A COMPARATIVE STUDY BETWEEN DISCRETE AND CONTINUUM MODELS TO SIMULATE CONCRETE FRACTURE

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Abstract. We present a comparative study between models that follow the two main trends to study fracture of quasi-brittle materials like concrete. On the one hand we focus on a discrete model that represents the fracture process by cohesive elements that are inserted in the original mesh only when the opening condition is met. Such elements also implement contact and friction algorithms. Besides, mesh size is selected so as to represent the inter-locking effect between the crack surfaces. Everything considered, this approach leads to an explicit and multiscale modeling of fracture. On the other hand we analyze a continuum model based on the strong discontinuity approach. It localizes damage in bands that are narrowed to the limit of having null width and thus simulate the fracture surface. The initiation and propagation processes are modeled by a bifurcation analysis that searches for the surfaces where damage can be localized at every step. Finally, we use both approaches to do 3-D simulations of fracture tests in concrete that allow an evaluation of their relative performance.

Resumen. Esta comunicación estudia comparativamente modelos que siguen las dos tendencias para abordar el estudio numérico de la fractura de materiales cuasi-frágiles como el hormigón. Nos centramos por un lado en un modelo discreto en el que la fractura se representa por medio de elementos cohesivos que se insertan entre los elementos del la malla original a medida que se propaga. Los elementos incorporan algoritmos de contacto y fricción. Además, el tamaño de la malla se selecciona de modo que se reproduzca el efecto de engranaje mecánico entre las superficies rotas. Todo ello hace que el proceso de fractura se simule de modo explícito y que esta aproximación pueda enmarcarse dentro de los modelos multiescala. También analizamos un modelo continuo basado en la aproximación de las discontinuidades fuertes. En ella se localiza el daño en bandas que llegan a tener un ancho nulo y que, consecuentemente, simulan la superficie de fractura. El proceso de iniciación y propagación se simula por medio de algoritmos de bifurcación que identifican las superficies sobre las que se formulan las discontinuidades, lo cual permite ofrecer un modelo autoconsistente. Por último, se presenta una simulacion en tres dimensiones de ensayos de fractura de hormigón con objeto de comparar los resultados de ambos métodos.

1 INTRODUCTION

Since linear elastic fracture mechanics showed its limitations when applied to high toughness materials (for example, tough steels, which are able to develop large plastic zones near the crack tip before tearing off) or quasi-brittle materials like concrete (whose internal length scale for fracture processes is much larger than for most materials), various approaches have emerged to take into account the nonlinear mechanisms of the fracture process zone.

One straightforward way to deal with the fracture phenomena is the discrete approach, which identifies the new crack as newly-emerged boundaries of the bulk material but still transfers traction in its early stage through a constitutive relation called cohesive law. This methodology was originally applied to ductile fracture by Dugdale and Barenblatt and adapted to concrete by Hillerborg and his coworkers (Hillerborg *et al.* 1976 [1]; Hillerborg 1985 [2]). It provides clear criteria for fracture initiation and growth, but the insertion of cracks represents a topological problem that is not easy to handle. For long years cohesive models were restricted to modeling cracks whose path was known *a priori*. There were also attempts of studying fracture processes with multiple cracks by embedding the cohesive elements into the mesh from the very beginning of the calculation, but such procedure was a source of numerical instabilities (Planas, 2003 [3]). Pandolfi and Ortiz ([4], [5]) came up with a fragmentation algorithm that solved the problem by inserting cohesive elements when and where they are needed. In principle it restricts the possible crack path to pre-existing element boundaries, although this hindrance can be overcome by using remeshing procedures. The versatility of the cohesive fracture model plus the fragmentation algorithm used for propagating dynamic cracks has been well demonstrated by Ortiz and his coworkers (see Camacho and Ortiz, 1996 [6]; Ortiz and Pandolfi, 1999 [7]; Ruiz *et al.* 2000 [8]; Ruiz *et al.* 2001 [9]; Pandolfi *et al.* 2000

[10]; Yu *et al.* (2002) [11]). So we would like to consider the fragmentation algorithm as part of the discrete cohesive fracture model which we are going to abbreviate as DCFF from now on. The simplicity of the model and its compatibility with the standard finite element framework make it very attractive for studying complex fracture processes.

An alternative way of looking at fracture is to incorporate strain or displacement discontinuities into standard finite element interpolations. The development of such techniques was pioneered by the work of Ortiz (Ortiz *et al.*, [12]). His work triggered the development of various powerful methods that allow the efficient modeling of regions with highly localized strains (see Jirásek [13], for a systematic comparative study of embedded-crack modeling). One of them, termed as the strong discontinuity approach (SDA), considers fracture as the limit case of a strain localization in a band of null bandwidth. The SDA refers to the capture of jumps in the displacement field (strong discontinuities) by using standard solid mechanics models equipped with stress vs. strain relationships (continuum constitutive equations). By identifying the main features that make the standard constitutive equations consistent with the appearance of strong discontinuities, going through the process of re-evaluating the kinematics to include the discontinuous displacement fields, enhanced strain fields, the SDA naturally brings on its link with the cohesive fracture mechanics (Oliver *et al.*, 2000 [14]). Discrete constitutive models are automatically induced through a continuum damage model in the 1D case. For general 2D-3D cases, the weak discontinuity concept is introduced to precede the strong discontinuity condition and at the same time connects with the physics of the fracture process zone. Another way of embedding strong discontinuities is the recently developed extended finite element method (termed XFEM; for instance, see Melenk and Babuska, 1996 [15]; Moës and Belytschko, 1999 [16] or Chessa and Belytschko, 2003 [17]), which utilizes nodal enrichments of the displacement field based on a local partition of unity. It was motivated by minimizing re-meshing; efforts are therefore devoted to various enrichment techniques (Belytschko, 2003 [18, 19]) to resolve the crack initiation and propagation.

In this paper we are going to focus on two advanced models that are quite representative of their respective class: the discrete cohesive fracture model companied by the fragmentation algorithm (DCFF) and the strong discontinuity approach (SDA) embedded into the element formulations. In particular, we are interested on how do the two models tackle the initiation and propagation of cracks in a quasi-brittle material like concrete.

The organization of the rest of the paper is as follows. The boundary value problem for a cracked body is presented in Section 2; a brief review of both models is depicted in Section 3. Numerical examples applied to fracture in concrete are presented in Section 4. Finally in Section 5 some conclusions are drawn.

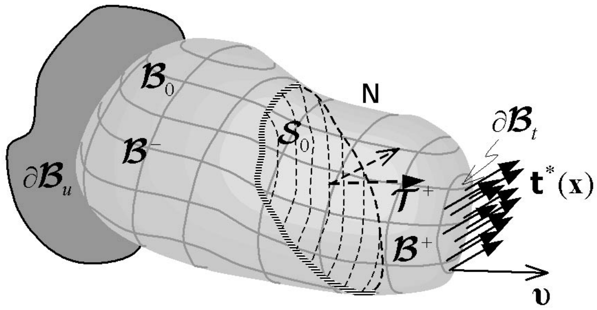

Figure 1: Three dimensional body and discontinuity interface S_0.

2 THE BOUNDARY VALUE PROBLEM (BVP)

By way of a general framework, we start by considering a deformable body occupying an initial configuration $B_0 \subset R^3$. The boundary of the body is partitioned into a displacement boundary ∂B_u and a traction boundary ∂B_t. The body undergoes a motion described by a deformation mapping $\varphi : B_0 \times [0,T] \to R^3$, where $[0,T]$ is the duration of the motion, under the action of body forces $\rho_0 \mathbf{b}$ and prescribed boundary tractions $\mathbf{t}^*$ applied over ∂B_t. The attendant deformation gradients are denoted $\mathbf{F}$ and the first Piola-Kirchhoff stress tensor $\mathbf{P}$. In addition, the solid contains a collection of cohesive cracks (or displacement discontinuities). The locus of these cracks on the undeformed configuration is denoted S_0, Fig. 1.

Under these conditions, the weak form of linear momentum balance, or virtual work expression, takes the following form:

$$\int_{B_0} \left[\rho_0(\mathbf{b} - \ddot{\varphi}) \cdot \eta - \mathbf{P} \cdot \nabla_0 \eta\right] dV_0 - \int_{S_0} \mathbf{t} \cdot [\![\eta]\!]\, dS_0 + \int_{\partial B_t} \mathbf{t}^* \cdot \eta \, dS_0 = 0 \quad (1)$$

where a superposed dot denotes the material time derivative, ∇_0 is the material gradient, η is an arbitrary virtual displacement satisfying homogeneous boundary conditions on ∂B_u, $\mathbf{t}$ is the cohesive traction over S_0, and $[\![\cdot]\!]$ denotes the jump across an oriented surface.

3 HOW DOES EACH MODEL SOLVE THE BVP?

3.1 The discrete cohesive fracture model + the fragmentation algorithm

From Eq. (1), it is clear that the presence of a cohesive surface results in the addition of a new term to the virtual work expression. In order to complete the definition of the problem, a set of constitutive relations for the cohesive tractions $\mathbf{t}$ has to be provided, in addition to the conventional constitutive relations describing the bulk behavior of the material.

Ortiz and Pandolfi (1999) [7] postulated a general form of a free energy density ϕ per unit undeformed area over S_0, which is a function of the opening displacements, the local temperature, some suitable collection of internal variables describing the current state of decohesion of the surface, as well as the unit normal $\mathbf{n}$ to the cohesive surface in the deformed configuration. The explicit dependence of ϕ on $\mathbf{n}$ is required to allow for differences in cohesive behavior for opening and sliding.

A potential structure of the cohesive law furnishes its scalar dependence on the free energy density ϕ. By assuming that ϕ depends on the opening displacements only through an effective opening displacement and, at the same time, introducing a parameter β which assigns different weights to the sliding and normal opening displacements, a simple class of mixed-mode cohesive laws accounting for tension-shear coupling (see Camacho and Ortiz [6]) is obtained:

$$\mathbf{t} = \frac{t}{\delta}(\beta^2 \delta_s \mathbf{s} + \delta_n \mathbf{n}), \tag{2}$$

where

$$t = \sqrt{\beta^{-2} t_s^2 + t_n^2} \tag{3}$$

$$\delta = \sqrt{\beta^2 \delta_s^2 + \delta_n^2} \tag{4}$$

The unit vector of the tangential direction of the displacement jump is denoted by $\mathbf{s}$; t_s and t_n are the shear and the normal traction components, respectively and t is an effective cohesive traction; δ_s and δ_n are the sliding and the opening components of the displacement jump, and δ is an effective opening displacement. The two effective quantities are going to be related by an irreversible cohesive law, say, for example, Fig. 2.

Contact and friction are regarded as independent phenomena to be modelled outside the cohesive law. Notice that the presence of friction may significantly increase the sliding resistance in closed cohesive surfaces.

3.1.1 Constitutive models for the bulk material

Cohesive models furnish a complete theory of fracture, and permit the incorporation into the material description of *bona fide* fracture parameters such as the fracture energy and the tensile strength. By focusing specifically on the separation process, a sharp distinction is drawn in cohesive theories between fracture, which is described by recourse to cohesive laws, and bulk material behavior, which is described through an independent set of constitutive relations. The use of cohesive models is therefore not limited by any consideration of material behavior, finite kinematics, non-proportional loading, dynamics, or the geometry of the specimen.

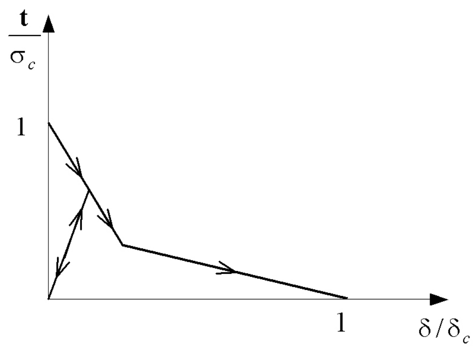

Figure 2: Bi-linear irreversible cohesive law.

3.1.2 The crack initiation and propagation

In calculations, decohesion is allowed to occur along element boundaries only. Initially, all element boundaries are perfectly coherent (and all of them could be considered as possible cracks) and the elements conform in the usual sense of the displacement finite element method. When the critical value for the effective cohesive traction is attained at the interface between two volume elements, a cohesive element is inserted using a fragmentation algorithm (Pandolfi and Ortiz, 2002 [5]) at that location. The cohesive element with its proper cohesive law subsequently governs the opening of the cohesive surface.

The crack propagation and initiation are not considered as distinct events in the DCFF. For each loading step, the fragmentation algorithm checks for possible cracks. Thanks to this feature, the initiation and nucleation of cracks can be predicted with ease.

3.2 The strong discontinuity approach

Originated from its precedence strain localization, the main goal of SDA has been to approach the limit case of a strain localization in a band of null bandwidth, whereas the general strain localization case is matched by a weak discontinuity, characterized by continuous displacement fields and discontinuous but bounded strain fields which localize in a band of finite bandwidth. See Simo and Rifai (1990), Simo *et al.* (1993), Simo and Oliver (1994), Oliver *et al.* (2002) [20, 21, 22, 23].

3.2.1 Constitutive model for the bulk material

The SDA was introduced as a basic tool to derive a general framework in which different families of constitutive equations for bulk materials can be adopted, Oliver (1996) [24]. For inelastic quasi-brittle materials an isotropic damage model is often adopted. The term damage mechanics has been used to refer to models that are characterized by a loss of stiffness or a reduction of the secant constitutive modulus. First introduced by Kachanov (1958) [25] along the concept of effective tension, the damage variable was treated as a scalar (isotropic damage), whose value ranged from 0 to 1. More details about this model can be found in Chaboche (1979), Carol *et al.* (1998), Oliver *et al.* (1990) [26, 27, 28]. A representative continuum damage model in the finite deformation range is presented in Oliver *et al.* (2003) [29], in which a free energy density function in terms of the deformation gradient tensor and a set of internal variables is defined. The constitutive equation is presented through a scalar strain-like internal variable r and a stress-like internal variable q. The variable r determines the damage level of the material through the damage variable $d = 1 - q(r)/r$, and $q(r)$ sets the evolution of the elastic domain through a damage function. The rate form of the softening law is defined through the softening modulus as

$$\dot{q} = \mathscr{H}\dot{r}. \tag{5}$$

In terms of the stress-strain response, four distinct loading phases can be identified, see Figs.3 and 4.

I. **Elastic phase:** the stress-state before the point Y (the yielding point in plasticity, the initiation of inelastic behavior in general inelastic solids). In this phase the material obeys generalized Hooke's law.

II. **Inelastic phase:** the state between point Y and B. B is the bifurcation point when the general bifurcation conditions (the loss of uniqueness) is achieved. The hardening/softening modulus takes the value $\mathscr{H}_Y$, the material behavior is still continuous.

III. **Weak discontinuity phase:** the state up to point SD. From the mechanics viewpoint, the weak discontinuity regime defines a zone where the discontinuity is processed. Physically it signals a change in the behavior of the bulk material due to the formation of the fracture process zone. Numerically speaking this transition avoids an unexpected artificial elastic loading (see Oliver *et al.* (2003) [29] for detailed discussion). Finally, from an analytical standpoint, this phase is predicted by a region between the loss of uniqueness (general bifurcations) and the loss of ellipticity (discontinuous bifurcations) of the stress-strain response, see Ottosen and Runesson (1991) [30, 31].

In this stage a variable bandwidth model is activated, whose initial width h_B (Fig. 4), defined as the ratio between a critical softening modulus $\mathscr{H}_{crit}$ and the discrete softening modulus $\bar{\mathscr{H}}$, see Oliver *et al.*(1999) [32], Manzoli(1998) [33], Oliver *et al.* (2000) [14].

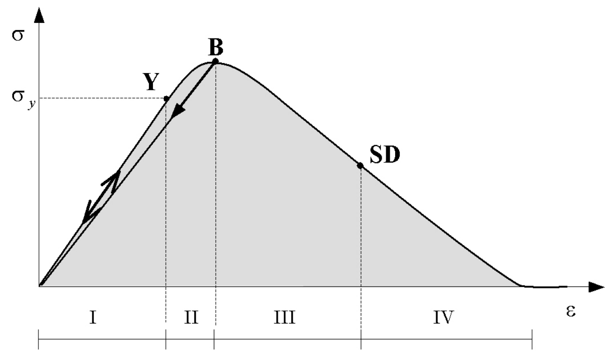

Figure 3: Characteristic points during the loading process.

IV. **Strong discontinuity phase:** The point SD corresponds to the onset of the strong discontinuity (the loss of ellipticity of the stress-strain response). It is characterized by the appearance of a jump in the displacement field, Oliver *et al.* (2000) [14].

3.2.2 The fracture initiation

The fracture initiation is identified as the appearance of material instability, or the loss of uniqueness of the solution (point B in fig. 3). In the mathematical sense, this is signaled by the singularity of the characteristic tangent stiffness modulus tensor Q defined as $Q_{il} = n_j D_{ijkl} n_l$ (or the so-called acoustic tensor following the fluid dynamics terminology), where D_{ijkl} is the tangent stiffness tensor, $\mathbf{n}$ is the unit normal vector of the surface S_0, see Fig. (1). A critical value $\mathscr{H}$ and a critical direction of the discontinuity surface $\mathbf{n}$ are obtained to define the fracture initiation.

3.2.3 The crack propagation

Unlike the DCFF, in which all element boundaries are possible cracks, the SDA needs to define a series of failure surfaces for crack propagation. For this purpose an efficient method called the *overall tracking* has been proposed by Oliver *et al.* (2002) to obtain a continuous failure surface. A family of level curves (in 2D) or level surfaces (in 3D) enveloping the propagation direction can be constructed in analogy to a heat conduction problem. This methodology proves itself a powerful tool especially in simulating multiple cracks (Samaniego and Oliver 2003 [34]).

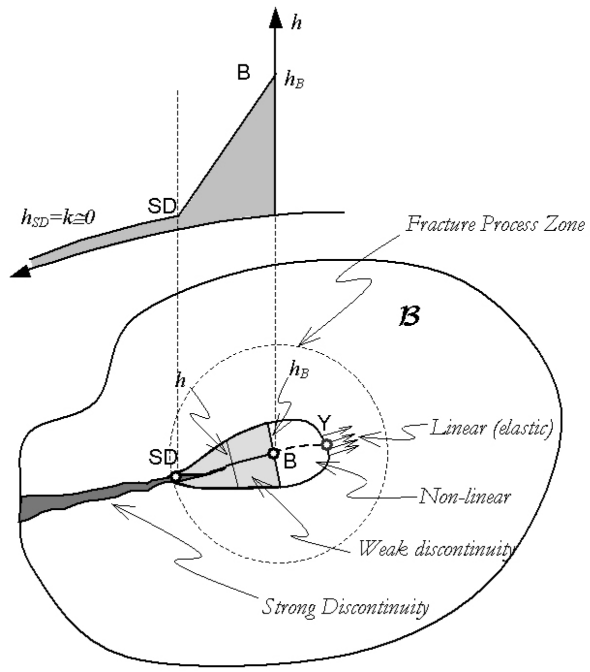

Figure 4: Fracture process zone modelled by the strong discontinuity approach.

4 APPLICATION OF THE TWO MODELS TO THE PREDICTION OF FRACTURE IN CONCRETE

In this section, we proceed to simulate the static behavior of concrete using the two aforementioned models. Our aim is to check their relative performance against several very different specimens and load configurations. We are starting here by a mode I test in which the path of the crack is known in advance. DCFF and SDA are used to simulate the same experimental test conducted with the same material. Efforts are made to assure the same boundary value problem is being solved.

For details on the implementation and on the discretization for both methods, the readers are directed to Ortiz and Pandolfi (1999) [7], Pandolfi and Ortiz (2002) [5], Yu and Ruiz [35], Oliver (1996) [24], Chaves [36] and the references within. Nevertheless, we would like to mention that DCFF uses 12-node quadratic cohesive elements composed of two surfaces that are inserted between 10-node quadratic tetrahedra, while SDA is optimized for 5-node linear tetrahedra. This implies that different meshes have to be used to get the same relative accuracy in the solid representation.

4.1 Numerical example

The particular configuration contemplated in the study is the three point bend test (TPB) performed in a quasi-static regime. We specifically aim to simulate experiments con-

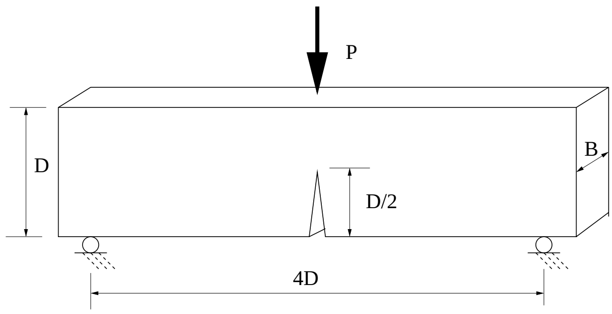

Figure 5: Geometry of a half-notched concrete beam subjected to three point bending, where $D = 75$ mm, $B = 50$ mm.

ducted over a micro-concrete (with maximum aggregate size 5 mm) by Ruiz (1998) [37]. The size of the specimens and the testing method are described in Fig. 5. The characterization of the concrete is as follows: specific fracture energy $G_F = 62.5$ N/m, tensile strength $f_t = 3.8$ MPa, Young's modulus $E = 30.5$ GPa, Poisson's ratio $\nu = 0.2$. The density is $\rho = 2402$ kg/m^3. A bi-linear cohesive law according to the Model Code [38] is adopted for the DCFF. The softening modulus $\mathscr{H}$ in SDA is adjusted accordingly. The β parameter in DCFF is derived as 8.4 although in this particular example its influence in the results is negligible for it is a pure mode I test. In SDA we make a choice of 1 mm for h_B, which is proven to represent adequately the width of the proccess zone at the initial state [29].

4.2 The three-point-bending test

Two meshes were adopted in the modeling. DCFF used a mesh composed of 8282 nodes, 5183 10-node quadratic tetrahedrons. The mesh size was chosen to scale the maximum aggregate size. The second mesh, used by the SDA model consists of 6412 nodes and 5183 5-node linear tetrahedrons. Both meshes have the same appearance for they share the shape and location of the tetrahedra, i.e. the vertex nodes are the same, DCFF puts one middle node at every edge and SDA adds one interior node inside every tetrahedron. Figure 6 depicts the visible tetrahedra. It should be noticed that the middle surface of the specimen is not physically represented by element boundaries which forces DCFF to choose a rough path.

Figures 6 and 7 show some of the numerical results. The crack pattern is adequately predicted by both methods although we only draw the deformed mesh given by SDA. The load-displacement curves in Fig. 7 show that the maximum load prediction is also very good for both methods. The DCFF run had convergence problems soon after the load peak. We should have in mind that the mesh is very refined and implies a rough crack path, which imposes a great computational effort for the solver at each

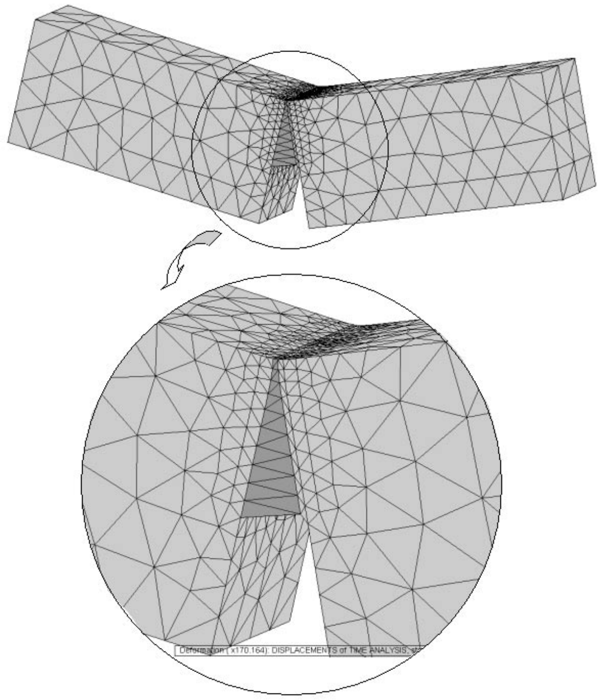

Figure 6: The fracture patterns at loading displacement 0.25 mm.

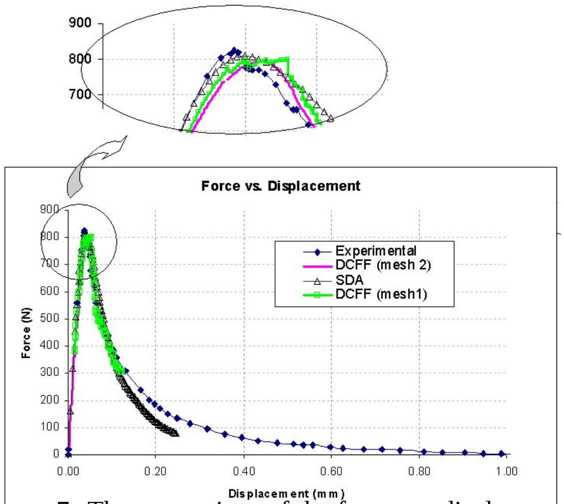

Figure 7: The comparison of the force vs. displacement curves obtained by the DCFF, SDA and the experimental data.

loading step. The SDA model is more stable for this particular mesh, provided that it allows the crack to be located in the middle of the element. In fact, we have tried an alternative mesh in which the crack surface is fully contained in inter-tetrahedron boundaries and the SDA was not able to get to the peak load. This alternative mesh favors DCFF because it implies a smooth crack propagation. Actually DCFF run up to the insertion of the last cohesive element in this case.

5 SUMMARY AND CONCLUSIONS

We have briefly compared two distinct finite element approaches to non-linear fracture mechanics for quasi-brittle materials like concrete.

On the one hand we have focused on a discrete approach that represents cracks by means of cohesive elements. The model uses a fragmentation algorithm that inserts the cohesive elements within the original mesh where and when the opening condition is met. The elements are also provided with contact and friction routines that enable them to simulate explicitly physical phenomena that may condition the macroscopic response. This also implies that the process zone has to be adequately resolved which may lead to take recourse to re-meshing techniques. It is precisely this kind of topological problems what increases the computational cost and may fade the appeal of the method. This approach to study fracture is compatible with any bulk constitutive law. Indeed, it has been used successfully to simulate both ductile and brittle fracture. The ability of simulating separately events that are of different nature gives this model a multi-scale character.

On the other hand the strong discontinuity approach studies fracture within a continuous framework. The adjective *strong* refers to the ability of capturing jumps in the displacement field across a surface with zero bandwidth. Doing so implies an enhancement of the kinematics of the governing equations. The strain localization starts when a failure surface is reached in the space of the principal stresses. From then on there is a softening of the properties of the material and a localization of the strain over a band whose width tends to zero, the whole process being controlled by a damage law. The search for the surface that is likely going to hold the fracture in the next step is done by a standard bifurcation analysis.

Both approaches have been used to model a simple mode I TPB test in concrete. The mesh arrangement plays an important role in both models. DCFF works better when element boundaries are placed in the track trajectory (which in this case is known beforehand) and may not converge when dealing with many cracks and fragments. Likewise, SDA prefers mesh orientations that allow the main crack going through the elements and is not able so far to handle multi-cracking processes (in 3D). The element size is chosen in DCFF to represent the aggregate size and consequently works as a material length that determines some of the mechanisms of concrete fracture. SDA uses the width of the weak discontinuity transient zone as a parameter to model the nucleation of the process zone. The results of both models are quite close to their experimental counterparts. Nevertheless, some more cases in a wider variety of geometries and loading conditions should be run in order to complement this study.

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