A truly–mixed method for cohesive crack propagation in quasi–brittle materials

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SUMMARY. An alternative approach for cohesive crack growth in elastic media is proposed. Standard methods resort to the enrichment of displacement–based formulations to model the cohesive crack through ad hoc displacement jump interpolations. The proposed method is conversely based on a mixed variational principle that inherently allows for regular traction while discontinuous displacements both in the continuous and discrete form. An extension of the truly–mixed formulation for macro–cracked media is herein presented along with a growth algorithm that is able to cope with pure mode I and mixed mode propagation in quasi–brittle materials. To assess the capabilities of the method a few numerical simulations are performed on different kinds of concrete specimens. The size effect with respect to three–point bending beams is firstly investigated through pure mode I simulations. Predictions of crack paths in mixed mode growth are subsequently addressed assessing the mesh independence of the procedure.

1 INTRODUCTION

An alternative approach for cohesive crack growth in quasi–brittle materials is addressed. Classical methods move from displacement–based formulations that are enriched to handle discontinuities in the inherently continuous displacement field (see e.g. the extended finite element method XFEM [1] or the embedded discontinuity [2] approaches).

The herein adopted formulation is conversely based on a truly–mixed discretization [3] that has stresses as main regular variables, while discontinuous displacements play the role of Lagrangian multipliers. The approach directly handles the propagation of cohesive cracks in elastic media through the appropriate inclusion of interface energy terms that enrich the formulation when a crack is growing. Notably, no edge element is introduced but simply the inherent discontinuity of the displacement field is taken advantage of. Furthermore, stress–flux continuity is imposed in an exact fashion within the formulation and not as an additional weak constraint, as classically done.

An algorithm capable of solving the variational setting is therefore derived, having the aim of handling the propagation of a discrete crack within a continuum medium. The evolution of the cohesive zone makes the problem nonlinear, thus calling for ad hoc procedures that manage numerical simulations. To this purpose the crack length is assumed as the controlling parameter, i.e. a monotonically increasing function that drives the loading process. Since the discontinuity of the displacement field is only allowed at the mesh edges in the discrete formulation, a remeshing technique is proposed to align the element sides to the evolving crack path. Step–wise loads and growth directions are computed resorting to the classical MTS (maximum tensile stress) criterion [4], that may exploit the accuracy in the evaluation of the stress field peculiar to the truly–mixed setting.

A few simulations are provided along with comparisons with numerical results and experimental data from established literature of the field. Pure mode I analysis are used to assess the capability of the method to handle the size effect phenomenon. Global mixed mode simulations are therefore performed to investigate the robustness of the results and the capability of the method to deal with

different meshes.
Concerning the ongoing research, reference is made to the development of XFEM-like techniques to allow crack propagation within the JM element and to the extension of the presented framework to the case of elasto–plastic media.

2 THE CONTINUOUS PROBLEM

Section 2.1 reports fundamentals on the truly–mixed finite element formulation, as modified to cope with the presence of a cohesive crack. The variational formulation for the isotropic elastic problem is detailed in [3], while modifications in case of cracked media are also discussed in [5]. To complete the general framework, Section 2.2 discusses the cohesive constitutive laws as included in the presented formulation and implemented in the numerical algorithms.

2.1 *Truly–mixed formulation for cohesive–cracked media*

As detailed in Section 1, the peculiar benefits of the adoption of a truly–mixed method in the description of cohesive–cracked media mainly descend from the nature of the fields involved in the analysis of the elastic problem.
To introduce the continuous formulation let firstly consider the case of a homogeneous domain $\Omega \in R^2$, with regular boundary $\partial\Omega$, making also the assumption of a linear elastic isotropic material whose elasticity tensor is further denoted as $\underline{\underline{\underline{\underline{C}}}}$. As usual, $\partial\Omega$ is made of two complementary parts, i.e. Γ_d and Γ_t, where prescribed displacements $\underline{u}_d$ and stresses $\underline{f}_t$ are respectively enforced. Let $\underline{\underline{\sigma}}$ denote the unknown stress fields and $\underline{u}$ the unknown displacement field, while $\underline{g}$ is the square integrable vector body load. The "truly–mixed" weak formulation reads: find $(\underline{\underline{\sigma}}, \underline{u}) \in H \times W$ such that $\underline{\underline{\sigma}} \cdot \underline{n} \,|_{\Gamma_t} = \underline{f}_t$ and

$$\begin{cases} \displaystyle\int_\Omega \underline{\underline{\underline{\underline{C}}}}^{-1} \underline{\underline{\sigma}} : \underline{\underline{\tau}} dx + \int_\Omega \underline{\text{div}}\, \underline{\underline{\tau}} \cdot \underline{u} dx = \int_{\Gamma_d} \underline{u}_d \cdot (\underline{\underline{\tau}} \cdot \underline{n}) ds, & \forall \underline{\underline{\tau}} \in H, \\ \displaystyle\int_\Omega \underline{\text{div}}\, \underline{\underline{\sigma}} \cdot \underline{v} dx = -\int_\Omega \underline{g} \cdot \underline{v} dx, & \forall \underline{v} \in W. \end{cases} \tag{1}$$

where $\underline{n}$ denotes the normal to the boundary and the relevant functional spaces H and W may be derived in a fairly natural way so that the integrals involved in the above equations make sense. One has that the stress field $\underline{\underline{\sigma}}$ is the main variable of the formulation and must belong to the regular space:

$$H = H(\underline{\text{div}}\,; \Omega) = \left\{ \underline{\underline{\tau}} : \tau_{ij} = \tau_{ji},\ \tau_{ij} \in L^2(\Omega),\ \underline{\text{div}}\, \underline{\underline{\tau}} \in W \right\}. \tag{2}$$

Conversely, displacements play the role of Lagrangian multipliers and may also be discontinuous, since the square–integrability is the only requirement on regularity properties of the functionals, i.e.:

$$W = \left[L^2(\Omega)\right]^2. \tag{3}$$

From a mathematical point of view, the presence of a cohesive crack implies that a localized discontinuity arises in the displacement field, while continuity of the stress–flux is preserved. This means that two opposite sides, Γ_{c1} and Γ_{c2}, must be taken into account when a crack is developing along Γ_c, while the same $\underline{\underline{\sigma}} \cdot \underline{n}$ characterizes both the edges. Due to the continuity of the stress–field, one may specialize the right hand side of Eqn. $(1)_1$, thus deriving the following term on Γ_c:

$$\int_{\Gamma_{c1}} \underline{u} \cdot (\underline{\underline{\tau}} \cdot \underline{n}) ds - \int_{\Gamma_{c2}} \underline{u} \cdot (\underline{\underline{\tau}} \cdot \underline{n}) ds = \int_{\Gamma_c} [\![\underline{u}]\!] \cdot (\underline{\underline{\tau}} \cdot \underline{n}) ds, \tag{4}$$

where $[\![\,\cdot\,]\!]$ denotes the jump of the relevant quantity. Eqn. (4) clearly shows that the displacement jump is computed as a difference between the values of the relevant field on adjacent elements and does not call for any enrichment of the discretization, see e.g. XFEM or the embedded discontinuity approaches. In the framework of cohesive fracture one may therefore introduce a (rate–independent) law, that is a generally nonlinear vector relation between the stress flux $\underline{\underline{\sigma}} \cdot \underline{n}$ and the displacement jump vector $[\![\underline{u}]\!]$, i.e.

$$\underline{\underline{\sigma}} \cdot \underline{n} = \mathcal{F}([\![\underline{u}]\!]). \tag{5}$$

Proceeding on a purely formal ground one may introduce the inverse of the operator $\mathcal{F}$ and merging Eqns. (4) and (5), thus writing:

$$\int_{\Gamma_c} [\![\underline{u}]\!] \cdot (\underline{\underline{\tau}} \cdot \underline{n}) ds = \int_{\Gamma_c} \mathcal{F}^{-1}(\underline{\underline{\sigma}} \cdot \underline{n}) \cdot (\underline{\underline{\tau}} \cdot \underline{n}) ds. \tag{6}$$

Eqn. (6) turns out to be a complementary energy term that takes into account the presence of a cohesive crack on Γ_c. Eqn. (1) may be therefore re–written according to the classical compact form of saddle point problems. In the specific case of "truly–mixed" formulation for cohesive crack media one has the generally nonlinear statement: find $(\underline{\underline{\sigma}}, \underline{u}) \in H \times W$ such that $\underline{\underline{\sigma}} \cdot \underline{n} \,|_{\Gamma_t} = \underline{f}_t$ and:

$$\left\{ \begin{array}{lll} a(\underline{\underline{\sigma}}, \underline{\underline{\tau}}) + b(\underline{\underline{\tau}}, \underline{u}) & = f(\underline{u}_d, \underline{\underline{\tau}} \cdot \underline{n}), & \forall \underline{\underline{\tau}} \in H, \\ b(\underline{\underline{\sigma}}, \underline{v}) & = g(\underline{g}, \underline{v}), & \forall \underline{v} \in W, \end{array} \right. \tag{7}$$

where scalar products $(\cdot, \cdot)$ may be straightforwardly derived from a comparison with Eqn. (1) that refers to the uncracked medium. The only modification needed to take into account the complementary energy in Eqn. (6) affects the bilinear term, that now reads:

$$a(\underline{\underline{\sigma}}, \underline{\underline{\tau}}) = \int_{\Omega} \underline{\underline{\underline{\underline{C}}}}^{-1} \underline{\underline{\sigma}} : \underline{\underline{\tau}} dx - \int_{\Gamma_c} \mathcal{F}^{-1}(\underline{\underline{\sigma}} \cdot \underline{n}) \cdot (\underline{\underline{\tau}} \cdot \underline{n}) ds. \tag{8}$$

Both the bulk elastic law and the nonlinear cohesive crack law are enforced in strong form according to the above truly–mixed setting, depending on stress and stress–flux, respectively. The bulk integral takes into account the energy contributions of the elastic material, while the line one refers to the cracked path. The presence of both energy contributions on Ω and Γ_c is the key to capture size effect behaviors, see e.g. [4].

2.2 *The cohesive law*

At least in rate form, one may write the following matrix expression, that linearizes the traction–separation relationship introduced in Eqn. (5):

$$\left\{ \begin{array}{c} |\, \underline{\underline{\sigma}} \cdot \underline{n} \,|_{\perp} \\ |\, \underline{\underline{\sigma}} \cdot \underline{n} \,|_{\parallel} \end{array} \right\} = \left[\begin{array}{cc} \mathcal{C}_{11} & \mathcal{C}_{12} \\ \mathcal{C}_{21} & \mathcal{C}_{22} \end{array} \right] \left\{ \begin{array}{c} [\![\underline{u}]\!]_{\perp} \\ [\![\underline{u}]\!]_{\parallel} \end{array} \right\} + \left\{ \begin{array}{c} |\, \underline{\underline{\sigma}} \cdot \underline{n} \,|_{\perp} \\ |\, \underline{\underline{\sigma}} \cdot \underline{n} \,|_{\parallel} \end{array} \right\}^{*}, \tag{9}$$

In the above equation, $|\, \underline{\underline{\sigma}} \cdot \underline{n} \,|_{\perp}$ is the normal traction and $|\, \underline{\underline{\sigma}} \cdot \underline{n} \,|_{\parallel}$ the shear stress. The threshold vector is denoted as $|\, \underline{\underline{\sigma}} \cdot \underline{n} \,|^{*}$, whose entries are the the tensile strength of material σ_t^* and the shear strength of material σ_s^*. $[\![\underline{u}]\!]_{\perp}$ stands for the opening displacement and $[\![\underline{u}]\!]_{\parallel}$ denotes the sliding one, while the entries of the matrix $\mathcal{C}$ define the softening behavior in case of mode I, mode II or mixed mode fracture.

Towards the assessment of an algorithm based on the truly–mixed formulation, the inverse of Eqn. (9) may be plugged in Eqn. (6) to write the relevant energy integral on Γ_c in case of a linearized traction–separation relationship:

$$\int_{\Gamma_c} [\![\underline{u}]\!] \cdot (\underline{\underline{\tau}} \cdot \underline{n}) ds = \int_{\Gamma_c} \mathcal{C}^{-1}(\underline{\underline{\sigma}} \cdot \underline{n}) \cdot (\underline{\underline{\tau}} \cdot \underline{n}) ds - \int_{\Gamma_c} \mathcal{C}^{-1}(\underline{\underline{\sigma}} \cdot \underline{n})^* \cdot (\underline{\underline{\tau}} \cdot \underline{n}) ds. \tag{10}$$

According to notations introduced in Eqn. (7), the right hand side of the above statement may be divided into two different parts. The first integral is in fact the expected contribution to the complementary energy in the bilinear form $a(\underline{\underline{\sigma}}, \underline{\underline{\tau}})$. The second one has conversely the form of a natural boundary condition where $\underline{u}_d = \mathcal{C}^{-1}(\underline{\underline{\sigma}} \cdot \underline{n})^*$, and may be therefore grouped in the term $f(\underline{u}_d, \underline{\underline{\tau}} \cdot \underline{n})$.
In the following studies it will be assumed to cope with pure mode I growth or free–sliding conditions in mixed mode propagation, in agreement with [6, 7]. This means that $\mathcal{C}_{11} \neq 0$, while $\mathcal{C}_{22} = \mathcal{C}_{12} = \mathcal{C}_{21} = 0$. Referring to the shape of the cohesive law, a bi-linear softening curve for concrete is assumed in agreement with the Peterson model, see e.g. [4].

3 THE DISCRETE PROBLEM

This section refers to the finite element discretization of the formulation above presented. Fundamentals of the adopted discrete scheme are discussed in Section 3.1, while Section 3.2 presents the algorithm used in the numerical simulations to handle the crack growth.

3.1 *Discrete matrix vector equations*

The "truly–mixed" setting calls for the non–trivial issue of providing a suitable robustness to the numerical scheme, since not so many finite element discretizations are available in literature that fully pass the inf–sup condition, see e.g. [3]. Within a bidimensional framework, the herein adopted JM composite element, introduced in [8], is one of the very few that are robust towards the stability requirement.
The JM element is a triangular element T, that is further subdivided into three sub-triangles T_j. Due to the mixed nature of the variational principle, both stress and displacement fields are separately approximated. Within each sub-triangle T_j, the stress is linearly interpolated, while the continuity of the stress–flux between inner edges is a priori imposed. This means that fifteen stress dofs are needed. Three dofs are computed as the components of the average stress tensor on the whole triangle T. The remaining twelve dofs are derived from the stress–flux on the edges of T, i.e. two stress–flux vectors are defined as dofs on each boundary of the main triangle.
Moving to the approximation of the globally discontinuous displacement field, an element–wise linear discretization is adopted, i.e. two dofs at each node of the main triangle completely represent the cartesian components of the displacement field.
According to the discretization above introduced, Eqn. (7) and Eqn. (10) generate the following nonlinear discrete setting:

$$\begin{bmatrix} A_{\sigma\sigma}(\Omega, \Gamma_c) & B_{\sigma u}(\Omega) \\ B_{u\sigma}(\Omega) & 0 \end{bmatrix} \begin{Bmatrix} \sigma \\ u \end{Bmatrix} = \begin{Bmatrix} f(\Gamma_d, \Gamma_c) \\ g(\Omega) \end{Bmatrix}. \tag{11}$$

Eqn. (11) highlights the dependence of each term on the relevant domain of integration, i.e. the whole domain Ω, the boundary with prescribed displacements Γ_d or the cohesive path Γ_c. The entries may be easily recovered from the bilinear forms of the continuous problem that were presented in Section 2.1. The only terms that contain contributions computed on the cohesive path Γ_c are the bilinear forms $A_{\sigma\sigma}$ and f. Denoting by $A_{\sigma\sigma}(\Omega)$ and $A_{\sigma\sigma}(\Gamma_c)$ the relevant components of the complementary energy depending on the domain of integration, one has:

$$A_{\sigma\sigma}(\Omega, \Gamma_c) = A_{\sigma\sigma}(\Omega) + A_{\sigma\sigma}(\Gamma_c) = \int_\Omega \underline{\underline{\underline{\underline{C}}}}^{-1} \underline{\underline{\sigma}} : \underline{\underline{\tau}} dx - \int_{\Gamma_c} \mathcal{C}^{-1}(\underline{\underline{\sigma}} \cdot \underline{n}) \cdot (\underline{\underline{\tau}} \cdot \underline{n}) ds. \tag{12}$$

Similarly, the right hand side f may be written as:

$$f(\Gamma_d, \Gamma_c) = f(\Gamma_d) + f(\Gamma_c) = \int_{\Gamma_d} \underline{u}_d \cdot (\underline{\underline{\tau}} \cdot \underline{n}) ds - \int_{\Gamma_c} \mathcal{C}^{-1}(\underline{\underline{\sigma}} \cdot \underline{n})^* \cdot (\underline{\underline{\tau}} \cdot \underline{n}) ds. \tag{13}$$

Notwithstanding the contributions due to the cohesive path, Eqn. (11) preserves the classical compact form of saddle–point problems. As a peculiar feature of mixed methods, the solving matrix is non–positive definite and suitable solvers are needed to handle the arising indefinite linear systems, see [9].

3.2 *An algorithm for quasi–static cohesive crack propagation*

This section points out the main features of an algorithm capable of solving the variational setting previously derived, in the case of a discrete crack growth within a continuum medium. During the process, the evolution of the cohesive zone makes the problem nonlinear, thus calling for ad hoc procedures that manage numerical simulations.
According to [10], the crack length is assumed as the controlling parameter, i.e. a monotonically increasing function that drives the loading process. The bi–linear cohesive law allows for a step–wise linear procedure that computes, via an iterative scheme, the elemental loads that open edge–wise crack segments.
A local remeshing procedure is needed for mixed mode growth where the crack path is not aligned with the mesh. This procedure involves only a few elements around the evolving mathematical tip of the cohesive crack, thus requiring limited modifications to the overall stiffness matrix at each step–wise growth. The well–known maximum tensile stress criterion [4] is herein adopted to manage the fracture propagation, exploiting moreover the accuracy of the JM–based discretization in the evaluation of the stress field. The crack growth is assumed to take place when the principal stress at the tip is equal to the the tensile strength of the material σ_t^*, while the direction of propagation is derived as the perpendicular to the corresponding principal axis of greatest tension.

4 NUMERICAL RESULTS

This section presents numerical simulations referring to crack propagation in pure mode I and mixed mode with the free–sliding assumption, as defined in Section 2.2. Firstly the capability of capturing the deterministic size effect on a three–point bending beam is investigated. Afterwards the features of mesh independence of the proposed procedure are tested on mixed mode crack paths.

4.1 *Size effect in mode I propagation*

The first set of investigations focuses on the three–point bending specimen depicted in Figure 1 that has been discretized according to a mesh of about 8.000 triangular JM elements, with 30 element sides along the depth of the beam. The following mechanical parameters are considered:

$$E = 25127MPa, \;\; \nu = 0.1, \;\; \sigma_t^* = 2.81MPa, \;\; G_f = 72Nm^{-1}.$$

The beam is used to perform numerical investigations for different values of the beam depth d in a wide range of experimental significance. The well–known behavior of concrete specimens that

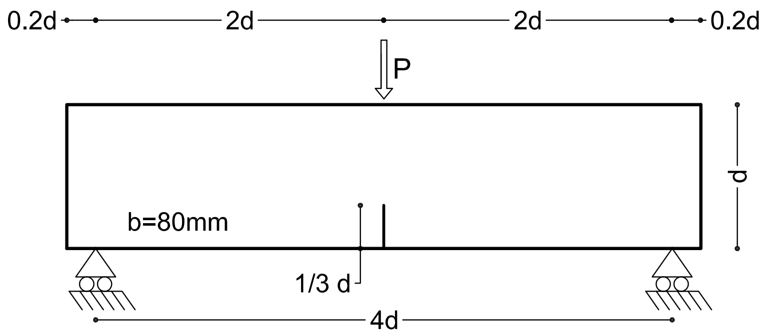

Figure 1: A three–point bending specimen.

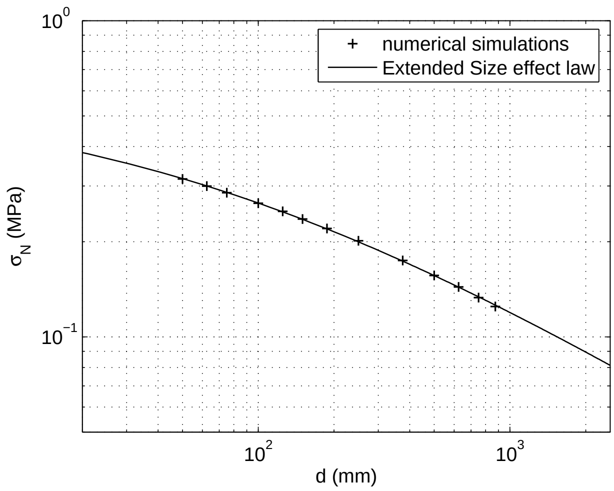

Figure 2: Extended size effect law vs. numerical simulations.

are geometrically similar, see e.g. [4], may be resumed stating that large size beams have a lower non–dimensional load–carrying capacity with respect to small size ones. These issues have been intensively investigated via numerical methods, as in the case of displacement–based formulations [11] or X–FEM approaches [7].

To assess the capabilities of the method, the peak loads reported from the performed numerical simulations are compared with an established analytical representation of the size effect. The so–called extended form of the size effect law [12] ties the nominal strength of the material $\sigma_N = P_{max}/bd$, i.e. its ultimate nominal stress, to the size parameter d. It may be written as:

$$\sigma_N = B_0 \left[1 + \left(\frac{d}{D_0} \right)^r \right]^{-1/2r}, \tag{14}$$

where B_0 and D_0 are constants that characterize the material and the geometrical shape of the structure, while r is a parameter tied to the range and type of the data to be fitted.

In the case $r = 1$ Eqn. (14) reduces to the classical size effect law [13] that allows to fit experimental

results with a very good approximation for a range up to about $1:20$.
Dealing with numerical predictions achieved via piece–wise linear softening equations the accuracy may be gradually lost for wider intervals, due to the asymptotic behavior of the adopted interpolation for small sizes, as pointed out in [14]. To cope with this issue, the choice $r = 0.5$ has been suggested in [12] to produce the best fitting in the case of notched beams that are analyzed via the cohesive crack model.
Figure 2 shows that the achieved numerical results approximate with high accuracy the curve derived from Eqn. (14) along with $r = 0.5$, over a wide range of sizes. This assesses the capabilities of the proposed truly–mixed approach to deal with the deterministic size effect in quasi–brittle materials.

4.2 *Mixed mode propagation*

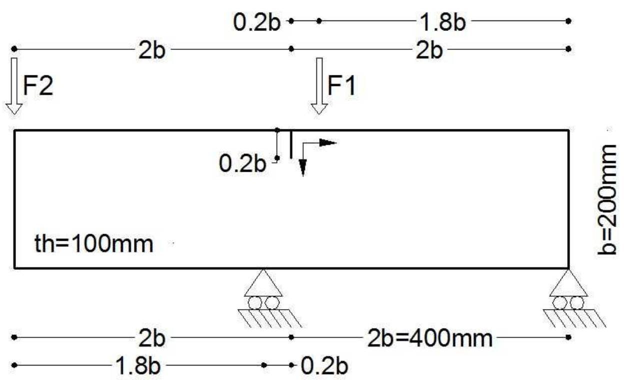

Figure 3: A four–point bending specimen.

The analysis herein presented refer to the non–symmetric four–point bending specimen depicted in Figure 3. This geometry was originally studied in the work [6] via a displacement–based technique and, subsequently, by [7], that implemented an enriched XFEM–based procedure coupled with a J–integral scheme to predict the crack growth.
The beam is herein analyzed by the proposed truly–mixed formulation and adopts the following mechanical parameters from the above literature:

$$E = 28000MPa, \;\; \nu = 0.1, \;\; \sigma_t^* = 2.40MPa, \;\; G_f = 145Nm^{-1}.$$

Experimental evidences reported in [6] show that a curved crack is expected to propagate from the notch, if the load F is applied according to the scheme presented in Figure 3, assuming $F1 = 10/11F$ and $F2 = 1/11F$. The crack starts with a strong deviation from the vertical notch, while progressively turns towards the lower side of the beam following a smoother path. As detailed e.g. in [4], similar specimens are used as a benchmark to assess numerical methods for mixed mode propagation, due to the difficulties that may be experienced in the prediction of this curved trajectory.
The numerical simulations herein presented are performed on two different structural meshes: a coarse discretization, called mesh 40x10, that has 851 nodes and 10 edge–wise segment on the beam

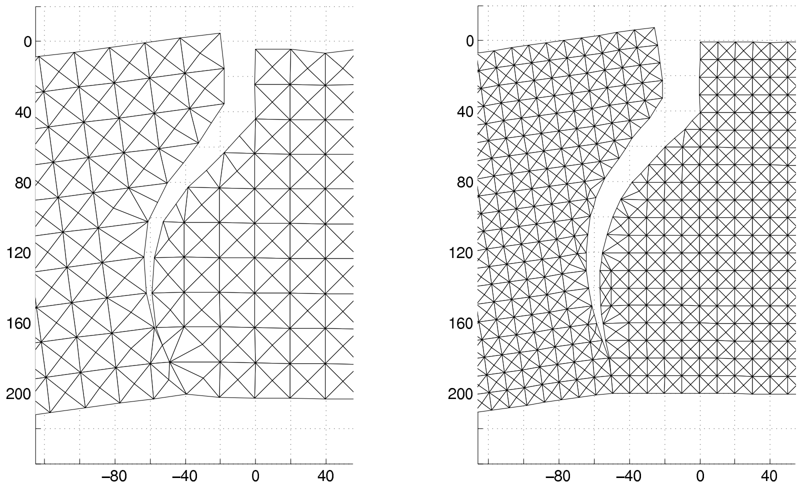

Figure 4: Detail of the deformed meshes in the region of the crack path: discretization 40x10 (L); discretization 80x20 (R).

depth and a finer grid, called mesh 80x20, that has 3301 nodes and 20 vertical edge–wise segments. Figure 4 shows a direct comparison of the predicted crack pathes for each one of the two meshes herein considered. Notwithstanding the remarkable difference in terms of mesh refinement, the achieved results exhibit a similar approximation of the crack trajectory, that is in full agreement with the referenced literature.

According to the above results, the proposed algorithm exhibits a remarkable robustness towards the refinement of the mesh used in the simulations. This means that the truly–mixed discretization allows for a suitable approximation of the stress field at the crack tip in both the considered cases.

5 CONCLUSIONS

An alternative approach for cohesive crack growth in elastic media has been addressed, based on the adoption of a truly–mixed discretization. While most of the methods that are available in literature call for ad hoc enrichments to model displacement jumps, the adopted formulation seems ideally tailored to cope with cohesive crack propagation. The regular traction and discontinuous displacements peculiar to both the continuous and discrete schemes straightforwardly allow for the extension of the truly–mixed formulation to macro–cracked media. A growth algorithm that is able to cope with pure mode I and mixed mode propagation under the free-sliding assumption has also been presented and commented on.

The proposed procedure has been tested on concrete specimens testing the capability of capturing the deterministic size effect for the load–carrying capacity and the mesh independence towards the prediction of crack paths in mixed mode growth. Further developments include the implementation of XFEM-like techniques to allow crack propagation within the JM composite and extensions to more complex dissipation modes.

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