ON OPTIMIZATION OF SYSTEMS GOVERNED BY IMPLICIT COMPLEMENTARITY PROBLEMS*

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Abstract. We consider a class of parameter-dependent implicit complementarity problems possessing for each value of the parameter (control) from a given set a unique solution. Then an optimization problem can be formulated in which such an implicit complementarity problem arises as a constraint. We analyze these optimization problems with the tools of nonsmooth analysis and propose an approach to their numerical solution, using a bundle method from nondifferentiable optimization and a nonsmooth variant of the Newton method. As a test example, the so-called packaging problem, known from the optimum shape design is taken, in which, however, the standard rigid obstacle is replaced by an elastic one.

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Introduction

The implicit complementarity problem (ICP) represents an important case of the quasi-variational inequality, useful in modelling of different complicated

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equilibria ([1, 12]). In the literature these problems are mostly discussed within the theory of quasi-variational inequalities; however, in many respects they indeed deserve a special treatment. The works devoted exclusively to ICP's are, as to our knowledge, not very numerous. To mention at least some of them, there is a two-part paper by Pang ([15, 16]) in which the questions of existence and uniqueness are examined and some iterative algorithms are proposed. In [11] the behaviour of the solution of a parameter-dependent ICP is investigated using a general implicit function theorem from [20] and in [14] a nonsmooth variant of the Newton method is applied to the numerical solution of some ICP's. Some other works may be found in the references of [15].

In the present paper we investigate an optimization problem in which a parameter-dependent ICP arises as a constraint. It can also be viewed as optimal control of a system governed by a parameter-dependent ICP, whereby the parameter plays a role of the control (or design) variable. The organization of the paper is as follows. In Section 1 we formulate the problem, collect the fundamental assumptions and present some basic facts which may be directly derived from the known results. Section 2 is devoted to the analysis of the "system" map which assigns to each parameter from a given set the unique solution of the corresponding ICP. We characterize this map by generalized Jacobians ([3]) and explain how this characterization can be utilized in applying a bundle method from nondifferentiable optimization (NDO) (cf. [7]) to the numerical solution of our optimization problem. For the numerical solution of single ICP's (with fixed parameters) we use a nonsmooth variant of the Newton method as proposed in [18] and [14] which is, under the assumptions being imposed, locally convergent. This is explained in Section 3, where finally the whole method is described and numerical tests are reported. As a nonacademic test example we have chosen the packaging problem ([6]) in which the rigid obstacle has been replaced by an elastic one. In such a way we obtain a shape optimization problem in which the system is governed by an ICP satisfying our assumptions.

1 Problem formulation and preliminaries

Throughout the paper, we employ the following notation: Functions from infinite dimensional spaces are denoted by boldface italic letters $(\boldsymbol{x}, \boldsymbol{y}, \boldsymbol{\lambda}, \ldots)$ and vectors from $\mathbb{R}^n$ by italic letters $(x, y, \lambda, \ldots)$. $\mathrm{Proj}_\Gamma(z)$ is the (metric) projection of the point z on the set Γ, $f'(x_0; v)$ is the directional derivative of the function f at the point x_0 in the direction v, $\partial f(x_0)$ is the generalized gradient or the generalized Jacobian of f at x_0 and for a function $g(x, y)$, differentiable at (x_0, y_0), the partial gradients with respect to x and y at (x_0, y_0) are denoted by $\nabla_1 g(x, y)$ and $\nabla_2 g(x, y)$, respectively. $\triangle$ denotes the Laplacian operator. Further, A^i is the i^{th} row of a matrix A, x^i is the i^{th} component of a vector $x \in \mathbb{R}^n$, $\mathbb{R}^n_+$ is the nonnegative orthant of $\mathbb{R}^n$ and e_i is the i^{th} vector of the canonical basis in $\mathbb{R}^n$. For x, $y \in \mathbb{R}^n$, the inequality $x \geq y$ means $x^i \geq y^i$ for all i.

For a proper understanding of Sections 2 and 3 certain basic knowledge of Lipschitz analysis is required; we state here at least the definition of the generalized gradient/Jacobian and the critical cone and refer the reader to [3] for further helpful information.

Definition 1.1 *Let the operator $H[\mathbb{R}^n \to \mathbb{R}^m]$ be Lipschitz near $x_0 \in \mathbb{R}^n$ and let σ_H denote the set of points at which H fails to be differentiable. The generalized Jacobian of H at x_0 is the set of $[m \times n]$ matrices, given by*

$$\partial H(x_0) = \operatorname{conv}\left\{\lim_{i\to\infty} \nabla H(x_i) \,|\, x_i \to x_0,\ x_i \notin \sigma_H\right\}. \tag{1.1}$$

For $m = 1$, $\partial H(x_0)$ is termed the generalized gradient of H at x_0.

The set (1.1) is nonempty due to the Rademacher's Theorem and the boundedness of the derivatives $\nabla H(x_i)$.

Definition 1.2 *Let $\Gamma \subset \mathbb{R}^n$ be a polyhedral set, $z \in \mathbb{R}^n$ and $x = \operatorname{Proj}_\Gamma(z)$. Then the intersection of the tangent cone to Γ at x (denoted by $T_\Gamma(x)$) with the subspace orthogonal to $z - x$ is called the critical cone of Γ corresponding to z and $z - x$.*

Assume now that U_{ad} is a nonempty and compact set in $\mathbb{R}^n$ and $\mathcal{A} \supset U_{ad}$ is an open bounded set in $\mathbb{R}^n$. Let $G, F[\mathcal{A} \times \mathbb{R}^m \to \mathbb{R}^m]$ be two continuously differentiable operators and consider the ICP:

For a given $x \in \mathcal{A}$ find a vector $y \in \mathbb{R}^m$ such that

$$F(x, y) \geq 0, \quad y \geq G(x, y), \quad \langle F(x, y), y - G(x, y)\rangle = 0. \tag{1.2}$$

Throughout the whole paper we assume that

(A1) $F(x, \cdot)$ is strongly monotone on $\mathbb{R}^m$ (cf. [13]) and (globally) Lipschitz on $\mathbb{R}^m$ for each $x \in \mathcal{A}$.

Let $x_0 \in \mathcal{A}$ be fixed. Under (A1), $F(x_0, \cdot)$ is a homeomorphism of $\mathbb{R}^m$ onto $\mathbb{R}^m$ ([13]) and its inverse is continuously differentiable and strongly monotone on $\mathbb{R}^m$. In what follows this inverse is denoted by $F^{-1}(x_0, \cdot)$.

Proposition 1.1 *Let $x = x_0 \in \mathcal{A}$ and assume that*

$$\begin{gathered}\left\langle h,\, (\nabla_2 F^{-1}(x_0, z))^{\mathrm{T}}\, \nabla_2 G(x_0, F^{-1}(x_0, z))\, h\right\rangle \leq 0 \\ \text{for each } z \in \mathbb{R}^m_+ \text{ and each } h \in \mathbb{R}^m.\end{gathered} \tag{1.3}$$

Then the ICP (1.2) with $x = x_0$ possesses a unique solution.

Proof. Let $y \in \mathbb{R}^m$ and denote $z = F(x_0, y)$. In variable z the ICP (1.2) for $x = x_0$ attains the form

$$\begin{gathered} z \geq 0, \quad F^{-1}(x_0, z) - G\,(x_0,\, F^{-1}(x_0, z)) \geq 0, \\ \langle z,\, F^{-1}(x_0, z) - G(x_0,\, F^{-1}(x_0, z))\rangle = 0, \end{gathered}$$

which is a standard nonlinear complementarity problem. It is equivalent to the variational inequality:

Find $z \in \mathbb{R}^m_+$ such that

$$\left\langle F^{-1}(x_0, z) - G(x_0,\, F^{-1}(x_0, z)),\, w - z \right\rangle \geq 0 \quad \text{for all } w \in \mathbb{R}^m_+. \tag{1.4}$$

Due to Corollary 3.2 in [5], (1.4) possesses a unique solution z_0 whenever the operator

$$\Psi_{x_0}(z) = F^{-1}(x_0, z) - G\left(x_0,\, F^{-1}(x_0, z)\right)$$

is strongly monotone over $\mathbb{R}^m_+$. However, this is ensured by (A1) and the condition (1.3) and so $y_0 = F^{-1}(x_0, z_0)$ is the unique solution of (1.2) (for $x = x_0$). □

To guarantee that the statement of Proposition 1.1 holds on the *whole* set $\mathcal{A}$, we will henceforth suppose that the condition (1.3) is satisfied for each $x_0 \in \mathcal{A}$. Then the ICP (1.2) defines a "system" map $S[\mathcal{A} \to \mathbb{R}^m]$ assigning to each $x \in \mathcal{A}$ the (unique) solution of (1.2) and we turn next our attention to the properties of this operator. The following statement is an easy consequence of the standard results for variational inequalities applied to (1.4).

Proposition 1.2 *The operator S is locally Lipschitz over $\mathcal{A}$ and directionally differentiable at each $x_0 \in \mathcal{A}$. If $h \in \mathbb{R}^n$ is an arbitrary direction, $y_0 = S(x_0)$ and $z_0 = F(x_0, y_0)$, then one has*

$$S'(x_0; h) = -\left(\nabla_2 F(x_0, y_0)\right)^{-1} \nabla_1 F(x_0, y_0)\, h + \left(\nabla_2 F(x_0, y_0)\right)^{-1} v; \tag{1.5}$$

thereby v is the (unique) solution of the linear generalized equation (cf. [19])

$$\begin{aligned} 0 \in \Big[&\nabla_1 F^{-1}(x_0, z_0) - \nabla_1 G(x_0, y_0) - (\nabla_1 F^{-1}(x_0, z_0))^{\mathrm{T}} \nabla_2 G(x_0, y_0)\Big]\; h + \\ &\Big[\nabla_2 F^{-1}(x_0, z_0) - (\nabla_2 F^{-1}(x_0, z_0))^{\mathrm{T}} \nabla_2 G(x_0, y_0)\Big]\; v + N_{K(x_0, z_0)}(v) \end{aligned} \tag{1.6}$$

with $K(x_0, z_0) = T_{\mathbb{R}^m_+}(z_0) \cap (F^{-1}(x_0, z_0) - G(x_0, y_0))^{\perp}$ (critical cone to $\mathbb{R}^m_+$ corresponding to $z_0 - F^{-1}(x_0, z_0) + G(x_0, y_0)$ and $-F^{-1}(x_0, z_0) + G(x_0, y_0)$).

Proof. Under our assumptions the variational inequality (1.4) satisfies the Strong Regularity Condition (SRC) of Robinson at all pairs (x_0, z_0) with $x_0 \in$

$\mathcal{A}$ and $z_0 = F(x_0, S(x_0))$ ([19, 10]). Therefore (cf. [10, Thm. 2.1]), there exists a locally Lipschitz and directionally differentiable operator $Q[\mathcal{A} \to \mathbb{R}^m_+]$ which assigns to each $x \in \mathcal{A}$ the unique solution z of (1.4) with x_0 being replaced by x. Further, due to (A1), the equation $F(x, y) - z = 0$ defines a continuously differentiable implicit function $\mu[\mathcal{A} \times \mathbb{R}^m \to \mathbb{R}^m]$ such that

$$y_0 = \mu(x_0, z_0) \quad \text{and} \quad F(x, \mu(x, z)) - z = 0 \quad \text{on } \mathcal{A} \times \mathbb{R}^m.$$

As $S(x) = \mu(x, Q(x))$, the first assertion follows.

Concerning the second assertion, $Q'(x_0; h)$ is the unique solution of (1.6) again due to [10, Thm. 2.1]. As

$$S'(x_0; h) = -\left(\nabla_2 F(x_0, y_0)\right)^{-1} \nabla_1 F(x_0, y_0)\, h + \left(\nabla_2 F(x_0, y_0)\right)^{-1} Q'(x_0; h),$$

the proof is complete. □

Remark. The partial derivatives $\nabla_1 F^{-1}(x_0, z_0)$ and $\nabla_2 F^{-1}(x_0, z_0)$ in (1.6) may be replaced by $-(\nabla_2 F(x_0, y_0))^{-1} \nabla_1 F(x_0, y_0)$ and $(\nabla_2 F(x_0, y_0))^{-1}$, respectively.

Let $f[\mathcal{A} \times \mathbb{R}^n \to \mathbb{R}]$ be our objective function and assume that f is continuously differentiable. This function together with U_{ad} and the ICP (1.2) define the optimization problem

$$\begin{aligned} &\text{minimize} && f(x, y) \\ &\text{subject to} && y = S(x) \\ & && x \in U_{ad}. \end{aligned} \tag{1.7}$$

It is clear that due to Proposition 1.2 this problem possesses a solution. Another way to write it is

$$\begin{aligned} &\text{minimize} && \Theta(x) := f(x,\, S(x)) \\ &\text{subject to} && u \in U_{ad}. \end{aligned} \tag{1.8}$$

As S and thus also Θ are nondifferentiable in general, standard optimization methods cannot be applied to the numerical solution of (1.8) and we have to refer to methods from NDO, in particular to the effective bundle methods. Such methods typically require that Θ is locally Lipschitz and directionally differentiable and that we dispose of a subgradient[1] of Θ at each iterate. In our situation, Θ evidently satisfies the first two requirements due to Proposition 1.2 and the continuous differentiability of f. The question of the computation of subgradients will be addressed in the next section.

[1]The term subgradient is borrowed from convex analysis, where it is used for the vectors belonging to the subdifferential. Recently, however, it is frequently used also in a nonconvex setting for the elements of various generalized gradients, e.g., the generalized gradient of Clarke.

2 Generalized Jacobians of S

As observed in [17], (1.2) is equivalent to the nonsmooth equation

$$H(x,y) := \min\{F(x,y),\, y - G(x,y)\} = 0, \tag{2.1}$$

where the minimum is taken componentwise. Propositions 1.1, 1.2 imply that (2.1) defines on $\mathcal{A}$ a unique, locally Lipschitz and directionally differentiable implicit function — the operator S.

Let a pair $(x_0, y_0) \in \mathcal{A} \times \mathbb{R}^m$ be fixed and denote

$$\begin{aligned}
&M := \{1, 2, \ldots, m\},\\
&I(x_0,y_0) := \left\{ i \in M \mid F^i(x_0,y_0) < y_0^i - G^i(x_0,y_0) \right\},\\
&J(x_0,y_0) := \left\{ i \in M \mid F^i(x_0,y_0) > y_0^i - G^i(x_0,y_0) \right\},\\
&L(x_0,y_0) := \left\{ i \in M \mid F^i(x_0,y_0) = y_0^i - G^i(x_0,y_0) \right\}.
\end{aligned}$$

Obviously,

$$M = I(x_0,y_0) \cup J(x_0,y_0) \cup L(x_0,y_0).$$

Theorem 2.1 *Let $x_0 \in \mathcal{A}$, $y_0 = S(x_0)$ and assume the existence of a direction $h \in \mathbb{R}^n$ and two index sets L_1, L_2, $L_1 \cup L_2 = L(x_0,y_0)$, such that*

$$\begin{aligned}
&\langle \nabla_1 F^i(x_0,y_0),\, h\rangle + \langle \nabla_2 F^i(x_0,y_0),\, S'(x_0;h)\rangle > 0 \quad \textit{for } i \in L_1\\
&\textit{and}\\
&\langle -\nabla_1 G^i(x_0,y_0),\, h\rangle + (S'(x_0;h))^i -\\
&\qquad\qquad \langle \nabla_2 G^i(x_0,y_0),\, S'(x_0;h)\rangle > 0 \quad \textit{for } i \in L_2.
\end{aligned} \tag{2.2}$$

Further suppose that the $[m \times m]$ matrix $P(x_0)$, given by

$$P^i(x_0) = \left\langle \begin{array}{ll} (\nabla_2 F^i(x_0,y_0))^{\mathrm{T}} & \textit{for } i \in I(x_0,y_0) \cup L_2,\\ (e_i - \nabla_2 G^i(x_0,y_0))^{\mathrm{T}} & \textit{for } i \in J(x_0,y_0) \cup L_1, \end{array}\right. \tag{2.3}$$

is nonsingular. Then one has

$$\Xi(x_0) := -(P(x_0))^{-1}\, T(x_0) \in \partial S(x_0), \tag{2.4}$$

where the $[m \times n]$ matrix $T(x_0)$ is given by

$$T^i(x_0) = \left\langle \begin{array}{ll} (\nabla_1 F^i(x_0,y_0))^{\mathrm{T}} & \textit{for } i \in I(x_0,y_0) \cup L_2,\\ (-\nabla_1 G^i(x_0,y_0))^{\mathrm{T}} & \textit{for } i \in J(x_0,y_0) \cup L_1. \end{array}\right. \tag{2.5}$$

Proof. It is evident that for $i \in L(x_0, y_0)$ and any direction $k \in \mathbb{R}^n$ one has

$$(H'(x_0, y_0;\ k,\ S'(x_0; k))^i = \min\left\{\langle \nabla_1 F^i(x_0, y_0),\ k\rangle + \langle \nabla_2 F^i(x_0, y_0),\ S'(x_0; h)\rangle\ ,\right.$$
$$\left.\langle -\nabla_1 G^i(x_0, y_0),\ h\rangle + (S'(x_0; h))^i - \langle \nabla_2 G^i(x_0, y_0),\ S'(x_0; h)\rangle\right\} = 0.$$

Therefore the inequalities (2.2) imply the existence of a positive number ϑ_1 such that

$$\begin{aligned} L(x_0 + \vartheta h,\ S(x_0 + \vartheta h)) &= \emptyset, \\ I(x_0 + \vartheta h,\ S(x_0 + \vartheta h)) &= I(x_0, y_0) \cup L_2, \\ J(x_0 + \vartheta h,\ S(x_0 + \vartheta h)) &= J(x_0, y_0) \cup L_1 \end{aligned}$$

for all $0 < \vartheta < \vartheta_1$. From the nature of H it is clear that there is an open set $\mathcal{O}$ in $\mathcal{A} \times \mathbb{R}^m$ containing the set

$$\{(x_0 + \vartheta h,\ S(x_0 + \vartheta h))\,|\,0 < \vartheta < \vartheta_1\}$$

where H is continuously differentiable. As $P(x_0)$ is nonsingular and S is continuous, there exists a positive number $\vartheta_2 \leq \vartheta_1$ such that the matrices

$$\nabla_2 H(x_0 + \vartheta h,\ S(x_0 + \vartheta h))$$

are also nonsingular for all $0 < \vartheta < \vartheta_2$. For such ϑ's, the classical implicit function theorem may be applied to the equation $H(x, y) = 0$ at the pairs $(x_0 + \vartheta h,\ y_0 + \vartheta h)$, which yields

$$\nabla S(x_0 + \vartheta h) = -\left(P(x_0 + \vartheta h)\right)^{-1}\ T(x_0 + \vartheta h);$$

thereby

$$P^i(x_0 + \vartheta h) = \begin{cases} (\nabla_2 F^i(x_0 + \vartheta h,\ S(x_0 + \vartheta h)))^{\mathrm{T}} & \text{for } i \in I(x_0, y_0) \cup L_2, \\ (e_i - \nabla_2 G^i(x_0 + \vartheta h,\ S(x_0 + \vartheta h)))^{\mathrm{T}} & \text{for } i \in J(x_0, y_0) \cup L_1, \end{cases}$$

and

$$T^i(x_0 + \vartheta h) = \begin{cases} (\nabla_1 F^i(x_0 + \vartheta h,\ S(x_0 + \vartheta h)))^{\mathrm{T}} & \text{for } i \in I(x_0, y_0) \cup L_2, \\ (-\nabla_1 G^i(x_0 + \vartheta h,\ S(x_0 + \vartheta h)))^{\mathrm{T}} & \text{for } i \in J(x_0, y_0) \cup L_1. \end{cases}$$

If we let now $\vartheta \downarrow 0$, we get formula (2.4) by the definition of the generalized Jacobian. □

Remark. It is obvious that if $L(x_0, y_0) = \emptyset$, then we may directly conclude that S is differentiable at x_0 and $\nabla S(x_0) = -(P(x_0))^{-1}\, T(x_0)$.

For the computation of one arbitrary vector from $\partial\Theta$ at $x_0 \in \mathcal{A}$ we need to know one arbitrary matrix $\Xi(x_0) \in \partial S(x_0)$. Then by the generalized Jacobian Chain Rule (cf. [3]) one has

$$\nabla_1 f(x_0, y_0) + (\Xi(x_0))^{\mathrm{T}}\, \nabla_2 f(x_0, y_0) \in \partial\Theta(x_0), \tag{2.6}$$

where $y_0 = S(x_0)$. However, the verification of the requirements of Theorem 2.1 is usually a difficult task. One possibility could be to choose an arbitrary direction $k \in \mathbb{R}^m$, compute first $S'(x_0; k)$ and then the expressions on the left-hand sides of the inequalities (2.2). If for all $i \in L(x_0, y_0)$ one of these two expressions is positive, the index sets L_1, L_2 may be identified and formula (2.4) holds true. Unfortunately, the computation of $S'(x_0; k)$ is rather cumbersome and additionally, for a randomly chosen k, it could happen that for some $i \in L(x_0, y_0)$ both expressions in (2.2) are zero. We return to this subject in the Conclusion.

To compute a subgradient of Θ at x_0, one actually does not need to compute a matrix from $\partial S(x_0)$ and proceed directly according to (2.6). It is substantially easier to use the adjoint-equation technique, known from the classical optimal control theory. This way is again based on Theorem 2.1.

Proposition 2.1 *Let $x_0 \in \mathcal{A}$, $y_0 \in S(x_0)$ and suppose that the assumptions of Theorem 2.1 hold with index sets L_1, L_2. Let p_0 be the solution of the adjoint linear equation*

$$(P(x_0))^{\mathrm{T}}\, p + \nabla_2 f(x_0, y_0) = 0. \tag{2.7}$$

Then one has

$$\xi := \nabla_1 f(x_0, y_0) + (T(x_0))^{\mathrm{T}}\, p_0 \in \partial\Theta(x_0). \tag{2.8}$$

Proof. By (2.4)

$$\left(\Xi(x_0))^{\mathrm{T}}\, \nabla_2 f(x_0, y_0)\right) = -\,(T(x_0))^{\mathrm{T}} \left((P(x_0))^{-1}\right)^{\mathrm{T}} \nabla_2 f(x_0, y_0) = (T(x_0))^{\mathrm{T}}\; p_0.$$

Thus, $\xi \in \partial\Theta(x_0)$ due to (2.6.) $\square$

3 The numerical method and applications

3.1 Nonsmooth Newton method

At each evaluation of Θ we have to solve (1.2) for the appropriate value of x with a high accuracy. A suitable solver of (1.2) can thus speed up the whole optimization in a decisive way. We have implemented to this purpose a nonsmooth variant of the Newton method, proposed originally in [18]. In [14], this method has been applied to the numerical solution of some quasi-variational inequalities and in particular to ICP's (1.2), whereby a surprisingly fast convergence has been observed.

Let $x = \bar{x} \in \mathcal{A}$ and denote $\Phi_{\bar{x}}(y) := H(\bar{x}, y)$. $\Phi_{\bar{x}}$ is evidently locally Lipschitz and in [14] it has been shown that it is even *semismooth* at each $y \in \mathbb{R}^m$, i.e. that the limit

$$\lim_{\substack{V \in \partial\Phi_{\bar{x}}(y + th') \\ h' \to h,\; t \downarrow 0}} \{V\, h\}$$

exists for each $h \in \mathbb{R}^m$. Consider for a given $y_0 \in \mathbb{R}^m$ the iterative process

$$y_{k+1} = y_k - V_k^{-1}\Phi_{\bar{x}}(y_k), \quad k = 0, 1, \ldots, \tag{3.1}$$

with $V_k \in \partial\Phi_{\bar{x}}(y_k)$. If $\bar{y} = S(\bar{x})$ and all matrices from $\partial\Phi_{\bar{x}}(\bar{y})$ are nonsingular, then this iterative process would be well-defined and convergent in a neighbourhood of $\bar{y}$ ([18]). For $\partial\Phi_{\bar{x}}(\bar{y})$ we have the following estimate.

Proposition 3.1 *Let $V(\bar{x}, \bar{y}) \in \partial\Phi_{\bar{x}}(\bar{y})$. Then one has*

$$V^i(\bar{x}, \bar{y}) = \left\langle \begin{array}{ll} (\nabla_2 F^i(\bar{x}, \bar{y}))^{\mathrm{T}} & \textit{for } i \in I(\bar{x}, \bar{y}), \\ (e_i - \nabla_2 G^i(\bar{x}, \bar{y}))^{\mathrm{T}} & \textit{for } i \in J(\bar{x}, \bar{y}) \end{array} \right. \tag{3.2}$$

and

$$V^i(\bar{x}, \bar{y}) \in conv\left\{ \left(\nabla_2 F^i(\bar{x}, \bar{y})\right)^{\mathrm{T}}, \left(e_i - \nabla_2 G^i(\bar{x}, \bar{y})\right)^{\mathrm{T}} \right\} \quad \textit{for } i \in L(\bar{x}, \bar{y}).$$

Proof. By [3, Prop. 2.6.2 (e)],

$$\partial\Phi_{\bar{x}}(\bar{y}) \subset \partial\Phi^1_{\bar{x}}(\bar{y}) \times \partial\Phi^2_{\bar{x}}(\bar{y}) \times \ldots \times \partial\Phi^m_{\bar{x}}(\bar{y}).$$

As

$$-\Phi^i_{\bar{x}}(\bar{y}) = \max\left\{ -F^i(\bar{x}, \bar{y}), -\bar{y}^i + G^i(\bar{x}, \bar{y})) \right\},$$

it suffices to apply [3, Prop. 2.3.12] (pointwise maxima). □

To ensure the convergence of (3.1), we will thus assume that

(A2) At each pair $(\bar{x}, \bar{y})$ with $\bar{x} \in \mathcal{A}$ and $\bar{y} = S(\bar{x})$, all matrices $V(\bar{x}, \bar{y})$ given by (3.2) are nonsingular.

In this way we ensure simultaneously that for each decomposition of $L(\bar{x}, \bar{y})$ into L_1, L_2, the matrix $P(\bar{x})$ given by (2.3) (which is also of the type (3.2)) is nonsingular. Unfortunately, a matrix given by (3.2) may evidently not belong to $\partial\Phi_{\bar{x}}(\bar{y})$ and then, if we use it in (3.1), the process need not converge. This is in fact a similar hurdle as in Theorem 2.1 with the choice of L_1, L_2. However, in the numerical tests we have not observed L to be nonempty at the points $(\bar{x}, y_k)$, y_k being generated by (3.1), even if $L(\bar{x}, \bar{y}) \neq \emptyset$. Therefore we had no difficulties in solving our ICP's by the mentioned Newton variant.

Let $\pi_y\partial H(\bar{x}, \bar{y})$ denote the set of all $[m \times n]$ matrices $\mathbb{M}$ such that, for some $[m \times n]$ matrix $\mathbb{N}$, the $[m \times (m+n)]$ matrix $[\mathbb{N}, \mathbb{M}]$ belongs to $\partial H(\bar{x}, \bar{y})$. If we estimate $\partial H(\bar{x}, \bar{y})$ in the same way as $\partial\Phi_{\bar{x}}(\bar{y})$ in Proposition 3.1, we may conclude that due (A2) all matrices from $\pi_y\partial H(\bar{x}, \bar{y})$ are nonsingular whenever $\bar{x} \in \mathcal{A}$, $\bar{y} = S(\bar{x})$. Consequently, the assumptions of the implicit function theorem of Clarke hold, which implies for each $\bar{x}$ the existence of a Lipschitz selection of the system map on a neighbourhood of $\bar{x}$ even without (A1) and (1.3). This generalizes the first assertion in [11, Thm. 2]. However, in this way we get neither the single-valuedness of the system map nor the existence of a locally Lipschitz selection on the whole set $\mathcal{A}$.

The oracle (cf. [7]) which computes for the applied bundle code the values and the subgradients of Θ might be organized according to Fig. 1.

3.2 Packaging problem with elastic obstacle

As an application of the numerical method described in the previous subsection, we consider an example from shape optimization of a mechanical structure described by an ICP. We define the problem, show that it fulfills our theoretical assumptions and report on results of a numerical example.

First we describe the (infinite dimensional) implicit complementarity problem which, after discretization, leads to an ICP of type (1.2). Let us introduce the set of admissible design variables

$$\mathbf{U}_{ad} := \left\{ \boldsymbol{x} \in C^{0,1}([0,1]) \,|\, 0 < c_1 \leq \boldsymbol{x}(\xi^2) \leq c_2,\ |\frac{\mathrm{d}}{\mathrm{d}\xi^2}\boldsymbol{x}(\xi^2)| < c_3 \text{ a.e. in } (0,1) \right\},$$

where c_1, c_2, c_3 are given real positive numbers such that $\mathbf{U}_{ad} \neq \emptyset$. Consider a family of admissible domains $\Omega(\boldsymbol{x})$ with variable right "vertical" part of the boundary:

$$\Omega(\boldsymbol{x}) := \left\{ (\xi^1, \xi^2) \in \mathbb{R}^2 \,|\, 0 < \xi^1 < \boldsymbol{x}(\xi^2) \text{ for all } \xi^2 \in (0,1) \right\}.$$

Denote by $\widehat{\Omega} = (0, c_2) \times (0,1)$ the largest domain from this family. Let $\boldsymbol{\psi} \in H^1(\mathrm{cl}\,\widehat{\Omega})$ be the obstacle function such that $\boldsymbol{\psi} \leq 0$ on $\partial\widehat{\Omega} \cup ((c_1, c_2) \times (0,1))$, and $\boldsymbol{b} \in L^2(\widehat{\Omega})$. Denote by V the Sobolev space $H_0^1(\widehat{\Omega})$. Let $k \in \mathbb{R}_+$ and set formally for $\boldsymbol{y} \in V$

$$\boldsymbol{G}(\boldsymbol{y}) = k(\triangle \boldsymbol{y} + \boldsymbol{b}) + \boldsymbol{\psi}. \tag{3.3}$$

The generalized ICP (cf. [5]) reads as follows:

Find $\boldsymbol{y} \in V$ such that

$$\left.\begin{array}{r} -\triangle \boldsymbol{y} \geq \boldsymbol{b}, \quad \boldsymbol{y} \geq \boldsymbol{G}(\boldsymbol{y}) \\ (\triangle \boldsymbol{y} + \boldsymbol{b})(\boldsymbol{y} - \boldsymbol{G}(\boldsymbol{y})) = 0 \end{array}\right\} \text{in } \Omega(\boldsymbol{x}) \tag{3.4}$$
$$\boldsymbol{y} = 0 \text{ on } \partial\Omega(\boldsymbol{x}).$$

The boundary condition does not fit the standard structure of an ICP. However, after discretization the problem is reduced and we get a standard ICP. The solution $\boldsymbol{y}$ of (3.4) represents the deflection of a membrane fixed on its boundary given by $\partial\Omega(\boldsymbol{x})$, loaded by the pressure $\boldsymbol{b}$ and supported from below

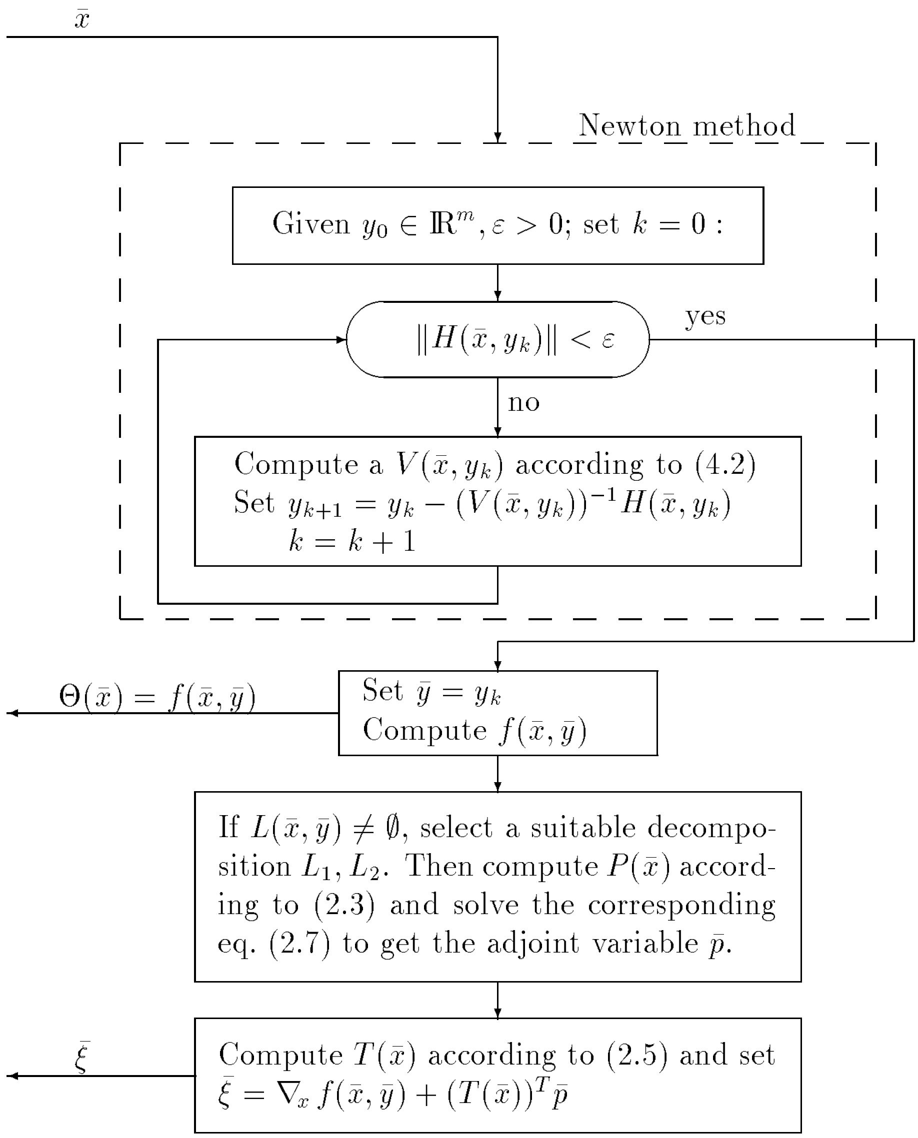

Figure 1: The oracle supplying the bundle code with the value and a subgradient of Θ

by an obstacle made of an elastic (compliant) material. Here $\boldsymbol{\psi}$ describes the original shape of the obstacle and $1/k$ is the coefficient of compliance (e.g., $1/k \approx 0.4$ for sand). The term $\triangle \boldsymbol{y} + \boldsymbol{b}$ represents the force acting on the obstacle. We remark that, when setting $k = 0$ in (3.3), problem (3.4) becomes a standard contact problem with a rigid obstacle given by the function $\boldsymbol{\psi}$ (cf., e.g. [8]).

Let us show that there exists a unique solution of (3.4) for any $\boldsymbol{x} \in \mathbf{U}_{ad}$. Putting $\boldsymbol{\lambda} := \triangle \boldsymbol{y} + \boldsymbol{b}$, we can formally rewrite (3.4) as

$$\left.\begin{aligned} -\triangle \boldsymbol{y} + \boldsymbol{\lambda} &= \boldsymbol{b} \\ \boldsymbol{y} &\geq k\boldsymbol{\lambda} + \boldsymbol{\psi} \\ \boldsymbol{\lambda} &\leq 0 \\ \boldsymbol{\lambda}(\boldsymbol{y} - k\boldsymbol{\lambda} - \boldsymbol{\psi}) &= 0 \end{aligned}\right\} \text{in } \Omega(\boldsymbol{x})$$
$$\boldsymbol{y} = 0 \text{ on } \partial\Omega(\boldsymbol{x}),$$

which can further be rewritten as a nonlinear equation

$$\begin{aligned} -\triangle \boldsymbol{y} + \frac{1}{k}\min\{0, \boldsymbol{y} - \boldsymbol{\psi}\} &= \boldsymbol{b} \quad \text{in } \Omega(\boldsymbol{x}) \\ \boldsymbol{y} &= 0 \quad \text{on } \partial\Omega(\boldsymbol{x}). \end{aligned} \tag{3.5}$$

The existence and uniqueness of a solution to (3.5) is guaranteed by a corollary of Theorem 26.14 from [4] which, in our notation and for a general Ω, can be stated as follows.

Proposition 3.2 *Let $\boldsymbol{g}(\xi)$ be a continuous nondecreasing function on $\mathbb{R}$, $\boldsymbol{b} \in L_2(\Omega)$. Assume that there exists a real number $c > 0$ such that*

$$|\boldsymbol{g}(\xi)| \leq c(1 + |\xi|^\tau) \qquad \textit{for all } \xi \in \mathbb{R}$$

with an arbitrary real positive τ. Then there exists a unique solution (in the weak sense) to the equation

$$\begin{aligned} -\triangle \boldsymbol{y} + \boldsymbol{g}(\boldsymbol{y}) &= \boldsymbol{b} \quad \textit{in } \Omega \\ \boldsymbol{y} &= 0 \quad \textit{on } \partial\Omega. \end{aligned}$$

Setting $\boldsymbol{g}(\xi) := \frac{1}{k}\min\{0, \xi - d\}$ with $k > 0$ and d an arbitrary constant, we can immediately apply the proposition to the problem (3.5). Recall that the case $k = 0$ leads to a linear complementarity problem which can be treated in the standard way (cf. [8]).

In the packaging problem introduced in [2] and [6] we try to find such a control $\boldsymbol{x}^*$ for which the contact of the membrane with the obstacle occurs on a whole given set $\Omega_0 \subset \widehat{\Omega}$, while the surface of the membrane (i.e., the measure of $\Omega(\boldsymbol{x}^*)$) is minimized.

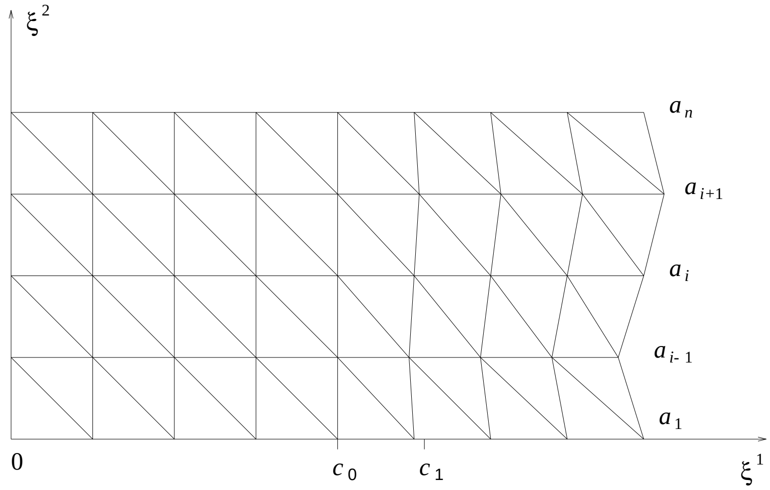

Figure 2: Triangulation of $\Omega(x)$

Let Ω_0 be a closed simply connected subset of $[0, c_0] \times [0, 1]$. For $\boldsymbol{x} \in \mathbf{U}_{ad}$, denote by $\mathbf{Z}(\boldsymbol{x})$ the contact region which is the set $\{\xi \in \Omega(\boldsymbol{x}) \mid \boldsymbol{y}(\xi) = \boldsymbol{G}(\boldsymbol{y})(\xi)\}$, where $\boldsymbol{y}$ is the solution of (3.4). The packaging problem is defined as follows:

$$\begin{array}{ll} \text{minimize } \boldsymbol{E}(\boldsymbol{x}) := & \text{meas } \Omega(\boldsymbol{x}) \\ \text{subject to } & \mathbf{Z}(\boldsymbol{x}) \supset \Omega_0, \\ & \boldsymbol{x} \in \mathbf{U}_{ad}, \\ & \boldsymbol{y} \text{ solves (3.4).} \end{array} \tag{3.6}$$

For the treatment of the state constraint $\mathbf{Z}(\boldsymbol{x}) \supset \Omega_0$, an exact penalty technique has been proposed in [9], leading to an augmented objective functional

$$\boldsymbol{E}_r(\boldsymbol{x}, \boldsymbol{y}) := \text{meas } \Omega(\boldsymbol{x}) + r \int_{\Omega_0} (\boldsymbol{y} - \boldsymbol{G}(\boldsymbol{y}))\, d\xi, \tag{3.7}$$

where $r > 0$ is the penalty parameter.

We discretize our problem by the finite element method in the standard way (cf. [6], [9] for details). The control variable $\boldsymbol{x}$ (one-dimensional real function) is approximated by a piece-wise linear function; the discrete control variable x is a vector of values of this function at n nodes $a_1, \ldots, a_n$, i.e., a vector of ξ^1-coordinates of these boundary nodes (cf. Figure 2). Thus the set $\mathbf{U}_{ad}$ is replaced by the finite-dimensional set

$$U_{ad} := \{x \in \mathbb{R}^n \mid x^i = \boldsymbol{x}(a_i), \boldsymbol{x} \in \mathbf{U}_{ad} \text{ piece-wise linear}\}.$$

The domain $\Omega(\boldsymbol{x})$ is discretized by triangular elements as shown in Figure 2: the triangulation is fixed in a rectangle $[0, c_0] \times [0, 1]$ with $c_0 < c_1$, the rest is triangulated by means of principal moving nodes (control variable) and associated moving nodes, ξ^1-coordinates of which are given by an equidistant division of corresponding line segments. Thus the triangulation depends continuously on x.

For the discretization of the state problem (3.4) we use piece-wise linear basis functions. In the standard way we obtain the stiffness matrix $A(x) \in \mathbb{R}^{m\times m}$ (m is the number of nodes of the mesh) and the right-hand side vector $b(x) \in \mathbb{R}^m$, both continuously depending on $x \in U_{ad}$. The discretized obstacle ψ is the vector of values of the function $\boldsymbol{\psi}$ at the nodes of the triangulation.

The discretized state problem can be written as the following ICP of type (1.2):

For a given $x \in U_{ad}$ find $y \in \mathbb{R}^m$ such that

$$\begin{aligned} &A(x)y - b(x) \geq 0, \quad y \geq G(x,y) \\ &\langle A(x)y - b(x), y - G(x,y)\rangle = 0 \end{aligned} \tag{3.8}$$

with

$$G(x,y) := k(b(x) - A(x)y) + \psi(x). \tag{3.9}$$

Note that while the function $\boldsymbol{G}(\boldsymbol{y})$ does not depend on the control $\boldsymbol{x}$, its discretization $G(x,y)$ does.

The discretization of the optimization problem

$$\begin{aligned} &\text{minimize } \boldsymbol{E}_r(\boldsymbol{x},\boldsymbol{y}) \\ &\text{subject to } \ \boldsymbol{x} \in \mathbf{U}_{ad}, \\ &\qquad\qquad\quad \boldsymbol{y} \text{ solves (3.4)} \end{aligned}$$

is straightforward. Let $\mathcal{D}_0$ be the set of indices of nodes lying in Ω_0. The discretized problem attains the form:

$$\begin{aligned} &\text{minimize } E_r(x,y) := \text{meas } \Omega(x) + \frac{r}{h^2}\sum_{i\in\mathcal{D}_0} y^i \\ &\text{subject to } \ x \in U_{ad}, \\ &\qquad\qquad\quad y \text{ solves the ICP (3.8)}, \end{aligned} \tag{3.10}$$

where $r > 0$, h is the discretization parameter and $\Omega(x)$ the polygonal computational domain. Problem (3.10) is now exactly of type (1.7), with

$$f(x,y) := E_r(x,y).$$

Let us show that the assumptions of Sections 1,2 are satisfied. Due to the definition of U_{ad}, the boundary $\partial\Omega(x)$ is uniformly Lipschitz for all $x \in U_{ad}$, hence the stiffness matrix $A(x)$ is positive definite on U_{ad} and the assumption

(A1) holds. Since $G(x,y)$ is a linear function of y, assumption (1.3) simplifies to

$$\langle h, A^{-1}(-kA)h\rangle = -k\langle h,h\rangle \leq 0 \quad \text{for all } h \in \mathbb{R}^m,$$

which follows from $k \geq 0$. From the definition of the discretization follows the continuous differentiability of $f(x,y)$. It remains to verify the assumption (A2). The matrix $V(x,y)$ is composed from the rows

$$(\nabla_2 F^i(x,y))^T = A^i(x) \tag{3.11}$$

and

$$(e_i - \nabla_2 G^i(x,y))^T = e_i^T + kA^i(x). \tag{3.12}$$

Since $k \geq 0$ and $A(x)$ is nonsingular for all $x \in U_{ad}$, $V(x,y)$ is also nonsingular for all $x \in U_{ad}$ and (A2) holds. Thus the only open question remains the validity of the first assumption of Theorem 2.1. According to the equivalence of the ICP with a nonlinear complementarity problem, the question of convergence of the discretized solutions to the "continuous" one may be treated in the same way as in [6].

Example. Consider the packaging problem in which $\Omega = [0.25, 0.5]\times[0.25, 0.75]$, $b(\xi^1,\xi^2) \equiv -1.0$ and $\psi(\xi^1,\xi^2) = -0.04[(\xi^1)^2 + ((\xi^2)^2 - 0.25)^2]$. The set U_{ad} is specified by the parameters $c_1 = 0.6$, $c_2 = 1.0$, $c_3 = 3.0$, the parameter c_0 (determining the triangulation) was set to 0.5. The discretization parameter was chosen $h = 1/32$, i.e., we used $33 \times 33 = 1089$ discretization nodes and 2048 finite elements. Figure 3 shows the isolines of the initial obstacle. For the parameter of compliance $k = 2$ we obtained the optimal shape shown in Figure 4. The penalty parameter was $r = 10^6$, the resulting value of the objective functional $E_r = 0.6918$. We compared this result with that obtained for $k = 0$, i.e. for a rigid obstacle, by the technique described in [9]. In this case the resulting objective value was $E_r = 0.7616$ and the optimal shape is depicted in Figure 5. One easily sees that both the objective values as the shapes differ substantially from each other. $\square$

Finally, let us make some remarks on the numerical algorithms used for solving the previous example. The "upper-level" nonsmooth optimization problem (3.10) was solved by the bundle algorithm BT ([21]). To solve the above example, we needed 69 BT iterations. The ICP (3.8) was solved by the nonsmooth Newton method described in the beginning of this section. This method was surprisingly efficient — the average number of iterations was 5 in the first ten BT iterations and 3 in the rest; recall that the dimension of the problem was $m = 1089$. The Newton iterations were stopped when either the norm $\|H(\bar{x}, y_k)\|$ or the difference of two successive iterates $\|y_k - y_{k-1}\|$ was less then 10^{-11}. At each Newton step (3.1), one has to solve a system of linear equations with the matrix $V(x_k, y_k)$ from (3.2). In our application, this matrix

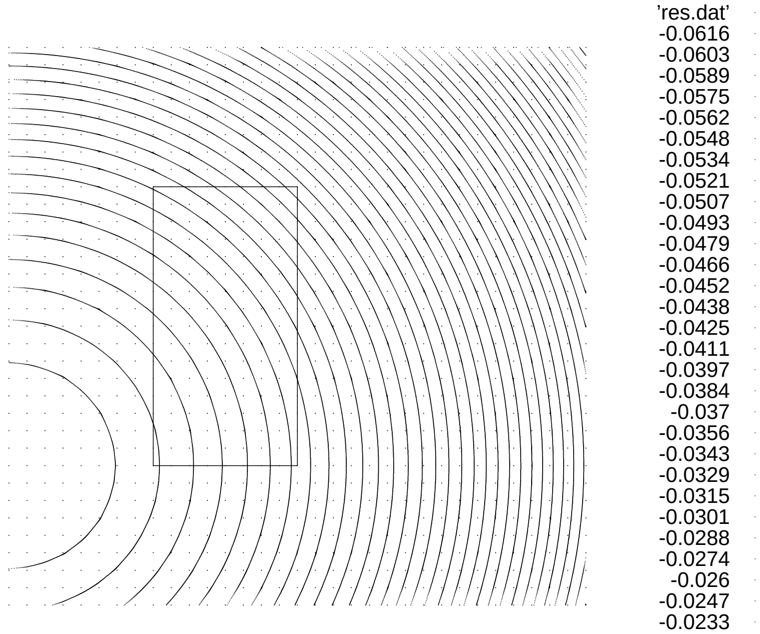

Figure 3: Isolines of the initial obstacle ψ

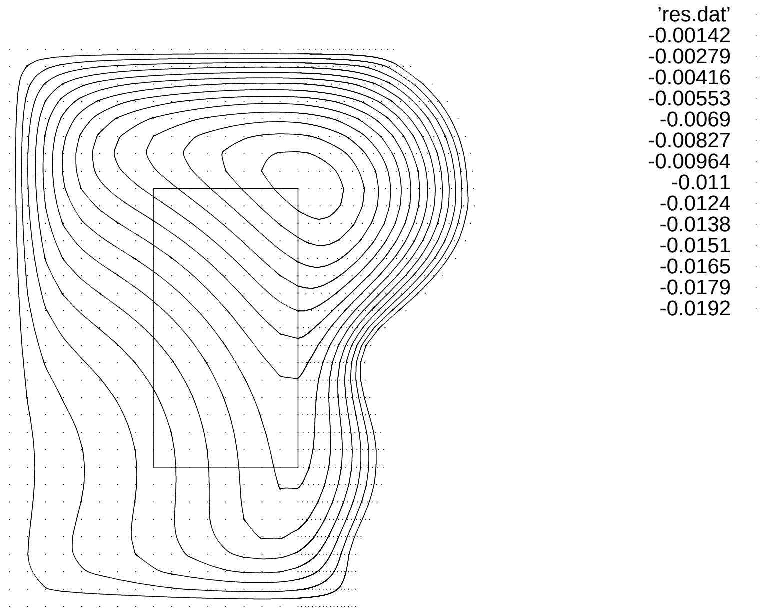

Figure 4: Optimal shape for an elastic obstacle

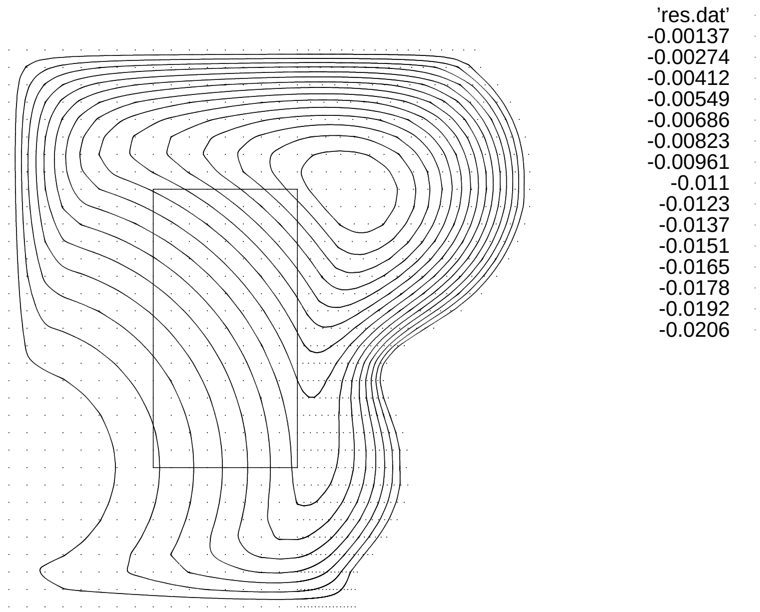

Figure 5: Optimal shape for a rigid obstacle

is given by (3.11), (3.12), i.e., it is sparse, symmetric and positive definite, as the stiffness matrix A. Therefore, for solving this linear system we used the conjugate gradient method with preconditioning by incomplete factorization. This method preserves the sparsity of V and contributes significantly to the efficiency of the overall algorithm.

Conclusion

At solving nonacademic examples, one can hardly compute the index sets L_1, L_2 satisfying with a direction h the inequalities (2.2), whenever the index set L is (numerically) nonempty. It would be too time-consuming. Therefore the used bundle method need not converge or may converge to a wrong point. As the cardinality of L is usually very low and in most iterates $L = \emptyset$, one can change the choice of L_1, L_2 interactively, which can rescue the convergence in some cases. To check the obtained solution, suitable necessary optimality conditions should be derived, which, however, goes beyond the aims of this paper. Another source of an undesirable numerical behaviour might be the fact that in the proposed technique, one "nonsmooth" solver (Newton method) is embedded in another "nonsmooth" solver (BT) and additionally, in the Newton method, we solve a large linear system by a conjugate gradient method. Therefore a very high accuracy is required on the lower levels to ensure that the BT code on the upper level is supplied by sufficiently precise data.

On the other hand, with respect to the complexity of problem (1.7), one can hardly expect that a fast and reliable technique to its numerical solution could easily be developed and implemented. Therefore our approach should be considered as a first attempt in this direction.

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