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Parametric Study of the SUR Method for the Simulation of Quasi-Brittle Materials

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Abstract—**In this paper, the authors study the influence the form of the smooth unloading-reloading function on the nonlinear solution characteristics of the recently developed smooth unloading-reloading (SUR) approach for nonlinear finite element simulation of quasi-brittle materials. The SUR method uses a target function and a smooth unloading-reloading function to compute an approximate tangent matrix with an incremental-iterative Newtown type solution scheme. The smooth unloading-reloading function has two main parameters a_p and ν which affect the form of the SUR function. The study is illustrated using different values of the two main parameters of the SUR curve. A Mathcad code has been written to carry out the nonlinear finite element analysis of the numerical example presented in this paper.**

Index Terms: **Nonlinear finite element analysis, smooth unloading-reloading method, quasi-brittle materials, damage model.**

I. INTRODUCTION

The development, growth and coalescence of micro-cracks in quasi-brittle materials, such as concrete, induce degradation in mechanical performance in both strength and stiffness of the material when loaded beyond its elastic limit. The degradation is reflected macroscopically as strain-softening behavior. This behavior gives rise to the issue of stability and convergence difficulties. Therefore, the nonlinear finite element analysis of such materials is still a truly numerical challenging undertaking [1, 2].

The nonlinear systems of equations resulting from the finite element simulation of quasi-brittle structures are frequently solved using incremental-iterative solution schemes based on Newton-Raphson algorithm. However, existing Newton-based incremental-iterative schemes, such as standard Newton-Raphson, modified Newton-Raphson, Quasi-Newton-Raphson, line search algorithms and arc-length procedures, often suffer from stability and convergence difficulties and thus can be inappropriate for the numerical simulation of many quasi-brittle materials problems [3].

None of the aforementioned incremental-iterative solution schemes based on Newton-Raphson are completely robust, nor do they fully resolve all the stability and convergence difficulties encountered when analysing quasi-brittle structures. In an attempt to avoid such difficulties, a number of researchers have developed solution procedures that either avoid (or limit) the use of iterations. These methods include 'implicit-explicit' approach of Oliver et al [4], 'modified implicit-explicit' method [5] and 'Sequentially Linear Approach' (SLA) [6-9].

Although there are considerable benefits to using these non-iterative approaches, they can result in non-smooth responses, and would require further development if they are to be applicable to problems that include multiple materials and several non-linear processes [10].

Recently, Alnaas and Jefferson [11] developed a novel incremental-iterative numerical approach, called smooth unloading-reloading 'SUR', for the nonlinear finite element analysis of quasi-brittle structures. This method improves the robustness and convergence properties of solutions to fracture problems in quasi-brittle materials. The SUR approach uses a target function and a smooth unloading-reloading function to compute an approximate tangent matrix in an incremental-iterative Newton type solution procedure. The target function gives the equivalent uniaxial stress, which in 1D is directly proportional to the maximum strain experienced and the smooth unloading-reloading function has a small positive gradient at its intersection with the target softening curve. A key feature of the SUR method is that it is always uses a positive definite stiffness matrix and never resulted in a breakdown of the nonlinear solution procedure. See **section 3** for more details of the SUR method.

In this paper, two main parameters ν and a_p of the SUR function, which affect the form of the SUR function, are investigated and their effects on the on the convergence characteristics of the developed smooth unloading-reloading method are explored.

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II. CONSTITUTIVE MODEL

In this study, the isotropic damage model of Oliver et al. [12] is employed. This isotropic damage model is based on the simplifying assumption that stiffness degradation is isotropic and the loss of material stiffness is characterised by a scalar damage variable ($\omega \in [0, 1]$), in which ω =0 for undamaged material and ω =1 for fully damaged materials. The constitutive equation for the isotropic damage model is expressed as:

$$\boldsymbol{\sigma} = (1-\omega)\, \mathbf{D_0} : \boldsymbol{\varepsilon} \tag{1}$$

The where $\boldsymbol{\sigma}$ and $\boldsymbol{\varepsilon}$ are the stress and strain tensors respectively; $\mathbf{D_0}$ donates the elastic stiffness of the undamaged material and the damage variable ω is a function of a damage evolution parameter r_p. The effective stress is defined as follows:

$$\boldsymbol{\sigma_0} = \mathbf{D_0} : \boldsymbol{\varepsilon} \tag{2}$$

r_{eff} is a scalar measure of the current 'effective' stress and is computed by:

$$r_{eff} = \sqrt{\boldsymbol{\sigma_0}^{+} : \mathbf{D_0}^{-1} : \boldsymbol{\sigma_0}^{+}} \tag{3}$$

where $\boldsymbol{\sigma_0}^{+}$ denotes the positive part of the effective stress tensor, and is given by the following form:

$$\boldsymbol{\sigma_0}^{+} = \sum_{i=1}^{3} \langle \boldsymbol{\sigma_0}_i \rangle \mathbf{p}_i \otimes \mathbf{p}_i \tag{4}$$

where $\langle \boldsymbol{\sigma_0}_i \rangle$ stands for the positive part of the i^{th} principal effective stress $\boldsymbol{\sigma_0}_i$, $\mathbf{p}_i$ represents the i^{th} stress eigenvector. Symbol $\otimes$ denotes the tensor product, and symbol $\langle \mathbf{x} \rangle$ is the Macaulay bracket, in which

$$\langle x \rangle = x,\ \ if\ x \geq 0; \quad \langle x \rangle = 0,\ \ if\ x < 0$$

The damage loading function is expressed in terms of the effective stress and the scalar damage evolution parameter (r_p). The damage loading function is given by:

$$f(r_{eff}, r_p) = r_{eff} - r_p \tag{5}$$

r_p is a measure of the largest effective stress reached in the history of the material up to the current state. Initially, r_p is equal to r_k, which is the damage evolution parameter at the peak of the uniaxial stress curve and is related to the peak stress f_t of the material in uniaxial tension. The expression used to compute r_k is described in section 3.

Damage evolution is controlled via the standard Kuhn-Tucker loading/unloading conditions, as follows:

$$\dot{r}_p \geq 0; \qquad f \leq 0; \qquad \dot{r}_p f = 0; \tag{6}$$

The constitutive tensor takes the form:

$$\mathbf{D}_{tan} = \begin{cases} (1-\omega)\mathbf{D_0} & \forall\, r_{eff} < r_p \\ (1-\omega)\mathbf{D_0} - \dfrac{d\omega}{dr_p}\boldsymbol{\sigma_0} : \left(\mathbf{D_0} \otimes \dfrac{dr_p}{d\boldsymbol{\sigma}}\right)^T & \forall\, r_{eff} \geq r_p \end{cases} \tag{7}$$

III. THE SUR METHOD

The smooth unloading-reloading approach uses a target function $f_s(r_p)$ and a smooth unloading-reloading function $\sigma_p(r_p, r_{eff})$, as illustrated in Figure 1. It may be seen that the SUR function has two parts; **(i)** when $r_{eff} < a_p r_p$, for which linear unloading-reloading with a slope $(1 - \omega_{pf})E$ is assumed, and **(ii)** when $r_{eff} \geq a_p r_p$, for which nonlinear unloading-reloading is assumed, according to the function $\sigma_p(r_p, r_{eff})$.

$$f_s(r_p) = \begin{cases} f_t & \forall \quad r_p < r_k \\ f_t \cdot e^{-c_1 \cdot \left(\frac{r_p - r_k}{r_0 - r_k}\right)} & \forall \quad r_p \geq r_k \end{cases} \tag{8}$$

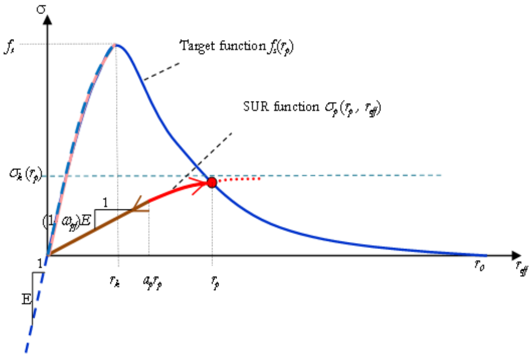

Figure 1: Target and unloading-reloading damage evolution functions

$$\sigma_p(r_p, r_{eff}) = \sigma_k(r_p) \cdot \left[1 - (1 - \frac{a_p}{v}) \cdot e^{-\left[\frac{r_{eff} - a_p r_p}{(v - a_p) r_p}\right]} \right] \tag{9}$$

where r_{eff} is the effective damage parameter, E is Young's modulus, f_t is the tensile strength, r_0 is the effective end of the softening curve, r_k is the damage evolution parameter at the peak of the uniaxial stress curve and c_1=5 [11].

The two main input parameters of the SUR function a_p and v are studied in this paper to examine the effect of varying these parameters on the numerical performance of the SUR model. It should be mentioned that Ref [11] used the values of 0.70 and 0.75 for the constants a_p and v, respectively.

The SUR function is tangential to the secant curve with modulus [(1-ω_{pf}) E], and σ_p depends upon the asymptotic stress function σ_k , which is defined as follows;

$$\sigma_k(r_p) = \begin{cases} f_s(r_k)\cdot v\cdot a_k & \forall \quad r_p \le r_k \\ f_s(r_p)\cdot v\cdot a_k & \forall \quad r_p > r_k \end{cases} \tag{10}$$

noting that $f_s(r_k) = f_t$, and that the expression a_k is defined in equation (11) below;

$$a_k = \frac{1}{v\cdot\left[1-(1-\frac{a_p}{v})\cdot e^{-\left[\frac{1-a_p}{v-a_p}\right]}\right]} \tag{11}$$

The damage parameter that controls the linear part of the SUR function is computed as:

$$\omega_{pf}(r_p) = \begin{cases} 0 & \forall \quad r_p \le r_k \\ 1-\frac{\sigma_k}{v\cdot r_p\cdot\sqrt{\mathrm{E}}} & \forall \quad r_p > r_k \end{cases} \tag{12}$$

and the damage parameter for the SUR function is given by:

$$\omega_p(r_p, r_{eff}) = \begin{cases} \omega_{pf} & \forall \quad r_{eff} \le a_p r_p \\ 1-\frac{\sigma_p(r_p, r_{eff})}{\sqrt{E}\cdot r_{eff}} & \forall \quad r_{eff} > a_p r_p \end{cases} \tag{13}$$

The introduction of the SUR function results in changes to two of the model equations presented in equations 1 and 7; these being the overall constitutive equation (14) and the expression for the tangent **D** matrix (15), as follows:

$$\boldsymbol{\sigma} = \left(1-\omega_p(r_p, r_{eff})\right)\mathbf{D_0} : \boldsymbol{\varepsilon} \tag{14}$$

$$\mathbf{D}_{tan} = \begin{cases} (1-\omega_{pf})\mathbf{D_0} & \forall \quad r_{eff} < a_p r_p \\ (1-\omega_p)\mathbf{D_0} - \frac{d\omega_p}{dr_p}\boldsymbol{\sigma_0} : \left(\mathbf{D_0}\otimes\frac{dr_p}{d\boldsymbol{\sigma}}\right)^T & \forall \quad r_{eff} \ge a_p r_p \end{cases} \tag{15}$$

The overall stress-strain relationship (14) now depends on ω_p, rather than ω, which in turn is governed by the value of SUR function σ_p. The new form of the matrix $\mathbf{D}_{tan}$ is evaluated using the SUR function and therefore is always positive definite. See references [10] and [11] for more details of the SUR method.

IV. NUMERICAL EXAMPLE

A one dimensional bar example shown in Figure 2 is used in the present study. The purpose of this study is not to examine the robustness of the SUR method, but rather to explore the effect of varying the two main parameters of SUR function (a_p and v) on the convergence characteristics of the new SUR approach.

Eight cases with different values of a_p and v for the SUR function were considered in the present study, as shown in table 1. It should be mentioned that more cases (with different parameters of a_p and v) of the SUR model can be studied; however, the authors' experience of the SUR model is that the cases given in table 1 are the most recommended cases that should be used for the SUR method.

Table 1:.Different values of a_p and v for the sur function

Case No.	a_p	v
Case 1	0.60	0.65
Case 2	0.65	0.70
Case 3	0.70	0.75
Case 4	0.75	0.80
Case 5	0.60	0.75
Case 6	0.70	0.80
Case 7	0.60	0.80
Case 8	0.80	1.0

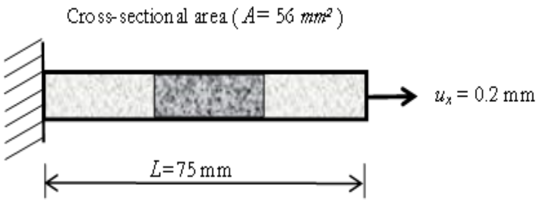

Figure 2: One-Dimensional bar problem

The 1D bar problem considered in this paper was fixed at one end and loaded by prescribed displacement of 0.2 mm at the other end. The prescribed displacement was applied evenly over 100 increments in the analysis. The 1D bar was divided into 3 linear elements of equal length, with the middle element being assigned a small amount of initial damage such that damage only occurred in this central element.

The material properties used for the analysis were: Young's modulus (E=20000 MPa), Poisson's ratio (υ=0.2), tensile strength (f_t=2.5 MPa) and the fracture energy (G_f= 0.1 N/mm).

A convergence tolerance of 10^{-6}, based on L2 norms of iterative displacement and out of balance force was used in the analysis of this example.

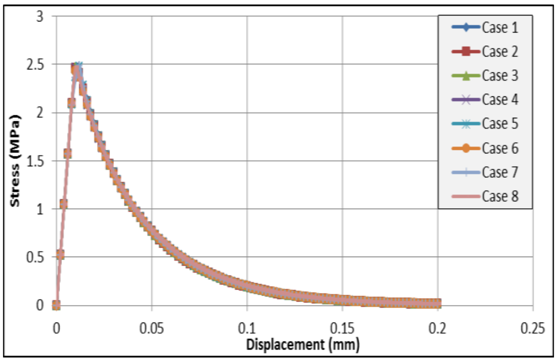

Figure 3: Displacement-stress responses of the SUR solution with different cases of SUR function

The resulting stress-displacement responses, from the analyses using eight different cases of SUR function parameters (a_p and v), are shown in Figure 3 and, as expected, the stress-displacement results from the various cases are indistinguishable from each other. Indeed, the form of the unloading-reloading curve would not be expected to have a major influence on the overall predicted stress-displacement response but predominantly affect the convergence characteristic of the solution, as can be seen in Figures 3 and 4.

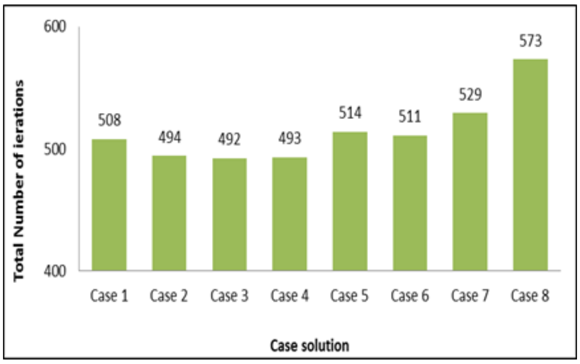

Figure 4: Total number of iterations that are needed for each case of the SUR solution

The convergence performance of the SUR method with different parameters (a_p and v) to form the SUR function is illustrated in Figure 4 by showing the total number of iterations required for completing the SUR solution for each case. Results showed that cases (2, 3 and 4) achieved converged solutions in fewer iterations than to the rest of cases (1, 5, 6, 7 and 8), as it can be clearly seen from the bar charts in Figure 4. Thus, for the SUR function, using the parameters of cases 2, 3 and 4 can give a noticeable reduction in the total number of iterations relative to those required by parameters of cases 1, 5, 6, 7 and 8.

The better performance of the SUR solution using the parameters of cases 2, 3 and 4 is attributed to the fact that the SUR curve of these cases has a much smaller gradient at the intersection with the target curve than does the SUR curve of cases 1, 5, 6, 7 and 8. This means that the 'tangent matrix' used in cases 2, 3 and 4 solutions was closer to the true (negative) tangent and therefore resulted in less drift from the target solution in each iteration than the solutions of cases 1, 5, 6, 7 and 8. studied case has different form of the SUR function.

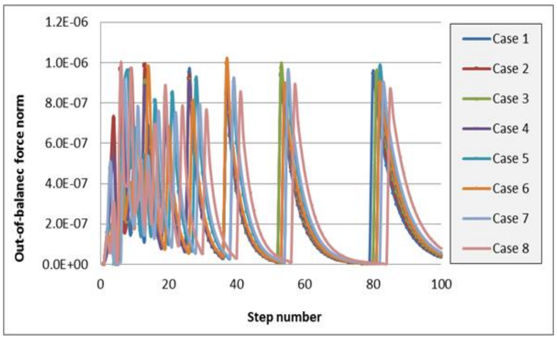

Figure 5: Convergence history of SUR solutions with different forms of the SUR function

The convergence history for each studied case of the SUR solution is plotted in Figure 5. The information provided in Figure 5 includes the out of balance force norm at the end of each load increment for the eight cases, in which each studied case has different form of the SUR function.

V. CONCLUSIONS

Effect the form of the SUR function on the convergence performance of the recently developed smooth unloading-reloading (SUR) method is studied by using different values of the two main parameters (a_p and v) of the SUR curve. The convergence characteristics are illustrated by showing the total number of iterations required to achieve convergence for the SUR solution. The following conclusions can be drawn from this work:

- The form of the SUR curve does not affect the overall predicted structural response, but only affect the convergence characteristics of the SUR solution, with SUR functions that have small gradients at the intersection with the target softening curve performing best.
- For the SUR function, using the parameters of case 2 [a_p =0.65 and v =0.70], case 3 [a_p =0.70 and v =0.75] or case 4 [a_p =0.75 and v =0.80] provide the best efficiency for the SUR method as they result in substantial savings in terms of the total number of iterations required for a complete solution, relative to any other suggested parameters.
- The SUR method was robust and never resulted in a breakdown of the nonlinear solution procedure.

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