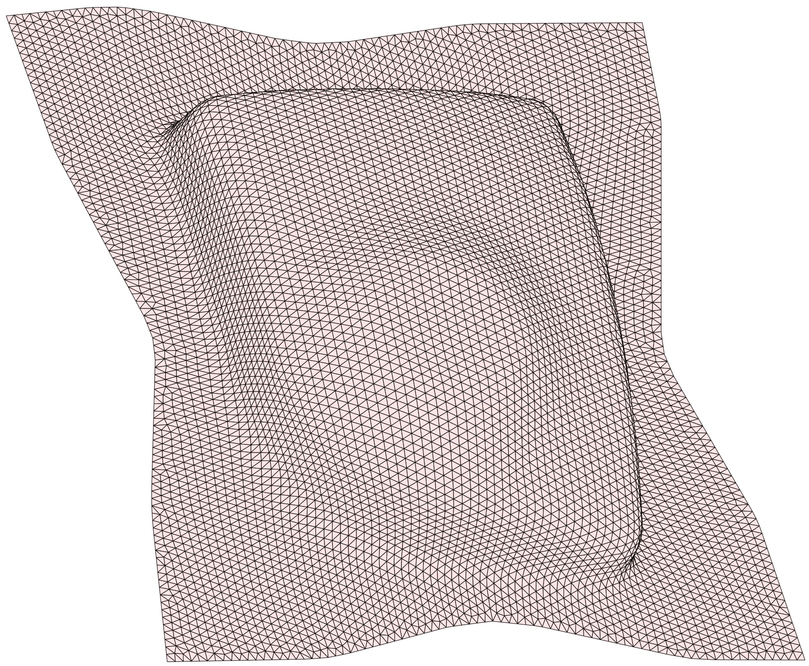

Fig. 10. Optimized surface mesh.

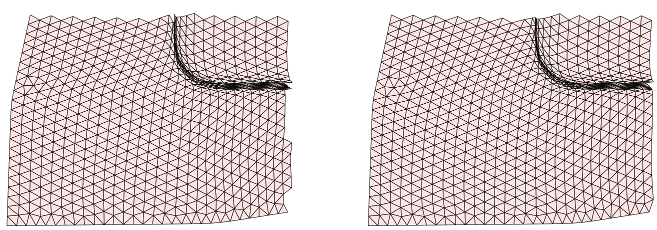

Fig. 11. Surface mesh fragments: left - no patch test, right - patch test is satisfied.

Numerical experience suggests that not bad quality facets, but surface wrinkles, especially needle-like are fatal for flattening quality. In this case Gaussian curvature of surface is very large and flattening with low metric distortion simply does not exist. So a key operation in repair of geometry is smoothing of parasitic wrinkles which by itself is quite nontrivial. The wrinkles can be created during assembly of surface from CAD patches. An example of fault tolerant meshing procedure is shown on Figures 8, 9, 10, 11. In this case the flattening procedure is very good, but still mapping $y(x)$ is nonsmooth due to slightly different flattening of very large facets. In the optimized mesh shown on Fig.10 the quasi-isometry constant C_1 is about 1.6 which seems to be quite close to unimprovable result.

9. Conclusions

Unsolved problems in grid generation were considered and some solutions and hypotheses were suggested. The main conclusion is that grid generation field along with other methods should use ideas and methods from theory of mappings and theory of manifolds of bounded curvature.

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