

On a Branch and Bound Algorithm for the Solution of a Family of Softening Material Problems of Mechanics with Applications to the Analysis of Metallic Structures

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Abstract. The variational formulation of mechanical problems involving nonmonotone, possibly multivalued, material or boundary laws leads to hemivariational inequalities. The solutions of the hemivariational inequalities constitute substationarity points of the related energy (super)potentials. For their computation convex and global optimization algorithms have been proposed instead of the earlier nonlinear optimization methods, due to the lack of smoothness and convexity of the potential. In earlier works one of us has proposed an approach based on the decomposition of the solutions space into convex parts resulting in a sequence of convex optimization subproblems with different feasible sets. In this case nonconvexity of the potential was attributed to (generalized) gradient jumps. In order to treat ‘softening’ material effects, in the present paper this method is extended to cover also energy functionals where nonconvexity is caused by the existence of concave sections. The nonconvex minimization problem is formulated as d.c. (difference convex) minimization and an algorithm of the branch and bound type based on simplex partitions is adapted for its treatment. The partitioning scheme employed here is adapted to the large dimension of the problem and the approximation steps are equivalent to convex minimization subproblems of the same structure as the ones arising in unilateral problems of mechanics. The paper concludes with a numerical example and a discussion of the properties and the applicability of the method.

Key words: Hemivariational inequalities, nonconvex superpotentials, softening materials, d.c. minimization.

1. Introduction

The equilibrium conditions of classical nonlinear mechanics problems are systems of partial differential equations which are usually formulated as variational equalities involving smooth potentials with the aid of the calculus of variations (the well known ‘principles’ of minimum potential or complementary energy) [1]. Finding the equilibrium configuration of a structural system is then equivalent to minimizing a quadratic potential functional in the displacement space (usual primary variables) in the case of linear elasticity or a smooth and convex functional when

a more general smooth and monotone material law is employed. This is valid as long as the structure remains in a normal operational framework, i.e. the loads are not severe enough to cause structural damage or change the response mode of the structural members (e.g. buckling of slender steel columns) and no other complex physical mechanisms (material behaviour, unilateral contact etc.) contribute to the energy balance of the system.

Modern engineering applications made necessary the introduction of material laws and interface conditions that include complete ascending and descending vertical branches and inclined decreasing branches. Such stress-strain (material) and force-displacement (boundary) laws describe macroscopically a variety of response changes such as locking or the gradual loss of strength [2–7]. When the material law is monotone and multivalued the corresponding potential is convex but nonsmooth and the equilibrium problem is expressed as a variational inequality or equivalently as a convex minimization problem [3, 8]. Nonmonotone laws, i.e. laws containing vertical or inclined descending branches describe various aspects of strength degradation. In this case the corresponding superpotentials are nonconvex and maybe nonsmooth (depending on the existence of vertical branches) and the variational form of the equilibrium problem is a hemivariational inequality [3, 5, 6, 9]. The study of the variational inequalities is based on monotonicity arguments [3], while the study of hemivariational inequalities is based on weak compactness arguments due to the lack of convexity of the superpotentials involved [6]. If some mild conditions on the growth of the nonsmooth superpotentials are fulfilled, then the corresponding potential and complementary energy functionals can be obtained for the whole structure [3, 6], whose substationarity points (all the local minima, local maxima or saddle points) provide all the solutions of the hemivariational inequality. This is a generalization of the minimum potential and complementary energy theorems which hold for the case of monotone material laws leading to variational equalities and inequalities [3, 10]. We note that in the absence of these growth conditions the hemivariational inequality may have solutions that are not substationarity points.

Recently, the notion of the quasidifferential of a general nonsmooth and nonconvex functional has been employed for the formulation of a new kind of variational expressions that generalize the variational equations and inequalities and provide a useful tool for the treatment of the hemivariational inequalities [5, 11–13]. The quasidifferential is set-valued generalization of the gradient operator of smooth potentials and coincides with the subdifferential for the case of convex (nonsmooth) functionals. Convexity and concavity are described separately by the two sets comprising the quasidifferential. The difference convex (d.c.) approximation of nonconvex functionals, where the functional is written as a difference of two convex components [14], is also covered by the quasidifferential as a special case. For an extensive analysis and discussion see [13].

Although the progress in the theoretical study of the existence and approximation questions for the hemivariational inequalities is considerable [6, 9, 15] relatively few efficient methods exist for their numerical treatment.

The determination of the full set of solutions of a substationarity problem, even when only smooth functionals are involved, remains an as yet open problem and constitutes an area of active research in the field of computational mechanics. This indeed holds for a global optimization problem as well, the latter being a particular case of the general substationarity problem [16, 17]. However, in the majority of engineering problems instead of the complete set of solutions only a subset is sought that contains the stable and unstable solutions on a loading path: the external action (load) is applied gradually on the structure in a quasistatic way (in the sense that the application is slow enough that the structure has the time to equilibrate) and the resulting path of equilibrium points must be traced [18–20]. Using small load increments the path-following problem is broken down into a sequence of equilibrium subproblems each having a single or restricted number of mechanically acceptable solutions at most. Since many types of mechanical behaviour are history or path dependent the ‘acceptable’ substationarity point is affected by intermediate stages of the mechanical process. Consequently, the existing nonconvex optimization algorithms that locate some local or the global minimum provide only a partial remedy for engineering problems, unless appropriately adapted. In the following we focus our attention to the treatment of a quasistatic subproblem where the load level remains constant and the starting point in the displacement space (initial configuration of the structure) is acceptable but non-equilibrating.

An additional restriction arises from the fact that problems encountered in mechanics usually have a very large dimension, of the order of several thousands of degrees of freedom, which limits significantly the applicability of the available methods and makes necessary the exploitation of all particular characteristics of the problem (e.g. possible partial convexity, sparsity etc.).

Among the methods that have been proposed until now for the treatment of the nonsmooth and nonconvex problems of mechanics, two lines of approach have been proved most fruitful: the quasi-differentiability approximation and the sequential approximation of the hemivariational inequality by variational inequalities. The former resolves in the solution of a sequence of steepest descent finding subproblems using polyhedral approximations of the quasidifferential or codifferential set that contains local gradient information [5, 11, 13]. In the latter approach the solution of the hemivariational inequality (nonconvex problem) is approximated by a sequence of appropriately formulated variational inequalities (nonsmooth convex problems) that are treated by existing efficient convex minimization algorithms [21–26]. The major advantage of the quasi-differentiability approach is the accurate representation of the gradient information that makes it particularly efficient for the treatment of points where nonconvexity and nonsmoothness are combined (crisps). In contrast, the sequential approximation methods are employing rules based on mechanical reasoning for the management of crisps. However, a signif-

icant advantage of the latter is the high convergence rate attained in the parts of the solutions space where the functionals are convex even if they are nonsmooth. This is due to the fact that these methods exploit efficiently the second order information available that is a controlling factor for the majority of the mechanical problems. Indeed the former procedure has proved efficient for the treatment of problems where multiple crisps have to be passed along the loading path while the second in cases where the number of the monotonicity changes in the material laws employed are relatively few (e.g. in the case of zig-zag stress-strain laws) [13, §4]. We note that both procedures can be combined with modern nonlinear finite element methods and are able to treat problems of large dimension arising in structural modelling.

In the present paper we attempt to combine the positive characteristics of the first and second order approximations with the aid of d.c. minimization methods. A method of the sequential approximation type proposed earlier by one of us [22, 24] and based on the multilevel decomposition of the solution space is extended here by the hypodifferential descent method for the treatment of crisps [12, 13] and a d.c. minimization procedure for the treatment of the sections of the domain where some parts of the potential functional are concave [14, 16, 27]. While the original procedure was applicable to problems where the nonconvex energy terms can be decomposed into convex constituents, the method proposed here is able to treat efficiently a more general family of nonconvex functionals, roughly speaking, these that can be decomposed into convex or concave parts, e.g. arising from material laws composed of (vertical or inclined) ascending or descending (softening) branches. More than the significantly wider range of application, a particularly useful characteristic of the method from the engineering point of view is the possibility it offers to attribute mechanical meaning to the approximation steps employed, making thus easier the correlation of the mathematical and mechanical model.

In the following section we discuss the mathematical problem of equilibrium in mechanics for the general case of a nonmonotone and nonsmooth material or interface law. An algorithm is proposed for the treatment of the resulting substationarity problem for a wide class of energy functionals. In Section 3 we focus our attention to the main subproblem of the algorithm, that is reformulated as a d.c. minimization problem and is solved through a branch and bound type of procedure based on simplex subdivision. The solution is approximated by a sequence of convex minimization problems identical to the monotone material problems of mechanics. The final section concludes with a numerical example and a discussion of the properties and the implementation of the method.

2. The Energy Optimization Problem and the Feasible Domain Decomposition

We consider a structure which occupies $\Omega \subset \mathbb{R}^3$ in the initial state (assumed undeformed or equilibrating under the previous load increment). Let $\mathbf{e} = \{e_{ij}\}$, $\mathbf{s} = \{s_{ij}\} \in \mathbb{R}^6$ denote the strain and stress tensors and $\mathbf{u}(\mathbf{x})$, $\mathbf{p}(\mathbf{x}) \in \mathbb{R}^3$, $\mathbf{x} \in \Omega$ the displacements and external loads. For simplicity of the mathematical expressions we consider here only unconstrained structures (i.e. the kinematically admissible displacement set is $U_{ad} = \mathbb{R}^3$). The application range of the developed procedure is not affected since equality and inequality boundary constraints of the same type as the material laws described next can be easily incorporated in the model.

The behaviour of each element of the structure is described by the material law:

$$\mathbf{s} \in \bar{\partial}w(\mathbf{e}) \tag{1}$$

where w is the nonconvex and nonsmooth strain energy density. Here $\bar{\partial}$ denotes the generalized gradient of Clarke which constitutes an extension of the usual differential to nonsmooth and nonconvex functionals [3, 5]. We recall that (1) is by definition equivalent to: $w^0(\mathbf{e}, \mathbf{e}^*) \geq s_{ij}e_{ij} \forall \mathbf{e} \in \mathbb{R}^6$ where $w^0(\cdot, \cdot)$ denotes the directional derivative of Clarke. Under the assumption of small deformations each equilibrium state of the structure fulfills the expression:

$$\int_{\Omega} s_{ij}[e_{ij}(\mathbf{v}) \Leftrightarrow e_{ij}(\mathbf{u})] \, d\Omega = (\mathbf{p}, \mathbf{v} \Leftrightarrow \mathbf{u}) \quad \forall \mathbf{v} \in \mathbb{R}^3. \tag{2}$$

This is the expression of the ‘principle’ of virtual work characterizing the equilibrium position where the bilinear form (\mathbf{p}, \mathbf{v}) expresses the virtual work of the external forces. Using the inequality form of (1) we transform (2) to the following hemivariational inequality [9]:

$$\underline{\mathcal{P}}_v : \quad \text{find } \mathbf{u} \in \mathbb{R}^3 : \int_{\Omega} w^0[\mathbf{e}(\mathbf{u}), \mathbf{e}(\mathbf{v} \Leftrightarrow \mathbf{u})] \, d\Omega \geq (\mathbf{p}, \mathbf{v} \Leftrightarrow \mathbf{u}) \quad \forall \mathbf{v} \in R^3 \tag{3}$$

Next we introduce the ‘potential energy’ functional:

$$\Pi(\mathbf{u}) = W(\mathbf{u}) \Leftrightarrow (\mathbf{p}, \mathbf{u}), \quad W(\mathbf{u}) = \int_{\Omega} w(\mathbf{e}) \, d\Omega. \tag{4}$$

The following substationarity problem is now considered:

$$\underline{\mathcal{P}}_w : \quad \text{find } \mathbf{u} \in \mathbb{R}^3 : \quad \mathbf{0} \in \bar{\partial}\Pi(\mathbf{u}). \tag{5}$$

If Π is convex then $\bar{\partial}\Pi$ coincides with the subdifferential $\partial\Pi$ of convex analysis and $\underline{\mathcal{P}}_w$ becomes a convex minimization problem [3]. If the functional w is locally Lipschitz and satisfies a growth assumption [6, proposition 4.1] and a regularity assumption ($\bar{\partial}$ -regularity) then every solution of the substationarity problem $\underline{\mathcal{P}}_w$ is a solution of the hemivariational inequality $\underline{\mathcal{P}}_v$ and conversely.

As it has been mentioned in the introduction the numerical solution of $\underline{\mathcal{P}}_w$ in the general case is yet an open problem. Thus, in the following we will focus to a class

of nonsmooth and nonconvex functionals which are able to model a wide range of locking, cracking and crushing effects that are encountered in mechanics. We assume that the strain space ($\mathcal{D}(w) = \mathbb{R}^6$) can be partitioned into a finite number of subsets A_1, \dots, A_k having common boundaries such that within each subset $\bar{\partial}w$ is monotone or equivalently w is convex or concave only. We note that a similar but more restricted class of functionals decomposable into convex parts has been employed in [22, 24].

For a given displacement field $\mathbf{u}(\mathbf{x})$ we derive the corresponding strain field $\mathbf{e}(\mathbf{u}(\mathbf{x}))$ and create a complete decomposition of the structure Ω into nonoverlapping subsets $\Omega_1, \dots, \Omega_m$ whose contents have strains belonging to the same strain space partition. Each subset Ω_j is characterized by the index i of the corresponding partition A_i :

$$\mathcal{I}(\Omega_j) = i \quad \Leftrightarrow \quad \Omega_j = \{\mathbf{x} \in \Omega : \mathbf{e}(\mathbf{u}(\mathbf{x})) \in A_i\}. \quad (6)$$

The determination of the properties of the sets A_i, Ω_j is a difficult, still open, mathematical problem of mechanics. We assume that A_i 's are convex closed sets with common boundaries since this condition assures solution uniqueness for the substationarity problem in the simplest convex case. Let each partition be described by set of inequalities: $A_i = \{\mathbf{e} : \mathbf{f}_i(\mathbf{e}) \leq 0\}$ where each \mathbf{f}_i is a set of convex functions. Although the theory does not exclude the possibility of very complicated decomposition topologies for Ω , in most numerical applications a 'certain continuity' of mechanical behavior leads to rather simple topological forms for the decomposition of the structure. We assume here that subsets with common borders correspond to neighboring partitions of the strain space. We denote by $\partial A_i, \partial \Omega_j$ the boundaries of the sets A_i, Ω_j 's. Since these boundaries separate subsets with opposite w 'curvature', they mark the position of nonconvexity 'crisps' in the strain space and within the structure Ω_j .

We consider the case of variation of the displacements only on Ω_j 's such that the decomposition of Ω is kept unchanged or equivalently the position of the subset boundaries $\partial \Omega_j$ is constant. Under this assumption the admissible displacements set of \mathcal{P}_w is restricted to:

$$\tilde{U}_{ad} = \{\mathbf{u} : \mathbf{e}(\mathbf{u}(\mathbf{x})) \in A_{\mathcal{I}(\Omega_j)} \quad \forall \mathbf{x} \in \Omega_j \quad j = 1, \dots, m\}. \quad (7)$$

Using the decomposition of Ω we may write at any step of the calculation the functionals $\tilde{\Pi}, \tilde{W}$ of (4) as:

$$\tilde{\Pi}(\mathbf{u}) = \tilde{W}(\mathbf{u}) \Leftrightarrow (\mathbf{p}, \mathbf{u}) \quad \tilde{W}(\mathbf{u}) = \sum_{j=1}^m \int_{\Omega_j} w(\mathbf{e}) \, d\Omega. \quad (8)$$

By definition w is either convex or concave for $\mathbf{e}(\mathbf{u}) \in A_i$ and consequently if Ω_j remains unchanged for a variation of the displacement field the corresponding term in the sum becomes either convex or concave. Furthermore, for $\mathbf{u} \in \tilde{U}_{ad}$ we

can separate the convex and concave terms of $\tilde{\Pi}$, \tilde{W} and express them as a sum of two parts having opposite ‘curvature’ or equivalently as a difference of convex functions.

Concerning the properties of the constraint set \tilde{U}_{ad} we observe that the strains are affine functions the displacements (small strain theory) and the strain space partitions are convex sets by definition. Consequently the constraints $\mathbf{f}_i(\mathbf{e}(\mathbf{u})) \leq 0$ are convex in the displacement space and their intersection \tilde{U}_{ad} is also a convex set.

The initial substationarity problem \mathcal{P}_w when solved over \tilde{U}_{ad} is reduced to:

$$\underline{\mathcal{P}}_r : \quad \text{find } \mathbf{u} \in \tilde{U}_{ad} : \quad \mathbf{0} \in \partial \tilde{\Pi}(\mathbf{u}). \quad (9)$$

According to the previous observation this is a d.c. minimization problem that can be treated by existing global minimization algorithms.

Obviously, if the assumed decomposition of Ω is correct, at the solution of \mathcal{P}_r the inclusions of (7) are satisfied automatically and all the constraints in the definition of \tilde{U}_{ad} must be inactive or weakly active at most. Conversely, a solution that activates strongly some constraints of (7) signifies that the decomposition of Ω is not accurate. Since the Lagrange multiplier of a constraint in mechanics expresses the corresponding reaction force, the ‘reactions’ of the constraints imposed through \tilde{U}_{ad} can be thought as the part of the load that has not been transferred to the material of the structure but is supported by the artificial internal boundaries $\partial\Omega_j$. Thus the strongly active constraints of \tilde{U}_{ad} offer an indication of the boundaries between the current subsets Ω_j that must be moved and of new subsets that must be added to the decomposition.

Attempting to exploit the particular form of $\tilde{\Pi}$ as a d.c. function we are led to the following iterative algorithm for the treatment of the initial substationarity problem \mathcal{P}_w :

1. Compute an initial decomposition of Ω for \mathbf{u}^0 .
Define \tilde{U}_{ad}^1 for \mathbf{u}^0 according to (7) and set $k = 1$
2. Solve the restricted form \mathcal{P}_r^k of \mathcal{P}_w on \tilde{U}_{ad}^k to derive \mathbf{u}^k .
3. If \mathbf{u}^k in the interior of \tilde{U}_{ad}^k stop.
else: modify the decomposition of Ω , define a new \tilde{U}_{ad}^{k+1}
set $k = k + 1$ and restart from step 2.

While at the end of each iteration the kinematical conditions imposed through \tilde{U}_{ad}^k are satisfied, the static conditions are not (there exist some non zero reactions of the artificial internal boundaries). The static condition violations are reduced at step 3 with each adaptation of the decomposition of Ω or equivalently the movement of the subset boundaries $\partial\Omega_j$.

Since our purpose is not to find the global minimum of Π but the equilibrium configuration that is nearest to the origin, at the beginning we set $\mathbf{u}^0 = \mathbf{0}$, i.e. we consider an initially undeformed structure. In this case definition (7) results in: $\Omega_1 \equiv \Omega$ and $\tilde{U}_{ad}^0 = \{\mathbf{u} : \mathbf{f}_1(\mathbf{e}(\mathbf{u})) \leq 0\}$. Furthermore, the purpose of the

decomposition modifications performed at the step 3 is the determination of the ‘nearest’ minimum in the mechanical sense. The procedure is terminated when the first ‘interior’ minimum is found (with respect to \tilde{U}_{ad}^k).

The modification of the Ω decomposition can be performed in various ways depending on the complexity of the curvature changes in the energy density functional (indicated by the number of the strain space partitions). In simple cases, direct mechanical reasoning may be employed based on the aforementioned interpretation of the Lagrange multipliers of the activated constraints [22, 25]. More complicated functionals can be treated by the the procedure of [24, 26] where the position of each internal boundary is computed by solving a sequence of variational inequality pairs. A mathematically oriented alternative is the derivation of the quasidifferential of the potential for the current point at the displacement space (see the introduction for discussion and references). It is followed by the computation of a descent direction (first order approximation) defining the internal boundary modifications and concludes with a line search along this direction.

The treatment of the large size d.c. minimization problems \mathcal{P}_r arising at step 2 will be discussed in the following section in detail since they are critical for the applicability and the effectiveness of the procedure.

We note that the mechanical model described at the beginning of this section is based on a holonomic assumption, i.e. that the effects of the applied external actions are fully reversible. Although this condition is not satisfied in the general case where the material may undergo permanent damage and the load distributed to some parts of the structure may decrease, it becomes unnecessary if we assume that unloading does not occur in any part of the structure as it happens in many cases. For an alternative model taking into consideration an additional ‘damage’ parameter we refer to [26, §5].

3. Treatment of the D.C. Minimization Subproblem

The major part of the computational effort in the procedure of the previous section is spend at the repeated solution of subproblem \mathcal{P}_r of step 2. Obviously, the efficient treatment of \mathcal{P}_r will decide the applicability of the algorithm. As it has already been noted in the introduction the large size of \mathcal{P}_r is of critical importance, since it restricts significantly the range of the applicable methods and makes necessary the exploitation of all existing sparsity patterns.

First we reformulate \mathcal{P}_r as a d.c. minimization problem and then we adapt a typical algorithm of the branch and bound family for its treatment. The global minimum of $\tilde{\Pi}(\mathbf{u})$ over \tilde{U}_{ad} is determined by a sequence of steps where a linear underestimator of a concave function is minimized over a convex domain. We show that each step of the approximation sequence can be formulated as a minimization of a convex potential energy term over \tilde{U}_{ad} which expresses the kinematical constraints. This last problem can be seen as the equilibrium problem for the ‘resisting’ part of the initial structure subject to some unilateral constraints

and under the action of the initial load combined with an additional load due to the softening of the rest of the structure.

For the sake of clarity, instead of the continuous form of \mathcal{P}_r in this section we discuss its discrete form. We assume that the structure has been discretized by finite elements. In the following vector quantities will be printed boldface. Let $\mathbf{u}, \mathbf{p} \in \mathbb{R}^n$ denote the nodal displacement and force vectors respectively, while $\mathbf{e}_i, \mathbf{s}_i$ are the strain and stress vectors for element i . Here $W_j(\mathbf{u})$ denote the integrals $\int_{\Omega_j} w(\mathbf{e}(\mathbf{u})) \, d\Omega$ where the integrals imply summation over the finite elements composing Ω_j and the integration volumes are kept constant according to the definition of \mathcal{P}_r (7)–(9). The admissible displacement set is defined by sets of convex constraints $\mathbf{g}_j(\mathbf{u}) \leq 0$ corresponding to each subset Ω_j of the structure, derived from $\mathbf{f}_i(\mathbf{e}_i(\mathbf{u})) \leq 0$ for $i = \mathcal{I}(\Omega_j)$ (see discussion following the definition (6)). Then the subproblem \mathcal{P}_r takes the form:

$$\underline{\mathcal{P}}_1 : \min_{\mathbf{u} \in \mathbb{R}^n} \{ \tilde{\Pi}(\mathbf{u}) = \sum_{j=1}^m W_j(\mathbf{u}) \Leftrightarrow \mathbf{p}^T \mathbf{u} : \mathbf{u} \in \tilde{U}_{ad} \} \quad (10)$$

$$\text{where: } \tilde{U}_{ad} = \{ \mathbf{u} \in \mathbb{R}^n : \mathbf{g}_j(\mathbf{u}) \leq 0 \quad j = 1, \dots, m \}. \quad (11)$$

We are reminded that W_j 's are either convex or concave functionals of \mathbf{u} according to the definition of the respective strain space partitions A_j . After a renumbering of W_j 's, the sum in $\tilde{\Pi}$ can be separated into two parts: Φ, Ψ where the convex and concave components are collected:

$$\Phi(\mathbf{u}) = \sum_{j=1}^l W_j(\mathbf{u}) \Leftrightarrow \mathbf{p}^T \mathbf{u} \quad \Psi(\mathbf{u}) = \sum_{j=l+1}^m W_j(\mathbf{u}). \quad (12)$$

Here Φ expresses the potential energy of the ‘resisting’ part of the structure under the action of a load \mathbf{p} , while Ψ is the potential of the elements in the ‘softening’ regime. Finally, \mathcal{P}_1 takes the form:

$$\underline{\mathcal{P}}_2 : \min_{\mathbf{u} \in \mathbb{R}^n} \{ \tilde{\Pi}(\mathbf{u}) = \Phi(\mathbf{u}) + \Psi(\mathbf{u}) : \mathbf{u} \in \tilde{U}_{ad} \} \quad (13)$$

where Φ, Ψ are the convex and concave parts of $\tilde{\Pi}$ and \tilde{U}_{ad} is given by (11). Introducing an independent variable t we rewrite \mathcal{P}_2 as [28]:

$$\underline{\mathcal{P}}_3 : \min_{\tilde{\mathbf{u}} \in D} \{ \Pi'(\tilde{\mathbf{u}}) = t + \Psi(\mathbf{u}) \} \quad (14)$$

$$\text{where: } \tilde{\mathbf{u}} = (\mathbf{u}, t) \in \mathbb{R}^{n+1} \\ D = \{ \tilde{\mathbf{u}} : \mathbf{u} \in \tilde{U}_{ad}, \Phi(\mathbf{u}) \Leftrightarrow t \leq 0 \} \quad (15)$$

where the function to be minimized is concave while the feasible domain D remains convex due to the convexity of \tilde{U}_{ad} and Φ .

For the treatment of \mathcal{P}_3 we adapt an algorithm of the branch and bound type proposed by R. Horst [28, 29], [16, §6.2]. We define initially a simplex $S_1 \in \mathbb{R}^{n+1}$

containing the solution set and subsequently we partition it into subsimplices S_n . Over each simplex we derive the (linear) convex envelope $L(\tilde{\mathbf{u}})$ of $\Pi'(\tilde{\mathbf{u}})$ which is then minimized over $S_n \cap D$, thus providing a nondecreasing sequence of lower bounds for the global minimum of Π' .

The starting simplex $S_1 = [\nu^0, \nu^1, \dots, \nu^{n+1}]$ is constructed such that it is the smallest one containing the solution set. Its edges $(\nu^0, \nu^1), \dots, (\nu^0, \nu^{n+1})$ parallel the coordinate axes. We observe that Π' is a linearly increasing function of t and that Ψ depends on \mathbf{u} only. Consequently, for a particular \mathbf{u} , Π' takes a minimum value at $\Phi(\mathbf{u}) = t$ and the solution set of \mathcal{P}_3 may be reduced to $D' = \{\tilde{\mathbf{u}} : \mathbf{u} \in \tilde{U}_{ad}, \Phi(\mathbf{u}) = t\}$ instead of D .

In the case of a general admissible displacement set \tilde{U}_{ad} we define the coordinates for the origin ν^0 of the starting simplex as the solutions of $n + 1$ linear programs over a convex set:

$$\nu_j^0 = \arg \min_{\tilde{\mathbf{u}} \in D} \tilde{u}_j \quad j = 1, \dots, n + 1. \tag{16}$$

If \tilde{U}_{ad} has a special structure, exploitation of its particular characteristics may offer a direct way for deriving the extrema, avoiding the solution of linear subproblems (e.g. \tilde{U}_{ad} polyhedral or defined as the intersection of strips lying between parallel hyperplanes, as in the case of a rectangular decomposition of the strain space).

The remaining vertices are chosen as the intersection of rays emanating from ν_0 parallel to the coordinate axes with a hyperplane: $\sum_{i=1}^{n+1} (\tilde{u}_i \Leftrightarrow \nu_i^o) = c$, where c is computed from:

$$\begin{aligned} c + \sum_{i=1}^{n+1} \nu_i^o &= \arg \max_{\tilde{\mathbf{u}} \in D'} \sum_{i=1}^{n+1} \tilde{u}_i = \arg \max_{\substack{\mathbf{u} \in \tilde{U}_{ad} \\ \Phi(\mathbf{u})=t}} \left\{ \sum_{i=1}^n u_i + t \right\} \\ &= \arg \max_{\mathbf{u} \in \tilde{U}_{ad}} \left\{ \sum_{i=1}^n u_i + \Phi(\mathbf{u}) \right\}. \end{aligned} \tag{17}$$

Problem (17) is a convex maximization problem and only an overestimator of its solution is needed. An appropriate overestimator is the maximum of the same function over a simplex containing \tilde{U}_{ad} which in turn is smaller than the maximum of a linear function with the same values at the vertices of the simplex. Thus (17) is reduced to the solution of a linear program [16, §1.5]. An appropriate simplex in \mathbb{R}^n can be constructed by the same technique as before by employing the first n solutions of (16) for the location of the origin μ^0 and setting the remaining vertices to: $\mu^i = \mu^0 + c' \mathbf{e}^i \quad i = 1, \dots, n$ where: $c' = \max_{\mathbf{u} \in \tilde{U}_{ad}} \sum_{j=1}^n u_j$ and \mathbf{e}^i is the i th unit coordinate vector.

After deriving c , the vertices of S_1 are computed by:

$$\nu^i = \nu^0 + c \mathbf{e}^i \quad i = 1, \dots, n + 1. \tag{18}$$

For S_1 thus defined, ν^{n+1} (corresponding to the t direction) is the only feasible vertex with respect to the constraint $\Phi(\mathbf{u}) \Leftrightarrow t \leq 0$, while ν^0, \dots, ν^n and the whole facet of S_1 defined by them are infeasible. We note that this method for constructing S_1 requires the solution of $n + 3$ linear programs of dimension n or $n + 1$ over \tilde{U}_{ad} or D respectively. Linear problems of this type constitute the main subproblem of the iterative procedure used for the solution of \mathcal{P}_3 and their numerical treatment will be discussed after the outline of the main minimization algorithm.

Considering that the solution of \mathcal{P}_3 lies on the boundary D' of D , in the following we adapt the simplex subdivision method such that the search in the $n + 1$ 'st direction of the $\tilde{\mathbf{u}}$ -space is avoided ($u_{n+1} \equiv t$). Let $S = [\nu^0, \dots, \nu^{n+1}]$ be a simplex and $T = [\nu^0, \dots, \nu^n]$ one facet of it. Initially we find the longest edge of T that is an edge of S also. Subsequently we construct two subsimplices S', S'' of S by replacing the vertices of S defining this edge by its midpoint. In this partitioning of S all subsimplices have a common vertex ν^{n+1} .

The convex envelope of the concave function Π' of \mathcal{P}_3 over a simplex S is a linear function $L(\tilde{\mathbf{u}})$ which agrees with Π' at all vertices of S . Let $S_1, S_2, \dots, S_\kappa$ be sequence of simplices where each element is derived by subdividing its predecessor as above and let $L_1, L_2, \dots, L_\kappa$ be the corresponding convex envelopes. It is not difficult to extend Theorem 6.2.2 of [16] to show that for such a sequence exists an 'accumulation' line (ν_{n+1}, ν) with $\nu \in T$ satisfying: $\lim_{\kappa \rightarrow \infty} S_\kappa = \bigcap_{k=1}^\infty S_k = (\nu_{n+1}, \nu)$. Furthermore, the sequence of convex envelopes is nondecreasing: $L_{\kappa-1}(\tilde{\mathbf{u}}) \leq L_\kappa(\tilde{\mathbf{u}}) \leq \Pi'(\tilde{\mathbf{u}}) \quad \forall \tilde{\mathbf{u}} \in S_\kappa$ for $\kappa = 1, 2, \dots$.

The current definition of the starting simplex and the modification of the subdivision method of [16, §6.2] introduced here, do not alter the structure of the original algorithm for the treatment of the concave minimization problem \mathcal{P}_3 . For completeness, we outline next the main steps of the procedure (J^k denotes the set of the indices of the candidate simplices at each iteration k):

1. Set $k = 1, J^k = \{1\}$ and construct S_1
2. For all $i \in J^k$ solve the linear program:

$$\underline{\mathcal{P}}_4 : \quad \tilde{\mathbf{u}}_i = \arg \min_{\mathbf{u} \in D \cap S_i} \{L_i(\tilde{\mathbf{u}})\} \tag{19}$$

and find $j = \arg \min_{i \in J^k} L_i(\tilde{\mathbf{u}}_i)$

3. If $|\Pi'(\tilde{\mathbf{u}}_j) \Leftrightarrow L_j(\tilde{\mathbf{u}}_j)| \leq \epsilon$ stop, $\tilde{\mathbf{u}}_j$ solves problems \mathcal{P}_1 - \mathcal{P}_3 .

else: partition S_j into subsimplices $S_{j'}, S_{j''}$, set $J^{k+1} = J^k \cup \{j', j''\} \Leftrightarrow \{j\}$, $k = k + 1$ and restart from step 2.

We note that for each iteration only the pair of subproblems \mathcal{P}_4 defined on the new simplices have to be solved since the minima on the remaining simplices with indices in J^k have been derived in previous iterations.

We discuss next the numerical treatment of the main subproblem \mathcal{P}_4 . We are reminded that linear problems with a feasible set of a similar structure arose also during the construction of the starting simplex. \mathcal{P}_4 is a linear minimization problem with objective function $L(\tilde{\mathbf{u}}) = \tilde{\mathbf{b}}^T \tilde{\mathbf{u}} + d = \mathbf{b}^T \mathbf{u} + b^t t + d$ subject to the following

sets of convex constraints:

$$\begin{aligned} \mathcal{C}_1 : \quad & \tilde{\mathbf{u}} \equiv (\mathbf{u}, t) \in S \\ \mathcal{C}_2 : \quad & \mathbf{u} \in \tilde{U}_{ad} \stackrel{(11)}{\Leftrightarrow} \mathbf{g}_j(\mathbf{u}) \leq 0 \quad j = 1, \dots, m \\ \mathcal{C}_3 : \quad & \Phi(\mathbf{u}) \Leftrightarrow t \leq 0 \end{aligned}$$

The characteristics of each group are quite different and call for a particular treatment. The simplex constraint \mathcal{C}_1 can be expressed as a system of linear inequalities, while the admissible displacement constraints \mathcal{C}_2 give rise to a system of convex but possibly nonsmooth inequalities. Since only the strain of a single element is involved in each inequality of the latter group ($\mathbf{g}_j(\mathbf{e}_j(\mathbf{u})) \leq 0$) and the element strain is expressed as a function of a few nodal displacements only (these of the nodes connected with this element), each inequality involves a small number of displacement variables. Furthermore, as it was noted earlier, there exist cases where these inequalities may have the form of simple bounds on element strains and result in a polyhedral \tilde{U}_{ad} . In contrast, the last constraint \mathcal{C}_3 involves the strains of numerous elements ($1, \dots, l$) or equivalently a large part of the displacement variables, thus resulting in a quite complex expression. The availability of curvature information for \mathcal{C}_2 and particularly for \mathcal{C}_3 may also be exploited for the acceleration of the solution procedure. We note that the expression of the constraints in separable form, even if not impossible, is not considered a practical option.

We assume that an iterative minimization algorithm will be used, leading to a sequence of points approximating the minimum of \mathcal{P}_4 . At each iteration a descent direction is first defined and then a line minimization is performed along it. Here we focus our attention in the derivation of the search direction at a feasible point since it will determine largely the efficiency of the overall procedure. Because the common vertex ν^{n+1} of all subsimplices is feasible, we examine initially if it constitutes a solution of \mathcal{P}_4 , a fact that can be tested directly. If this is not the case and since no other vertex of S may be a solution (due to infeasibility with respect to \mathcal{C}_3) at least one of the last two sets of constraints must be active at the solution. We examine now the most complicated case, i.e. the case of \mathcal{C}_3 being active together with \mathcal{C}_1 and \mathcal{C}_2 . The following discussion applies also to the simpler case where \mathcal{C}_1 and \mathcal{C}_2 are active, but not \mathcal{C}_3 .

Facets of S active at the solution (\mathcal{C}_1) may be used to reduce the dimension of \mathcal{P}_4 directly by variable elimination or be employed as linear inequality constraints. Assuming either that a variable elimination has been performed or that the current approximation in an iterative solution procedure belongs to the interior of S , problem \mathcal{P}_4 will have the general form: $\arg \min_{\tilde{\mathbf{u}} \in D} L(\tilde{\mathbf{u}})$. Considering that \mathcal{C}_3 is active, we reformulate \mathcal{P}_4 using the equality form $\Phi(\mathbf{u}) = t$ of \mathcal{C}_3 :

$$\min_{\tilde{\mathbf{u}} \in \tilde{U}_{ad}} \{\mathbf{b}^T \mathbf{u} + b' \Phi(\mathbf{u}) + d\} \Leftrightarrow \min_{\tilde{\mathbf{u}} \in \tilde{U}_{ad}} \{\Phi(\mathbf{u}) \Leftrightarrow \mathbf{q}^T \mathbf{u}\} \quad \text{where } \mathbf{q} = \Leftrightarrow \mathbf{b}/b' \quad (20)$$

Using the definition (12) of $\Phi(\mathbf{u})$, we rewrite (20) as:

$$\underline{\mathcal{P}}_5 : \min_{\mathbf{u} \in \tilde{U}_{ad}} \left\{ \sum_{j=1}^l W_j(\mathbf{u}) \Leftrightarrow (\mathbf{p} + \mathbf{q})^T \mathbf{u} \right\}. \tag{21}$$

From the engineering viewpoint \mathcal{P}_5 expresses the equilibrium of a structure consisting of the resisting elements of the initial structure with indices $1, \dots, l$ (cf. the definition (12)) subject to a set of unilateral constraints (i.e. the assumed positions of the internal boundaries $\partial\Omega_j$). On this structure act the initial external loads augmented by ‘load’ vector \mathbf{q} induced by the softening part of the structure (elements with indices $l + 1, \dots, m$) [26, discussion of §5].

Large nonsmooth minimization problems with the same sparsity pattern and dimension of the same order as \mathcal{P}_5 , have been studied extensively in recent years because they constitute the typical form of the equilibrium problem arising when monotone (maybe nonsmooth) material or interface laws are employed. For their treatment efficient algorithms have already been developed exploiting their particular sparsity pattern and the availability of second order information for the potentials and the constraints involved. Methods of the nonsmooth quadratic approximation family (*NSQP*) have been proved to be robust and effective for this kind of problems, due to their global convergence and the superlinear convergence rate [9, 22, 30].

Summarizing the present section we see that the discrete form \mathcal{P}_1 of \mathcal{P}_r was first transformed into a d.c. minimization problem \mathcal{P}_3 that is then solved by an algorithm of the branch and bound type. Each iteration of this procedure requires the solution of a linear minimization problem \mathcal{P}_4 that is approximated by a sequence of convex minimization problems \mathcal{P}_5 whose efficient treatment is made possible, despite the large size, by the special structure of the potential and the constraints.

4. Discussion and Numerical Application

The method described in the previous sections has been applied to an illustrative example. We consider a metallic rod embedded in an elastic material, glued to it by a resinous adhesive having a smooth softening response (Figure 1a). An increasing tensile force is applied to the free end of the rod until it is extracted from the surrounding mass. A similar example was examined in [24, §4] and it used for comparison.

The materials of both the cylinder and the surrounding mass are assumed linearly elastic and simple quadrilateral constant stress elements are employed for modeling both bodies. In [24] the softening behavior of the binding material in the tangential direction was described by the sawtooth nonmonotone laws (graphs **a**, **b** of Figure 1b) while here the adhesive material is modelled by the continuously softening law (graph **c** of Figure 1b).

For the application of the proposed method the strain space for the interface elements is divided into three partitions: ($e \leq 2.5 \cdot 10^{-3}$), ($2.5 \cdot 10^{-3} \leq e \leq$

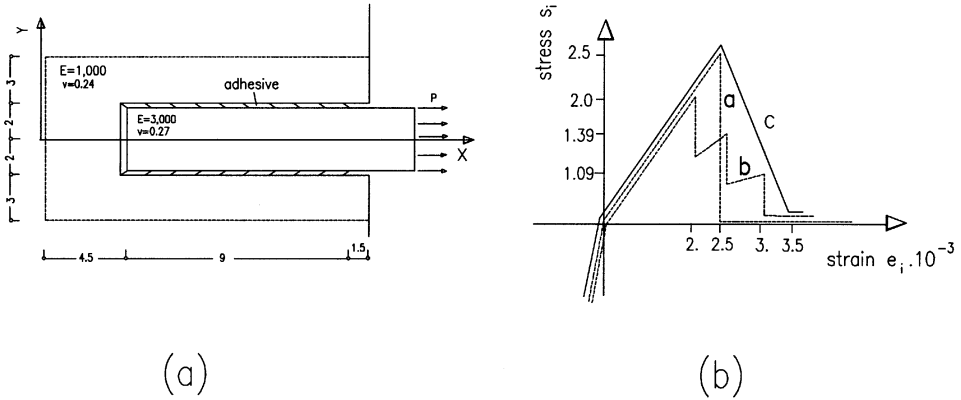


Fig. 1. **a.** Embedded rod under tensile load. **b.** Nonmonotone interface law (a, b: sawtooth laws, c: smooth softening law.)

$3.5 \cdot 10^{-3}$), ($3.5 \cdot 10^{-3} \leq e$). We note that the softening behavior of the structure as a whole made necessary the introduction of some kind of direct displacement control through a bound on the displacements of the free end. The load-displacement graphs obtained with the present method up to the complete release of the rod compare quite well with the results given in the reference, when the different deformation energy capacity of the stress-strain graphs is taken into account.

Concerning the requirements of computational resources for the implementation of the proposed method, we note that if an *NSQP* type of approach is used for the solution of the convex minimization subproblems \mathcal{P}_5 , then the computational memory needed increases linearly only with the size of the problem (a property that is critical for large scale problems of mechanics).

In Figure 2 we have depicted the computation time required by the present method (as implemented on an HP750 workstation) for the solution of the equilibrium problem for different extraction lengths (line c). The extraction length offers a indication of the complexity of the problem since the number of the interface elements operating in the softening regime increases with it. In the same figure are shown the computation times given in the reference for the treatment of the sawtooth interface laws. Observing that the computation time increases significantly with the number of decreasing vertical branches of the stress-strain graph we see that the present method is better suited for the treatment of nonmonotone material laws where the gradual loss of strength prevails while the distinct vertical branches are few. We note that the trials performed until now indicate that the computational effort tends to increase linearly with the complexity of the problem (number of nonmonotone elements, complexity of the laws used etc.).

In Figure 2 is also shown the time spent by the procedure in the solution of quadratic programming (QP) problems required for the treatment of \mathcal{P}_5 . From this graph it becomes evident that the solution of the QP problems is taking up a major

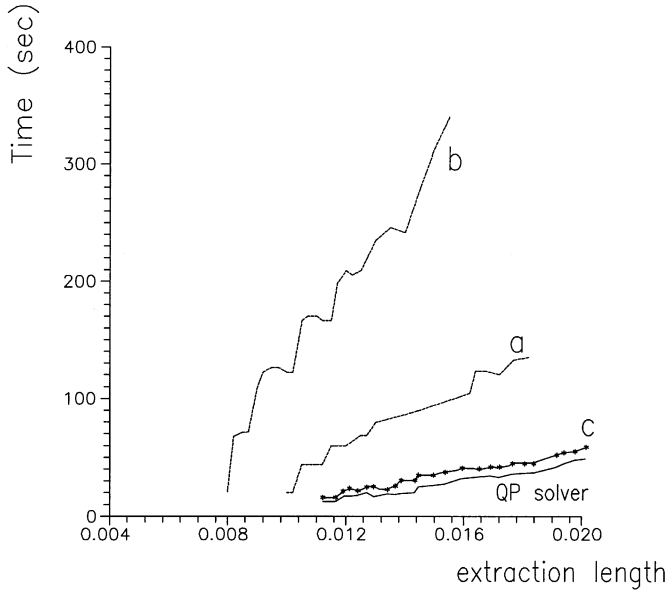


Fig. 2. Total computation time (c), time spend by the QP solver and computation times from reference [24] (a,b).

part of the total computation time. Considering that a general purpose sparse QP solver has been employed in our implementation, we expect significant time savings from its replacement by a solver that exploits the band structure of the curvature matrices involved in the computation. We note that for a particular application the computation time can be further reduced if some specific characteristics of the problem are used for simplification of the intermediate approximation steps [22, §4,5].

5. Conclusions

A numerical method for the treatment of a family of hemivariational inequalities has been presented. The method uses a multilevel decomposition of the solution space and the appropriate structure decomposition to solve the hemivariational inequality through a sequence of d.c. minimization problems. The latter resolve into a sequence of convex minimization problems of large dimension which can be solved by existing efficient algorithms. Since the requirements for the multilevel decomposition are minimal, this approach can be applied to a wide range of hemivariational inequalities. Moreover, the structure decomposition can be easily automated.

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