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Quasidifferentiability in Nonsmooth, Nonconvex Mechanics

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Abstract. Nonconvex and nonsmooth optimization problems arise in advanced engineering analysis and structural analysis applications. In fact the set of inequality and complementarity relations that describe the structural analysis problem are generated as optimality conditions by the quasidifferential potential energy optimization problem. Thus new kind of variational expressions arise for these problems, which generalize the classical variational equations of smooth mechanics, the variational inequalities of convex, nonsmooth mechanics and give a solid, computationally efficient explication of hemivariational inequalities of nonconvex, nonsmooth mechanics. Moreover quasidifferential calculus and optimization software make this approach applicable for a large number of problems. The connection of quasidifferential optimization and nonsmooth, nonconvex mechanics is discussed in this paper. A number of representative examples from elastostatic analysis applications are treated in details. Numerical examples illustrate the theory.

Key words: quasidifferentiability, codifferentiability, d.c. optimization, nonconvex energy, nonsmooth mechanics, variational inequalities, hemivariational inequalities

1 Introduction

Advanced structural analysis and engineering mechanics applications require the study of structures with boundary or interface conditions and with material laws and constitutive equations which involve complete ascending and descending vertical branches with monotone and generally nonmonotone graphs. Adhesive contact mechanics, softening and locking effects in concrete and geomaterials, tension cracking effects in masonry structures and delamination effects in composites belong to this category of problems, to name but a few of the areas where delicate nonsmooth structural analysis methods are used [10], [14], [17]. A general scheme used in structural analysis and computational mechanics, which also covers the majority of applications, consists in first defining a potential energy function and then producing the governing relations (equations and inequalities) of the initial problem by writting down the optimality (or critical point) conditions for this potential function, possibly taking into account subsidiary equality or inequality constraints. This general scheme will be adopted in the present paper which examines new extensions of structural analysis methods based on quasidifferential and codifferential optimization.

Lack of convexity and differentiability properties are the main obstackles which must be treated in an appropriate way, if potential energy optimization methods

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are to be used in the aforementioned advanced applications. Accordingly appropriate definition of the "generalized gradient" operator must be used in order to derive the optimality conditions and extend the applicability of gradient-like, steepest descent numerical optimization algorithms. The multiplicity of the solution, which recalls for the use of "global optimization" [11] methods must also be addressed, since multiple solutions do arise in these applications and a possibility of finding more than one of them (optimally all of them or the "best" one with respect to a given critetion) is of interest.

The concept of the quasidifferential and its computationally more appealing concept of the codifferential tackle both problems in an appropriate way [5], [4], [6], [3], [2]. A function is called quasidifferentiable if its directional derivative can be constructed as a sum of two terms which are in turn the maximum and minimum of linear functions of the direction multiplied by elements of two convex, compact subsets of $\mathbb{R}^n$. This ordered pair of sets, the subdifferential and the superdifferential in the sense of Demyanov and Rubinov, constitute the quasidifferential of the function at the sought point. The set-valued nature of this generalization of the gradient operator treats the complete vertical branches of the mechanical laws and boundary conditions in our application, analogously to the classical subdifferential operator of convex analysis [12], [10], [14]. In fact the two notions coincide for convex, nondifferentiable applications. Moreover convexity and concavity is treated separately by the two sets that comprise the quasidifferential. This is a generalization of the difference convex approximation [20], [11] where the function is written as a difference of two convex functions, the second constituent of the ordered set being actually the concave counterpart. The case of difference convex decomposition is covered, as a special case by the quasidifferential [4], [20]. In an analogous way sets defined by equations and inequalities involving quasidifferentiable functions are called quasidifferentiable sets. A systematic definition of the normal and the tangential cones of these sets (the strict, nonconvex ones, not some convex approximation of them) is among the interesting aspects of this approach with significant applications in structural analysis (e.g. in plasticity theory with nonconvex yield functions [15], [16]).

The codifferentiability concept extends the notion of quasidifferentiability in a way advantageous for numerical applications [2], since the arising operators are Hausdorff continuous (cf. the various ϵ-subdifferential generalizations of the convex subdifferential operator, see e.g. [4]).

For convex, nondifferentiable problems the adoption of the convex subdifferential gave rise to the formulation and study of variational inequality problems in mechanics [10], [14]. For nonconvex, nondifferentiable problems the explication of the arising optimality conditions gives rise to systems of variational inequalities [24], [16] which can be solved either by quasidifferential and codifferential optimization algorithms, as it will be described in this paper, or in some specific cased by appropriate multilevel decomposition techniques that resemple the sub- and supergradient optimization of mathematical programming [26], [16], [24], [17]. Note here that the hemivariational inequality approach (after P.D. Panagiotopoulos [14], [15], [17]) which is based on the generalized subgradient operator in the sense of F.H. Clarke, is connected to the systems of variational inequalities approach advocated in this paper. In fact Clarke's generalized gradient is derived by the quasidifferential calculus in a systematic way [22], [8], while the latter concept permit us effectively differentiate local minima and local maxima from critical points.

It should also be mentioned here that a complete quasidifferential calculus exists, which covers the most frequently arising cases of maximum and minimum type functions and of composite functions [6], [22].

The aim of this paper is to review the parallel developments in nonsmooth mechanics and quasidifferentiable and codifferentiable optimization, to give model formulations of variational inequality problems and systems of variational inequality problems in mechanics and to demonstrate by numerical examples its impact on computational mechanics and nonsmooth modelling in mechanics and engineering (see also [9]).

2 Quasidifferentiable and codifferentiable optimization. Optimality conditions

A function f defined on an open set $X \in \mathbb{R}^n$ is called quasidifferentiable at $x \in X$ if it is directionally differentiable at x and its directional derivative $f'(x, g)$ along the direction $g \in \mathbb{R}^n$ can be written as:

$$f'(x,g) = \max_{h_1 \in U} < h_1, g > + \min_{h_2 \in V} < h_2, g > \tag{1}$$

Here U and V are convex compact sets in $\mathbb{R}^n$. The ordered pair $Df(x) = [U, V]$ is called the quasidifferential of f at x, U is called the subdifferential of f at x and is denoted by $\underline{\partial} f(x)$ and V is the superdifferential of f at x, denoted by $\overline{\partial} f(x)$.

EXAMPLE 2.1. For a differentiable function f either $Df = [\nabla f, \{0\}]$ or $Df = [\{0\}, \nabla f]$ can be used as the quasidifferential of f.

EXAMPLE 2.2. For a convex, nondifferentiable function f, $Df = [\partial f, \{0\}]$, where ∂f denotes the classical subdifferential of convex analysis [21].

EXAMPLE 2.3. For a concave function f, $Df = [\{0\}, \partial f]$, where ∂f denotes the superdifferential of the concave function f.

EXAMPLE 2.4. For a difference convex (d.c.) function, i.e. a function f written as $f(x) = f_1(x) - f_2(x), \forall x \in X$ with $f_1(x)$ and $f_2(x)$ appropriate convex functions, one may take $Df(x) = [\partial f_1(x), \partial f_2(x)]$, where the convex subdifferentials of the constituent functions $f_1(x)$ and $f_2(x)$ are used.

For the calculation of the quasidifferential of given structured functions, (i.e. functions that are composed from simple components by taking the classical rules of addition, subtraction, multiplication and division, and beyond them certain finite combinations of maximum and minimum operators), and of composite functions calculus rules exist (see [6], [3], [7], [8], p.121).

We should mention here that the quasidifferential is not uniquelly defined, since addition of a given compact convex set to each element of the ordered pair $[\underline{\partial} f, \overline{\partial} f]$, does not change the result in (1). Thus it should be considered as class of equivalent pairs of convex compact sets.

A set $A \subset \mathbb{R}^n$ defined by a finite number of equalities and inequalities involving quasidifferential functions is called quasidifferential [4]. For these kind of generally nonconvex sets with nonsmooth boundaries, normal and tangential vectors are exactly defined by the quasidifferentiability concept. Thus a potential for applications in mechanical theories exists (e.g. in plasticity and damage theories with nonconvex and nondifferentiable yield sets, see also [16], [15]). In this article we will restrict ourselfes to unconstrained problems due to lack of space.

Since the concept of the quasidifferential gives rise to polyhedral approximations of general nonconvex and nonsmooth, but directionally differentiable functions, necessary and in some cases sufficient conditions for a point $x \in X$ to be an extremum poit for f can be written [19], [4], [8], Chapt. V. First-order conditions for unconstrained minima will be reviewed here. For more complicated cases the reader is referred to the above given literature. The basic local necessary (resp. sufficient) conditions for a directionally differentiable function f to admitt a local minimum (resp. a strict local minimum) at point $x^* \in \mathbb{R}^n$ read:

$$f'(x^*, \Delta) \geq (\text{resp.} >)\ 0,\ \forall \Delta \in \mathbb{R}^n \tag{2}$$

For a subdifferentiable function f, relation (2) is equivalent to the satisfaction of the convex set-valued inclusion:

$$0 \in \partial f(x^*) \text{ (resp. } 0 \in \text{int}\partial f(x^*) \text{ if } x^* \text{ is a nondifferentiable point)} \tag{3}$$

For f quasidifferentiable relation (2) is equivalent to relation

$$-\overline{\partial}\, \overline{f}(x^*) \subset \underline{\partial}\, \underline{f}(x^*) \tag{4}$$

If f is in addition locally Lipschitz continuous and the following relation holds:

$$-\overline{\partial}\, \overline{f}(x^*) \subset \text{int}\underline{\partial}\, \underline{f}(x^*) \tag{5}$$

then point $x^* \in \mathbb{R}^n$ is a strict local minimum of f at X. For extensions of the above given optimality conditions to constrained optimization problems the reader is referred to [4], [8].

It should be noted here that in the course of checking optimality conditions (4), (5) (for instance in a numerical algorithm) the question of finding an optimal representative element among the equivalent class of quasidifferentials arise. For most applications this choise does not pose serious problems in practical numerical implementations. For a discussion of current research and open questions related to this subject we refer the reader to [8], [13].

The notion of the quasidifferential gives rise to the following local polyhedral approximation of $f(x)$ around point x^* (quasilinearization):

$$f(x^* + \Delta) = f(x^*) + \max_{v \in \underline{\partial} f(x^*)} < v, \Delta > + \min_{w \in \overline{\partial} f(x^*)} < w, \Delta > + o_x(\Delta) \quad (6)$$

with $\frac{O_x(\alpha\Delta)}{\alpha} \to 0$, as $\alpha \downarrow 0$, $\forall \Delta \in \mathbb{R}^n$.

Unfortunately the approximation (6) is not a continuous function of x^* (cf. the convex subdifferential operator which has the same deficiency). This problem, which is essential for the efficiency of numerical algorithms, led to the definition of the codifferential [2], [8], an operator which is a continuous function of both x and Δ. A function f is called codifferentiable at x, if it admits a first order approximation of the form (see e.g. [8], p.189):

$$f(x+\Delta) = f(x) + \max_{[\alpha, h_1] \in \underline{d} f(x)} [\alpha + < h_1, \Delta >] + \min_{[\beta, h_2] \in \overline{d} f(x)} [\beta + < h_2, \Delta >] \quad (7)$$

The ordered pair of convex compact sets of $\mathbb{R}^{n+1}$, $\mathcal{D} f(x) = [\underline{d} f(x), \overline{d} f(x)]$, is called the codifferential of f at point x. $\underline{d} f(x)$ is called the hypodifferential and $\overline{d} f(x)$ is called the hyperdifferential of f at x. Clearly α, $\beta \in \mathbb{R}^1$ and h_1, $h_2 \in \mathbb{R}^n$. Note here that the set of quasidifferentiable and codifferentiable functions coincide (in fact by setting $\alpha = \beta = 0$ in (7) we get the expression (6) of the quasidifferential), and that calculus rules and optimality conditions are written analogously to the ones written for the quasidifferentials (see e.g. [8], Chapter IV and the section of the numerical algorithms of this paper).

EXAMPLE 2.5. (see [8], p.193) The advantages of using the notion of the codifferential instead of the quasidifferential and the similarities with other approaches concerning the convex subdifferential are demonstrated here by means of the convex nondifferentiable function f(x) = — x — The directional derivative of $f(x)$ and the convex analysis subdifferential of f, which coincides with the subdifferential in the quasidifferential sense) read

$$f'(x,g) = \begin{cases} g, \text{ if } x > 0 \\ -g, \text{ if } x < 0 \\ \|g\|, \text{ if } x = 0 \end{cases}, \quad \partial f(x) = \underline{\partial} f(x) = \begin{cases} 1, \text{ if } x > 0 \\ -1, \text{ if } x < 0 \\ [-1,1], \text{ if } x = 0 \end{cases} \quad (8)$$

Here $g \in \mathbb{R}^1$ and the superdifferential is $\overline{\partial} f(x) = \{0\}$. The hypodifferential of f reads:

$$\underline{d}f(x) = \begin{cases} \text{co}\{(0,1),(-2x,-1)\}, \text{ if } x > 0 \\ \text{co}\{(2x,1),(0,-1)\}, \text{ if } x < 0 \end{cases} \tag{9}$$

while the hyperdifferential is $\underline{d}f(x) = \{(0,0)\}$. One may observe that the mapping $\mathcal{D}f(x) = [\overline{d}f(x), \underline{d}f(x)]$ is Hausdorff continuous in x and that it contains in some sense "global" information which would allow to a numerical scheme to detect and treat the nondifferentiability of the function appropriately, even from points different from the point $x = 0$ where the function is nondifferentiable (a case which appears with probability one in a numerical scheme).

3 Quasidifferentiable energy optimization in mechanics

A large number of nonlinear problems in mechanics can be derived by differentiation from appropriate potential energy functions (called from this fact potential problems). The classical system of nonlinear equations (e.g. compatibility, equilibrium, material laws in elasticity) and the boundary conditions result as optimality (or in general critical point) conditions from this potential. The classical gradient operator permit one consistently linearize these expressions and write them as a linear variational inequality. Extensions to nondifferentiable, convex and nonconvex potentials are described in this paper. Nonsmooth elastostatic structural analysis applications will serve as model problems here. The need for considering these extensions comes from problems with complete vertical branches (multivalued relations) in their constitutive laws or in the boundary conditions. The concept of the quasidifferential permit us define a consistent quasilinearization of the nonlinear relations. In this general framework variational inequality problems [10], [14] and hemivariational inequality problems [14], [17] are included.

Let us give a concrete application by considering a discretized elastic structure in a displacement based finite element formulation where $\mathbf{u}$ is the n-dimensional vector of displacement degrees of freedom and $\mathbf{e}$ is the m-vector of element deformations. A fairly general discrete potential energy optimization problem in elastostatics reads:

$$\min_{\mathbf{u} \in U_{ad}} \quad \{\overline{\Pi}(\mathbf{u}) = \Pi(\mathbf{e}(\mathbf{u})) + \Phi(\mathbf{u}) + p(\mathbf{u})\} \tag{10}$$

where $\Pi(\mathbf{e})$ is the elastic energy stored in the system due to deformation, $\Phi(\mathbf{u})$ is the potential that counts for various boundary, interface or skin effects and $p(\mathbf{u})$ is the potential that generates the external loading vector. The geometric compatibility transformation is written in the form of a generally nonlinear but differentiable operator $\mathcal{A}(\mathbf{u}) : \mathbb{R}^n \to \mathbb{R}^m$,

$$\mathbf{e} = \mathcal{A}(\mathbf{u}) \tag{11}$$

Multibranch elasticity or holonomic plasticity models with ascending and descending complete vertical branches that count for crashing, cracking and locking effects in a phenomenological way are covered by this model, by using nonsmooth and possibly nonconvex superpotential energy functions $\Pi(\mathbf{e})$ in (10). Analogously nonmonotone relations, like stick-slip boundary or interface laws, frictional or softening frictional laws etc., introduce nonsmooth and nonconvex potential functions $\Phi(\mathbf{u})$ in (10) (see [14], [17], [9] among others). The set of kinematically admissible displacements is in general a quasidifferentiable set, defined by:

$$U_{ad} = \{\mathbf{u} \in \mathbb{R}^n \ : \ \mathcal{H}(\mathbf{u}) \leq \mathbf{0}, \ \mathcal{G}(\mathbf{u}) = \mathbf{0} \ \} \tag{12}$$

where $\mathcal{G}(\mathbf{u}) \ : \ \mathbb{R}^n \rightarrow \mathbb{R}^{n_1}$, $\mathcal{H}(\mathbf{u}) \ : \ \mathbb{R}^n \rightarrow \mathbb{R}^{n_2}$ and $n_1+n_2 < n$ are general nonlinear and possibly nondifferentiable (but quasidifferentiable) equality and inequality constraints. Bilateral and unilateral contact effects and locking behaviour in a large displacement setting leads to relations of the (12) type. For simplicity only unconstrained structural analysis problems, i.e. $U_{ad} = \mathbb{R}^n$ are considered in this paper. Nevertheless note here that the generality of the developed theory is not seriously affected, since by the method of exact penalty functions (see e.g. [8], p.301, [9]) constraints (12) can be included in the goal function of the minimization problem (10), and thus they lead to an unconstrained quasidifferendiable optimization problem.

Variational formulations for the elastostatic analysis problem described by (10) will be produced in the sequel by writting down the optimality conditions for this quasidifferentiable minimization problem and using the quasidifferential calculus for the derivation of the quasidifferential of the composite function $\overline{\Pi}(\mathbf{u})$. Variational equalities for classical smooth problems, variational inequalities for nonsmooth, subdifferentiable problems (cf. [10], [14], [17]) and systems of variational inequalities for general quasidifferentiable problems (cf. [24], [16], [17], [9]) are thus derived in a systematic way.

3.1 Smooth case

Let $\Pi(\mathbf{e})$ be a smooth function. Then optimality condition for problem (10) leads to the variational equality

$$\overline{\Pi}'(\mathbf{u}, \Delta\mathbf{u}) = [\frac{\partial \mathcal{A}(\mathbf{u})}{\partial \mathbf{u}}]^T \frac{\partial \Pi(\mathbf{e})}{\partial \mathbf{e}} \Delta\mathbf{u} + [\frac{\partial \Phi(\mathbf{u})}{\partial \mathbf{u}}]^T \Delta\mathbf{u} + [\frac{\partial p(\mathbf{u})}{\partial \mathbf{u}}]^T \Delta\mathbf{u} = 0 \tag{13}$$

Since (13) hold true for every $\Delta\mathbf{u} \in \mathbb{R}^n$ the system of nonlinear equalibrium equations of the classical large displacement elasticity are produced.

3.2 Subdifferentiable case

Let the composite function $\overline{\Pi}(\mathbf{u})$ in (10) be subdifferentiable. In this case the optimality condition for problem (10) leads to the variational inequality: Find $\mathbf{u} \in \mathbb{R}^n$ such that

$$\mathbf{0} \in \partial\overline{\Pi}(\mathbf{u}), \ \text{or equivalently} \ 0 \leq \overline{\Pi}(\mathbf{u}^*) - \overline{\Pi}(\mathbf{u}), \ \forall \mathbf{u}^* \in \mathbb{R}^n \tag{14}$$

Note here that $\overline{\Pi}(\mathbf{u}^*)$ is subdiferentiable either if $\mathcal{A}(\mathbf{u})$ is a linear transformation (e.g. in small displacement theory), $\Pi(\mathbf{e})$ is convex and possibly nondifferentiable (subdifferentiable) and $\Phi(\mathbf{u})$, $p(\mathbf{u})$ are convex (subdifferentiable) functions, or in the general quasidifferentiable case if certain relations hold true (see [8]).

3.3 Quasidifferentiable case

Let $\Pi(\mathbf{e})$ of (10) be quasidifferentiable and let $D\Pi(\mathbf{e}) = [\underline{\partial}\Pi(\mathbf{e}), \overline{\partial}\Pi(\mathbf{e})] \in \mathbb{R}^m \times \mathbb{R}^m$. Then by using the rules of the quasidifferential calculus (see [8], p.127) for the composite function $\Pi(\mathbf{e}(\mathbf{u}))$ we get a representation of the $D\overline{\Pi}(\mathbf{u}) = [\underline{\partial}\,\overline{\Pi}(\mathbf{u}), \overline{\partial}\,\overline{\Pi}(\mathbf{u})] \in \mathbb{R}^n \times \mathbb{R}^n$ with

$$\underline{\partial}\,\overline{\Pi}(\mathbf{u}) = \{\mathbf{q} \in \mathbb{R}^n \mid \mathbf{q} = \sum_{i=1}^{m}(\nu^{(i)}) - \frac{1}{2}\underline{\nu}^{(i)} - \frac{1}{2}\overline{\nu}^{(i)})[\frac{\partial \mathcal{A}(\mathbf{u})}{\partial \mathbf{u}}]\} \tag{15}$$

with $\nu = (\nu^{(1)}, \ldots, \nu^{(m)}) \in \underline{\partial}\Pi(\mathbf{e})$,

$$\overline{\partial}\,\overline{\Pi}(\mathbf{u}) = \{\mathbf{l} \in \mathbb{R}^n \mid \mathbf{l} = \sum_{i=1}^{m}(\nu^{(i)}) - \frac{1}{2}\underline{\nu}^{(i)} - \frac{1}{2}\overline{\nu}^{(i)})[\frac{\partial \mathcal{A}(\mathbf{u})}{\partial \mathbf{u}}]\} \tag{16}$$

with $\nu = (\nu^{(1)}, \ldots, \nu^{(m)}) \in \overline{\partial}\Pi(\mathbf{e})$, and $\underline{\nu}, \overline{\nu} \in \mathbb{R}^m$ such that

$$\underline{\nu} < \nu < \overline{\nu},\ \forall \nu \in \underline{\partial}\Pi(\mathbf{u}) \cup (-\overline{\partial}\Pi(\mathbf{u})) \tag{17}$$

Moreover, on the assumption that $\Phi(\mathbf{u})$ and $p(\mathbf{u})$ are differentiable we get

$$D\overline{\Pi}(\mathbf{u}) = [\underline{\partial}\,\overline{\Pi}(\mathbf{u}), \overline{\partial}\,\overline{\Pi}(\mathbf{u})] = [\underline{\partial}\Pi(\mathbf{u}) + \nabla\Phi(\mathbf{u}) + \nabla p(\mathbf{u}), \overline{\partial}\Pi(\mathbf{u})] \tag{18}$$

The optimality conditions for the quasidifferentiable unconstrained optimization problem, i.e. find $\mathbf{u} \in \mathbb{R}^n$ such that

$$\underline{\partial}\,\overline{\Pi}(\mathrm{u}) \subset \overline{\partial}\,\overline{\Pi}(\mathrm{u}) \tag{19}$$

lead to the equivalent problem of solving the system of variational inequalities: find $\mathbf{u} \in \mathbb{R}^n$ such that

$$\mathrm{w} \subset \underline{\partial}\,\overline{\Pi}(\mathbf{u}),\ \forall w \in \overline{\partial}\,\overline{\Pi}(\mathbf{u}) \tag{20}$$

3.4 Difference convex (d.c.) case

Let a small displacement problem be considered, i.e. linear compatibility relations hold with (11) replaced by $\mathcal{A}(\mathbf{u}) = \mathbf{G}^T\mathbf{u}$, with $\mathbf{G}^T$ an $(m \times n)$ matrix and accordingly $p(\mathbf{u}) = \mathbf{p}^T\mathbf{u}$, with $\mathbf{p}$ the n-dimensional loading vector. Let moreover $\Pi(\mathbf{e})$ in (10) be convex and differentiable, e.g. consider for instance the linear elasticity problem (Hookean law) with $\Pi(\mathbf{e}) = \frac{1}{2}\mathbf{e}^T\mathbf{K}_0\mathbf{e}$, where $\mathbf{K}_0$ is the $(m \times m)$ natural stiffness matrix of the structure. Let the only cause of nonconvexity and nondifferentiability in the problem be introduced by a difference convex boundary potential energy function, i.e. $\Phi(\mathbf{u})$ is written as a difference of convex, possibly nondifferentiable terms [24], [25]

$$\Phi(\mathbf{u}) = \Phi_1(\mathbf{u}) - \Phi_2(\mathbf{u}) \tag{21}$$

In this case by using the quasidifferential calculus on the d.c. potential energy function one has:

$$\underline{\partial}\,\overline{\Pi}(\mathbf{u}) = \mathbf{K}\mathbf{u} + \mathbf{p} + \partial\Phi_1(\mathbf{u}),\ \overline{\partial}\,\overline{\Pi}(\mathbf{u}) = -\partial\Phi_2(\mathbf{u}) \tag{22}$$

Optimality conditions for the d.c. potential lead to the following system of variational inequalities that describe the nonsmooth and nonconvex structural analysis problem: Find $\mathbf{u} \in \mathbb{R}^n$ such that

$$\mathbf{0} \in \mathbf{K}\mathbf{u} + \mathbf{p} + \partial\Phi_1(\mathbf{u}) - \mathbf{w} \tag{23}$$

for each $\mathbf{w} \in \mathbb{R}^n$ with

$$\mathbf{w} \in \partial\Phi_2(\mathbf{u}) \tag{24}$$

REMARK 3.1. Relations (23) , (24), which are convex differential inclusions, or multivalued relations, are equivalent to the discrete variational inequalities:

$$\mathbf{u}^T\mathbf{K}(\mathbf{u}^* - \mathbf{u}) + (\mathbf{p} - \mathbf{w})^T(\mathbf{u}^* - \mathbf{u}) + \Phi_1(\mathbf{u}^*) - \Phi_1(\mathbf{u}) \geq 0,\ \forall \mathbf{u}^* \in \mathbb{R}^n \tag{25}$$

and

$$\Phi_2(\mathbf{u}^*) - \Phi_2(\mathbf{u}) \geq \mathbf{w}^T(\mathbf{u}^* - \mathbf{u}),\ \forall \mathbf{u}^* \in \mathbb{R}^n \tag{26}$$

REMARK 3.2. The system of variational inequalities (20) is explicitly defined due to the global d.c. representation of the potential energy function. Unfortunately this is not possible in the general quasidifferential case, where the system of variational inequalities (20) are implicitly defined, i.e. they are defined at each point of an iterative scheme.

4 Nondifferentiable numerical optimization methods

Quasidifferential and codifferential optimization algorithms are based on gradient-like, descent, iterative techniques whereas gradient information is replaced by the set-valued quasidifferential or the codifferential and the steepest descent finding subproblems are appropriately replaced by quadratic programming subproblems with a polyhedral approximation of the aforementioned set-valued quantities. Since supergradients (resp. hyperdifferentials) pose a combinatorial problem in the descent direction finding subproblem, which can be effectively treated after making the polyhedral approximation by repeated solution of a number of similar subproblems or simply by solving one of them (supergradient-like technique) the basic methods used are the ones of hypodifferential optimization. These techniques will be described in the sequel (for more details we refer to [4], [20], [7], [8], [9]) and for applications in mechanics to [15], [26], [24], [17], [9]). It should be mentioned here that first order quasidifferential and codifferential optimization schemes treat more effectively, in a correct way vertical branches of laws and boundary conditions in mechanical problems, or equivalently, the nonsmoothness of the respective potentials. If at a neighborhood of the solution the problem is essentially smooth, i.e. the solution lies far away from a point of nondifferentiability, classical methods of nonlinear computational mechanics (e.g. Newton methods and it's derivatives [1]) can be used for the refinement of the accuracy and for speeding up the rate of convergence. Nevertheless if multiple points of nondifferentiability (crisps) have to be passed along a given loading path (probably the incremental loading in a more general incremental scheme) the here proposed schemes have more advantaghes compared with the classical approaches (e.g. quasi-Newton techiques).

4.1 The method of hypodifferential descent.

Let f be a locally Lipschitz function defined on an open set X from the Euclidean space $\mathbb{R}^n$ and be hypodifferentiable there. Since the class of hypodifferentiable functions coincides with the class of subdifferentiable functions, then in this case for every point $x \in X$ the following relation holds:

$$\partial f(x) = \{v \in \mathbb{R}^n \mid [0, v] \in df(x) \subset \mathbb{R}^1 \times \mathbb{R}^n\} \tag{27}$$

where $\partial f(x)$ is the subdifferential of f at x and $df(x)$ is the hypodifferential of f at x.

Both the subdifferential $\partial f(x)$ and the hypodifferential $df(x)$ are convex sets, but they belong to different Euclidean spaces.

It is well known that for a point x to be a local minimum point of a subdifferentiable function f, it is necessary that

$$0_n \in \partial f(x) \tag{28}$$

Making use of (27) it is easy to check that for any local minimum point it is necessary that the following inclusion be true:

$$0_{n+1} \in df(x) \tag{29}$$

A point x for which the condition (27) is satisfied will be called a stationary point of the function f on the set X.

Let a point x be a nonstationary point for f on X, that is (29) does not hold true. Then we can project 0_{n+1} on the set $df(x)$, i.e. we can find the solution of the subproblem:

$$\min_{z \in df(x)} \quad \|z\| = \|z(x)\|, \; z(x) = [t(x), w(x)] \in \mathbb{R}^1 \times \mathbb{R}^n \tag{30}$$

Here and in the sequel we consider the Euclidean metric $\|.\|$. Note that, if $0_{n+1} \in df(x)$, then $w(x)$ is not equal to 0_n.

The direction $g(x) = -w(x)$ is called a direction of hypodifferential descent of the function f at the point x on X. This direction is unique. Moreover if $f'(x, g)$ is the directional derivative of f at x in the direction g, it is not difficult to prove that if x is not a stationary point of f at x, then

$$f'(x, g(x)) \leq -\|z(x)\|^2 \tag{31}$$

Let f be continuously differentiable, that is, the hypodifferential mapping $df : \mathbb{R}^{n+1} \to 2^{R^n}$ is Hausdorff continuous, then the direction of hypodifferential descent is continuous in x. This property makes it possible to construct methods for minimizing continuously hypodifferentiable functions like the gradient methods in the smooth case. Note that this development can not be based on the classical convex analysis subdifferential notion, since the subdifferential mapping is not Hausdorff continuous, even if the function is continuously hypodifferential. Most of the iterative numerical methods generate minimizing sequences by the rule:

$$x_{k+1} = x_k + \alpha_k d_k \tag{32}$$

where d_k is a descent direction (if d_k is not equal to 0_n), and α_k is a positive step size. All gradient descent methods use (32).

Let us show that a direction of hypodifferential descent can be used for minimizing continuously hypodifferentiable functions analogously to the direction of the antigradient in the smooth case. The step-size can be choosen in several ways. Let us consider some alternatives as in the smooth case:

– one-dimensional minimization: the step-size is choosen to satisfy the following condition

$$\alpha_k = \underset{\alpha > 0}{argmin}\, f(x_k - \alpha w_k) \tag{33}$$

– one-dimensional minimization in the presence of constraints: in this case the step-size is choosen from the following condition

$$\alpha_k = \underset{\alpha \in (0,q]}{argmin}\; f(x_k - \alpha w_k),\; q > 0 \tag{34}$$

– the Armijo step-size rule: let us fix a parameter $\theta \in (0, 0.5]$. Find the first value $i_k = 0, 1, \ldots$ under which the following inequality holds true

$$f(x_k - (0.5)^{i_k} w_k) \leq f(x_k) - (0.5)^{i_k}\theta\|w_k\| \tag{35}$$

and set $\alpha_k = (0.5)^{i_k}$

Suppose that $X = \mathbb{R}^n$. Since the function f is directionally differentiable at x, then

$$f(x + \alpha g) - f(x) = f'(x, g) + o(\alpha, g) \tag{36}$$

where $\frac{o(\alpha,g)}{\alpha} \to 0$, as $\alpha \to +0$

Assume that the convergence in (31) is uniform with respect to $g \in \mathbb{R}^n$, $\|g\| = 1$. The method of hypodifferential descent for minimizing f on $\mathbb{R}^n$ has the following steps:

- Choose $x_0 \in \mathbb{R}^n$
- If $0_{n+1} \in df(x_0)$, then x_0 is a stationary point for f and the process is finished.
- Otherwise, for $k \geq 0$ set

$$x_{k+1} = x_k + \alpha_k g(x_k) = x_k + \alpha_k g_k \tag{37}$$

where g_k is the direction of hypodifferential descent, and the step-size is choosen either by the Armijo rule or as the result of one-dimensional minimization.

If the sequence $\{x_k\}$ is finite then by construction the latter point is the stationary point of f. Consider the case where this sequence is infinite. By virtue of inequality (31) the sequence $\{f(x_k)\}$ is decreasing. Let the Lebesgue set

$$\mathcal{L}(x_0) = \{x \in \mathbb{R}^n \mid f(x) \leq f(x_0)\} \tag{38}$$

be bounded.

THEOREM 1. *Every accumulation point of the sequence $\{x_k\}$ is a stationary point of the function f.*

Let us clarify the above given theory by some examples of continuously hypodifferentiable functions.

EXAMPLE 4.1. Any continuously differentiable function is a continuously hypodifferentiable function because we can take the point $[0, f'(x)] \in \mathbb{R}^1 \times \mathbb{R}^n$ as a continuous hypodifferential of f at x, where $f'(x)$ is the gradient of f at x. In this case the direction of hypodifferential descent coincides with the antigradient of f.

EXAMPLE 4.2. Let f be a maximum function, i.e.

$$f(x) = \max_{y \in Y} \phi(x, y) \tag{39}$$

where $Y \subset \mathbb{R}^m$ is a compact set and the function ϕ and its derivative are both continous on $X \times Y$, where $X \subset \mathbb{R}^n$ is an open set. Then function f is directionally differentiable at $x \in X$ and

$$f'(x,g) = \max_{y \in R(x)} \left\{ \frac{\partial \phi(x,y)}{\partial x}, g \right\} \tag{40}$$

where $R(x) = \{y \in Y | f(x) = \phi(x,y)\}$. From (40) follows that $f'(x,g)$ is a convex function in g. The set

$$df(x) = \text{ co } \left\{ [t,w] \in \mathbb{R}^1 \times \mathbb{R}^n \mid t = \phi(x,y) - f(x),\ w = \phi'_x(x,y),\ y \in Y \right\} \tag{41}$$

can be considered as a continuous hypodifferential of f at x. Therefore f is continuous hypodifferentiable. In particular, if we consider the maximum function then Y contains a finite collection of points, i.e.

$$Y = \{y_i\},\ i \in I = \{1, \dots, m\} \tag{42}$$

then the set $df(x)$ is polyhedral

$$df(x) = \text{ co } \{ \alpha_i(x) \mid i \in I \}, \tag{43}$$

where

$$\alpha_i = [\phi(x,y_i) - f(x), \phi'_x(x,y_i)] \in \mathbb{R}^1 \times \mathbb{R}^n \tag{44}$$

EXAMPLE 4.3. Let f be the sum of maximum functions

$$f(x) = \sum_{j \in J} f_j(x),\ J = \{1, \dots, p\} \tag{45}$$

$$f_j = \max_{y \in Y} \phi_j(x,y) \tag{46}$$

where $Y \subset \mathbb{R}^m$ is a compact set and all functions ϕ_j, $j \in J$, and their derivatives are continuous on $X \times Y$. Since all $\phi_j(x,y)$ are continuously hypodifferentiable, by using appropriate calculus rules [6] we get

$$df(x) = \sum_{j \in J} df_j(x) \tag{47}$$

4.2 Finding the direction of hypodifferential descent.

For practical application of the method of hypodifferential descent it is necessary to solve effectively the problems of finding the direction of descent and the step-size. The problem of definding the step-size is a one-dimensional minimization problem and a lot of effective methods are available to solve it. The problem of finding the direction of hypodifferential descent can be successfully solved if a hypodifferential is a polyhedron, which is discretized by its vertices or a sum of such polyhedrons, because in these cases we have to solve a quadratic programming subproblem under simple constraints. This subproblem reads:

$$\min_{z \in df(x)} \quad < z, z >= min\|z\|^2 = \|z(x)\|^2$$

$$z(x) = [t(x), w(x)] \in \mathbb{R}^1 \times \mathbb{R}^n \tag{48}$$

EXAMPLE 4.4. Let us consider the function $f(x) = max_{i \in I} f_i(x)$, $I = \{1, \ldots, m\}$, where f_i are continuously differentiable on $\mathbb{R}^n$, then $df(x) = \text{co}\{\alpha_i(x) \mid i \in I\}$, where $\alpha_i(x) = [f_i - f(x),\ f_i'(x)] \in \mathbb{R}^1 \times \mathbb{R}^n$, $i \in I$, $f_i'(x)$ is the gradient of f_i at x. Since any point of the convex hull can be presented by a convex combination of points $\alpha_i(x)$, $i \in I$, we get

$$z = \sum_{i \in I} \lambda_i \alpha_i(x) = \sum_{i \in I} \lambda_i c_i(x) + p(x) \tag{49}$$

where $\sum_{i=1}^{m} \lambda_i = 1$, $\lambda_i \geq 0$, $i \in I$, with $c_i(x) = [f_i(x), f_i'(x)]$ and $p(x) = [-f(x), 0_n]$. Thus the problem (48) is equivalent to the following problem:

$$min \frac{1}{2} < G(x)\lambda, \lambda > + < q(x), \lambda >, \ \sum \lambda_i = 1, \ \lambda_i \geq 0, \ i \in I \tag{50}$$

where $\lambda = [\lambda_1, \ldots, \lambda_m] \in \mathbb{R}^m$ and $G(x)$ is a Gram matrix of vectors $c_i(x)$, i.e.

$$G(x) = \left\{ \begin{array}{ccc} < c_1(x), c_1(x) > & \ldots & < c_1(x), c_m(x) > \\ < c_m(x), c_1(x) > & \ldots & < c_m(x), c_m(x) > \end{array} \right\} \tag{51}$$

with $q(x) = [q_1(x), \ldots, q_m(x)] \in \mathbb{R}^m$ and $q_i(x) = -f_i(x)f(x)$, $i \in I$. By solving problem (50) we find multipliers λ_i, $i \in I$, such that

$$w(x) = \sum_{i=1}^{m} \lambda_i f_i'(x)$$

$$t(x) = \sum_{i=1}^{m} \lambda_i (f_i'(x) - f(x)) = \sum_{i=1}^{m} \lambda_i f_i'(x) - f(x)$$

Note that instead of problem (50) se can solve the following problem:

$$min\frac{1}{2} < G_1(x)\lambda, \lambda >, \sum_{i=1}^{m} \lambda_i = 1, \ \lambda_i \geq 0 \tag{52}$$

where $\lambda = [\lambda_1, \ldots, \lambda_m] \in \mathbb{R}^m$ and $G_1(x)$ is a Gram matrix of vectors $\alpha_i(x)$, $i \in I$.

EXAMPLE 4.5. Let

$$f(x) = \sum_{i \in I} |f_i(x)|, \ i \in I = \{1, \ldots, m\} \tag{53}$$

and $f_i, i \in I$ are continuously differentiable on $\mathbb{R}^n$. Then

$$df(x) = \sum_{i \in I} d\phi_i(x) \tag{54}$$

where $\phi_i(x) = \max\{f_i(x), -f_i(x)\}, i \in I$ and $d\phi_i(x) = \text{co}\{\alpha_i(x), \beta_i(x)\}$, $\alpha_i(x) = [f_i(x) - \phi_i(x), f_i'(x)] \in \mathbb{R}^1 \times \mathbb{R}^n$, $\beta_i(x) = [-f_i(x) - \phi_i(x), f_i'(x)] \in \mathbb{R}^1 \times \mathbb{R}^n$. In this case problem (50) is equivalent to

$$\min_{z \in df(x)} < z, z >= min||z||^2 = ||z(x)||^2$$

$$z = z_1 + \ldots + z_m, z \in df(x) \subset \mathbb{R}^1 \times \mathbb{R}^n, z_i \in d\phi_i(x) \subset \mathbb{R}^1 \times \mathbb{R}^n, i \in I. \tag{55}$$

Since each set $d\phi_i$ is an interval on $\mathbb{R}^1 \times \mathbb{R}^n$, the set $df(x)$ is a sum of intervals. Therefore $z_i = 2\lambda_i[f_i(x), f_i'(x)] + [-f_i(x) - f(x), -f_i'(x)], \lambda_i \in [0,1], i \in I$, and $z = \sum_{i=1}^m 2\lambda_i[f_i(x), f_i'(x)] + [-f_i(x) - f(x), -f_i'(x)] = \sum_{i=1}^m 2\lambda_i[f_i(x), f_i'(x)] - [f_i(x), f_i'(x)] + [-f(x), 0]$, $0 \leq \lambda_i \leq 1, i \in I$. In the notation used previously we have $z = \sum_{i \in I}(2\lambda_i - 1)c_i(x) + p(x)$. By denoting by $\mu_i = 2\lambda_i - 1$ we get the problem:

$$min\frac{1}{2} < G(x)\mu, \mu > + < q(x), \mu >, \ \mu_i \in [-1,1], \ i \in \{1, \ldots, m\} \tag{56}$$

where $\mu = [\mu_1, \ldots, \mu_m] \in \mathbb{R}^m$, $G(x)$ is the Gram matrix of vectors $c_i(x), i \in I$, and $q(x) = [q_1(x), \ldots, q_m(x)] \in \mathbb{R}^m$, $q_i(x) = -f_i(x)f(x)$. By solving problem (56) we find multipliers $\mu_i, i \in I, \mu_i \in [-1,1]$, such that

$$w(x) = \sum_{i \in I} \mu_i f_i'(x), \ t(x) = \sum_{i \in I} \mu_i f_i(x) - f(x). \tag{57}$$

Note that prolems (50) and (56) differ only in the constraints, while the objective function remains the same. As the Gram matrix is a nonnegative matrix, there always exist solutions to these problems. These solutions may not be unique when the Gram matrix is non positive.

5 Quasi- and co-differentiable computational mechanics and examples

Within the general potential energy minimization scheme of section three, concrete examples of computational mechanics applications of quasidifferentiable and codifferentiable optimization will be given here. A remark of general validity on the connection with traditional computational mechanics techniques should be given first. Nonlinearity is usually treated by step-wise linearization techniques (e.g. by the generalized Newton method or the method of linear iterations as described among others in [1], Chap.3). Nonsmoothness requires the introduction of special nonsmooth approximation schemes (e.g. quasi-Newton techniques) while no general effective scheme for treating nonconvexity has been proposed undil now. Both issues require nonsmooth mechanics methods for their effective treatment [14], [17]. The concepts of the quasidifferential and the codifferential address both problems in a systematic and elegant way since the set valued substitutes of the derivative treat nondifferentiability while convex and concave parts are treated separately by the sub- and the super-differential (resp. the hypo- and the hyper-differential).

Characteristic applications of the general scheme discussed in section three and an example solved by the algorithms of section four are given here. A frictional skin effect, where a monotone Coulomb friction law is considered to hold at eadh d.o.f. of the adhesive joint of Fig.1 is considered first. On the assumption that boundary supports are treated explicitly (i.e. inequality constraints in (14) are considered in the effective stiffness matrix $\mathbf{K}$) and in the framework of small displacement and deformation theory the potential energy minimization problem (12) reads:

$$\overline{\Pi}(\mathbf{u}) = \frac{1}{2}\mathbf{u}^T\mathbf{K}\mathbf{u} + cc\sum_{i=1}^{n}|u_i| - \mathbf{p}^T\mathbf{u} \tag{58}$$

In (58) cc stands for the *frictional force limit* and, for notational simplicity, unidirectional frictional joints along each d.o.f. direction are considered separately. Obviously the convex, nondifferentiable potential $\Pi(\mathbf{u})$ in (58) is subdifferentiable (thus also hypodifferentiable) and the static analysis problem, which requires the numerical solution of (58) can be tackled by the hypodifferential descent algorithms given in section four (see also [4], [8], [9]). The results, in the form of displacement contours for various cc's are given in Figs.2,3 (for load $p = 10.$ and $cc = 0.1$, $cc = 0.5$ resp.).

Nonmonotone skin effects can be tackled by replacing the second term in the potential energy function of (58) by the nonconvex term

$$cc\sum_{i=1}^{N} min\{\frac{1}{2}k_i(u_i - u_0)^2, \frac{1}{2}k_iu_i^2, \frac{1}{2}k_i(u_i + u_0)^2\} \tag{59}$$

A problem like the one in (22) arises, for which either a conjugate super and subgradient method can be used, or a difference convex decomposition that leads to

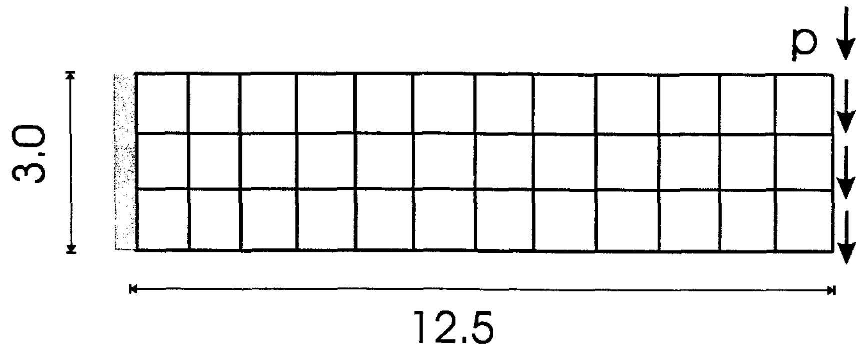

Fig. 1. Configuration of the example adhesive joint.

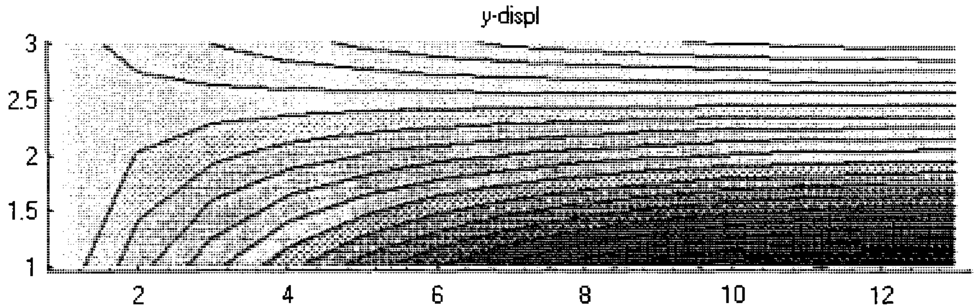

Fig. 2. Monotone frictional law of (58) with $cc = 0.1$.

problems (26), (27) or (28), (29) must be solved (see also [16], [24], [25], [26], [9]). Sample results for a problem of this kind are given in Figs. 4,5 (with $cc = 10., u_0 = 0.01, k_i = 1500.$ and load $p = 0.1$, $p = 1.0$ resp.).

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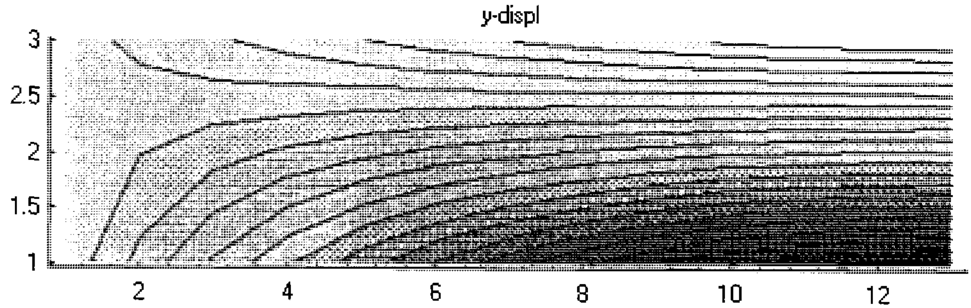

Fig. 3. Monotone frictional law of (58) with $cc = 0.5$.

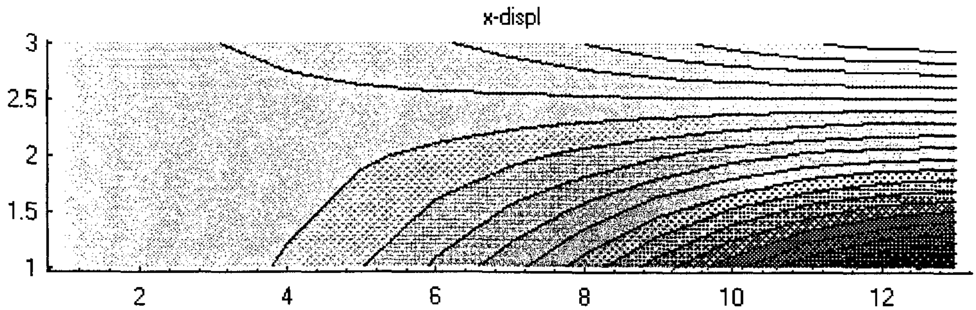

Fig. 4. Nonmonotone adhesion law of (59) with $p = 0.1$.

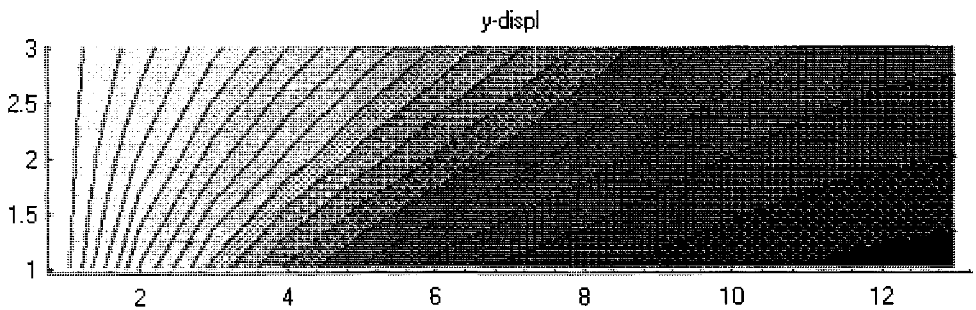

Fig. 5. Nonmonotone adhesion law of (59) with $p = 1$.

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