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Special methods for shape optimization problems

by

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Abstract: The state equations in the shape optimization problems have in general singular solutions, and exact representation of changing shapes by smooth transformations is troublesome. We propose the combination of special approximation method and harmonic transformation to overcome these difficulties. The example solved by specially developed package is presented.

1. Introduction

In the paper we shall consider a method of harmonic transformation applied to the shape optimization problems in plane elasticity, together with special approaches improving its implementation. We shall present also a numerical example ilustrating the performance of the method.

Let us consider a plane domain Ω_t satisfying uniform cone condition (Chenais, 1975), with boundary consisting of finite number of smooth arcs. Uniform cone condition excludes too narrow necks. We split the boundary into two parts: $\partial\Omega = \Gamma_c \cup \Gamma_t$, where Γ_c is constant and Γ_t may change, thus allowing for shape variation. We assume additionally, that all the domains Ω_t, as parametrized by t, fulfil the above stated conditions and additionally $\Omega_{low} \subset \Omega_t \subset \Omega_{upp}$, where sub- and supersets are given. This defines the set of admissible domains Π_{ad}.

In such a domain we define a plane elasticity problem for the state variable $\mathbf{u}_t$ representing displacement:

$$\begin{aligned} A^T \cdot D \cdot A\mathbf{u}_t &= \mathbf{f} \quad \text{in } \Omega_t, \\ \mathbf{u}_t &= \mathbf{g} \quad \text{on } \Gamma_t^1, \\ B^T \cdot D \cdot A\mathbf{u}_t &= \mathbf{h} \quad \text{on } \Gamma_t^2, \end{aligned} \tag{1}$$

where

$$A = \begin{bmatrix} \frac{\partial}{\partial x_1} & , & 0 \\ 0 & , & \frac{\partial}{\partial x_2} \\ \frac{\partial}{\partial x_2} & , & \frac{\partial}{\partial x_1} \end{bmatrix}, \quad B = \begin{bmatrix} n_1 & , & 0 & , & n_2 \\ 0 & , & n_2 & , & n_1 \end{bmatrix},$$

$\mathbf{n}$ - outer normal vector on the boundary, and D - matrix of material constants (Lame coefficients). We assume here, that the boundary data do not introduce additional singularities, i.e. the components of **f, g, h** are in the Sobolev spaces $L_p(\Omega_t)$, $W_p^{2-1/p}(\Gamma_t^1)$, $W_p^{1-1/p}(\Gamma_t^2)$ respectively. The decompositions $\Gamma_c \cup \Gamma_t = \Gamma_t^1 \cup \Gamma_t^2$ in general do not coincide.

Next we consider the domain functional

$$J(t) \;=\; \int_{\Omega_t} F(\mathbf{u}_t)\, d\Omega, \tag{2}$$

which may represent for example a stiffness of the elastic structure or average stress, and formulate the optimization problem

$$\min_{\Omega_t \in \Pi_{ad}} \qquad J(\Omega_t) \tag{3}$$

subject to state constraints (1).

In connection with this there appear three questions:
– how to represent the domain variations?
– what is the sensitivity of the functional (3) with respect to the domain variations?
– how to compute these sensitivities accurately enough?

2. Domain parametrization – harmonic transformations

In general we can take a family of invertible, smooth mappings

$$\Phi_t \,:\, \mathbf{R}^2 \longrightarrow \mathbf{R}^2, \qquad \Phi_0 = \mathrm{id},$$

and define $\Omega_t = \Phi_t(\Omega_0)$, where Ω_0 constitutes some given initial domain. Without loss of generality we may for small t consider only mappings of the form

$$\Phi_t(\mathbf{x}) \;=\; \mathbf{x} \,+\, t\cdot \mathbf{w}, \tag{4}$$

where $\mathbf{w}=[w_1, w_2]$ is a regular enough vector field on $\mathbf{R}^2$. This is the essence of the speed method, see the review in Sokołowski, Zolesio (1992). Since $\mathbf{w}$ is given globally, it may be difficult to ensure, that Γ_c remains exactly in place and Γ_t is exactly as we want it. Therefore it is advantageous to define $\mathbf{w}$ first on the boundary, and to extend it on the whole $\mathbf{R}^2$ next. To this goal we have proposed (Żochowski, 1992) the method of harmonic transformation.

Let $\mathbf{d}= [d_1, d_2]$ defined on Γ_t represents the desired movement of the boundary for $t\,:\,0 \rightarrow t_1$. Then we construct the vector field $\mathbf{v}=[v_1, v_2]$ on Ω_0 as a solution of Laplace equations

$$\begin{aligned} \Delta v_i &= 0 \quad \text{in} \;\; \Omega_0, \\ v_i &= 0 \quad \text{on} \;\; \Gamma_c, \\ v_i &= d_i \quad \text{on} \;\; \Gamma_t, \quad i = 1, 2. \end{aligned} \tag{5}$$

Of course we assume continuity of boundary movement, i.e. $d_i = 0$ at $\partial\Gamma_t$. Due to the uniform cone condition satisfied by Ω_0, each component v_i may be now extended without loss of regularity (Chenais, 1975) on the whole $\mathbf{R}^2$. If we denote these extensions by w_i, the global field $\mathbf{w}$ is thus obtained and the mapping (4) transforms the domain as desired.

The regularity of the field $\mathbf{v}$ requires more detailed specification. Our assumptions concerning domains admit reentrant corners. It means, that v_i may have at a boundary vertex a singularity of the form r^λ, where $\lambda = 1/2 + \delta$, $\delta > 0$, (Grisvard, 1985). Therefore for some neighbourhood V of the given vertex,

$$v_i \in W_p^s(\Omega_0 \cap V), \tag{6}$$

where $s = \lambda + 2/p - \varepsilon$, $\varepsilon > 0$ and W_p^s is a Sobolev space in standard notation, see e.g Grisvard (1985). Since $\delta > 0$ depends on the measure of the reentrant corner, the number of corners is finite and ε may be arbitrarily small, we have finally, after extension on the whole $\mathbf{R}^2$,

$$\mathbf{w} \in [W_p^{s_1}(\mathbf{R}^2)]^2, \tag{7}$$

where $s_1 = 1/2 + 2/p + \delta_1$, $\delta_1 > 0$.

3. Sensitivity computations

The solutions of the state equations depend on Ω_t, i.e. $\mathbf{u}_t = \mathbf{u}(\Omega_t; \mathbf{x})$. In order to characterize this dependence, we make use of the so called material derivative, which is defined as

$$\dot{\mathbf{u}}(\Omega_0; \mathbf{x}) = \frac{d}{dt}\mathbf{u}(\Omega_t; \Phi_t(\mathbf{x}))|_{t=0}. \tag{8}$$

The above equation is understood in the sense of the Sobolev space W_p^1, that is the norm of the difference between $\dot{\mathbf{u}}$ and the difference quotient corresponding to the right–hand side tends to 0 as t goes to 0. There exists also another type of derivative, namely shape derivative (Sokołowski, Zolesio 1992), which is less regular and more difficult to approximate.

Our main goal consists in the following: given the vector field $\mathbf{w}$ in definition (4) of Φ_t find $\dot{J}$,

$$\dot{J} = \frac{d}{dt}J(\Omega_t)|_{t=0}. \tag{9}$$

Before presenting sensitivity results let us observe that our set of admissible domains admit reentrant corners which may coincide with points, where the type of boundary conditions changes. Therefore the solutions of elasticity system (1) may have singularities similarly as $\mathbf{v}$, also of the type r^λ, where $\lambda = 1/2 + \delta$

in points having the same types of conditions on both sides, and $\lambda = 1/4 + \delta$, if the type changes (Vasilopoulos, 1988, Żochowski, 1992). Therefore

$$\mathbf{u}_t \in [W_p^{s_2}(\mathbf{R}^2)]^2, \tag{10}$$

where $s_2 = 1/4 + 2/p + \delta_2, \quad \delta_2 > 0$.

If we take the vector field $\mathbf{w}$ regular enough (e.g. C^2), then it turns out (Sokołowski, Zolesio 1992, Żochowski, 1992), that the material derivative $\dot{\mathbf{u}}$ has the same regularity as $\mathbf{u}$.

In order to write down the final formulae, additional notation must be introduced. Let

$D_x\mathbf{f}$ – Jacobian matrix of the vector function,

$\tilde{\nabla}\mathbf{f} = diag\{\nabla f_1, \nabla f_2\}$,

and

$$\dot{Q} = \begin{bmatrix} -D_x\mathbf{w}^T & 0 \\ 0 & -D_x\mathbf{w}^T \end{bmatrix}, \quad N = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 1 & 1 & 0 \end{bmatrix},$$

$$D(\mathbf{w}) = (\nabla \cdot \mathbf{w})N^T DN + \dot{Q}^T N^T DN + N^T DN\dot{Q},$$

$$S(\mathbf{w}) = \nabla \cdot \mathbf{w} - \mathbf{n} \cdot D_x\mathbf{w} \cdot \mathbf{n}.$$

Let now $\mathbf{u}_0$ correspond to Ω_0 and $\mathbf{q}_0$ be the corresponding adjoint function satisfying the system of equations

$$\begin{array}{rcl} A^T \cdot D \cdot A\mathbf{q}_0 & = & D_u F(\mathbf{u}_0) \ \text{ in } \ \Omega_0, \\ \mathbf{q}_0 & = & 0 \ \text{ on } \ \Gamma_0^1, \\ B^T \cdot D \cdot A\mathbf{q}_0 & = & 0 \ \text{ on } \ \Gamma_0^2, \end{array} \tag{11}$$

Then, exploiting the regularity of $\dot{\mathbf{u}}$ in the intermediate steps, we may eliminate it from the final formulae and obtain the following theorem, Żochowski (1992):

THEOREM 1 *Given* $\mathbf{d}$ *defined on the variable part of the boundary, the derivative* $\dot{J}$ *may be computed as*

$$\begin{array}{rcl} \dot{J} & = & \int_{\Omega_0} [F(\mathbf{u}_0) \cdot (\nabla \cdot \mathbf{v}) + (\tilde{\nabla} \cdot \mathbf{q}_0)^T \cdot D(\mathbf{v}) \cdot \tilde{\nabla}\mathbf{u}_0] \, d\Omega + \\ & + & \int_{\Omega_0} [(\mathbf{f} \cdot \mathbf{q}_0)(\nabla \cdot \mathbf{v}) + (D_x\mathbf{f}) \cdot \mathbf{q}_0] \, d\Omega + \\ & - & \int_{\Gamma_2^0} [(D_x\mathbf{h} \cdot \mathbf{v}) \cdot \mathbf{q}_0 + S(\mathbf{v})(\mathbf{h} \cdot \mathbf{q}_0)] \, dS + \\ & + & \int_{\Gamma_1^0} (D_x\mathbf{g} \cdot \mathbf{v})^T \cdot B^T \cdot D \cdot A\mathbf{q}_0 \, dS \end{array} \tag{12}$$

where the field $\mathbf{v}$ *is the solution of (5). The admissible types of functions* F *correspond to functionals*

$$J_u(t) = \left(\int_{\Omega_t} ||\mathbf{u}_t - \mathbf{u}_d||^{2p} \, d\Omega\right)^{1/2p}, \quad p > 0,$$

$$J_\sigma(t) = (\int_{\Omega_t} ||DA\mathbf{u}_t - \sigma_d||^2 \, d\Omega)^{1/2}.$$

□

Here $\mathbf{u}_d$ denotes a given function, $\mathbf{u}_d \in [W_p^{s_2}(\mathbf{R}^2)]^2$, and $\sigma_d = [\sigma_{11}^d, \sigma_{22}^d, \sigma_{12}^d]^T \in [W_p^{s_2-1}(\mathbf{R}^2)]^3$, see (10).

Let us observe, that the smooth field $\mathbf{w}$ has been replaced in (12) by $\mathbf{v}$. It is a consequence of the fact, that smooth functions are dense in $W_p^{s_1}(\Omega_t)$. We may therefore take the sequence $\mathbf{w}_n$ converging to $\mathbf{v}$ and take the limit in formula (12). However, it is to be noticed (Żochowski, 1992), that the convergence in $W_p^{s_1}$–norm is very nearly the weakest possible for the Theorem 1 to hold. If the reentrant corners are nearly cracks, there is very little surplus of regularity. This indicates, that the expression for $\dot{J}$ is sensitive to the convergence rate of the approximation used in numerical computations.

4. Approximation of singular problems

For finding the field $\mathbf{v}$ and functions $\mathbf{u}, \mathbf{q}$ (state variable, adjoint state) we shall use finite element method. It is well known (Grisvard, 1985), that in standard case one may expect, due to the limited regularity of the above mentioned functions, the convergence rate in $L_2(\Omega_0)$:
- $h^{1/2+}$ for derivatives of $\mathbf{v}$,
- $h^{1/4+}$ for derivatives of $\mathbf{u}, \mathbf{q}$.

This contrasts with full h^1 rate in W_2^2 – regular case. Moreover, the convergence is spoilt not only in the neighbourhood of singular point, but in the whole domain. Since this convergence is quite weak, it is neccessary to improve it in order to apply formula (12) with confidence.

The standard way of dealing with such problems is to refine locally the discretization at the cost of increasing dimensionality (Grisvard, 1985). For changing shapes this has many drawbacks. In Żochowski (1996a) we have proposed another approach. Note similar results derived slightly differently in Ying (1995).

Let us create the star shaped domain encompassing all the triangles having the point of singularity as vertex, Fig.1. Next we decompose this domain S into similar rings, $R_0, R_1, \ldots$ having at $\mathbf{x}_s$ the similarity centre. They are related by the ratio $0 < r < 1$, so that $R_{i+1} = r \cdot R_i$ and $S = \overline{\bigcup_i R_i}$.

Let us now assume for simplicity, that each ring has been triangulated and linear finite elements on triangles used. Denote the nodal values of $\mathbf{u}$ on the outer boundary of R_i by $\mathbf{u}_i$. Then the elastic energy of the ring may be expressed in the discrete form as

$$E_i(\mathbf{u}_i, \mathbf{u}_{i+1}) = \frac{1}{2}[\mathbf{u}_i^T, \mathbf{u}_{i+1}^T] \cdot M \cdot \begin{bmatrix} \mathbf{u}_i \\ \mathbf{u}_{i+1} \end{bmatrix},$$

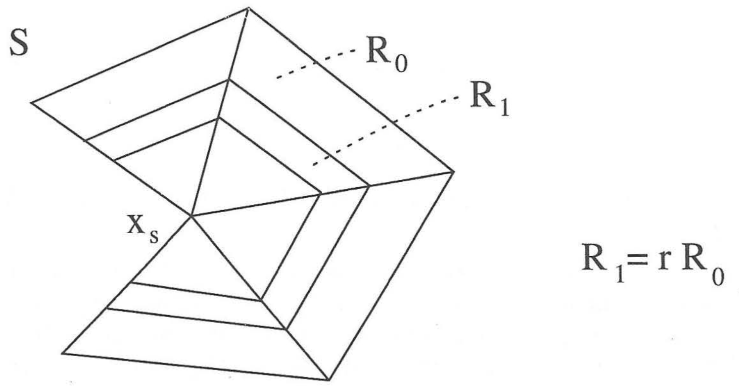

Figure 1. Ring–like discretization around singularity

where the symmetric, semipositive matrix M has the block form

$$M = \begin{bmatrix} M_{d1} & , & M_n \\ M_n^T & , & M_{d2} \end{bmatrix},$$

and does not depend on i. In the subsequent derivations we assume homogeneous and/or traction–free conditions on outer parts of the boundary around $\mathbf{x}_s$ and homogeneous equations, but the method may be generalized on any type of discretization, boundary conditions or constant differential operator.

Now the energy of the whole domain S may be expressed as

$$E = \sum_{i=0}^{\infty} E(\mathbf{u}_i, \mathbf{u}_{i+1}),$$

what leads, if we take $\mathbf{u}_0$ as given, to the infinite system of equations, written in the block form:

$$M_\infty \cdot \mathbf{u}_\infty = \begin{bmatrix} M_d & M_n & & & \\ M_n^T & M_d & M_n & & \\ & M_n^T & M_d & M_n & \\ & & M_n^T & \ddots & \\ & & & & \ddots \end{bmatrix} \cdot \begin{bmatrix} \mathbf{u}_1 \\ \mathbf{u}_2 \\ \mathbf{u}_3 \\ \vdots \\ \vdots \end{bmatrix} = \begin{bmatrix} -M_n^T \\ 0 \\ 0 \\ \vdots \\ \vdots \end{bmatrix} \cdot \mathbf{u}_0, \quad (13)$$

where $M_d = M_{d1} + M_{d2}$.

Infinite systems of linear equations have in general whole family of solutions, but imposing the condition of boundedness on $\mathbf{u}_\infty$ makes it in our case unique. Using the formal series approach (Żochowski, 1996a) one may derive the following procedure. We consider the eigenvalue problem

$$det(\ M_n\lambda^2 + M_d\lambda + M_n^T\ ) = 0,$$

which has $2n$ roots, where $n = dim\, \mathbf{u}_i$. However, they appear in pairs $(\lambda_i, 1/\lambda_i)$, so we always may take half of them satisfying condition $\lambda \leq 1$. Eigenvalues equal to 1 must be considered separately:
- $\lambda = 1$, with multiplicity 2, and only one eigenvector $\mathbf{e}_1 = [1, 0]^T$,
- $\lambda = 1$, with multiplicity 2, and only one eigenvector $\mathbf{e}_2 = [0, 1]^T$,

see more detailed discussion in Żochowski (1996b). For our purpose we shall state only that we take two of them with eigenvectors $\mathbf{e}_1, \mathbf{e}_2$.
Next we create the matrices

$$\Lambda = \mathrm{diag}[\lambda_1, ..., \lambda_n],$$

$$R_\lambda = [\mathbf{r}_{\lambda_1}, ..., \mathbf{r}_{\lambda_n}],$$

where $\mathbf{r}_\lambda$ is a right eigenvector corresponding to λ:

$$(M_n \lambda^2 + M_d \lambda + M_n^T) \cdot \mathbf{r}_\lambda = 0,$$

and finally the matrix

$$Q = R_\lambda \cdot \Lambda \cdot R_\lambda^{-1}.$$

The following theorem may be proved, Żochowski (1996a,1996b):

THEOREM 2 *The total elastic energy of the discretized displacement field over the domain S may be expressed as*

$$E = \frac{1}{2} \cdot \mathbf{u}_0^T \cdot K \cdot \mathbf{u}_0, \tag{14}$$

where $K = M_{d1} + M_n \cdot Q$.
□

This theorem allows us to compute the stiffness matrix of the superelement surrounding the singularity, which takes into account the infinite local refinement, but does not increase the dimensionality. One may say, that it contains already the discrete singular solution.

As it has been shown in Żochowski (1996a), Ying (1995), such treatment of singularities does indeed raise the L_2 convergence rate to h^2, as in case of regular problems.

5. Implementation

The methods described above have been implemented as a package in the MATLAB environment. Since Theorem 1 gives a procedure for computing sensitivities of any integral functionals, they may appear not only as goals, but constraints as well. A third functional has been added

$$J_v(t) = \int_{\Omega_t} d\Omega,$$

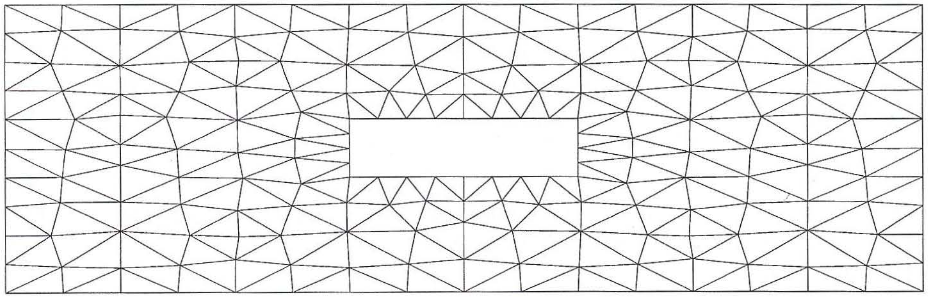

Figure 2. Initial shape of the optimized domain.

and a vector created

$$\mathbf{J}(t) = [J_v(t), J_u(t), J_\sigma(t)].$$

Hence the goal functional could be expressed as

$$G(t) = \mathbf{c}^T \cdot \mathbf{J}(t), \tag{15}$$

and global constraints as (A – 3×3 matrix):

$$A \cdot \mathbf{J}(t) \leq \mathbf{b}. \tag{16}$$

The local geometrical constraints have been imposed in the following way: at each movable node of the discretized boundary the direction of movement (given by a line) has been defined, and on it two limiting points given. Finally, some simplification have been made. It was assumed, that $\mathbf{g} \equiv 0$, $\mathbf{f} \equiv 0$ (only boundary load) and the variable part of boundary is unloaded. This reduces the formula (12) to

$$\dot{J} = \int_{\Omega_0} [F(\mathbf{u}_0) \cdot (\nabla \cdot \mathbf{v}) + (\tilde{\nabla} \cdot \mathbf{q}_0)^T \cdot D(\mathbf{v}) \cdot \tilde{\nabla} \mathbf{u}_0] \, d\Omega. \tag{17}$$

For solving the discrete optimization problems a variant of Pschenichny linearization method has been used. As an ilustration we show here the optimization results for the domain with the initial shape given in Fig.2. The upper edge is uniformly loaded by vertical downward force, both left and right edges are clamped. The lower edge and the hole boundary is traction free and simultanouosly serve as design parameters, i.e. they are allowed to vary. The geometrical constraints are not shown, but they simply allow back and forth movement of the boundary points by a common for all points distance in the direction perpendicular to the initial edge. We wanted to obtain the most "stiff" structure of the given weight, what corresponds to the problem:

$$\min J_u(t), \qquad (p = 5)$$

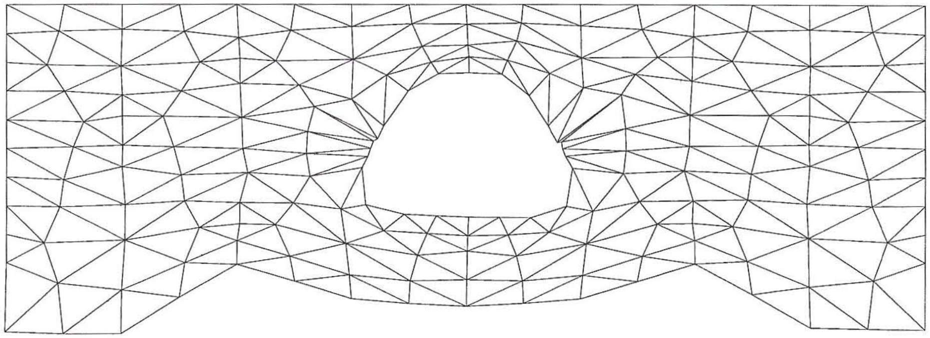

Figure 3. Optimal, i.e. most rigid shape.

subject to

$$\begin{array}{rcr} J_v(t) & \leq & V_0, \\ -J_u(t) & \leq & -V_0, \end{array}$$

and state equation constraints. After 5–6 iterations of the optimization process we have obtained convergence and 15% improvement in the goal function for the shape shown in Fig.3. Experience with many other examples, goal functionals and constraints show that the methods work very reliably.

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