

ITERATIVE STRATEGIES BASED ON CONSTITUTIVE DISSIPATION

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Key words: Arc-length control, non-linear analysis, Indirect Displacement Control Strategy, dissipation, concrete

Abstract. FE formulation of solid mechanics problems typically require iterative strategies to solve the resulting nonlinear system. Basic strategies with prescribed load values, such as the Newton-Raphson method, are not valid in the presence of structural snap-back due to material or geometric non-linearity. In this case, the most common strategy is the cylindrical Arc-length method, which prescribes the norm of displacements as constraint, in order to obtain the load factor increment. However, because the constraint is quadratic, additional non-trivial criteria need to be introduced for choosing the appropriate solution, and the wrong choice may lead to potential spurious unloading among other problems. As a way to overcome these shortcomings, alternative methods have been proposed which are based on an energy dissipation constraint. Constitutive dissipation may be considered as an always increasing “time” parameter with the advantage that the corresponding constraint equation is always linear. Iterative methods based on a dissipation constraint can be found in the literature.]. But most of those formulations are based on specific constitutive models. In contrast, the present formulation is general in the sense that it is valid for any constitutive model, as long as the model subroutine provides, additional to the standard output, also the appropriate values of dissipation and dissipation derivatives. Some application examples in concrete structures with progressive fractures are also provided to illustrate the performance of the model proposed.

1 INTRODUCTION

Discontinuities such as cracks or fractures play a fundamental role in the mechanical behavior of concrete, rock and other quasi-brittle materials. Other sources of non-linearity may be plasticity or distributed damage. The numerical solution of those problems inevitably require iterative methods. The Newton-Raphson (NR) method has been extensively used in the analysis of non-linear solid mechanics problems because it is an effective and intuitive method, relatively simple to implement, and with different variants or adaptations such as full Newton-Raphson, quasi-Newton-Raphson or modified Newton-Raphson [1]. However, in NR methods, the loading factor is always monotonically increasing, and therefore these methods cannot follow load-displacement curves exhibiting “snap-back” behavior that may take place in very brittle materials or structures. For these situations, more sophisticated iterative techniques such as Arc-Length (AL) or Indirect Displacement Control (IDC) methods have been proposed.

Arc-Length technique was originally developed by Wempner and Riks [2,3], and relevant alternative formulations were extensively used such as [1,4,5]. In particular, Crisfield [1] developed a cylindrical Arc-Length strategy, probably the most popular of these methods and

widely used even in commercial codes. Arc-Length strategy has been modified or adapted by [6-8], among others. Arc-Length (AL) strategy is based on the calculation of the load factor at each iteration with the objective of satisfying a prescribed "constraint", the increment of the norm of the overall nodal displacement vector. As a result, a quadratic polynomial expression is generally obtained, this complicates the solution with possibility of negative discriminant or bad solution selection (for example, spurious unloading). Similarly, in Indirect Displacement Control (IDC) methods the constraint control can be adapted to a region e.g. near the crack mouth [7, 9, 10], although this requires some *a priori* knowledge of the precise location of such crack.

Alternatively, another family of methods with variable load step size has been proposed using as a constraint the dissipation energy. This may be an advantageous choice in inelastic dissipative problems, because dissipation is an always-growing magnitude and it leads to a linear constraint, thus avoiding the introduction of additional criteria to choose the correct solution. Gutiérrez [11] introduced the use of constitutive dissipation as a parameter to control the loading process in non-linear solid mechanics; in particular, he developed a formulation based on energy release control, for the numerical simulations of failure in quasi-brittle solids using a scalar damage model. Later, the formulation has been expanded in the literature [12-18] to generalize it in different context such as geometrically linear and non-linear damage, or for plasticity models. Recently, Özdemir [19] has adapted May et al. (2016)'s formulation to be used in commercial software packages, and in particular in Abaqus.

The above considerations motivate the development and implementation of a new Indirect Displacement Control method based on energy dissipation in the framework of quasi-brittle materials with discrete fractures represented by elasto-plastic zero-thickness interface elements.

2 IDC METHOD BASED ON ENERGY DISSIPATION

Generally speaking, when the mechanical behavior of the domain or structure is nonlinear, an incremental-iterative procedure is required to solve the nonlinear equations. The iterative procedure may be seen as a sequence of trials (iterations) of the displacement vector increment (${}^i\Delta\mathbf{u}$), and for each of those iterations a correction of the displacement vector is introduced (${}^i\delta\mathbf{u}$) until the solution satisfies mechanical equilibrium and constraints. This may be expressed as:

$${}^i\Delta\mathbf{u} = {}^{i-1}\Delta\mathbf{u} + {}^i\delta\mathbf{u} \quad (1)$$

where i represents the current iteration and the correction ${}^i\delta\mathbf{u}$ is calculated as a linear solution of residual forces from previous iteration ${}^{i-1}\mathbf{t}$, plus the variation of external forces in the current iteration ${}^i\delta\lambda\mathbf{q}$:

$${}^i\delta\mathbf{u} = ({}^{i-1}\mathbf{K})^{-1} ({}^i\delta\lambda\mathbf{q} + {}^{i-1}\mathbf{t}) \quad (2)$$

Rearranging terms as follows ${}^i\delta\mathbf{u}^I = ({}^{i-1}\mathbf{K})^{-1}\mathbf{q}$ and ${}^i\delta\mathbf{u}^{II} = ({}^{i-1}\mathbf{K})^{-1}{}^{i-1}\mathbf{t}$, equation (2) may be expressed as:

$${}^i\delta\mathbf{u} = {}^i\delta\lambda {}^i\delta\mathbf{u}^I + {}^i\delta\mathbf{u}^{II} \quad (3)$$

Until here, the incremental-iterative strategy depends on the load factor ${}^i\delta\lambda$, which has to be determined as the result of the imposed constraint, and therefore may have different expressions. For example, Crisfield uses the norm of the incremental displacement as the Arc-Length constraint,

$${}^i\Delta l^2 = {}^i\Delta\mathbf{u}^T {}^i\Delta\mathbf{u} \quad (4)$$

and developing this equation the classical second-degree expression for the load increment is obtained (see e.g. [1,20]), from which the choice has to be made of the correct solution (or alternative strategy provided if discriminant negative, i.e. no solution exists). In the present study, these choices have been made according to the criterion proposed in [1].

The Arc-Length method is very robust and has been used and implemented in a wide variety of codes due to its effectiveness, especially in the description of Snap-Back (SB) and Snap-Through (ST). However, in situations with Snap-Back, where the softening slope is very sharp and similar in magnitude to the elastic unloading, the root associated to an elastic/spurious unloading can be mistakenly chosen. As a way to remedy these shortcomings, this article focuses on the use of a dissipation constraint (alternative to Crisfield's displacement norm constraint). If done properly, this energy constraint approach leads to a linear equation with a single solution valid in principle for any dissipative constitutive model [21]:

$${}^i\delta\lambda = \frac{\Delta\bar{W}^D - {}^{i-1}\Delta W^D - \left(\frac{\partial W^D}{\partial \mathbf{u}}\right) {}^i\delta\mathbf{u}^{II}}{\left(\frac{\partial W^D}{\partial \mathbf{u}}\right) {}^i\delta\mathbf{u}^I} \quad (5)$$

In this expression, the prescribed increment of dissipation is $\Delta\bar{W}^D$, ${}^{i-1}\Delta W^D$ represents the total energy dissipation accumulated during the current iterative process since the last converged state, and $\partial W^D / \partial \mathbf{u}$ is the vector of derivatives of total element dissipation with respect to nodal displacements, which is calculated as an integral of the derivative of constitutive dissipation w.r.t. strain (or relative displacements, in interfaces), which is a new magnitude to be derived from the constitutive model.

The evaluation of constitutive dissipation derivatives also makes it possible to calculate the dissipation rate associated to each of the two roots of the classical AL method, which in turn may be used as alternative criterion to choose between the two roots, in the case of using the traditional cylindrical AL method. This option is labeled as "AL(D)" in the example of the next section.

3 NUMERICAL EXAMPLE

The three-point bending (TPB) test is used to validate and compare the load control strategies based on dissipation energy. The example consists of a beam of 5x1m simply supported at the two lower corner nodes, with the left corner totally restrained. The loading consists of an increasing prescribed vertical displacement at the top central point of the beam (Fig. 1). This domain is discretized into a regular mesh of 100x20 linear quadrangles and 20 zero-thickness

interface elements (Fig. 2).

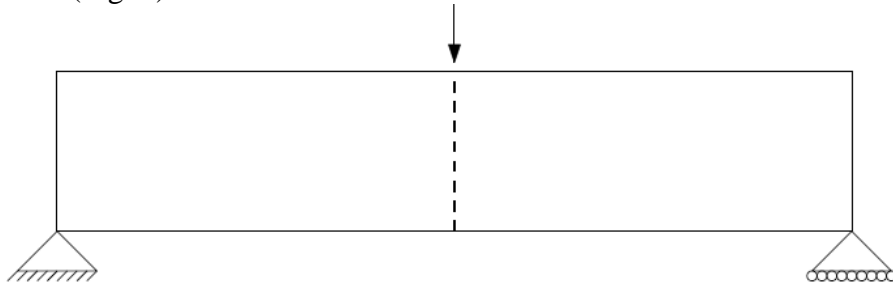


Figure 1: TPB test Boundary conditions.

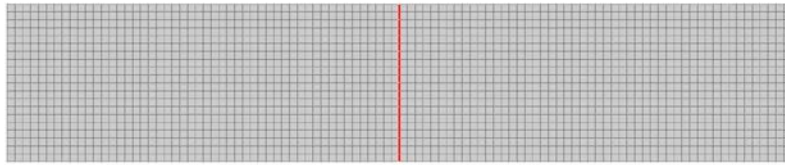


Figure 2: TPB test mesh discretization. Zero-thickness interface elements are inserted between continuum elements and are represented in red

Small strain and linear elasticity are assumed for the continuum, with Poisson's ratio $\nu = 0.0$ and Young's modulus taking one of the three following values depending on the case: $E = 6000$ MPa (Case A), $E = 7000$ MPa (Case B) and $E = 8000$ MPa (Case C). A single line of interface elements is pre-inserted along the central vertical cross-section of the beam (dashed line). These elements are equipped with the fracture-based elastoplastic constitutive law developed in [24], with the following parameter values: normal and tangential elastic stiffness $K_N = K_T = 10^7$ MPa/m, tensile strength $\chi = 2$ MPa and mode I fracture energy $G_f^I = 4 \cdot 10^{-4}$ MPa·m. Other model parameters not relevant in this case are cohesion $c = 10$ MPa, friction angle $\tan \Phi = 0.7$, limit stress dilatancy $\sigma_{dil} = 20$ MPa and fracture energies in mode IIa $G_f^{IIa} = 4 \cdot 10^{-3}$ MPa·m.

In Fig.3, the load-displacement curve obtained for the TPB problem in the three cases with different elastic modulus (A, B or C), and with the four iterative strategies mentioned above, are represented. These strategies were: Newton-Raphson (“NR”, upper-left diagram (a)), proposed IDC-dissipation (labelled “IDC-D”, upper-right diagram (b)), cylindrical arc-length (labelled “AL”, lower left diagram (c)) and cylindrical arc-length with selection of root based on constitutive dissipation (labeler “AL(D)”, lower right diagram (d)). As shown in Figure 3, the proposed strategies based on dissipation lead to consistent load-displacement curves in the three cases with different elastic modulus, while the traditional Newton-Raphson and Cylindrical Arc-Length strategies are not able of correctly reproducing the snap-back response of cases A and B. The Newton-Raphson strategy simply cannot follow a snap back curve which implies a negative load-factor increment, while the cylindrical Arc-Length strategy, which in general allows for negative-load factors, in these two cases fails in making the right choice among the two solutions of the quadratic constraint equation, thus leading to spurious unloading (Case B) or lack of convergence (Case C).

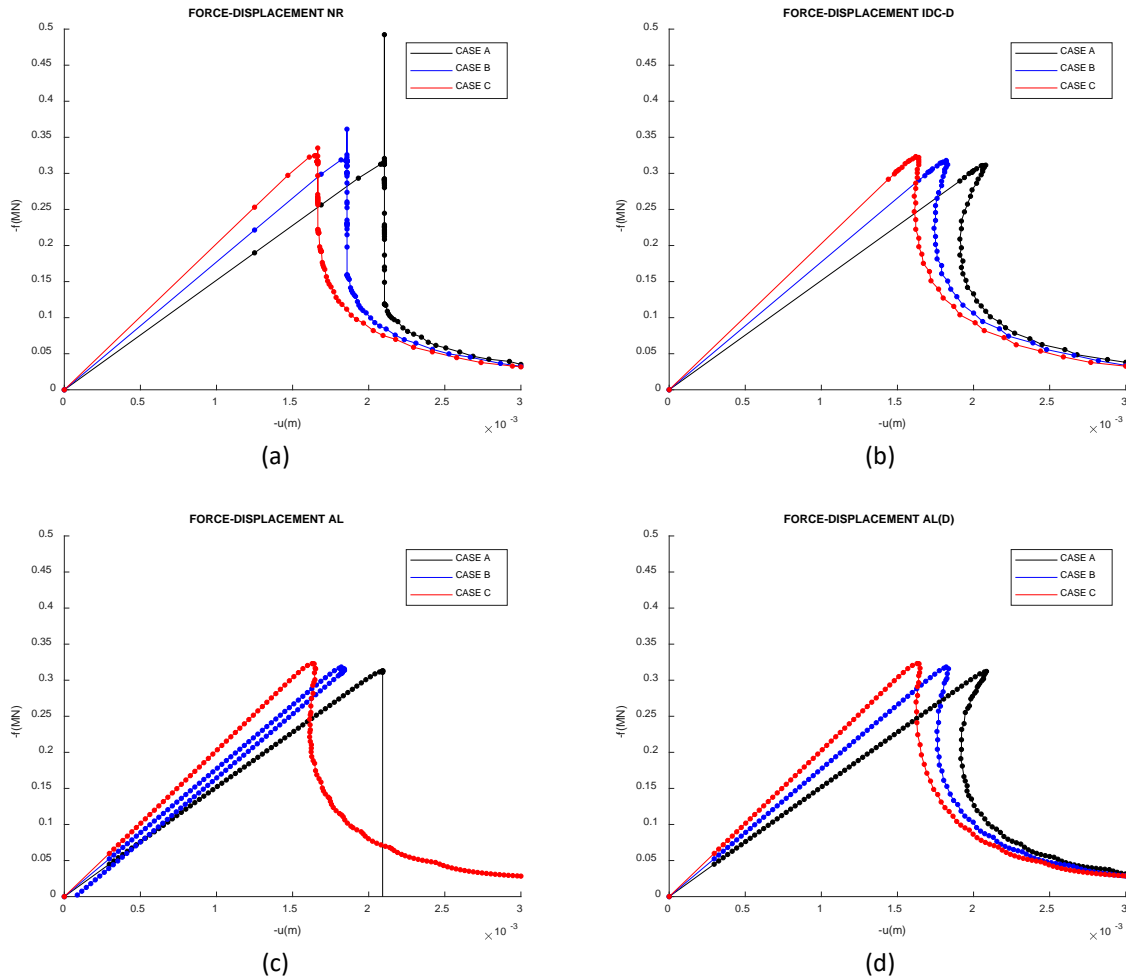


Figure 3: Three-point bending (TPB) test for the different cases: in black Case A ($E = 6000$ MPa), depicted in blue Case B ($E = 7000$ MPa) and represented in red Case C ($E = 8000$ MPa). The load-displacement curves are solved with the following strategies: (a) Newton-Raphson, (b) Indirect Displacement Control based on energy dissipation, (c) Cylindrical Arc-Length, root selection based on the closest solution to the old incremental direction, and (d) Cylindrical Arc-Length, root selection based on energy dissipation.

Figures 3(b) and 3(d) based on dissipative-control strategies, exhibit both practically the same load-displacement curves; however note that the IDC strategy does it using fewer increments because, using only energy dissipation norm to define the load increment, the elastic loading branch (which does not cause any dissipation) is entirely included in the first increment which extends to the point of the curve at which dissipation has reached the target value.

In order to compare the efficiency of the various methods, the same calculation has been solved using an automatic adjustment of the constraint size so that the calculation takes a certain desired number of iterations. In this example, the desired number of iterations has been set to $n_{iter} = 10$, and Table 1 summarizes the number of increments needed by AL(D) and IDC-D strategies. The first three columns show the number of increments needed in the AL(D) strategy (first column for the total, second for the elastic part of the curve, and third for the post-peak part), while the last column shows the total number of increments needed for the IDC-D strategy, which is always much lower than the AL(D). But even if, for not taking into account

the elastic branch (for which the IDC-D strategy does not need any increment) only the post peak part of the AL(D) is considered, still the IDC-D turns out more efficient in this particular calculation.

Table 1: Number of increments of a variable step strategy based on the number of iterations, which is needed in strategy AL(D) (AL with root selection based on energy dissipation) and in strategy IDC-D (IDC based on energy dissipation), for the three cases A, B and C (different elastic modulus).

	AL(D)			IDC-D
	Total N.increments = N.incrs. elastic part + N.incrs. post-peak			Total N.incrs.
Case A	128	56	72	46
Case B	115	46	69	46
Case C	110	40	70	45

4 CONCLUDING REMARKS

This article compares different iterative-incremental strategies used in non-linear material calculations for concrete and geomaterials. In particular, it focuses on the effectiveness of using dissipation energy as a control variable, taking advantage of the fact that the fracture process in quasi-brittle materials is controlled precisely by this magnitude. The strategy has been developed as an Indirect Displacement Control (IDC) method based on energy dissipation, in the framework of quasi-brittle materials with discrete fractures represented by elasto-plastic zero-thickness interface elements. In this context a TPB test example has been run with the different strategies to show and validate dissipation-based strategies in a case with snap-back. A practical advantage of the strategy developed, is that it has similar structure as the traditional cylindrical AL strategy, and therefore its implementation in an existing FE code is quite direct. A second advantage is that it is applicable to any constitutive law with energy dissipation (elasto-plasticity, damage, etc.), as long as the required magnitudes (dissipation increments, and their derivatives with respect to constitutive deformations) are provided as outputs by the constitutive subroutine.

ACKNOWLEDGMENTS

This work was partially supported by research grants BIA2016-76543-R from MEC (Madrid), which includes FEDER funds, and 2017SGR-1153 from Generalitat de Catalunya. The FPI fellowship from MEC (Madrid) to the first author is also gratefully acknowledged.

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