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On the Numerical Treatment of Nonconvex Energy Problems of Mechanics

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Abstract. The present paper presents three numerical methods devised for the solution of hemivariational inequality problems. The theory of hemivariational inequalities appeared as a development of variational inequalities, namely an extension foregoing the assumption of convexity that is essentially connected to the latter. The methods that follow partly constitute extensions of methods applied for the numerical solution of variational inequalities. All three of them actually use the solution of a central convex subproblem as their kernel. The use of well established techniques for the solution of the convex subproblems makes up an effective, reliable and versatile family of numerical algorithms for large scale problems. The first one is based on the decomposition of the contigent cone of the (super)-potential of the problem into convex components. The second one uses an iterative scheme in order to approximate the hemivariational inequality problem with a sequence of variational inequality problems. The third one is based on the fact that nonconvexity in mechanics is closely related to irreversible effects that affect the Hessian matrix of the respective (super)-potential. All three methods are applied to solve the same problem and the obtained results are compared.

Key words: hemivariational inequalities, nonconvex superpotentials, convex minimization

1 Introduction

The present paper intents to present three numerical methods for the treatment of non-convex, non-smooth minimization problems arising in structural and continuum solid mechanics.

The usual problem in structural analysis consists in finding an equilibrium point in the space of primary variables (displacement field) under a given value of the dual variable (field of forces) and boundary conditions.

Along the process of imposing a field of displacements, the mechanical system undergoes mechanical distortions (strains), resists by developing local counteractive forces at an infinitesimal level (stresses) and absorbs the work supplied by the loading field : this process can be described by means of a potential functional.

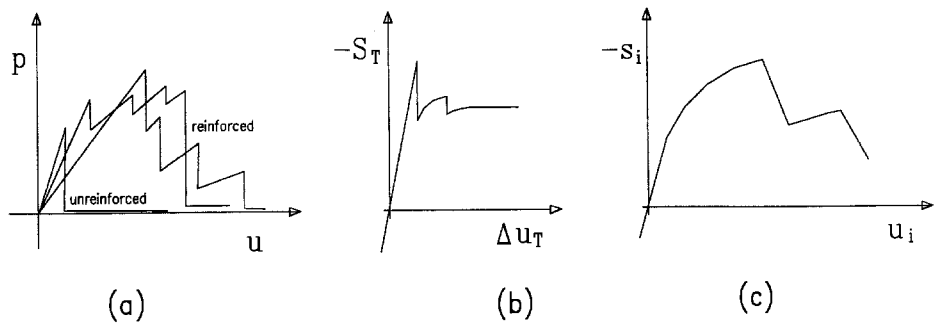


Fig. 1. Examples of nonmonotone laws : (a) Slow pull-off test of composite laminate, (b) Real and Coulomb friction, (c) Reinforced concrete in tension.

Finding the equilibrium of a structural system is equivalent to finding the minimum of the potential functional expressing the total work of the system, i.e. that absorbed by the structure minus that supplied by the loading field.

When the mechanical system remains in the normal operational framework, i.e. the loads are not severe enough to cause structural damage and no other complex physical mechanisms (material behaviour, unilateral contact etc) contribute to the energy balance of our system, the potential functional is quadratic and the respective unconstraint quadratic minimization problem constitutes a simple, everyday practice problem for the engineering community.

It is noteworthy that the geometric form and properties of the epigraph set of the potential functional is directly associated to types of mechanical behaviour.

Foregoing the quadratic form of the epigraph of the potential functional necessitates the use of Newton-Raphson type non-linear solution strategies.

An excellent account of the structure of the formulation of the equilibrium problem in mechanics suitable for a reader rather mathematically than mechanically oriented, can be found in the book by G.Strang [1].

However there is often the case that the classical methods of linear or linearized analysis encounter forbidding difficulties both in the formulation and in the numerical approximation of problems involving nonmonotone, possibly multivalued stress - strain or reaction - displacement laws [2, 3, 4, 5, 6, 7, 8, 9, 10]. (cf. Fig.1).

This can be due to the fact that either the stress-strain laws in the interior of the elastic body or the respective non-linear boundary condition is multivalued, i.e. complete vertical branches may be present in the one-dimensional case. Then, the respective energy functionals (superpotentials) involved are nonconvex and nonsmooth.

The variational forms for such problems are termed hemivariational inequalities [5, 6, 8, 9, 11] The respective nonconvex energy functions, are called nonconvex superpotentials in accordance to the case of monotone mechanical behaviour

described by convex superpotentials, where variational inequalities are obtained [12, 13, 6].

The theory of variational (resp. hemivariational) inequalities is closely related to the notion of convex superpotentials (resp. of nonconvex superpotentials) introduced into Mechanics by J. J. Moreau [14, 15] (resp. P. D. Panagiotopoulos [5, 6, 16]) for monotone (resp. for nonmonotone) possibly multivalued boundary conditions and constitutive laws.

The lack of convexity of the energy functions necessitates that the mathematical study regarding the existence of solution for the so-called hemivariational inequalities be exclusively based on weak compactness arguments [6, 9]; this makes things a bit more difficult than the case of variational inequalities where monotonicity and respectively arguments can be applied [12, 6].

If some additional, mild, growth assumptions for the nonsmooth superpotentials involved are imposed [14, p.167], then, nonsmooth, nonconvex potential or complementary energy functions can be obtained. The substationarity points hence obtained (all the local minima, certain local maxima or saddle points) supply all the possible solutions of a hemivariational inequality.

This is a generalization of the minimum potential or complementary energy theorems which hold in the case of variational equalities and inequalities [12, 6]. In the absence of the mentioned growth conditions the hemivariational inequality may have solutions, i.e. points of equilibrium, that are not substationarity points.

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 only a particular case of the general substationarity problem [17, 18, 19, 20].

In addition, the problems encountered in mechanics usually have a very large dimension, of the order several thousands of degrees of freedom. Moreover, all the stable and unstable solutions on the loading path are sought as the global minimizer is affected by intermediate stages of the mechanical process (many types of mechanical behaviour are history or path dependent due to the irreversibility involved). Consequently, the existing nonconvex optimization algorithms can provide only a partial remedy for engineering problems.

Although the progress in the theoretical study of the existence and approximation questions for hemivariational inequalities is considerable (cf. [9, 16, 21, 22, 23, 24, 25] and the references given therein), relatively few methods exist for the numerical treatment. The following lines of approach have appeared in the literature :

1. Iterative processes with a convex analysis origin :

   - Penalization by means additional terms in the energy functional [26],
   - Bundle - type methods of Nonsmooth Optimization [20],

- Regularization techniques resulting in a sequence of variational equalities [21].

These methods can find only very limited use in practical applications, due to the fact that they fail too rapidly with increasing problem size (order of one hundred of unknowns), due mainly to stability problems.

2. Special methods dealing only with special classes of nonconvex problems [16] :

   a) nonlinear solver with step - length control to remain stable around limit points [27, 28, 29, 30],

   b) nonconvex problem substitution by appropriate combination of convex problems by means of quasidifferentiability [31],

   c) local approximation of the hemivariational inequality by appropriately chosen sequence of convex problems [32, 33].

All the methods of the second group lead to sequences of subproblems amenable by means of existing optimization algorithms. The verified reliability and high convergence rates of the latter make a precious advantage. An additional advantage is that their combination with the methods developed in nonlinear finite element analysis, with efficient iterative minimization procedures and specialized preconditioning schemes may lead to the construction of algorithms that are able to operate on large scale systems (order of thousands of unknowns) for any kind of nonmonotonicity. Note that the last three methods are especially efficient in the case of nonconvex energy functions resulting from zig - zag (i.e. multivalued) stress-strain and reaction displacement laws.

In the present paper we describe three methods that reduce a hemivariational inequality (nonmonotone problem) into a number of variational inequalities (monotone problems). The first one decomposes the hemivariational inequality into a number of variational inequalities by replacing partially the nonconvex superpotential by convex cones (see for preliminary information Fig. 3). Then the problem is formulated as a finite set of variational inequalities or convex optimization problems on differing domains of the displacements space. Subsequently each variational inequality can be treated effectively by specialized convex minimization algorithms (based on Nonsmooth Sequential Quadratic Programming in most cases [17, 33, 34]). The robustness of this method constitutes its major advantage. An additional acceleration of the procedure may be achieved, if some simplifying assumptions on the form of the nonmonotone laws involved are made.

The second method which will be studied here replaces the hemivariational inequality problem with a sequence of variational inequality problems. This is achieved using an iterative procedure which approximates in every step the nonmonotone force-displacement diagram corresponding to the nonconvex energy function by a monotone diagram. Based on the solution of this monotone problem a

new convex energy problem is formulated until convergence is achieved. Each variational inequality problem that arises is then treated with a convex minimization algorithm. This way we extend the advantages of the robust algorithms employed in convex minimization, in the area of nonconvex minimization.

The third method makes use of the irreversibility of mechanical degradation and attempts to formulate a condition for global optimality based on certain rather strict assumptions on the part of the potential that is responsible for the lack of convexity (dissipation potential).

2 The mathematical problem

In this section we outline the mathematical formulation of a general hemivariational inequality that governs a large class of nonconvex energy problems of Mechanics. In the following vector quantities will be printed boldface to distinguish from scalars.

We consider a structure which occupies a subset Ω of $\mathbb{R}^3$ in its undeformed state and let Γ be the total boundary of the structure which consists of the nonoverlapping parts Γ_f, Γ_u and Γ_c. On Γ_f (resp. Γ_u) the forces (resp. displacements) are prescribed and on Γ_c nonmonotone possibly multivalued laws hold between the normal (resp. tangential) tractions $\mathbf{S}_N$ (resp. $\mathbf{S}_T$) and the boundary normal (resp. tangential) displacements $\mathbf{u}_N$ (resp. $\mathbf{u}_T$) which can be expressed through the nonconvex superpotential relations :

$$-\mathbf{S}_N \in \bar{\partial} j_N(\mathbf{u}_N) \quad , \quad -\mathbf{S}_T \in \bar{\partial} j_T(\mathbf{u}_T) \tag{1}$$

Here $\bar{\partial}$ denotes the generalized gradient of Clarke [6, 8, 35]. This symbol constitutes an extension of the usual differential to nonsmooth and nonconvex functionals while j_N, j_T are nonconvex, generally nonsmooth energy functions (Fig. 1). We assume also that the behaviour of Ω is governed by an analogous nonconvex energy law :

$$\sigma \in \bar{\partial} w(\epsilon) \tag{2}$$

where $\sigma = \{\sigma_{ij}\}, \epsilon = \{\epsilon_{ij}\}$ are the stress and strain tensors and w is the nonconvex strain energy density. We recall that (2) - analogous holds also for (1) is by definition equivalent to : $w^0(\epsilon, \epsilon^*) \geq \sigma_{ij}\epsilon_{ij} \ \forall \ \epsilon \in \mathbb{R}^6$ where $w^0(.,.)$ denotes the directional derivative of Clarke. Under the assumption of the small deformations each equilibrium state of the structure fulfills the expression :

$$\int_\Omega \sigma_{ij}(\epsilon_{ij}(\mathbf{v}) - \epsilon_{ij}(\mathbf{u}))d\Omega = \int_{\Gamma_c} [\mathbf{S}_N(\mathbf{v}_N - \mathbf{u}_N)d\Gamma + \mathbf{S}_T(\mathbf{v}_T - \mathbf{u}_T)d\Gamma] + (\mathbf{l}, \mathbf{v} - \mathbf{u}) \quad \forall \mathbf{v} \in U_{ad} \tag{3}$$

This is the expression of the "principle" of virtual work characterizing each equilibrium position. There the bilinear form $(\mathbf{l}, \mathbf{v})$ expresses the virtual work of the

external forces $\mathbf{l}(\mathbf{x}) \in \mathbb{R}^3$ and $U_{ad} = \{\mathbf{u} : u_i = U_i(\mathbf{x}) \ , \ \mathbf{x} \in \Gamma_u\}$ is the kinematically admissible displacement set. Using the inequality form of (1,2) we transform (4) to the following problem :

Problem $\mathcal{P}_v$: Find $\mathbf{u} \in U_{ad}$ satisfying the inequality :

$$\int_\Omega w^0[\epsilon(\mathbf{u}), \epsilon(\mathbf{v}-\mathbf{u})]\, d\Omega \ + \ \int_{\Gamma_c} j_N^0[\mathbf{u}_N(\mathbf{u}), \mathbf{u}_N(\mathbf{v}) - \epsilon_N(\mathbf{u})]\, d\Gamma \ +$$

$$\int_{\Gamma_c} j_T^0[\mathbf{u}_T(\mathbf{u}), \mathbf{u}_T(\mathbf{v}) - \mathbf{u}_T(\mathbf{u})]\, d\Gamma \ \geq \ (\mathbf{l}, \mathbf{v}-\mathbf{u}) \quad \forall \mathbf{v} \in U_{ad} \tag{4}$$

Expression (4) is a hemivariational inequality due to the appearance of the energy variation terms $\int_\Omega w^0[\ldots]\, d\Omega$, $\int_{\Gamma_c} j_N^0[\ldots]\, d\Gamma$ and $\int_{\Gamma_c} j_T^0[\ldots]\, d\Gamma$ [11, 16].

Next we introduce the 'potential energy' functional :

$$\Pi(\mathbf{u}) = W(\mathbf{u}) + J(\mathbf{u}) - (\mathbf{l}, \mathbf{u}) \tag{5}$$

where :

$$W(\mathbf{u}) = \int_\Omega w(\mathbf{e})\, d\Omega \quad J(\mathbf{u}) = \int_{\Gamma_c} j_N(\mathbf{u}_N)\, d\Gamma + \int_{\Gamma_c} j_T(\mathbf{u}_T)\, d\Gamma \tag{6}$$

The following 'substationarity' [36] problem is now considered :

Problem $\mathcal{P}_w$: Find $\mathbf{u} \in U_{ad}$ such that :

$$\mathbf{0} \in \bar{\partial}\Pi(\mathbf{u}). \tag{7}$$

If Π is convex then $\bar{\partial}\Pi$ coincides with the subdifferential $\partial\Pi$ of convex analysis and $\mathcal{P}_w$ becomes a convex minimization problem [6].

If the functionals w, j_N and j_T are locally Lipschitz and satisfy a growth assumption [9, proposition 4.1] and a regularity assumption ($\bar{\partial}$-regularity) then every solution of the substationarity problem $\mathcal{P}_w$ is a solution of the hemivariational inequality $\mathcal{P}_v$ and conversely. One can verify that for the unidimensional laws of Fig. 1 both the growth and the $\bar{\partial}$-regularity assumptions hold.

We note that if instead of (1,2) the boundary forces (resp. stress) are expressed as generalized gradients of the displacements (resp. strain) then a hemivariational inequality similar to (4) will be derived (in terms of stress variations) and we are led to a substationarity problem for a complementary energy functional analogous to $\mathcal{P}_w$.

3 Convex decomposition based on the contingent cone

In this section we will discuss a wide subclass of nonsmooth and nonconvex functionals which are encountered in many engineering applications especially related to the laws depicted in Fig.1 : we assume that for w in relation (2) a set of auxiliary nonsmooth convex functionals $w_i, i \in L(w) = \{1, 2, \ldots, l\}$ exists such that for

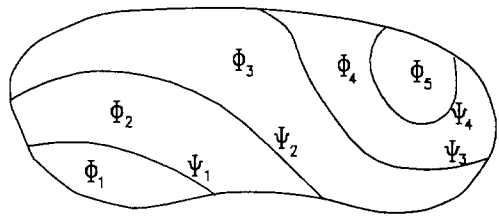


Fig. 2. Decomposition of Ω in sections with common indices.

every admissible displacement $\mathbf{u}$ at all points $\mathbf{x} \in \Omega$ the value of w equals to the value of one or more w_i's and an 'active function' index set can be defined :

$$\alpha(w(\mathbf{u},\mathbf{x})) = \{i \in L(w) : w_i(\mathbf{u},\mathbf{x}) = w(\mathbf{u},\mathbf{x})\} \tag{8}$$

Since the following discussion can be easily extended to functionals j_N, j_T also, for the sake of clarity in the following we will assume that j_N, j_T in $\mathcal{P}_v$ and $\mathcal{P}_w$ are zero.

For a given displacement field $\mathbf{u}$ the indices $\alpha[w(\mathbf{u},\mathbf{x})]$ create a partitioning of Ω in $m \geq l$ subsets Ω_i with common indices :

$$\Omega = \bigcup_{i=1}^{m} \Omega_i \quad \Omega_j = \{\mathbf{x} | \mathbf{x} \in \Omega, \quad j \in \alpha[w(\mathbf{u},\mathbf{x})]\} \quad j = 1,\ldots,m \tag{9}$$

We denote by $\Phi_i, i = 1,\ldots,m$ the corresponding open sets and by Ψ_ρ, $\rho = 1,\ldots,\mu$ the boundaries between the Φ_i's, $i = 1,\ldots,m$ (see Fig. 2) : $\Psi_i = \Omega_i \cap \Omega_{i+1}$ and $\Phi_i = \Omega_i - \Psi_{i-1} - \Psi_i$. If we assume that Φ_i is the interior of a partition with 'borders' Ψ_i and Ψ_{i+1} then $\Phi_i \cap \Phi_j = \Psi_i \cap \Psi_j = \Phi_i \cap \Psi_j = \emptyset \quad i \neq j \quad i,j = 1,\ldots,m$. For all points in Φ_i i is the only active index while in the common boundary Ψ_ρ between Φ_i and Φ_{i+1} both i and $i+1$ are active. The determination of the properties of the sets Φ_i and Ψ_ρ is a difficult, still open, mathematical problem for the general case of 3D -nonmonotone possibly multivalued relations. Although the theory does not exclude the possibility of very complicated partitioning topologies, in most numerical applications a 'certain continuity' of mechanical behaviour leads to rather simple topological forms for the partitioning of Ω.

Using this decomposition of Ω we write the functional W in (6) as :

$$\tilde{W}(\mathbf{u}) = \sum_{i=1}^{m} \int_{\Phi_i} w_i(\mathbf{e}(\mathbf{u}))d\Omega + \sum_{\rho=1}^{\mu} \int_{\Psi_\rho} w|_{\Psi_\rho}(\mathbf{e}(\mathbf{u}))d\Psi \tag{10}$$

where $w|_{\Psi_\rho} = w_i|_{\Psi_\rho}$ or $w|_{\Psi_\rho} = w_{i+1}|_{\Psi_\rho}$. We assume that all the integrals in (10) make sense. Next we introduce the superpotential $\tilde{\Pi}$ that is derived by replacing

W in (5) by $\tilde{W}$. Although the equivalence :

$$\mathbf{0} \in \bar{\partial}\tilde{\Pi}(\mathbf{u}) \quad \Leftrightarrow \quad \mathbf{0} \in \bar{\partial}\Pi(\mathbf{u}) \tag{11}$$

is obvious, the generalized gradient $\bar{\partial}\tilde{\Pi}$ is easier to compute than $\bar{\partial}\Pi$. Similarly it is easier to compute feasible descent directions for $\tilde{\Pi}$ than for Π. Thus, in the following instead of Π we will use the "decomposed" form $\tilde{\Pi}$ and will adapt accordingly problem $\mathcal{P}_v$ by means of an iterative scheme. Let us assume that after the k-th iteration a solution $\mathbf{u}^k$ is known and we want to determine $\mathbf{u}^{k+1}$. $\mathbf{u}^k$ is used to derive the active index sets (8) that lead to a decomposition Ω_i^k, Ψ_ρ^k. For the $k+1$ iteration we consider the hemivariational inequality :

Find $\mathbf{u}^{k+1} \in \tilde{U}_{ad}$ satisfying the inequality :

$$\sum_{j=1}^{m} \int_{\Omega_j^k + \Delta_j} w_j^0(\mathbf{e}(\mathbf{u}^{k+1}), \mathbf{e}(\mathbf{v} - \mathbf{u}^{k+1}))d\Omega \geq (\mathbf{l}, \mathbf{v} - \mathbf{u}^{k+1}) \quad \forall \mathbf{v} \in \tilde{U}_{ad} \tag{12}$$

Here $\Delta_1, \Delta_2, \ldots$ must be determined and

$$\tilde{U}_{ad} = \{\mathbf{u} | \mathbf{u} = \{\mathbf{u}_i\}, \mathbf{u} \in U_{ad} \quad \mathbf{u}|_{\Omega_j^{k+1}}(\mathbf{x}) = \mathbf{u}|_{\Omega_{j+1}^{k+1}}(\mathbf{x}) \text{ for } \mathbf{x} \in \Psi_\rho^{k+1},\ \rho = 1, \ldots, \mu\} \tag{13}$$

Ψ_ρ^{k+1} is the common boundary of $\Omega_j^{k+1} = \Omega_j^k + \Delta_j$ and $\Omega_{j+1}^{k+1} = \Omega_{j+1}^k + \Delta_{j+1}$. Setting in (12) $\mathbf{v} = \mathbf{u}^{k+1}$ on Ω_j^{k+1} $j = 1, \ldots, i-1, i+1, \ldots, m$ we obtain, due to the convexity of w_i, the variational inequality :

Find $\mathbf{u}^{k+1} \in \tilde{U}_{ad}$ such as :

$$\int_{\Omega_i^k + \Delta_i} \left[w_i(\mathbf{e}(\mathbf{v})) - w_i(\mathbf{e}(\mathbf{u}^{k+1}))\right] d\Omega_i \geq (\mathbf{l}, \mathbf{v} - \mathbf{u}^{k+1})|_{\Omega_i^k + \Delta_i} \quad \forall \mathbf{v} \in \tilde{U}_{ad} \tag{14}$$

for $i = 1, 2, \ldots, m$. The corresponding minimum problems for the subsets Ω_j^{k+1} and Ω_{j+1}^{k+1} with common boundary Ψ_ρ^{k+1} together with the kinematical compatibility condition on Ψ_ρ^{k+1} read :

Find $\mathbf{u}_j^{k+1}, \mathbf{u}_{j+1}^{k+1} \in \tilde{U}_{ad}$ such as :

$$\Pi_j(\mathbf{u}_j^{k+1}) = \min\Big\{ \int_{\Omega_j^k + \Delta_j} w_j(\mathbf{e}(\mathbf{v}))d\Omega_j - (\mathbf{l}, \mathbf{v})\,|_{\Omega_j^k} \Big| \mathbf{v} \in \tilde{U}_{ad}\Big\} \tag{15}$$

$$\Pi_{j+1}(\mathbf{u}_{j+1}^{k+1}) = \min\Big\{ \int_{\Omega_{j+1}^k + \Delta_{j+1}} w_{j+1}(\mathbf{e}(\mathbf{v}))d\Omega_{j+1} - (\mathbf{l}, \mathbf{v})\,|_{\Omega_{j+1}^k} \Big| \mathbf{v} \in \tilde{U}_{ad}\Big\} \tag{16}$$

$$\text{subject to :} \quad \mathbf{u}_{j+1}^{k+1}(\mathbf{x}) = \mathbf{u}_j^{k+1}(\mathbf{x}) \quad \text{on} \quad \Psi_\rho^{(\delta+1)} \tag{17}$$

Now we consider the following problem :

Find $\mathbf{u}_j^{k+1}$ and $\mathbf{u}_{j+1}^{k+1}$ as a solution of :

$$\min\{\Pi_j(\mathbf{u}_j^{k+1})+\Pi_{j+1}(\mathbf{u}_{j+1}^{k+1})-\int\limits_{\Psi_\rho^{k+1}}\lambda_\rho(\mathbf{u}_{j+1}^{k+1}(\mathbf{x})-\mathbf{u}_j^{k+1}(\mathbf{x}))d\Psi_\rho\,|\,\mathbf{u}_j^{k+1},\mathbf{u}_{j+1}^{k+1}\in\tilde{U}_{ad}\} \tag{18}$$

For the solution of (18) we follow according to [16] a modification of the 'nonfeasible gradient controller' method of Lasdon and Schoeffler [37], [6, p.356]). Suppose that λ_ρ has a given value, say $\lambda_{\rho,\nu}$ for $\nu=1,2,\ldots$ and that Ψ_ρ^{k+1} (or equivalently Δ_j or Δ_{j+1}) have a given geometry say $\Psi_{\rho,\nu}^k$. The first level problems have he form :

$$\min\{\Pi_j(\mathbf{u}_{j,\nu}^{k+1})+\int\limits_{\Psi_{\rho,\nu}^k}\lambda_{\rho,\nu}\mathbf{u}_{j,\nu}^{k+1}d\Psi_\rho\;\Big|\;\mathbf{u}_{j,\nu}^{k+1}\in U_{ad}\} \tag{19}$$

$$\min\{\Pi_{j+1}(\mathbf{u}_{j+1,\nu}^{k+1})-\int\limits_{\Psi_{\rho,\nu}^k}\lambda_{\rho,\nu}\mathbf{u}_{j+1,\nu}^{k+1}d\Psi_\rho\;\Big|\;\mathbf{u}_{j+1,\nu}^{k+1}\in U_{ad}\} \tag{20}$$

while the corresponding second level corrections for the Lagrange multipliers and the free boundary geometry read :

$$\lambda_{\rho,\nu+1}=\lambda_{\rho,\nu}+\kappa(\mathbf{u}_{j+1,\nu}^{k+1}-\mathbf{u}_{j,\nu}^{k+1})\quad\Psi_{\rho,\nu+1}^k=\Psi_{\rho,\nu}^k+\bar{\kappa}(\mathbf{u}_{j+1,\nu}^{k+1}-\mathbf{u}_{j,\nu}^{k+1})\quad\kappa,\bar{\kappa}>0 \tag{21}$$

where $\kappa,\bar{\kappa}$ are appropriately chosen constants [37]. First (19),(20) are solved, then $\lambda_{\rho,\nu}$ (resp. $\Psi_{\rho,\nu}^k$) is corrected through (21), the new value $\lambda_{\rho,\nu+1}$ (resp. the new geometry of the interface $\Psi_{\rho,\nu+1}^k$) is passed to (19),(20) and so on until the differences $|\mathbf{u}_{j,\nu+1}^{k+1}-\mathbf{u}_{j,\nu}^{k+1}|$, $|\lambda_{\rho,\nu+1}-\lambda_{\rho,\nu}|$ become appropriately small for every $\mathbf{x}$ within Ω. This procedure is continued until $|\mathbf{u}_j^k-\mathbf{u}_j^{(k-1)}|$ becomes appropriately small and the sets $\Omega_i^k\ i=1,\ldots,m$ do not vary considerably from step to step. We note that at the points belonging to the borders Ψ_ρ the compatibility condition (17) must be satisfied. The values of the corresponding Lagrange multipliers provide the constraint forces.

The method outlined here includes two interrelated iterations: the first with respect to the decomposition of the energy functions and the second with respect to a partitioning of the structure Ω into parts corresponding to common indices. To explain this by means of a simple example let us consider Fig. 3.a-c. The energy function (3.a) is decomposed into two convex parts w_1 and w_2. The first (resp. the second) part introduces the inequality $e\le e_0$ (resp. $e\ge e_0$). We denote the set of points of Ω, where the first (resp. the second) inequality if fulfilled by Ω_1 (resp. by Ω_2). The idea of the proposed algorithm is the following : iterations with respect to the problems $0\in\partial w_1(u), 0\in\partial w_2(u)$ ($\partial\equiv\bar{\partial}$ due to the convexity) and also with respect to the partitioning of Ω into Ω_1 and Ω_2 (i.e. by changing the position

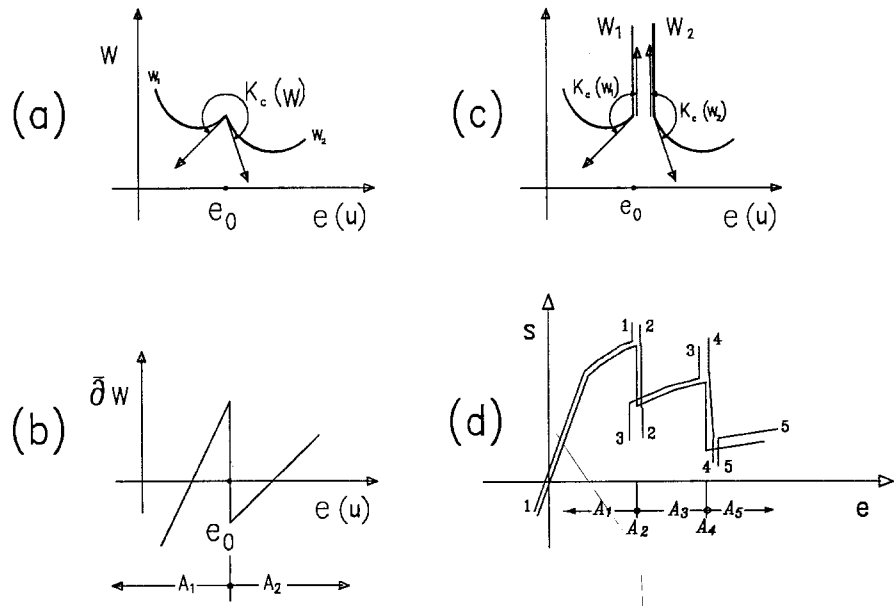


Fig. 3. (a-b) nonsmooth potential with nonmonotone generalized gradient, (c) Convex decomposition using indicator functions. (d) A nonmonotone - nonsmooth law and its 'complete' decomposition using monotone graphs.

of the boundary between Ω_1 and Ω_2 we try to find a better local minimum) lead to the solution set.

The decomposition of the nonconvex functionals w, j_N, j_T in the manner described at the beginning of this section is not uniquely defined because the epigraph of any given functional may be divided in convex parts in many different ways. The number of the auxiliary convex functionals employed must be minimized in order to keep the partitioning of Ω as simple as possible. In [33] a decomposition scheme has been proposed based on the analysis of the contingent cone of the functionals into convex parts. We note that the contingent cone $K_c(w)$ of a functional w provides a measure of its nonsmoothness and nonconvexity [35]. An important practical advantage of this approach is that it can easily be automated, a fact that greatly facilitates programming.

In many problems of Mechanics the position of the nonconvexity kinks in the displacement space is predefined by affine relations of the form : $f(\mathbf{e}) = 0$ (eg. in Fig. 3.b by : $e(u) - e_0 = 0$). We use these hypersurfaces to divide the domain of w into sections $A_i, i = 1, \ldots, l$. Each section is bounded by a set of inequalities of the form : $f(\mathbf{e}) \geq 0$. Since each A_i is a convex cone, w is also convex within it. A family of auxiliary convex functions can now be produced by adding an indicator

function to w (Fig. 3.c) :

$$w_i(\mathbf{e}) = w(\mathbf{e}) + I_i(\mathbf{e}) \quad I_i(\mathbf{e}) = \begin{cases} 0 & \text{for } \mathbf{e} \in A_i \\ \infty & \text{for } \mathbf{e} \notin A_i \end{cases} \quad i = 1, \ldots, l \tag{22}$$

This decomposition is able to provide a single active function index at either side of a kink and pairs of active indices along it, as required by (8). Since $w_j(\mathbf{e}) \geq w_k(\mathbf{e}) \quad \forall \mathbf{e} \notin A_k$ the auxiliary potentials w_i are related to w by : $w(\mathbf{e}) = \min_l\{w_1(\mathbf{e}), \ldots, w_l(\mathbf{e})\}$.

The mechanical meaning of the contingent cone decomposition approach and the usefulness of the auxiliary functionals w_i can be demonstrated easily in terms of stress - strain (or displacement - reaction) graphs. Roughly speaking, the contingent cone decomposition described corresponds to the analysis of the nonmonotone stress - strain curves (e.g. of Fig. 1) into monotone parts.

The decomposition method described here has already been applied as an independent procedure to the study of delamination of laminated composites in [38] with satisfactory results. Both algorithms outlined there are special cases of the approximation scheme described in this section for the discretized form of the problem.

4 The approximation of the nonconvex superpotential by a sequence of convex superpotentials

In this section we will describe the second method for the solution of the hemivariational inequality problem $\mathcal{P}_v$. As it was mentioned in Section 2, the problem is nonconvex possibly nonsmooth, due to the appearance of the nondifferentiable terms $\int_\Omega w^0[\ldots]\, d\Omega$, $\int_{\Gamma_c} j_N^0[\ldots]\, d\Gamma$ and $\int_{\Gamma_c} j_T^0[\ldots]\, d\Gamma$. We shall propose a method consisting in the approximation of the solution of the hemivariational inequality by the solutions of certain appropriately defined variational inequalities. Let us consider instead of the nonconvex energy terms w, j_N, j_T the convex energy terms w', j'_N, j'_T. Then instead of (4) the following variational inequality problem arises: Problem $\mathcal{P}'_v$: Find $\mathbf{u} \in U_{ad}$ such that

$$\int_\Omega [w'(\epsilon(\mathbf{v})) - w'(\epsilon(\mathbf{u}))] d\Omega + \int_{\Gamma_c} [j'_N(\mathbf{u}_N(\mathbf{v})) - j'_N(\mathbf{u}_N(\mathbf{u}))] d\Gamma_i + \int_{\Gamma_c} [j'_T(\mathbf{u}_T(\mathbf{v})) - j'_T(\mathbf{u}_T(\mathbf{u}))] d\Gamma_i \geq (\mathbf{l}, \mathbf{v} - \mathbf{u}) \ \forall \mathbf{v} \in U_{ad}. \tag{23}$$

This problem is convex and can be solved using convex minimization algorithms. Let us write now problem $\mathcal{P}_v$ in (4) in the form: Find $\mathbf{u} \in U_{ad}$ such that

$$\int_\Omega [w'(\epsilon(\mathbf{v})) - w'(\epsilon(\mathbf{u}))] d\Omega + \int_{\Gamma_c} [j'_N(\mathbf{u}_N(\mathbf{v})) - j'_N(\mathbf{u}_N(\mathbf{u}))] d\Gamma + \int_{\Gamma_c} [j'_T(\mathbf{u}_T(\mathbf{v})) - j'_T(\mathbf{u}_T(\mathbf{u}))] d\Gamma \geq (\mathbf{l}, \mathbf{v} - \mathbf{u}) + R(\mathbf{v}, \mathbf{u}) \ \forall \mathbf{v} \in U_{ad} \tag{24}$$

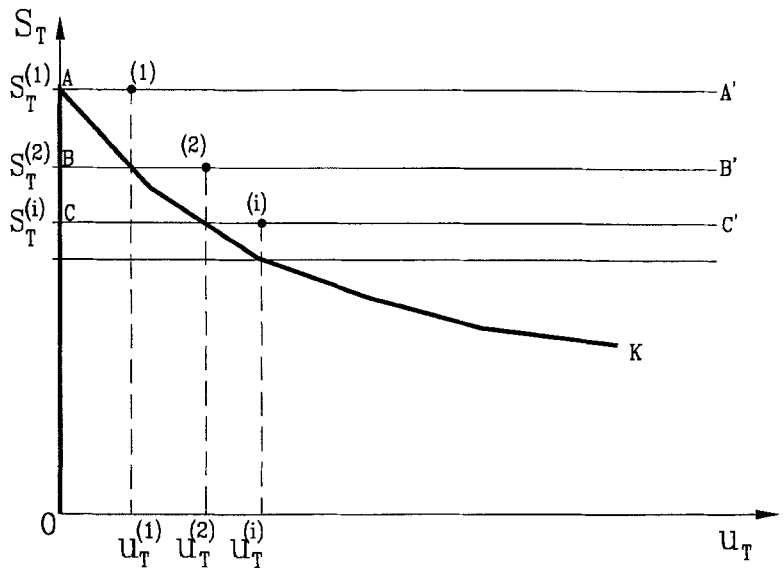


Fig. 4. Parametric partial decomposition of a nonmomonotone law.

where

$$R(\mathbf{v},\mathbf{u}) = \int_\Omega [w'(\epsilon(\mathbf{v})) - w'(\epsilon(\mathbf{u}))]d\Omega + \int_{\Gamma_c} [j'_N(\mathbf{u}_N(\mathbf{v})) - j'_N(\mathbf{u}_N(\mathbf{u}))]d\Gamma +$$
$$\int_{\Gamma_c} [j'_T(\mathbf{u}_T(\mathbf{v})) - j'_T(\mathbf{u}_T(\mathbf{u}))]d\Gamma - \int_\Omega w^0[\epsilon(\mathbf{u}), \epsilon(\mathbf{v}-\mathbf{u})]\, d\Omega -$$
$$\int_{\Gamma_c} j^0_N[\epsilon_N(\mathbf{u}), \mathbf{u}_N(\mathbf{v}) - \mathbf{u}_N(\mathbf{u})]\, d\Gamma - \int_{\Gamma_c} j^0_T[\mathbf{u}_T(\mathbf{u}), \mathbf{u}_T(\mathbf{v}) - \mathbf{u}_T(\mathbf{u})]\, d\Gamma] \quad (25)$$

Using the previous formulation we propose the following iterative scheme for the solution of the hemivariational inequality problem.

Find $\mathbf{u}^{(k)} \in U_{ad}$ such that

$$\int_\Omega [w'(\epsilon(\mathbf{v})) - w'(\epsilon(\mathbf{u}^{(k)}))]d\Omega + \int_{\Gamma_c} [j'_N(\mathbf{u}_N(\mathbf{v})) - j'_N(\mathbf{u}_N(\mathbf{u}^{(k)}))]d\Gamma +$$
$$\int_{\Gamma_c} [j'_T(\mathbf{u}_T(\mathbf{v})) - j'_T(\mathbf{u}_T(\mathbf{u}^{(k)}))]d\Gamma_i \geq (\mathbf{l}, \mathbf{v} - \mathbf{u}^{(k)}) + R(\mathbf{v}, \mathbf{u}^{(k-1)})\ \forall \mathbf{v} \in U_{ad}. \quad (26)$$

This heuristic iterative scheme can be justified by means of Fig. 4. Starting the iterations we assume that instead of the nonmonotone law OAK, the simple monotone law OAA′ holds. Then the structure has a unique solution as it is well known from the solution of the variational inequality of the monotone friction

problem with given normal reaction. Let us denote this solution by $u_T^{(1)}$. Obviously this is not a solution of the hemivariational inequality problem because the solution does not lie on the nonmonotone law (point (1)). In the next step we try to find a better estimation of the solution by solving a new monotone problem but with the assumption that the simple monotone law OBB′ holds. This new problem gives as a solution $u_T^{(2)}$. Then a new variational inequality problem arises assuming that the law OCC′ holds and so on until the solution $u_T^{(i-1)}$ coincides with the solution $u_T^{(i)}$. We must note at this point that the nonlinear term R of (25) represents from the mechanical point of view the difference of the area variations under the two graphs – the nonmonotone one and the monotone one – i.e. it measures the differences of the reaction forces corresponding to the two laws.

Based on the above simplified concept, a large class of algorithms can be formulated in order to treat the particularities of each problem. For example it is possible to formulate algorithms in order to treat the unilateral contact problem with nonmonotone friction or the debonding problem and so on. The complexity of the algorithms increases together with the number of the introduced nonlinearities. For a complete description of the developed algorithms and their applications the reader is referred to [39].

In general, using the iterative scheme (26), the following basic algorithm can be formulated.

1. Select the appropriate convex functionals w', j'_N, j'_T to approximate locally the given nonconvex problem. Select initial values for $\mathbf{u}$.
2. Set k=1
3. Solve the arising convex problem (26). This gives as a solution $\mathbf{u}^{(k)}$.
4. If the solution $\mathbf{u}^{(k)}$ equals to the solution $\mathbf{u}^{(k-1)}$ within some predefined accuracy, terminate the algorithm.
5. Update the convex functionals with the new values for $\mathbf{u}$, set $k = k + 1$ and go to step 3.

The convex superpotentials w', j'_N, j'_T that approximate the nonconvex superpotentials can be selected in such a way that the computational effort will be minimum. But this task depends on the particular nonmonotone functions to be approximated. For this reason we prefer to approximate the nonconvex functions with simple convex ones. This task is much easier to be programmed and it can be done in a quite general way to include any kind of nonmonotone functions.

All the algorithms yielded from the basic algorithm presented here, proved to be very efficient. Indeed, the fact that at every step we solve a convex minimization problem gives us the ability to treat large scale problems taking advantage of the robustness, the speed and the high convergence rate of the convex minimization algorithms.

5 An approach based on the irreversibility of softening

In this section we shall present a numerical method, mainly developed by the first author, that uses the fact of the irreversibility of softening as a basis for some numerical methods. It is quite straightforward even to those lacking an engineering background, that structural damage is irreversible i.e. no healing of cracked parts of an elastic body might spontaneously happen. Softening behaviour may be an abstract way of describing what is called "structural degradation" or "damage" i.e. phenomena that happen in the microscale of the structure. Nevertheless the essential trait of irreversibility of degradation is retained. Our main problem is still the computation of one (or possibly a set of) solutions for the inclusion (7). It may be noted that Π does not only depend on $\mathbf{u}$ but on the load $\mathbf{p}$ as well, acting as a parameter.

Let us consider the discrete case and assume the superpotential Π to be Lipschitz continuous. Following a known methodology of convex analysis, (see [40, 41]) we express the non-convex, non-smooth potential Π of the energy absorbed by the mechanical system, as the difference of two convex potentials Ψ and Φ :

$$\Pi(\mathbf{u}) = \Psi(\mathbf{u}) - \Phi(\mathbf{u}) \quad , \quad \mathbf{u} = \{u_1, ..., u_n\} \quad . \tag{27}$$

Here one can see that, as both Ψ and Φ are convex, the second function acts in a way that causes energy to be taken out of the elastic system. What happens to the part of energy dissipated in this way needs not concern us; in general it is converted to heat, acoustic emission and is lost in the environment without (in the context, of course, of the present paper) causing any further, i.e. thermal or other, effects to the mechanical system. Taking note of the previous remark about irreversibility, one can deduce that there has to exist at least one more parameter in this function.

$$\Phi = \Phi(\mathbf{u}, \lambda) \quad , \quad \lambda = \{\lambda_1, ..., \lambda_m\} \tag{28}$$

where m is the number of degrees of freedom where a softening mechanical law is assumed to exist. We will further refer to Ψ as the free energy potential and to Φ as the irreversible dissipation potential.
An important trait of Φ, is that

$$|\Phi(\mathbf{u}_1) - \Phi(\mathbf{u}_2)| = 0 \quad \text{for} \quad \mathbf{u}_1 \, , \, \mathbf{u}_2 \in \mathcal{I} = \{\mathbf{u} \, / \, \mathcal{F}(u_i) < \mathcal{F}(\lambda_j) \, j \in \alpha_i\} \tag{29}$$

α being an appropriate index set. The meaning of this, is that we assert that $|\Phi|$ always remains constant inside a region $\mathcal{I}$, wherein a certain measure of the displacements $\|\mathbf{u}\|_{\mathcal{F}(u,\lambda)}$ remains negative; $|\Phi|$ strictly increases outside $\mathcal{I}$.
A natural and simple choice for λ is to consider the maximum value of the primary variable (displacement) a certain point has undergone :

$$\lambda_i = \max_{\mu}(u_i^{(\mu)}) \, , \, u_i^{(\mu)} = u_i(\mathbf{p}^{(\mu)}) \tag{30}$$

where $\mathbf{p}^{(\mu)}$ are loading states that out mechanical system was forced to undergo. Other choices for λ are associated to various mechanical theories (see e.g. [42]). For the present form, one can have in mind the *simple fracturing solid* of Dugill introduced as a displacement relation in the boundary of the mechanical system. The definition of (30), brings forth the difference in nature of the sense of a "load" in the case of the presence of an irreversible dissipation potential. In the classical sense a "load" is a point in the dual space of the primary variable (i.e. the displacement u) and usually appears in the right hand side of the equilibrium equations constituting the sole cause for any effects on our system.

In the case of presence of irreversible dissipation, all points of the set

$$\mathcal{P} = \{(p_1^{min}, p_1^{max}) \times ... \times (p_n^{min}, p_n^{max})\} \tag{31}$$

have to be considered, as all of them represent possible actions excercized on our mechanical system at an *arbitrary sequence.* By specifying just a load vector $\mathbf{p}$, an engineer makes the tacit assumption that all p_i^{min} are null.
Looking a bit further into the nature of the parameter λ, we can see that the greater λ is, the less costy it is, in energy terms, to bring the mechanical system to the same status of displacement $\bar{\mathbf{u}}$:
Let $\lambda^{(1)}$ be equal to $\lambda^{(2)}$ except for a certain, say the l-th component : $\lambda_l^{(2)} > \lambda_l^{(1)}$. Then, as $\Pi(\lambda^{(1)}) > \Pi(\lambda^{(2)})$, we have that

$$|\Phi(\lambda^{(1)})| < |\Phi(\lambda^{(2)})| \quad \text{for} \quad \lambda^{(1)} < \lambda^{(2)} \quad . \tag{32}$$

It is therefore clear that, in view of (27), it is possible, in the context of an iterative procedure, to write a reaction - displacement relation of the form $s_i \in \bar{\partial}\pi(u_j), j \in \alpha_i$ where α_i is an index set (like e.g. in (2), in the new form

$$S_i^{(j)} = S(u_j, \lambda_i^{(j)}) \quad \text{where} \quad \lambda_i^{(j)} = \max_{k=1,...,j} \lambda_i^{(k)} \, , \, j \in \alpha_i \tag{33}$$

i.e. $\lambda_i^{(j)}$ is our j-th estimate for the ultimate value of λ_i.
Denoting by $\mathbf{K}$ and $\mathbf{\Lambda}$ the Hessians of Ψ and Φ, we can therefore propose a basic iterative scheme that is made up of the following steps :

Iterative scheme 1

1. set initial values : $\lambda^{(0)}$, $\mathbf{\Lambda}^{(0)} = \mathbf{\Lambda}(\lambda^{(0)})$; set iteration counter $i = 0$
2. $i = i + 1$; compute $\mathbf{u}^{(i)} = \arg\{\mathbf{K} - \mathbf{\Lambda}^{(i-1)}\}\mathbf{u} = \mathbf{p}$
3. update $\lambda^{(i-1)}$'s according to relation (30)

4. *if* $\exists\, k \,/\, \lambda_k^{(i-1)} < \lambda_k^{(i)}$, update $\mathbf{\Lambda}^{(i-1)}$ and goto *step 2*;
   else postprocess and stop

Note that *step 2* is presented as linear. Should this not be the case, it is straightforward that we would have to iterate over $\mathbf{K}(\mathbf{u})$ keeping $\mathbf{\Lambda}^{(i-1)}$ constant.
Having computed a solution of our system does not indeed settles things: to put the problem in mechanical terms, one has to eliminate the possibility that alleviation of an action p_j on the system might cause an increase on the measure of Φ according to (32). In fact, we set forth the following

Criterion 1 For a solution obtained by *iterative scheme 1* to be immune to any future load paths (trajectories of the load point inside the set $\mathcal{P}$, the relation

$$\partial\lambda_i/\partial p_j \;<\; 0 \tag{34}$$

must hold for all load components and all softening parameters λ.
The necessity therefore arises for us to compute a set $\mathcal{U}$ in the space of λ so that

$$\mathcal{U} \;=\; \{(\bar{\lambda}_1^{inf}, \bar{\lambda}_1^{sup}) \times \ldots \times (\bar{\lambda}_m^{inf}, \bar{\lambda}_m^{sup}) \,/\, \bar{\lambda}_i^{sup} = \max_{p\in\mathcal{P}} u_i(\mathbf{p})\,,\; \bar{\lambda}_i^{inf} = \min_{p\in\mathcal{P}} u_i(\mathbf{p})\} \tag{35}$$

i.e. the Cartesian product of the intervals between the maximum and the minimum values any component of λ is ever going to assume. The idea behind $\mathcal{U}$ is that although it is not possible to reach some of its point with one element of $\mathcal{P}$, it may be possible to reach it with a certain succession of applications of loads (in terms of mechanics a "load path"). This is a consequence of the irreversibility of structural degradation each single application of a load may cause.

Given the *iterative scheme 1* the computation of the set $\mathcal{U}$ is, although tedious, rather straightforward.

Iterative scheme 2

1. $i = 0$; run *scheme 1* and compute $\bar{\lambda}^{(0)}$;

2. $i = i + 1$;
   using the current estimate of $\lambda^{(i-1)}$ form $\mathbf{M}^{(i)} = \mathbf{K} - \mathbf{\Lambda}^{(i-1)}$ and compute the inverse $\mathbf{M}^{-1} = \mathbf{N}$

3. For $j = 1, \ldots, m$ do :
   compute the max and the min values $\mathbf{p}$ may cause to u_j:
   $u_j = N_{jk}p_k = (N_{jk}p_k)_{pos} + (N_{jk}p_k)_{neg}$ i.e. $u_j^{(+)} = (N_{jk}p_k)_{pos}$, $u_j^{(-)} = (N_{jk}p_k)_{neg}$ so that we can have $\bar{\lambda}_j^{inf,(i)} = \min(\bar{\lambda}_j^{inf,(i-1)}, u_j^{(-)})$ and $\bar{\lambda}_j^{sup,(i)} = \max(\bar{\lambda}_j^{sup,(i-1)}, u_j^{(+)})$

4. *if* $|\lambda_j^{(i)}| - |\lambda_j^{(i-1)}| > \epsilon$ goto 2
   else stop

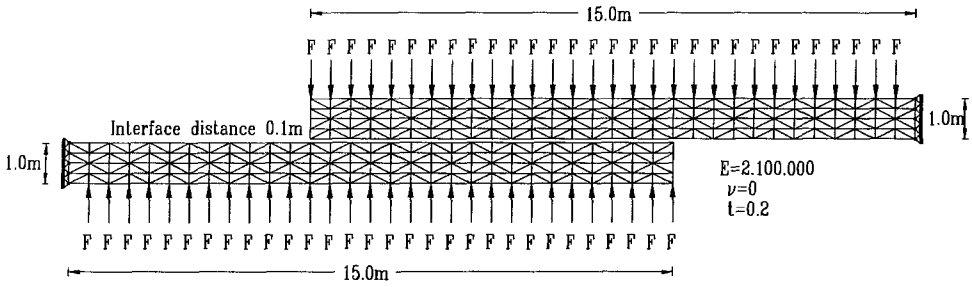


Fig. 5. Finite element discretization of the structure.

This scheme along with (35) can supply an estimate for the set $\mathcal{U}$ therefore allowing for a "worst case" computation of our mechanical system based on the simple idea of the irreversibility of structural degradation.

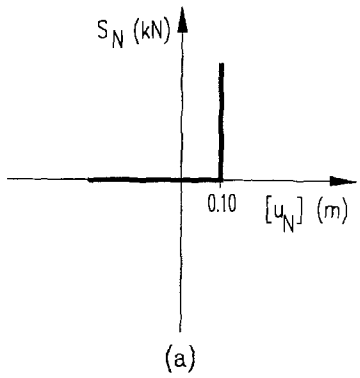
6 Discussion and numerical example

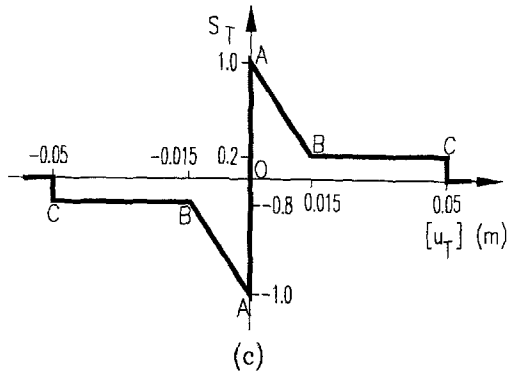
The methods described in the previous Sections have been applied to the analysis of a simple structure. A linearity assumption is made for the material and a two-dimensional constant stress model was employed instead of a more realistic nonlinear material law and a three-dimensional representation, with the purpose of pronouncing the effects of interface's nonmonotone behaviour.

The simple structure of Fig. 5 is examined. The structure data are shown in the figure. On the interface unilateral contact conditions are assumed for the normal to the interface direction(Fig. 6a) . For the tangential direction, the nonmonotone law of Fig. 6b is assumed to hold. The various load cases for which the structure was analysed are given in Fig. 6c.

The results obtained by the three methods differ slightly. The main reason of these differences is that the three algorithms use different finite element schemes to solve the problem. The first and the third use the displacement's method whereas the second uses a combination of the displacement's and of the force method. Another factor affecting the results is the kind of the finite elements which are used for the solution of the problem. The first method uses quadrilateral elements to discretize the structure, whereas the second and the third use triangular elements. Taking the above into account, the results of the three methods are found to be in good accordance. Indeed, the differences between the results given by the three methods at every calculated point, are less than 2 percent. For this reason, here we present only the results obtained by the second method.

Fig. 7a (resp. Fig. 7b) gives the distribution of the contact (resp. the frictional) forces along the interface. We observe that the values of the contact forces increase linearly with respect to the loading (the curves (a) ... (h) are almost parallel).





Load case	F (kN)
(a)	100.0
(b)	110.0
(c)	120.0
(d)	130.0
(e)	140.0
(f)	150.0
(g)	160.0
(h)	170.0

(c)

Fig. 6. The adopted interface laws and the analysed load cases.

This is not the case with the frictional forces where the effect of the nonlinearity introduced by the nonmonotone diagram of Fig. 6b is obvious.

In curves (a) and (b) and for some nodes (3,17), the solution lies on branch OA of the nonmonotone diagram. This is easily verified from Fig. 8 that gives the values of the relative tangential displacements along the interface. The increase of the load (load case (c)) has as a result the realization of the softening part of the diagram in all the nodes of the interface and a sudden reduction of the values of the frictional forces. Further increase of the load (load cases (d) ... (g)) has as a

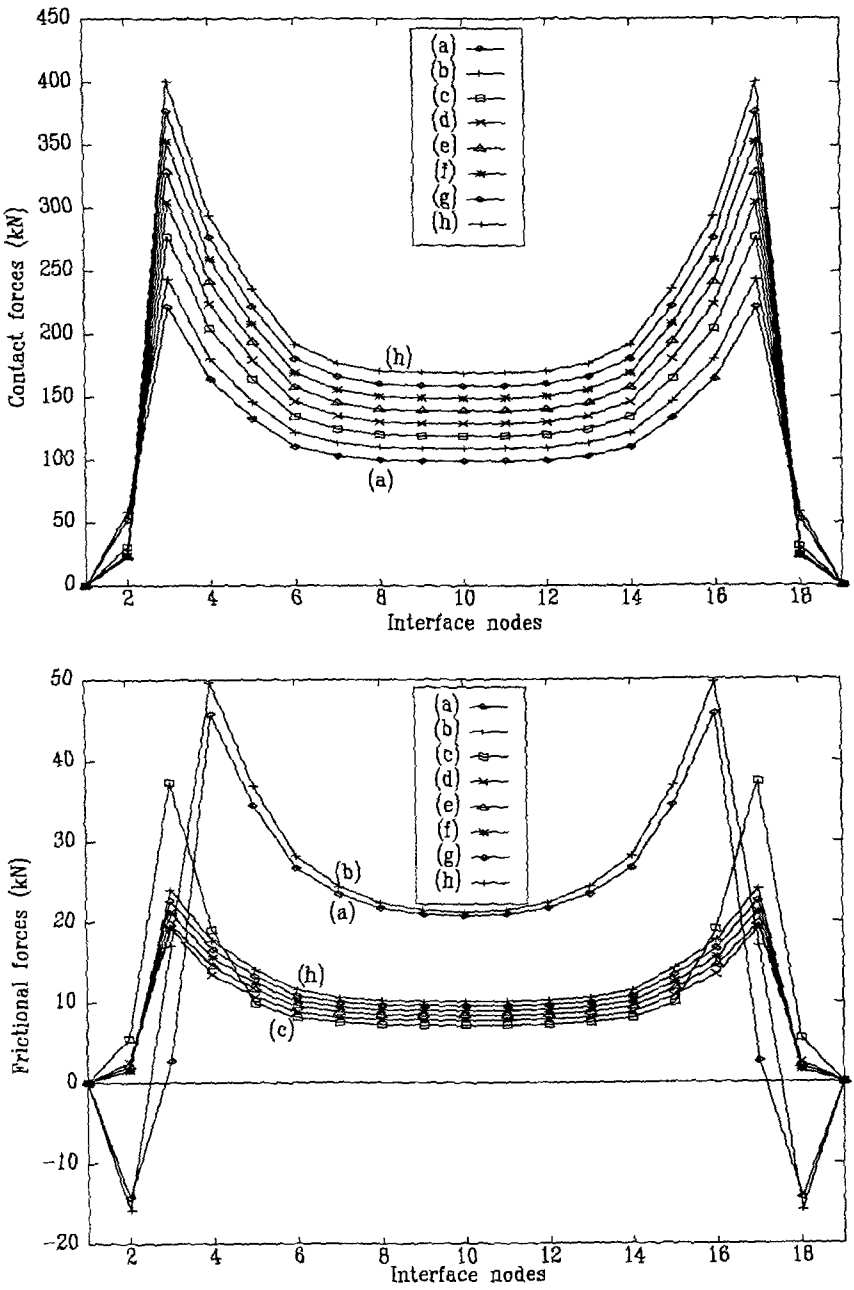


Fig. 7. Distribution of the contact and frictional forces along the interface.

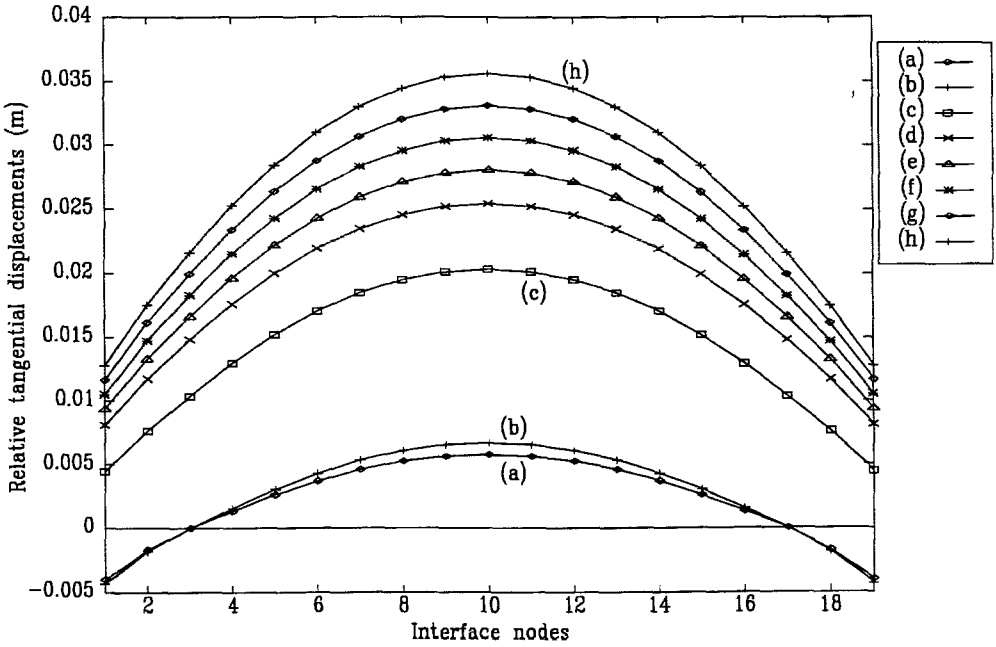


Fig. 8. Relative tangential displacements along the interface.

result the realization of branch BC in almost all the nodes of the interface and consequently, the frictional forces increase almost linearly with respect to the load.

7 Conclusions

A family of numerical method for the treatment of hemivariational inequalities has been presented. All the methods approximate the corresponding nonconvex energy problem with convex subproblems. The advantages of this approach are obvious as these methods can be applied for the solution of a wide range of hemivariational inequalities. The more or less heuristic character of these methods should be takeninto account as well as their excellent numerical performance for large scale engineering problems. A full mathematical discussion is still needed.

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