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HOLONOMIC AND NONHOLONOMIC SIMULATIONS OF QUASI-BRITTLE FRACTURE: A COMPARATIVE STUDY OF MATHEMATICAL PROGRAMMING APPROACHES

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Abstract

The cohesive-crack idealization of quasi-brittle fracture processes, if supplemented by a piecewise linear constitutive law for the interfaces, leads to linear complementarity problems (LCPs) as recurrent mathematical model governing both time-stepping (nonholonomic) and single-step (holonomic) analysis whenever the crack propagation path is a priori known. This paper is devoted to a preliminary investigation of typical linear complementarity solution algorithms, as for their ability to capture the expected multiplicity of solutions and for their main computational potentialities in quasi-brittle fracture mechanics.

1 Introduction

The cohesive-crack model widely used for the engineering analysis of fracture processes in quasi-brittle structures, rests on the following assumptions (cf. Fig. 1): (i) a locus Γ of potential displacement discontinuities (briefly called "interfaces") is characterized by a softening constitutive law relating tractions $\mathbf{p}$ to displacement jumps $\mathbf{w}$ across Γ, so

that Γ can be conceived as the union of cracks Γ_c (where $\mathbf{p} = \mathbf{0}$), process zone Γ_z (where $\mathbf{p} \neq \mathbf{0}$ and $\mathbf{w} \neq \mathbf{0}$) and undamaged material (where $\mathbf{w} = \mathbf{0}$); (ii) outside Γ, in the whole domain Ω occupied by the structure, Hookean (hyper-)elasticity holds in a regime of linear (infinitesimal) kinematics.

At least in mode I fracture, experimental investigations (cf. e.g. Alvaredo and Torrent, 1987; Wittmann and Hu, 1991) show that a piecewise linear decay of traction p for increasing opening displacement w provides an accurate description of the interface law for concrete and concrete-like materials. In this case, the tensile strength $\overline{\sigma}$ and the critical opening displacement $\overline{w}$ are the only parameters needed for the usually adopted linear decay (Fig. 1b), with the addition of the "break-point" coordinates in the case of bilinear decay.

The nonlinear interface law can be interpreted as holonomic (i.e. path-independent, reversible, nonlinear elastic) whenever regularly progressive yielding can be reasonably conjectured under monotonically increasing loads. This hypothesis confers practical meaning to non-evolutive single-step fracture analysis in finite terms, in the spirit of the so-called "deformation theory" of plasticity. The piecewise linearity of the interface behavior along Γ can be analytically described by a linear complementarity problem (LCP), i.e. by a mathematical construct which consists of a linear relationship between two orthogonal vectors with sign-constrained components. The linearity of the surrounding structure in Ω leads, through space discretization, to an LCP with the role of mathematical model governing fracture phenomena as overall structural responses.

Nonholonomic (path-dependent, irreversible) interpretation of the current process zone Γ_z and consequent incremental descriptions (in rates or finite steps) are required whenever significant local "elastic unloadings" are expected, e.g. under non-proportional loading. Then the LCP format still shows up at the constitutive level and, hence, at the structural level.

In all the above cases the LCP generally exhibits an indefinite matrix and may admit a multiplicity (in particular, a discrete set) of solutions. This

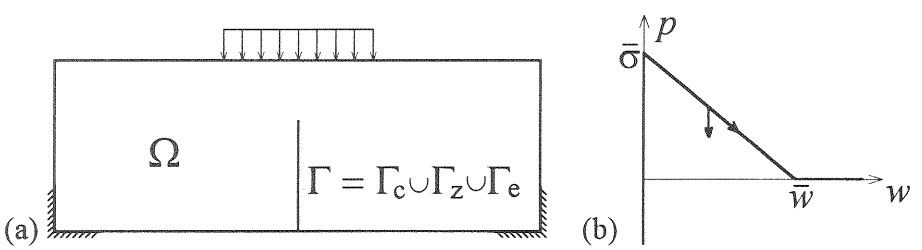


Fig. 1. Illustration of some symbols.

essential mathematical circumstances reflect mechanically crucial phenomena, such as response bifurcations and loss of overall stability.

The above outlined LCP formulations of quasi-brittle fracture analysis have been presented by Maier et al. (1993) and by Bolzon et al. (1994) on the basis of boundary element and of finite element discretizations.

This paper focuses on some computational techniques potentially apt to efficiently solve the general LCP arising in the present context and possibly to provide the complete set of alternative solutions. It is worth noting that LCP with symmetric positive-semidefinite matrices admit either one or infinite or none solution, are equivalent to convex quadratic programming problems and can be solved by traditional algorithms. They have been extensively studied since the late Sixties with reference to structural plasticity and unilateral contact (cf. e.g. Maier, 1970; Maier and Munro, 1982; Wakefield and Tin-Loi, 1990; Cottle et al., 1992).

2 Problem formulation

The following restrictions are assumed here for brevity since they preserve the essential features of the problems in point: (a) the locus Γ of possible displacement discontinuities is a priori known; (b) shear tractions and tangential relative displacements vanish along Γ (e.g. because of symmetry, as in the examples presented later), i.e. the fracture processes considered occur in mode I only; (c) a linear sloping-down branch describes the softening relationship between normal traction p and opening displacement w. Assumption (a) is not very restrictive since Γ can be formed by a set of interfaces between finite elements or cells (like in Xu and Needleman, 1994) with decreasing mesh dependence and alignment subjectivity for increasing mesh finesse.

With reference to Fig. 1b, the holonomic version of the interface law on Γ under restriction (c) can be expressed in the form:

$$\boldsymbol{\varphi} = \mathbf{a}p + \mathbf{h}\boldsymbol{\lambda} - \mathbf{b}\,\overline{\sigma} \le \mathbf{0}, \quad \boldsymbol{\lambda} \ge \mathbf{0}, \quad \boldsymbol{\varphi}^{\mathrm{T}}\boldsymbol{\lambda} \le \mathbf{0} \quad \forall \mathbf{x} \in \Gamma \tag{1}$$

$$\boldsymbol{\varphi} = \begin{Bmatrix} \varphi \\ -r \end{Bmatrix}, \quad \boldsymbol{\lambda} = \begin{Bmatrix} \lambda \\ w \end{Bmatrix}, \quad \mathbf{a} = \begin{Bmatrix} 0 \\ 1 \end{Bmatrix}, \quad \mathbf{b} = \begin{Bmatrix} 1 \\ 1 \end{Bmatrix}, \quad \mathbf{h} = \begin{bmatrix} h & -h \\ h & -h \end{bmatrix} \tag{2}$$

where φ, r, λ are auxiliary variables and $h = -\overline{\sigma} / \overline{w}$ represents a measure of softening. These relations are discussed and generalized to bilinear softening (with "break-point") in Bolzon et al. (1994).

The nonholonomic version (in rates, denoted by dots) of the interface law for the current process zone $\Gamma_z \subset \Gamma$ can be derived from (1) and reads:

$$\dot{\varphi} = \dot{p} - h\dot{w} \leq 0,\ \dot{w} \geq 0,\ \dot{\varphi}\dot{w} = 0 \text{ , on } \Gamma_z;\quad \dot{w} = 0 \text{ on } \Gamma_c;\quad \dot{p} = 0 \text{ on } \Gamma_e \qquad (3)$$

The Green function $G(\mathbf{x}, \xi)$, $\mathbf{x}, \xi \in \Gamma$, which relates tractions p to opening displacements w with homogeneous boundary conditions, could in principle be constructed on the basis of the geometric and elastic properties of the structure, so that one can write:

$$p(\mathbf{x}) = \int_\Gamma \mathbf{G}(\mathbf{x},\xi) w(\xi) d\Gamma + p^E(\mathbf{x}) \qquad \mathbf{x},\xi \in \Gamma \qquad (4)$$

where p^E denotes tractions generated by the external actions in the absence of displacement jumps, i.e. in a fictitious elastic regime.

The holonomic response of the system (in terms of p and w) to given loads is fully governed by the association of Eqs. (1) and (4). Similarly, the continuum formulation of nonholonomic analysis is achieved by associating Eqs. (3) to Eq. (4) re-written in rates.

Either a boundary element (BE) approach or a finite element (FE) method supplemented by condensation of out-of-Γ (or out-of-Γ_z) variables generates a discrete counterpart to the linear integral equation (4), namely

$$\mathbf{P} = \mathbf{Z}\,\mathbf{W} + \mathbf{P}^E \qquad (5)$$

The influence matrix $\mathbf{Z}$ preserves essential features of the kernel $\mathbf{G}$ it approximates (i.e. symmetry and semi-negativeness), provided the space modeling is such that the field-governing variables in vectors $\mathbf{W}$ and $\mathbf{P}$ be "generalized variables" in Prager's sense and, for BE discretization, a symmetric Galerkin approach is adopted (Maier et al., 1993). Consistently, let the same concept of generalized variables be adopted in the semi-discretization of the interface laws (1) and (3). Thus these laws acquire the forms, respectively:

$$\mathbf{\Phi} = \mathbf{A}\mathbf{P} + \mathbf{H}\mathbf{\Lambda} - \mathbf{B}\overline{\mathbf{P}} \leq \mathbf{0}, \quad \mathbf{\Lambda} \geq \mathbf{0}, \quad \mathbf{\Phi}^T\mathbf{\Lambda} = 0 \qquad (6)$$

$$\dot{\mathbf{\Phi}}' = \dot{\mathbf{P}}' + \mathbf{H}'\dot{\mathbf{W}}' \leq 0, \quad \dot{\mathbf{W}}' \geq \mathbf{0}, \quad \mathbf{\Phi}'^T\dot{\mathbf{W}}' = 0 \qquad (7)$$

where $\mathbf{A}^T \equiv [\mathbf{0}\ \mathbf{I}]$, $\mathbf{B}^T \equiv [\mathbf{I}\ \mathbf{I}]$, $\mathbf{I}$ being the identity matrix of order equal to the node number on iterface Γ, primes denote the restriction of all variables

to the current process zone Γ_z and to the currently active yield modes, and with self-evident meaning of the other symbols. The discretized holonomic (single-step) analysis of quasi-brittle solids is formulated by combining Eqs. (6) and (5) to obtain the following LCP:

$$\mathbf{\Phi} = (\mathbf{AZA}^{\mathrm{T}} + \mathbf{H})\mathbf{\Lambda} + (\mathbf{AP}^{E} - \mathbf{B}\overline{\mathbf{P}}) \leq \mathbf{0}, \quad \mathbf{\Lambda} \geq \mathbf{0}, \quad \mathbf{\Phi}^{\mathrm{T}}\mathbf{\Lambda} = 0 \tag{8}$$

Similarly, semi-discretization of the nonholonomic analysis turns out to be centered on the LCP arising from Eqs.(5) and (7) combined, namely on:

$$\dot{\mathbf{\Phi}}' = (\mathbf{Z}' + \mathbf{H}')\,\dot{\mathbf{W}}' + \dot{\mathbf{P}}'^{E} \leq \mathbf{0}, \quad \dot{\mathbf{W}}' \geq \mathbf{0}, \quad \dot{\mathbf{\Phi}}'^{\mathrm{T}}\,\dot{\mathbf{W}} = 0 \tag{9}$$

Matrices $\mathbf{H}$ in Eqs. (8) and $\mathbf{H}'$ in (9) reflect the softening (unstable) nature of the interface constitution, so that $\mathbf{AZA}^{\mathrm{T}}+\mathbf{H}$ and $\mathbf{Z}'+\mathbf{H}'$ may be sign-indefinite.

Evolutive analysis resting on a sequence of time steps, each of which consisting of solution to LCP (9) and linear scaling, was described in Bolzon et al. (1994). Alternatively, the finite-step problem can be formulated by a backward-difference scheme (De Donato and Maier, 1972) which again leads to a LCP in finite increments.

What precedes shows that both single-step holonomic and evolutive nonholonomic analyses are amenable to a common LCP format:

$$\mathbf{y} = \mathbf{M}\,\mathbf{z} + \mathbf{q} \leq \mathbf{0}, \quad \mathbf{z} \leq \mathbf{0}, \quad \mathbf{z}^{\mathrm{T}}\mathbf{y} = 0 \tag{10}$$

where as crucial feature (in contrast to what occurs in traditional plasticity and contact problems), matrix $\mathbf{M}$ is not positive semidefinite (nor symmetric) in general. Clearly, this conclusion holds also outside the restrictions listed earlier, provided a piecewise linear model is adopted for the interface law.

3 Examples

Two familiar cases are analyzed below for reference in the subsequent discussion of solution algorithms.

Fig. 2 shows results concerning a 3-Point-Bending (3PB) test characterized by the following parameters: length 400 mm; height and depth 100 mm; Young's modulus E = 14700 MPa; Poisson's ratio $\nu = 0.1$; tensile strength $\overline{\sigma} = 1.285$ MPa; critical opening displacement

$\overline{w} = 0.03$ mm. Solid lines represent the solutions obtained from evolutive analyses with a coarse mesh (5 nodes retained on the interface Γ) and a refined mesh (80 nodes on the same interface); circles visualize the single-step solutions of the holonomic problem based on 5-node discretization. Analyses with different numbers of pairs of complementary variables (ranging between 5 and 160) have been carried out but are not documented here; the mesh designed for giving the elastic response represented by integral equation (4) uses 3600 nodes for modeling half the specimen.

The main features of the 3PB test (namely: the initial elastic branch; the limit point or peak; the unstable behaviour beyond the peak) can be well captured with only few variables on the interface; increasing the number of unknowns mainly smoothes the asperities of the load-displacement curves. Excellent agreement was found between the results of evolutive and single-step analyses for the same interface discretization. In fact, in this case fracture develops with regularly progressive yielding (no crack closure), so that the holonomic and the nonholonomic description of the process are fully equivalent.

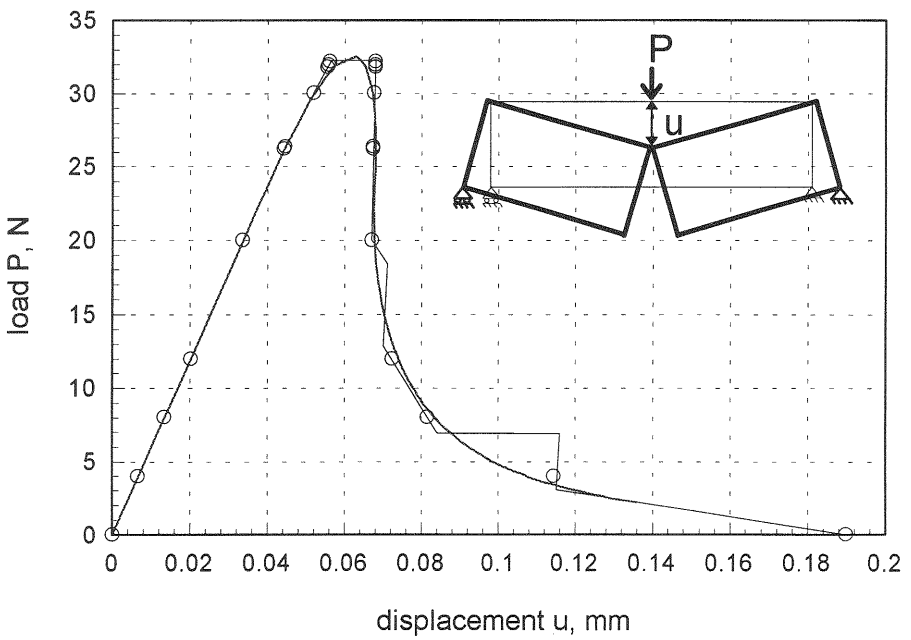
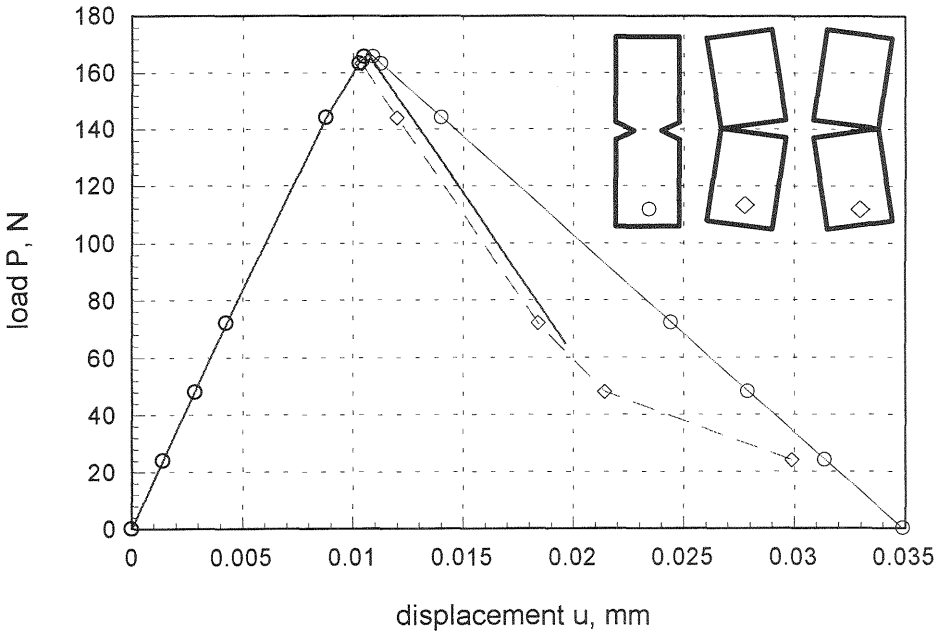
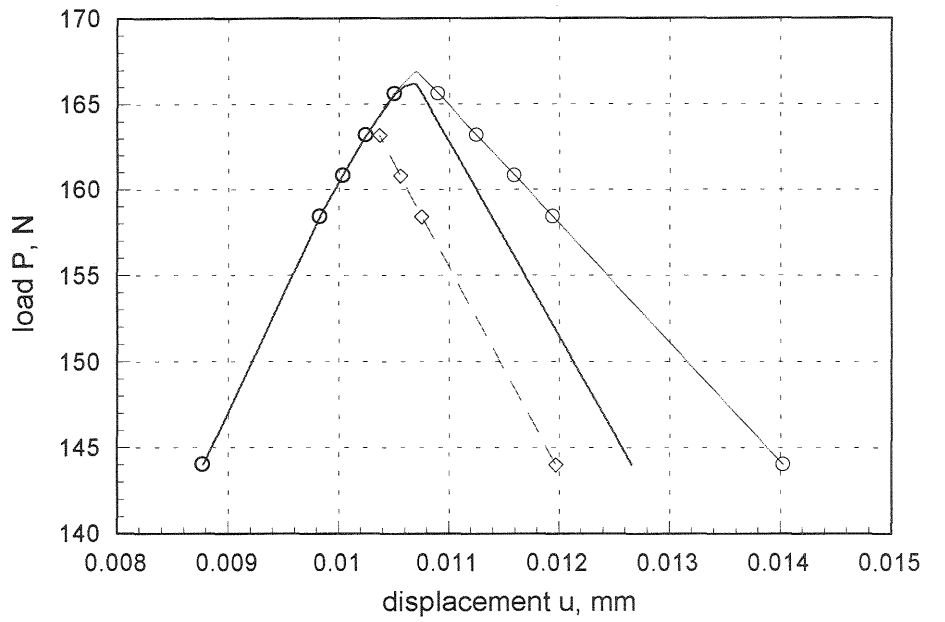


Fig. 2. Simulations of 3-Point-Bending tests: evolutive (light line: 5 interface nodes; heavy line: 80 interface nodes); holonomic single-step (circles).



(a)



(b)

Fig. 3. Simulations of 2-Notch-Tensile tests: (a) evolutive nonsymmetric (heavy line); evolutive symmetric holonomic or nonholonomic (light line); holonomic single-step (symmetric solutions: circles; nonsymmetric solutions: rhombs); (b) details by zooming (a).

Results for the 2-Notch-Tensile (2NT) test are shown in Fig. 3, geometry and elastic properties being the same as in Rots and de Borst (1989), with $\overline{\sigma} = 3.4$ MPa and $\overline{w} = 0.0698$ mm. The resultant of the end tractions isplotted versus the relative displacement of the mid-points of the specimen end sides. Solid lines represent the results of the evolutive analyses, circle and rhombs refer to the single-step holonomic solutions, all based on a 21-node discretization in space of the interface.

Bifurcation of the overall response into a symmetric and two nonsymmetric configurations is observed, starting from a point on the ascending branch of the load-displacement plot and leading to different peak loads. Local unloading occurs for increasing overall load, so that the equivalence between holonomic and nonholonomic description is invalid. This is evidenced by Fig. 4, where the opening displacement profiles are drawn for the symmetric response on the ascending branch and for the nonsymmetric configurations resulting from holonomic and nonholonomic analyses, under a load just below the peak resulting from the holonomic description of the fracture process.

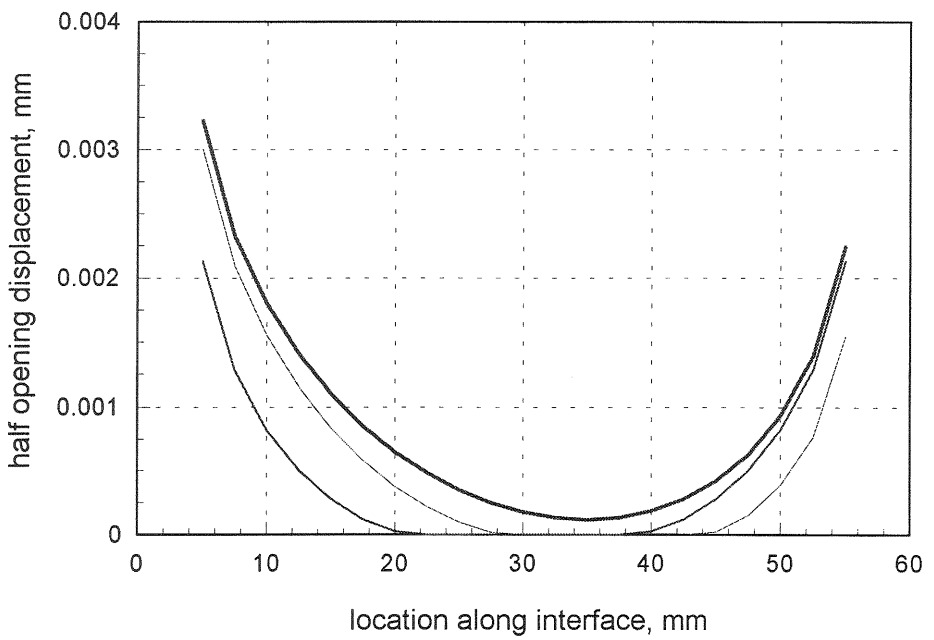


Fig. 4. Opening displacements in 2-Notch-Tensile test simulation for P = 163 N: the symmetric response on the ascending branch (light line); nonsymmetric nonholonomic analysis (heavy line); nonsymmetric holonomic analysis (very thin line).

4 Solution methods

The general LCP (10) turns out to be equivalent to: a nonconvex quadratic program (QP) (cf. e.g. Harker and Pang, 1990); a system of non-smooth nonlinear equations (Harker and Xiao, 1990; Pang and Gabriel, 1993; Ralph, 1994); a hemivariational inequality (Panagiotopoulos, 1994). These equivalencies will not be considered herein explicitly but are often useful for the theoretical foundations of LCP algorithms.

The spectrum of algorithms now available in the literature, but largely untested in the present engineering context, include the following categories: (a) enumerative, branch-and-bound methods with finite termination; (b) Newton-type algorithms with asymptotic termination; (c) genetic algorithms for direct search optimization (cf. e.g. Goldberg, 1989); (d) neural networks (cf. e.g. Avdelas et al., 1995); (e) sequential convex optimizations (Mistakidis and Panagiotopoulos, 1994).

In this paper, for paucity of space, only algorithms representative of the approaches (a) and (b) will be tested and briefly discussed to the present purposes, while others will be investigated elsewhere.

The enumerative method (Judice and Mitra, 1988) is based on the observation that the solution of an LCP can be found by an exhaustive exploration of a binary tree. The tree can be generated as follows: the first node corresponds to an initial "basic feasible solution" (satisfying the linear constraints of the LCP; if no such a solution exists, then LCP has no solution); other nodes are generated by solving in each case a linear programming sub-problem, namely by minimizing, through a modified simplex method, either y_i or z_i subject to the linear constraints of the original LCP and the constraints $y_j = 0$ or $z_k = 0$ fixed in upper level nodes. Two cases can then occur: either the minimized variable assumes a positive value at optimum, then the corresponding node is pruned and the node is fathomed; or the minimized variable is zero at optimum, then it is fixed to zero in all descendent paths of the tree and (in the case of non-degeneracy) the variable has become unbasic and is no longer eligible to become basic.

In this manner, by maintaining feasibility in each iteration, the procedure attempts to find a complementary solution $(\mathbf{z}, \mathbf{y})$ satisfying the constraint $\mathbf{z}^T \mathbf{y} = 0$ by generating successive nodes of the tree. However, generating and exploring all 2^{n+1}-1 nodes of the tree cannot be achieved in reasonable computer time for most practical problem sizes n. Success depends primarily on the nature of the problem and on the efficiency of heuristics to fathom nodes (leading to a termination of the relevant branches).

To assess the numerical performances of the method, analyses have been performed on the 3PB and 2NT specimens of Section 3, and computing

times for the holonomic analyses on an HP735 workstation are plotted in Fig. 5 versus the number of unknowns. It can be seen that time consuming grows almost exponentially with the problem size n. Therefore, holonomic description seems to be particularly disadvantageous, since the nodes of the interface discretization are considered all together, and the number of unknowns for each node is at least two and increases with the complexity of the assumed piecewise linear interface law. However, this method can give sure answer at limited costs when no solution exists, as it happens when the limit load of the structure is exceeded by the applied load.

Al-Khayyal (1987) discussed the use of various heuristics, coupled with a reduced gradient method, designed to speed up the basic tree search algorithm; these are however aimed at obtaining one solution to the general LCP. More promising future approaches would be to exploit the peculiarity of the expected solutions (made of subsets of consecutive zeros either of the vector **z** or of the vector **y**) and to implement a parallel version, possibly without communication between the subproblems of the enumerative scheme (Laursen, 1994).

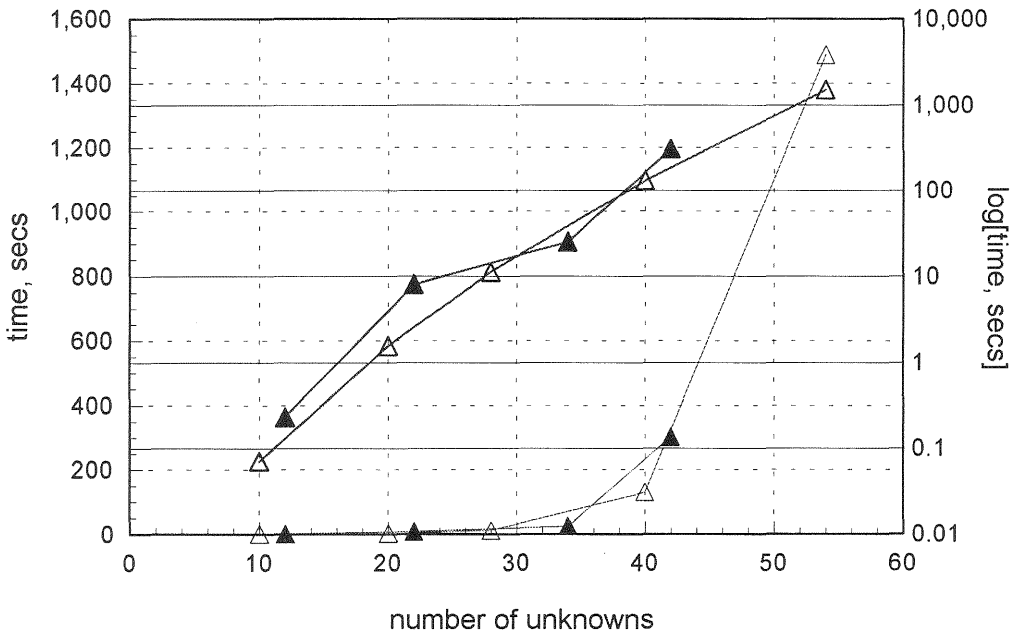


Fig. 5. Computing time versus number of unknowns in simulations of 3-Point-Bending test (white triangles) and 2-Notch-Tension test (black triangles) by the enumerative method: Cartesian scale (left; light lines) and logarithmic scale (right; heavy lines).

Classical algorithms, such as pivoting-based Lemke method or other methods proposed for computing solutions to LCPs with semidefinite matrices, can still be tried although not much is known about their ability to solve a general LCP (see the survey by Harker and Pang, 1990). One of the most powerful schemes is a generalization, to the nonsmooth case, of the classical Newton's method for solving systems of nonlinear equations. Specific computer implementations include: (i) the B-DIFF code of Harker and Xiao (1990) in which the search direction is determined by solving a system of equations; (ii) the NE/SQP program of Pang and Gabriel (1993) which makes use of the "min" operator and solves a quadratic programming subproblem to find a search direction; and (iii) PATH, the path-following code of Dirkse and Ferris (1993).

The PATH solver is an implementation of a stabilized Newton method for solving the Mixed Complementarity Problem (MCP) which requires the solution $\mathbf{z}$, $\mathbf{y} \geq \mathbf{0}$, and $\mathbf{v} \geq \mathbf{0}$ to the following set of relations:

$$\mathbf{F}(\mathbf{z}) = \mathbf{y} - \mathbf{v}, \quad l\mathbf{1} \leq \mathbf{z} \leq u\mathbf{1}, \quad (\mathbf{z} - l\mathbf{1})^{\mathrm{T}}\mathbf{y} = 0, \quad (u\mathbf{1} - \mathbf{z})^{\mathrm{T}}\mathbf{v} = 0 \tag{11}$$

where: $\mathbf{F}(\mathbf{z})$ is a given function $\Re^n \rightarrow \Re^n$; l, u are given lower and upper bounds, respectively, and $\mathbf{1}$ is the vector with all entries equal to 1. The LCP is a special case of the MCP obtained by setting $\mathbf{F}(\mathbf{z}) = \mathbf{M}\mathbf{z} + \mathbf{q}$, $l = 0$ and $u = +\infty$.

In the standard linesearch-damped Newton's method for solving smooth equations, three steps are distinguishable: linearization, direction-finding and linesearching. The PATH solver similarly involves three analogous steps: approximation, path generation and pathsearch damping.

In order to apply a damped Newton method, the MCP is rewritten as a zero-finding problem by using the nonsmooth "normal" equation (NE)

$$\mathbf{F}_{\mathrm{B}}(\mathbf{x}) = \mathbf{F}(\mathbf{x}_{\mathrm{B}}) + \mathbf{x} - \mathbf{x}_{\mathrm{B}} = \mathbf{0} \tag{12}$$

where $\mathbf{x}_{\mathrm{B}}$ is the Euclidean projection of $\mathbf{x}$ onto the rectangular set or "box" $\mathrm{B} = [l, u]$. In the case of LCP, $\mathbf{x}_{\mathrm{B}}$ is the vector in $\Re^n_+$ whose i-th component is $\max(x_i, 0)$. It can be seen that if a vector $\mathbf{x}$ solves NE (12) then $\mathbf{z} = \mathbf{x}_{\mathrm{B}}$ solves the MCP and, conversely, a solution $\mathbf{z}$ of the latter yields a solution $\mathbf{x} = \mathbf{z} - \mathbf{F}(\mathbf{z})$ of the former. The normal map $\mathbf{F}_{\mathrm{B}}$ is a piecewise smooth map, continuous on $\Re^n$; in case of our LCP, $\mathbf{F}_{\mathrm{B}}$ is only nonsmooth on the boundaries of orthants in $\Re^n$.

Typical of Newton approach, in the general case $\mathbf{F}_B$ is approximated, through a standard first-order approximation at $\mathbf{x}_k$, by a piecewise linear normal map $\mathbf{A}_k$, which obviously coincides with $\mathbf{F}_B$ itself for the LCP.

For finding a Newton point, i.e. a zero of function (12) or of its approximation $\mathbf{A}_k$ at $\mathbf{x}_k$, a path is constructed between the current point $\mathbf{x}_k$ and the corresponding Newton point by pivotal techniques using a parametric (in t) extension of Lemke method. Each linear portion of the path is identified by a new pivot step, and the whole path generation scheme involves forcing parameter t from 1 down to 0 (details in Dirkse and Ferris, 1993).

The robustness and efficiency of PATH is due both to its theoretical soundness and to its implementation details. The PATH solver was tried on the 3PB and 2NT problems in Section 3, of size $n = 42$ and $n = 146$, respectively, using the default setting in all instances. All runs were carried out on a Sun-Sparc2.

Algorithm PATH is able to generate one solution each run. An attempt was then made to capture all solutions by trying different starting vectors $\mathbf{z}$. The crude scheme adopted to generate these vectors is as follows. The starting $\mathbf{z}$ vector was divided into 6 subvectors $\{\mathbf{z}_1, ..., \mathbf{z}_6\}$ (a different size can of course be used); in the case of $n = 42$, each subvector was of length 7×1, while for $n = 146$ each was of length 24×1 except for $\mathbf{z}_6$ being of length 26×1. All elements of a subvector were assigned a value of either 0 or $z^* = 0.001$ in both cases. This gave rise to an obvious 64 (or 26) combinations to try for each problem. The main reasons for choosing such a scheme were that: (i) 6 subvectors do not lead to an unduly large number of trials; (ii) it is expected that any cracking occurs in definite patterns, with either non zero z-values occurring in consecutive or alternate sequences.

For all cases ran, the above scheme managed to capture all solutions (the numbers of which were known in advance). As a typical example: for the 42-variable case, solutions were obtained after 9 runs; for the 64 runs, the number of times the same solution was obtained were 36, 11, 7 and 6, with 4 failed runs; and the average time taken for each successful run was about 0.2 sec. The larger 146-variable case was similarly encouraging: both solutions being obtained after 4 runs; one solution was obtained 41 times, the other 17 times, with 6 failures. The average computing time for obtaining a solution was about 1.7 secs.

5 Conclusion

Holonomic (single-step) and nonholonomic (time-stepping) analyses of quasi-brittle fracture based on the cohesive-crack idealization with piecewise linear interface law can be formulated as a general linear complementarity problem. Among recent ad hoc solution algorithms, an enumerative technique and a Newton-type method have been investigated and found apt to provide the possible multiplicity of solutions, but from the computing burden standpoint, still improvements are needed which exploit the peculiarities of the specific context.

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