A Comparative Review of
XFEM, Mixed FEM and Phase-Field Models
for quasi-brittle cracking

M. Cervera¹, G. B. Barbat¹, M. Chiumenti¹ and J.-Y. Wu²

¹ International Center for Numerical Methods in Engineering (CIMNE),
Technical University of Catalonia – BarcelonaTech,
Edificio C1, Campus Norte, Jordi Girona 1-3, 08034 Barcelona, Spain
² State Key Laboratory of Subtropic Building Science,
South China University of Technology,
510641 Guangzhou, China
miguel.cervera@upc.edu, gbarbat@cimne.upc.edu, michele@cimne.upc.edu, jyw@scut.edu.cn

Abstract

In this work, a critical comparison between three different numerical approaches for the computational modelling of quasi-brittle structural failure is presented. Among the many finite element approaches devised to solve the problem, both within continuous and discontinuous methods, the present study examines the relative performance of the XFEM, the Mixed strain/displacement FE and Phase-Field models. These numerical techniques are selected as the current representatives of embedded, smeared and regularized models for analyzing the phenomenon of fracture with different mathematical descriptions for the cracking induced discontinuities in the displacement and strain fields. The present investigation focusses on the main differences of the formulation of these models both at the continuum and discrete level and discusses the main assets and burdens that ensue in their practical application. The relative advantages and difficulties related to their use in the computation of localized structural failure in engineering practice are evaluated against a 10-point checklist that cover the main challenges met by these models.

The paper includes an extensive comparison of selected numerical benchmark problems analyzed with the three examined methods. Relative performance is assessed in terms of load capacity, force-displacement curves, crack paths, collapse mechanisms, cost-efficiency and other key issues.

Keywords: Cracking, structural failure, XFEM, Mixed Finite Elements, Phase-field models.
1. Introduction

The finite element is regularly used for assessing structural behavior in engineering practice. In this endeavor, the calculation of the structural capacity and the determination of collapse mechanisms require the accurate numerical simulation of localized failure.

In computational mechanics, two different formats exist to model the phenomenon of tensile cracking in the context of finite element analysis: the discontinuous and the continuous crack approaches. In the discontinuous crack models, displacement jumps across the crack are explicitly considered and the nonlinear cohesive behavior is usually established through a softening traction-jump law. In the continuous crack models, displacement jumps across the crack are smeared over the affected elements and the behavior of the crack is established through a softening stress–(total) strain law.

However, when modelling cracking in quasi-brittle materials, the standard displacement based FE formulation of solid mechanics has shown to produce spuriously mesh dependent collapse mechanisms and crack paths [1, 2, 3, 4], raising ensuing safety concerns. It is therefore necessary to find a computational method able to produce mesh objective results regarding cracking and localized failure.

During the last 50 years, an enormous effort has been devoted to this task and many different strategies for crack modelization have been proposed. The extension and the dispersity of these attempts make it impossible to cover them in a single work. However, since the beginning of the century, three new methodologies have appeared that have the necessary merits to be considered concurrently: the Extended Finite Element Method (XFEM), the Mixed strain/displacement FE formulation (MFEM) and the Phase-field model (PFM). They are the current representatives of the embedded, smeared and regularized approaches to the numerical modeling of quasi-brittle failure. As such, their comparative review becomes a digest of most of the aspirations and achievements in the field of computational failure mechanics.

The objectives of this work are: (1) to identify the main challenges that the numerical modelling of cracking faces and how these have been addressed historically, (2) to outline the main differences in the theoretical models and practical application of the three methods considered in this work, XFEM, MFEM and PFM, in the numerical modelling of quasi-brittle structural failure, (3) to critically compare these three methods against a common checklist that focuses on the identified challenging points, (4) to investigate the relative performance of these three methods for the same benchmark problems.

The outline of this paper is the following. In Section 2, the concepts of embedded, smeared and regularized cracks are presented; both the continuous description and the corresponding discrete setting are introduced. In Section 3, the main challenges of the numerical modelling of cracking are discussed, namely, crack representation, a challenge for the approximability capabilities of the discrete approximation, crack propagation, a test for uniqueness and mesh-bias independence, and balance between fracture strength and toughness, a requisite for the modelization of structural size effect. Features related to these issues are compiled in a 10-point checklist. Sections 4, 5 and 6 are devoted to the XFEM, the MFEM and the PFM, respectively. In each section, a brief introduction, a historical perspective, the continuous formulation, the FE approximation and the appraisal of the corresponding method is given. Each of them is evaluated against the proposed checklist. Section 7 presents sharp numerical simulations of localized structural failure comparing the relative performance of the three examined methods. Section 8 closes the paper with some conclusions and the outlook for future developments.
2. Embedded, smeared and regularized cracks

Since the earliest applications of the FEM to concrete structures, back in the 1960s, the modelling of cracks has been a hot topic in the FE literature, both professional and academic. Many approaches have been suggested and new terminology has been coined. In this section, we distinguish between the formulation at continuum level and its discrete counterpart, the FE implementation.

2.1. Continuous setting

Consider the solid $\Omega$, shown in Figure 1, crossed by a discontinuity $S$, which shows two alternative crack representations in the continuum setting. Regions $\Omega^+$ and $\Omega^-$ are the parts of the solid located “in front” and “behind” the crack. Figure 2 shows the corresponding displacement and strain field, up and bottom, respectively.

A sharp crack is represented in Figure 1a. The top graph in Figure 2a shows the normal displacement along a line normal to the crack, with a discontinuous jump $w$, which represents the normal opening of the crack, occurring at $S$. The corresponding normal strain component is shown in the bottom graph, with a singularity occurring at $S$.

A regularized crack is represented in Figure 1b and Figure 2b. Here, $S'$ and $S$ are two lines that run parallel to $S$, at a relative distance $b$, and forming an in-between band $B$ of small, but finite, thickness. Here, the normal jump $w$ occurring at $S$ is regularized over the distance $b$. The top graph in Figure 2b shows the normal displacement along a line normal to the crack, with the normal jump $w$ increasing continuously between $S'$ and $S$. The corresponding normal strain is shown in the bottom graph, with no discontinuity occurring at $S$.

In the regularized crack, the bandwidth $b$ is a “localization limiter”, introduced in the continuous setting so that the formation of a sharp crack is prevented. Therefore, postulating the existence of a length scale regularizes the problem, but it also changes the problem being solved. For this model to represent the physical problem fracture it must happen that when reducing the regularizing length, that is, for $b \to 0$, the regularized crack converges to a sharp crack.

Figure 1. Crack representations in the continuous setting: (a) sharp and (b) regularized
Figure 2. Crack representations in the continuous setting: (a) sharp and (b) regularized approaches in terms of the displacement (up) and strain (bottom) fields

Regarding the cohesive behavior of the crack, both sharp and regularized cracks follow what are described as Fictitious Crack Models, presented in Hillerborg et al., 1976 [5] and further developed in [6, 7, 8, 9], following the original work of Rashid in 1968 [10]. According to this, the crack is not realized as a topological discontinuity but rather through its constitutive behavior. The sudden drop in strength and stiffness across the crack is replaced by a continuous degradation function; this avoids the singularity at the tip of the crack [11, 12]. In sharp cracks, the behavior of the crack is established through a softening traction-jump law. In regularized cracks, softening stress–strain laws are used.

Cervera and Wu demonstrate in references [13, 14] how the embedded and smeared crack models relate to each other in the continuous setting and the conditions for them to be conforming.

2.2. Discrete setting

Let us now consider a FE discretization of the body $\Omega$, as shown in Figure 3, crossed by a discontinuity $S$. There is the option of discretizing either the sharp or the regularized continuous approaches. Figure 4 shows the corresponding displacement and strain field, up and bottom, respectively.

The embedded crack model in Figure 3a and Figure 4a reproduces the behavior of the sharp crack. The embedded crack model incorporates the behavior of the crack inside the finite elements crossed by it in order to reproduce the displacement and strain behavior of its continuous parent model, as shown in Figure 4a. The displacement field inside the affected elements is discontinuous, and the strain field is composed of a regular part outside the crack, and a singular part at the crack. This is the idea behind the EFEM, Embedded Finite Element Method, also called Strong Discontinuity Approach [15, 16, 17, 18], derived in the Computational Mechanics community and the XFEM, eXtended Finite Element Method [19, 20, 21, 22], and originated from Computational Fracture Mechanics.
Alternatively, the *smeared crack model* is shown in Figure 3b and Figure 4b. In this discrete model, the behavior of the crack is smeared across the elements traversed by the crack, over a bandwidth $b = h$, $h$ related to the element size. The displacement field inside the affected elements is discontinuous, and the strain field is regular part inside and outside the crack. The strains inside the crack are inversely proportional to the bandwidth $b$. The smeared approach was first used by Rashid in 1968 [10] to study pre-stressed concrete pressure vessels. As the behavior of the crack is established through a softening stress–strain law, this approach can be implemented in any nonlinear FE code by simply writing a routine for a new material constitutive model.

In 1983, Bazant and Oh [23] introduced the *crack band theory* (CBT) that used energy considerations to link the softening behavior of the smeared cohesive crack to Griffith’s theory of fracture. The ratio $\Pi = h/L$ between the bandwidth $h$ and Irwin’s material length $L = E G_f / f_t^2$ ($E$ is the Young’s modulus, $f_t$ is the tensile strength and $G_f$ is the fracture energy) determines the brittleness of the element. This coupling between continuum and fracture
mechanics allowed obtaining mesh-size objective results with the smeared crack approach. Even today, more than 35 years later, most of the commercial FE codes use this approach.

Note that, on mesh refinement, that is, as the size of the elements representing the crack reduces, $b = h \to 0$, the discrete smeared crack band model should converge to a sharp crack. This means that strains localize and approach the singular distribution of the sharp crack; also, the energy dissipated in the band must approach the energy release in Griffith’s theory of fracture.

Figure 4. Crack representations in the discrete setting: (a) embedded (b) standard crack band model, (c) mixed crack band model and (d) regularized model in terms of the displacement (up) and strain (bottom) fields
Regrettably, the application of the CBT is plagued by mesh-bias dependency, that is, the computed crack trajectory is spuriously dependent on the alignment of the FE mesh employed; that is, instead of according to the physics of the problem, cracks tends to form parallel to the boundaries of the elements, in an obvious unphysical fashion. Early reports of this issue, shown in Figure 5, can be found in [2, 1, 4, 3].

This lack of consistency between the continuum and the discrete problem of fracture when using the standard FE formulation is caused by its lack of local convergence for the stress and strain fields [24, 25]. Near quasi-singular points, such as in the vicinity of the tip of a crack, the norm of the error of the strains in the standard FE solution, computed as the gradients of the displacements, becomes unbounded [26]. The path of the propagating crack is determined by stress and strain fields that are incorrectly computed at these critical locations, and so the resulting trajectories are spuriously dependent on the FE mesh orientation bias [27]. The problem of mesh-bias dependency displayed by the CBT is solved by enhancing the accuracy of the underlying FE formulation.
The enhanced smeared crack model is shown in Figure 3c and Figure 4c. In this method, proposed and developed by Cervera and coworkers [24, 25, 28, 29, 30, 31, 32, 33], the strain field is no longer computed by local differentiation at element level; instead, strains are treated as additional primary unknowns of the problem, interpolated independently from the displacements. Note that in Figure 4c both the displacement (top) and the strains are linearly interpolated. In particular, the strains field is continuous, differently from the one in Figure 4b for the standard FE interpolation, where the strains are inter-element discontinuous. This added degree of regularity in the strain definition enhances the order of convergence and the accuracy of the computed strain and stress fields. More notably, it achieves local convergence of the discrete problem. Consequently, the method is shown to be mesh-bias independent.

In this discrete model, the behavior of the crack is smeared over an effective bandwidth $b = 2h$, $h$ related to the element size.

The regularized crack model is shown in Figure 3d and Figure 4d. Here, a length scale is introduced at continuum level that acts as a “localization limiter”. As the problem is regular at continuum level, the ensuing FE discretization can be constructed following standard procedures. Clearly, the FE discretization needs the resolution to solve the strain localization that occurs localizing band; this requires an extremely fine mesh, $h \leq b/(4 - 10)$. This strategy has been followed by nonlocal [34, 35, 36, 37, 38], gradient-enhanced [39, 40, 41, 42, 43, 44] and phase-field models [45, 46, 47, 48, 49, 50].

Correspondence of the numerical solutions obtained with these approaches and the physical problem of fracture was not addressed until phase-field models for brittle fracture were proposed. In the original nonlocal and gradient-enhanced models, the length scale was considered a material parameter, dependent on the internal micro or mesostructured, and not as a regularization length. Therefore, the setting of the problem was not that of a fracture problem. Contrariwise, phase-field models are a regularized variational approach to brittle fracture [51, 52, 46], and for vanishing regularizing length, that is, for $b \to 0$, the solution converges to the LFM solution, according to the $\Gamma$-convergence theorem [53]. This property is the definitive advantage of PFM over previous regularized models. The updated geometrically regularized phase-field models, the regularizing length can made dependent on the FE, $b = (5 - 10)h$, so that the crack bandwidth tends to zero upon mesh refinement, guaranteeing the consistency with the original problem.

3. The challenges of the numerical modelling of cracking

As demonstrated by the vast literature devoted to the topic during the last five decades, the numerical modelling of quasi-brittle fracture addresses numerous challenges. In this Section a digest of these is offered grouped in three categories: crack representation, crack propagation and strength and fracture toughness. The Section closes with a proposed checklist to be verified by numerical models of fracture discussed in this work.

3.1. Crack representation. Approximability

The first challenge posed to the numerical models of cracking is the representation of the crack, that is, the ability of the discrete model to reproduce the crack. This comprises several aspects, namely geometry, kinematics, statics and constitutive behavior.

‘Realistic’ crack appearances may be obtained using different models. Figure 6 shows results from a 3D simulation of a pull-out test using the embedded crack model, XFEM [54], and the
enhanced smeared crack, the mixed FEM [55]. In both cases, the direct output of the model has been post-processed to produce an adequate geometrical representation of the opening crack.

Figure 6. 3D simulation of a pull-out test using (a) XFEM, by [54] and (b) mixed FE by [55]

The basic fabric of the stiffness method is the approximation spaces used for the displacement and strains fields. Regarding cracking, the fundamental difference and relative merits between the different methods available lies in the approximation spaces used for the separation modes.

Figure 7. Finite element simulation of a crack: (a) well-aligned and (b) mis-aligned meshes

The very limited ability of standard finite elements to reproduce separation modes in general circumstances is well known. Consider, for instance, a mesh of linear P1 constant strain
triangles, such as the one in Figure 7, subjected to a separation motion in which the nodes located in the $\Omega^+$ part of the domain have a relative displacement of $w$ with respect the $\Omega^-$ part of the domain. Consider also, as in Figure 7a, that $S^+$ and $S^-$ are two lines that run parallel to $S$ (with normal $n$), at a relative distance $b = h$, this being the typical height of the triangular elements. Surfaces $S^+$ and $S^-$ delimit a localization band of width $b$ inside which strain localization may occur. In this case, $w = u^+ - u^-$ is the difference between the displacements at $S^+$ and $S^-$ and $\beta = \partial w / \partial n$ is a deformation vector defined by differentiation with respect to the normal coordinate $n$. With linear elements, the deformation vector $\beta$ can only be approximated satisfactorily as $\approx w / h$. This will, in fact, be the result obtained by projecting the exact separation mode on the finite element mesh of Figure 7a. However, projecting the exact separation mode onto the finite element mesh of Figure 7b, in which lines of nodes $S^+$ and $S^-$ are not parallel to the intended discontinuity line, will not yield the same (correct) results. This is because $P1$ elements can only reproduce a constant deformation mode of the form required by Maxwell’s compatibility condition if $n$ is normal to one of the sides of the triangles. The bilinear quadrilateral element $Q1$ shows similar shortcomings.

The reason for this is that discrete solution spaces built from piecewise continuous polynomials cannot represent displacement discontinuities with arbitrary orientations inside the element, not even in a smeared fashion. This is purely an approximability shortage of the discrete solution spaces used for interpolating the displacement field, which translates in the strain modes. Moreover, this approximability error is not eliminated nor reduced on mesh refinement.

In the embedded methods, the way of correcting this approximability local discretization error is to enrich the approximation spaces with additional deformation modes that enhance the desired capacities for representing embedded displacement and/or strain discontinuities. Thus, the EFEM and the XFEM strategies aim to represent strong discontinuities as such, via elemental or nodal enhancements of the displacement solution space. As pointed out by [56] and shown in Figure 8, the difference between the EFEM and the XFEM is that EFEM accounts for constant (i.e. the relative rigid body translations) and special linear discontinuity modes (i.e. the relative rigid body motions and the self-stretching), whereas XFEM considers a more general relative displacement field that is at least, of linear precision.

In practice, both formulations are often applied in a regularized manner [57, 58], and in these regularized versions, the discrete solution considers embedded strain localization bands rather than actual displacement discontinuities. The width of the regularized band is regarded as a numerical parameter of the implementation, chosen to be small. An obvious choice for this width is the size of the element, which, on mesh refinement, can be made as small as desired. This suggests representing strong discontinuities in a smeared mesh-corrected framework [59, 60].

Using an enhanced formulation requires to specify the orientation of the modeled discontinuity. This poses the question of when, along the deformation process, calculating and fixing this orientation. Selecting the direction of the discontinuity according to some ad hoc condition and fixing it afterwards may become a superimposed condition on the constitutive behavior.

In the smeared methods, as pointed out by [24, 25] and shown in Figure 9, one of the differences between the standard and the mixed FEM is the superior capacity of the second one to represent the strain fields corresponding to pure separation modes. As mentioned, low-order standard FEs are only capable of reproducing separation modes which are parallel to one of their sides. This is also one of the main reasons for the mesh-bias results that they produce. The independent interpolation of the strain field in the mixed FEs increases considerably the corresponding approximating space.
In a variationally consistent formulation, the statics of the discrete crack model is very much linked to the kinematics. In embedded formulations, the outcome of this consistency is that the formulation is symmetric, but also that the condition of traction continuity is not ‘naturally’ satisfied. If this condition is enforced, non-symmetric Petrov-Galerkin formulations ensue, both for EFEM and XFEM [61, 56]. In smeared formulations, statics of the crack emanate from the projection of the crack plane of the constitutive behavior adopted for the cracking solid. Symmetry is ensured in a secant format of the constitutive equation, as the secant matrix needs to be symmetric from thermodynamic considerations.

Regarding the constitutive behavior of cracks, this is complex, even in monotonic loading conditions. The decohesive behavior of cracks yields that their opening is accompanied by stress distribution, which may cause the occurrence of shear stresses across the cracks. Even if the crack has been initiated in pure Mode I conditions, complex mixed mode situations may arise that require contemplating the sliding of the open crack. Additionally, a model for a crack subjected to cyclic loading needs to have closing-reopening capabilities. These are requirements not easily incorporated in the numerical models.

Traction-separation models adopted for embedded cracks are phenomenologically derived and comparatively simple [62, 63, 64]. Stress-strain models adopted for smeared models are usually derived in the Continuum Damage Mechanics framework, with varying degrees of sophistication [28, 29]. Orthotropic behavior, sliding, closing-reopening and irreversible straining are already realistically considered [31]. Regularized crack models relate almost exclusively to scalar damage models under monotonic loading, although they are progressively considering the mentioned effects [65, 66, 67].
Cervera and Wu address in references [13, 14] how traction- and stress- based constitutive models are related.

3.2. Crack propagation. Uniqueness and mesh-bias independence

The second challenge posed to the numerical models of cracking is the propagation of the crack, that is, the ability of the discrete model to reproduce the onset of cracking and the direction of propagation. Both the continuous and the discrete settings of the model contribute to this challenge. Not least important are the implementation prospects.

From the engineering standpoint, this is a crucial aspect of the problem. Crack propagation determines failure mechanisms and carrying capacity of a structure. Not surprisingly, the inability of FEM models to produce physically realistic crack pattern arouse awareness of academics and practitioners at the beginning on the 1990’s. Since then the issue has received a great deal of attention, and promoted numerous research lines.

In the continuous setting, it is necessary to distinguish the Fracture Mechanics (FM) and the Continuum Mechanics (CM) traditions.

FM follows Griffith’s theory of fracture, which establishes an energy based criterion for fracture propagation; it does not provide a direction for propagation, which has to be established as a separate ingredient of the problem statement [68, 69]. Several phenomenological criteria are used in FM for crack propagation and they have been used in the embedded crack models derived from FM.

The CM community uses a variety of stress based criteria for the onset of damage, and they have been used in the smeared crack models derived from Continuum Damage Mechanics (CDM). Here, the cohesive behavior of the crack works as a quasi-brittle version of Griffith’s theory, ensuring the energy dissipated in the formation of the crack is objectively defined. The more recent regularized phase-field approach to fracture is based in the same energy conserving concept.

In the stress based model for fracture, the initiation of cracking and the direction of propagation are implicit in the underlying constitutive model. This connection has been thoroughly investigated by Cervera and Wu [14, 70, 71, 72, 73]. A generalization of Morh’s maximization postulate [74] is invoked to determine the direction of propagation. Weihe and coworkers have also used similar arguments [75, 76, 77].

Figure 10. Crack patterns corresponding to different cracking criteria using mixed FE [29]
Figure 11. 3D simulation of a torsion test on a solid cylindrical specimen and comparison with a piece of chalk using mixed FE [29]

Figure 10, shows the crack patterns in the same discretization of a cylindrical piece of chalk subjected to pure torsion according to different cracking criteria, obtained with the enhanced smeared crack model and mixed FEM [29]. The Beltrami criterion produces a planar horizontal crack surface. This is accountable to the fact that, for pure torsion, this criterion coincides with the Von Mises criterion, which would yield exactly such a planar crack in the plane of maximum shear stress. The Positive Beltrami and Rankine models produce very similar results, a helicoidal crack, as these two criteria are only sensitive to tensile stress. Of all the isotropic models considered, the only one that is able to reproduce the helicoidal crack with 45° slope that occurs in the piece of chalk is the Drucker-Prager criterion. The computed crack surfaces obtained with the orthotropic Rankine and Drucker-Prager criteria produce noticeably different results than their isotropic counterparts, even if they are driven by the same failure criteria. The reason for this is that the corresponding inelastic deformations are different.

All the orthotropic criteria produce slightly different crack surfaces, all similar to the crack produced in the real piece of chalk, but the one that reproduces better the actual crack in Figure 11 is the orthotropic Rankine constitutive law.

In the discrete setting, the major specific challenge in crack initiation and propagation is the lack of local convergence of the standard displacement based FE formulation that is commonly used in both in the embedded and the smeared approaches. Using linear elements, local convergence for the stresses (or strains) cannot be guaranteed in the irreducible formulation. Using higher order elements in problems involving strong gradients and/or discontinuities does not improve the convergence estimates, since higher order derivatives involved in these estimates are not bounded in such situations. In fact, if the continuous solution is singular, not even the first order derivatives are going to be point-wise bounded.

Given the intrinsic local nature of the fracture problem, the discrete solution is largely affected by the local discretization error. Additionally, strongly nonlinear constitutive behavior yields a
nonlinear problem and lack of uniqueness of the solution. Using the standard formulation in 2D and 3D situations local discretization error together with material nonlinearity commonly produce that, from the multiple solutions that the nonlinear discrete model has, the one obtained is mesh-biased and, therefore, apparently unrelated to the continuous case.

Consider the stress field obtained at the tip of a notch subjected to mixed mode bending test as shown in Figure 12. The solution of the associated continuous elastic problem using standard FEs depends strongly on the actual detail geometry of the tip of the notch. The strain and stress fields are regular if the tips are rounded, but they become singular if the notches present sharp corners. In this case, the corresponding discrete model will perform satisfactorily in terms of a global error norm, but will approximate very poorly the actual behavior at the singular points. In fact, local error estimates will be unbounded, as can be appreciated in Figure 12a.

![Figure 12. Contours of major principal stress at the tip of a notch in a mixed mode bending test obtained with (a) standard P1 FEs (b) mixed P1P1 FEs](image)

The local discretization error in the elastic or pre-cracking regime observed in Figure 12a cannot be circumvented by mesh refinement nor by regularization of the geometry of the notch so that singular points are eliminated. Even if the tips of the notches in the specimen are rounded and the discrete elastic solution is reasonably accurate, the problem of a local discretization error will reappear as soon as sudden, brittle and irreversible cracks progress through the finite element mesh. This may be of crucial importance in a nonlinear analysis if the criteria for initiation of inelastic behavior are established in terms of local values and directions or strains or stresses, see Figure 14 (left). Propitiously, the mixed formulation can guarantee local convergence of the strain field and for a region around the singularity (Figure 12b) and, therefore, converged solutions are produced using this method, see Figure 14 (right).

Figure 13 presents an in depth mesh dependency study taken from [30] where the performance of the standard and mixed FE formulations are thoroughly compared. On the one hand, it can be seen that the computed crack trajectory of the standard displacement based formulation in solid mechanics is pathologically dependent on the orientation of the finite elements. On the other hand, the mixed FE method is producing mesh objective results for all the different FE alignments considered, due to its enhanced accuracy in stresses and strains. Additional comparisons between the standard and the mixed formulations can be found in reference [32].

Figure 14 also shows that with standard FE and orthotropic damage severe stress oscillations appear along the sides of the crack. Using orthotropic damage models, the discontinuous approximation of the strain field and the meagerness of the kinematic description of low order standard FE produces strain oscillations and spurious stresses that make their implementation
unpractical. This is known in the literature as spurious shear stress locking and it caused the almost complete abandonment of orthotropic models for cracks in favor of isotropic models. The above problem is greatly alleviated by the enhanced kinematical description of the mixed finite elements, so that with mixed FE orthotropic models no stress oscillations appear along the crack path. The reason for this is the inter-elemental continuity of the strain interpolation.

The difficulties associated to the local discretization error of the standard FE formulation are avoided if the problem of fracture is regularized at continuous level. This is the reason why models portrayed as regularized are not affected by them. The regularity injected in the continuum problem is naturally inherited by the discrete problem, at the cost of achieving the required level of resolution of the strain localization band.

![Fig. 13. Mesh dependency study comparing crack trajectories computed with standard FE (left) and mixed FE (right) with varying element orientations and sizes [30](image)](image)
Conversely, the local discretization error characteristic of the standard FEM in quasi-singular simulations also plagues the embedded crack FE models. The introduction of the enriched separation modes requires the a priori determination of the location and orientation of the crack. This is done from the established criterion for crack propagation and from the approximated fields of strain and stress. The lack of local convergence has two consequences, as it pollutes the determination of the required magnitudes and may also affect the geometrical continuity of the crack.

In relation to this, and the implementation prospects of the FE procedures, it is noteworthy to remark on the use of auxiliary tracking techniques in cracking problems (see Figure 15). In the last decade, these procedures, originated in the context of FE applications of the Fracture Mechanics, have been introduced in Continuum Mechanics based approaches, even if there is no variational justification for their use. Successful application of the EFEM and the XFEM requires their use to determine the direction of crack propagation [78, 79, 80, 81, 22]. Mosler and Meschke [80] have reported that, without tracking, the EFEM leads to the same spurious mesh bias dependence as the standard weak discontinuity approach. Cervera and coworkers [26, 27, 82, 83, 84, 85] have reported in the reciprocal sense that if tracking is used, the weak discontinuity formulation produces results that do not suffer from mesh bias dependence in an evident spurious way.

There are at least two reasons to explain why the use of auxiliary tracking procedures is useful. On one hand, global tracking techniques help to overcome the local discretization error, particularly if coarse meshes are used. On the other hand, more fundamentally, the use of seeding and tracking techniques, either local or global, is determinant in eliminating undesired alternative solutions of the nonlinear discrete problem. The tracking procedures not only “label” the elements along the potential localization path; they also “cross out” the elements outside that path, overriding the possibility of, supposedly spurious, alternative solutions. In this sense, they are useful in selecting the appropriate solution among the many possible ones. Regretfully, and disregarding their heuristic introduction, crack tracking techniques are simply not robust enough in cases like bending, where the trajectories of tensile principal strains stop at the neutral axis; and they are intrinsically unable to deal with branching situations which may have physical meaning.
3.3. **Strength and fracture toughness. Structural Size Effect**

Structural size effect refers to the variation, motivated by a change of size, of the load capacity of a structure from estimations made using stress failure criteria [87]. The observed behavior of quasi-brittle specimens in laboratory tests does not correlate with the one perceived in real sized structures, because the latter are usually much bigger. This phenomenon has a profound impact in many practical applications [88, 89, 90, 91, 92]. Although several sources of structural size effect have been observed, the study of the size effect phenomenon is principally related to energetic considerations [93, 94, 95, 96, 97, 98]. When the fracture develops the stored elastic energy in the structure is released into the crack front. This energy is dissipated and engaged into the process of the crack surface formation. The ratio between the elastic energy stored in the structure and the energy dissipated through the crack tip varies when size changes. This is the main cause for structural size effect.

According to the dimensional analysis derived in reference [96], in situations involving materials with softening, the brittleness of the problem is governed by the brittleness number \(\Pi_B\), the ratio \(L/L_0\) between the characteristic size of the structure \(L\) and Irwin’s material length \(L = E G_f / f_t^2\) where \(E\) is Young’s modulus, \(f_t\) is the (tensile) strength and \(G_f\) is the fracture energy of the material, which is the energy dissipated per unit of area of the fracture surface.

Thus, from energy considerations, the brittleness of the problem is size-dependent. Consequently, collapse in smaller specimens occurs in a more ductile way while larger specimens fail in a more brittle manner. In the small limit case, the formation of a failure mechanism takes place as a result of the yielding of an extensive area. In the large scale limit, perfect brittle failure occurs. For intermediate sizes failure is due to the formation of a crack that gradually develops in the structure while stress redistribution and the release of stored energy into the crack front takes place [87, 95].

From experimental observations and theoretical considerations [94] Bazant’s size effect law has been proposed to represent the phenomenon. It describes the relationship between the load capacity of the structure and its characteristic size. It is defined in its simplest form as [87, 99, 98]:

\[
\sigma_{Nu} = B f_t \left(1 + \frac{L}{L_0}\right)^{-\frac{1}{2}}
\]

(1)
where $\sigma_{Nu}$ is the nominal strength, defined as

$$
\sigma_{Nu} = c_n \frac{P_u}{Lt} \quad \text{(2D Scaling)}; \quad \sigma_{Nu} = c_n \frac{P_u}{L^2} \quad \text{(3D Scaling)}
$$

where $L$ is the characteristic size of the structure, $t$ is its thickness, $P_u$ is the ultimate/failure load of the structure, $f_t$ is the strength of the material and $L_0$ is a reference structural size; $B$ is a dimensionless constant which depends on the shape and the loading of the structure but not on its size and $c_n$ is a dimensionless constant that can be arbitrarily chosen. Assuming that the reference structural size $L_0$ is linearly dependent with Irwin’s characteristic length $L$, $L_0 = A^{-2} L$, $A$ being a constant similar to $B$, allows to rewrite Bazant’s law in Eq. (1) as

$$
\sigma_{Nu} = B f_t \left(1 + A^2 \frac{L}{\Pi_B} \right)^{-1/2}
$$

where $\Pi_B = L/L_0$ is the brittleness number defined in [96].

In Figure 16 the size effect behavior described by Bazant’s law in Eq. (1) is shown, where the role of the reference size $L_0$ is appreciated.

![Figure 16. Bazant's size effect law](image)

The law indicates how for small structures, when $L/L_0$ is much smaller than 1, $\Pi_B \to 0$, the structure collapses following the predictions of limit analysis, which does not contemplate size effect, as the nominal strength of the structure is explicitly independent from size: $\sigma_{Nu}(\Pi_B \to 0) = B f_t$. Note that this nominal strength depends directly on the tensile strength of the material $f_t$. Material strength and strength envelopes are typically determined in laboratory tests performed on small scale samples.

For large structures, when $L/L_0$ is much larger than 1, $\Pi_B \to \infty$, the structure fails following the LEFM theory, with the strongest possible size effect, the nominal strength being inversely proportional to the square root of the structural size [91]: $\sigma_{Nu}(\Pi_B \to \infty) = \frac{B}{A\sqrt{EGf(L)}}^{-1/2}$. Note that this nominal strength depends on the stress intensity factor (or fracture toughness) $K_c = \sqrt{EGf}$ of the material, but it is independent of its strength $f_t$. For large specimens, criteria based on critical stress intensity factors, such as the those used in LEFM, are applicable.
For intermediate size cases a gradual transition from one failure mode to the other takes place, as it typically happens in most applications involving quasi-brittle fracture [95]. Such situations require the consideration of both the strength and the fracture energy and material properties.

It is noteworthy that even though the size effect law is generally defined in terms of the nominal strength $\sigma_{Nu}$, this is in fact an indirect way of describing the peak load $P_u$ sustainable by the structure in terms of its characteristic size. Therefore, the nominal stress is not a real stress but a load parameter, useful to depict in a clearer way the deviation from limit analysis due to size effect [93].

![Figure 17. Force-displacement curves, normalized with size, of geometrically similar structures exhibiting size effect. Grégoire Tests for the fifth-notched beams [37]](image)

Experimental evidence shows that, in addition to the consequences that it has on the structural load capacity, size effect also governs the ductility and post-peak behavior of the structure. For loading under displacement control, failure in larger sized structures occurs closer to the peak load [87, 91], as shown in Figure 17. The fact that the post-peak curves of large structures descend more steeply than in smaller ones [93, 95] is also due to the fact that, once properly normalized, the energy dissipated in the failure process is comparatively smaller in larger structures.

When considering the scaling of structures in general, several other factors do not scale geometrically apart from their brittleness. For example, in dynamic analysis, a big concern is the fact that the strain rate is influenced by the scaling factor, affecting the predictions of the stresses obtained from scaled models [100, 101, 102]. This issue, which requires specific attention, is not treated in this work which focusses on structural size effect under quasi-static loading. It should also be noted that weight forces do not scale geometrically neither. Even if considering them in FE analysis is straightforward, they can be effectively neglected in laboratory tests of small concrete specimens. Regarding scale modelling, it should also be taken into consideration that in laboratory tests the possibilities of scaling the aggregate inside concrete are limited.

Regarding energy dissipation, at the continuous level, when considering sharp cracks, the total energy dissipated during the fracture process is proportional to the area of the crack surface. However, when the regularization of the cracks is introduced, at continuous level, the total energy dissipation is proportional to the volume of the localization band [13, 14]. Therefore, for ensuring consistency between the regularized and non-regularized problems, the fracture energy
per unit area $G_f$ is substituted by $g_f = G_f/b$ as the energy dissipated by unit volume, $b$ being the width of the regularized crack. In such case, the same brittleness number as in the original problem holds

$$\Pi_B = \frac{L}{b} \cdot \frac{b}{L} = \frac{L}{L}$$  \hspace{1cm} (4)

In the discrete FE problem, the embedded, smeared and regularized models need to be considered separately.

Figure 18. Structural Size Effect: Force-CMOD curves of the Grégoire Tests for the fifth-notched beams [32]

In **embedded crack models** the adopted traction-jump laws define the softening behavior in terms of the fracture energy of the material. Therefore, size effect is straightforwardly considered.

In **smeared crack models** the crack bandwidth $b$ is related to the FE size $h$ ($b = \alpha h$, $\alpha$ being a constant, $\alpha = 1$ for standard FE, $\alpha = 2$ for mixed FE) and the same brittleness number is recovered

$$\Pi_B = \frac{L}{ah} \cdot \frac{ah}{L} = \frac{L}{L}$$  \hspace{1cm} (5)

guaranteeing the consistency between the continuum and the discrete problems with respect to fracture energy dissipation and mesh-size objectivity.

In regularized crack models two interpretations of the crack bandwidth $b$ have been proposed. In the original nonlocal models, the scale length is a material property that acts as a localization limiter, so that the interpretation of Eq. (4) holds. Phase-field models introduce $b$ as a regularizing length, so that Eq. (4) also applies. If this regularizing length is linked to the resolution of the mesh, then Eq. (5) also applies. In any of the cases, regularized cracks model size effect accurately.

In Figure 18 the enhanced (mixed) smeared crack model is used to numerically reproduce the behavior of three series of notched beams under bending. One series differs from the other in the notch to depth ratio. It can be appreciated how the structural size effect displayed by the experimental test is match remarkably by the numerical results. Furthermore, Figure 19 shows...
how the numerical computed nominal strengths of the notched beam over a large range of sizes fit the size effect behavior described by Bazant’s law in Eq. (3).

Figure 19. Computed predictions of the nominal strength vs beam depth for the notched beam [32]

3.4. A 10-Point Checklist for the modelling of fracture

According to the challenges that the numerical modelling of fracture poses to the diverse approaches that have been put forward in the last 5 decades and continue to be presented, the following 10-Point Checklist is proposed:

1. **Variational formulation in the continuous setting**
   The definition of the problem of cracking in the continuous setting should rely on a rigorous physical foundation and mathematical framework.

2. **Convergence of the FE formulation**
   Commonly, regularity of the solution is assumed and convergence of a FE formulation is proved at global level. In the problem of fracture, local regularity of the continuous problem is lost and convergence is not guaranteed for the FE procedure. The approximation spaces for displacements and strains need to be designed so that convergence is attained.

3. **Strength, toughness and energy dissipation**
   The initiation and propagation of cracks depend on material strength and toughness and on stress and energy release rate criteria. Structural size effect in brittle and quasi-brittle failure depends on the adequate blending of both.

4. **Criterion for direction of propagation**
   Classical Linear Fracture Mechanics does not incorporate a criterion for the propagation of cracking, so one needs to be provided and assessed.

5. **Constitutive behavior generality**
   Additionally to their cohesive behavior, cracks may slide, close and reopen. The stress and stiffness changes associated to the evolution of the crack need to be considered.

6. **Generality and implementation effort**
A crack model should be applicable in conjunction with any linear interpolation basis (triangles, quadrilaterals, tetrahedra, hexahedra, prisms) with as few necessary variations as possible. Implementation of element-dependent specific procedures for numerical integration, sampling or averaging is undesirable.

7. **Cost-efficiency**
   Different FE procedures have different unknown variables in different sets of nodes, but they also require different mesh resolution. Also alternative FE formulations have different accuracy and order or convergence.

8. **Multiple, intersecting and branching cracks**
   Practical applications of fracture often involve multiple, intersecting and/or branching cracks. Different crack models have considerable shortcomings in addressing these situations.

9. **Auxiliary tracking techniques**
   Crack tracking techniques are required in embedded FE formulations. This a seriously limiting drawback.

10. **Application in 3D**
    Engineering applications require crack procedures that can be applied in 3D problems. Smeared crack models are implemented in commercial codes and applied routinely. A substitute model should be able to address the same sort of applications.

In the following Sections three numerical methods for modelling quasi-brittle fracture are discussed: (i) the XFEM, (ii) the mixed FEM and (iii) the Phase-Field method, as representative techniques of the embedded, smeared and regularized crack models, respectively. They have been selected because of their outstanding merits. For each method, its historical perspective, continuum formulation, FE approximation and performance on the checklist is offered.

4. **XFEM**

**Introduction**
In the Extended Finite Element Method (XFEM), the standard displacement based FE formulation in solid mechanics is enriched, extended, with the introduction of additional degrees of freedom and discontinuous interpolation functions to explicitly represent an embedded sharp crack in the body without the need of performing remeshing operations. The study of the propagation of sharp cracks is a realm of Fracture Mechanics and remeshing techniques are very much used there, but they are difficult to implement and computationally burdensome. The XFEM was born to be applied in LEFM, and then jumped to more general Computational Mechanics. The XFEM enjoyed wide acceptance in academic circles during the first decade of the millennium, but it is now rarely used due to its intrinsic limitations.

**Perspective**
The XFEM [19, 20, 21, 22, 103] was introduced by Belytschko and coworkers at the end of the 20th century as an advance with respect to the previous embedded discontinuous approaches that had been proposed previously. The strategy employed for enriching the FE solution was first proposed by Babuska and coworkers [104, 105] for the so-called Generalized Finite Element Method (GFEM) [106, 107, 108]. Nowadays, there is general consensus that the GFEM and the XFEM are basically identical [109, 110, 111, 112, 113, 114] and they are often referred to as the GFEM/XFEM.
Regarding cracking and fracture, the XFEM contributes with an original FE formulation of a conforming embedded strong discontinuity in the displacement field. This is the last of a long history of attempts to incorporate sharp cracks in FE models.

First, sharp cracks were modelled through a separation of the FEs along their edges by doubling the nodes. Clough [115] and Ngo and Scordelis [116] analyzed pre-defined cracks, while Nilson [117] was the first to evaluate fracture propagation according to a criterion set in terms of stress. Later, remeshing approaches were proposed [118, 119, 120, 121] where the crack is introduced by remeshing elements that are encountered along its trajectory. These approaches were found to be spuriously mesh dependent and, more importantly, involved a change in the mesh topology, this increasing their computational cost. Similarly, techniques involving the inclusion of cohesive interface elements [122, 123, 64, 124, 125, 126] representing the crack have been developed. However, all these techniques suffer from spurious mesh dependency unless a crack tracking technique or the smoothing of the FE solution is introduced [127, 128]. See the reviews in references [129, 130] for more details.

An improved technique proposed to consider sharp cracks is the embedded finite element method (EFEM) in which the approximation of the displacement field is enriched to introduce the discontinuous displacements due to the crack. Pioneering work by Ortiz [15] was followed by Belytschko [16] and others [17, 131, 86, 60, 132, 133]; see reference [61] for an extensive review. Similarly to the XFEM, the main advantage of the EFEM with respect to previous techniques is that no remeshing is required.

In reference [56], Wu presented a unified framework that encompasses both the EFEM and the XFEM for modeling cohesive cracks. A fine scale refinement is hierarchically added to the regular approximation of the displacement field to model the effect of the crack; the added degrees of freedom constitute a parametrization of this fine scale. The difference between the EFEM and the XFEM is the way of constructing the discrete subspace for the fine scale. Different possibilities exist for this, but generally the extra space used in the XFEM is larger than in the EFEM.

As generally used, the main difference between the EFEM with respect to the XFEM is the conformity of the extended displacement field. In Figure 20 a comparison regarding inter-elemental displacement continuity between conforming and non-conforming embedded formulations is shown. In the EFEM extra degrees of freedom and correspondent static relations are introduced and established at element level; in this way the additional unknowns may be locally condensed at the cost of inter-element displacement continuity. In the XFEM, the enrichment is introduced at nodal level and equilibrium is satisfied at global level; conformity is preserved. In references [134, 61] a comparative study between EFEM and XFEM is made.

For the numerical implementation of the embedded crack, via the XFEM or the EFEM, it is necessary to introduce a specific criterion to check whether an element is crossed by the crack, and if it is, to determine the orientation of the crack segments within that element. This auxiliary procedure is known as crack tracking technique. Several such procedures have been proposed and their relative merits assessed (see reference [82] for a detailed review), but they are invariably defined in discretionary fashion, alien to the variational structure of the problem and violating the assumed constitutive behavior outside of the track. The necessity of recurring to auxiliary crack tracking techniques is the largest frailty in the application of the XFEM.

The application of the XFEM to the problem of fracture is founded in two keystones: the Partition of Unity property applied to hierarchically enhance the FE approximation space so that conforming discontinuous displacements may be included and the ensuing variational form of the problem according to the embedded crack concept accommodating Griffith’s theory of
fracture. The enrichment in the FE approximation space is done a priori; Griffith’s theory does not include a criterion for the orientation of the advancement of the crack.

Figure 20. (top) non-conformity in the EFEM: (a) computed crack path with the EFEM and (b) detail, (bottom) comparison of (a) non-conforming and (b) conforming embedded formulations [135]

**Continuous formulation**

In the following, the principal characteristics of the improved-stable XFEM (is-XFEM) model developed by Wu [136, 137, 138, 139], referred to in the comparisons of this work, are laid out. The method follows the mathematical approach to fracture employed in the strong discontinuity approach [140, 18, 141, 79]. For additional details, references [136, 137, 138, 139] are recommended.

The domain $\Omega$ is divided in two parts by the crack, denoted $\Omega^+$ and $\Omega^-$, so that $\mathbf{u}^+$ and $\mathbf{u}^-$ are the displacement fields in their respective parts and $\mathbf{u}$ is the relative displacement field of one part with respect to the other, as shown in Figure 21.

\[ \mathbf{u} = \mathbf{u}_+ - \mathbf{u}_- \]  \hspace{1cm} (6)

The embedded crack $S$ causes a discontinuity in the displacement field $\mathbf{u}$ that is explicitly considered. According to the variational multiscale method [142, 143], the displacement field can be expressed as

\[ \mathbf{u} = \mathbf{u} + \mathbf{u} \]  \hspace{1cm} (7)
where $\tilde{\mathbf{u}}$ represents the coarse scale displacement field that satisfies the standard regularity conditions, and $\bar{\mathbf{u}}$ denotes the fine scale displacement field that is discontinuous across the crack $S$, so that it can be further expressed as

$$\tilde{\mathbf{u}} = H_S \bar{\mathbf{u}} - \mathbf{u}'$$  \hspace{1cm} (8)

where $H_S$ is a unit step function which is equal to 0 in $\Omega^-$ and to 1 in $\Omega^+$, and $\mathbf{u}'$ is the regular part of the fine scale. It is also assumed that the fine scale vanished at the boundary.

The strain field is obtained as the symmetric gradient of the displacements

$$\varepsilon = S\mathbf{u}$$  \hspace{1cm} (9)

where $S$ is the differential symmetric gradient operator. And, therefore,

$$\varepsilon = \varepsilon + \varepsilon = S \tilde{\mathbf{u}} + S \bar{\mathbf{u}} = S \tilde{\mathbf{u}} + H_S S \bar{\mathbf{u}} - S \mathbf{u}'$$  \hspace{1cm} (10)

Outside of the crack, the material is assumed to have a linear elastic behavior, so the following constitutive law can be written in $\Omega \setminus S$

$$\sigma = D_0 \varepsilon$$  \hspace{1cm} (11)

where $D_0$ is the elastic constitutive matrix and $\varepsilon$ is the regular strain field in $\Omega \setminus S$

$$\varepsilon = S \tilde{\mathbf{u}} - S \mathbf{u}'$$  \hspace{1cm} (12)

The nonlinear behavior of the crack is introduced as a traction-separation law [137, 138]. Let $\omega$ be the displacement jump at the crack, equal to $\tilde{\mathbf{u}}$ evaluated at the crack, $\omega = \llbracket \mathbf{u} \rrbracket = \tilde{\mathbf{u}}(\mathbf{x} \in S)$.

$$\mathbf{t} = E_S \omega = \phi E_0 \omega$$  \hspace{1cm} (13)
where $E_s$ and $E_0$ are the secant and reference stiffness of the discontinuity, respectively, relating the displacement jump of the crack $\omega$ and the traction on the crack surface $t$. The localized integrity variable $\phi$ describes the decohesion of the crack; $\phi$ is initially infinite and monotonically decreases to zero as the crack opens.

The evolution of localized integrity variable $\phi$ depends on the opening of the jump. A failure criterion, expressed in terms of the normal displacement jump across the crack $\omega_n$, is introduced

$$F(\omega_n, r) = \omega_n - \kappa = 0$$

where $\kappa$ is an equivalent displacement jump threshold. Its current value at time $t$ is computed from the Kuhn-Tucker conditions, so that the irreversibility of the process is guaranteed

$$\kappa = \max \omega_n(\hat{t}) \quad \hat{t} \in [0, t]$$

The localized integrity variable $\phi$ can follow several evolution laws. In [138], both exponential and Cornelissen [62] softening functions, shown in Figure 22, are considered.

$$\phi = \frac{f_t}{E} \frac{1}{\kappa} \exp \left( - \frac{f_t}{G_f} \kappa \right) \quad \text{Exponential}$$

$$\phi = \frac{f_t}{E} \frac{1}{\kappa} \left[ (1 + \eta_1^2 \kappa^3) \exp(-\eta_2 \kappa) - \kappa (1 + \eta_1^2) \exp(-\eta_2) \right] \quad \text{Cornelissen}$$

where $E$ is the initial elastic Young’s modulus, $f_t$ is the tensile strength and $G_f$ is the fracture energy. The variable $\kappa$ is defined as $\kappa = \kappa f_t / (5.1361 G_f)$. The parameters considered in [138] for the Cornelissen softening law are $\eta_1 = 3.0, \eta_2 = 6.93$.

Equilibrium is enforced as usual through the Cauchy momentum equation

$$S^T \sigma + f = 0$$

where $S^T$ is the differential divergence operator, adjoint to the $S$ in Eq. (9) and $f$ is the body forces vector.

From these considerations, the principle of virtual work is rewritten considering separately the work of the internal forces corresponding in $\Omega \setminus S$ and $S$ in which $\Omega$ is divided

$$\int_{\Omega \setminus S} \delta \epsilon^T \sigma d\Omega + \int_S \delta \omega^T t dS = \int_{\Omega} \delta u^T f d\Omega + \int_{\Gamma_t} \delta u^T \bar{t} d\Gamma$$

Figure 22. Constitutive behaviors considered for XFEM and PFM in [138]:

(a) exponential and (b) Cornelissen softening laws
where \( \mathbf{t} \) is the vector of tractions acting on the boundary \( \Gamma_t \) of the domain.

**FE approximation**

The spatial domain is discretized into FE. The coarse/fine scale decomposition is adopted also in the FE spaces, so the displacement \( \mathbf{u} \) is approximated with a discrete interpolation \( \mathbf{\hat{u}} \) defined as

\[
\mathbf{u} \cong \mathbf{\hat{u}} = \mathbf{N}_u \mathbf{U} + \mathbf{\tilde{N}}_u \mathbf{\tilde{U}}
\]

where \( \mathbf{U} \) is the vector of the nodal displacements of the coarse scale, \( \mathbf{\tilde{U}} \) is the vector of the nodal displacements of the fine scale. Note that bar used in the previous subsection for the coarse scale is here dropped and only the curl used for the fine scale is retained. \( \mathbf{N}_u \) and \( \mathbf{\tilde{N}}_u \) are the matrices containing the interpolation functions adopted in the FE approximations. The coarse scale is interpolated on all the nodes of the domain, while the fine scale is interpolated only on the elements cut by the crack \( S \). Therefore, \( \mathbf{\tilde{U}} \) are hierarchical enriched degrees of freedom representing the displacement jump.

![Figure 23. Crack path and enriched nodes in XFEM [144]](image)

The interpolation functions in \( \mathbf{\tilde{N}}_u \) for the discretization of the fine scale are chosen \textit{a priori} as to incorporate the enrichment functions and satisfying the partition of unity property [104, 105].

![Figure 24. Interpolation functions for the coarse and fine scale employed by [56]](image)

The enriched interpolation functions \( \mathbf{\tilde{N}}_{u,j} \) incorporated in \( \mathbf{\tilde{N}}_u \) are

\[
\mathbf{\tilde{N}}_{u,j}(\mathbf{x}) = N_{u,j}(\mathbf{x}) \theta_j(\mathbf{x})
\]

where \( N_{u,j} \) are the standard linear shape functions which satisfy the partition of unity property and \( \theta_j \) are the enrichment functions, defined as

\[
\theta_j(\mathbf{x}) = H_{S}(\mathbf{x}) - H_{S}(\mathbf{x}_j)
\]
where the Heaviside function $H_S(x)$ is defined as $H_S(x) = 1$ if $(x - x_S) \cdot n > 0$ and $H_S(x) = 0$ otherwise. The last shifter item is introduced so that the essential boundary conditions can be enforced directly on the standard element nodes.

$$
\theta_f(x) = H_S(x) - c_S \varphi(x) - (1 - c_S)H_S(x_f); \quad \varphi(x) = \sum_{j \in A^*} N_f(x)H_S(x_f)
$$

Figure 25. Embedding strong discontinuities in the discrete FE approximation: (a) [145], (b) [146], (c) [147] and (d) [80]

To construct the interpolations functions, the nodes of a particular element located in $\Omega^+$ and $\Omega^-$ need to be identified. That is, the crack has to be exactly located and oriented inside the element, see Figure 23, Figure 24 and Figure 25.

The direct use of the Heaviside function for the enrichment causes the ill-conditioning of the problem when the crack trajectory gets too close to the elemental nodes. For this reason, in Is-XFEM, a stabilization term is added to the Heaviside functions used as enrichment [138]
where sub-set $A^*$ groups only those nodes in the elements in which the crack is embedded and $c_s \in [0,1]$ is the stabilization parameter. The case $c_s = 0$ recovers the Heaviside enrichment used in the standard XFEM. References [138, 136, 137] recommend the adoption of values for $c_s \in [0.01,0.1]$.

From Eq. (20), the following interpolation of the strain field $\varepsilon$ in $\Omega \setminus S$ is derived

$$\varepsilon \equiv \hat{\varepsilon} = B_u U + \tilde{B}_u \tilde{U}$$

(24)

where $B_u$ is the regular compatibility matrix, $B_u = SN_u$ and $\tilde{B}_u$ is the enriched compatibility matrix, consistent with the definition of the strain field $\varepsilon^e$ in Eq. (12) and with the choice of the enrichment functions for the discrete displacement field. Note that the matrix $\tilde{B}_u$ is discontinuous inside the element and this requires specific sampling techniques to be devised, see Figure 26.

![discontinuity](image)

**Figure 26. Integration scheme for a quadrilateral element crossed by a discontinuity [146]**

Introducing the FE approximation of Eqs. (20) and (24) in the weak form in Eq.(19), and splitting the discrete problem into standard and enriched degrees of freedom (or regular and fine scales), results the following system of two equations

$$\int_{\Omega \setminus S} B_u^T \sigma \, d\Omega = \int_{\Omega} N_u^T f \, d\Omega + \int_{\Gamma_t} N_u^T t \, d\Gamma$$

(25)

$$\int_{\Omega \setminus S} \tilde{B}_u^T \sigma \, d\Omega + \int_{S} N_u^T t \, dS = \int_{\Omega} \tilde{N}_u^T f \, d\Omega + \int_{\Gamma_t} \tilde{N}_u^T \tilde{t} \, d\Gamma$$

(26)

Introducing the constitutive relations (13) and (18) and operating results in

$$\int_{\Omega \setminus S} B_u^T DB_u U \, d\Omega + \int_{\Omega \setminus S} B_u^T \tilde{D} \tilde{B}_u \tilde{U} \, d\Omega = \int_{\Omega} N_u^T f \, d\Omega + \int_{\Gamma_t} N_u^T \tilde{t} \, d\Gamma$$

(27)

$$\int_{\Omega \setminus S} \tilde{B}_u^T DB_u U \, d\Omega + \int_{\Omega \setminus S} \tilde{B}_u^T \tilde{D} \tilde{B}_u \tilde{U} \, d\Omega + \int_{S} N_u^T E_s N_u \tilde{U} \, dS = \int_{\Omega} \tilde{N}_u^T f \, d\Omega + \int_{\Gamma_t} \tilde{N}_u^T \tilde{t} \, d\Gamma$$

(28)

and the following discrete FE formulation can be obtained

$$\begin{bmatrix}
K_{UU} & K_{U\bar{U}} \\
K_{\bar{U}U} & K_{\bar{U}\bar{U}}
\end{bmatrix}
\begin{bmatrix}
U \\
\bar{U}
\end{bmatrix} = \begin{bmatrix}
F \\
\bar{F}
\end{bmatrix}$$

(29)

with
\[ K_{\theta u} = \int_{\Omega \backslash S} B_u^T DB_u \, d\Omega \]  
\[ K_{\theta \theta} = \int_{\Omega \backslash S} B_u^T DB_u \, d\Omega \]  
\[ K_{\theta u} = \int_{\Omega \backslash S} B_u^T DB_u \, d\Omega \]  
\[ K_{\theta \theta} = \int_{\Omega \backslash S} B_u^T DB_u \, d\Omega + \int S N_u^T E_s N_u \, dS \]  
\[ F = \int_{\Omega} N_u^T f \, d\Omega + \int_{\Gamma_t} N_u^T \bar{t} \, d\Gamma \]  
\[ \bar{F} = \int_{\Omega} \bar{N}_u^T f \, d\Omega + \int_{\Gamma_t} \bar{N}_u^T \bar{t} \, d\Gamma \]  

Note that the system in Eq. (29) is symmetric. This is a consequence of the variational consistency of the procedure followed and but it translates in a poor description of the traction continuity condition at the crack and ensuing poor stress approximation. This statical limitation is overcome in some EFEM formulations using a Petrov–Galerkin approximation, but it yields a non-symmetric global matrix.

**Crack propagation and orientation criteria. Tracking algorithm**

Instead of the local stress \( \sigma \), the is-XFEM uses the following modified stress \( \bar{\sigma}_e \), computed as the average of the stresses over an element, to check if crack propagation occurs

\[ \bar{\sigma}_e = \frac{1}{V_e} \int_{\Omega_e} \sigma \, d\Omega \]  

where \( V_e \) is the volume of element \( \Omega_e \). According to the Rankine criterion employed, a crack propagates into the element \( \Omega_e \) if the major principal stress of \( \bar{\sigma}_e \) is larger than the material strength \( f_t \). In such a case, the following adjusted nonlocal smoothed stress \( \bar{\sigma}_e \) is adopted to compute the direction of crack propagation

\[ \bar{\sigma}_e = \int_{\Omega_e} \varphi_0(r) \sigma \, d\Omega \approx \sum_{e=1}^{n_{Ve}} \varphi_0(r_e) V_e \bar{\sigma}_e \]  

with \( \varphi_0 \) being a weighting function depending on the distance \( r_e \) between the centroids of the element considered for crack propagation and neighboring ones

\[ \varphi_0(r_e) = \exp \left( -\frac{r_e^2}{r_0^2} \right) \]  

where \( r_0 \) is a numerical parameter provided by the program user. \( n_{Ve} \) denotes the number of elements \( e \) present within a certain distance, \( r_e \leq 2.5r_0 \). In accordance to the Rankine criterion employed, the crack propagates perpendicular to the major principal stress of \( \bar{\sigma}_e \). The averaged nonlocal stress \( \bar{\sigma}_e \) is not normalized, but this does not affect the ensuing direction of advance of the crack.
The tracking algorithm adopted in [138, 139] is based on element connections/graph. Crack propagation within elements is done following straight lines and intersecting discontinuities cannot be considered. For additional details, see references [138, 139].

**Appraisal**

The major strong point of the XFEM with respect previous discontinuous approaches is that it is able of explicitly modelling the strong discontinuity caused by the crack without the need of remeshing. The major frailty of XFEM is that this modelling requires the a priori knowledge of the location and orientation of the crack, therefore its necessity of auxiliary crack tracking techniques.

**Assets:**

A1. **Generality.** The partition of unity concept at the basis of the XFEM is a robust and general numerical procedure that enables the conforming local enrichment of the approximation spaces. The preservation of conformity makes the method attractive in many applications, including fracture mechanics.

A2. **Strength, toughness and energy dissipation.** The introduction of traction-separation laws, following the Fictitious Crack Model, in which both the strength and the fracture energy are included allows to successfully represent softening quasi-brittle failure and structural size effect.

A3. **No need of remeshing.** XFEM requires no mesh adaptivity to adequately capture strong discontinuities in the displacement field.

A4. **Reduced computational cost.** The XFEM only increases the number of degrees of freedom in the nodes intersected by the crack; therefore, a very small part of the total number of nodes. Even if these additional dofs have to be assembled and solved at global level, the increase in overall computational cost is small.

**Drawbacks:**

D1. **Constitutive behavior of crack in terms of traction-separation laws.** Rather than standard stress-strain models, methods representing sharp cracks, such as the XFEM, require to express the traction across the crack in terms of the displacement jump. These laws are postulated in different ways, not necessarily corresponding to the constitutive laws adopted for the bulk material [148].

D2. **Need for criterion for the determination of the orientation of crack propagation.** The construction of the extended approximation space used by the XFEM requires the a priori determination of the location and orientation of the crack. This needs to be done from an established criterion for crack propagation and from the approximated fields of strain and stress. On the one hand, there is not general consensus on the criterion to be used for the orientation of crack propagation. On the other hand, the local convergence of strain and stress fields cannot be guaranteed at the tip of a crack using the standard FEM.

D3. **Need for specific analytical developments and element dependent implementations.** Dealing with discontinuous fields inside a finite element requires the development of specific sampling and integration schemes that need to be applied differently for each FE interpolation basis (triangles, quads, etc.) [149, 150, 19, 151, 152, 153, 154, 155, 156]. Also, implementation in 2D and 3D needs to be separately considered. This makes the implementation of the XFEM rather involved. As noted in reference [157], “the implementation of customized integration schemes is possibly the most time-consuming part of an implementation of the XFEM”. Different approaches have been proposed to alleviate these difficulties. The regularized XFEM, or REXFEM, presents the use of embedded but regularized discontinuities in the finite
elements, avoiding the utilization of discontinuous interpolation functions [58, 158, 159]. In the so-called phantom node method [160, 161, 162, 163, 164], two overlapping elements are introduced, each representing the displacement field in one side of the cracked element. This prevents as well using discontinuous interpolation functions for representing the crack.

**D4. Multiple, intersecting and branching cracks.** Although dealing with these situations is allegedly possible using the XFEM [165, 166, 167, 168, 169, 170, 171], it is certainly not easy, and the number of attempts to it is scant.

**D5 Need for crack tracking techniques.** Even if the displacement interpolation of the XFEM is conforming, it is necessary to ensure the spatial continuity of the crack and to label those elements crossed by it. Several auxiliary crack tracking techniques, using local, global and partial domain strategies, have been proposed. The need and the use of these procedures lies outside the variational setting of the problem and is not rightly justified. Applying some tracking techniques in 3D problems is far from straight-forward [172, 173, 174, 138].

**Checklist:**

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5. **Mixed FE**
Introduction

The mixed strain/displacement $\varepsilon/\mathbf{u}$ FE formulation fits within the well established framework of the smeared crack approach and the crack band theory, but attains mesh-objective solutions in quasi-brittle fracture. The crack is modelled as a band of small but finite thickness and the discontinuous displacement across it is smeared producing localized but bounded strains inside the band. This means that the setting of the fracture problem in the continuum framework remains unaltered.

On the one hand, the mixed formulation differs from the standard displacement-based FE in the fact that the strain and the displacement fields are interpolated independently; this represents a kinematical enhancement that attains the necessary mesh independence of the discrete solution. This avoids the use of ad-hoc crack tracking techniques. On the other hand, the local format of the cracking problem is preserved, without introducing gradient or higher order terms in the constitutive law or regularizing terms in the variational form.

Perspective

Using a mixed FE formulation, with both stress and displacement as unknowns, and based on the Hellinger-Reissner variational principle [175], was for the first time discussed in detail by Fraeijs de Veubeke in 1965 [176]. In the same year, Herrmann [177] proposed the use of a mixed FE formulation for incompressible and nearly incompressible materials with displacements and a variable depending on the pressure as primary variables. From 1968 onwards, the first numerical implementations and applications appeared [178, 179, 180, 181, 182], and the terms mixed finite element and mixed variational principle started being used for this approach [183, 184, 185].

The advantage of a mixed FE formulation over the irreducible one is that it allows increasing the order of convergence, and therefore the accuracy, of the fields selected as additional primary unknowns [186]. This feature has proven to be crucial in many applications where standard formulations have been proven to fail: incompressible and nearly-incompressible problems in computational solid [187, 188, 177, 189] and fluid [186, 190, 191, 192] mechanics, shear locking in thin plates [193, 194] and shear and membrane locking in shells [179, 180, 182], to name just those better known [178, 179, 180, 181, 182].

Regarding quasi-brittle fracture, adopting a mixed strain/displacement FE formulation serves two purposes, one concerning crack initiation and propagation and the other concerning crack representation.

Adopting a continuum mechanics framework, cracks are initiated and propagate according to a stress-based criterion. Conformance to Griffith’s theory is made via the energy dissipated during the later decohesive (softening) stage. Therefore, the capability of the FE formulation to propagate cracks adequately depends crucially on the accuracy of the strain and stress field evaluated prior to the formation of the crack and at the tip of the advancing crack.

Regrettably, the standard FE formulation cannot guarantee local convergence of these fields in the quasi-singular near-tip of the crack. This is the reason behind the spurious mesh dependency that the standard approach displays when the mesh is not appropriately aligned with the crack path. PFM do not exhibit such mesh dependency because they regularize the problem at continuum level, so that these near-singular never arise on the discretized problem. Mixed FEM are designed to gain order of convergence on the strain and stress fields, so that convergence may be guaranteed where it is most needed and yield mesh independent results. The enforced continuity of the strain field in the mixed interpolation is in fact a projection on the FE space of the discontinuous strain field of the standard interpolation. This projection enhances the
accuracy and provides, naturally and at discrete level, the regularity needed to ensure convergence [24, 25].

With respect to the reproducibility of the strain and stress fields once the crack is formed, the mixed interpolation also provides a significant enhancement. Low order standard FE perform extremely poorly when reproducing “smeared” separation modes; higher order standard FE perform even worse. This is the reason behind stress locking in crack problem. This is so serious that the “obvious” orthotropic crack models had to be abandoned in favor of the obviously limited isotropic damage models [3].

Although the underlying strain field is continuous in the mixed formulation, low order mixed FE reproduce separation modes far better. Ensuing, the discrete stress field is practically free from locking. Orthotropic crack models can be restated [29, 31].

As most of the nonlinear constitutive laws are defined in a strain-driven structure, in which the stress is evaluated in function of the strain, the adoption of a mixed strain/displacement formulation is more convenient than a stress/displacement one. Therefore, the mixed ε/φ FEM allows to readily adopt the large number of constitutive laws already established under this format [28]. Symmetry of the formulation is ensured when the constitutive equation is introduced in secant form [28, 29, 30, 32].

The application of mixed FEM to the problem of fracture is founded in two keystones: the variational form of the problem of fracture according to the mixed Hellinger-Reissner principle and the spatial regularization according to the smeared crack concept. The mixed variational formulation of the problem is established in the continuum setting, while the smearing of the crack links the energy dissipated in the smeared crack with the resolution of the FE mesh. The coupling of these two components constitutes a mixed FE formulation of Griffith’s theory of fracture, which naturally furnishes a criterion for crack propagation.

Continuous formulation

In the following, the mixed strain/displacement ε/φ FE formulation employed in this work is briefly introduced. Additional details can be found in references [24, 25, 195, 28, 29, 31, 196].

The variational keystone of the Mixed FEM is the mixed Hellinger-Reissner principle, formulated as follows.

The displacements φ and the strains ε are taken as primary unknowns of the nonlinear solid mechanics problem. First, the compatibility equation relates these two fields

\[ \varepsilon = S \phi \]  \hspace{1cm} (39)

where \( S \) is the differential symmetric gradient operator. Secondly, the Cauchy momentum equation relates the stresses \( \sigma \) and the body forces \( f \)

\[ S^T \sigma + f = 0 \]  \hspace{1cm} (40)

where \( S^T \) is the differential divergence operator, adjoint to the \( S \) in Eq. (39). And thirdly, the constitutive equation connects the stress and strain vectors

\[ \sigma = D \varepsilon \]  \hspace{1cm} (41)

where \( D = D(d) \) is the (nonlinear) secant constitutive matrix. From thermodynamic considerations, the secant constitutive matrix needs to be symmetric and positive semidefinite.

Eq. (39) is pre-multiplied by \( D \) and Eq. (41) is introduced into Eq. (40), resulting in the following system of PDEs.
\[-D\varepsilon + DSu = 0 \tag{42}\]
\[S^T(D\varepsilon) + f = 0 \tag{43}\]

The corresponding weak form of the mixed problem is obtained by: (i) multiplying Eq. (42) by a virtual strain vector, (ii) multiplying Eq. (43) by a virtual displacement vector, (iii) integrating both equations over the spatial domain and (iv) applying the Divergence Theorem in the first term of Eq. (43). The resulting system of equations is

\[-\int_\Omega \delta\varepsilon^T D\varepsilon \, d\Omega + \int_\Omega \delta\varepsilon^T DSu \, d\Omega = 0 \quad \forall \delta\varepsilon \tag{44}\]
\[\int_\Omega (S\delta u)^T (D\varepsilon) \, d\Omega = \int_\Omega \delta u^T f \, d\Omega + \int_{\Gamma_t} \delta u^T \bar{t} \, d\Gamma \quad \forall \delta u \tag{45}\]

where the boundary \(\Gamma\) of the domain is divided in two parts: \(\Gamma_u\), corresponding to the Dirichlet boundary condition and \(\Gamma_t\) corresponding to the Newmann boundary condition. The variational form of the problem consists in finding the \(u\) and \(\varepsilon\) fields full satisfying the system of Eqs. (44)-(45) and complying with the boundary condition \(u = 0\) in \(\Gamma_u\), for the arbitrary virtual displacement vector \(\delta u\), which is also null on \(\Gamma_u\), and the arbitrary virtual strain vector \(\delta\varepsilon\). Note that the problem is symmetric.

The regularization keystone of mixed FEM follows exactly the crack band model [23], and consists in the smearing of the sharp crack \(S\) over a band \(B\) of small, but finite, thickness \(b\). In this crack band, the Continuum Damage Mechanics apply. In this case, the constitutive behavior inside the smeared crack reads

\[\sigma = D(d) \varepsilon = (1 - d) D_0 \tag{46}\]

where \(D = D(d)\) is the secant constitutive matrix, written as a function of the internal scalar damage variable \(d\) that describes the degradation of the material and \(D_0\) is the initial elastic constitutive matrix. In an initially isotropic elastic material, \(D_0\) is defined in function of the undamaged elastic values of Young’s modulus \(E\) and Poisson’s ratio \(\nu\). The secant constitutive matrix is symmetric and positive semidefinite if \(0 \leq d \leq 1\).

Cracks have an unquestionable directional character and orthotropic damage models have recently been re-assessed by the authors in relation with brittle failure in references [29, 31]. However, an isotropic damage model is used hereafter in order to compare results obtained with XFEM and the PFM.

The effective stress \(\bar{\sigma}\) is stipulated as \(\bar{\sigma} = D_0 \varepsilon\), according to the hypothesis of strain equivalence. In this work, only tensile damage is considered. The Rankine damage criterion for tension, whose surface is plotted in Figure 27a, is introduced as

\[F(\bar{\sigma}_{eq}, r) = \bar{\sigma}_{eq}(\bar{\sigma}) - r = \langle \bar{\sigma}_1 \rangle - r = 0 \tag{47}\]

Where the positive the major principal effective stress is taken as the equivalent effective stress, \(\bar{\sigma}_{eq}(\bar{\sigma}) = \langle \bar{\sigma}_1 \rangle\), and \(r\) is the current damage threshold. The initial value of the damage threshold is the tensile strength of the material \(f_t\). The current value at time \(t\) of the damage threshold \(r\) is computed from the Kuhn-Tucker optimality and consistency conditions, guaranteeing the irreversibility of damage and the positiveness of the dissipation

\[r = \max \left(f_t, \max \bar{\sigma}_{eq}(\bar{t}) \right) \quad \bar{t} \in [0, t] \tag{48}\]
In this work, the evolution of the internal damage variable $d$ follows an exponential softening law, shown in Figure 27b. Other functions can be alternatively contemplated if considered necessary. The only requirement for the damage function is that the evolution of $d$ monotonically progresses from 0 to 1 as the damage threshold $r$ varies from $f_t$ to infinity. Therefore

$$d = 1 - \frac{f_t}{r} \exp \left( -2H_d \frac{(r - f_t)}{f_t} \right)$$  \hspace{1cm} (49)$$

where $H_d$ is a softening parameter controlling the rate of degradation of the material.

From energy conservation considerations, in the crack band theory $H_d$ is linked to material properties through Irwin’s material length $L = EG/f_t^2$ and the crack bandwidth $b$

$$H_d = \frac{b}{2L - b}$$  \hspace{1cm} (50)$$

This approach allows to achieve independence of the results with respect to the size of the crack bandwidth and to guarantee the correct energy dissipation during the fracture process. Note that this is very similar to the uses in PFM. In crack band theory, the crack bandwidth $b$ is linked to the FE discretization: in mixed FE, $b = 2h$, $h$ being the finite element size.

**FE approximation**

The discrete form of the mixed problem is obtained by discretizing the spatial domain $\Omega$ into nonintersecting FE $\Omega_e$, such that $\Omega = \cup \Omega_e$. The displacement $\mathbf{u}$ and the strain $\mathbf{\varepsilon}$ are substituted with discrete FE approximations $\mathbf{\bar{u}}$ and $\mathbf{\bar{\varepsilon}}$ defined element-wise as

$$\mathbf{u} \equiv \mathbf{\bar{u}} = \mathbf{N}_u \mathbf{U}$$  \hspace{1cm} (51)$$

$$\mathbf{\varepsilon} \equiv \mathbf{\bar{\varepsilon}} = \mathbf{N}_e \mathbf{E}$$  \hspace{1cm} (52)$$

$\mathbf{U}$ and $\mathbf{E}$ are vectors containing the values of the displacements and the strains at the nodes of the finite element mesh. $\mathbf{N}_u$ and $\mathbf{N}_e$ are the matrices composed of the interpolation functions adopted in the FE approximation.
In mixed FE, the choice of the interpolation functions for the primary variables must satisfy the inf-sup stability condition, also known as the Ladyzhenskaya-Babuska-Brezzi (LBB) condition, to avoid spurious oscillations in the solution [197, 198, 199, 200, 201, 202, 203].

The Inf-Sup condition is not fulfilled when equal order interpolation functions are used for \( N_u \) and \( N_\varepsilon \) [202, 203, 199]. Solutions computed with such interpolation functions are unstable, presenting spurious oscillations in the displacement and strain fields. To use equal order interpolation functions for both fields, a stabilization technique for the discrete mixed problem is required. The procedure employed in this work follows the Orthogonal Subscales Method, conceived within the Variational Multiscale Stabilization approach [204, 142, 205, 206, 207, 143].

The process consists in replacing the FE approximation of the strain field in Eq. (52) with the following

\[
\tilde{\varepsilon} \equiv \varepsilon = N_\varepsilon E + \tau_\varepsilon (B_u U - N_\varepsilon E) = (1 - \tau_\varepsilon) N_\varepsilon E + \tau_\varepsilon B_u U
\]  

(53)

where \( \tau_\varepsilon \) is a stabilization parameter such that \( 0 \leq \tau_\varepsilon \leq 1 \) and \( B_u = S N_u \) is the standard compatibility matrix. Note that \( \tau_\varepsilon = 0 \) corresponds to the strain interpolation of the non-stabilized problem, while \( \tau_\varepsilon = 1 \) corresponds to the strain interpolation from the standard displacement-based formulation.

It is shown in references [24, 25, 208] that an optimal convergence rate of the problem is achieved by choosing \( \tau_\varepsilon = c_\varepsilon h/L \), with \( c_\varepsilon \) an arbitrary constant, \( L \) a reference size of the structure. In this work, \( c_\varepsilon = 1 \) is adopted.

Taking into consideration this stabilization procedure, the value of the crack bandwidth introduced in Eq. (50) is

\[
b = (1 - \tau_\varepsilon) 2h + \tau_\varepsilon h = (2 - \tau_\varepsilon) h
\]  

(54)

The ensuing algebraic system of equations is:

\[
\begin{bmatrix}
-M_T & G_T \\
G_T^T & K_T
\end{bmatrix}
\begin{bmatrix}
E \\
U
\end{bmatrix} = \begin{bmatrix}
0 \\
F
\end{bmatrix}
\]  

(55)

where \([E \ U]^T\) is the vector containing the nodal values of the unknowns if the problem, strains and displacements, and \( M_T = (1 - \tau_\varepsilon) M, G_T = (1 - \tau_\varepsilon) G \) and \( K_T = \tau_\varepsilon K \). \( M \) is a mass like projection matrix, \( G \) is the discrete gradient matrix, \( K \) is a stiffness like matrix and \( F \) is the vector of external nodal forces:

\[
M = \int_\Omega N_\varepsilon^T D N_\varepsilon \, d\Omega
\]  

(56)

\[
G = \int_\Omega N_\varepsilon^T D B_u \, d\Omega
\]  

(57)

\[
K = \int_\Omega B_u^T D B_u \, d\Omega
\]  

(58)

\[
F = \int_\Omega N_u^T f \, d\Omega + \int_{\Gamma_t} N_u^T \tilde{t} \, d\Gamma
\]  

(59)
Appraisal
The major strong point of Mixed FEM with respect to previous smeared approaches is that it constitutes an extended mixed FE formulation of Griffith’s theory of fracture able to achieve mesh independent and convergent solutions. The weakest point is that it is not straightforwardly implementable in a standard FE code.

Assets:

A1. Rigorous physical fundamentals. The method is based on the mixed Hellinger-Reissner, together with Griffith’s theory of fracture implemented through the crack band theory. It applies both to quasi-static as well as dynamic problems, in 2D or in 3D.

A2. Rigorous mathematical foundation. The adoption of a mixed formulation of the FE problem is soundly based, as this guarantees that the FE solution converges in quasi-singular situations.

Figure 28. Damage contours of a cubic metal specimen subjected to monotonic loading resulting from an isotropic Drucker-Prager using different compressive vs tensile strength ratios: (a) \( f_c/f_t = 1 \), (b) \( f_c/f_t = 5 \), (c) \( f_c/f_t = 8 \) and (d) \( f_c/f_t = 100 \), computed with mixed FE by [31]
A3. Generality of implementation. The strain/displacement $\varepsilon/u$ FE formulation does not require any specific FE interpolation basis, so it can equally be used with linear or quadratic, triangles or quads. It does not require any particular development to be implemented in 3D.

A4. Mesh-bias and mesh-size independence. Because adopted mixed FE formulation has better convergence rate than the standard FE one, convergence of the discrete problem of fracture to the continuous solution can be expected. Results of the FE problem are therefore mesh-bias independent. Application of the CBT guarantees mesh-size independence.

A5. Generality of the crack constitutive behavior. The mixed FEM accommodates any suitable constitutive behavior. In the secant format of here presented, isotropic and orthotropic damage models have been considered [29, 31], demonstrating that they not yield identical solutions. Also, crack closing-reopening effects can be considered, as well as irreversible straining, both features essential under cyclic loading [31]. Furthermore, other constitutive frameworks can be contemplated. Computational Plasticity has been used for the modelling of fracture [195, 55] and other strain localization problems [209, 71]. Figure 28 and Figure 29 illustrate this remarkable features.

A6. Strength, toughness and energy dissipation. Both material strength and toughness are included can be included in the material description.

A7. Branching and intersecting cracks. Mixed FEM can deal with branching and intersecting cracks as a matter of course if they spring in the solution of the specific problem.

A8. No tracking of cracks procedures are required. Griffith’s theory for fracture consisted of a criterion for crack growth but did not address the prediction of the direction of advance of the crack [210, 211, 129, 212]. In Mixed FEM the direction of crack advance is implicitly incorporated in the variational formulation model. Crack directions follow from the underlying damage model adopted.
A9. Computational cost. An apparent weak point of the Mixed FE formulation is the computational cost. The formulation requires the independent interpolation of strains and displacement and, thus, the number of nodal degrees of freedom is considerably increased with respect the standard formulation. Regarding this, it needs to be considered that the mixed formulation has a higher convergence rate that standard FE. This means that, for a given required bound of the discretization error, the mixed method requires less elements that the standard one. The difference is larger the smaller the required discretization error. In fact, it can be shown [213] than in practical applications, the mixed method is less costly that the standard one in terms of elements, dofs and CPU time.

Regarding the fineness that the Mixed Fem requires for cracking problems, the method smears the crack over a band of 2 elements, with bandwidth $b = 2h$, $h$ being the mesh size. A proper definition of the crack requires a relation $L/b > 100$, $L$ being the a characteristic length of the problem. This requires that $L/h > 200$, so that a 2D domain requires meshes in the order of $10^{64}$ of elements and 3D domains requires $10^6 - 10^7$ of elements. This computational cost is smaller than that required by PFM by several orders of magnitude.

**Drawbacks:**

**D1. Implementation.** Mixed FE formulations cannot be straightforwardly implemented in a standard FE code, as they require a multi-field structure to be implemented.

**Checklist:**

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6. Phase-field model

Introduction
The phase-field model can be included, together with the nonlocal and gradient-enhanced models, in a broader family of “regularized” methods in which the continuous statement of the problem is modified so that the strong displacement discontinuity associated to a sharp crack are avoided by transforming it into a band of finite bandwidth of highly, but regularly, localized strains. The regularized continuous problem is amenable to discretization via the standard FEM achieving mesh objectivity.

Perspective
In nonlocal integral models [34, 35, 36, 37, 38, 214] the common continuum mechanics theory is altered by replacing the locally evaluated strain field, the state variable driving the constitutive behavior, by a nonlocal counterpart evaluated as a weighted integral average over a predefined spatial domain of finite diameter. This results in a smoothing of the strains, with intensity dependent on the range of the spatial averaging. Promoters of nonlocal models claim that this range is an internal length, a material property, see Bazant and Jirasek [215] for a review and references therein.

In gradient-enhanced models [39, 40, 41, 42, 43, 44, 214], the common continuum mechanics formulation is altered by changing the definition of an originally locally defined variable, e.g. the equivalent strain, by its nonlocal counterpart, whose definition involves higher order derivatives (usually a Laplacean). The methods may be explicit, involving the Laplacean of the local variable or implicit, involving the Laplacean of the nonlocal variable and requiring the solution a Helmholtz-type BVP. A length scale is required in the definition of the nonlocal variable for dimensional consistency. This length regularizes the continuous statement of the problem and determines the width of the localization band. Backers of gradient-enhanced models advocate that this length is an internal length, a material property.

Considering the length scale as a “localization limiter” does regularize the problem, but alters radically its continuous statement; that is, changes the problem being solved and deviates from the physical problem of cracking. This accounts for the many inconsistencies found by the users of this type of models.

In reference [216] it was analytically proven and numerically shown that the nonlocal model in [34] and the gradient-enhanced model in [39] produce non-physical results. Specifically, it was shown that in mode I fracture situations: (i) the stress at the crack tip is not infinite, its value being dependent on the chosen material length, (ii) the maximum stress is not located at the crack tip but at a certain distance which changes according to the chosen material length and (iii) the value of the maximum stress is not infinite and also varies according to the material length employed. Consequently, in reference [216] it was proven that these methods predict damage initiation inside the specimen and not at the crack tip. Additionally, it was also shown that they produce incorrect crack trajectories, also dependent on the material length.

In reference [41] another unintended consequence of introducing a localization limiter was reported: when using the gradient-enhanced formulation [39] the damage spreads out spuriously, and the pretension of a localization band for damage is very much lost. This effect has also been detected in the nonlocal integral model [217].

To avoid the aforementioned issues, several modifications of the original nonlocal and gradient-enhanced models, have been proposed, reported and discussed in references [218, 219, 220].
These include quaint fixes like evolving weighted averaging of the local and nonlocal variables [221, 220], the so-called “over-nonlocal” approach, with weights larger than one for the nonlocal variable and negative weights for the local one [219, 222] or evolving internal lengths dependent on the degradation of the material [223, 41, 218].

More recently, Phase-Field Models (PFM) for brittle fracture have appeared and become widely used [212, 45, 46, 47, 48, 49]. PFM s are based on the regularization of Griffith’s theory of Linear Fracture Mechanics, where the sharp crack topology is regularized by a diffuse damage band thanks to the introduction of a scalar phase-field that discriminates the intact and broken material, with a smooth transition from the intact material to the completely degraded material. Also, irreversibility of the fracture process is ensured. Phase-Field models for fracture are very closely link to Continuum Damage Mechanics Models (CDM, as the scalar phase-field is easily identifiable with a scalar damage field. The evolution of the damage field is solved using an additional PDE which involves the gradient of damage; a length scale is required in this equation for dimensional consistency.

The name phase-field comes from the original application for which the basis of the method was developed: multiphase problems regarding the creation, evolution, destruction and merging of interfaces (i.e. the boundaries of phases, regions with homogeneous physical properties that can be solid, fluid, etc.) in microstructures within computational material science. It was developed pursuing a similar idea: avoiding the difficulties resulting from the treatment of sharp interfaces and the use of models requiring to explicitly tracking these interfaces [224].

PFM can be considered as a regularized variational approach to brittle fracture [51, 52, 46], as the formulation introduces a small positive length scale parameter which characterizes the width of the localization band; when this length tends to zero, the solution of the problem converges to the LFM solution, according to the $\Gamma$-convergence theorem [53]. This property is the definitive advantage of PFM over previous regularized models.

Note that originally, in the references [45, 47, 48], the length scale introduced in equation for damage evolution is understood as a mathematical regularization of the sharp crack. This length tends to zero for the diffuse crack to “\(\Gamma\) convergence” to the original sharp crack, see . However, this length is sometimes defined as an “intrinsic material parameter”; this conception misinterprets the original concept and it is as misleading as the localization limiters of the previously discussed approaches.

Lately, the geometrically regularized phase-field models, or phase-field regularized cohesive zone model (PF-CZM), has been introduced [225, 226, 227] in which the incorporated length scale affects the localization bandwidth, but it has negligible effects on the global responses, so long as the regularized localization band can be sufficiently resolved. Therefore, the length scale is considered as a numerical parameter which value can be taken as small as possible. In FE analysis, the regularizing length can be made dependent on the FE, so that the crack bandwidth tends to zero upon mesh refinement, guaranteeing the consistency with the original problem. Reference [228] performs a sensitivity study of various phase-field models with respect the internal length scale where it is shown that only the PF-CZM is able to yield solutions independent of the regularizing lengths chosen.

The PFM is founded in two keystones: the variational form of the problem of fracture and the spatial regularization of cracks. Both are established in the continuous formulation of the problem. The adoption of CDM for the behavior of the damaged material provides a criterion for the direction of propagation of the crack, an ingredient lacking in Griffith’s theory for fracture [68].
Continuous formulation

In the following, the main characteristics of the geometrically regularized phase-field model, developed by [225, 226, 227, 229, 230, 138, 228, 231, 232, 233] [234, 235, 236], and used in the numerical comparisons of this work is briefly introduced. For additional details on the method, the original references are recommended.

In the phase-field model for brittle fracture, the damage $d$ that develops in the solid is treated as an additional field variable, together with the displacement field $u$. Irreversibility of damage is assumed, so that damage cannot decrease.

The variational keystone of the PFM is Griffith’s theory for fracture [51], which says that during the cracking process the principle of minimum energy holds. This principle is essentially a restatement of the second law of thermodynamics. It states that for a closed system, with constant external parameters and entropy, the internal energy will decrease and approach a minimum value at equilibrium. Therefore, in a closed system, the variation of the total energy when the crack develops vanishes. Griffith also assumed that the formation of a crack involved a certain energy dissipation that must be accounted for in the process. The total energy of the system $E_T$ is expressed as

$$ E_T = W_e + W_S - W_{ext} \quad (60) $$

where $W_e$ is the strain energy stored in the body, $W_S$ is the energy dissipation required for the creation of the crack surface and $W_{ext}$ is the work done by the external forces.

According to Griffith, the energy dissipated by the crack formation is proportional to the area of the developing fracture, $A_S$, through a material property, $G_f$, called the fracture energy, the dissipated fracture energy per unit of area [51], so that

$$ W_S = G_f \int_S dS = G_f A_S \quad (61) $$

For an elasto-damaging solid, the strain energy is

$$ W_e = \int_{\Omega} \Psi(d, \epsilon) d\Omega \quad (62) $$

with $\Psi(d, \epsilon)$ being the strain energy density per unit of volume.

The work done by the external forces, body forces $f$ and tractions $\mathbf{t} \overline{\mathbf{t}}$ acting on the corresponding boundary, $\Gamma_t$, has the standard expression

$$ W_{ext} = \int_{\Omega} \mathbf{u}^T \mathbf{f} d\Omega + \int_{\Gamma_t} \mathbf{u}^T \mathbf{t} d\Gamma \quad (63) $$

In equilibrium, the variation of the total energy $E_T$ with respect to the crack growth $a$ is zero [129]:

$$ \frac{\partial E_T}{\partial a} = 0 \quad (64) $$

From this, Griffith’s criterion for fracture ensues: a crack will develop in a body only if the release of stored elastic energy caused by its growth is greater than the energy required to create its surface [210].
The regularization keystone of PFM consists in the smoothing of the sharp crack $S$ over a band $B$ of small, but finite, thickness $b$, where the material is damaged, see Figure 30. Consequently, the area of the crack $A_S$ that appears in Eq. (61) is approximated as

$$A_S = \int_S dS = \int_B \delta_s d\Omega \approx \int_B \gamma(d, \nabla d) d\Omega \quad (65)$$

so that the Dirac-delta $\delta_s$ describing the sharp crack is approximated with the crack surface density function $\gamma$, which is expressed in terms of the damage $d$ and its gradient $\nabla d$. The gradient of the damage is inserted in the definition of $\gamma$ to introduce the necessary regularity to the problem, see Figure 31. The relation of the previous gradient-enhanced formulations with the phase-field models is evident [237, 238, 239]. The thickness $b$ of the regularized crack is included in the expression of $\gamma$ for dimensional consistency

$$\gamma(d, \nabla d) = \frac{1}{\pi b} \left[ \frac{1}{b} (2d - d^2) + b|\nabla d|^2 \right] \quad (66)$$

Note that $b$ is a regularizing length in a purely mathematical sense; it does not carry any material significance. In phase-field models, reducing the crack bandwidth must ensure $\Gamma$-convergence to the sharp crack problem, see Figure 32 [240].

The strain energy density $\Psi$ is written in terms of the strain $\varepsilon$ and the damage index $d$ as

$$\Psi(d, \varepsilon) = \omega(d) \Psi_0(\varepsilon) \quad (67)$$

where $\omega(d)$ is a monotonically decreasing function, ranging from 1 to 0, describing the degradation of the material in terms of the damage and $\Psi_0(\varepsilon)$ is the elastic strain energy of the elastic material.

![Figure 30. Representation of cracks using (a) embedded and (b) regularized models, taken from [241], with $4l = b$](image)
Figure 31. Damage profile of the 2nd and 4th order phase-field model, taken from [242], with \( \phi(x) \) being the phase-field variable identified with damage \( d(x) \) and \( l = b/2 \).

Figure 32. \( \Gamma \)-convergence: reducing the crack bandwidth in phase-field models in [240] with

\[
\Psi_0(\varepsilon) = \frac{1}{2} \varepsilon^T D_0 \varepsilon
\]  \hspace{1cm} (68)

where \( D_0 \) is the elastic constitutive matrix. From this, the constitutive law is obtained as

\[
\sigma = \frac{\partial \Psi}{\partial \varepsilon} = \omega(d) \frac{\partial \Psi_0}{\partial \varepsilon} = \omega(d) D_0 \varepsilon
\]  \hspace{1cm} (69)

Note that the standard format of an isotropic damage model is recovered if the degradation function \( \omega(d) \) written as:

\[
\omega(d) = (1 - d)
\]  \hspace{1cm} (70)

Instead, the geometric phase-field adopts a degradation function
\[ \omega(d) = \frac{(1 - d)^p}{(1 - d)^p + a_1 d (1 + a_2 d + a_3 d^2)} \]  

(71)

This function depends on a number of parameters, see Figure 33 [240]. Exponent \( p \geq 2 \) defines the softening behavior of the material: linear, exponential, hyperbolic, etc. Parameter \( \alpha_1 \) is proportional to the relation between Irwin’s material length \( L = EG_f/f_t^2 \) and the crack bandwidth \( b \); parameters \( \alpha_2 \) and \( \alpha_3 \) are dependent on the tensile strength \( f_t \) and the fracture energy \( G_f \).

![Figure 33. Softening laws adopted in phase-field simulations by [240]](image)

The crack driving force \( Y \), conjugate to the damage index, is

\[ Y = - \frac{\partial \Psi(d, \varepsilon)}{\partial d} = - \frac{\partial \omega(d)}{\partial d} \psi_0(\varepsilon) \]  

(72)

In PFM, it is common to substitute the crack driving force in Eq. (72) with the following

\[ Y = - \frac{\partial \omega(d)}{\partial d} \bar{Y}(\varepsilon) \]  

(73)

where \( \bar{Y} \) is a modified reference energy defined in function of the equivalent effective stress \( \sigma_{eq} \), which allows to introduce an appropriate damage surface to define damage initiation

\[ \bar{Y} = \frac{1}{2E} \sigma_{eq}^2 \]  

(74)

where the elastic Young modulus \( E \) is introduced for dimensional consistency. Taking \( \sigma_{eq} = \langle \sigma_1 \rangle \) corresponds to the Rankine damage surface, \( \sigma_1 \) being the maximum normal effective stress, evaluated as \( \sigma = D_0 \varepsilon \). Other damage surfaces may be adopted by changing the expression of \( \sigma_{eq} \) in terms of \( \sigma \), see [243]. Note that Eqs. (72), and the substitute Eq. (73), are strain-driven, another feature that PFM have in common with CDM.

The damage flux vector \( \mathbf{q} \) and the net damage supply per unit of volume \( r \) are defined as

\[ \mathbf{q} = G_f \frac{\partial y(d, \nabla d)}{\partial \nabla d} = \frac{2b}{\pi} G_f \nabla d \]  

(75)

\[ r = Y - G_f \frac{\partial y(d, \nabla d)}{\partial d} = - \frac{\partial \omega(d)}{\partial d} \bar{Y}(\varepsilon) - \frac{2}{\pi b} G_f (1 - d) \]  

(76)

Using both the variational and the regularizing keystones, the expression of the total energy is rewritten as
\[ E_F = \int_{\Omega} \omega(d) \Psi_0(\epsilon) \, d\Omega + G_f \int_{B} \gamma(d, \nabla d) \, d\Omega - \int_{\Omega} \mathbf{u}^T \mathbf{f} \, d\Omega - \int_{\Gamma_t} \mathbf{u}^T \mathbf{t} \, d\Gamma \]

(77)

And its minimization, Eq. (64), yields

\[ \int_{\Omega} \delta \epsilon^T \omega(d) \frac{\partial \Psi_0(\epsilon)}{\partial \epsilon} \, d\Omega + \int_{B} \delta d \frac{\partial \omega(d)}{\partial d} \Psi_0(\epsilon) \, d\Omega + G_f \int_{B} \delta d \frac{\partial \gamma(d, \nabla d)}{\partial d} \, d\Omega 
+ G_f \int_{B} \delta \nabla d \frac{\partial \gamma(d, \nabla d)}{\partial \nabla d} \, d\Omega - \int_{\Omega} \delta \mathbf{u}^T \mathbf{f} \, d\Omega - \int_{\Gamma_t} \delta \mathbf{u}^T \mathbf{t} \, d\Gamma = 0 \]

(78)

Eq. (78) can then be split into a system of two equations, the first one corresponding to the classical Principle of Virtual Work, and the second one governing the evolution of damage

\[ \int_{\Omega} \delta \epsilon^T \sigma \, d\Omega = \int_{\Omega} \delta \mathbf{u}^T \mathbf{f} \, d\Omega + \int_{\Gamma_t} \delta \mathbf{u}^T \mathbf{t} \, d\Gamma \]

(79)

\[ \int_{B} \nabla \delta d \mathbf{q} \, d\Omega = \int_{B} \delta d \mathbf{r} \, d\Omega \]

(80)

where the divergence theorem has been applied the term \( \int_{B} \delta \nabla d \frac{\partial \gamma(d, \nabla d)}{\partial \nabla d} \, d\Omega \)

The corresponding strong form of the problem is the following system

\[ \mathbf{S}^T \sigma + \mathbf{f} = \mathbf{0} \]

(81)

\[ \mathbf{G}^T \mathbf{q} + \mathbf{r} = \mathbf{0} \]

(82)

A most unsettling issue related to the use of discrete regularized crack models is the appearance of spurious stress oscillations in the computed solution, as shown in Figure 34 and Figure 35. This problem has been reported in nonlocal integral [244, 245], gradient-enhanced [246, 247, 248, 249] and phase-field models [68, 250, 241]. References [244, 247, 249, 241] detail how the choice of the approximation spaces for the variables selected as nodal unknowns influences the performance of these methods with regard to the representation of the discrete stress field. In particular, the use of linear interpolation functions for all the primary variables causes spurious oscillations in the computed stress profile. The reason for these wild oscillations is not yet properly explained, but several alternative alleviating procedures have been proposed. Firstly, the use of higher order elements has been considered: references [247, 251] suggest the use of quadratic-linear interpolations for the gradient-enhanced model. In the same way, references [250, 241] show how the use of cubic-linear-linear interpolations in their phase-field models prevents the spurious oscillations. Secondly, the reduced integration technique has been employed as a remedy for this issue [245]. Thirdly, smoothing and post-processing techniques for the raw discrete stresses have been employed [247, 249, 230].
FE approximation
Once the spatial domain is discretized into FE, the displacement $\mathbf{u}$ and damage $d$ fields and are approximated by independent interpolations $\mathbf{\bar{u}}$ and $\mathbf{\bar{d}}$

$$\mathbf{u} \approx \mathbf{\bar{u}} = N_u \mathbf{U} \tag{83}$$
$$d \approx \mathbf{\bar{d}} = N_d \mathbf{D} \tag{84}$$

where $\mathbf{U}$ and $\mathbf{D}$ are the vectors of the nodal values of the displacements and the damage in the whole domain, and $N_u$ and $N_d$ are the matrices containing the interpolation functions adopted in the FE approximations.

The following discrete approximations for the strain and the damage gradient fields ensue

$$\mathbf{\varepsilon} \approx \mathbf{\bar{\varepsilon}} = B_u \mathbf{U} \tag{85}$$
$$\nabla d \approx \nabla \mathbf{\bar{d}} = B_d \mathbf{D} \tag{86}$$
where $\mathbf{B}_d$ is the discrete gradient operator, defined as $\mathbf{B}_d = \mathbf{G}\mathbf{N}_d$.

Introducing the FE approximation in Eqs. (83), (84), (85) and (86) into the weak form in Eq.(79)-(80) results in the following system of two equations

$$
\int_{\Omega} \mathbf{B}_u^T \mathbf{\sigma} \, d\Omega = \int_{\Omega} N_u^T \mathbf{f} \, d\Omega + \int_{\Gamma} N_u^T \mathbf{t} \, d\Gamma \tag{87}
$$

$$
\int_{\mathcal{B}} N_d^T \mathbf{r} \, d\Omega = \int_{\mathcal{B}} \mathbf{B}_d^T \mathbf{q} \, d\Omega \tag{88}
$$

Several alternatives have been proposed for solving the nonlinear system of Eqs. (87)-(88) [230, 232]. For example, a staggered scheme may be used, so that the resulting algebraic system is

$$
\begin{bmatrix}
K_{UU} & 0 \\
0 & K_{DD}
\end{bmatrix}
\begin{bmatrix}
\Delta \mathbf{U} \\
\Delta \mathbf{D}
\end{bmatrix} =
\begin{bmatrix}
\mathbf{r}_u \\
\mathbf{r}_d
\end{bmatrix}
\tag{89}
$$

with

$$
K_{UU} = \int_{\Omega} \mathbf{B}_u^T \left( \frac{\partial \mathbf{\sigma}}{\partial \mathbf{\varepsilon}} \right) \mathbf{B}_u \, d\Omega \tag{90}
$$

$$
K_{DD} = \int_{\mathcal{B}} \left( -N_d^T \left( \frac{\partial \mathbf{r}}{\partial \mathbf{d}} \right) N_d + \frac{2b}{\pi} \mathbf{G}_d \mathbf{B}_d \right) \, d\Omega \tag{91}
$$

and $\mathbf{r}_u$ and $\mathbf{r}_d$ are the residuals related to Eqs. (87) and (88) respectively

$$
\mathbf{r}_u = \int_{\Omega} N_u^T \mathbf{f} \, d\Omega + \int_{\Gamma} N_u^T \mathbf{t} \, d\Gamma - \int_{\Omega} \mathbf{B}_u^T \mathbf{\sigma} \, d\Omega \tag{92}
$$

$$
\mathbf{r}_d = \int_{\mathcal{B}} N_d^T \mathbf{r} \, d\Omega - \int_{\mathcal{B}} \mathbf{B}_d^T \mathbf{q} \, d\Omega \tag{93}
$$

The off-diagonal terms have been removed in the system (89), neglecting the inter-field coupling, according to the discussion in references [232, 240]. Alternative approaches for computing the nonlinear problem have been proposed in [230, 232, 240].

**Appraisal**

The major strong point of the Phase-Field Method with respect previous regularized approaches is that it very rigorously founded in its two keystones: the variational formulation of fracture and the rigorous regularization of the crack. The major weakness of the PFM is extreme level of mesh refinement that it requires and its colossal computational cost.

**Assets:**

**A1. Rigorous physical fundamentals.** The method is based on the principle of minimum energy or, equivalently, the second law of thermodynamics, together with Griffith’s theory of fracture. It applies both to quasi-static as well as dynamic problems, in 2D or in 3D.

**A2. Rigorous mathematical foundation.** The regularization of the sharp crack into a diffuse crack is soundly based, and this allows proving that the regularized problem converges to the original one in a certain sense.

**A3. Easiness of implementation.** PFM is easy to implement in any standard FE code, and straightforward to do in a multi-field FE code. It does not require any specific FE interpolation.
basis, so it can equally be used with linear or quadratic, triangles or quads. It does not require any particular development to be implemented in 3D.

Figure 36. Comparison of damage contours obtained with isotropic, anisotropic and hybrid phase-field models, displayed in [252]

Figure 37. 3D mixed mode I and III fracture surface obtained with phase-field by [253]
A4. Mesh-bias independence. Because the problem of fracture is regularized at continuous level, the corresponding discrete FE behaves according to the standard rates of convergence. Results are therefore mesh-bias independent.

A5. Strength, toughness and energy dissipation. PFM were originally devised to model brittle fracture but, as such, they could not incorporate the material strength, nor quasi-brittle failure. This serious drawback is overcome in more recent formulations incorporating the material strength and crack nucleation [69, 227].

A6. Branching and intersecting cracks. PFM can deal with branching and intersecting cracks as a matter of course if they spring in the solution of the specific problem.

A7. No tracking of cracks procedures is required. Griffith’s theory for fracture consisted of a criterion for crack growth but did not address the prediction of the direction of advance of the crack [210, 211, 129, 212]. In PFM the direction of crack advance is implicitly incorporated in the variational formulation model. Crack directions follow from the underlying damage model adopted. Similarities can be found between the PFM formulation and the energy-based crack tracking strategy in references [254, 132] where the path of the crack is chosen as the direction which minimizes the total mechanical energy.

A8. Allows for extensions of the crack constitutive behavior. PFM represents the process of fracture using a scalar damage variable. In its original formulation, the model does not discriminate tension from compression. Extension have been made through the split of the strain energy density into positive and negative or volumetric and deviatoric parts using the so-called “anisotropic” [255, 47, 48] or “hybrid” formulations [252, 243, 256]. This is a basic requirement to apply the model to materials such as concrete. Furthermore, crack closing-reopening effects need also to be considered [257]. See Figure 36 for some of these developments [252].

Drawbacks:

D1. Generality with respect to constitutive behavior. From the original scalar isotropic damage model, PFM has been extended to consider anisotropic brittle fracture [65, 66, 231] including several damage mechanisms [67]. Effects such as irreversible straining and plasticity are also being considered [258, 259]. Stiffness recovery due to crack closure and reopening have not yet been included, even if it is possible [257]. Anyhow, PFM stems from the CDM framework, and it cannot encompass other settings such as Computational Plasticity.

D2. Extremely high computational cost. The weak point of PFM is the computational cost. This method achieves mesh objectivity by regularizing the crack over a band of FEs, with a minimum bandwidth \( b \in [4h, 10h] \), \( h \) being the mesh size. A proper definition of the crack requires a relation \( L/b > 100 \), \( L \) being the a characteristic length of the problem. This requires that \( L/h > 1000 \), so that a 2D domain requires meshes with in the order of \( 10^6 \) of elements and 3D domains requires \( 10^9 \) of elements. This colossal computational cost prevents PFM from being used in engineering applications at present. Figure 37, Figure 38 and Figure 39 show some of the few 3D applications presented so far [253, 260, 261, 262, 263, 264, 265, 266]. This issue has been addressed via the implementation of adaptive mesh refinement techniques in references [49, 267, 268, 48, 269, 270] and by computing the nodal phase-field variables only in a reduced sub-domain where damage develops rather than in the whole structure [138], see Figure 47.

The requirement of fine mesh densities is a common issue in methods introducing a high regularization of the localization band. Figure 41 shows the mesh density involved in the
computation of a problem using a gradient enhanced damage model and Figure 42 presents the discrete damage and strain profiles employed in simulations using several nonlocal damage models.

D3. **Strength, toughness and energy dissipation.** PFM were originally devised as a regularized version of LEFM. As such, they could not represent the material strength, nor quasi-brittle failure. This serious drawback is being overcome in some recent models.

D4. **Spurious oscillations in the discrete stress field.** This issue, reported in many regularized crack models, is not fully explained. Alleviating auxiliary procedures have been proposed.

**Checklist:**

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<tr>
<th>Checklist for PFM</th>
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<tbody>
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<tr>
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<td></td>
<td></td>
<td>D4</td>
<td></td>
</tr>
<tr>
<td>3 Strength, toughness and energy dissipation</td>
<td>A2, A5</td>
<td></td>
<td>D3</td>
<td></td>
<td></td>
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<tr>
<td>4 Criterion for direction of propagation</td>
<td>A4, A7</td>
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<td>5 Constitutive behavior generality</td>
<td>A8</td>
<td></td>
<td>D1</td>
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<tr>
<td>6 Generality and implementation effort</td>
<td>A1, A3</td>
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<td>7 Cost-efficiency</td>
<td></td>
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<td>D2</td>
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<td>8 Multiple, intersecting and branching cracks</td>
<td>A6</td>
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<td>9 Auxiliary tracking techniques</td>
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<td>10 Application in 3D</td>
<td></td>
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<td>D2</td>
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Figure 38. Crack propagation in a thick-walled cylinder computed with phase-field by [260]

Figure 39. Cracking sequence of a hollow notched cylinder with tear straps under internal pressure computed with phase-field by [261]
Figure 40. Mesh densities required in phase-field: three-point bending test of a notched beam: (a) model and (b) detail of the damage contour [138]

Figure 41. Mesh employed and evolution of the computed damage field in a four-point bending test using a gradient damage model with (top) constant and (bottom) evolving length scale [44]
7. Numerical simulations of localized structural failure

In this section some of the numerical simulations reported in references [138, 227] using the is-XFEM and PF-CZM models are contrasted with the results obtained with the mixed FE formulation. The study cases selected are some of the most popular in the community, having been considered many times for the validation of numerous numerical models. The objectives of this section are (i) to assess the relative performance of the mixed FE approach when compared to XFEM and phase-field techniques, (ii) to reproduce the results of references [138, 227] obtained with is-XFEM and PF-CZM as best as possible.

The mixed FE numerical simulation are computed with an enhanced version of the finite element code COMET [271]. Pre- and post-processing are performed with GID [272], developed at CIMNE (International Center for Numerical Methods in Engineering). Convergence in each load step is reached when the ratio between the norm of residual forces and the norm of total external forces is lower than $10^{-3}$%.

7.1. Wedge splitting test

In this section, the numerical analysis of a wedge splitting test reported in [273] is considered. In reference [273] multiple series of geometrically similar specimens of varying sizes are tested and numerically simulated using the fictitious crack model. Other numerical simulations of these tests can be found for example in reference [274], where a gradient plasticity model is employed, in reference [54], which used XFEM, in references [81, 275, 276] where EFEM is considered, in reference [277] which used cohesive interface elements, and in reference [278] which used the peridynamic theory to model the crack propagation.
In the following, the computations in reference [138], where a comparison of the results obtained with is-XFEM and PF-CZM is made, are contrasted with the results obtained with mixed FE. In this mode I fracture test the computed crack trajectory is a straight line. Therefore, this case is not used here to assess the mesh-objectivity of the examined FE formulations. However, it is employed as an initial reference test for comparing the three models in terms of the material nonlinear softening behavior. All the methods should converge to the same solution if the same properties and constitutive laws are employed. Note that the objective of this study is to compare the results with respect to the XFEM and phase-field solutions in [138] and not to reproduce the original experimental results. The interested reader can find a comparison with the experiment in reference [28], where mixed FE have been already employed to replicate the wedge splitting test.

The geometry and boundary conditions of the test are shown in Figure 43. It is a specimen of dimensions 0.8 m x 0.8 m x 0.4 m with a vertical notch in the upper half. Two horizontal loads are applied close to the notch mouth. The same material properties as in [138] are considered and shown in Table 1. The simulation is performed under arc length control of the CMOD until it reaches 4 mm.

![Figure 43. Geometry of the wedge splitting test (mm)](image)

<table>
<thead>
<tr>
<th>Material Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Young’s Modulus</td>
<td>$28.3 \cdot 10^9$ Pa</td>
</tr>
<tr>
<td>Poisson’s Ratio</td>
<td>0.18</td>
</tr>
<tr>
<td>Tensile Strength</td>
<td>$2.12 \cdot 10^6$ Pa</td>
</tr>
<tr>
<td>Tensile Fracture Energy</td>
<td>373 J/m2</td>
</tr>
</tbody>
</table>

Table 1. Material parameters of the wedge splitting test
The simulation is performed in 2D under the plane strain assumption using a structured mesh of quadrilateral elements with a size of 1 cm, resulting in a 6,276 element mesh, shown in Figure 44. On the one hand, reference [138] used a similar FE size for the elements in the area where damage develops in the corresponding XFEM simulations. On the other hand, for the phase-field computations a mesh size of 1 mm, 10 times smaller, was adopted, which in 2D increases the number of elements employed in the simulation by a factor on the order of $10 \times 10 = 100$.

Figure 44. Mesh used for the wedge splitting test in the mixed FE simulations
Figure 45. Computed crack paths in the wedge splitting test with: (a) XFEM, (b) mixed FE and (c) phase-field. (a) and (c) taken from [138]
Figure 45 shows the computed crack paths for the three methods examined in this work. Specifically, Figure 45a displays the trajectory obtained with XFEM, while Figure 45c depicts the computed damage with the phase-field approach, both taken from [138] and Figure 45b the computed maximum principal strain with mixed FE. In all the cases the fracture follows the same straight vertical line.

In Figure 46 the force-displacement curves for the three methods are shown. The results for XFEM and phase-field, which are almost overlapping, are taken from reference [138]. It can also be seen that the results produced by the mixed FE formulation are also practically the same. This shows that the constitutive laws introduced in the three methods are consistent with each other and are able of producing the nonlinear cohesive behavior when the same material properties are introduced. Note that if distinct constitutive laws are used for each method, the results would no longer be the same.

It should also be noted that the computational cost involved in each method to produce the same result is not the same. In particular, the computational cost involved in the phase-field method is much larger, as it requires a much finer FE mesh.

![Figure 46. Force-CMOD curve of the wedge splitting for the three methods considered](image)

### 7.1.1. Mesh refinement analysis

The objective of this section is to assess the capacity of the mixed FE formulation of producing the same results with different mesh sizes using both triangular and quadrilateral elements. For this, the simulation of the wedge splitting test is performed using the four different meshes detailed in Figure 47, where the FE size is taken as 10 mm and 3.33 mm both for triangles and quads. It can be seen that these meshes, as well as all the other ones employed for mixed FE throughout this work, are much coarser than the ones employed in phase-field, as is shown in Figure 40.
Figure 47. Detail of the meshes used for the mesh convergence analysis around the tip of the notch: (up) quadrilateral and (bottom) triangular FE, using (left) $h = 10$ mm and (right) $h = 3.33$ mm

Figure 48. Mesh refinement analysis of the wedge splitting test: Computed crack paths with (up) quadrilateral and (bottom) triangular FE, using (left) $h = 10$ mm and (right) $h = 3.33$ mm
Figure 49. Mesh refinement analysis: Force-CMOD curve of the wedge splitting test for (a) quadrilateral elements, (b) for triangular elements and (c) quadrilateral vs triangular comparison.
The obtained maximum principal strain field, depicting the computed crack paths is shown in Figure 48 for the four meshes, where it can be seen that the crack bandwidth is reduced when mesh size decreases. In Figure 49 the force-CMOD curves obtained with the different meshes are assessed against each other. It can be seen, in Figure 49a, that the results obtained with quadrilateral elements are practically overlapping, while the ones computed with triangular elements in Figure 49b require a finer mesh to reach a converged solution. In Figure 49c it is verified that, when the FE size is reduced enough, both quadrilateral and triangular elements produce the same solution. It can be seen that suitable results can be reached with mixed FE without using the fine meshes required in phase-field. In reference [138] the convergence analysis featured for phase-field compares meshes with elements of 1 mm and 0.5 mm. As displayed in Figure 47, in the mixed formulation the FE size can be set equal to the width of the notch, which is in this case of 1 cm. In the corresponding phase-field simulation in reference [138], the crack bandwidth is equal to 10 elements, so that at least 1 mm elements are required, seriously increasing the computational cost of the method.

### 7.1.2. 2D vs 3D simulations

3D applications are usually prevented in phase-field by the high computational cost involved and in XFEM by the additional effort required to implement it. The generality and the reduced computational cost of mixed FE allows to readily perform the same simulations in 3D.

![Figure 50. Force-CMOD curves of the wedge splitting test in 2D and 3D](image)

With the intent of showing the capacity of the mixed FE method to accurately produce results in 3D, in this section the computed results obtained in 2D are compared with corresponding 3D simulations. The same material properties are employed than in 2D, shown in Table 1. The simulation is performed with a mesh of 6,276 hexahedral elements of 10 mm size with one element through the thickness.

The computed force-CMOD curves for the 2D and 3D analyses are shown in Figure 50. It can be seen that both results are very close to each other and also very similar to the XFEM and phase-field simulations by [138]. The crack surface obtained in the 3D simulation is shown in Figure 51.
7.2. **Arrea and Ingraffea mixed mode bending test**

In this section, the numerical simulation of the Arrea and Ingraffea experiment, reported in reference [279], is considered. Other numerical simulations of the tests can be found for instance in reference [1, 280], where a smeared crack model is employed, in reference [281], where the fictitious crack model is considered, in references [131, 86], where a model with a transition from smeared nonlocal formulation to a discontinuous embedded finite element method is proposed, in reference [282], which employed cohesive interface elements, in references [283, 214] where a nonlocal damage model is used, in references [18, 78, 284, 285], where EFEM is applied, in [134], where EFEM and XFEM are compared, in [286] which compares rotating and fixed smeared crack models, in references [287, 288] where a meshfree method is introduced, in reference [289] where an approach coupling the finite element method and the discrete element method is proposed and in reference [290] where a model featuring a transition from a smeared crack damage model to XFEM is used. Also, the numerical modelling of a beam with a similar geometry and boundary conditions, experimentally tested in reference [291] can be found in [291], which considered a lattice model, a method which considers a network of 1D beam finite elements to model the 2D structure, in reference [40], where a gradient-enhanced model is used and in reference [292], which employed XFEM to compute the problem.

Again, the results obtained with XFEM and phase-field in [138] are taken as references for the present comparison with mixed FE. In the experiment an eccentricity was introduced in the load and the boundary conditions of a notched beam, so that it is subjected to mixed mode fracture. Therefore, this example can also be employed to assess the mesh objectivity in terms of crack trajectory of the three methods contrasted in this work.

Figure 51. Computed crack surfaces of the wedge splitting test
Table 2. Material parameters of the Arrea and Ingraffea tests

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
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<tbody>
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<td>Poisson’s Ratio</td>
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<tr>
<td>Tensile Strength</td>
<td>$2.8 \cdot 10^6$ Pa</td>
</tr>
<tr>
<td>Tensile Fracture Energy</td>
<td>100 J/m$^2$</td>
</tr>
</tbody>
</table>

Figure 52. Geometry of the Arrea and Ingraffea experimental tests (mm)

Figure 53. Meshes used for the Arrea and Ingraffea simulations in the mixed FE simulation with (a) $h = 5$ mm and (b) $h = 2.5$ mm

The details of the geometry and boundary conditions of the experiment can be found in Figure 52. The dimensions of the beam are $1.322 \, m \times 0.306 \, m$ and the notch length is $82 \, mm$. The thickness of the beam is $0.156 \, m$ and the two eccentric loads $F$ and $0.13 \, F$ are applied. The simulations are done under CMOD control. For comparing purposes, the same material properties as in reference [138], shown in Table 2, are used. Note that they were not chosen with the intent of reproducing the experimental response but rather to compare the results of the XFEM and phase-field techniques. An actual comparison between the mixed FE formulation and the experimental results of this test can be found in reference [29].
The mixed FE simulations are performed under the plane stress hypothesis using quadrilateral elements of sizes 5 mm and 2.5 mm, which correspond to the sizes used for the XFEM simulations in reference [138] in the refined region where damage appears. This results in a mesh of 16173 and 64976 elements respectively, shown in Figure 53. Again, the size of the elements used for the corresponding phase-field simulations in [138] are 10 times smaller, of 0.5 mm and 0.25 mm. This increases the number of elements as well as the number of degrees of freedom in 2D by a factor of around 100.

Figure 54. Comparison of the results of the Arrea and Ingraffea beam: (a) crack trajectory obtained with XFEM and damage contour computed with (b) mixed FE using $h = 5$ mm, (c) mixed FE using $h = 2.5$ mm, and (d) phase-field. (a) and (d) taken from [138]

Figure 54b and c depict the computed damage contours of the Arrea and Ingraffea beam obtained with mixed FE. It can be seen that the path of the fracture, starting at the notch, turns influenced by the mixed mode loading of the beam. It can be compared with computations using XFEM and phase-field in Figure 54a and d, taken from [138]. A detailed comparison of the crack trajectories is delivered in Figure 55. It can be clearly observed that the solutions obtained with the three methods are almost identical. In particular, it can be seen that results acquired with phase-field and mixed FE are practically the same. Note also that the results computed
with mixed FE with both meshes are practically overlapping, showing that convergence has been reached.

Figure 56 shows the computed Force F vs CMSD curves with the three methods. It can be seen that they are very similar, even if they are not exactly the same. This is because, even if everything else in the three methods is equivalent in the Rankine damage constitutive law employed, the XFEM and phase-field simulations were obtained in [138] using the Cornelissen softening curve [62] while for the mixed FE exponential softening was considered. It should be noted that in reference [138] the Cornelissen softening law, which is a more complicated expression, defined in terms of the crack opening, produced different general curves when applied with XFEM and phase-field. However, the ability of the three methods to produce the same results is demonstrated again. This is remarkable as the difference in the computed results obtained by the three different methods for quasi-brittle cracking and with different FE codes is minimal.

![Figure 55. Comparison of the Arrea and Ingraffea beam crack trajectories (a) in the whole structure and (b) in detail](image)

Note that while the phase-field and mixed FE are able of producing practically the same results in terms of crack trajectory, the computed fracture path in XFEM is slightly different. Interestingly, the results obtained with the two meshes sizes considered in [138] for XFEM produce practically overlapping results. This small difference between the models is caused by a bias introduced by the crack tracking algorithm employed in XFEM, while no hypotheses are implanted in the determination of the crack trajectory in mixed FE and phase-field.
7.2.1. Comparison of the results obtained with different damage surfaces

To obtain the same results with both phase-field and mixed FE, equivalent constitutive laws should be employed. For this reason, an isotropic Rankine damage model, the same one as employed in reference [138] for phase-field, is considered in the previous simulations. However, as shown in references [29, 31], mixed FE can be readily used in conjunction with any constitutive law defined in the traditional stress vs strain format. In particular, the generality of the mixed FE method allows to easily consider different damage surfaces when performing the numerical simulations. This allows to study the effect that they have on the crack trajectory. Note that XFEM, requires the implementation of crack tracking algorithms specific to each damage surface. See for example reference [85] where a tracking criterion consistent with the Mohr-Coulomb damage surface is developed. However, usually the criterion employed in XFEM is Rankine exclusively. This differs from the mixed FE approach, were the direction of crack propagation is implicitly provided by the constitutive law and does not require tracking. Other studies comparing the behavior of several damage surfaces with mixed FE are made in references [29, 31].

In this section, the Rankine, Positive Beltrami and Drucker-Prager surfaces, depicted in Figure 57 for plane stress, are considered. The same material properties, given in Table 2, are used for all the cases. The compressive vs tensile strength ratio is taken as 10. The computed damage contours are shown in Figure 58 and a detailed comparison of the crack trajectories is provided in Figure 59. On the one hand, it can be seen that the Rankine and Positive Beltrami criteria produce practically the same results. This is because their damage surfaces, portrayed in Figure 57, are the same in the traction-compression quadrant. On the other hand, the Drucker-Prager criterion produces a slightly more curved trajectory. In Figure 60, the corresponding force-CMSD results are provided. Again, the behavior of Rankine and Positive Beltrami is very similar, while a somewhat larger difference can be appreciated for the Drucker-Prager curve, which is caused by the deviation of the crack trajectory.
Figure 57. Rankine, Beltrami Positive and Drucker Prager damage surfaces

Figure 58. Damage contours computed with mixed FE of the Arrea Ingraffea beam using (a) Rankine, (b) Positive Beltrami and (c) Drucker Prager ($f_c/f_t = 10$) surfaces
Figure 59. Comparison of the crack trajectories for the Rankine, Positive Beltrami and Drucker-Prager surfaces in the Arrea and Ingraffea beam (a) in the whole structure and (b) in detail

Figure 60. Computed Force F vs CMSD curves of the Arrea and Ingraffea beam with the three damage surfaces considered
7.2.2. 2D vs 3D simulations

The generality and the reduced computational cost of mixed FE allows to produce the same results in 3D as well without any difficulty, while 3D simulations are more challenging in XFEM and phase-field for the reasons already discussed. This is the motivation for the next section, where the computed results in 2D are contrasted to corresponding 3D simulations.

The same material properties of Table 2 are employed, and the 3D solution is obtained using a 16,173 hexahedral element mesh of 5 mm size and one element through the thickness.

Figure 61. Damage contour of the 3D simulation of the Arrea and Ingraffea beam computed with mixed FE:
(a) front view, (b) side view and (c) deformed shape (x 200)

Figure 61 shows the computed damage contours in 3D simulations, comparable to the 2D results in Figure 54b and c. A detailed comparison of the crack trajectories is provided in Figure 62. It can be seen that the 2D and 3D results are practically overlapping, and also almost the same as the phase-field results from reference [138] while the XFEM solution is, as previously mentioned, slightly different.
The computed force vs CMSD curves in 2D and 3D are compared in Figure 63. They are almost the same. It can be concluded that the plane stress hypothesis assumed for computing the beam in 2D is correct. The computed crack surface ensuing from the 3D calculation is shown in Figure 64.

Figure 62. Comparison of the computed crack trajectories in 2D and 3D for the Arrea and Ingraffea beam with mixed FE (a) in the whole structure and (b) in detail
7.3. Garcia-Alvarez beams

This section covers the numerical modelling of the Garcia-Alvarez experiments reported in [293]. Reference [293] also includes the computational modelling of the experiments using interface elements. Other FEM simulations of the tests are given in reference [227] using the PF-CZM model, which are compared to mixed FE in this work. Note that in this case, no equivalent is-XFEM results are available in the literature.
Table 3. Material parameters of the Garcia-Alvarez beams

<table>
<thead>
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<tbody>
<tr>
<td>Young’s Modulus</td>
<td>$3.38 \times 10^9$ Pa</td>
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<tr>
<td>Poisson’s Ratio</td>
<td>0.2</td>
</tr>
<tr>
<td>Tensile Strength</td>
<td>$3.5 \times 10^6$ Pa</td>
</tr>
<tr>
<td>Tensile Fracture Energy</td>
<td>80 J/m²</td>
</tr>
</tbody>
</table>

In this experiment the phenomenon of structural size effect is studied. For this reason, geometrically similar beams with depths $D$ of 80 mm, 160 mm and 320 mm are subjected to three-point bending. A constant span-to-depth ratio of 2.5 is used. A notch of varying eccentricity is included, so that a mixed mode fracture develops. Specifically, notch eccentricities $\mu D$ of $0.625D$, $0.3125D$ and $0.0D$ are introduced. In all the cases, the notch-to-depth ratio $\lambda$ is 0.25 and the thickness of the beams is 50 mm. The details of the geometry can be examined in Figure 65. The material properties introduced are displayed in Table 3. The beams are subjected to a vertical force at the top midpoint and the numerical simulations are made under CMOD control.
The objective of this section is again to contrast the results achieved with phase-field and mixed FE and not to reproduce the experimental results. Only the medium-sized specimens, with depth $D = 160$ mm, are considered in the present comparison, because these are the only cases for which reference [227] provided the computed crack trajectories with phase-field. The comparison between the original experimental results and the corresponding mixed FE simulations for all the beam sizes can be found in reference [32], where the capacity of mixed
formulation in modelling the size effect phenomenon is demonstrated. Also, a mesh independence study as well as a comparison between standard and mixed FE solutions are provided in reference [32] for this case.

The mixed FE simulations of the 0.3125D eccentricity case of this section have been made under the plane stress hypothesis using a mesh of 36,714 triangular elements, shown in Figure 66, which results from using a finite element size $h$ of $10^{-2}D$ in the central area where damage develops. For the other eccentricity cases, the same FE size is used and similar meshes ensue. Note that in the phase-field results obtained in reference [227] the thickness $b$ of the regularized crack is equal to $10^{-2}D$ and that the finite element size is taken as $b = 10h$. This results in an element size of $10^{-3}D$, 10 times smaller, increasing approximately 100 times the number of elements used in 2D.

In Figure 67 a comparison between the phase-field and mixed FE results in terms of computed damage contours is shown. Specifically the medium-sized specimens with depth $D = 160 \text{ mm}$ and all three eccentricities are considered. It can be seen how the computed crack trajectories of the cases with notch eccentricities deviate towards the center of the beam while in the case without eccentricity the crack follows a vertical straight line. The results obtained with the two methods are very similar for all the cases. These computed crack trajectories are compared in detail in Figure 68. It can be seen that the results computed with phase-field and mixed FE are practically overlapping for all the eccentricities. The minimal difference existing between the solutions obtained with phase-field and mixed FE is remarkable. However, it must be pointed out that the phase-field method requires a much finer mesh density to achieve them.
Figure 69. Comparison of the force-CMOD curves of the Garcia-Alvarez tests for a depth $D = 160 \text{ mm}$ with eccentricities of (a) 0.625$D$, (b) 0.3125$D$ and (c) 0.0$D$
Figure 69 compares the force-CMOD curves computed for the medium-sized specimens with depth $D = 160 \text{ mm}$ for the three eccentricities considered with phase-field and mixed FE. It can be seen that the results are not exactly the same for both methods. The small differences that can be seen are caused by the fact that reference [227] used a damage evolution law with Cornelissen softening to compute the phase-field results while exponential softening is considered here for mixed FE. This only causes minor differences in the computed force-CMOD curves. The resemblance between the results obtained with the two methods in terms of force-CMOD curves as well as crack trajectories, for all the eccentricities, using the same material properties, is noteworthy.

### 7.3.1. 2D vs 3D simulations

Once again the corresponding 3D simulations are performed to show the capabilities of the mixed FE formulation for accurately producing 3D results.

The material properties are taken from Table 3. For this study, unstructured meshes tetrahedral elements are used. For the case with eccentricity $0.625D$ the FE size is $1.875 \cdot 10^{-2} D = 3 \text{ mm}$ in the area where damage develops, resulting in a mesh with 35,149 nodes and 192,279 tetrahedral elements. In the case with an eccentricity of $0.3125D$ the FE size is $2.8125 \cdot 10^{-2} D = 4.5 \text{ mm}$ in the region where damage appears, and the corresponding FE mesh is of 7,666 nodes and 38,593 elements. And the case with no eccentricity, has a FE size of $10^{-2} D = 1.6 \text{ mm}$ in the central region where the crack progresses, ensuing a 4,168 node and 18,546 element mesh.

![Figure 70. Damage contours, front view, from the 3D analyzes of the Garcia-Alvarez tests for a depth $D = 160 \text{ mm}$ with eccentricities of (a) $0.625D$, (b) $0.3125D$ and (c) $0D$](image-url)
Figure 71. Damage contours: (left) lateral view and (right) deformed shape (x 50) from the 3D analyzes of the Garcia-Alvarez tests for a depth \( D = 160 \text{ mm} \) with eccentricities of (a) 0.625\( D \), (b) 0.3125\( D \) and (c) 0.0\( D \)

In Figure 70 the computed damage contours resulting from the 3D simulations is shown. They are to be compared with the corresponding 2D results in Figure 67. Figure 71 provides a lateral view of the 3D analyzes as well as the deformed shape (x 50) of the Garcia-Alvarez beams. A detailed comparison between the 2D and 3D crack trajectories is included in Figure 72. It can be seen that despite using much coarser meshes in 3D, the computed results practically match the 2D simulations obtained with the phase-field and mixed FE formulations. This shows how powerful the mixed FE technology is, as it provides mesh objective results with a poor level of mesh refinement.
Figure 72. Detailed comparison of the computed crack trajectories in 2D and 3D of the Garcia-Alvarez tests, \( D = 160 \text{ mm} \) for the (a) 0.625\( D \) and (b) 0.3125\( D \) eccentricities.

The resulting force-CMOD curves from the 3D analyzes are contrasted in Figure 73 against the 2D counterparts previously shown. It can be seen that the 2D and 3D results are practically overlapping. It is inferred again that the plane stress hypothesis commonly assumed to perform the simulations of the beams is accurate enough. Figure 74 and Figure 75 show the computed fracture surfaces obtained from the 3D calculations, showing the aptness of the mixed FE model to produce accurate 3D crack surfaces without spurious mesh dependency.
Figure 73. Comparison of the 2D and 3D computed force vs CMOD curves of the Garcia-Alvarez beams for eccentricities (a) 0.625D, (b) 0.3125D and (c) 0.0D
Figure 74. Computed crack surfaces of the Garcia-Alvarez beams, medium sizes, with eccentricities (a) 0.625\(D\) and (b) 0.3125\(D\)
In this section, the numerical simulation of a fracture propagating in the Koyna dam is considered. After the beginning of the dam filling in 1962, the region, previously considered nearly nonseismic, started experiencing a serious increase in earthquake activity. In December 1967 a 6.5 magnitude earthquake caused some damage to the structure, raising the concern of the community. An overview of the history of the dam, located in India, is given for example in reference [294]. The seismic analysis of the Koyna dam has been performed many times, like for example in reference [294], which conducted a linear elastic FEM analysis, in [295, 296, 297, 298, 299, 300, 301], where different smeared crack models are employed, in reference [302] which used XFEM and in reference [303] where XFEM, the crack band model and a plasticity model are compared. At the same time, the quasi-static analysis of the dam overflow has become a reference benchmark in the community, see for example references [304], where a comparison between linear elastic fracture mechanics (LEFM) and plasticity theories is made, in [286] which compares rotating and fixed smeared crack models, in [305] which also employed a smeared crack model, in references [131, 86], where a model with a transition from smeared nonlocal formulation to a discontinuous embedded finite element method is proposed, in reference [290], where a model featuring a transition from a smeared crack damage model to XFEM is used, in [306], which employed cohesive interface elements, and in [307], where phase-field is used to model fracture.

Again, the numerical results of [138] are taken here as references for comparison with the XFEM and phase-field techniques. The geometry of the Koyna dam is shown in Figure 76. It is a gravity dam made of concrete and has a height of 103 m. In the simulation an initial crack of

7.4. Koyna dam

In this section, the numerical simulation of a fracture propagating in the Koyna dam is considered. After the beginning of the dam filling in 1962, the region, previously considered nearly nonseismic, started experiencing a serious increase in earthquake activity. In December 1967 a 6.5 magnitude earthquake caused some damage to the structure, raising the concern of the community. An overview of the history of the dam, located in India, is given for example in reference [294]. The seismic analysis of the Koyna dam has been performed many times, like for example in reference [294], which conducted a linear elastic FEM analysis, in [295, 296, 297, 298, 299, 300, 301], where different smeared crack models are employed, in reference [302] which used XFEM and in reference [303] where XFEM, the crack band model and a plasticity model are compared. At the same time, the quasi-static analysis of the dam overflow has become a reference benchmark in the community, see for example references [304], where a comparison between linear elastic fracture mechanics (LEFM) and plasticity theories is made, in [286] which compares rotating and fixed smeared crack models, in [305] which also employed a smeared crack model, in references [131, 86], where a model with a transition from smeared nonlocal formulation to a discontinuous embedded finite element method is proposed, in reference [290], where a model featuring a transition from a smeared crack damage model to XFEM is used, in [306], which employed cohesive interface elements, and in [307], where phase-field is used to model fracture.

Again, the numerical results of [138] are taken here as references for comparison with the XFEM and phase-field techniques. The geometry of the Koyna dam is shown in Figure 76. It is a gravity dam made of concrete and has a height of 103 m. In the simulation an initial crack of
1.93 m of length is located at a height of 66.5 m, representing the cracking that was discovered after the 1967 earthquake. The dam is made of concrete and the material parameters employed in the simulation are provided in Table 4. The load in the dam is introduced in three stages: first the self-weight is applied, secondly the hydrostatic pressure corresponding to the full reservoir situation is imposed and thirdly a constant pressure corresponding to the dam overflow is assigned. Gravitational acceleration $g$ is taken as $9.81 \text{ m/s}^2$. In the third stage, the applied load uniformly increases while the analysis is performed under arc length control of the horizontal displacement at the top of the dam until it reaches 75 mm.

![Figure 76. Geometry of the Koyna dam (m)](image)

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<table>
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<tr>
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<td>Poisson’s Ratio</td>
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<td>Water Density</td>
<td>$1000 \text{ kg/m}^3$</td>
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Table 4. Material parameters of the Koyna dam
The dam is computed using an unstructured mesh. Triangular elements of a size of 0.1 m are employed in the area where the crack develops and of 1 m in the rest, resulting in a 84,465 element mesh, shown in Figure 77. The notch width is set equal to zero. In reference [138], slightly larger FEs of size 0.3 m and 0.2 m are considered for XFEM, while for phase-field 0.06 m and 0.04 m sized elements are employed in the refined area.
Figure 78. Comparison of the Koyna dam results: (a) crack trajectory obtained with XFEM, (b) damage contour computed with mixed FE and (c) damage contour captured with the phase-field method, (a) and (c) taken from [138]
Figure 78 shows the results obtained with the mixed FE formulation collated with the XFEM and phase-field computations performed by [138]. It can be seen how the crack trajectory branches several times when using mixed FE and phase-field but that this phenomenon is not captured with XFEM. The employed XFEM formulation does not have branching implemented. As mentioned before, branching requires the handling of specific enrichment functions, integration schemes, tracking algorithms that include a branching criterion, etc. All of this involves a significantly large implementation effort. In contrast to XFEM, branching in phase-field and mixed FE does not require special additional attention. It seems that a consequence of the inability of branching is that the crack computed with XFEM is longer, in order to reach the

Figure 79. Comparison of the Koyna dam crack trajectories (a) in the whole structure and (b) in detail.
imposed horizontal displacement at the top of the dam of 75 mm. Aside from this, a direct comparison of the main fracture path in Figure 79 shows that the three methods produce almost overlapping results in terms of crack trajectory.

Figure 80 shows the overflow height vs top horizontal displacement curves of the Koyna dam with the three methods considered. It can be seen that the phase-field and mixed FE produce practically the same results while the ones obtained with XFEM are slightly apart. This is likely due to the inability of XFEM in capturing the branching of the crack. The computed results with phase-field and mixed FE are remarkably close and the overall phenomenon is well captured by both models.

Once again, after using equivalent materials laws and seeing that the obtained results are practically the same, it should be noted that the computational cost of phase-field is much larger than in mixed FE, which may become a great concern especially for the simulation of large structures like in the present case.

![Figure 80. Computed overflow height vs horizontal displacement at the top of the Koyna dam with the three methods considered](image)

7.5. **Buchholz skew notched beam**

In this section, the numerical simulation of a skew notched beam subjected to three-point bending is considered. Computations with mixed FE for this case have already been presented in reference [28], and they are here reexamined to compare them with the results recently obtained with PF-CZM, reported in reference [253]. No corresponding simulations using the is-XFEM are available in the literature so far.

This test, reported in reference [308], was carried out in a beam made of acrylic glass (PMMA). References [309, 310] performed the same experiment under cyclic loading to study fatigue crack growth. References [308, 309, 310] completed as well the numerical modelling of the test using the modified virtual crack closure integral (MVCCI) method. One member of the team who originally conducted the experiments is the coauthor of reference [311], which compares computations using the dual boundary element method (DBEM) and the MVCCI. This case has
also been simulated in [312, 313, 314, 315, 316], using the XFEM and in reference [317], where an eigenerosion approach to fracture is proposed.

Details of the geometry and boundary conditions of beam are presented in Figure 81. The beam has a span of 240 mm and a depth of 60 mm. Its thickness is 10 mm. The specimen has a notch of 20 mm x 2 mm with a deviation of 45° with respect to the surface of the specimen. The insertion of a skew notch causes the development of a twisting crack under mixed mode I and III fracture in the beam. For this reason, a 3D simulation is required.

In the computations, the load is applied imposing increments of vertical displacement at the top midpoint of the beam.

The material properties are shown in Table 5. The same material properties as in reference [253] are used to allow a direct comparison.

![Figure 81. Geometry of the Buchholz skew notched beam (mm), (a) front view and (b) top view](image)

<table>
<thead>
<tr>
<th>Material Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
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<td>Young’s Modulus</td>
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<td>Poisson’s Ratio</td>
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<td>Tensile Strength</td>
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<td>Tensile Fracture Energy</td>
<td>500 J/m²</td>
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</table>

Table 5. Material parameters of the Buchholz skew notched beam
Figure 82. (a) Mesh used for the Buchholz skew notched beam and (b) detail of the refined area

Figure 83. Computed damage profile of the Buchholz skew notched beam with (a) mixed FE and (b) phase-field
Figure 82 shows the 3D structured mesh used to perform the simulation with mixed FE. It is made of hexahedral and tetrahedral elements of approximately 0.7 mm size in the central area where damage develops, resulting in a total of 66,044 nodes and 218,946 elements. Reference [253] solved the problem using a structured mesh of brick elements with a size of 0.2 mm in the central part, which, divided into tetrahedra, which results in a mesh of 1,355,613 elements.

Figure 83 shows a comparison of the computed damage profiles with mixed FE and the phase-field model. It can be observed how the crack starts at the notch and deviates towards the center due to the mixed mode I and III loading conditions. Both methods are able of producing the skew-symmetric and twisting pattern of the crack in agreement with the test. No sign of spurious mesh dependency can be appreciated in the results.
Figure 84 displays a detailed comparison of the computed crack trajectories from Figure 83. It can be seen how both methods produce the same results, even if the phase-field method produces a smoother solution due to the higher resolution used.

The computed crack resulting from the 3D calculation is shown in Figure 85. The detail of the structured mesh used to compute the problem can be perceived through the fracture surface generated by the mixed FE method.

8. **Outlook**

XFEM, the MFEM and the PFM are the currently most promising methods used in computational failure mechanics of quasi-brittle materials. They are representatives of the embedded, smeared and regularized crack approaches, respectively.

From the independent appraisal of the XFEM, the MFEM and the PFM in Sections 4, 5 and 6 and the performance displayed in the numerical simulations in Section 8, the following comparative assessment is made using the 10-point checklist.

<table>
<thead>
<tr>
<th>Checklist</th>
<th>XFEM</th>
<th>MFEM</th>
<th>PFM</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 Variational formulation in the continuous setting</td>
<td>✗</td>
<td>✓✓</td>
<td>✓✓</td>
</tr>
<tr>
<td>2 Convergence of the FE formulation</td>
<td>✗✓</td>
<td>✓✓</td>
<td>✓✓</td>
</tr>
<tr>
<td>3 Strength, toughness and energy dissipation</td>
<td>✓✓</td>
<td>✓✓</td>
<td>✓✓</td>
</tr>
<tr>
<td>4 Criterion for direction of propagation</td>
<td>✗✓</td>
<td>✓✓</td>
<td>○</td>
</tr>
<tr>
<td>5 Constitutive behavior generality</td>
<td>✗✓</td>
<td>✓✓</td>
<td>✗</td>
</tr>
<tr>
<td>6 Generality and implementation effort</td>
<td>✗✓</td>
<td>✓✓</td>
<td>✓</td>
</tr>
<tr>
<td>7 Cost-efficiency</td>
<td>✓✓</td>
<td>○</td>
<td>✗</td>
</tr>
<tr>
<td>8 Multiple, intersecting and branching cracks</td>
<td>✗✓</td>
<td>✓✓</td>
<td>✓✓</td>
</tr>
<tr>
<td>9 Auxiliary tracking techniques</td>
<td>✗✓</td>
<td>✓✓</td>
<td>✓✓</td>
</tr>
<tr>
<td>10 Application in 3D</td>
<td>✗✓</td>
<td>✓✓</td>
<td>○</td>
</tr>
</tbody>
</table>

One salient observation is that all three methods get a double tick in modelling the physical aspects of *strength, toughness and energy dissipation*. The three have also the capacity of producing realistic failure mechanisms that are mesh-independent. These are undoubtedly the main reasons for their adoption.

Notwithstanding, it is clear that in the XFEM the burdens far out-weight the benefits, with shortcomings common to all methods in the discontinuous crack approach.
The MFEM and the PFM are the contestants for future developments, as they accomplish a double or single tick in many of the check points. In the above checklist, MFEM has several advantages, while not sporting any disqualifier.

On the one hand, MFEM allows full generality regarding constitutive behavior. On the other hand, the PFM requires a degree of mesh resolution that makes it comparatively very expensive and applications in 3D rather impracticable.

The reason for these two features lays is the fundamental difference between MFEM and PFM. PFM is conceived as a regularization of the problem of linear fracture at continuous level. The resolution to reproduce this regularity at discrete level requires very fine meshes, 10 to 30 elements across the crack. Also, only one isotropic damage index is represented by the phase-field, with very limited constitutive capabilities. Conversely, MFEM is a fully general framework for solving the mechanical problem that enhances the accuracy of the discrete strain field and introduces the required regularity to solve fracture at discrete level. On the one side, the resolution needed for this is about 3 elements across the crack, far fewer than for the PFM; on the other side, orthotropic behavior and irreversible strains can be considered straightforwardly.

The cost-efficiency issues of MFEM and PFM can be addressed by selectively and adaptively applying them in the relatively small parts of the structure where cracking is actually developing. Also, more general crack material behavior is progressively being incorporated into PFM, at the price of increasing its cost and complexity. For instance, introducing orthogonal damage requires the computation of three separate phase fields. These developments will highlight the advantages of MFEM, directly addressing the problem at strain level.

9. Acknowledgements

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