Pré-Publicações do Departamento de Matemática
Universidade de Coimbra
Preprint Number 03–18

A CLASS OF MATHEMATICAL PROGRAMS WITH EQUILIBRIUM CONSTRAINTS: A SMOOTH ALGORITHM AND APPLICATIONS TO CONTACT PROBLEMS

ISABEL N. FIGUEIREDO, JOAQUIM J. JÚDICE AND SILVÉRIO S. ROSA

ABSTRACT: We discuss a special mathematical programming problem with equilibrium constraints (MPEC), that arises in material and shape optimization problems involving the contact of a rod or a plate with a rigid obstacle. This MPEC can be reduced to a nonlinear programming problem with independent variables and some dependent variables implicity defined by the solution of a mixed linear complementarity problem (MLCP). A projected-gradient algorithm including a complementarity method is proposed to solve this optimization problem. Several numerical examples are reported to illustrate the efficiency of this methodology in practice.

KEYWORDS: Nonlinear programming, complementarity problems, contact problems, finite elements, structural optimization.

1. Introduction

In this paper we address the following optimization problem

$$\left[\begin{array}{l} \min g(x,u) \\ \text{subject to : } \left[\begin{array}{l} u = h(x) \\ x \in X, \quad u \in U \end{array}\right. \end{array}\right. \tag{1}$$

where X and U are nonempty closed subsets of $\mathbb{R}^k$ and $\mathbb{R}^n$, respectively, $g : \mathbb{R}^k \times \mathbb{R}^n \to \mathbb{R}$ is the objective function and $h : X \to \mathbb{R}^n$ is a map which assigns to each $x \in X$ the solution u of a inner level Mixed Linear Complementarity Problem (MLCP).

This type of problems arise in many fields of applications. In particular problem (1) may be the mathematical formulation of a structural optimization problem, discretized by the finite element method, where the objective function is the performance criterion of the structure, the inner level optimization problem represents the equilibrium state of the structure, the outer variable x is the design variable (for instance, the material and/or geometric parameters of the structure), the inner variable u is the state variable (representing, for each design x, the displacement of the structure at the equilibrium state), and X and U are the sets of admissible designs and admissible (constrained) states, respectively.

The optimization problem (1) is a special case of a *Mathematical Programming Problem with Equilibrium Constraints* (in short MPEC) (see Luo, Pang and Ralph [14] and Outrata, Kočvara and Zowe [17]). For a general function g, the non-smoothness of u with respect to x, or the non-smoothness of the objective function, requires the use of non-smooth optimization techniques, such as subgradients and bundle methods (see Outrata, Kočvara and Zowe [17]) to solve the MPEC. In this paper, we show that for a particular objective function of the MPEC, the resulting function $g(x, u(x))$ is continuously differentiable in an open set containing X. Therefore the MPEC problem can be processed by a smooth projected-gradient algorithm, which includes a block pivoting complementarity algorithm to get the information concerning the variable u. Moreover we apply this solution method to some real material and shape optimization problems, involving the contact of a rod or a plate with a rigid obstacle.

This paper extends the contents of a previous synopsis paper (see Figueiredo, Júdice and Silvério [9]). The outline of the paper is as follows. In section 2 the MPEC is introduced. The differentiation of the objective function is discussed in section 3. The description of the projected-gradient algorithm is presented in section 4. The case studies are introduced in section 5. The numerical results of the solution of the corresponding MPECs and some conclusions about the efficiency of the proposed methodology are reported in the last section of the paper.

2. Description of the problem

In this section we define the exact formulation of problem (1). Let ψ be a vector with n components, independent of x. For each $x \in X \subset \mathbb{R}^k$, let $A(x)$ be a symmetric, positive definite matrix of order n and $F(x)$ a vector with n components, depending on x. Consider the following Mixed Linear Complementarity Problem (in short MLCP)

$$\text{MLCP} \quad \left[\begin{array}{l} \text{Find} \quad u \in \mathbb{R}^n, \quad w \in \mathbb{R}^n \quad \text{such that:} \\ A(x)u - F(x) = w \\ u_J \geq \psi_J, \quad w_J \geq 0, \quad w_I = 0 \\ (u_J - \psi_J)^T w_J = 0, \end{array} \right. \tag{2}$$

where the upper index ^{T} denotes transposition, $\{I, J\}$ forms a partition of $\{1, 2, ..., n\}$, and u_J, ψ_J, w_J, w_I are subvectors of u, ψ and w, whose components have indices in J and I. We assume that the admissible set X is nonempty, closed and convex. In the sequel we often write $u(x)$ and $w(x)$ instead of u and w, if we want to emphasize that u and w implicitly depend on x.

The particular optimization problem considered in this paper, is the following Mathematical Programming Problem with Equilibrium Constraints (MPEC)

$$\textit{MPEC} \quad \left[\begin{array}{l} \min g(x,u) = \min \frac{1}{2}(u-\psi)^T A(x)(u-\psi) \\ \text{subject to :} \\ x \in X \quad \text{and} \quad \left[\begin{array}{l} u = u(x) \in \mathbb{R}^n, \quad w = w(x) \in \mathbb{R}^n \\ A(x)u - F(x) = w \\ u_J \geq \psi_J, \quad w_J \geq 0, \quad w_I = 0 \\ (u_J - \psi_J)^T w_J = 0, \end{array}\right. \end{array}\right. \tag{3}$$

where the inner level problem is the MLCP (2).

The following theorem states a sufficient condition for the existence of a solution to the MPEC.

Theorem 2.1. *If $X \subset \mathbb{R}^k$ is compact, $A : X \to \mathbb{R}^{n^2}$ and $F : X \to \mathbb{R}^n$ are continuous, and $A(x)$ is positive definite uniformly with respect to $x \in X$, then the MPEC (3) has at least one solution.*

Proof - The hypotheses required for A and F assure that, for each x, the unique solution pair of the MLCP (2), $(u, w) : X \to \mathbb{R}^n \times \mathbb{R}^n$, is a continuous function, on the admissible set X (see theorem 4.1, page 70, Haslinger and Neittaanmäki [11]). Then, the existence of a solution to the MPEC (3) is a consequence of the Weierstrass theorem, as (3) reduces to the following problem

$$\left[\begin{array}{l} \min f(x) = \min \frac{1}{2}(u(x)-\psi)^T A(x)(u(x)-\psi) \\ \text{subject to} \quad x \in X \end{array}\right. \tag{4}$$

where the function $f(x)$ is continuous over the set X. •

The next result gives two other expressions for the objective function $g(x,u)$, that will be used in section 5.

Theorem 2.2. *For each (x,u),*

$$\begin{array}{l} g(x,u) = \frac{1}{2}(u(x)-\psi)^T(F(x) - A(x)\psi) \\ g(x,u) = \frac{1}{2}\|u(x)-\psi\|^2_{A(x)} \end{array} \tag{5}$$

where $\|.\|_{A(x)}$ *is a norm defined by* $A(x)$ *for each* x.

Proof - By adding and subtracting ψ in the first equation of (2), the MLCP is equivalent to

$$\left[\begin{array}{l} \text{Find} \quad u \in \mathbb{R}^n, \quad w \in \mathbb{R}^n \quad \text{such that:} \\ A(x)(u-\psi) - (F(x) - A(x)\psi) = w \\ u_J - \psi_J \geq 0, \quad w_J \geq 0, \quad w_I = 0 \\ (u_J - \psi_J)^T w_J = 0. \end{array}\right. \tag{6}$$

It then follows from the first equation of (6) and the complementarity condition $(u-\psi)^T w = 0$, that

$$\begin{aligned} g(x,u) &= \tfrac{1}{2}(u-\psi)^T A(x)(u-\psi) = \tfrac{1}{2}(u-\psi)^T (w + (F(x) - A(x)\psi)) \\ &= \tfrac{1}{2}(u-\psi)^T (F(x) - A(x)\psi), \end{aligned} \tag{7}$$

and the first expression is proved. On the other hand, as $A(x)$ is a positive definite matrix for each x, the following norm $\|.\|_{A(x)}$ can be defined in $\mathbb{R}^n$

$$\|v\|_{A(x)} = \sqrt{v^T A(x) v}, \qquad \text{for all} \quad v \in \mathbb{R}^n. \tag{8}$$

Therefore

$$g(x,u) = \frac{1}{2}(u(x)-\psi)^T A(x)(u(x)-\psi) = \frac{1}{2}\|u(x)-\psi\|^2_{A(x)}. \bullet \tag{9}$$

3. Differentiation of the objective function

In this section the differentiation of the objective function with respect to x is studied. In order to do this, the dependence of the solution $u = u(x)$ of the MLCP on the variation of the outer variable x is first analyzed.

Since the matrix $A(x)$ is symmetric positive definite for each $x \in X$, the MLCP has a unique solution for each $x \in X$, and therefore it is possible to write the MPEC (3) as the following optimization problem in the variable x

$$\left[\begin{array}{l} \min f(x) = \min g(x, u(x)) \\ \text{subject to} \quad x \in X \end{array}\right. \tag{10}$$

where u depends implicitly and uniquely on x through the MLCP.

In general, the non-smoothness of $u(x)$ with respect to the variable x implies the non-smoothness of the objective function f. As stated in theorem

2.1, u is a continuous function on the admissible set X and it is also possible to prove, under additional assumptions, that the directional derivative $u'(x, \tilde{x})$ of u at x in the direction $\tilde{x}$ exists; however, the gradient $\nabla_x u(x)$ of u at x does not exist when the coincidence set $\{j \in J : \ w_j(x) = 0, \ u_j(x) = 0\}$ is not empty (see, Harker and Pang [10] or Haslinger and Neittaanmäki [11] for a justification of these statements).

The next theorem shows that the gradient $\nabla_x f$ of f exists for the particular objective function f defined in (10).

Theorem 3.1. *For each x, let $(u(x), w(x))$ be the solution of the MLCP. Assume that F, A, $\nabla_x F$ and $\nabla_x A$ are continuous with respect to each $x \in X$, where $\nabla_x F$ and $\nabla_x A$ are the gradients of F and A defined by*

$$\nabla_x F(x) = (\nabla_x F_i(x))_{i=1,\ldots,n}, \quad \nabla_x A(x) = (\nabla_x A_{ij}(x))_{i,j=1,\ldots,n} \tag{11}$$

and F_i and A_{ij} are the elements of F and A, respectively. Then $\nabla_x f$ is a continuous function of x and

$$\left[\begin{array}{l} \nabla_x f(x) = (\nabla_x F(x) - \nabla_x A(x)\psi)^T (u(x) - \psi) \\ \qquad\qquad\qquad -\frac{1}{2}(u(x) - \psi)^T \nabla_x A(x)(u(x) - \psi). \end{array} \right. \tag{12}$$

Proof - The following proof is based on an analogous argument of Haslinger and Neittaanmäki [11] for another framework, and is included here to facilitate the reading of the paper. As remarked in theorem 2.1, the mappings $x \to u(x)$ and $x \to w(x)$ are continuous on X, where, for each x, $(u(x), w(x))$ is the solution of the MLCP. Moreover, under the hypotheses of the theorem, these mappings are also Lipschitz-continuous on X (see remark 4.2, page 70, Haslinger and Neittaanmäki [11]). It can also be proven (see pages 83-84, Haslinger and Neittaanmäki [11]), that there exist the directional derivatives $u'(x, \tilde{x})$ and $w'(x, \tilde{x})$ of u and w, at the point x in the direction $\tilde{x}$, which are defined by

$$\begin{aligned} u'(x, \tilde{x}) &= \big(u_i'(x, \tilde{x})\big)_{i=1}^n = \Big(\lim_{t \to 0} \frac{u_i(x + t\tilde{x}) - u_i(x)}{t}\Big)_{i=1}^n \\ w'(x, \tilde{x}) &= \big(w_i'(x, \tilde{x})\big)_{i=1}^n = \Big(\lim_{t \to 0} \frac{w_i(x + t\tilde{x}) - w_i(x)}{t}\Big)_{i=1}^n . \end{aligned} \tag{13}$$

In particular, for each $i \in \{1, 2, \cdots, n\}$

$$(u(x) - \psi)_i w_i'(x, \tilde{x}) = 0, \tag{14}$$

and thus

$$(u(x)-\psi)^T w'(x,\tilde{x})=0. \tag{15}$$

To show (14-15), we first note that, for each $i \in I$, $w_i(x)=0$ for any $x \in X$, so $w_i'(x,\tilde{x})=0$ and $(u(x)-\psi)_i w_i'(x,\tilde{x})=0$. On the other hand, for each $i \in J$, the inequality $(u(x)-\psi)_i \geq 0$ is always satisfied. If $(u(x)-\psi)_i = 0$, it is obvious that $(u(x)-\psi)_i w_i'(x,\tilde{x})=0$. If $(u(x)-\psi)_i > 0$, then $(u(x+t\tilde{x})-\psi)_i > 0$ for t small enough (due to the Lipschitz-continuity of u), and $w_i(x+t\tilde{x})=0$, by the complementarity condition. So, for each $i \in J$, $w_i'(x,\tilde{x})=0$ and $(u(x)-\psi)_i w_i'(x,\tilde{x})=0$.

The formula (12) can now be obtained by calculating the directional derivative $f'(x,\tilde{x})$ of f at the point x in the direction $\tilde{x}$, and using (15). In fact, it follows from the definition of f that

$$f'(x,\tilde{x})=(u(x)-\psi)^T A(x) u'(x,\tilde{x})+\frac{1}{2}(u(x)-\psi)^T A'(x,\tilde{x})(u(x)-\psi) \tag{16}$$

where $A'(x,\tilde{x})$ is the directional derivative of A at x in the direction $\tilde{x}$. By writing the complementarity problem (6) for x and $x+t\tilde{x}$ and subtracting these equations and dividing by t, we obtain

$$A(x)u'(x,\tilde{x})=w'(x,\tilde{x})+(F'(x,\tilde{x})-A'(x,\tilde{x})\psi)-A'(x,\tilde{x})(u(x)-\psi) \tag{17}$$

where $F^{'}(x,\tilde{x})$ is the directional derivative of F at x in the direction $\tilde{x}$. Introducing (17) in (16) and using (15), the term $u'(x,\tilde{x})$ disappears. Since A and F are continuously differentiable, then $A'(x,\tilde{x})=\nabla_x A^T \tilde{x}$ and $F'(x,\tilde{x})=\nabla_x F^T \tilde{x}$, and the expression (12) of the gradient of f follows. •

Consider now the special case of the MPEC, where the outer variable x has only one component, that is $x=(x_1) \in R$, $X=[x_1^{\min}, x_1^{\max}]$, with $x_1^{\min}$ and $x_1^{\max}$ two real numbers, and $\nabla_x F(x)-\nabla_x A(x)\psi=0$. It then follows from (12) that the derivative of f is given by

$$\frac{df}{dx}(x)=-\frac{1}{2}(u(x)-\psi)^T \frac{dA}{dx}(x)(u(x)-\psi). \tag{18}$$

If in addition we suppose that $\frac{dA}{dx}(x)$ is a positive definite matrix, then

$$\frac{df}{dx}(x) \leq 0, \qquad \forall x \in X. \tag{19}$$

This means that for this particular instance of the MPEC, the function f is a monotone decreasing function in the admissible set $X=[x_1^{\min}, x_1^{\max}]$, and so f attains its minimum at $x_1^{\max}$. Thus, the solution of the MPEC is $x_1^{\max}$, in this case, and the minimum value of the objective function is equal to

$$f(x_1^{\max}) = g(x_1^{\max}, u(x_1^{\max})). \tag{20}$$

So, for this quite special case, the solution $u(x_1)$ of the MLCP (2), with $x_1 = x_1^{\max}$, is sufficient to get the minimum of the objective function. However, this is a very particular case, as in general x has more than one component, the difference $\nabla_x F(x) - \nabla_x A(x)\psi$ is not zero and depends on x and $\nabla_x A(x)$ is not a positive definite matrix in general. This implies the need of an algorithm to obtain the solution of the MPEC (10).

4. A projected-gradient algorithm

In the previous section, we have been able to show that the MPEC under consideration reduces into a nonlinear program (10), where the function f is continuously differentiable on an open set containing the set X. However, the computation of the values of the objective function and of its gradient require the knowledge of the dependent variables u of the original MPEC (3). The values of these variables can be obtained by processing the MLCP (2), which has a unique solution for each $x \in X$. Due to these properties of the problem, a projected-gradient algorithm is quite recommended for this particular application. In this section, we first introduce the steps of this algorithm. Then we explain how all the information required by the algorithm can be computed through the solution of the MLCP (2).

If P_X denotes the projection operator on the convex set X, then the steps of the projected-gradient algorithm are as follows.

Projected-Gradient Algorithm

- Let $x^0 \in X$ and $\epsilon > 0$ be a given tolerance.
- For $k = 0, 1, 2, \ldots$
  - Compute $\nabla_x f(x^k)$, $y^k = P_X(x^k - \nabla_x f(x^k))$ and $p^k = y^k - x^k$.
  - If $\|p^k\| < \epsilon$, stop with $(x^k, u(x^k))$ a solution of the MPEC.
  - Compute the stepsize $\alpha_k \in]0, 1]$ by using the Armijo Criterion

$$f(x^k + \alpha_k p^k) \leq f(x^k) + c\,\alpha_k \nabla_x f(x^k)^T p^k, \quad \text{with } 0 < c < 1. \tag{21}$$

- Update $x^{k+1} = x^k + \alpha_k p^k$.

As discussed in Bertsekas [1] and Nocedal and Wright [16], the projected-gradient algorithm possesses global convergence into a stationary point of the function f on the convex set X under mild assumptions on f. The implementation of the algorithm for the solution of the nonlinear program (10) requires three types of information, namely the computation of the projections $P_X(y)$, the values of the objective function $f(\bar{x})$ and the gradients $\nabla_x f(\bar{x})$. These issues are discussed below.

(i) *Computation of the projected vector* $P_X(y)$ - This vector is the unique solution of the following optimization problem

$$\begin{array}{l} \min ||y-x||_2 \\ \text{subject to } x \in X \end{array} \tag{22}$$

where $||.||_2$ denotes the euclidean norm. In the case studies discussed in section 6, X consists of simple lower and upper bounds, that is

$$X = \left\{ x = (x_1, ..., x_k) \in \mathbb{R}^k : \quad x_i^{\min} \le x_i \le x_i^{\max}, \quad 1 \le i \le k \right\} \tag{23}$$

where $x_i^{\min}$ and $x_i^{\max}$ are real numbers, for each i. For this particular choice, the projection $P_X(y)$ is quite easy to compute and is given by

$$P_X(y)_i = \begin{cases} y_i, & \text{if} \quad x_i^{\min} < y_i < x_i^{\max} \\ x_i^{\max}, & \text{if} \quad y_i \ge x_i^{\max} \\ x_i^{\min}, & \text{if} \quad y_i \le x_i^{\min}. \end{cases} \tag{24}$$

In some interesting applications, the set X can also contain one linear constraint. In this case the nonlinear program (22) is replaced by a strictly convex quadratic knapsack problem, which can be processed by a number of quite efficient polynomial algorithms (see Helgason, Kennington and Lall [12], Pardalos and Kovoor [18] and Robinson, Jiang and Lerme [21]).

(ii) *Computation of* $f(\bar{x})$ *and* $\nabla_x f(\bar{x})$ *and implementation of the Armijo Criterion* - It follows from (10) and (12) that, for each $\bar{x} \in X$,

$$\begin{array}{l} f(\bar{x}) = g(\bar{x}, \bar{u}) \\ \left[\begin{array}{l} \nabla_x f(\bar{x}) = (\nabla_x F(\bar{x}) - \nabla_x A(\bar{x})\psi)^T(\bar{u} - \psi) \\ \qquad\qquad -\frac{1}{2}(\bar{u}-\psi)^T \nabla_x A(\bar{x})(\bar{u}-\psi) \end{array} \right. \end{array} \tag{25}$$

where $\bar{u}$ is the unique solution of the MLCP (2) for $x = \bar{x}$, that is, $\bar{u} = u(\bar{x})$. So for each $\bar{x} \in X$ the values of the objective function f and of its gradient require the solution of one MLCP, for a fixed $x = \bar{x}$. Therefore the implementation of the Armijo criterion needs exactly a number of MLCPs to be solved equal to the number of trials that are performed in order to find the stepsize α_k used in (21) by the projected-gradient algorithm.

It follows from this discussion that the implementation of the projected-gradient algorithm requires an efficient solver for processing the MLCP (2) for each $x \in X$. Since $A(x)$ is symmetric definite positive for each x, then for each $x \in X$ the MLCP (2) is equivalent to the following strictly convex quadratic program

$$\begin{array}{l} \min \left\{ \frac{1}{2} u^T A(x) u - F^T(x) u \right\} \\ \text{subject to} \quad \{ u \in \mathbb{R}^n : \quad u_J \geq \psi_J \}. \end{array} \tag{26}$$

This optimization problem can be processed by a number of efficient algorithms (see Bertsekas [1], Cottle, Pang and Stone [5], Fernandes, Júdice and Patrício [7] and Nocedal and Wright [16]). Among these, the so-called block principal pivoting algorithm (see Júdice and Pires [13]) is quite recommend to process this MLCP, due to its efficiency for solving quite large MLCPs with positive definite matrices and its ability to start with an advanced basic solution (see Fernandes, Júdice and Patrício [7]). Next, we briefly describe the steps of this procedure.

A block principal pivoting algorithm

Consider again the MLCP (2)

$$\left[\begin{array}{l} A(x) u - F(x) = w \\ u_J \geq \psi_J, \quad w_J \geq 0, \quad w_I = 0 \\ (u_J - \psi_J)^T w_J = 0 \end{array} \right. \tag{27}$$

where I and J form a partition of the set $\{1, 2, \ldots, n\}$. We denote by $|P|$ the number of elements of the set P and by C_{PS} the submatrix of a generic matrix C whose elements have indices in the subset $P \times S$, that is, $C_{PS} = (c_{ps})_{(p,s) \in P \times S}$.

The principal pivoting algorithms use in each iteration a complementary basic solution $(\overline{u}, \overline{w})$ of the MLCP (27) (see Fernandes, Júdice and Patrício [7] and Júdice and Pires [13]). If P and S are subsets of $\{1, 2, ..., n\}$ such that $P \cup S = \{1, 2, ..., n\}$, $P \cap S = \emptyset$ and $A_{PP}(x)$ is nonsingular, such a solution satisfies $\overline{u}_i = \psi_i$, for all $i \in S$ and $\overline{w}_i = 0$, for all $i \in P$. This implies that the remaining components are uniquely given by

$$\begin{array}{l} A_{PP}(x)\overline{u}_P = F_P(x) - A_{PS}(x)\psi_S \\ \overline{w}_S = -F_S(x) + A_{SP}(x)\overline{u}_P + A_{SS}(x)\psi_S. \end{array} \tag{28}$$

It is important to add that as $A(x)$ is a symmetric positive definite matrix there is a complementary basic solution for each possible partition $\{P, S\}$ of $\{1, 2, ..., n\}$. Since $w_I = 0$ in any solution of the MLCP (27), then we force I to be always included in the set P of any complementary basic solution that is used by the algorithm. If such a solution $(\overline{u}, \overline{w})$ satisfies

$$\overline{u}_{P\cap J} \geq \psi_{P\cap J} \quad \text{and} \quad \overline{w}_S \geq 0 \tag{29}$$

then it is said to be feasible and is a solution of the MLCP (27). Otherwise, the so-called set of infeasibilities is considered :

$$H = \{i \in P \cap J : \quad \overline{u}_i < \psi_i\} \cup \{i \in S : \quad \overline{w}_i < 0\}. \tag{30}$$

The number of elements of this set H is called the infeasibility count of the complementary basic solution. We note that $0 \leq |H| \leq |J|$ and $|H| = 0$ if and only if $(\overline{u}_P, \psi_S)$ is the unique solution of the MLCP (27).

Each iteration of a principal pivoting algorithm simply consists of replacing the sets P and S associated with a complementary basic infeasible solution $(H \neq \emptyset)$ to another sets $\overline{P}$ and $\overline{S}$ corresponding to another solution of the same type. This is done by using the following formulas

$$\begin{array}{l} \overline{P} = P \setminus (P \cap H_1) \cup (S \cap H_1) \\ \overline{S} = \{1, 2, ..., n\} \setminus \overline{P} \end{array} \tag{31}$$

where $H_1 \subseteq H$. The principal pivoting algorithms differ on the choice of the set H_1. As is discussed in Fernandes, Júdice and Patrício [7], the use of

$$H_1 = \big\{ \min\{i \in H\} \big\} \tag{32}$$

in each iteration guarantees finite termination to the algorithm. However, these modifications of a unique element usually lead to too many iterations for large-scale MLCPs, where the initial and final partitions $\{P, S\}$ are quite different. On the other hand, the all-change modification $H_1 = H$ usually leads to small number of iterations in practice (Fernandes, Júdice and Patrício [7]). However, there is no theoretical guarantee that an algorithm solely based on these latter changes possesses finite termination. As is discussed in Fernandes, Júdice and Patrício [7], it is possible to design a principal pivoting method algorithm that combines these two features presented before.

The resulting method performs all-changes modifications (31) with $H_1 = H$ in general, and one-element changes (32) are only included for assuring finite termination. The switch from one form of iterations to the other one, is done by controlling the infeasibility count, that is, the number of elements $|H|$ of the set H given by (30).

The steps of the algorithm are presented below.

Block Principal Pivoting Algorithm

(1) Let $P = I$, $S = \{1, 2, ..., n\} \setminus P$, $p > 0$, $ninf = |\{1, 2, ..., n\}| + 1$ and $nit = 0$.

(2) Compute $\overline{u}_P$ and $\overline{w}_S$ by (28) and the infeasibility set H by (30). Let $|H|$ be the number of elements of H. Then
   - If $|H| = 0$, terminate with $\overline{u} = (\overline{u}_P, \psi_S)$ the unique solution of the MLCP.
   - If $ninf > |H|$, set $ninf = |H|$ and $nit = 0$. Go to 3.
   - If $ninf \leq |H|$ and $nit \leq p$, go to 3. (if $nit = 1$ set $\tilde{P} = P$ and $\tilde{H} = H$).
   - If $ninf \leq |H|$ and $nit \geq p + 1$, go to 4 (if $nit = p + 1$ set $P = \tilde{P}$ and $H = \tilde{H}$).

(3) Set $P = P \setminus (P \cap H) \cup (S \cap H)$, $S = \{1, 2, ..., n\} \setminus P$, $nit = nit + 1$ and go to 2.

(4) Let $t = \min\{i \in H\}$. Set $nit = nit + 1$,

$$P = \begin{cases} P \setminus \{t\}, & \text{if } t \in P \\ P \cup \{t\}, & \text{if } t \in S \end{cases} \tag{33}$$

and $S = \{1, 2, ..., n\} \setminus P$ and go to 2.

It follows from the description of the steps of the algorithm that the integer constant p plays an important role on the efficiency of the algorithm. This value represents the maximum number of block iterations ($H_1 = H$) that are allowed to be performed without an improvement of the infeasibility count. It is obvious that this value should be small. However, too small values for p may lead to the performance of one-element modifications too often with an increase on the number of iterations. Extensive computational experience reported in Fernandes, Júdice and Patrício [7] has shown that $p = 10$ is usually a good choice in practice.

As is discussed in Fernandes, Júdice and Patrício [7], and Júdice and Pires [13], this block principal pivoting algorithm can be efficiently implemented for the solution of large scale MLCPs with symmetric positive definite matrix. In the experiments to be reported in the last section of this paper, we have implemented the algorithm in MATLAB [15]. It should be added that such an implementation is quite simple to do, as MATLAB contains efficient procedures to solve the system of linear equations in (28), even when the cardinal $|P|$ of the set P is large.

As remarked in Júdice and Pires [13], the block principal pivoting algorithm possesses finite termination for each choice of initial partition $\{P, S\}$ of the set $\{1, \ldots, n\}$, when the matrix of the MLCP is positive definite. On the other hand, the implementation of the Armijo criterion explained in this section requires in each iteration, the solution of a number of MLCPs equal to the number of trials that are necessary to obtain the stepsize for the projected-gradient algorithm. Therefore the final partition of one application of the block principal pivoting algorithm should be the initial partition for the next application of the procedure. The results of the experiments to be reported in section 6, show that this strategy works quite well in practice. It is also important to add that this feature of the block principal pivoting algorithm is not shared by other quite efficient alternative methods to process large scale MLCPs or its equivalent strictly convex quadratic programs, such as interior-point or active-set based methods. This feature together with its simplicity and efficiency in practice (see Fernandes, Júdice and Patrício [7]) leads to our recommendation of the block principal pivoting algorithm for the solution of the MLCP associated to the case studies of this paper.

5. Case studies

We have applied the previous projected-gradient algorithm to structural optimization models for two types of solids, a rod and a plate. More exactly, we have considered four problems, involving the contact, without friction, of one of these solids (the rod or the plate) with a rigid obstacle. Each one of these four problems is formulated as a MPEC of the type (3). The inner level problem represents the contact between the solid and the obstacle. The differences among these problems rely on the geometry of the solid and on the definition of the outer variable $x \in X$, as discussed below.

- In problems 1, 2, 3 the solid is a rod and for problem 4 the solid is a plate.

- In problems 1 and 4 the outer variable x has only one component which is related to the material (of the rod or of the plate), and thus problems 1 and 4 are material optimization problems.
- In problems 2 and 3 the outer variable x has two components, one related to the material and the other one to a geometric feature of the rod (the side and shape of the cross section of the rod for problem 2, and the length of the rod axis for problem 3); therefore problems 2 and 3 are material and shape optimization problems.

In the next subsection we define the contact problem between the solid and the obstacle. Then, we define the structural optimization MPEC and we give its mechanical interpretation in mathematical terms. In the last section the problems 1, 2, 3 and 4 are described in more detail and the experiments on the solutions of these problems are reported.

5.1. The contact problem. Let ω and Ω be two open, bounded and connected subsets of $\mathbb{R}^2$. Let $L > 0$ and $t > 0$ be two constants. We denote by $\overline{\omega} \times [0, L]$ the set occupied by the rod, in its reference configuration, with length L and cross section ω. The reference configuration of the plate is denoted by $\overline{\Omega} \times [-\frac{t}{2}, \frac{t}{2}]$, where Ω is the middle plane of the plate and t is its thickness. We assume that the material of both the rod or the plate is an unidirectional fiber reinforced composite material. For the rod, the fiber direction is parallel to the direction of the rod axis. For the plate, the fiber direction is parallel to one of the axis of the reference system of the middle plane Ω. We denote by $x = (x_1, x_2, ..., x_k) \in \mathbb{R}^k$ the vector whose k components specify the type and the number of material and/or geometric features of either the rod or the plate under consideration. Moreover we assume that the rod is clamped at its extremities and the plate is clamped at its lateral surface. The rod or the plate are subjected to the action of applied forces that force a part of the boundary to be in contact with a rigid obstacle. By using the finite element method, the discrete formulation for each x of this contact problem (either the rod or the plate contact problem) constitutes the following discrete variational inequality

$$\left\{ \begin{array}{l} \text{Find} \quad u \in \overline{C} = \{v \in \mathbb{R}^n : \quad v_{\tilde{J}} = 0, \quad v_J \geq \overline{\psi}_J\}, \quad \text{such that} \\ (v-u)^T(B(x)u - F(x)) \geq 0, \quad \forall v \in \overline{C}. \end{array} \right. \tag{34}$$

In (34), n denotes the number of global degrees of freedom of the finite element mesh (the mesh of the rod axis $[0, L]$, for the rod contact problem or the mesh of the middle plane Ω, for the plate contact problem). The sets $\tilde{J}$ and J are subsets of the global degrees of freedom $\{1, 2, ..., n\}$. The matrix $B(x)$ is the stiffness matrix and $F(x)$ is the vector associated to the applied forces. $B(x)$ depends explicitly on x and $F(x)$ may also depend on the components of x. The vector u is the solution of the contact model and represents the approximate displacement of the solid. For the rod contact problem the vector u contains two subvectors $\overline{u}_J = (\overline{u}_j)_{j\in J}$ and $\hat{u}_J = (\hat{u}_j)_{j\in J}$, representing the bending displacement of the rod axis (in the direction perpendicular to the rod axis) and the stretch displacement of the rod axis (in the direction of the rod axis), respectively, at the nodes $j \in J$ of the mesh. For the plate contact problem the vector u corresponds to the finite element approximation of the vertical displacement of the middle plane of the plate (there are only applied forces in the direction perpendicular to the middle plane of the plate); in particular the subvector $u_J = (u_j)_{j\in J}$ is the vertical displacement of the middle plane of the plate at the nodes $j \in J$ of the mesh. We remark that in (34) u depends implicitly on x. The set $\overline{C}$ is the set of admissible displacements. The condition $v_{\tilde{J}} = 0$ corresponds to the clamped rod or plate condition. The vector $\overline{\psi}_J = (\overline{\psi}_j)_{j\in J}$ is independent on x and defines the rigid obstacle at the nodes $j \in J$. The condition $v_J \geq \overline{\psi}_J$ states that the solid (either the rod or the plate) can touch but should not penetrate the rigid obstacle at each node $j \in J$.

The rod and the plate contact problems have the common mathematical formulation (34), but they differ in the definitions of the matrix $B(x)$ and of the vector $F(x)$. In order to clarify these differences and to give the explicit the dependence of B and F on x, we describe next the element stiffness matrix and the element vector force, for the two problems and for particular choices of finite elements.

5.1.1. *Element stiffness matrix and element vector force for the rod contact problem.* We denote by h_i the amplitude of the generic finite element $[y_i, y_{i+1}] \subset [0, L]$, and we choose cubic Hermite polynomials as shape functions (see Ciarlet [4]) for the bending displacements, and affine functions for the stretching displacements. Then, in each interval $[y_i, y_{i+1}]$ there are six degrees of freedom, namely the bending displacement, its first derivative and the stretch displacement at the extremities of $[y_i, y_{i+1}]$. The corresponding element stiffness matrix B_i is

$$B_i = B_i(x) = E \begin{bmatrix} \frac{|w|}{h_i} & 0 & 0 & -\frac{|w|}{h_i} & 0 & 0 \\ 0 & \frac{12I}{h_i^3} & \frac{6I}{h_i^2} & 0 & -\frac{12I}{h_i^3} & \frac{6I}{h_i^2} \\ 0 & \frac{6I}{h_i^2} & \frac{4I}{h_i} & 0 & -\frac{6I}{h_i^2} & \frac{2I}{h_i} \\ -\frac{|w|}{h_i} & 0 & 0 & \frac{|w|}{h_i} & 0 & 0 \\ 0 & -\frac{12I}{h_i^3} & -\frac{6I}{h_i^2} & 0 & \frac{12I}{h_i^3} & -\frac{6I}{h_i^2} \\ 0 & \frac{6I}{h_i^2} & \frac{2I}{h_i} & 0 & -\frac{6I}{h_i^2} & \frac{4I}{h_i} \end{bmatrix} \tag{35}$$

where E, $|w|$ and I depend on x and represent the longitudinal modulus of the material, the area of the cross section and the moment of inertia, respectively. In particular E is defined by

$$E = E_f V_f + E_m(1 - V_f) \tag{36}$$

with E_f the Young's modulus of the fiber, E_m the Young's modulus of the matrix, V_f the fiber volume fraction and V_m the matrix volume fraction. The volume fractions verify $V_m = 1 - V_f$, with $V_f,\ V_m \in [0, 1]$.

Assuming that q and p are the uniformly distributed forces per unit of length in the direction of the rod axis and in the direction perpendicular to the rod axis, respectively, then the element vector force F_i is defined by

$$F_i^T = F_i(x)^T = \begin{bmatrix} \frac{qh_i}{2} & \frac{ph_i}{2} & \frac{ph_i^2}{12} & \frac{qh_i}{2} & \frac{ph_i}{2} & -\frac{ph_i^2}{12} \end{bmatrix}. \tag{37}$$

As h_i depends on the rod axis (which is a geometric feature, that can be included in the definition of the outer variable x) and the applied forces p or q may depend on x, the previous vector may also depend on x.

5.1.2. *Element stiffness matrix and element vector force for the plate contact problem.* We suppose that the middle plane $\Omega \subset \mathbb{R}^2$ of the plate is a square and we denote by (y_r, y_s) an arbitrary point of Ω and by Ω_i a generic finite element of the finite element mesh of Ω. In addition, we choose a mesh built with Adini-Clough-Melosh finite elements (see Ciarlet [4]). Therefore there are twelve degrees of freedom, in each rectangle Ω_i, namely the vertical displacement and its two first partial derivatives at each vertice of Ω_i. The corresponding element stiffness matrix B_i is defined by

$$B_i = B_i(x) = \frac{t^3}{12} \int_{\Omega_i} N_i^T D N_i \, d\Omega \tag{38}$$

where N_i is a 3×12 matrix of the second order derivatives of the 12 local shape functions S_i^1, S_i^2,..., S_i^{12} of the Adini-Clough-Melosh finite element. These functions depend on the geometry of Ω_i, and then on x, but are independent on the material of the plate. The definition of N_i is

$$N_i = \begin{bmatrix} S^1_{i,11} & S^2_{i,11} & \cdots & S^{12}_{i,11} \\ S^1_{i,22} & S^2_{i,22} & \cdots & S^{12}_{i,22} \\ 2S^1_{i,12} & 2S^2_{i,12} & \cdots & 2S^{12}_{i,12} \end{bmatrix}_{3\times 12} . \tag{39}$$

The functions S_i^1, S_i^2,..., S_i^{12} are defined in $\Omega_i \subset \Omega \subset \mathbb{R}^2$ and $S^j_{i,rs}$ denotes the second derivative of S_i^j with respect to the variables y_r and y_s, for $j = 1, ..., 12$ and $r,\ s \in \{1, 2\}$. The matrix D is the constitutive matrix, which depends on the material and then on x, and its definition is

$$D = \begin{bmatrix} Q_{11} & Q_{12} & 0 \\ Q_{21} & Q_{22} & 0 \\ 0 & 0 & Q_{33} \end{bmatrix}_{3\times 3} . \tag{40}$$

Denoting by 1 and 2 the directions of the axis of the reference system of the middle plane of the plate, the elastic coefficients Q_{11}, Q_{22}, Q_{12}, Q_{33} in (40) are related to the engineering constants E_1, E_2 (Young's modulus in directions 1 and 2 respectively) ν_{12}, ν_{21} (Poisson's ratio), G_{12} (shear modulus in the 1-2 plane, respectively). These engineering constants E_1, E_2, ν_{12}, ν_{21}, G_{12} depend on E_m (the Young's modulus of the matrix), υ_f (Poisson's ratio of the fiber), υ_m (Poisson's ratio of the matrix), V_f (fiber volume fraction) and V_m (matrix volume fraction which verifies $V_m = 1 - V_f$). Their definitions are (see Bertholet [2]) as follows:

$$\begin{aligned} Q_{11} &= \frac{E_1}{1-\nu_{12}\nu_{21}}, & Q_{22} &= \frac{E_2}{1-\nu_{12}\nu_{21}} \\ Q_{21} &= \frac{\nu_{12}E_2}{1-\nu_{12}\nu_{21}} = \frac{\nu_{21}E_1}{1-\nu_{12}\nu_{21}} = Q_{21}, & Q_{33} &= G_{12}, \end{aligned} \tag{41}$$

and

$$\begin{aligned}
&E_1 = E_f V_f + E_m V_m, \quad E_2 = \frac{E_f E_m}{E_f V_m + E_m V_f} \\
&\nu_{12} = \nu_f V_f + \nu_m V_m, \quad \frac{\nu_{21}}{\nu_{12}} = \frac{E_2}{E_1} \\
&G_{12} = \frac{G_f G_m}{G_f V_m + G_m V_f}, \ G_f = \frac{E_f}{2(1+\nu_f)}, \quad G_m = \frac{E_m}{2(1+\nu_m)}.
\end{aligned} \tag{42}$$

Assuming that p is the intensity of the density (per unit area) of the force acting in the direction perpendicular to the middle plane of the plate, the element vector force F_i in the finite element Ω_i is defined by

$$F_i = F_i(x) = \int_{\Omega_i} p M_i^T \, d\Omega \tag{43}$$

where $M_i = [S_i^1, S_i^2, ..., S_i^{12}]_{1\times 12}$ is the vector of local shape functions already introduced. We observe that $F_i(x)$ may depend on x if either M_i or p depend on x.

5.2. The structural MPEC. We remark that (34) is an obstacle problem. In particular it can be reformulated as a mixed complementarity problem. To see this, we denote by I and H the subsets of indices defined by $I = \{1, 2, ...n\} \setminus \{\tilde{J} \cup J\}$ and $H = I \cup J$, respectively. By performing the change of variables

$$v \in \overline{C} \Longleftrightarrow v - \psi \in C = \{v \in \mathbb{R}^n : \quad v_{\tilde{J}} = 0, \quad v_J \geq 0\} \tag{44}$$

where the vector $\psi \in \mathbb{R}^n$ is defined by

$$\psi = (\psi_j)_{j\in\mathbb{R}^n} \quad \text{and} \quad \psi_j = 0, \quad \text{if } j \notin J, \quad \psi_j = \overline{\psi}_j, \quad \text{if } j \in J, \tag{45}$$

then problem (34) is equivalent to the following parametric Mixed Linear Complementarity Problem

$$\left[\begin{array}{l}
\text{Find} \quad u \in \mathbb{R}^{|H|}, \quad w \in \mathbb{R}^{|H|} \quad \text{such that} \\
A(x)(u - \psi) - \overline{F}(x) = w \\
u_J \geq \psi_J, \quad w_J \geq 0, \quad w_I = 0, \\
(u_J - \psi_J)^T w_J = 0.
\end{array}\right. \tag{46}$$

The number $|H|$ is the cardinal of H, A is a submatrix of B and $\overline{F}$ is a subvector of $F - B\psi$, whose elements have indices in H, that is,

$$A(x) = B_{HH}(x) \qquad \text{and} \qquad \overline{F}(x) = F_H(x) - B_{HH}(x)\psi_H. \tag{47}$$

It should be added that for both the rod and the plate, the matrix $A(x)$ is a symmetric positive definite matrix, for each x.

After this definition of the contact problem, we can consider the following structural optimization MPEC:

$$\left[\begin{array}{l} \min f(x) = \min g(x,u) = \min \frac{1}{2}(u-\psi)^T A(x)(u-\psi) \\ \text{subject to :} \\ x \in X \quad \text{and} \quad \left\{\begin{array}{l} u = u(x) \in \mathbb{R}^{|H|}, \quad w = w(x) \in \mathbb{R}^{|H|} \\ A(x)(u-\psi) - \overline{F}(x) = w \\ u_J - \psi_J \geq 0, \quad w_J \geq 0, \quad w_I = 0 \\ (u_J - \psi_J)^T w_J = 0. \end{array}\right. \end{array}\right. \tag{48}$$

As a consequence of theorem 2.2 there are two mechanical interpretations of the objective function f of (48), which are next explained.

(1) For each x, $f(x) = \frac{1}{2}(u(x)-\psi)^T \overline{F}(x)$ is the compliance of the solid (either the rod or the plate), constrained by the zero obstacle and subjected to the action of loads represented by the vector $\overline{F}$, and with material and geometric features defined by the vector x. The compliance of a solid, when it is subjected to the action of applied loads, is a measure of its stiffness (see Petersson [19], for a justification of other definitions of stiffness measure in structural optimization). In this case the loads $\overline{F}(x) = (F_H(x) - B_{HH}(x)\psi)$ are functions of the vector x and depend on the obstacle ψ and the stiffness matrix $B(x)$. Therefore MPEC (48) is a compliance minimization problem.

(2) For each x, $f(x) = \|u(x)-\psi\|_{A(x)}$ represents (in rigorous mathematical terms) the distance between the deformed solid (represented by the vector $u(x)$) and the obstacle (defined by ψ) measured in the norm $\|.\|_{A(x)}$. So the objective function is a distance and the MPEC (48) corresponds to the maximization of the contact region between the deformed solid and the obstacle (the smaller the distance $\|u(x) - \psi\|_{A(x)}$ is, the bigger is the contact region).

6. Numerical experiences

In this section we report some numerical experiments with the projected-gradient algorithm on the solutions of four MPECs of the form (48), where a rod is considered in the first three problems and a plate in the remaining one.

In the case of a rod, its axis $[0, L]$ has been discretised successively by 30, 40 and 50 finite elements. Denoting by n the number of finite elements of the mesh, the length of each finite element is constant and equal to $h = \frac{L}{n}$, for problems 1, 2, 3. Moreover we consider a fixed two-dimensional coordinate system OST and assume that in this system the rod axis occupies in its reference configuration the position defined by the function

$$\psi_0(s) = ms + b, \qquad \forall s \in [0, L], \tag{49}$$

where m and b are constants. In problems 1, 2, 3 we have chosen (without loss of generality) $m = 0$ and $b = 0.001$, that is, the rod axis is horizontal with respect to the fixed coordinate system. Furthermore, for the rod problems 1, 2, 3, and for the same fixed coordinate system OST, the following two obstacles ψ_1, ψ_2 have been considered

$$\begin{aligned} &\psi_1(s) = 0 \\ &\psi_2(s) = -0.001(\tfrac{2s}{5} - 1)^2 - 0.0008(\tfrac{2s}{5} - 1) - \frac{0.001}{1+30(\frac{2s}{5}-1)^2} + 0.0008, \end{aligned} \tag{50}$$

for $s \in [0, L]$. The obstacle ψ_1 is a straight line segment and ψ_2 is the curve represented in figure 1.

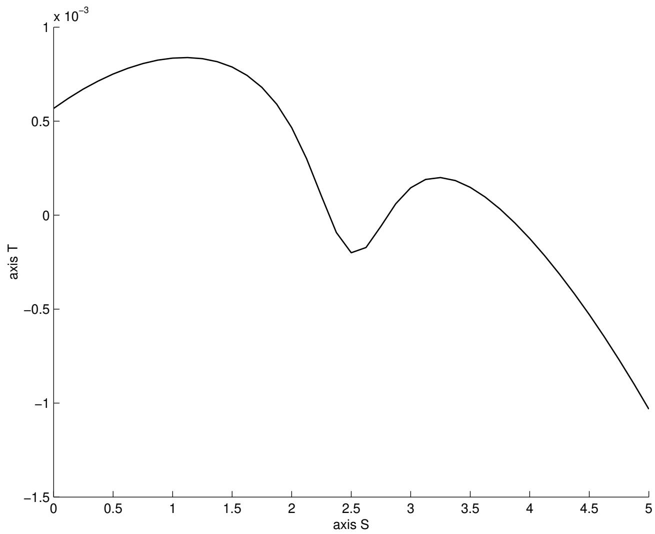

FIGURE 1. Obstacle ψ_2 for the rod

For the plate problem we suppose that the middle plane Ω is a square whose side has length $0.1m$, that is, $\Omega = [0, 0.1] \times [0, 0.1]$ in a fixed three-dimensional coordinate system $OSTW$. Moreover, Ω is discretized successively by 10×10, 15×15 and 20×20 finite elements (the Adini-Clough-Melosh, with 12 degrees

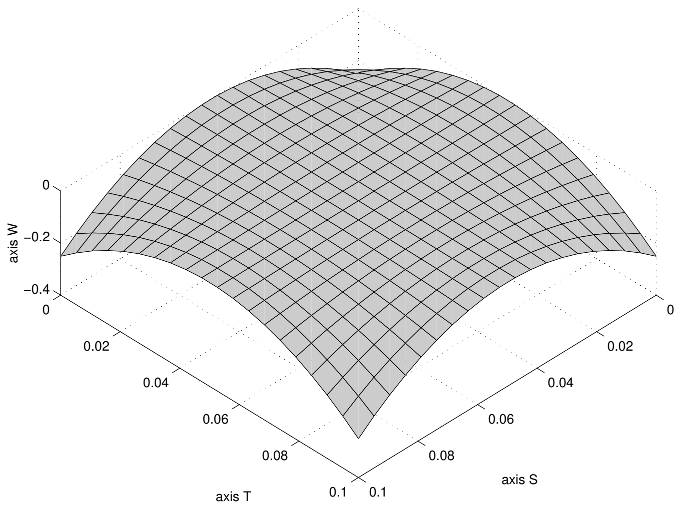

FIGURE 2. Obstacle ψ_4 for the plate

of freedom, was adopted for the approximation of the vertical displacement of the middle plane of the plate). The following two obstacles have been considered

$$\begin{aligned} \psi_3(r,s) &= -0.0008 \\ \psi_4(r,s) &= -0.0008 - (20r-1)^2(10s-0.5)^2, \end{aligned} \tag{51}$$

with $(r,s) \in [0,0.1] \times [0,0.1]$. The obstacle ψ_3 is a plane and ψ_4 is a surface which is depicted in figure 2.

As stated before, the material of the rod and of the plate is assumed to be an unidirectional fiber reinforced composite material, with E_f the modulus of the fiber, E_m the modulus of the matrix and V_f the fiber volume fraction, which belongs to $[0,1]$ (as defined before V_m denotes the matrix volume fraction that verifies $V_m + V_f = 1$). The remaining data of the problems 1, 2, 3, 4 are displayed in the table 1, where the symbols (GPa) and (m) denote the units Giga Pascal and meter, respectively.

In the sequel the tables 2, 3, 4, 5, 6, 7, 8 report the results of problems 1, 2, 3, 4, respectively, with the projected-gradient algorithm, and for the different obstacles ψ_i, $i = 1,2,3,4$. In these tables n represents the number of finite elements considered in the mesh, q is the intensity of the force (in the direction of the rod axis, per unit of length, in problems 1, 2, 3), p is the intensity of the force (perpendicular to the rod axis, per unit of length, in problems 1, 2, 3, and perpendicular to the middle plane of the plate, per unit of area, in problem 4), x^* is the solution of the structural

TABLE 1. Data of the Problems 1, 2, 3, 4

Parameter	*Value*
E_m (GPa) – modulus of the matrix (problems 1, 2, 3, 4)	3.45
E_f (GPa) – modulus of the fiber (problems 1, 2, 3, 4)	86
$V_f^{\min}$, $V_f^{\max}$ – lower and upper bounds for V_f (problems 1, 2, 3)	0.01, 0.99
L (m) – length of the rod (problems 1, 2)	5
$L^{\min}$, $L^{\max}$ (m) – lower and upper bounds for L (problem 3)	3, 5
$b^{\min}$, $b^{\max}$ (m) – lower and upper bounds (problem 2)	0.05, 0.07
$\lvert w\rvert$ (m^2) – area of the cross section (problems 1, 2, 3)	0.004
I (m^4) – moment of inertia (problems 1, 3)	2.1×10^{-6}
t (m)– thickness of the plate (problem 4)	0.002
ν_f – Poisson's ratio of the fiber (problem 4)	0.22
ν_m – Poisson's ratio of the matrix (problem 4)	0.30
G_m (GPa) – shear modulus of the matrix (problem 4)	1.33
G_f (GPa) – shear modulus of the fiber (problem 4)	35.2

problem (48), $MLCP$ denotes the total number of MLCPs solved by the block principal pivoting algorithm (BPP), $it\,BPP$ represents the medium number of iterations of this last BPP algorithm per iteration of the projected gradient method and $it\,PG$ the number of iterations of the projected-gradient algorithm. In these tables the intensities q and p of the forces are measured in the unit Newton (N), per unit of length for problems 1, 2, 3, and per unit of area for problem 4. Moreover in problems 1, 2, 4 the forces q and p are constants independent of the outer variable x, but q and p depend on x in problem 3.

In all the tests, the stiffness matrix B and the force vector F of the rod or of the plate contact problem have been evaluated with the subroutines *beam 2e* or *platre*, respectively, of the CALFEM [3] toolbox of MATLAB. As stated before, the block principal pivoting algorithm has been implemented in MATLAB [15].

6.1. Problem 1 (material optimization for a rod). For problem 1 the admissible set X of outer variables is defined by

$$X = \Big\{x \in [0,1] : \quad V_f^{\min} \le x \le V_f^{\max}\Big\}. \tag{52}$$

So, the outer variable x has only one component, which represents the fiber volume fraction V_f. Thus the objective of problem 1 is to find the fiber volume fraction of the rod that minimizes the objective function of the MPEC (48). The rod is subjected to the action of external loads with intensities $q(N)$ and $p(N)$, that are independent on x. The modulus of the matrix is $E_m = 3.45GPa$, the modulus of the fiber is $E_f = 86GPa$, the axis length is $L = 5m$, the area of cross section is $|w| = 0.004m^2$ and the moment of inertia is $I = 2.1 \times 10^{-6} m^4$. Moreover the longitudinal modulus E of the material is a function of x defined by

$$E(x) = E_f x + E_m(1 - x). \tag{53}$$

The results obtained with the projected-gradient algorithm for the two obstacles ψ_1, ψ_2 and different forces are displayed in tables 2, 3 and indicate that the solution x^* found by the algorithm is equal to $V_f^{\min}$.

TABLE 2. Results for Problem 1, for $q = -100N$

Obstacle	q (N)	n	p (N)	x^*	$MLCP$	$it\,BPP$	$it\,PG$
ψ_1	-100	30	-25	0.01	2	7	2
			-80	0.01	2	8	2
			-120	0.01	2	9	2
		40	-25	0.01	2	8	2
			-80	0.01	2	8.5	2
			-120	0.01	2	11	2
		50	-25	0.01	2	9.5	2
			-80	0.01	2	12	2
			-120	0.01	2	15	2
ψ_2	-100	30	-25	0.01	2	8	2
			-80	0.01	2	10.5	2
			-120	0.01	2	6	2
		40	-25	0.01	2	8.5	2
			-80	0.01	2	10.5	2
			-120	0.01	2	7.5	2
		50	-25	0.01	2	9.5	2
			-80	0.01	2	15.5	2
			-120	0.01	2	9	2

So for a fixed force, the contact zone between the rod and the obstacle is maximized when the fiber volume fraction is as minimum as possible. This agrees with the expected behaviour of the rod. In fact, if the material contains less fiber, then it is softer and the deformation of the rod is bigger. This implies that the region of contact between the rod and the obstacle is larger.

TABLE 3. Results for Problem 1, for $q = -20000N$

Obstacle	q (N)	n	p (N)	x^*	$MLCP$	$it\,BPP$	$it\,PG$
ψ_1	-20000	30	-25	0.07571	64	1.953	9
			-80	0.07575	87	2.494	11
			-120	0.07577	77	2.584	10
		40	-25	0.03454	53	2.245	7
			-80	0.03456	56	3.054	7
			-120	0.03456	73	2.795	9
		50	-25	0.01282	31	2.71	5
			-80	0.01282	31	4	5
			-120	0.01285	32	3.594	5
ψ_2	-20000	30	-25	0.04176	70	1.686	9
			-80	0.04174	56	1.696	8
			-120	0.04173	69	2.043	9
		40	-25	0.01188	20	2	4
			-80	0.01188	20	2.4	4
			-120	0.01188	20	2.45	4
		50	-25	0.01	2	7.5	2
			-80	0.01	2	11.5	2
			-120	0.01	2	8.5	2

It follows from the results displayed in tables 2 and 3, that if the forces q and p are more or less of the same order, then the projected-gradient algorithm achieves the minimum value in two iterations. But if q is much bigger than p, the projected-gradient algorithm requires more iterations and the minimum value 0.01 is achieved only for a more refined mesh. The table 3 also illustrates the convergence of the method to the value 0.01, as the number of finite elements increases.

The figures 3 and 4 represent the displacement $u = u(x^*)$ of the rod axis for the two different perpendicular forces $p = -25N$ and $p = -120N$, and for the solution $x^* = 0.01188$, with the obstacle ψ_2, $n = 40$ and $q = -20000N$. The contact region increases with the intensity of p.

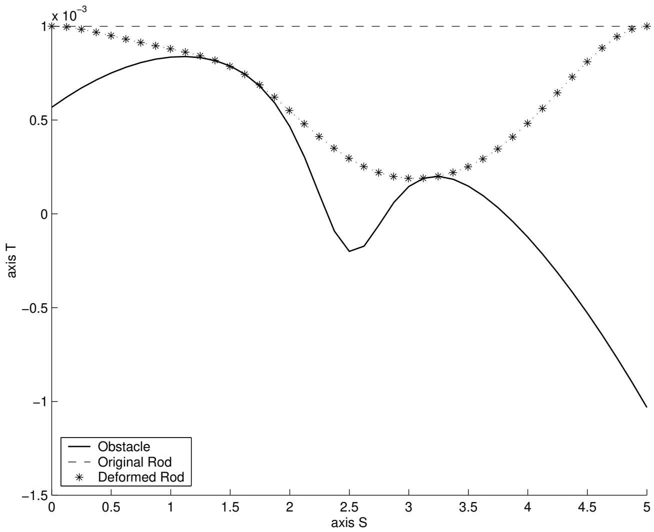

FIGURE 3. Displacement u for Problem 1, $p = -25N$

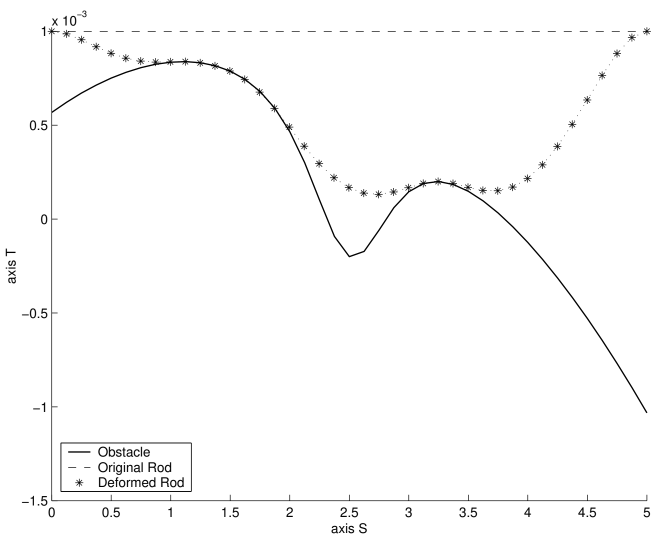

FIGURE 4. Displacement u for Problem 1, $p = -120N$

By using formula (12) and, as since F_H is independent on x, it is easy to see that the gradient of the objective function f is given by

$$\left[\begin{array}{l} \frac{df}{dx}(x) = -\left(\frac{dB_{HH}}{dx}(x)\psi_H\right)^T (u(x)-\psi) \\ \qquad\qquad\qquad -\frac{1}{2}(u(x)-\psi)^T \frac{dB_{HH}}{dx}(x)(u(x)-\psi), \end{array}\right. \tag{54}$$

where

$$\frac{dB_{HH}}{dx}(x) = \frac{E_f - E_m}{E_f x + E_m(1-x)} B_{HH}(x). \tag{55}$$

Since the reference configuration of the rod axis, in the fixed coordinate system is defined by ψ_0, then in (54) $\psi = \psi_1 - \psi_0$ or $\psi = \psi_2 - \psi_0$, if the displacement of the rod axis is constrained by the obstacle ψ_1 or ψ_2, respectively. To obtain the formula (55) it is enough to derive with respect to x, the element stiffness matrix (35), that is, to derive the longitudinal modulus of the material $E(x)$ defined in (53).

In the right side of (54), the second term is always positive, for any $x \in X$, as the matrix $\frac{dB_{HH}}{dx}(x)$ is symmetric and positive definite, $B_{HH}(x)$ is also symmetric, positive definite and $\frac{E_f - E_m}{E_f x + E_m(1-x)} > 0$. But it is impossible to predict the sign of the first term. So, the sign of the derivative $\frac{df}{dx}(x)$ is not known in advance and the projected-gradient algorithm is required to solve problem 1.

6.2. Problem 2 (material and cross section optimization for a rod). The admissible set X of outer variables in problem 2 is defined by

$$X = \left\{ x = (x_1, x_2) \in \mathbb{R}^2 : \; V_f^{\min} \le x_1 \le V_f^{\max}, \; b^{\min} \le x_2 \le b^{\max} \right\} \tag{56}$$

The outer variable $x = (x_1, x_2)$ has now two components, where x_1 represents the fiber volume fraction V_f and x_2 the length of a side of the rectangular cross section of the rod in a direction perpendicular to the rod axis. Moreover we suppose that the area of the cross section is constant $|w| = 0.004m^2$. Hence the longitudinal modulus of the material E is a function of x_1 and the moment of inertia I is a function of x_2, and are defined by

$$E(x_1) = E_f x_1 + E_m(1 - x_1), \qquad I(x_2) = \frac{x_2^2}{12}|w|. \tag{57}$$

If the rectangular cross section has length sides a and x_2, the area is $|w| = ax_2$, $I(x_2) = \frac{x_2^3 a}{12}$ and I verifies the formula (57). Thus, the objective of this problem 2 is to find both the fiber volume fraction $V_f = x_1$ in the material and the shape of the cross section (a rectangle if $x_2 \neq a$ or a square if $x_2 = a = \sqrt{|w|}$) which minimize the objective function of the MPEC (48). In addition for this rod, the modulus of the matrix is $E_m = 3.45GPa$, the modulus of the fiber is $E_f = 86GPa$, the axis length is $L = 5m$, and the external loads have intensities $q(N)$ and $p(N)$, that are independent of x.

The tables 4 and 5 include the results of problem 2 with the projected-gradient algorithm. The solution produced is $x^* = (x_1^*, x_2^*) = (V_f^{\min}, b^{\min})$. The value $x_1^* = V_f^{\min}$ means that the percentage of fiber in the material is the minimum, and so, as in problem 1, the material is softer. The value $x_2^* = b^{\min}$ indicates that the length of a side of the rectangular cross section of the rod must be the minimum, which means that the cross section must be very thin. This solution corresponds to the expected mechanical properties of the rod, as a soft material and a very thin rectangular cross section lead to a big deformation, which increases the contact region between the rod and the obstacle and decreases the value of the objective function.

A direct observation of tables 4 and 5, with respect to the value x_1^* of the first component of x^*, leads to the following conclusion analogous to that of problem 1 (when observing tables 2 and 3): if q is considerably bigger than p, the number of iterations of the projected-gradient algorithm increases, and the expected solution is only obtained for a sufficiently refined mesh. On the contrary, the value x_2^* of the second component of x^* is always the minimum value of x_2, that is $x_2 = 0.05 = b^{\min}$, independently of the relation between the intensities of the forces q and p.

The figures 5 and 6 illustrate the influence of the force p. They represent the displacement $u = u(x^*)$ of the rod axis for the value $x^* = (0.01048, 0.05)$, for the two different perpendicular forces $p = -10N$ and $p = -80N$, with the obstacle ψ_1, for $n = 50$ and $q = -12000N$.

For this problem 2, it follows from (12) that the gradient of f is defined by

$$\nabla_x f(x) = \Big(\frac{\partial f}{\partial x_1}(x), \frac{\partial f}{\partial x_2}(x)\Big) \tag{58}$$

Table 4. Results for Problem 2 with $q = -12000N$ and $q = -20000N$

Obstacle	q (N)	n	p (N)	$x^* = (x_1^*, x_2^*)$	$MLCP$	$it\,BPP$	$it\,PG$
ψ_1	-12000	30	-10	$(0.07101, 0.05)$	17	2.706	4
			-80	$(0.07101, 0.05)$	17	3.529	4
			-150	$(0.07113, 0.05)$	18	3.444	4
		40	-10	$(0.03153, 0.05)$	37	2.568	6
			-80	$(0.03154, 0.05)$	37	3.649	6
			-150	$(0.03154, 0.05)$	37	3.676	6
		50	-10	$(0.01048, 0.05)$	15	3.133	3
			-80	$(0.01048, 0.05)$	15	4.733	3
			-150	$(0.01048, 0.05)$	15	4.733	3
ψ_2	-20000	30	-25	$(0.09159, 0.05)$	36	2.222	8
			-80	$(0.09159, 0.05)$	36	2.278	8
			-120	$(0.09152, 0.05)$	37	2.649	8
		40	-25	$(0.04407, 0.05)$	26	2.577	5
			-80	$(0.04407, 0.05)$	26	2.346	5
			-120	$(0.04407, 0.05)$	26	2.346	5
		50	-25	$(0.01926, 0.05)$	27	2.815	5
			-80	$(0.01926, 0.05)$	27	2.444	5
			-120	$(0.01926, 0.05)$	27	2.963	5

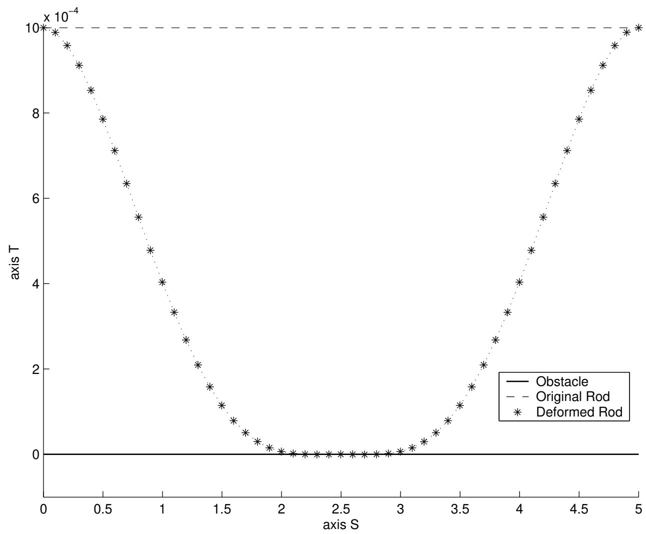

Figure 5. Displacement u for Problem 2, $p = -10N$

TABLE 5. Results for Problem 2, for $q = -50N$

Obstacle	$q\ (N)$	n	$p\ (N)$	$x^* = (x_1^*, x_2^*)$	$MLCP$	$it\,BPP$	$it\,PG$
ψ_1	-50	30	-10	$(0.01, 0.05)$	2	6	2
			-80	$(0.01, 0.05)$	2	10	2
			-150	$(0.01, 0.05)$	2	9	2
		40	-10	$(0.01, 0.05)$	2	7.5	2
			-80	$(0.01, 0.05)$	2	10	2
			-150	$(0.01, 0.05)$	2	11	2
		50	-10	$(0.01, 0.05)$	2	8.5	2
			-80	$(0.01, 0.05)$	2	13.5	2
			-150	$(0.01, 0.05)$	2	13.5	2
ψ_2	-50	30	-25	$(0.01, 0.05)$	2	7.5	2
			-80	$(0.01, 0.05)$	2	6	2
			-120	$(0.01, 0.05)$	2	7	2
		40	-25	$(0.01, 0.05)$	2	10.5	2
			-80	$(0.01, 0.05)$	2	9	2
			-120	$(0.01, 0.05)$	2	7.5	2
		50	-25	$(0.01, 0.05)$	2	11.5	2
			-80	$(0.01, 0.05)$	2	9.5	2
			-120	$(0.01, 0.05)$	2	9.5	2

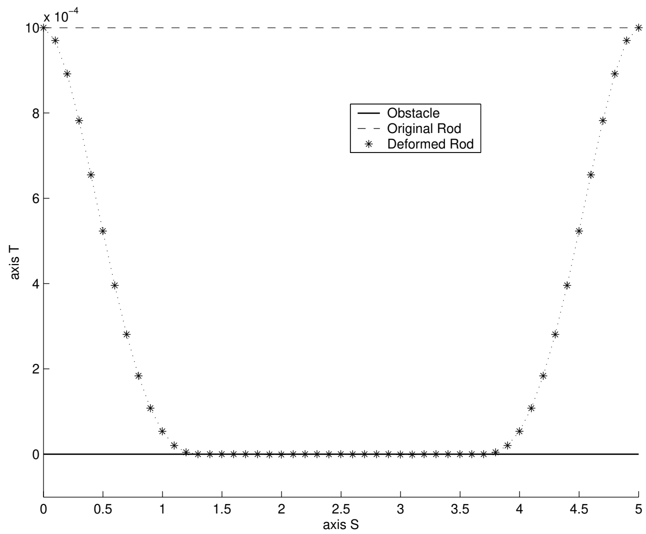

FIGURE 6. Displacement u for Problem 2, $p = -80N$

where

$$\left[\begin{array}{l} \dfrac{\partial f}{\partial x_1}(x) = -\Big(\dfrac{\partial B_{HH}}{\partial x_1}(x)\psi_H\Big)^T (u(x)-\psi) \\ \qquad\qquad\qquad -\frac{1}{2}(u(x)-\psi)^T \frac{\partial B_{HH}}{\partial x_1}(x)(u(x)-\psi), \end{array}\right.$$

$$\left[\begin{array}{l} \dfrac{\partial f}{\partial x_2}(x) = -\Big(\dfrac{\partial B_{HH}}{\partial x_2}(x)\psi_H\Big)^T (u(x)-\psi) \\ \qquad\qquad\qquad -\frac{1}{2}(u(x)-\psi)^T \frac{\partial B_{HH}}{\partial x_2}(x)(u(x)-\psi), \end{array}\right. \tag{59}$$

as F_H is independent of x. As observed before in problem 1, the function ψ in (59) is defined by $\psi_i - \psi_0$, for $i = 1$ or $i = 2$, depending on the choice of the obstacle ψ_1 or ψ_2. In order to compute the partial derivatives $\frac{\partial B_{HH}}{\partial x_j}(x)$ for $j = 1, 2$, it is enough to calculate the derivatives $\frac{dE}{dx_1}$, $\frac{dI}{dx_2}$, in the definition of the element stiffness matrix B_i (35). So, analogously to problem 1 (see (55))

$$\frac{\partial B_{HH}}{\partial x_1}(x) = \frac{E_f - E_m}{E_f x_1 + E_m(1-x_1)} B_{HH}(x), \tag{60}$$

and for a generic finite element $[y_i, y_{i+1}]$ the derivative $\frac{\partial B_{HH}}{\partial x_2}(x)$ is equal to $\frac{\partial B_i}{\partial x_2}(x)$, where

$$\frac{\partial B_i}{\partial x_2}(x) = E(x_1)\frac{dI}{dx_2}(x_2) \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{12}{h_i^3} & \frac{6}{h_i^2} & 0 & -\frac{12}{h_i^3} & \frac{6}{h_i^2} \\ 0 & \frac{6}{h_i^2} & \frac{4}{h_i} & 0 & -\frac{6}{h_i^2} & \frac{2}{h_i} \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -\frac{12}{h_i^3} & -\frac{6}{h_i^2} & 0 & \frac{12}{h_i^3} & -\frac{6}{h_i^2} \\ 0 & \frac{6}{h_i^2} & \frac{2}{h_i} & 0 & -\frac{6}{h_i^2} & \frac{4}{h_i} \end{bmatrix}, \tag{61}$$

h_i is the amplitude of the element $[y_i, y_{i+1}]$ and, according to (57), $\frac{dI}{dx_2}(x_2) = \frac{1}{6}x_2|w|$.

Since the matrices $\frac{\partial B_{HH}}{\partial x_j}(x)$, for $j = 1, 2$, are symmetric and positive definite, in the right-hand sides of the two formulas (59) each second term is positive, for any $x \in X$, but the sign of the first term is not known. So, it is impossible to know *a priori* the sign of each partial derivative in the definition of the gradient $\nabla_x f(x)$ and the projected-gradient algorithm is necessary to obtain this information and to compute the minimum.

6.3. Problem 3 (material and axis length optimization for a rod). The admissible set X of outer variables is now defined by

$$X = \Big\{ x = (x_1, x_2) \in \mathbb{R}^2 : \quad V_f^{\min} \le x_1 \le V_f^{\max},\ L^{\min} \le x_2 \le L^{\max} \Big\} \quad (62)$$

The component x_1 represents the fiber volume fraction V_f and x_2 is the length of the axis of the rod, which belongs to $[L^{\min}, L^{\max}]$. It is also assumed that the uniformly distributed forces per unit of length q and p, in the direction of the rod axis and the direction perpendicular of the rod axis, respectively, depend on the length of the rod and satisfy

$$q = \frac{\overline{q}}{x_2} \qquad \text{and} \qquad p = \frac{\overline{p}}{x_2}, \quad (63)$$

with $\overline{q}$ and $\overline{p}$ constants. This means that for a rod whose axis length is x_2, $\overline{q}$ and $\overline{p}$ are the total constant forces applied to the rod. The longitudinal modulus of the material depends on x through x_1, that is $E(x_1) = E_f x_1 + E_m(1 - x_1)$, and the amplitude h_i of each finite finite element depends on the length of the rod so it depends on x_2 the second component of the outer variable x.

The aim of this problem 3 is to find both the fiber volume fraction $V_f = x_1$ in the material and the length of the axis rod $L = x_2$, which minimize the objective function of the MPEC (48), for a rod such that the modulus of the matrix is $E_m = 3.45GPa$, the modulus of the fiber is $E_f = 86GPa$, the area of the cross section is $|w| = 0.004m^2$ and the moment of inertia is $I = 2.1 \times 10^{-6} m^4$.

The tables 6 and 7 include the results of problem 3 with the projected-gradient algorithm. The solution obtained is $x^* = (x_1^*, x_2^*) = (V_f^{\min}, L^{\max})$.

Tables 6 and 7 lead to conclusions similar to those achieved for problems 1 and 2. In this case the value x_2^* of the second component of x^* is the maximum value of x_2, that is $x_2^* = L^{\max}$ (instead of the minimum value of x_2 as in problem 2). The solution $x^* = (x_1^*, x_2^*) = (V_f^{\min}, L^{\max})$ is precisely the expected value, because of the mechanical interpretation of the problem given immediately after theorem 2.2: the rod tends to become closer to the obstacle as the fiber volume fraction reduces and when the rod axis increases. In fact, with a soft material and a long axis, the deformation of the rod is bigger, which increases the contact region with the obstacle.

TABLE 6. Results for Problem 3 with $q = -40000N$ and $q = -100000N$

Obstacle	q (N)	n	p (N)	$x^* = (x_1^*, x_2^*)$	$MLCP$	$it\,BPP$	$it\,PG$
ψ_1	-40000	30	-25	$(0.01, 5)$	2	1	2
			-80	$(0.01, 5)$	2	7	2
			-150	$(0.01, 5)$	2	6.5	2
		40	-25	$(0.01, 5)$	2	1	2
			-80	$(0.01, 5)$	2	8	2
			-150	$(0.01, 5)$	2	8	2
		50	-25	$(0.01, 5)$	2	1	2
			-80	$(0.01, 5)$	2	9	2
			-150	$(0.01, 5)$	2	8	2
ψ_2	-100000	30	-25	$(0.04177, 5)$	84	1.488	10
			-80	$(0.04177, 5)$	84	1.94	10
			-150	$(0.04176, 5)$	70	1.871	9
		40	-25	$(0.01188, 5)$	20	1.8	4
			-80	$(0.01188, 5)$	20	2.35	4
			-150	$(0.01188, 5)$	20	2.6	4
		50	-25	$(0.01, 5)$	2	6.5	2
			-80	$(0.01, 5)$	2	7	2
			-150	$(0.01, 5)$	2	9	2

The figures 7 and 8 illustrate the influence of the refinement of the finite element mesh. They represent, for $q = -100000N$, $p = -80N$, the displacement u of the rod axis at the values $x = (0.04177, 5)$ and $x = (0.01188, 5)$, for $n = 30$ and $n = 40$ finite elements, respectively, with the obstacle ψ_2.

Now the gradient of the objective function f is defined by

$$\nabla_x f(x) = \Big(\frac{\partial f}{\partial x_1}(x), \frac{\partial f}{\partial x_2}(x)\Big) \tag{64}$$

TABLE 7. Results for Problem 3, for $q = -50N$

Obstacle	$q\ (N)$	n	$p\ (N)$	$x^* = (x_1^*, x_2^*)$	$MLCP$	$it\,BPP$	$it\,PG$
ψ_1	-50	30	-25	$(0.01, 5)$	2	1	2
			-80	$(0.01, 5)$	2	7	2
			-150	$(0.01, 5)$	2	7	2
		40	-25	$(0.01, 5)$	2	1	2
			-80	$(0.01, 5)$	2	8	2
			-150	$(0.01, 5)$	2	8	2
		50	-25	$(0.01, 5)$	2	1	2
			-80	$(0.01, 5)$	2	8.5	2
			-150	$(0.01, 5)$	2	8	2
ψ_2	-50	30	-25	$(0.01, 5)$	2	4.5	2
			-80	$(0.01, 5)$	2	6	2
			-150	$(0.01, 5)$	2	6.5	2
		40	-25	$(0.01, 5)$	2	5	2
			-80	$(0.01, 5)$	2	6.5	2
			-150	$(0.01, 5)$	2	8.5	2
		50	-25	$(0.01, 5)$	2	7	2
			-80	$(0.01, 5)$	2	7	2
			-150	$(0.01, 5)$	2	9	2

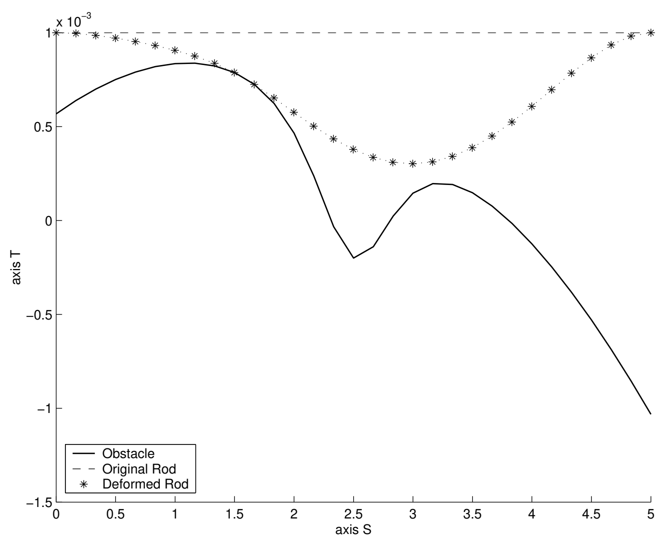

FIGURE 7. Displacement u for Problem 3, $n = 30$

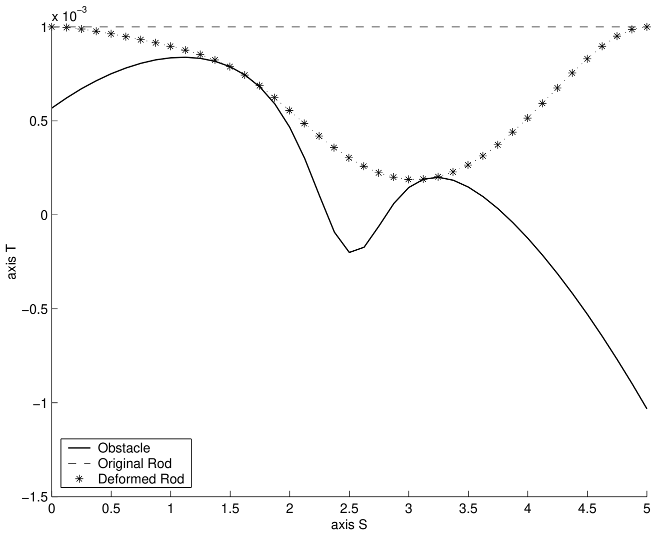

FIGURE 8. Displacement u for Problem 3, $n = 40$

where

$$\left[\begin{aligned} \frac{\partial f}{\partial x_1}(x) &= \Big(\frac{\partial F_H}{\partial x_1}(x) - \frac{\partial B_{HH}}{\partial x_1}(x)\psi_H\Big)^T (u(x)-\psi) \\ &\qquad -\tfrac{1}{2}(u(x)-\psi)^T \tfrac{\partial B_{HH}}{\partial x_1}(x)(u(x)-\psi), \\ \frac{\partial f}{\partial x_2}(x) &= \Big(\frac{\partial F_H}{\partial x_2}(x) - \frac{\partial B_{HH}}{\partial x_2}(x)\psi_H\Big)^T (u(x)-\psi) \\ &\qquad -\tfrac{1}{2}(u(x)-\psi)^T \tfrac{\partial B_{HH}}{\partial x_2}(x)(u(x)-\psi). \end{aligned}\right. \tag{65}$$

As observed before in problems 1 and 2, the function ψ in (65) is defined by $\psi_i - \psi_0$, for $i = 1$ or $i = 2$, depending on the choice of the obstacle ψ_1 or ψ_2. By examining the formulas (35) and (37) of the element stiffness matrix B_i and of the element vector force F_i (which by (63) is independent of x_1 but depends on x_2), we deduce that the above partial derivatives with respect to x_1 satisfy

$$\frac{\partial F_H}{\partial x_1} = 0, \qquad \frac{\partial B_{HH}}{\partial x_1}(x) = \frac{E_f - E_m}{E_f x_1 + E_m(1-x_1)} B_{HH}(x). \tag{66}$$

The derivatives with respect to x_2 are more complicated. The amplitude of each finite element is a function of x_2, that is, $h_i = h_i(x_2)$, where x_2 is the length of the axis rod. So in order to obtain the partial derivatives $\frac{\partial F_H}{\partial x_2}(x)$

and $\frac{\partial B_{HH}}{\partial x_2}(x)$ we must calculate the derivative $\frac{dh_i}{dx_2}$ and the derivatives $\frac{\partial F_i}{\partial x_2}(x)$ and $\frac{\partial B_i}{\partial x_2}(x)$ of the element vector F_i and of the element matrix B_i.

By (63), the elementary vector force F_i defined in (37) becomes

$$F_i(x)^T = \left[\frac{\overline{q}}{2x_2}h_i \quad \frac{\overline{p}}{2x_2}h_i \quad \frac{\overline{p}}{12x_2}h_i^2 \quad \frac{\overline{q}}{2x_2}h_i \quad \frac{\overline{p}}{2x_2}h_i \quad -\frac{\overline{p}}{12x_2}h_i^2\right], \tag{67}$$

where h_i depends on x_2, that is, $h_i = h_i(x_2)$. In particular, for a uniform mesh with n finite elements such that $h_i(x_2) = \frac{x_2}{n}$, we have that

$$\frac{\partial F_i(x)^T}{dx_2} = \left[0 \quad 0 \quad \frac{\overline{p}}{12n^2} \quad 0 \quad 0 \quad -\frac{\overline{p}}{12n^2}\right]. \tag{68}$$

Hence by assembling these elementary vector forces we obtain $\frac{\partial F_H}{\partial x_2}(x) = 0$. For the same mesh the derivative $\frac{\partial B_{HH}}{\partial x_2}(x)$ is computed by assembling the derivatives $\frac{\partial B_i}{\partial x_2}(x)$ for all the finite elements $i = 1, 2, ..., n$, with

$$\frac{\partial B_i}{\partial x_2}(x) = E(x_1)\begin{bmatrix} -\frac{|w|n}{x_2^2} & 0 & 0 & \frac{|w|n}{x_2^2} & 0 & 0 \\ 0 & -\frac{36In^3}{x_2^4} & -\frac{12In^2}{x_2^3} & 0 & \frac{36In^3}{x_2^4} & -\frac{12In^2}{x_2^3} \\ 0 & -\frac{12In^2}{x_2^3} & -\frac{4In^2}{x_2^2} & 0 & \frac{12In^2}{x_2^3} & -\frac{2In}{x_2^2} \\ \frac{|w|n}{x_2^2} & 0 & 0 & -\frac{|w|n}{x_2^2} & 0 & 0 \\ 0 & \frac{36In^2}{x_2^3} & \frac{12In}{x_2^2} & 0 & -\frac{36In^2}{x_2^3} & \frac{12In}{x_2^2} \\ 0 & -\frac{12In^2}{x_2^3} & -\frac{2In}{x_2^2} & 0 & \frac{12In^2}{x_2^3} & -\frac{4In}{x_2^2} \end{bmatrix}. \tag{69}$$

Note that it is not possible to conclude whether $\frac{\partial B_{HH}}{\partial x_2}(x)$ is a positive definite matrix in this case.

Similarly to problems 1 and 2, the sign of $\frac{\partial f}{\partial x_1}(x)$ is impossible to determine even when the matrix $\frac{\partial B_{HH}}{\partial x_1}(x)$ is positive definite, as the sign of the term $-(\frac{\partial B_{HH}}{\partial x_1}(x)\psi_H)^T(u(x)-\psi)$ is not known for each x. The sign of $\frac{\partial f}{\partial x_2}(x)$ is even more difficult to guess, since it is not known if $\frac{\partial B_{HH}}{\partial x_2}(x)$ is a positive definite matrix. Thus the projected-gradient algorithm is also needed to detect the increase or the decrease of the objective function $f(x_1, x_2)$.

6.4. Problem 4 (material optimization for a plate). This problem 4 is analogously to problem 1 and the admissible set X of outer variables is defined by

$$X = \Big\{ x \in [0,1] : \quad V_f^{\min} \leq x \leq V_f^{\max} \Big\}. \tag{70}$$

The variable x has only one component, which represents the fiber volume fraction V_f. The objective of this problem 4 is to find the fiber volume fraction of the plate which satisfies the data of table 1 ($E_m = 3.45GPa$, $E_f = 86GPa$, $t = 0.002m$, $\nu_m = 0.30GPa$, $\nu_f = 0.222GPa$, $G_m = 1.33GPa$, $G_f = 35.2GPa$) and minimizes the objective function of the MPEC (48). In addition the plate is subjected to the action of a vertical force, per unit of area, of intensity p independent on x.

Now, the coefficients of elasticity Q_{11}, Q_{12}, Q_{22}, Q_{33} defined in (41) are functions of x, as the Young's modulus E_1 and E_2 defined in (42) verify

$$E_1(x) = E_f x + E_m(1-x), \qquad E_2 = \frac{E_f E_m}{E_f(1-x) + E_m x}. \tag{71}$$

The table 8 presents the results for problem 4 with the projected-gradient algorithm and the solution obtained is $x^* = V_f^{\min}$.

The examination of this table 8 indicates that for the two obstacles ψ_3 and ψ_4, the solution $x^* = V_f^{\min} = 0.01$ is obtained in two iterations with the projected-gradient algorithm. This number of iterations does not change with the different intensities of the force and with the increase of the number of finite elements. Consequently the derivative $\frac{df}{dx}(x)$ in (72) must be always positive in these cases. As already remarked in the previous rod problems, this solution obtained with the projected-gradient method agrees with the expected mechanical properties of the plate, as the minimum value for the fiber means a soft material.

The figure 9 represents the deformed middle plane of the plate, represented by the displacement u for the constant obstacle ψ_3 with the force $p = -20000N$ and 225 finite elements. The figure 10 shows the displacement u of the middle plane of the plate for the obstacle ψ_4, with the force $p = -90000N$ and 400 finite elements.

By using formula (12) and since F_H defined in (43) is independent on x, the gradient of the objective function f satisfies

$$\left[\begin{aligned} \frac{df}{dx}(x) = -\Big(\frac{dB_{HH}}{dx}(x)\psi_H\Big)^T (u(x) - \psi) \\ -\frac{1}{2}(u(x)-\psi)^T \frac{dB_{HH}}{dx}(x)(u(x)-\psi), \end{aligned} \right. \tag{72}$$

TABLE 8. Results for Problem 4

Obstacle	n	$p\ (N)$	x^*	$MLCP$	$it\,BPP$	$it\,PG$
ψ_3	100	-10000	0.01	2	1	2
		-20000	0.01	2	2.5	2
		-30000	0.01	2	3	2
	225	-10000	0.01	2	1	2
		-20000	0.01	2	2.5	2
		-30000	0.01	2	4	2
	400	-10000	0.01	2	1	2
		-20000	0.01	2	4	2
		-30000	0.01	2	6	2
ψ_4	100	-20000	0.01	2	2	2
		-50000	0.01	2	3	2
		-90000	0.01	2	4	2
	225	-20000	0.01	2	2	2
		-50000	0.01	2	3.5	2
		-90000	0.01	2	3.5	2
	400	-20000	0.01	2	3.5	2
		-50000	0.01	2	4.5	2
		-90000	0.01	2	5	2

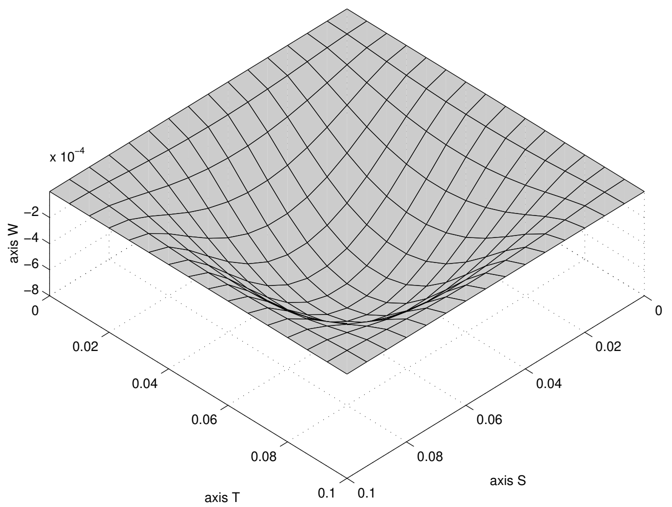

FIGURE 9. Displacement u for Problem 4 with obstacle ψ_3

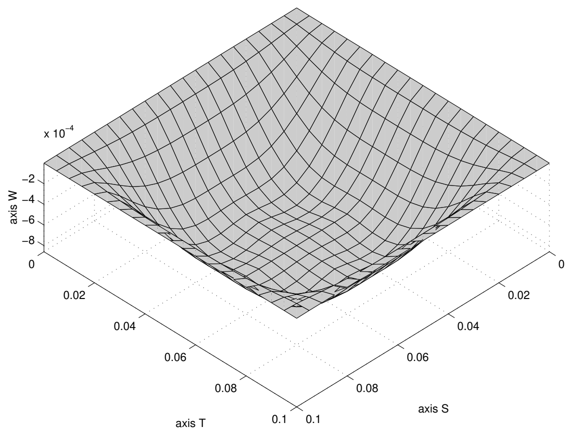

FIGURE 10. Displacement u for Problem 4 with obstacle ψ_4

where $\psi = \psi_i$ for $i = 3$ or $i = 4$. Similarly to the previous problems, in order to compute $\frac{dB_{HH}}{dx}(x)$ it is enough to calculate the derivative of the element stiffness matrix B_i defined in (38) and then to assemble all the element stiffness matrices, as is usual in the finite element method. Hence

$$\frac{dB_i}{dx}(x) = \frac{t^3}{12}\int_{\Omega_i} N_i^T \frac{dD}{dx}(x) N_i \tag{73}$$

and

$$\frac{dD}{dx}(x) = \begin{bmatrix} \frac{dQ_{11}}{dx}(x) & \frac{dQ_{12}}{dx}(x) & 0 \\ \frac{dQ_{21}}{dx}(x) & \frac{dQ_{22}}{dx}(x) & 0 \\ 0 & 0 & \frac{dQ_{33}}{dx}(x) \end{bmatrix}_{3\times 3} . \tag{74}$$

So to obtain the expression of $\frac{dB_{HH}}{dx}(x)$ it is sufficient to derive the elasticity coefficients with respect to x and to apply (73-74). Due to the complexity of the derivatives $\frac{dQ_{ij}}{dx}(x)$, for $i, j \in \{1, 2\}$ it is not possible to know *a priori* by a direct observation whether $\frac{dD}{dx}(x)$ is a positive definite matrix, and so it is not known if $\frac{dB_{HH}}{dx}(x)$ is a positive definite matrix. The projected-gradient algorithm is needed once more to compute the sign of $\frac{df}{dx}(x)$ and the solution of problem 4.

It follows from all these experiments that the results achieved with the projected-gradient algorithm confirm the expected mechanical properties of the rod or plate. Furthermore the number of iterations of the projected-gradient algorithm and of the block pivoting algorithm are always quite small. This indicates that these techniques are quite appropriate for their purposes.

More general structural optimization problems, whose solutions can not be predicted, both from the mathematical and mechanical view-point, may be determined by the iterative technique proposed in this paper. In fact, we can allow in the definition of the set X other linear constraints. As far as the implementation of the algorithm is concerned, this only affects the definition of the projection P_X. However, it may induce a significant alteration in the problem in such a way that it is impossible to guess in advance an acceptable mechanical solution. For instance, it would be interesting to consider a material optimization problem, such as problem 1, for a composite rod subjected to an applied load, which may come in contact with a rigid obstacle, and such that the rod is made of a variable Young's modulus E_j, in each finite element j, and with a constant global Young's modulus E. This implies that

$$\begin{cases} E_j = E_f x_j + E_m(1-x_j), \quad \text{for} \quad j=1,\dots,n \\ E = \sum_{j=1}^n E_j = \sum_{j=1}^n \left[E_f x_j + E_m(1-x_j)\right] \\ 0 \le x_j \le 1, \quad \text{for} \quad j=1,\dots,n, \end{cases} \tag{75}$$

where n is the number of finite elements in the mesh. The equation $E = \sum_{j=1}^n \left[E_f x_j + E_m(1-x_j)\right]$ is a linear constraint that should be included in the definition of the set X. The projected-gradient algorithm can also be applied in this case, but the projection operator P_X should be computed by one of the algorithms described in Helgason, Kennington and Lall [12], Robinson, Jiang and Lerme [21] and Pardalos and Kovoor [18] for this so-called strictly convex quadratic knapsack problem.

This process would give the amount of fiber volume fraction x_j in each finite element $j \in \{1,\dots,n\}$. This means that for a rod with a constant Young's modulus, we could know the distribution of the material in the rod (more or less fiber in the regions determined by the finite elements), which is not predictable in the majority of the cases.

Conclusion

A projected-gradient algorithm that includes a block principal pivoting algorithm is proposed in this paper for a particular MPEC whose objective function is differentiable. This technique has been applied to four material and shape optimization problems with constraints that include a contact problem with a rigid obstacle. The numerical results confirm the suitability of this method. The methodology discussed in this paper can also be very useful to solve more general material and shape optimization problems. This will certainly be one of the main objectives of our future research.

References

[1] Bertsekas, D.: *Nonlinear Programming.* Massachusetts: Athena Scientific, 1995.

[2] Bertholet, J.-M.: *Matériaux Composites, Comportement mécanique et analyse des structures.* Paris: Masson, 1992.

[3] *CALFEM (http://www.byggmek.lth.se/CALFEM), A finite element toolbox to MATLAB, Version 3.3.* Sweden: Structural Mechanics and Solid Mechanics, Department of Mechanics and Materials, Lund University, 2000.

[4] Ciarlet, P.G.: *Basic Error Estimates for Elliptic Problems.* In: P.G. Ciarlet and J.L Lions, editors. Handbook of Numerical Analysis. Vol.II, 17–135, Amsterdam: North-Holland, 1991.

[5] Cottle, R.W. ; Pang, J.S. and Stone, R.W.: *The Linear Complementarity Problem.* Boston: Academic Press, 1992.

[6] Duff, I. ; Erisman, A. and Reid, J.: *Direct Methods for Sparse Matrices.* Oxford: Claredon Press, 1986.

[7] Fernandes, L.M. ; Júdice, J. and Patrício, J.: An investigation of interior-point and block pivoting algorithms for large scale symmetric monotone linear complementarity problems. *Computational Optimization and Applications* 1996; 5: 49–77.

[8] Fernandes, L.M. ; Figueiredo, I.N. and Júdice, J.J.: On the solution of a finite element approximation of a linear obstacle plate problem. *International Journal of Applied Mathematics and Computer Science* 2002; 12(1): 101–114.

[9] Figueiredo, Isabel N. ; Júdice, Joaquim J. and Rosa, Silvério S.: *Solution Methods for Structural Optimization in Contact Rod Problems.* In: J.A.C. Martins and Manuel D.P. Monteiro Marques, editors. Contact Mechanics. 325-332, Amsterdam: Kluwer Academic Publishers, 2002.

[10] Harker, P.T. and Pang, J.S.: Finite-dimensional variational inequality and nonlinear complementarity problems: a survey of theory, algorithms and applications. *Mathematical Programming* 1990; 48(2): 161–220.

[11] Haslinger, J. and Neittaanmäki, P.: *Finite Element Approximation for optimal Shape Design, Theory and Applications.* Chichester: Wiley, 1997.

[12] Helgason, R. ; Kennington, J. and Lall, H.: A polynomially bounded algorithm for a singly constrained quadratic program. *Mathematical Programming* 1980; 18: 338–343.

[13] Júdice, J.J. and Pires, F.M.: A block principal pivoting algorithm for large-scale strictly monotone linear complementarity problems. *Computers and Operations Research* 1994; 21: 587–596.

[14] Luo, Z., Pang, J.-S., and Ralph, D.: *Mathematical Programs with Equilibrium Constraints.* Cambridge: Cambridge University Press, 1997.

[15] *MATLAB* - registered trademark of the MathWorks, Inc.

[16] Nocedal, J. and Wright, S.: *Numerical Optimization.* New York: Springer, 1999.

[17] Outrata, J. ; Kočvara, M. and Zowe, J.: *Nonsmooth Approach to Optimization Problems with Equilibrium Constraints.* Dordrecht: Kluwer Academic Publishers, 1998.

[18] Pardalos, P. and Kovoor, N.: An algorithm for a singly constrained class of quadratic programs subject to upper and lower bounds. *Mathematical Programming* 1990; 46: 321–328.

[19] Petersson, J.: *Optimization of Structures in Unilateral Contact.* Linköping Studies in Science and Technology, Dissertations n.397, Sweden: Linköping University, 1995.

[20] Reddy, J.N.: *Mechanics of Laminated Composite Plates, Theory and Analyis.* Boca Raton Florida: CRC Press, Inc., 1997.

[21] Robinson, A.G. ; Jiang, N. and Lerme, C.S.: On the continuous quadratic knapsack problems. *Mathematical Programming* 1992; 55: 99–108.

[22] Trabucho, L. and Viaño, J.M.: *Mathematical Modeling of Rods.* In: P.G. Ciarlet and J.L Lions, editors. Handbook of Numerical Analysis. Vol.IV, 487–974, Amsterdam: North-Holland, 1996.

Isabel N. Figueiredo
Departamento de Matemática, Universidade de Coimbra, Apartado 3008, 3001-454 Coimbra, Portugal
E-mail address: Isabel.Figueiredo@mat.uc.pt

Joaquim J. Júdice
Departamento de Matemática, Universidade de Coimbra, Apartado 3008, 3001-454 Coimbra, Portugal
E-mail address: Joaquim.Judice@co.it.pt

Silvério S. Rosa
Departamento de Matemática, Universidade da Beira Interior, 6201-001 Covilhã, Portugal
E-mail address: rosa@noe.ubi.pt