

UNIVERSIDADE DO PORTO

# Continuous-Discontinuous Approach for the Modelling of Ductile Fracture

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*“Crave for a thing, you will get it. Renounce the craving, the object will follow you by itself.”*

Swami Sivananda (1887-1963)



# *Abstract*

Ductile metals, such as aluminium or steel, are present in all sorts of industries, from aeronautical to automotive, construction to household goods. A deeper understanding of the fracture mechanisms associated to these type of materials is essential to optimize production processes as well as avoid catastrophic failures.

Traditional fracture theories generally rely on a single energetic parameter to trigger crack propagation, which may not be adequate for ductile metals, as there is a substantial amount of plastic deformation prior to failure. On the other hand, Continuum Mechanics theories successfully handle large straining and describe successfully the plastic-hardening and plastic-softening stages of material behaviour. Nevertheless in the final stages of failure, a discontinuous methodology is essential to represent surface decohesion and macro-crack propagation.

The aim of this work is to build a model for ductile fracture gathering the advantages of both continuous and discontinuous approaches. The Extended Finite Element Method (XFEM) is combined with the Lemaitre model for ductile damage in a way that crack initiation and propagation are governed by the evolution of damage. The model was built under a finite strain assumption and a non-local integral formulation is applied to avoid pathological dependency of results on the spatial discretisation. Special attention is given to the necessary adaptations of the XFEM to be used in a ductile fracture context, such as selection of the enrichment functions and numerical integration strategies. The energy consistency issue during the transition from damage to fracture is also addressed. The effects of the introduction of a cohesive law in the global ductile fracture model are analysed and a strategy to approximate the fully damaged material condition is proposed.

Throughout the work, the efficiency of the proposed model is evaluated through various numerical examples and general conclusions are outlined. To finalize this thesis, some comments on the overall performance of the model are given together with some suggestions for future work.



## *Resumo*

Os metais dúcteis, como o alumínio ou o aço, estão presentes nas mais diversas indústrias, da aeronáutica à automóvel, da construção aos bens de consumo. O aprofundamento dos conhecimentos relativos aos mecanismos de fractura associados a este tipo de metais é essencial para otimizar processos de produção e evitar falhas catastróficas.

As teorias clássicas da fractura baseiam-se num único parâmetro energético que pode não ser adequado a metais dúcteis, pois estes apresentam deformações plásticas significativas anteriores à propagação de fendas no material. Por outro lado, as teorias de Mecânica dos Meios Contínuos descrevem adequadamente as fases de endurecimento e amaciamento plásticos. Contudo, nas fases finais de degradação do material, uma formulação descontínua é fundamental para descrever a separação entre as superfícies de uma fenda em propagação.

Este trabalho tem como principal objectivo o desenvolvimento de um modelo de fractura dúctil, reunindo as vantagens dos modelos contínuos e descontínuos. O Método dos Elementos Finitos Estendidos (XFEM) é associado ao modelo de dano dúctil de Lemaitre, de forma a descrever a iniciação e propagação. O modelo considera grandes deformações e uma formulação não-local integral, de forma a evitar a dependência patológica dos resultados relativamente à discretização espacial.

Para conseguir uma transição energeticamente consistente entre o dano e a fractura, analisam-se os efeitos da introdução de uma lei coesiva no modelo de fractura dúctil global, o que permite o desenvolvimento de uma estratégia para aproximar a condição de total degradação do material.

Ao longo do trabalho, a eficiência do modelo proposto é avaliada através de vários exemplos numéricos. Encerra-se esta tese com importantes comentários gerais e sugestões de desenvolvimentos futuros.



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*Dedicated to my family and friends*



# Chapter 1

## Introduction

Ductile fracture has been regarded as a crucial issue in many industrial areas. Although it is usually associated to failure, as most of the metals, at room temperature, fail according to this mechanism, it may be an integrating part of production processes, such as machining, blanking or cutting. Numerous techniques have been developed to optimize operations and products, nevertheless, a deeper understanding of this phenomenon would lead to more efficient designs, which, in a first stage, prevents the use of unnecessary material and energy and, in a second stage, avoids catastrophic failures. More than ever, the responsible use of resources is essential, not only from the financial point of view but also for a sustainable world.

Up to the nineteenth century the design of structures and mechanical parts was mostly empirical and understanding of material behaviour quite poor. Nevertheless, with the massive production of iron and steel demanded by the Industrial Revolution came the need of defining feasible design laws. Thus, by the beginning of the twentieth century, the study of ductile metals gained a mathematical approach with the pioneering works of Tresca [2], Huber [3], von Mises [4] and Hencky [5], where there was an attempt of developing material laws able to reproduce the experimental observations. The main outcome of these contributions was the prediction of the onset of plastic behaviour through the establishment of yield functions. In these approaches, the material properties are described at the meso-scale and explained by a few energy mechanisms. As the material is regarded as a continuous media, these works later gave birth to the so-called *Continuum Mechanics*.

Although the dimensioning of structures using the yield criteria became quite popular in the engineering media between the World Wars, catastrophic failures of structures such

as ships or tanks were still frequent. In fact, for many situations, the material should not be considered as continuous but containing defects, which influence the service response and therefore should be considered for correct dimensioning. The first mathematical approach of the effect of flaws in the material is due to Inglis [6] that studied the stress distribution in a plate containing an elliptical hole, subjected to a uniform tensile stress. Later, Griffith [7] extended these works by applying energy conservation principles, however, as the fracture work was assumed to come exclusively from the surface energy of the material, this approach was only valid for ideally brittle solids. The application of the fracture concepts to metallic materials came with the works of Westergaard [8], Irwin [9, 10] and Orowan [11]. The first author studied the stress and displacements fields in the vicinity of a crack tip and the others extended Griffith's model by including the energy dissipation by plastic flow. Nevertheless, only in the sixties, the concepts of *Linear Elastic Fracture Mechanics* (LEFM) were well systematized. The incursion to ductile materials started with the works of Dugdale [12] and Barenblatt [13] that developed the *cohesive zone* model, in which the crack interface is governed by a traction-displacement law. In the same period, Wells [14] observed that the discontinuity surfaces moved apart with plastic deformation and proposed a failure criterion based on the *crack tip opening displacement* (CTOD). Another important parameter to evaluate the plastic behaviour ahead of a crack tip was proposed by Rice [15] and is known as the *J-integral*.

Although these models allowed a significant improvement in the engineering designs, they all assume that the flaws already exist in the material, which means that the initiation of new cracks is not considered and the plastic behaviour is confined to very restricted areas, when comparing with the total size of the structure or mechanical part.

Continuum theories, on the other hand, evolved separately from Fracture theories with the development of strategies to describe material progressive degradation, characteristic of ductile failure processes. Two main families of theories may be distinguished in this context, one oriented to micro-mechanical considerations and another oriented to phenomenological aspects.

At the micro-structural level ductile fracture is characterized by void nucleation growth and coalescence, induced by the weaker inclusions contained in a metal alloy. Therefore Gurson [16] developed a constitutive model which assumes the existence of spherical voids embedded in an elasto-plastic material matrix. This model was later extended by Tvergaard [17] and Tvergaard and Needleman [18], which introduced the evolution of porosity and modified the yield function of Gurson to account for the coalescence effect.

The GNT model became one of the most popular models to address ductile fracture, resulting in a vast number of publications [19–22].

In the late fifties, Kachanov [23] and Rabotnov [24] introduced the *damage* concept, as a measure of material internal degradation. The later theories originating from this concept constitute an alternative to the micro-mechanical models. Here, damage is treated as an internal variable and therefore the micro-mechanical phenomena are dealt with in an averaging way. Important contributions for the full establishment of the *Continuum Damage Mechanics* (CDM) are due to Lemaitre [25–27] and Chaboche [28, 29], in which damage and plasticity are strongly coupled in a thermodynamical framework. Numerous works also derive from the Lemaitre model, considering, for instance more or less complex descriptions of the damage variable or more or less complex straining paths [30–35].

Although the discussion whether GNT-type or Lemaitre-type of models are more adequate to describe the behaviour of ductile metals is still open, both are widely used, as they integrate elasticity, plastic-hardening and plastic-softening stages. Moreover, they are able to predict the areas where failure is likely to occur. Still, when it comes the final stages of failure they are incapable of representing macro-crack propagation.

Having in mind the potentialities of the continuum theories, in particular the Lemaitre based theories, and the advantages of the fracture theories in terms of description of macro-crack propagation, the main objective of this thesis is to build a numerical model for ductile fracture, blending continuum damage concepts with a discontinuous approach.

## 1.1 Continuous-discontinuous approach for ductile fracture

The description of ductile metals through constitutive modelling leads to a complex mathematical description, where the use of numerical methods, often the Finite Element Method (FEM) [36] is imperative. However, even in the numerical context, one of the most significant limitations of the Continuous models is the inability to represent surface decohesion and propagation of cracks in a structure.

Probably the most intuitive way of representing a discontinuity within a finite element formulation is to conform the finite element mesh to the geometry of the discontinuity. So far, the most successful simulations of ductile fracture processes lay in strategies

that involve relatively fine meshes and continuous remeshing [37–43]. Nevertheless, this method is still burdensome and extremely expensive in terms of computational costs. In addition, errors may be introduced due to the need of projecting the field variables.

Remeshing may be simplified applying the element deletion technique [44, 45], where the elements in which the fracture criterion is met are simply deleted from the mesh. However, this technique is highly dependent on the element size and orientation.

To overcome the disadvantages of remeshing, researches developed the smeared crack model [46], in which the effects of a discontinuity are incorporated in the stress field and not at the displacement or strain field level. However, due to poor kinematic representation, these models were mostly replaced by approaches in which, displacement or strain level discontinuities are placed intra-element.

A large number of intra-element discontinuity models follows within the *embedded discontinuities* class [47]. These models are in general characterized by the introduction of new deformation modes in the standard finite element. These deformation modes are able to represent discontinuities with an arbitrary orientation both at the strain level (weak discontinuity) [48] or at the displacement level (strong discontinuity) [49, 50]. Extensions to large strain plasticity [51] and large strain isotropic damage with application to ductile fracture [52, 53] are also available. Although the embedded discontinuity approach allows the efficient modeling of regions with highly localised strains, the two parts of the element separated by the discontinuity are not totally independent and often the deformation state needs to be taken to be constant across the discontinuity band.

Another powerful technique to represent discontinuities intra-element is the eXtended Finite Element Method (XFEM) [54] in which the standard displacement field approximation is enriched with functions able to capture the decohesion between two surfaces. Extra degrees of freedom are added to the nodes of the elements containing the discontinuity, allowing free propagation through the mesh. Although most of the existing literature on the XFEM is focused on brittle fracture, the method possesses the desired flexibility, at reasonable computer costs, to be employed in ductile fracture simulations and therefore is used in this thesis. The developments in the use of the XFEM in ductile fracture problems are still limited, especially when dealing with large strain yielding. The main contributions are outlined in the following paragraph.

Initially, the XFEM works dealing with cracks in elastic media were combined with cohesive zone models to describe crack propagation in elastic-damageable materials [55–57]. Cazes et al studied the conditions in which the transition from a continuous model to a continuous-discontinuous model is acceptable, firstly in elastic-damageable materials [58] and later in elasto-plastic-damageable materials [59]. However in those studies the methodology is only fully developed for 1D cases and the location of the crack has to be assumed *a priori*. It is also worth mentioning the extension of these works to a thermo-mechanical framework by Fagerström et al [60] and the thick level set approach by Moës et al [61], which incorporates the damage variable in the level set to model the behaviour of elastic-damageable solids in a new way.

Facing this scenario, the main goal of this thesis is to develop a robust continuous-discontinuous model for crack initiation and propagation in ductile metals, based on the XFEM, whose accuracy of results is competitive with remeshing. Thus, CDM is used to describe the material behaviour prior to critical damage and, once this stage is reached, a crack is inserted through the XFEM. The subsequent crack propagation is also governed by the evolution of damage until the final stage of failure. This work will focus both on the phenomenological description of a ductile fracture process and in all the necessary element technology developments required for successful numerical simulations.

## 1.2 Thesis organisation

In this section is outlined how this thesis is organised and which are the main subjects addressed in each chapter.

## Chapter 2

In this work material behaviour prior to crack initiation is described in a CDM framework, in particular by the Lemaitre model for ductile damage. This chapter begins with the review of the CDM, which is not intended to be exhaustive but rather present the necessary concepts to the description of the Lemaitre constitutive model. As continuum softening models suffer from pathological mesh dependence, when implemented in FEM formulation, a non-local extension of the original damage model is also presented.

### Chapter 3

As the use of a numerical method is imperative to solve the differential equations describing a ductile fracture problem, this chapter is devoted to the Finite Element Method. The main aspects associated to the method, such as the definition of the Initial Boundary Value Problem, displacement based discretization, and incremental iterative schemes are reviewed.

The modularity and repeatability of the tasks performed in a FEM computer program suggest that the generation of numerical code could be automated. Therefore, this chapter also addresses the automatic code generation, in particular the *AceGen* system, which combines symbolic and algebraic capabilities with automatic differentiation and optimization of numerical code.

### Chapter 4

The XFEM became one of the most popular techniques to address problems involving discontinuities and moving interfaces. This thesis is no exception, being this method essential for the global fracture model developed. This chapter is mostly devoted to element technology, beginning with a review of the basic features of the XFEM, such as the displacement field approximation and basic numerical implementation. As ductile metals undergo large strain processes without volume changes, it follows an intensive study on numerical integration in enriched elements, focusing in the ability of satisfying incompressibility constraints. Other numerical issues associated to the use of XFEM for ductile fracture, such as selection of the enrichment functions and variable transfer are also dealt with in this chapter.

### Chapter 5

In this chapter the CDM is associated to the XFEM to build the ductile fracture model. A damage based criterion for crack initiation and propagation is defined and illustrated through some various examples. The model requires the definition of a critical damage threshold and therefore its influence in the material response is analysed. Details on the numerical implementation, in particular, related to equilibrium recovery are also addressed. The interaction of the non-local damage model with the XFEM is inspected, analysing the effect of the regularization length in crack initiation and propagation.

## Chapter 6

From the theoretical point of view, an energetically transition from damage to fracture should occur for totally damaged material. Nevertheless, in terms of numerical simulation, this condition leads to a singularity in the constitutive equations. In this chapter, a cohesive law is inserted in the model developed in chapter 5, in order to overcome this limitation. An exponential type of cohesive law is assumed, but its defining parameters are not considered to be a characteristic of the material but are rather fitted to fulfil energetic requirements. The efficiency of the proposed approach is tested in various numerical examples.

## Chapter 7

In this chapter the main conclusions of this work are outlined. The the results obtained throughout the different chapters are analysed in a global way, emphasising the main contributions at the numerical and phenomenological levels. The thesis is finalised with the analysis of the potentialities of the developed ductile fracture model and some suggestions for future work.

### 1.3 Related publications

Most of the work developed in this thesis has been included in scientific contributions that have been published or are currently in final preparation for submission. A list relating these publications is given herein.

- M. Seabra, J. César de Sá, *ContinuousDiscontinuous Model for Ductile Fracture*, NUMIFORM 2010: Proceedings of the 10th International Conference on Numerical Methods in Industrial Forming Processes Dedicated to Professor O. C. Zienkiewicz (19212009).
- M. Seabra, J. César de Sá, F. Andrade, F. Pires, *Continuous-discontinuous formulation for ductile fracture*, Int. J. Material Forming 4(3), 271281 (2011)
- M. Seabra, J. César de Sá, P. Šuštarčič, T. Rodič, *Some Numerical Issues on the use of XFEM for Ductile Fracture*, Computational Mechanics (2012) DOI: 10.1007/s00466-012-0694-x.

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- M. Seabra, P. Šuštarich, J. César de Sá, T. Rodič, *Damage driven crack initiation and propagation in ductile metals using XFEM*, Computational Mechanics (accepted for publication).
  - M. Seabra P. Šuštarich, J. César de Sá, T. Rodič, *Towards energetically consistent transition from damage to fracture using XFEM*. (in preparation).
  - M. Seabra P. Šuštarich, J. César de Sá, T. Rodič, *Automatic generation of XFEM codes and application to crack propagation*, Technical note (in preparation).

## Chapter 2

# Standard Continuum Damage Mechanics

Ductile metals, which include iron and steel, aluminium and copper alloys, are characterized by the presence of moderate to large plastic deformations prior to failure. Plastic strains may result from crystalline slip through dislocation motion or from degradation of the mechanical properties and therefore both mechanisms are strongly coupled in this type of materials.

Classically, the material properties may be inferred from the study of the microstructure of the material, the so-called *Micro Mechanical* theories, or the material behaviour may be described in phenomenological way, based on a thermodynamic framework, referred as the *Continuum Damage Mechanics* (CDM).

In the first category, the probably most extensively used model was proposed by Gurson [16] and later extended by Tvergaard and Needleman [18], which considers the material as a porous media, where voids nucleate and coalesce.

On the other way, the model proposed by Lemaitre [25–27, 29] is the most representative of the CDM models, serving as a base for many other material laws. Here material progressive degradation is treated as an internal variable, acting in an averaging sense within a representative volume, corresponding to a scale where the material may be regarded as homogeneous.

In this work, the Lemaitre model is used to describe the degradation of the mechanical properties of a solid prior to the formation of macro cracks, capturing the elastic, plastic-hardening and plastic-softening stages of material behaviour. Therefore, in this chapter the basic concepts of CDM and constitutive modelling are reviewed, along with the Lemaitre model for isotropic damage, in both local and non-local formulations. Rather than presenting an intensive research on CDM models, this chapter intends to provide the basis theory for the broader model for ductile fracture built throughout this thesis. Among the existing literature on the subject, interested readers may consult the books [62–64].

This chapter is organized as follows. In the first section the basic kinematics of deformable bodies is introduced, followed by the main strain and stress measures. Next the balance equations and the principles of thermodynamics are presented. In section 2.3 the constitutive theory is derived, in particular the Lemaitre model for ductile damage, making use of the previously introduced concepts. This chapter finalizes with the re-formulation of the Lemaitre model following a non-local integral approach and some brief conclusions.

## 2.1 Kinematics

Kinematics provides the basic tools for motion and deformation description. In this section the fundamental quantities employed in the constitutive description of ductile metals are defined.

### Motion

Let  $\mathbf{B}$  be a deformable body occupying the domain  $\Omega \subset \mathcal{R}^3$ , with the positions of its particles defined by  $\mathbf{X}$ , referred as the *reference* configuration. The body may undergo a *motion* or *deformation*, within a certain time, corresponding to the transformation  $\mathcal{X} : \mathbf{B} \rightarrow \mathcal{R}^3$

$$\mathbf{x} = \mathcal{X}(\mathbf{X}, t) \quad (2.1)$$

where  $\mathbf{x}$  is the position at the *current* configuration, at time  $t$ .

Assuming that the motion  $\mathcal{X}$  is invertible, the position  $\mathbf{X}$  at a time  $t$  may be recovered as:

$$\mathbf{X} = \mathcal{X}^{-1}(\mathbf{x}, t) \quad (2.2)$$

and the *displacement* field may be introduced as

$$\mathbf{u}(\mathbf{X}, t) = \mathcal{X}(\mathbf{X}, t) - \mathbf{X} \quad (2.3)$$

The time derivative of the function  $\mathcal{X}(\mathbf{X}, t)$ , defined as

$$\mathbf{V}(\mathbf{X}, t) = \frac{\partial \mathcal{X}(\mathbf{X}, t)}{\partial t} \quad (2.4)$$

is the velocity of a particle at the position  $\mathbf{X}$ , and consequently, the velocity of a particle at the current configuration may be determined by applying equation 2.2:

$$\mathbf{v}(\mathbf{x}, t) = \mathbf{V}(\mathcal{X}^{-1}(\mathbf{x}, t), t) \quad (2.5)$$

## Deformation gradient

The derivative of the deformation,  $\mathbf{F}$ , is a second order tensor termed *deformation gradient*, relating  $\mathbf{X}$  and  $\mathbf{x}$  as follows:

$$\mathbf{F}(\mathbf{X}, t) = \frac{\partial \mathcal{X}(\mathbf{X}, t)}{\partial \mathbf{X}} = \frac{\partial \mathbf{x}}{\partial \mathbf{X}} = \nabla_{\mathbf{X}} \mathcal{X}(\mathbf{X}, t) \quad (2.6)$$

where  $\nabla_{\mathbf{X}}$  is usually termed *material gradient operator*. Alternatively, the deformation gradient may also be defined in the current configuration, making use of the *spatial gradient operator*,  $\nabla_{\mathbf{x}}$  as

$$\mathbf{F}(\mathbf{x}, t) = [\nabla_{\mathbf{x}} \mathcal{X}^{-1}(\mathbf{x}, t)]^{-1} \quad (2.7)$$

The displacement field may also be employed in the definition of the deformation gradient, leading to

$$\mathbf{F} = \mathbf{I} + \nabla_{\mathbf{X}} \mathbf{u} \quad (2.8)$$

where  $\mathbf{I}$  is the second order identity tensor.

From the definitions presented so far, it can be shown that line, surface and volume changes respectively transform according to:

$$\begin{aligned} d\mathbf{x} &= \mathbf{F} d\mathbf{X} \\ d\mathbf{a} &= J \mathbf{F}^{-T} d\mathbf{A} \\ dv &= J dV \end{aligned} \quad (2.9)$$

In the above equations,  $J$ , termed *Jacobian* of the deformation, is the determinant of the deformation gradient

$$J = \det \mathbf{F} \quad (2.10)$$

It follows that a volume-preserving or *isochoric* deformation is characterized by:

$$J = 1 \quad (2.11)$$

Moreover, any deformation can be locally decomposed into an isochoric deformation,  $\mathbf{F}_{vol}$  and a volumetric deformation,  $\mathbf{F}_{iso}$ , [65–67] as

$$\mathbf{F} = \mathbf{F}_{iso} \mathbf{F}_{vol} \quad (2.12)$$

where

$$\mathbf{F}_{iso} = (\det \mathbf{F})^{-\frac{1}{3}} \mathbf{F} = J^{-\frac{1}{3}} \mathbf{F} \quad (2.13)$$

$$\mathbf{F}_{vol} = (\det \mathbf{F})^{\frac{1}{3}} \mathbf{I} = J^{\frac{1}{3}} \mathbf{I} \quad (2.14)$$

and  $\mathbf{I}$  is the second order identity tensor.

Alternatively, a motion may be split in pure stretches and pure rotations, making use of the *polar decomposition*, that is,

$$\mathbf{F} = \mathbf{R} \mathbf{U} = \mathbf{V} \mathbf{R} \quad (2.15)$$

where  $\mathbf{U}$  and  $\mathbf{V}$  are unique, positive definite, symmetric tensors, termed, respectively *right* and *left stretch tensors*.  $\mathbf{R}$  is an unique proper orthogonal tensor, called *rotation* tensor. The tensors  $\mathbf{U}$  and  $\mathbf{V}$  may also be introduced as:

$$\mathbf{C} = \mathbf{U}^2 = \mathbf{F}^T \mathbf{F}, \quad \mathbf{b} = \mathbf{V}^2 = \mathbf{F} \mathbf{F}^T \quad (2.16)$$

where  $\mathbf{C}$  and  $\mathbf{b}$  are, respectively, the *right* and *left Cauchy-Green* strain tensors.

## Strain measures

The deformation gradient is the fundamental kinematic quantity characterizing the changes of each material point during motion. Nevertheless, to quantify the relative distance change between two material points, that is, to characterize the *straining*, proper strain measures have to be defined.

As the strains are not measurable quantities (such as the displacements) but a conceptual quantity to simplify analysis, there are numerous choices of strain tensors. An important

family of strain measures are the *Lagrangian* strain tensors:

$$\mathbf{E}^{(m)} = \begin{cases} \frac{1}{m}(\mathbf{U}^m - \mathbf{I}), & m \neq 0 \\ \ln \mathbf{U}, & m = 0 \end{cases} \quad (2.17)$$

Similarly, another family of strain tensors, called the Eulerian strain tensors, may be obtained using the left stretch tensor:

$$\mathbf{e}^{(m)} = \begin{cases} \frac{1}{m}(\mathbf{V}^m - \mathbf{I}), & m \neq 0 \\ \ln \mathbf{V}, & m = 0 \end{cases} \quad (2.18)$$

### Velocity gradient and strain rates

The velocity gradient,  $\mathbf{l}$ , is the spatial field defined as

$$\mathbf{l} = \nabla_x \mathbf{v}. \quad (2.19)$$

Alternatively,  $\mathbf{l}$  may be expressed as a function of the deformation gradient as

$$\mathbf{l} = \frac{\partial}{\partial t} \left( \frac{\partial \mathcal{X}}{\partial \mathbf{X}} \frac{\partial \mathbf{X}}{\partial \mathbf{x}} \right) = \dot{\mathbf{F}} \mathbf{F}^{-1} \quad (2.20)$$

The velocity gradient may also be split into a symmetric and skew part, originating two important tensors as follows:

$$\mathbf{d} = \frac{1}{2}(\mathbf{l} + \mathbf{l}^T) \quad (2.21)$$

$$\mathbf{w} = \frac{1}{2}(\mathbf{l} - \mathbf{l}^T) \quad (2.22)$$

The tensor  $\mathbf{d}$  is called the *rate of deformation* and is associated with the straining, while the tensor  $\mathbf{l}$  is termed *spin* tensor and is associated with rigid body velocity.

### Stress measures

In line with the previous sections, for each type of strain measure, it is possible to define a stress measure. One of the most important stress tensors is the *Cauchy* or *true stress* tensor,  $\boldsymbol{\sigma}$ , as:

$$\mathbf{t} = \boldsymbol{\sigma} \mathbf{n} \quad (2.23)$$

where  $\mathbf{t}$  is the surface traction and  $\mathbf{n}$  is the associated outward normal vector.

The Cauchy stress tensor may be split in a *deviatoric*,  $\mathbf{s}$ , and a *pressure*,  $p$ , contributions,

as follows

$$\boldsymbol{\sigma} = \mathbf{s} + p\mathbf{I} \quad (2.24)$$

where

$$p = \frac{1}{3}\text{tr}[\boldsymbol{\sigma}] \quad (2.25)$$

Another stress measure frequently used is the *Kirchhoff* stress tensor, given by

$$\boldsymbol{\tau} = J\boldsymbol{\sigma} \quad (2.26)$$

Other convenient stress tensors are the First and the Second Piola-Kirchhoff tensors, respectively introduced as

$$\mathbf{P} = \boldsymbol{\tau}\mathbf{F}^{-T} \quad (2.27)$$

and

$$\mathbf{S} = \mathbf{F}^{-1}\boldsymbol{\tau}\mathbf{F}^{-T} \quad (2.28)$$

## 2.2 Conservation principles

In the previous sections, the quantities used in the mathematical description of motion, straining and stress were introduced. In this section, these concepts are related in some fundamental conservation principles, which are essential to formulate a continuum mechanics problem. The detailed derivation of these principles is out of the scope of this thesis and may be found, for instance, in the references [62–64, 68].

### Conservation of mass

The first principle regards the mass conservation and may be expressed as

$$\dot{\rho} + \rho \text{div}_x \dot{\mathbf{u}} = 0 \quad (2.29)$$

where  $\rho$  is the mass density at the deformed configuration.

## Momentum balance

The momentum balance equation describes the equilibrium between internal and external forces in a body, as follows

$$\operatorname{div}_x \boldsymbol{\sigma} + \mathbf{b} = \rho \ddot{\mathbf{u}} \quad (2.30)$$

where  $\mathbf{b}$  denotes the body force vector at the deformed configuration. These equation is frequently referred as *strong form* of the equilibrium equation and has to fulfil the following boundary condition:

$$\bar{\mathbf{t}} = \boldsymbol{\sigma} \mathbf{n} \quad (2.31)$$

where  $\bar{\mathbf{t}}$  is a traction vector applied to the boundary of the body.

## First and second laws of thermodynamics

The first law of thermodynamics postulates that the energy must be conserved and may be mathematically expressed as:

$$\rho \dot{e} = \boldsymbol{\sigma} : \mathbf{d} + \rho r - \operatorname{div}_x \mathbf{q} \quad (2.32)$$

where  $e$  represents the specific internal energy,  $r$  represents the density of heat production and  $\mathbf{q}$  the heat flux. Throughout this thesis, only purely mechanical processes will be addressed, thus equation 2.32 reduces to

$$\rho \dot{e} = \boldsymbol{\sigma} : \mathbf{d} \quad (2.33)$$

This equation may be rewritten in terms of the Kirchhoff stress tensor, as follows

$$\bar{\rho} \dot{e} = \boldsymbol{\tau} : \mathbf{d} \quad (2.34)$$

where  $\bar{\rho} = J\rho$  is the reference mass density.

Second law of thermodynamics refers to the irreversibility of the entropy production, which may be expressed as

$$\rho T \dot{s} + \operatorname{div}_x \mathbf{q} - \rho r \geq 0 \quad (2.35)$$

where  $s$  represents the entropy and  $T$  the temperature. Similarly to the first law, for isothermal processes equation 2.35 reduces to

$$\rho T \dot{s} \geq 0 \quad (2.36)$$

Combining the first and the second laws and introducing the Helmholtz free energy concept,  $\psi$ , defined as

$$\psi = e - Ts \quad (2.37)$$

the so-called Clausius-Duhem inequality is obtained

$$\boldsymbol{\tau} : \mathbf{d} - \bar{\rho} \dot{\psi} \geq 0 \quad (2.38)$$

## 2.3 Finite strain damage mechanics

The laws presented are valid independently of the material considered. Therefore, to fully characterise the response of a solid body and distinguish between different materials, a constitutive model has to be formulated and boundary conditions have to be prescribed.

In this thesis, the chosen constitutive model, the Lemaitre model for ductile damage [25–27, 29], relies in the thermodynamics with internal variables, which means that at any instant, the thermodynamic state at any point is completely defined by the values of a given set of state variables. In order to successfully capture all the stages of material behaviour, the choice of the set of internal variables is crucial. In the particular case of ductile materials, the material degradation, that is damage occurs simultaneously with plastic deformations, and therefore, the internal energy function should reflect this dependency, as it will be shown throughout this section.

### 2.3.1 The damage variable

Failure in ductile metals initiates with the nucleation cavities and micro-cracks, which may grow and coalesce, eventually leading to macro-crack generation and propagation [27, 69]. The quantification of the micro-defects at the meso-scale level, may be taken in account in a averaging sense, defining the damage variable,  $D_{\hat{n}}$ , as:

$$D_{\hat{n}} = \frac{\partial S_D}{\partial S} \quad (2.39)$$

where  $\partial S$  is the area of intersection of a plane, with normal  $\hat{n}$ , with the representative volume element (RVE) and  $\partial S_D$  is the area that effectively intersects cavities or micro-cracks, as can be observed in figure 2.1. The RVE of a certain material is defined in such a way that all the properties are represented by homogenized variables (around  $0.1\text{mm}^3$

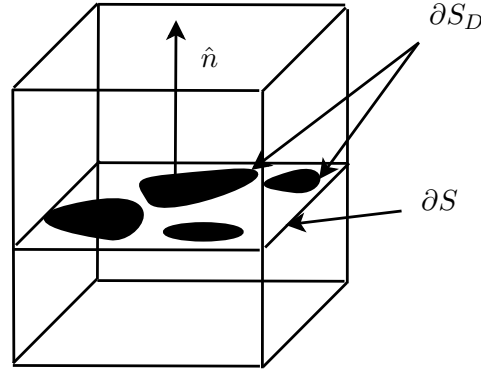


FIGURE 2.1: Representative volume element.

for metals [27]).

When only ductile damage is considered, the micro-defects density is often a weak function of the plane orientation. Therefore,  $D$  may be considered isotropic and represented by a scalar variable, ranging from 0 to 1, corresponding to undamaged to fully damage material, respectively, which is the case of this thesis. Nevertheless, a second or fourth order tensor representation may be adopted for other applications [27, 70].

### 2.3.2 Effective stress concept and strain equivalence principle

In the previous sections some strain and stress measures were introduced to be used in the constitutive equations that characterize a given material. These quantities were developed for plain material, however, in the presence of damage the resistant area is smaller and an the effective Cauchy stress tensor may be introduced as:

$$\bar{\sigma} = \frac{\sigma}{1 - D} \quad (2.40)$$

where  $\sigma$  is the Cauchy stress tensor for undamaged material. From this definition it follows the *strain equivalence principle*, which states that a damaged material is governed by the constitutive laws of the plain material, replacing the true stress by the effective stress [27].

### 2.3.3 Multiplicative plasticity framework

In ductile materials damage and plasticity are strongly connected, therefore the concepts associated with finite strain elasto-plasticity are now introduced.

The main assumption underlying the finite strain elasto-plasticity framework is the *multiplicative decomposition* of the deformation gradient [66, 71], as follows:

$$\mathbf{F} = \mathbf{F}^e \mathbf{F}^p \quad (2.41)$$

where  $\mathbf{F}^e$  and  $\mathbf{F}^p$  represent, respectively, the elastic and plastic deformation gradients. Consequently, this theory assumes the existence of a local, stress free, intermediate configuration, defined by  $\mathbf{F}^p$  alone.

This definition may be extended to other kinematic quantities, namely the right and left Cauchy-Green strain tensors, as:

$$\mathbf{C}^e = (\mathbf{F}^p)^{-1} \mathbf{C} (\mathbf{F}^p)^{-T} \quad (2.42)$$

$$\mathbf{b}^e = \mathbf{F} (\mathbf{C}^p)^{-1} \mathbf{F}^T \quad (2.43)$$

where  $(\bullet)^e$  and  $(\bullet)^p$  denote, respectively, the elastic and plastic contributions of each tensor. Analogously, the velocity gradient may be decomposed as:

$$\mathbf{l} = \mathbf{l}^e + \mathbf{F}^e \mathbf{l}^p (\mathbf{F}^e)^{-1} \quad (2.44)$$

### 2.3.4 State potential

The deformation process of a given body, within the thermodynamic framework, may be described by a sequence of constrained equilibrium states. Therefore, after introducing the background concepts, all the conditions are set to determine the thermodynamic state of a given point, at any time  $t$ , which, considering an isothermal process, is defined by the following set of variables:

$$\{\mathbf{C}, \mathbf{C}^p, R, D\} \quad (2.45)$$

where  $R$  is the isotropic hardening variable. The *Helmholtz free energy*,  $\psi$ , is considered to have the form:

$$\psi = \psi(\mathbf{C}, \mathbf{C}^p, R, D) \quad (2.46)$$

Nonetheless, if the tensor  $\mathbf{C}^p$  is known in a particular point, the tensor  $\mathbf{b}^e$  may be calculated through equation 2.43, and therefore, the set of internal variables may be reduced to:

$$\psi = \psi(\mathbf{b}^e, R, D) \quad (2.47)$$

From the free energy it is possible to derive the associated variables as follows:

$$\boldsymbol{\tau} = \rho 2\mathbf{b}^e \frac{\partial \psi}{\partial \mathbf{b}^e} \quad (2.48)$$

$$X = \rho \frac{\partial \psi}{\partial R} \quad (2.49)$$

$$Y = -\rho \frac{\partial \psi}{\partial D} \quad (2.50)$$

recalling that  $\boldsymbol{\tau}$  represents the Kirchhoff stress tensor,  $X$  are the thermodynamic forces conjugated with isotropic hardening,  $Y$  is the damage energy release rate and  $\rho$  is the mass density.

The analytical expression for  $\psi$  should reflect experimental observations, in which there is state coupling between damage and elastic strain but not between plasticity and elasticity nor between damage and plasticity. In addition, the strain equivalence principle should be recovered when equation 2.48 is applied, motivating the following decomposition of the state potential in elastic,  $\psi^e$ , and plastic,  $\psi^p$  contributions:

$$\psi = (1 - D)\psi^e(\mathbf{b}^e) + \psi^p(R) \quad (2.51)$$

### 2.3.5 Dissipative potentials and constitutive equations

To complete the description of a ductile damage process and derive the evolution equations, a complementary energy dissipation potential,  $\phi$ , has to be defined. From the micro-mechanical point of view, the damage dissipative process is associated to the irreversible rupture of atomic bonds, while plastic dissipation is a consequence of the movement and accumulation of dislocations, which cause irreversible deformations. Therefore, the effects of both mechanisms may be considered in a decoupled way, defining  $\phi$  as:

$$\phi = \phi^p + \phi^d \quad (2.52)$$

where  $\phi^p$  and  $\phi^d$  are the energy potentials associated with plasticity and damage, respectively. In order to determine the evolution equations of the constitutive models, these potentials have to be specified. For the plastic part, assuming the strain equivalence principle, the von Mises yield function may be adopted:

$$\phi^p = \frac{1}{1 - D} \sqrt{\frac{3}{2} \boldsymbol{\tau} : \boldsymbol{\tau}} - \tau_y(R) \quad (2.53)$$

where  $\tau_y$  is the uni-axial yield stress. For the damage dissipation potential, the following function based in the work of Lemaitre [27] will be employed:

$$\phi^d = \frac{r}{(s+1)(1-D)} \left[ \frac{-Y}{r} \right]^{s+1} \quad (2.54)$$

where  $r$  and  $s$  are scalar material parameters associated with damage evolution. Finally, making use of the normality rule it is possible to determine the evolution equations:

$$\mathcal{L}_v \mathbf{b}^e = -2\dot{\gamma} \frac{\partial \phi}{\partial \boldsymbol{\tau}} \mathbf{b}^e \quad (2.55)$$

$$\dot{D} = \dot{\gamma} \frac{\partial \phi}{\partial (-Y)} = \dot{\gamma} \frac{1}{1-D} \left( \frac{-Y}{r} \right)^s \quad (2.56)$$

$$\dot{R} = -\dot{\gamma} \frac{\partial \phi}{\partial X} = \dot{\gamma} \quad (2.57)$$

where  $\mathcal{L}_v$  represents the spatial velocity Lie derivative and  $\gamma$  is the plastic multiplier. The model is concluded with the Kuhn-Tucker conditions

$$\dot{\gamma}(\mathbf{x}) \geq 0; \quad \mathbf{F}^p \leq 0; \quad \dot{\gamma}(\mathbf{x}) \mathbf{F}^p = 0 \quad \forall \mathbf{x} \in V \quad (2.58)$$

which must hold globally in the domain,  $V$ .

## 2.4 Non-local integral model

The results obtained throughout this thesis required the implementation of the presented constitutive model in a Finite Element Method (FEM) code. However, when implemented in its purely local version, this formulation suffers from a pathological mesh dependence [72]. This behaviour, which is typical when softening is introduced at the constitutive level and that somehow may be related to material size effects, can be attenuated by the use of a non-local formulation that introduces an internal length parameter in the formulation, which acts as a localisation limiter for plasticity and damage [73, 74].

Non-local models can be divided into gradient-type [33, 75, 76] or integral-type formulations [77]. The first category is usually implemented in its implicit form, where the non-local variable is considered to be an additional degree of freedom of the structural problem, which has the advantage of keeping the local-like format of the problem, but requires additional FEM discretization. In other hand, the integral formulation keeps the non-locality entirely at the material level, requiring, however, a deeper change in the

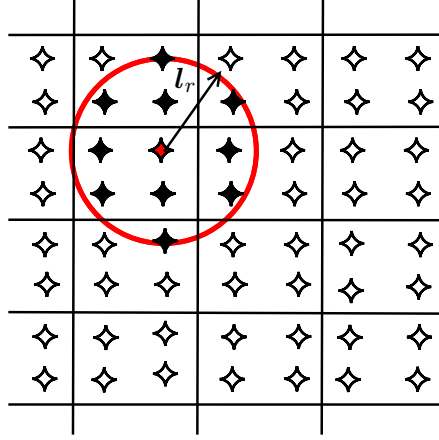


FIGURE 2.2: Definition of the non-local averaging volume.

local integration algorithms.

Having in view the combination of the constitutive model with XFEM, which introduces additional nodal variables and requires modified element kinematics, it is desirable to keep the non-locality at the material level. In a set of previous works [78, 79], an energetically consistent non-local integral approach has been developed for Lemaitre model, which will be summarized in the following paragraphs.

#### 2.4.1 Non-local damage variable

Failure in ductile metals is closely related to the localisation of damage. Therefore, damage is regarded as the optimal choice of variable to be enhanced by non-locality, that is, the damage variable of a certain point is averaged within a finite volume  $V$ , with radius  $l_r$ , as illustrated in figure 2.2. The radius  $l_r$  is often termed regularisation or characteristic length, as it acts as a localisation limiter.

Then, non-local damage,  $\bar{D}$ , may be defined in function of local damage,  $D$ , as follows:

$$\bar{D}(\mathbf{x}) = \int_V \beta(\mathbf{x}, \boldsymbol{\xi}) D(\boldsymbol{\xi}) dV(\boldsymbol{\xi}) \quad (2.59)$$

where  $\beta(\mathbf{x}, \boldsymbol{\xi})$  is an averaging operator defined as:

$$\beta(\mathbf{x}, \boldsymbol{\xi}) = \frac{\alpha(\mathbf{x}, \boldsymbol{\xi})}{\Omega(\mathbf{x})} \quad (2.60)$$

in which,  $\alpha(\mathbf{x}, \boldsymbol{\xi})$  is the following weighting function

$$\alpha(\mathbf{x}, \boldsymbol{\xi}) = \left(1 - \frac{\|\mathbf{x} - \boldsymbol{\xi}\|^2}{l_r^2}\right)^2 \quad (2.61)$$

and  $\Omega$  is usually designated as *representative* volume that may be defined as

$$\Omega(\mathbf{x}) = \int_V \alpha(\mathbf{x}, \boldsymbol{\xi}) dV(\mathbf{x}) \quad (2.62)$$

In these equations,  $\bar{D}(\mathbf{x})$  represents the damage measurement at a material generic point denoted by  $\mathbf{x}$ , which has been averaged over the defined finite volume  $V$ , containing the set of points  $\boldsymbol{\xi}$ .

*Remark 2.1.* The direct experimental measurement of  $l_r$  is not possible and thus it is usually obtained through inverse analysis [77, 79]. As the presented non-local formulation has proven to be able to alleviate pathological mesh dependence,  $l_r$  may be regarded as a numerical parameter.

### 2.4.2 Non-local constitutive model

The averaging operator defined in the previous section,  $\beta(\mathbf{x}, \boldsymbol{\xi})$ , is assumed to be independent of the deformation history. Therefore, the damage evolution  $\dot{\bar{D}}(\mathbf{x})$  can be readily determined:

$$\dot{\bar{D}}(\mathbf{x}) = \int_V \beta(\mathbf{x}, \boldsymbol{\xi}) \dot{D}(\boldsymbol{\xi}) dV(\boldsymbol{\xi}) \quad (2.63)$$

and, consequently:

$$\dot{\bar{D}}(\mathbf{x}) = \int_V \beta(\mathbf{x}, \boldsymbol{\xi}) \dot{\gamma} \frac{1}{1 - D(\boldsymbol{\xi})} \left(\frac{-Y}{r}\right)^s dV(\boldsymbol{\xi}) \quad (2.64)$$

In addition, as damage was chosen to be the only variable enhanced by non-locality, the local constitutive model presented can be directly extended to the non-local case, replacing the local damage variable by its non-local counterpart. In particular, the yield function reads:

$$\phi^p = \frac{1}{1 - \bar{D}} \sqrt{\frac{3}{2} \boldsymbol{\tau}(\boldsymbol{\xi}) : \boldsymbol{\tau}(\boldsymbol{\xi})} - \tau_y(R) \quad (2.65)$$

followed by the evolution equations

$$\mathcal{L}_v \mathbf{b}^e(\boldsymbol{\xi}) = -2\dot{\gamma}(\boldsymbol{\xi}) \frac{\partial \phi}{\partial \boldsymbol{\tau}(\boldsymbol{\xi})} \mathbf{b}^e(\boldsymbol{\xi}) \quad (2.66)$$

$$\dot{\bar{D}}(\mathbf{x}) = \int_V \beta(\mathbf{x}, \boldsymbol{\xi}) \dot{\gamma} \frac{1}{1 - D(\boldsymbol{\xi})} \left(\frac{-Y}{r}\right)^s dV(\boldsymbol{\xi}) \quad (2.67)$$

$$\dot{R}(\boldsymbol{\xi}) = \dot{\gamma}(\boldsymbol{\xi}) \quad (2.68)$$

The detailed thermodynamical derivation of the non-local integral constitutive model may be found in [79].

## 2.5 Conclusions

This chapter was devoted to the review of general concepts of continuum damage mechanics. Special attention was paid to the Lemaitre model, in its local and non-local formulations, which is well-established and widely used to model ductile materials, prior to macro-crack initiation. This model constitutes the reference theory which will be used throughout this thesis.



## Chapter 3

# Finite Element Distretization and Automatic Code Generation

The description of ductile materials following the damage model described in chapter 2 results in a complex system of differential equations. As only a very restricted set of analytical solutions are available, the use of numerical methods becomes imperative. In particular, the Finite Element Method (FEM) stands out as the most widely used numerical method for solving solid mechanics problems for its effective predictive capabilities.

The basis of the FEM are well established in the literature as, for instance, in the reference works of Zienkiewicz [36], Hinton and Owen [80], Hughes [81] or Crisfield [82]. Hence the method will be briefly reviewed in the first part of this chapter, which initiates by re-formulating the balance laws presented in chapter 2 in order to define a Initial Boundary Value Problem, suitable to be solved with the FEM. Next, the displacement-based discretisation is introduced, along with the non-linear incremental finite element equation.

The second part of this chapter will focus on the automatic generation of FEM codes. The computer science advances, in both software and hardware, had a significant impact in generalizing the use of the FEM, allowing the simulation of problems with higher number of variables, described by increasingly complex mathematical models . Moreover, the combination of modern Computer Algebra Systems with an automatic derivation technique, allows a faster and more efficient implementation of FEM formulations. In this chapter, special attention is paid to one of these systems, the *AceGen* system, which was used to develop a considerable amount of computer codes used in the context of

this thesis.

### 3.1 The quasi-static IBVP

In Chapter 2 the fundamental equilibrium laws were presented. However, to solve a problem using the FEM, these laws are often formulated as variational principles. Although this methodology is not mandatory, approximate solutions are often obtained through the weak forms of field equations.

Therefore, recalling the momentum balance equation:

$$\operatorname{div}_x \boldsymbol{\sigma} + \mathbf{b} = \rho \ddot{\mathbf{u}} \quad (3.1)$$

and considering the quasi-static case, as throughout this thesis the inertial effects will be neglected, we may write:

$$\operatorname{div}_x \boldsymbol{\sigma} = \mathbf{0} \quad (3.2)$$

Equation 3.2 may be multiplied by a virtual displacement,  $\boldsymbol{\eta}$ , and integrated over the domain, as:

$$\int_{\mathcal{X}(\Omega)} (\operatorname{div}_x \boldsymbol{\sigma})^T \boldsymbol{\eta} dv = 0 \quad (3.3)$$

After some algebra manipulation and making use of the divergence theorem, equation 3.3 may be written in the following form:

$$\int_{\mathcal{X}(\Omega)} \boldsymbol{\sigma} : \nabla_x \boldsymbol{\eta} dv - \int_{\mathcal{X}(\partial\Omega)} (\boldsymbol{\sigma} \cdot \mathbf{n})^T \boldsymbol{\eta} da = 0 \quad (3.4)$$

As introduced in chapter 3, the following boundary condition has to be fulfilled together with equation 3.1

$$\bar{\mathbf{t}} = \boldsymbol{\sigma} \mathbf{n} \quad (3.5)$$

where  $\bar{\mathbf{t}}$  is a prescribed traction at the boundary of the body. Therefore, replacing this relation in equation 3.4, the *weak form* of the equilibrium equation of obtained:

$$\int_{\mathcal{X}(\Omega)} \boldsymbol{\sigma} : \nabla_x \boldsymbol{\eta} dv - \int_{\mathcal{X}(\partial\Omega)} \bar{\mathbf{t}} \cdot \boldsymbol{\eta} da = 0 \quad (3.6)$$

The weak form of the equilibrium equation is equivalent to the strong form and allows the definition of the weak form of the Initial Boundary Value Problem (IBVP) associated with a certain deformation process, as follows.

*Find a kinematically admissible displacement function,  $\mathbf{u} \in \mathcal{K}$  such that the equation*

$$\int_{\mathcal{X}(\Omega)} \boldsymbol{\sigma} : \nabla_x \boldsymbol{\eta} dv - \int_{\mathcal{X}(\partial\Omega)} \bar{\mathbf{t}} \cdot \boldsymbol{\eta} da = 0 \quad (3.7)$$

is satisfied for all  $t \in [t_0, t_n]$  and for all  $\boldsymbol{\eta} \in \mathcal{V}_t$ . The set of virtual displacements and the set of kinematically admissible displacements, at time  $t$  are respectively defined as

$$\mathcal{V}_t = \{\boldsymbol{\eta} : \Omega \longrightarrow \mathcal{X}(\Omega) | \boldsymbol{\eta} = \mathbf{0} \in \partial\Omega(t)\} \quad (3.8)$$

$$\mathcal{K} = \{\mathbf{u} : \Omega \longrightarrow \mathcal{X}(\Omega) | \bar{\mathbf{u}}(\mathbf{X}, t), t \in [t_0, t_n], \mathbf{X} \in \partial\Omega\} \quad (3.9)$$

The Cauchy stress, at each point of the body is expressed as

$$\boldsymbol{\sigma}(t) = \boldsymbol{\sigma}(\mathbf{F}(t), \boldsymbol{\alpha}(t)) \quad (3.10)$$

where  $\boldsymbol{\alpha}$  represents the set of internal variables associated with the material and  $\mathbf{F}$  is a given prescribed deformation gradient history, defined as

$$\mathbf{F}(t) = \mathbf{I} + \nabla_X \mathbf{u}(\mathbf{X}, t) \quad (3.11)$$

The solution of the IBVP reflects how a solid body will behave when subjected to certain boundary conditions.

## Material description

Equation 3.6 reflects the spatial version of the *Principle of Virtual Work*, nevertheless, depending on the particular problem, the material version may provide a more efficient implementation. The first member of equation 3.6 is termed *internal work*,  $W_{int}$ , and may be written in the reference configuration, recalling the definition of the first Piola-Kirchhoff stress tensor:

$$\mathbf{P} = J \boldsymbol{\sigma} \mathbf{F}^{-T} \quad (3.12)$$

resulting in

$$W_{int} = \int_{\Omega} \mathbf{P} : \nabla_X \boldsymbol{\eta} dV \quad (3.13)$$

The first Piola-Kirchhoff tensor is not completely related to the material configuration but it may be replaced by the second Piola-Kirchhoff strain tensor as:

$$\mathbf{P} : \nabla_X \boldsymbol{\eta} = \mathbf{S} : \mathbf{F}^T \nabla_X \boldsymbol{\eta} = \mathbf{S} : (\mathbf{F}^T \nabla_X \boldsymbol{\eta} + \nabla_X \boldsymbol{\eta}^T \mathbf{F}) = \mathbf{S} : \partial \mathbf{E} \quad (3.14)$$

$$W_{int} = \int_{\Omega} \mathbf{S} : \partial \mathbf{E} dV \quad (3.15)$$

where  $\partial \mathbf{E}$  is the first variation of the Green-Lagrange strain tensor. The second member of equation 3.6, the *external work*,  $W_{ext}$  may be written in the material description simply by taking the applied traction in the initial configuration,  $\bar{\mathbf{t}}_0$

$$W_{ext} = \int_{\mathcal{X}(\partial\Omega)} \bar{\mathbf{t}} \cdot \boldsymbol{\eta} \, da = \int_{\partial\Omega} \bar{\mathbf{t}}_0 \cdot \boldsymbol{\eta} \, dA \quad (3.16)$$

Either in the material or spatial version, the IBVP is usually non-linear and therefore linearisation and discretisation are necessary to produce accurate solutions using the FEM, as described in the upcoming sections.

## 3.2 Displacement-based finite elements

The FEM for the numerical solution of the IBVP problem described in the previous section consists in replacing the sets  $\mathcal{V}_t$  and  $\mathcal{K}$ , defined in equations 3.8 and 3.9, respectively, by discrete subsets,  $\mathcal{V}_t^h$  and  $\mathcal{K}^h$  obtained from a finite discretization of the domain. In the case of displacement-based finite elements, the interpolated field variables are the displacements, which within a given element,  $e$ , assume the form:

$$\mathbf{u}(\mathbf{x}) = \sum_{i=1}^{nnode} N_i^{(e)}(\mathbf{x}) \mathbf{u}_i \quad (3.17)$$

where  $N_i^{(e)}$  is the *shape* or *interpolation* function associated with node  $i$  and  $nnode$  is the number of nodes of the element. Similarly, the interpolation function may be defined over the entire approximate domain, which is constituted by a total number of  $npoin$  nodal points, as

$$\mathbf{u}(\mathbf{x}) = \sum_{i=1}^{npoin} N_i^g(\mathbf{x}) \mathbf{u}_i \quad (3.18)$$

In equation 3.18,  $\mathbf{u}$  represents the global vector of nodal displacements, which, in a problem of dimension  $ndim$ , is given by

$$\mathbf{u}^h = [u_1^1, \dots, u_{ndim}^1, \dots, u_1^{npoin}, \dots, u_{ndim}^{npoin}] \quad (3.19)$$

and  $\mathbf{N}^g$  is the *global interpolation matrix* defined as:

$$\mathbf{N}_i^g = [ \text{diag}[N_1^g(\mathbf{x})] \quad \text{diag}[N_2^g(\mathbf{x})] \quad \cdots \quad \text{diag}[N_{npoin}^g(\mathbf{x})] ] \quad (3.20)$$

where  $\text{diag}[\mathbf{N}_1^g]$  represents a  $n_{dim} \times n_{dim}$  diagonal matrix as follows

$$\text{diag}[\mathbf{N}_1^g] = \begin{bmatrix} N_i^g & 0 & \cdots & 0 \\ 0 & N_i^g & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & N_i^g \end{bmatrix} \quad (3.21)$$

Equation 3.18 may be reformulated as:

$$\mathbf{u}^h(\mathbf{x}) = \mathbf{N}^g \mathbf{u} \quad (3.22)$$

Similarly, the field of virtual displacements may be written as:

$$\boldsymbol{\eta}^h(\mathbf{x}) = \mathbf{N}^g \boldsymbol{\eta} \quad (3.23)$$

Using the presented notation the discretized sets  $\mathcal{V}_t^h$  and  $\mathcal{K}^h$  may be defined as:

$$\mathcal{V}_t^h = \{ \boldsymbol{\eta}^h(\mathbf{x}) = \sum_{i=1}^{npoin} N_i^g \boldsymbol{\eta}_i \mid \boldsymbol{\eta}_i = \mathbf{0} \text{ if } \mathbf{x}_i \in \partial\Omega \} \quad (3.24)$$

$$\mathcal{K}^h = \{ \mathbf{u}^h(\mathbf{x}) = \sum_{i=1}^{npoin} N_i^g \mathbf{u}_i \mid \mathbf{u}_i = \bar{\mathbf{u}}(\mathbf{x}_i) \text{ if } \mathbf{x}_i \in \partial\Omega \} \quad (3.25)$$

Now, equation 3.6 may be replaced by its discretized version, as follows

$$\int_{\mathcal{X}(\Omega^h)} \boldsymbol{\sigma} : \nabla_x(\mathbf{N}^g \boldsymbol{\eta}^h) dv - \int_{\mathcal{X}(\partial\Omega^h)} \bar{\mathbf{t}} \cdot (\mathbf{N}^g \boldsymbol{\eta}^h) da = 0 \quad (3.26)$$

In classical FEM implementations it is usual to define the *global discrete symmetric gradient matrix*,  $\mathbf{B}$ , which for a plain strain problem has the form:

$$\mathbf{B}^g = \begin{bmatrix} N_{1,1}^g & 0N_{2,1}^g & 0 & \cdots & N_{npoin,1}^g & 0 & 0 \\ 0 & N_{1,2}^g & 0 & N_{2,2}^g & \cdots & 0 & N_{npoin,2}^g \\ N_{1,2}^g & N_{1,1}^g & N_{2,2}^g & N_{2,1}^g & \cdots & N_{npoin,2}^g & N_{npoin,1}^g \end{bmatrix} \quad (3.27)$$

where the following notation was employed

$$(\cdot)_{i,j} = \frac{\partial(\cdot)_i}{\partial x_j} \quad (3.28)$$

Finally, the discretized virtual work expression can be rearranged to

$$\int_{\mathcal{X}(\Omega^h)} [\boldsymbol{\sigma}^T \mathbf{B}^g \boldsymbol{\eta}^h - \mathbf{b} \cdot \mathbf{N}^g \boldsymbol{\eta}^h] dv - \int_{\mathcal{X}(\partial\Omega^h)} \bar{\mathbf{t}} \cdot \mathbf{N}^g \boldsymbol{\eta}^h da = 0, \forall \boldsymbol{\eta}^h \in \mathcal{V}_t^h \quad (3.29)$$

For completeness, when using the material version of the virtual work equation, the discretised form of the variation of the Green-Lagrange strain tensor is provided herein:

$$\partial \mathbf{E} = \frac{1}{2} \sum_{i=1}^{npoin} [\mathbf{F}^T (\boldsymbol{\eta}_i^h \otimes \nabla_X N_i) + (\nabla_X N_i \otimes \boldsymbol{\eta}_i^h) \mathbf{F}] \quad (3.30)$$

where

$$\mathbf{F} = \sum_{i=1}^{npoin} \mathbf{x}_i \otimes \nabla_X N_i \quad (3.31)$$

### The non-linear incremental finite element equation

The equilibrium equation is, in general, non-linear. For the particular case of material non-linearities, such as in the Lemaitre model where the Cauchy stress is dependent of the history of strains to which the solid has been subjected, a suitable temporal discretisation is required.

In this thesis, a pseudo-time discretisation between the time increments  $[t_n, t_{n+1}]$  will be considered, in a fully implicit scheme. The function,  $\hat{\boldsymbol{\sigma}}$ , defined as

$$\boldsymbol{\sigma}_{n+1} = \hat{\boldsymbol{\sigma}}(\mathbf{F}_{n+1}, \boldsymbol{\alpha}_n) \quad (3.32)$$

is assumed to exist and is associated with an integration algorithm that delivers the behaviour for a given deformation gradient,  $\mathbf{F}_{n+1}$ , and a set of internal variables,  $\boldsymbol{\alpha}_n$ , which are assumed to be constant within the one increment.

The Newton-Raphson algorithm is particularly attractive for the solution of this type of problems due to its robustness and quadratic rates of asymptotic convergence, and thus was used in this work. During a solution procedure in which equilibrium is not yet satisfied, there is a residual  $R$  between the internal work and the external work. As in the problems considered in this thesis, the applied traction is independent of the deformation, the individual element contribution to the residual may be defined as:

$$\mathbf{R}_e(\mathbf{u}_{n+1}) = R_{en+1} = \int_{\Omega_e} \mathbf{S}_{n+1} \frac{\partial \mathbf{E}_{n+1}}{\partial \mathbf{u}_{en+1}} d\Omega \quad (3.33)$$

where  $\Omega_e$  is the domain of the element. Following the general procedures of the Newton method, a system of equations of the the form

$$\mathbf{R}_{n+1} = \mathbf{0} \quad (3.34)$$

is obtained. However equation 3.34 is not satisfied unless convergence has occurred. Since the current global residual  $\mathbf{R}_{n+1}$  depends on the global displacement vector of the

previous time step,  $\mathbf{u}_n$ , and on the current global displacement vector,  $\mathbf{u}_{n+1}$ , that is,

$$\mathbf{R}_{n+1} = \mathbf{R}_{n+1}(\mathbf{u}_{n+1}, \mathbf{u}_n) \quad (3.35)$$

the  $(k)$ th iteration step may be written as

$$\mathbf{K}_{Tn+1}^k \Delta \mathbf{u}_n^k + \mathbf{R}_{n+1}^k = \mathbf{0} \quad (3.36)$$

where  $\mathbf{K}_T$  is the *global tangent stiffness matrix* given by

$$\mathbf{K}_{Tn+1}^k = \frac{\partial \mathbf{R}_{n+1}^k}{\partial \mathbf{u}_{n+1}^k} \quad (3.37)$$

Finally, the displacements are updated as follows:

$$\mathbf{u}_{n+1}^{k+1} = \mathbf{u}_{n+1}^k + \Delta \mathbf{u}_{n+1}^k \quad (3.38)$$

## Numerical integration

In a finite element implementation, the exact integrals are replaced by a numerical integration procedure. In general, standard Gaussian quadrature will be used for this purpose. The integral of a generic function  $f$  over a domain  $\Gamma$  is given by

$$\int_{\Gamma} f(\xi) d\xi \approx \sum_{i=1}^{ngaus} \omega_i f(\xi_i) \quad (3.39)$$

where  $ngaus$  is the number of approximation points, with coordinates  $\xi_i$  and weights  $\omega_i$ . At this stage, it should be remarked that in the following chapters of this thesis, some alternative methods for numerical integration will be addressed, in particular in the presence of discontinuities.

## 3.3 Automatic code generation

The implementation of a FEM code may be quite complicated and time consuming, especially when dealing with non-linear material models. In general, the discretisation and linearisation procedures described in the previous sections have to be performed prior to the actual code writing. The complexity of the required calculations increases the probability of error and, consequently, inefficient codes may result.

From another perspective, a new formulation represents essentially the coding of a different element kinematics and/or a different material model, which suggests that a large number of operations related to FEM programming could be automated.

In this context, the use of automatic differentiation tools and modern symbolic and algebraic computer systems may represent a considerable advantage. However, in most of these systems, the classical symbolic derivation leads to the exponential growth of expressions and inefficient codes. In order to overcome this limitation, the *AceGen* System [83] employs the *Simultaneous Stochastic Simplification of Numerical Code* approach [84, 85], which combines an automatic differentiation technique with the simultaneous optimization of symbolic expressions, allowing the automatic generation of efficient numerical codes. In the following subsections the main features of this system will be described and the application to the FEM will be illustrated.

### 3.3.1 Automatic code generation features

For an efficient code generation, the *AceGen* system gathers some important features characterized in the following paragraphs.

#### Differentiation

As shown in the beginning of this chapter, the development of a finite element formulation involves the calculation of numerous derivatives. Therefore a proper automatic differentiation tool, in which the dependence on intermediate quantities is correctly accounted for is essential.

The derivative of a general function,  $f$ , which depends on a set of mutually independent variables  $\mathbf{a}$  and a set of mutually independent intermediate variables  $\mathbf{b}$  (that is,  $\mathbf{b}$  depend on  $\mathbf{a}$ ) may be expressed as follows:

$$\nabla f = \frac{\partial f(\mathbf{a}, \mathbf{b}(\mathbf{a}))}{\partial(\mathbf{a})} \bigg|_{\frac{\partial(\mathbf{b})}{\partial(\mathbf{a})} = \mathbf{M}} \quad (3.40)$$

The total derivatives of the variables  $\mathbf{b}$  with respect to the variables  $\mathbf{a}$  may be written in the matrix form, where  $\mathbf{M}$  is the respective Jacobian matrix. During the differentiation procedure, when there exists an explicit algorithmic dependence between  $\mathbf{b}$  and  $\mathbf{a}$ , the derivatives may be obtained automatically by the chain rule without user intervention,

simply by replacing its value for the corresponding entrance of matrix  $\mathbf{M}$ . Nevertheless, for some situations, the direct application of the chain rule leads to erroneous results. In particular, when function  $f$  only depends explicitly on  $\mathbf{b}$ ,

$$\nabla f = \frac{\partial f(\mathbf{b})}{\partial(\mathbf{a})} \bigg|_{\frac{\partial(\mathbf{b})}{\partial(\mathbf{a})}=\mathbf{M}} \quad (3.41)$$

or the dependency between  $\mathbf{b}$  and  $\mathbf{a}$  has to be neglected,

$$\nabla f = \frac{\partial f(\mathbf{a}, \mathbf{b}(\mathbf{a}))}{\partial(\mathbf{a})} \bigg|_{\frac{\partial(\mathbf{b})}{\partial(\mathbf{a})}=\mathbf{0}} \quad (3.42)$$

a proper exception has to be considered by the automatic differentiation tool [84, 85]. A typical example of the first case is a differentiation that involves a transformation of coordinates, for instance, from a reference isoparametric finite element, to a global coordinate finite element. The introduction of the additional condition for the proper derivation of the deformation gradient is illustrated in section 3.3.2.

### Simplification of large mathematical expressions

After setting up a proper differentiation tool, the methodology to simplify mathematical expressions is of major importance. Most of the existing symbolic systems, such as *Mathematica* or *Matlab*, only search for common sub-expressions after all the formulae have been derived, using a pattern-matching technique. However this methodology is insufficient to obtain efficient codes for calculating typical FEM quantities like the internal force vector or the stiffness matrix, due to the excessive swell of the mathematical expressions [86, 87].

To overcome this problem, *AceGen* employs the *Simultaneous Stochastic Simplification of numerical code* [84, 85]. In this methodology the search of common sub-expressions is performed after each automatic derivation step, optimizing the introduction of intermediate variables. In addition, the equivalence between expressions is not only searched symbolically but also numerically [88]. It is a fact that the correctness of the simplified expressions can only be determined with a certain probability, nevertheless, when dealing with relatively smooth functions, as it is the case of the FEM, this can be neglected.

## Hybrid approach

As it has been referred throughout this section, the general Computer Algebra systems possess high symbolic and algebraic capabilities. Nevertheless, for intensive numerical tasks, these systems cannot compete with languages such as *C* or *Fortran* in terms of execution times. In fact, when testing a new formulation, a large number of flaws can be detected at the symbolic level or performing small examples, for which the first type of languages is preferred. However, for running large examples, the low-level languages are much more appealing.

In order to combine the advantages of both environments, *AceGen* includes two features. In one hand, it allows the generation of codes for different languages (Matlab, Fortran, C) and commercial FEM environments such as *Abaqus* or *FEAP*. Alternatively, *AceGen* is associated to its own FEM environment, *AceFEM* [89], where a hybrid approach is employed. Non-intensive numerical procedures (e. g. mesh generation, control of the solution procedures, post-processing) are run inside *Mathematica*, while intensive numerical procedures, such as assembly of the stiffness matrix or the internal force vector, are performed using a *C* language driver connected with *Mathematica*.

### 3.3.2 *AceGen/AceFEM* standard procedure

After a brief description of the *AceGen* and *AceFEM* systems, it will be now illustrated how these tools can be used to generate a FEM code.

Firstly, it must be noticed that *AceGen* is oriented to generate code at the single element level. The application of automatic differentiation procedures to a complete FEM environment may become inefficient, especially when fully implicit Newton-type procedures are used to solve highly non-linear problems. However, this problem is easily overcome by generating routines to evaluate specific quantities, at the individual element level, such as the consistent stiffness tangent matrix, the element force vector, the stress or strain tensors. Later, different elements may be combined for the analysis step in *AceFEM*.

Another fundamental aspect to generate automatically codes, which are as efficient as manually written codes, is the clearness of the formulation at the highest abstract level possible. The symbolical formulation often differs from the traditional computational

mechanics approach, which means that intermediate quantities manually defined may not appear explicitly in automatically generated codes (e.g. the  $\mathbf{B}$  matrix defined in equation 3.27). This type of formulation is more compressed resulting in fewer possibilities of error. Moreover, derivatives obtained automatically from the symbolic description are exact, leading to quadratically convergent Newton-type of iterative schemes.

Having in mind the above considerations, there are four main steps that should be considered in the generation of a finite element using *AceGen*, as follows:

1. **Initialization** - Major characteristics of the element are defined in a global set of constants, such as the element topology, the number of history variables, the material parameters or the finite element environment. The kinematics and the constitutive equations are also developed.
2. **Tangent and Residual** - Definition of the stiffness tangent matrix and element force vector for the discretization and material model defined in the **Initialization** step. It should be noticed that the element contribution to the global force vector,  $\mathbf{R}$ , considering the global set of unknowns,  $\mathbf{p}$ , is automatically derived using the relation:

$$\mathbf{R}_{en+1} = \int_{\Omega_e} \mathbf{S}_{n+1} \frac{\partial \mathbf{E}_{n+1}}{\partial \mathbf{p}_{en+1}} d\Omega_e \quad (3.43)$$

The contribution to the global stiffness matrix,  $\mathbf{K}$  is also automatically calculated as

$$\mathbf{K}_{Ten+1} = \frac{\partial \mathbf{R}_{en+1}}{\partial \mathbf{p}_{en+1}} \quad (3.44)$$

In the traditional FEM implementation, usually two separate routines have to be written for the internal force vector and the stiffness matrix. In addition, all the derivatives are calculated before the actual code writing. Here, on the contrary, the constitutive equations are only developed once, saving time and reducing the probability of error. Moreover, as in many material models the free parameters are uniquely the strain energy and the yield condition, the stress and strain tensors do not appear explicitly, and therefore the question of the optimal strain/stress pair does not arise. The choice between material and spatial descriptions is also not relevant.

3. **Post-processing** - This section is responsible for extrapolate the designated quantities (strains, stress, etc) from the Gauss points to the nodes and perform the graphic treatment of the results.

4. **Sensitivity** - This module allows the direct implicit analysis to get sensitivity of the global unknowns with respect to arbitrary parameters, however, it was not used in the FEM codes developed for this thesis.

In the *AceGen* user manual [83] all the stages are illustrated by a considerable number of examples, explained in detail. In the following paragraphs it will be briefly presented how the kinematics of a 2D quadrangular finite element may be derived.

Recalling section 3.2, the displacement field approximation, as well as the element coordinates, may be approximated by a set of shape functions. Then, the deformation gradient may be obtained using the gradient of the displacement field. In table 3.1 the *AceGen* input corresponding to this procedure is presented along with the corresponding mathematical description. For the correct calculation of the gradient of the displacement field an additional condition, relating the actual coordinates and the reference coordinates through the Jacobian matrix, had to be introduced. In table 3.1 this condition is represented by the "Dependency" option in *SMSD* comand, which is the command that denotes the automatic differentiation operation. The simple use of the *SMSD* comand would lead to erroneous results.

In a traditional FEM code, the presented derivatives are calculated by hand prior to the

TABLE 3.1: Calculation of the deformation gradient by deriving the displacement field approximation. The *SMSFreeze* command denotes the manual introduction of an intermediate variable, which in this situation is necessary to correctly define the dependencies in the automatic derivation procedure.

| AceGen                                                                                                                                       | Mathematical description                                                                                             |
|----------------------------------------------------------------------------------------------------------------------------------------------|----------------------------------------------------------------------------------------------------------------------|
| <pre>(* Shape Functions*) Ni = 1/4 * {(1 - ξ) (1 - η), (1 + ξ) (1 - η), (1 + ξ) (1 + η), (1 - ξ) (1 + η)};</pre>                             | $N_i = \frac{1}{4}(1 + \xi_i)(1 + \eta_i)$                                                                           |
| <pre>(* Global Coordinates*) X = SMSFreeze[Ni.Xi]; Y = SMSFreeze[Ni.Yi]; Z = SMSFreeze[ξ];</pre>                                             | $\mathbf{X} = \sum N_i \mathbf{X}_i$                                                                                 |
| <pre>(* Jacobian matrix and determinant *) Jm = SMSD[{X, Y, Z}, {ξ, η, ξ}]; Jd = Det[Jm];</pre>                                              | $\mathbf{J}_m = \partial \mathbf{X} / \partial \xi$<br>$J_d = \det \mathbf{J}_m$                                     |
| <pre>(* Displacement field approximation *) u = Ni.ui; v = Ni.vi;</pre>                                                                      | $\mathbf{u} = \sum N_i \mathbf{u}_i$                                                                                 |
| <pre>(* Deformation gradient *) D = SMSD[{u, v, 0}, {X, Y, Z}, "Dependency" → {{ξ, η, ξ}, {X, Y, Z}, Jmi}]; F = IdentityMatrix[3] + D;</pre> | $\nabla_X \mathbf{u} = \partial \mathbf{u} / \partial \mathbf{X}$<br>$\mathbf{F} = \mathbf{I} + \nabla_X \mathbf{u}$ |

code writing. Moreover, by changing the discretisation, that is, by changing the shape functions, the process has to be re-started from the beginning and a completely new code has to be written, while with *AceGen*, only the first line of the presented example

must be altered. This compact and clean notation reduces the probability of errors, especially when dealing with complex formulations.

### 3.4 Conclusions

The Finite Element Method is the chosen numerical approach to solve ductile fracture problem addressed in this thesis. In first part of this chapter its basic features were presented. Departing from the balance principles introduced in chapter 2, the Initial Boundary Value problem was defined along with the discretisation of the displacement field through shape functions. Time discetisation and general Newton-Raphson iterative scheme for solving non-linear problems was also addressed.

The second part of this chapter touches the new frontiers of implementation of a finite element formulation with the introduction of the concept of Automatic Code Generation. Motivated by the developments of computer science in the last decades, this approach allows a faster and more efficient development of numerical codes to solve complex problems, involving geometric and material non-linearities.

In particular, the *AceGen* system combines the symbolic and algebraic capabilities of the modern computer algebra systems with an automatic differentiation and optimization tools in a hybrid approach. This allows a faster development of numerical code, highly portable and efficient, offering fewer possibilities of error. In addition the system possesses multi-language and multi-environment capabilities, making it suitable for testing of new formulations and also to problems with a large number of finite elements. Complex problems, such as multi-field and multi-physics, are also easily handled.



## Chapter 4

# The Extended Finite Element Method

In the last decade, the Extended Finite Element Method (XFEM) became one of the most widely used numerical approaches to assess problems involving discontinuities and moving interfaces. Notwithstanding the fact that the pioneering works of the XFEM were devoted to fracture problems [54, 90, 91], this methodology spread through various areas, including metallurgy, phase-transformations and fluid mechanics, resulting in a considerable amount of available literature. A detailed review on the XFEM may be found in the bibliographic research papers [92–94] as well as in the the book [95] focused in the application of XFEM to linear elastic fracture.

As the objective of this thesis is to built a model for ductile fracture, having the XFEM as a tool to insert and propagate cracks in a continuous media, this chapter will focus on the basic formulation and the features which were developed specifically to deal with ductile fracture.

Thus, this chapter is organized in the following fashion. In the first section the essential theory of XFEM is reviewed, namely, the displacement field approximation, the selection of enriched nodes and the basic numerical implementation. Next, different numerical integration strategies are proposed and analysed, focusing in the ability of dealing with incompressibility constraints. Some numerical examples are also presented to illustrate the efficiency of the selected numerical integration strategies. The following section highlights other features developed for a successful combination of the XFEM with non-linear material models. Finally, some general conclusions are presented.

## 4.1 Formulation and basic numerical implementation

### 4.1.1 Displacement approximation and choice of the enrichment functions

The XFEM is a methodology which allows for the insertion of special features, such as discontinuities or interfaces, in a FEM problem, independently from the mesh, by enriching the displacement field,  $\mathbf{u}$ , with one or more functions  $\psi$ , as follows:

$$\mathbf{u}(\mathbf{x}) = \sum_{i=1}^n N_i(\mathbf{x}) \mathbf{u}_i + \sum_{j=1}^{n_{enr}} N_j(\mathbf{x}) \psi(\mathbf{x}) \boldsymbol{\psi}_j \quad (4.1)$$

where  $N_i$  represents the element shape functions and  $\boldsymbol{\psi}_j$  are the extra degrees of freedom associated to the function  $\psi$  in each one of the  $n_{enr}$  nodes.

The function  $\psi$ , termed *enrichment function*, contains the description of the desired feature and satisfies the *partition of unity principle*, which may be stated as,

$$\sum_j N_j(\mathbf{x}) \psi(\mathbf{x}) = 1. \quad (4.2)$$

It should be noticed that considering  $N_j$  as the standard FEM shape functions, this property is automatically satisfied, though this choice is not mandatory.

The mathematical expression of  $\psi$  varies greatly, as this method may be applied to very diverse scientific areas. In particular case of this thesis the XFEM is used in the context of fracture and therefore the enrichment function should be capable of capturing the decohesion between the two surfaces of a crack. Discontinuous functions such as the following Heaviside function,  $H(\hat{\eta})$ , defined in terms of the coordinate  $\hat{\eta}$  perpendicular to the crack plane (figure 4.1), are particularly suitable for this purpose.

$$H(\hat{\eta}) = \begin{cases} 1: & \hat{\eta} \geq 0 \\ -1: & \hat{\eta} < 0 \end{cases} \quad (4.3)$$

The displacement approximation then reads:

$$\mathbf{u} = \sum_{i=1}^n N_i \mathbf{u}_i + \sum_{j=1}^{n_{split}} N_j H \mathbf{a}_j \quad (4.4)$$

where  $\mathbf{a}_j$  are the degrees of freedom associated to the Heaviside function. When a finite element is totally cut by a crack is usually termed *split* element and therefore, has a number of  $n_{split}$  enriched nodes. An element only partially crossed by a crack, that is,

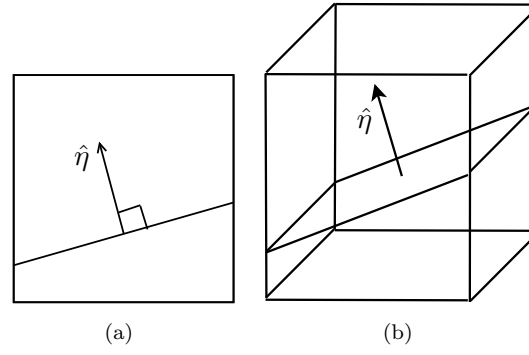


FIGURE 4.1: Definition of the coordinate perpendicular to the crack in a) 2D problem  
b) 3D problem.

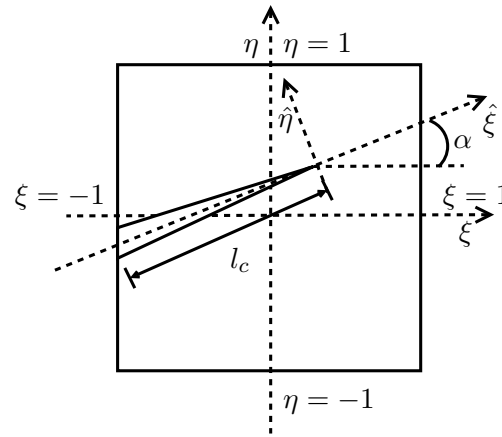


FIGURE 4.2: Crack tip coordinates for a 2D element or a cut along  $\hat{\zeta} = 0$  for a 3D element.

containing a crack tip is named *tip* element. A local coordinate system,  $\hat{\xi} = (\hat{\xi}, \hat{\eta}, \hat{\zeta})$ , centered at the crack tip, may be defined for these type of elements, as illustrated in figure 4.2, for a plane element or a cut along  $\hat{\zeta} = 0$  for a 3D element. In 2D problems  $\hat{\xi} = (\hat{\xi}, \hat{\eta})$ , where  $\hat{\xi}$  is in the crack direction and  $\hat{\eta}$  is perpendicular to the crack line. In 3D problems  $\hat{\xi} = (\hat{\xi}, \hat{\eta}, \hat{\zeta})$ , in which  $\hat{\xi}$  and  $\hat{\zeta}$  are in the crack plane, with  $\hat{\xi} = 0$  defining the crack tip line at the crack plane, and  $\hat{\eta}$  coordinate is normal to the crack plane.

Applying directly the displacement approximation of equation 4.4, in general  $\mathbf{u}(\mathbf{x}_i) \neq \mathbf{u}_i$ . This problem may be easily overcome by shifting the approximation around the node of interest, as follows:

$$\mathbf{u}(\mathbf{x}) = \sum_{i=1}^n N_i \mathbf{u}_i + \sum_{j=1}^{n_{split}} N_j [H(\mathbf{x}) - H(\mathbf{x}_j)] \mathbf{a}_j \quad (4.5)$$

Moreover, the shifted version of equation 4.5 prevents the enrichment of spreading to the neighbour elements, which contain standard and enriched nodes (figure 4.3), usually designated *blending elements*.

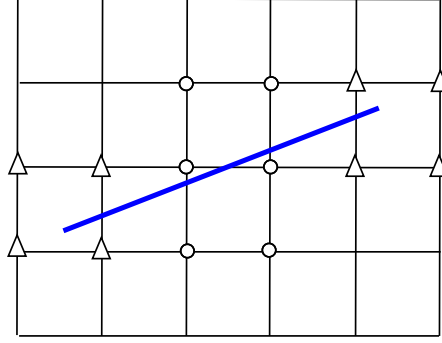


FIGURE 4.3: Crack inserted in the mesh through the XFEM. The nodes belonging to split elements are marked with circles, while the nodes belonging to tip elements are marked with triangles. Elements containing both enriched and standard nodes are designated *blending* elements.

Enriching finite elements only with the Heaviside function always causes the extension of the crack to the edge of an element. Nevertheless, to represent cracks truly mesh independent, it is desirable to define a strategy to deal with the closure of a crack away from the element edge, as can be observed in figure 4.3.

Elements containing crack tips, may then be enriched by a function, which has to ensure that the enrichment vanishes exactly at the crack tip. Some alternative definitions for this function are proposed and presented below, in terms of crack tip coordinates and the crack length inside the tip element,  $l_c$ . The first proposed form for the function, here named as  $R$ , is a Heaviside type function, defined as:

$$R(\hat{\xi}) = \begin{cases} 1 & \text{for } \hat{\xi} \leq 0 \\ 0 & \text{otherwise} \end{cases} \quad (4.6)$$

and determines that only Gauss points located behind the crack front should be enriched. The second proposed form is a linear type function, defined as:

$$R(\hat{\xi}) = \begin{cases} -\frac{\hat{\xi}}{l_c} & \text{for } \hat{\xi} \leq 0 \\ 0 & \text{otherwise} \end{cases} \quad (4.7)$$

A higher order function, defined in reference [96], is also adopted here as:

$$R(\hat{\xi}) = \begin{cases} 3\left(\frac{\hat{\xi}}{l_c}\right)^2 + 2\left(\frac{\hat{\xi}}{l_c}\right)^3 & \text{for } \hat{\xi} \leq 0 \\ 0 & \text{otherwise} \end{cases} \quad (4.8)$$

In this work, these functions are considered to be constant along the  $\hat{\zeta}$  coordinate, in the case of 3D elements.

Besides ensuring that the enrichment disappears exactly at the crack tip, the three forms of the  $R$  function are particularly suitable for ductile fracture problems, where plasticity is not only confined to the region around the crack tip but widely spread. Furthermore, as in the case of the Heaviside function, these polynomial enrichments vanish outside the elements containing discontinuities, which is not the case if other types of enrichments are employed [94, 97, 98].

The full displacement approximation may then be written as:

$$\begin{aligned} \mathbf{u}(\mathbf{x}) = & \sum_{i=1}^n N_i \mathbf{u}_i + \sum_{j=1}^{n_{split}} N_j [H(\mathbf{x}) - H(\mathbf{x}_j)] \mathbf{a}_j \\ & + \sum_{k=1}^{n_{tip}} N_k [R(\mathbf{x}) - R(\mathbf{x}_k)] [H(\mathbf{x}) - H(\mathbf{x}_k)] \mathbf{b}_k \end{aligned} \quad (4.9)$$

*Remark 4.1.* In the framework of linear elastic fracture mechanics, the most used enrichment functions to deal with crack tips are based in the asymptotic displacement fields derived from analytical solutions [54, 90, 99]. Therefore, the following set of four functions,  $\psi_{tip}^i$ , is employed:

$$\psi_{tip}^i = \left\{ \sqrt{r} \sin\left(\frac{\theta}{2}\right), \sqrt{r} \sin\left(\frac{\theta}{2}\right) \sin \theta, \sqrt{r} \cos\left(\frac{\theta}{2}\right), \sqrt{r} \cos\left(\frac{\theta}{2}\right) \sin \theta \right\} \quad (4.10)$$

These functions are widely used for brittle fracture problems, as they reproduce a singularity at the crack tip. Nevertheless, as previously referred, in a context of ductile fracture they may not be adequate.

Finally, for a successful implementation of the method it is essential to determine the split nodes and the tip nodes, which may be done through the *Level Set Method*, described in the next section.

#### 4.1.2 The level set method

The *Level Set Method* [100, 101] is the most frequently used complement of the XFEM to accurately determine the position of the discontinuities, that is, the set of nodes to be enriched [102, 103].

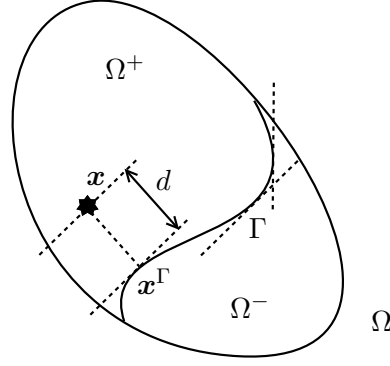


FIGURE 4.4: Domain

Considering a domain  $\Omega$ , divided in the regions  $\Omega^+$  and  $\Omega^-$  by the interface  $\Gamma$ , the level set function,  $\phi(\mathbf{x})$ , is defined in a such a way that

$$\phi(\mathbf{x}) = \begin{cases} 1: & \mathbf{x} \in \Omega^+ \\ 0: & \mathbf{x} \in \Gamma \\ -1: & \mathbf{x} \in \Omega^- \end{cases} \quad (4.11)$$

A common choice for  $\phi(\mathbf{x})$  is the signed distance function, defined as

$$\phi(\mathbf{x}) = \pm d = \pm \|\mathbf{x} - \mathbf{x}^\Gamma\| \quad (4.12)$$

where  $d$  is the distance between point  $\mathbf{x}$  and the closest point to  $\mathbf{x}$  laying in the interface,  $\mathbf{x}^\Gamma$ , as depicted in figure 4.4. The sign of  $d$  depends on which side of the interface is located point  $\mathbf{x}$ .

The function  $\phi(\mathbf{x})$  determines if a point lies *above* or *below* a crack. Nevertheless, as usually a crack does not cut the entire domain, a second function,  $\varphi(\mathbf{x})$ , has to be introduced to deal with the active crack tips. When a crack is defined by straight line segments, which is the case in this thesis, a function  $\varphi_i(\mathbf{x})$  may be defined by each active crack tip as follows:

$$\varphi(\mathbf{x}) = (\mathbf{x} - \mathbf{x}_i) \cdot \hat{\mathbf{t}}_i \quad (4.13)$$

where  $\hat{\mathbf{t}}$  is a unit vector tangent to the latest crack segment and  $\mathbf{x}_i$  is the location of the  $i$ th crack tip, as can be observed in figure 4.5.

Although, functions  $\phi$  and  $\varphi_i$  have to be updated at each crack growth step, the search for newly enriched elements is only required around the previous crack tip. Furthermore, in a ductile fracture problem the direction and magnitude of a crack increment are determined by the material model, as it will be described in the following chapters.

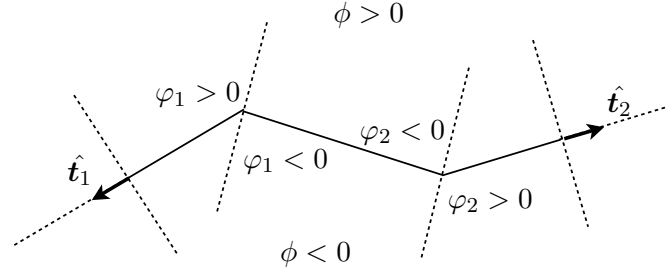


FIGURE 4.5: Level set functions.

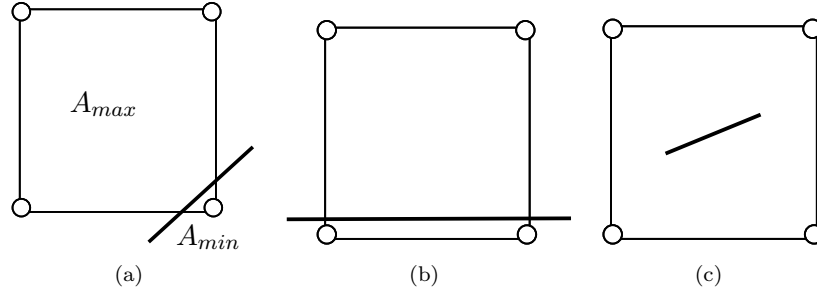


FIGURE 4.6: The crack is very close to a) a node b) an edge and totally contained in one element in c), possibly leading to ill-conditioned stiffness matrices.

Consequently, the level set functions are updated by simple geometrical considerations. The level set function described may also describe crack propagation for planar cracks in 3D problems. A more detailed description of the procedure may be found in the references [104–107].

#### 4.1.3 Basic implementation

The implementation of an XFEM formulation consists fundamentally in modifying the standard FEM displacement approximation and create a structure to deal with the extra degrees of freedom, introduced by the enrichment functions, when performing tasks such as the assembly of the internal force or the stiffness matrix.

Some linear dependencies or ill-conditioning may arise due, essentially, to elements where the ratio of the areas/volumes between the two sides of the crack is very high,  $A_{max}/A_{min}$ , as illustrated in figures 4.6(a) and 4.6(b), or when the discontinuity lies only inside one element (figure 4.6(c)). The first situation is usually prevented by setting a tolerance from which the crack should be converted into a inter-element crack while in the second situation, the mesh may be refined [94, 108].

Another key feature in the implementation of the XFEM is numerical integration. Due to its high importance the next section is fully devoted to this subject.

Other features that had to be developed to deal with the use of the XFEM with non-linear problems, such as transfer of history variables and non-locality, will be also addressed in the end of this chapter.

## 4.2 Numerical integration and the incompressibility issue

Numerical integration has to be carefully addressed when implementing a XFEM code, as the results produced by regular Gaussian quadrature rules are not accurate enough, due to the presence of discontinuous functions. Two main techniques were developed since the early stages of XFEM. Probably the most common of those techniques consists of dividing the elements containing discontinuities in sub cells conforming the discontinuity, usually triangles or tetrahedrons, for 2D and 3D problems respectively, and applying a regular rule to each sub cell [90, 91, 109]. Alternatively, some authors [110–112] prefer to keep fixed Gauss point positions, but largely increase their number inside an element to compensate for not adjusting the discontinuity pattern. As computationally this last method may become extremely expensive, other approaches were created to suppress the need of element subdivision, starting with the works of Iarve [113] and Ventura [114] who derived continuous polynomial functions which, integrated over an element, reproduce the integrals of the discontinuous XFEM functions. This method was extended for regularized discontinuities by Benvenuti et al. [115], but it is only exact for triangular or tetrahedral elements. Another integration rule was proposed by Holdych [116] for the same type of elements, where the drawback of having fixed positions for the Gauss points is compensated by adopting variable weights. The relation between these last two methods was established by Belytschko et al. [117] and, subsequently, the same authors developed a boundary integration method [118], applicable to quadrangular elements, in which all nodes are equally enriched. Recently, Natarajan et al. [119] proposed an integration technique based on the Schwarz-Christoffel conformal mapping valid for any type of 2D finite elements, and Mousavi et al. [120] made use of the node elimination technique to produce accurate integration rules with a reduced number of Gauss points.

As, so far, most of the XFEM applications are within the scope of brittle fracture, the accuracy of the methodologies described above is typically measured by the ability to reproduce the stress intensity factors, for particular problems that have an available analytical solution. Nevertheless, the direct extension of those methodologies to problems

involving ductile fracture may not be adequate. In fact, when ductile fracture is the issue, plastic deformation is widely spread and not just confined to the nearby zones around the crack, as it happens in brittle fracture. Furthermore it is well known that incompressibility of plastic deformation may lead to locking of the numerical solution, especially when low order finite elements are employed [121–126]. Consequently, in order to avoid it, adequate formulations or integration techniques must be used. Depending on the problem addressed solutions may include, for example, selective reduced integration techniques [122], mixed formulations [65], B-bar methods [123], F-bar methods [63, 127] or enhanced assumed strain methods [128], to name a few. Therefore when XFEM is used to model ductile fracture some questions emerge as important topics, namely those related with the discussion on the adequate number of Gauss points that should be used in the sub cells, when an element contains or is crossed by a crack, and the ability to satisfy the incompressibility constraints.

In the following sections, having in view the application of XFEM to ductile fracture problems, the efficiency of different integration rules is investigated, focusing on their ability to satisfy volumetric incompressible constraints in the context of both infinitesimal and finite strains. As a consequence, the conventional formulations for B-bar and F-bar are adapted to include the XFEM enrichment functions. Other alternatives to deal with incompressibility in XFEM elements include the adaptation of the assumed enhanced strain method by Dolbow et al [129] and the mixed formulation technique by Legrain et al [130]. Here, the efficiency of the proposed techniques is evaluated with some numerical examples and the performance of the F-bar method for XFEM is compared with the method developed by Dolbow et al [129].

#### **4.2.1 Methodology to assess the ability to alleviate locking**

The methodology here adopted to assess the tendency or the ability of a particular method to depict or to alleviate locking will follow closely some previous work that may be found in references [124–126]. This methodology is based on the analysis of the underlying sub-space of incompressible modes embedded in the approximation method adopted, rather than relying on mere constraint indexes which may be misleading, as they are defined independently of the boundary conditions. The aforementioned analysis may give information on how the dimension of this subspace can be enlarged or reduced as a function of the integration rule adopted. Consequently it may give precious hints on the ability of a particular method to reproduce incompressible deformations, on how

spurious modes may be prevented or on how over integration rules may be avoided.

Recalling equation 2.11 from chapter 2, an isochoric deformation is characterized by:

$$J = 1 \quad (4.14)$$

Taking into account that the material time derivative of the volume ratio may be written as a function of the rate of deformation tensor or of the velocity field:

$$\dot{J} = J \text{tr} \mathbf{d} = J \text{div} \mathbf{v} \quad (4.15)$$

and considering equation 4.14 and its time derivative, the incompressibility condition may alternatively be stated as:

$$\text{tr} \mathbf{d} = 0 \quad (4.16)$$

For a small strain problem, disregarding second and higher order terms, this condition may be simplified to:

$$\text{div} \mathbf{u} = 0 \quad (4.17)$$

where  $\mathbf{u}$  represents the displacement field.

Consequently, when imposing the incompressibility condition in a FEM framework via the Penalty Method or the Lagrange Multiplier technique [124], a local discretized form of equation 4.16 or equation 4.17 may be established at each numerical integration point of a particular element with the form

$$\mathbf{Q} \mathbf{w}^h = 0 \quad (4.18)$$

where  $\mathbf{w}^h$  is the vector of element nodal variables from which the rate of deformation tensor or the displacement field are approximated and  $\mathbf{Q}$  is a matrix  $i \times n$ , in which  $i$  is the number of integration points and  $n$  the number of unknowns in  $\mathbf{w}^h$ . Consequently, element wise, an admissible incompressible solution  $\mathbf{w}^h$  should belong to the null space of matrix  $\mathbf{Q}$ , which defines locally the space of incompressible deformations,  $I^h$

$$I^h = \{\mathbf{w}^h \in U : \mathbf{Q} \mathbf{w}^h = 0\} \quad (4.19)$$

Locking occurs, when for a given set of boundary conditions, the expected solution cannot be reproduced by a linear combination of a given basis of  $I^h$  [124–126]. Having applications on ductile fracture problems, in which extensive plastic deformations may be present, the analysis of this underlying sub-space and how it may be affected by adopting or altering a certain integration rule will be addressed in the following sections of this chapter.

### 4.2.2 Incompressible deformation modes in elements containing XFEM enrichments

A basis of  $I^h$  (equation 4.19), the space of admissible incompressible deformations, must be determined to study the vulnerability of the enriched elements to volumetric locking. It should be noticed that for the XFEM approximation, the nodal variables  $\mathbf{w}^h$  used in the approximation of the strain or the strain rate encompasses both the displacements  $\mathbf{u}^h$  and the extra variables  $\mathbf{a}^h$  or  $\mathbf{b}^h$  or their pseudo-time derivatives. Therefore, for simplicity and in line with the previous works of Cesar de Sa et al. [124–126], a basis of  $I^h$  of a particular element, in which global coordinates  $\mathbf{x}$  and natural coordinates  $\boldsymbol{\xi}$  are coincident, may be determined by obtaining a basis of the null space of matrix  $\mathbf{Q}$ . For this particular case equation 4.19 reads:

$$\mathbf{Q}\mathbf{w}^h = \left[ \begin{array}{ccc} \frac{\partial N_i}{\partial \xi} & \frac{\partial N_i}{\partial \eta} & \frac{\partial N_i}{\partial \zeta} \end{array} \frac{\partial(N_i\psi)}{\partial \xi} \frac{\partial(N_i\psi)}{\partial \eta} \frac{\partial(N_i\psi)}{\partial \zeta} \right]_{i=n_{nodes}} \left\{ \begin{array}{c} \mathbf{u}^h \\ \boldsymbol{\psi}^h \end{array} \right\} = 0 \quad (4.20)$$

where the number of lines in  $\mathbf{Q}$  equals the number of Gauss points,  $n_{Gauss}$ , used in the finite element,  $\psi$  represents the enrichment function associated with the extra variables  $\boldsymbol{\psi}^h$ , which may be  $\mathbf{a}^h$  or  $\mathbf{b}^h$  whether it is a *split element* or a *tip element*.

To determine the admissible incompressible deformations of an element containing a discontinuity, equation 4.20 has to be particularized for the displacement approximations of equation 4.5. For an element totally crossed by a discontinuity, only the Heaviside enrichment is considered leading to the displacement approximation, expressed locally as:

$$\mathbf{u}(\boldsymbol{\xi}) = \sum_{i=1}^n N_i \mathbf{u}_i + \sum_{j=1}^{n_{split}} N_j H_i^{Sh} \mathbf{a}_j \quad (4.21)$$

Therefore, the terms associated with the function  $R$  vanish and each line,  $g$ , of matrix  $\mathbf{Q}$  may be written as:

$$\mathbf{Q}_g = \left\{ \begin{array}{ccc} \frac{\partial N_i}{\partial \xi} & \frac{\partial N_i}{\partial \eta} & \frac{\partial N_i}{\partial \zeta} \end{array} \right\}_{i=n_{nodes}} \left\{ \begin{array}{ccc} \frac{\partial N_i}{\partial \xi} H_i^{Sh} & \frac{\partial N_i}{\partial \eta} H_i^{Sh} & \frac{\partial N_i}{\partial \zeta} H_i^{Sh} \end{array} \right\}_{i=n_{nodes}} \quad (4.22)$$

where  $H_i^{Sh}$  denotes the shifted version of the Heaviside function as:

$$\begin{aligned} H_i^{Sh} &= H(\boldsymbol{\xi}) - H(\boldsymbol{\xi}_i), \\ i &= 1, n_{nodes} \end{aligned} \quad (4.23)$$

For an element only partially cut by the crack, the displacement field approximation reads;

$$\mathbf{u}(\boldsymbol{\xi}) = \sum_{i=1}^n N_i \mathbf{u}_i + \sum_{j=1}^{n_{tip}} N_j R_i^{Sh} H_i^{Sh} \mathbf{b}_j \quad (4.24)$$

hence, the derivatives of the function  $R$  are required to evaluate each line of the matrix  $\mathbf{Q}$ , which may be written in the general form as:

$$\mathbf{Q}_g = \left\{ \begin{array}{ccc} \frac{\partial N_i}{\partial \xi} & \frac{\partial N_i}{\partial \eta} & \frac{\partial N_i}{\partial \zeta} \big|_{i=n_{nodes}} \end{array} \quad \begin{array}{c} (\frac{\partial N_i}{\partial \xi} R_i^{Sh} + N_i \frac{\partial R}{\partial \xi}) H_i^{Sh} \\ (\frac{\partial N_i}{\partial \eta} R_i^{Sh} + N_i \frac{\partial R}{\partial \eta}) H_i^{Sh} \\ (\frac{\partial N_i}{\partial \zeta} R_i^{Sh} + N_i \frac{\partial R}{\partial \zeta}) H_i^{Sh} \end{array} \right\} \quad (4.25)$$

where  $R_i^{Sh}$  denotes the shifted version of the function  $R$  as:

$$R_i^{Sh} = R(\boldsymbol{\xi}) - R(\boldsymbol{\xi}_i), \quad i = 1, n_{nodes} \quad (4.26)$$

When the step function (equation 4.6) is used,  $\mathbf{Q}$  general form is similar to equation 4.22, as the derivatives of this type of function are zero. However, when the linear function and the higher order polynomial function are used, their derivatives must be considered. Therefore, referring to figure 4.2, which may be interpreted as a cut along the plane  $\hat{\zeta} = 0$ , for the linear function it follows:

$$\begin{aligned} \frac{\partial R(\boldsymbol{\xi})}{\partial \xi} &= -\frac{1}{l_c} \frac{\partial \hat{\xi}}{\partial \xi} = -\frac{1}{l_c} \cos \alpha \\ \frac{\partial R(\boldsymbol{\xi})}{\partial \eta} &= -\frac{1}{l_c} \frac{\partial \hat{\xi}}{\partial \eta} = -\frac{1}{l_c} \sin \alpha \end{aligned} \quad (4.27)$$

and for the polynomial function

$$\begin{aligned} \frac{\partial R(\boldsymbol{\xi})}{\partial \xi} &= \frac{6}{l_c} \frac{\partial \hat{\xi}}{\partial \xi} \left( \frac{\hat{\xi}}{l_c} \right) + \frac{6}{l_c} \frac{\partial \hat{\xi}}{\partial \xi} \left( \frac{\hat{\xi}}{l_c} \right)^2 = \frac{6}{l_c} \cos \alpha \left( \frac{\hat{\xi}}{l_c} \right) + \frac{6}{l_c} \cos \alpha \left( \frac{\hat{\xi}}{l_c} \right)^2 \\ \frac{\partial R(\boldsymbol{\xi})}{\partial \eta} &= \frac{6}{l_c} \frac{\partial \hat{\xi}}{\partial \eta} \left( \frac{\hat{\xi}}{l_c} \right) + \frac{6}{l_c} \frac{\partial \hat{\xi}}{\partial \eta} \left( \frac{\hat{\xi}}{l_c} \right)^2 = \frac{6}{l_c} \sin \alpha \left( \frac{\hat{\xi}}{l_c} \right) + \frac{6}{l_c} \sin \alpha \left( \frac{\hat{\xi}}{l_c} \right)^2 \end{aligned} \quad (4.28)$$

In the case of 3D problems, we assume that there is no variation of these functions along the  $\hat{\zeta}$  coordinate and therefore the corresponding derivatives are zero.

As for both types of elements, partially or fully crossed by the crack, the number of lines of matrix  $\mathbf{Q}$  depends on the number of Gauss points of the finite element, consequently it also depends on the particular integration rule employed. In the next section some different strategies to define the distribution of the numerical integration points in XFEM

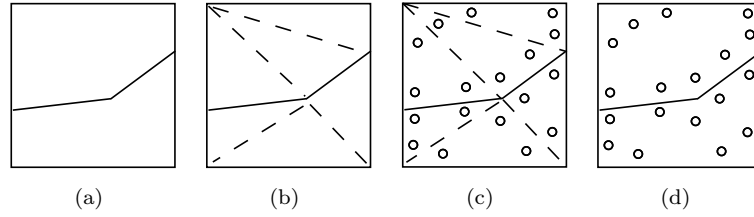


FIGURE 4.7: Possible triangulation process to determine the positions of the Gauss points.

elements are described and their influence in the incompressibility response, i. e. in the definition of the underlying sub-space of incompressibility deformations is analysed.

#### 4.2.2.1 Triangulation

The sub triangulation of elements crossed by a discontinuity [90, 91, 109] is perhaps the most used integration rule for the XFEM. It consists of dividing the existing elements into several smaller triangles or tetrahedrons, for 2D and 3D problems respectively and applying the regular Gaussian rules to each triangle. The weight of each Gauss point is a function of the area/volume of the corresponding sub cell.

The complete procedure used to obtain the positions of the Gauss points for a 2D quadrangular element is illustrated on figure 4.7. This methodology has the advantage of making the location of the Gauss points match the crack configuration inside the element. It is also easy to implement as the element division can be obtained by a Delaunay triangulation [131].

It is of common understanding that this process differs from the remeshing process because the triangles are only used for the determination of coordinates of the Gauss points. Consequently, the locations of the Gauss points have to be recalculated each time the crack configuration changes inside the element, as in the case of crack propagation.

Following the methodology described in the previous section it is possible to construct the matrix  $\mathbf{Q}$  and easily work out a basis for its null space, for the integration rule obtained through the triangulation procedure. Nevertheless, as there are endless possible crack configurations inside an element, it is necessary to group them in different categories, which are analysed in the following subsections. As the conclusions derived for 2D elements are straightforwardly extendible to 3D elements, the subsequent study will focus on three types of plane elements, namely elements totally crossed by a crack,

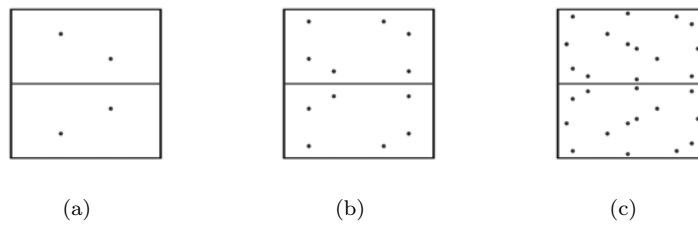


FIGURE 4.8: Integration rules for an element totally cut by a crack, subdividing into four triangles, two in each side of the crack, with: a) 1 Gauss point per triangle; b) 3 Gauss points per triangle; c) 7 Gauss points per triangle.

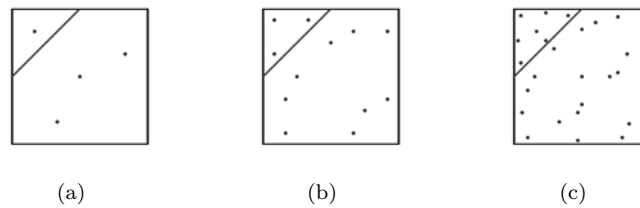


FIGURE 4.9: Integration rules for an element totally cut by a crack, subdividing the element into four triangles, one in one side of the crack and three in the other side, with: a) 1 Gauss point per triangle; b) 3 Gauss points per triangle; c) 7 Gauss points per triangle.

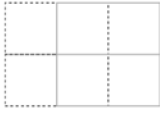
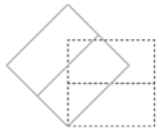
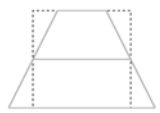
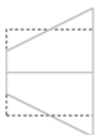
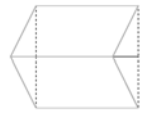
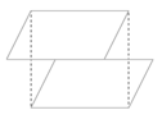
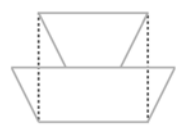
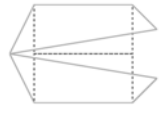
elements partially crossed by a crack and elements containing crack kinks. At the end of the section some comments on 3D elements will be also presented.

**Plane elements totally crossed by a crack:** Cracks crossing low order plane elements are usually represented by straight lines. Although there are endless possible crack directions, two main classes of configurations may be distinguished: elements divided in two quadrangles and elements divided in one triangle and one pentagon. Applying the triangulation procedure, considering four triangles in each element, it is possible to obtain integration points distributions as those illustrated in figures 4.8 and 4.9.

Either a crack crosses an element in two opposite edges (figure 4.8) or in two consecutive edges (figure 4.9), it is possible to find ten linearly independent incompressible deformation modes, including three rigid body motions, when three or more Gauss points per triangle are used. For a reduced integration rule, with one Gauss point per triangle, two more modes are added, giving a total of twelve linearly independent modes that define the basis of the subspace of incompressible deformations. A possible basis is illustrated in the figures of table 4.1, for the example of figure 4.8.

It is noteworthy that even changing the crack configuration, as exemplified in figure 4.10,  $I^h$  is characterized by a similar type of basis represented in table 4.1, consisting of ten linearly independent incompressible modes, for three Gauss points per triangle and twelve linearly independent incompressible modes, for one Gauss point per triangle. The

TABLE 4.1: A possible basis for the incompressible deformation space of an element totally crossed by a discontinuity.

| Incompressible deformation modes reproduced by all the integration rules           |                                                                                      |                                                                                    |                                                                                     |                                                                                     |
|------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------|------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------|
|   |     |   |  |  |
| m1                                                                                 | m2                                                                                   | m3                                                                                 | m4                                                                                  | m5                                                                                  |
|   |     |  |  |  |
| m6                                                                                 | m7                                                                                   | m8                                                                                 | m9                                                                                  | m10                                                                                 |
| Incompressible deformation modes only reproduced by a reduced integration rule     |                                                                                      |                                                                                    |                                                                                     |                                                                                     |
|  |  |                                                                                    |                                                                                     |                                                                                     |
| m11                                                                                | m12                                                                                  |                                                                                    |                                                                                     |                                                                                     |

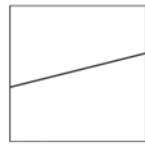
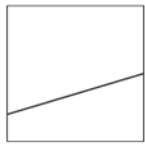
|                                                                                     |                                                                                      |
|-------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------|
|  |  |
| (a)                                                                                 | (b)                                                                                  |

FIGURE 4.10: Two possible crack configurations inside a finite element.

only difference lies in the resultant deformation patterns when the variables associated with the crack are active. As an illustration of this fact we represent in figure 4.11 how modes m9 and m10 of table 4.1 would appear in the example in figure 4.10(b).

In the remainder of this section it will be shown that the possibility of expanding  $I^h$  in a systematic way, when a reduced integration rule is used, is important to formulate strategies to alleviate volumetric locking.

**Tip elements:** The numerical integration on elements containing a crack tip may be performed with similar rules as those displayed on figure 4.12, in which Delaunay triangulation was performed in the set of points consisting of the nodes, the crack tip and the intersection of the crack and its extension with the element edges, resulting in

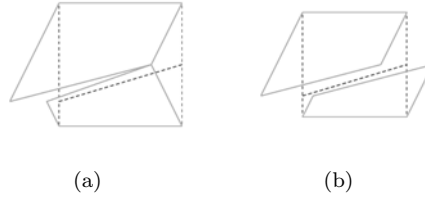


FIGURE 4.11: Deformation pattern obtained for the element 4.10(b): a) mode m9; b) mode m10.

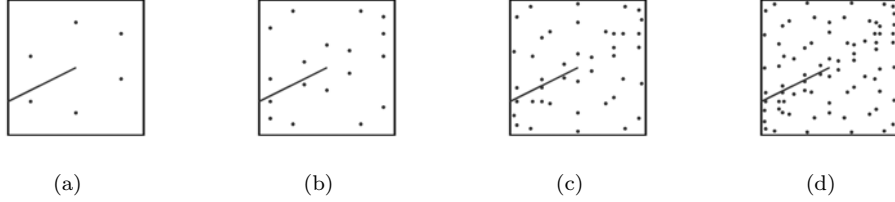


FIGURE 4.12: Integration rules for an element partially cut by a crack, considering subdivision into six triangles, with: a) one Gauss point per triangle; b) three Gauss points per triangle; c) seven Gauss points per triangle; d) thirteen Gauss points per triangle.

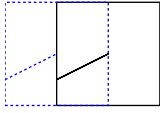
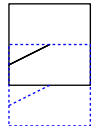
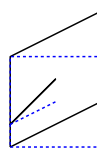
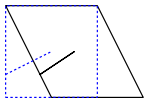
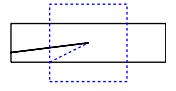
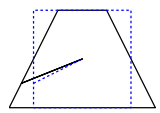
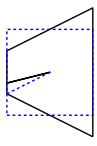
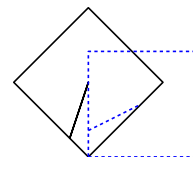
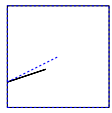
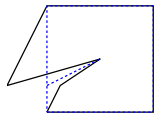
six triangles. A similar construction may be obtained by simply connecting the crack tip to the nodes, but with that construction, some Gauss points may be in line with the crack, which implies an undefined value for the Heaviside function.

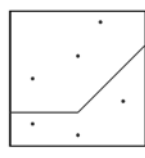
Independently of the type of tip enrichment used (order 0, 1 or 3), the basis of the null space of the matrix  $\mathbf{Q}$  contains ten linearly independent incompressible deformation modes, when one Gauss point per triangle is used, and only five linearly independent incompressible deformation modes when more than one Gauss point per triangle are employed. One possible basis for the null space of  $\mathbf{Q}$  is represented in table 4.2. It is interesting to observe that using a complete integration rule for the tip element, it is not possible to reproduce *bending* modes, similar to m6 and m7 in table 4.2, as in the standard 4-nodes element. Once more we verify that numerical integration with a reduced number of Gauss points expands the space of admissible incompressible deformations.

**Elements containing crack kinks:** When a discontinuity changes direction inside an element, usually the triangulation technique results in a larger number of triangles, and consequently, in a larger number of Gauss points on each side of the crack.

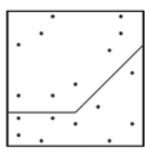
Therefore we start by analyzing the incompressible deformation modes of the crack configuration represented in figure 4.13. A possible basis for the space of admissible

TABLE 4.2: A possible basis for the incompressible deformation space of an element containing a discontinuity tip.

| Incompressible deformation modes reproduced by all the integration rules          |                                                                                   |                                                                                   |                                                                                     |                                                                                     |
|-----------------------------------------------------------------------------------|-----------------------------------------------------------------------------------|-----------------------------------------------------------------------------------|-------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------|
|  |  |  |  |  |
| m1                                                                                | m2                                                                                | m3                                                                                | m4                                                                                  | m5                                                                                  |
| Incompressible deformation modes only reproduced by a reduced integration rule    |                                                                                   |                                                                                   |                                                                                     |                                                                                     |
|  |  |  |  |  |
| m6                                                                                | m7                                                                                | m8                                                                                | m9                                                                                  | m10                                                                                 |



(a)



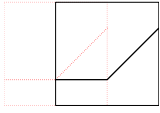
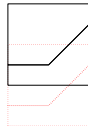
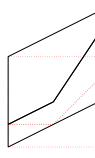
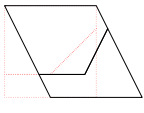
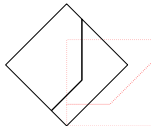
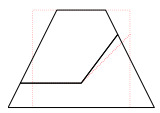
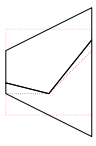
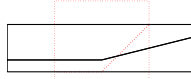
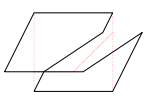
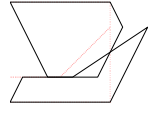
(b)

FIGURE 4.13: Possible crack configuration containing a kink, considering subdivision in to six triangles, three in each side of the crack, with a) one Gauss point per triangle, b) three Gauss points per triangle.

incompressible deformations of this type of element is represented in table 4.3, for either one Gauss point per triangle (figure 4.13(a)) and three Gauss points per triangle (figure 4.13(b)). It stands out that the structure of the basis is very similar to table 4.1, with exception of the modes m11 and m12 that are not reproducible by this type of element. Nevertheless, for some different configurations, as exemplified in figure 4.14, it is possible to add one mode, giving a total of eleven linearly independent incompressible deformations, when only one Gauss point per triangle is employed. In fact, this number depends on the total number of Gauss points inside the element and on the ratio between points above the crack and points below the crack.

**3D elements:** The study of incompressible deformation modes has been focusing on 2D elements, but, in fact, hexahedral elements follow the same pattern of the previously described elements, and we may say that similar observations as described so far are somehow extendable to 3D elements. As referred in the begining of this section, hexahedral finite elements crossed by discontinuity planes may be divided in tetrahedrons

TABLE 4.3: A possible basis for the incompressible deformation space of an element totally crossed by a discontinuity.

| Incompressible deformation modes reproduced by all the integration rules          |                                                                                   |                                                                                   |                                                                                    |                                                                                     |
|-----------------------------------------------------------------------------------|-----------------------------------------------------------------------------------|-----------------------------------------------------------------------------------|------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------|
|  |  |  |  |  |
| m1                                                                                | m2                                                                                | m3                                                                                | m4                                                                                 | m5                                                                                  |
|  |  |  |  |  |
| m6                                                                                | m7                                                                                | m8                                                                                | m9                                                                                 | m10                                                                                 |

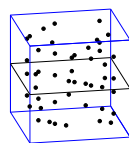


(a)

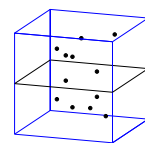


(b)

FIGURE 4.14: Possible crack configurations containing crack kinks, with integration rules obtained considering subdivision into six triangles, four in one side of the crack and two in the other side.



(a)

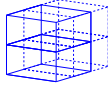
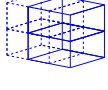
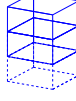
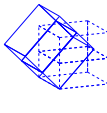
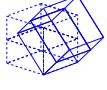
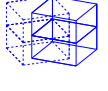
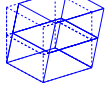
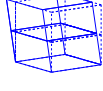
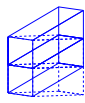
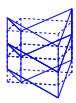
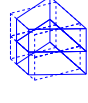
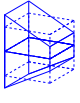
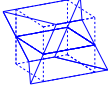
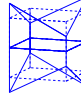
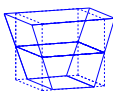
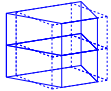
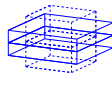
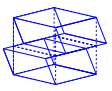
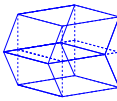
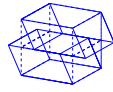
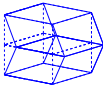
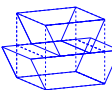
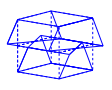
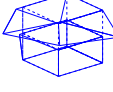
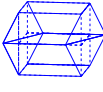
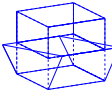
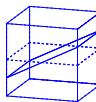
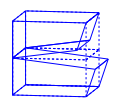
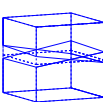


(b)

FIGURE 4.15: Examples of integration rules obtained for cracked hexahedrons: a) four points per tetrahedron; b) one point per tetrahedron.

conforming the crack plane, in which a regular Gaussian rule is applied, as shown in figure 4.15. For example, for an hexahedral element with  $1 \times 12$  Gauss points, corresponding to an element subdivision of twelve tetrahedrons, there are thirty seven linearly independent admissible incompressible deformation modes, whereas considering  $4 \times 12$  Gauss points, for the same subdivision in twelve tetrahedrons, it is only possible to reproduce thirty four linearly independent modes. A complete basis for  $I^h$  is represented in table 4.4.

TABLE 4.4: A possible basis for the incompressible deformation space of an element totally crossed by a discontinuity.

| Incompressible deformation modes reproduced by all the integration rules            |                                                                                     |                                                                                     |                                                                                       |                                                                                       |
|-------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------|
|    |    |    |    |    |
| m1                                                                                  | m2                                                                                  | m3                                                                                  | m4                                                                                    | m5                                                                                    |
|    |    |    |    |    |
| m6                                                                                  | m7                                                                                  | m8                                                                                  | m9                                                                                    | m10                                                                                   |
|    |    |    |    |    |
| m11                                                                                 | m12                                                                                 | m13                                                                                 | m14                                                                                   | m15                                                                                   |
|  |  |  |  |  |
| m16                                                                                 | m17                                                                                 | m18                                                                                 | m19                                                                                   | m20                                                                                   |
|  |  |  |  |  |
| m21                                                                                 | m22                                                                                 | m23                                                                                 | m24                                                                                   | m25                                                                                   |
|  |  |  |  |  |
| m26                                                                                 | m27                                                                                 | m28                                                                                 | m29                                                                                   | m30                                                                                   |
|  |  |  |  |                                                                                       |
| m31                                                                                 | m32                                                                                 | m33                                                                                 | m34                                                                                   |                                                                                       |
| Incompressible deformation modes only reproduced by a reduced integration rule      |                                                                                     |                                                                                     |                                                                                       |                                                                                       |
|  |  |  |                                                                                       |                                                                                       |
| m35                                                                                 | m36                                                                                 | m37                                                                                 |                                                                                       |                                                                                       |

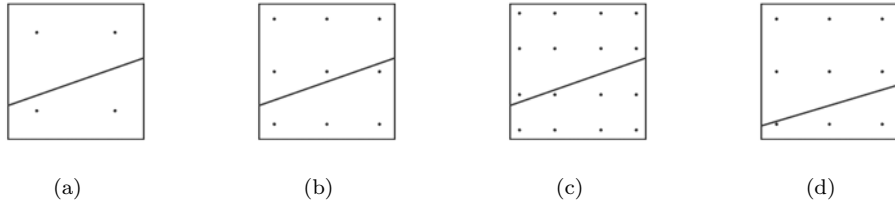


FIGURE 4.16: Regular Gaussian quadrature rules applied to an element crossed by a discontinuity: a) four Gauss points; b) nine Gauss points; c) sixteen Gauss points; d) nine Gauss points.

Once more, we conclude that is possible to expand the basis of incompressible deformation modes by using a reduced integration rule, which will be crucial to control volumetric locking.

#### 4.2.2.2 Regular Gauss point distribution

The simplest strategy to avoid the subdivision of the finite elements for integration purposes consists of placing a large number of Gauss points whose position is fixed in the element, and therefore does not adjust to the crack path [110–112], as illustrated in figure 4.16.

Although this technique is relatively simple, the characterization of the underlying space of incompressible deformations associated with each Gauss point distribution may not be as systematic as in the case of element subdivision. For example, in the configurations given in figure 4.16 it was expected that  $I^h$  could be characterized by the same basis for the cases in figure 4.16(b) and 4.16(d). Nevertheless the dimension of  $I^h$  is higher in the second case.

In fact, in this case, the number of linearly independent incompressible modes depends not only on the number of Gauss points but also on the particular crack configuration. In figure 4.16(a), the integration rule yields the same solution as the one in which only one Gauss point per triangle is used in the strategy defined in section 4.2.2.1, and the twelve modes represented in table 4.1 are reproducible; for higher number of Gauss points like in figures 4.16(b)-4.16(c), or even twenty-five or sixty-four Gauss points, only the first ten modes are included in the basis of  $I^h$ . Nevertheless, when the crack configuration is slightly changed, as illustrated in figure 4.16(d), the number of linearly independent incompressible deformation modes increases to eleven, when only ten modes were expected.

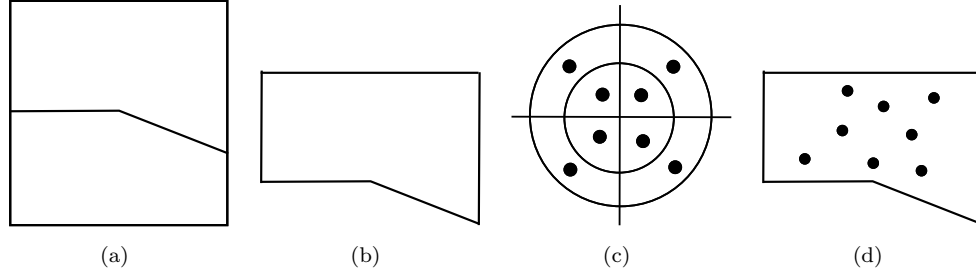


FIGURE 4.17: Application of the Schwarz-Christoffel conformal mapping to build an integration rule for elements crossed by a discontinuity: a) cracked element; b) polygon that will be mapped to the unit disk; c) unit disk containing the Gauss point positions; d) final Gauss point distribution on the upper part of element a).

These results suggest that when the integration rule does not conform the discontinuity, more likely spurious deformation modes may arise and the construction of strategies to avoid locking may not be so systematic as in the case of element subdivision. In addition, this strategy can become computationally more expensive than the referred subdivision due to the much larger number of Gauss points that has to be used to obtain the same accuracy.

#### 4.2.2.3 Schwarz-Christoffel conformal mapping

Another possible strategy used to avoid the subdivision of finite elements to perform numerical integration, based on the Schwarz-Christoffel conformal mapping was proposed by Natarajan et al. [18]. The Schwarz-Christoffel conformal mapping is an angle preserving transformation, which maps the complex upper half-plane,  $z = \{\zeta \in \mathbb{C} : \text{Im}\zeta > 0\}$  to the interior of a polygon. Mathematically it may expressed as a function  $f(\zeta)$ ,  $\zeta \in \mathbb{C}$ , as follows:

$$f(\zeta) = \int^{\zeta} \frac{K}{(w-a)^{\alpha/\pi}(w-b)^{\beta/\pi}(w-c)^{\gamma/\pi} \dots} dw \quad (4.29)$$

where  $K$  is a constant,  $\alpha, \beta, \gamma, \dots$  are the interior angles of the polygon and  $a, b, c, \dots$  are the values, along the real axis of the  $z$ -plane, of the vertices of the polygon.

To apply this transformation to enriched XFEM elements, each polygon belonging to an element cut or intersected by a crack is mapped onto a unit disk (figure 4.17) through the inverse of the described function. The unit disk contains equally spaced Gauss points on the complex plane, which are mapped back into the original polygon by the transformation function [119, 132].

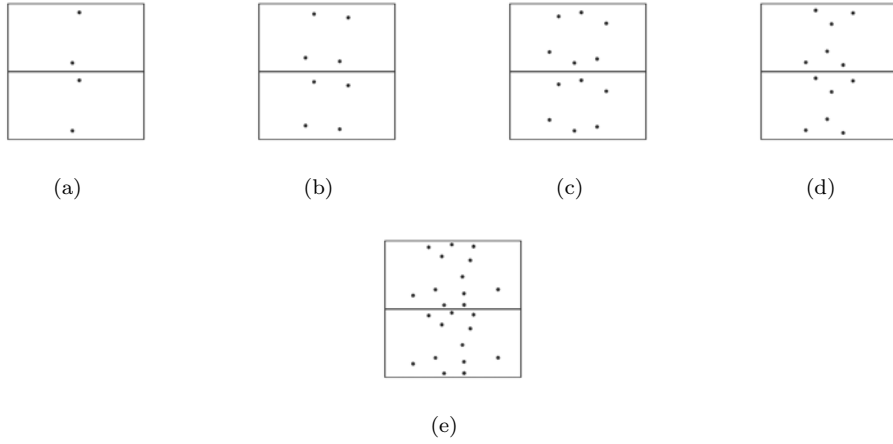


FIGURE 4.18: Integration rules built using the Schwarz-Christoffel conformal mapping: a) four Gauss points; b) eight Gauss points; c) twelve Gauss points; d) twelve Gauss points; e) twenty-four Gauss points. . These figures were created making use of the MATLAB SC Toolbox [1].

The Schwarz-Christoffel conformal mapping technique may be applied to an element totally crossed by a crack to construct the integration rules represented in figure 4.18. There is a certain freedom to distribute the Gauss points depending on the subdivision of the unit circle, as illustrated by figures 4.18(c) and 4.18(d), where twelve Gauss points are distributed in a different way. In line with the previous sections, equation 4.20 was applied to the integration rules of figure 4.18 to characterize the space of admissible incompressible deformations. Results exhibit the same structure of section 4.2.2.1, that is, twelve linearly independent incompressible deformation modes for four Gauss points (figure 4.18(a)), which corresponds to one Gauss point per triangle, when element subdivision is used, and ten linearly independent incompressible deformation modes when more than four Gauss points are employed (figures 4.18(b)-4.18(e)). A possible basis for  $I^h$  is also represented in table 4.1. Therefore, we conclude that the incompressible deformation modes associated to integration rules built with the Schwarz-Christoffel conformal mapping are exactly the same as the ones obtained with the subdivision in triangular sub cells technique, as long as the number of Gauss points above and below the crack is equal for both methods.

Although this methodology suppresses the need of sub cells, it does not bring any advantage in terms of incompressible problems. Moreover, it requires solving two differential equations for each element totally crossed by a crack, which is computationally more expensive than to subdivide the element in triangular sub cells, and, as additional disadvantage, it is not readily extendable to 3D problems.

### 4.2.3 Finite element formulations for incompressibility

The results previously obtained have shown, as expected, that it is possible to expand the space of admissible incompressible deformations, when an integration rule with a reduced number of Gauss points is used in the constraint equation which defines the incompressibility condition. Nevertheless these rules may introduce spurious deformation modes that should be controlled. This fact suggests that classical methods used to avoid locking in the framework of FEM, namely the B-bar method [123] and the F-bar method [127], should be used in conjunction with XFEM elements in order to prevent volumetric locking whilst preventing spurious deformation modes.

#### 4.2.3.1 B-bar method

The B-bar method [123] is based on the additive decomposition of the matrix of the shape functions derivatives,  $\mathbf{B}$ , into a volumetric component,  $\mathbf{B}_{dil}$  and a deviatoric component,  $\mathbf{B}_{dev}$ , as follows:

$$\mathbf{B}_{dev} = \mathbf{B} - \mathbf{B}_{dil} \quad (4.30)$$

To avoid volumetric locking,  $\mathbf{B}_{dev}$  is integrated with a complete Gaussian rule, whereas  $\mathbf{B}_{dil}$  is integrated with a reduced Gaussian rule, which is able to reproduce a larger number of admissible incompressible deformations than the complete counterpart. In 2D problems, the B-bar formulation is usually applied to low order quadrilateral elements and  $\mathbf{B}_{dev}$  is calculated using 4 Gauss points and  $\mathbf{B}_{dil}$  is calculated only for one Gauss point in the center of the element, as shown on figure 4.19(b), while in 3D problems, the complete integration rule consists of eight Gauss points and the reduced integration rule consists of one Gauss point in the center of the hexahedral element.

Here we propose to extend the B-bar methodology to elements crossed by discontinuities, based on the element subdivision procedure of section 4.2.2.1. Thus, in these finite elements the deviatoric part of the  $\mathbf{B}$  matrix is calculated using a 3 points per triangle rule or four points per tetrahedron in 2D and 3D problems, respectively, while the volumetric contribution of each Gauss point is calculated in the center of corresponding triangle (figure 4.19) or tetrahedron. As the numerical integration rule consisting of one point per triangle is able to reproduce more incompressible deformation modes than the higher order rules, this methodology efficiently alleviates the volumetric locking in infinitesimal strain problems, as will be later illustrated with some numerical examples.

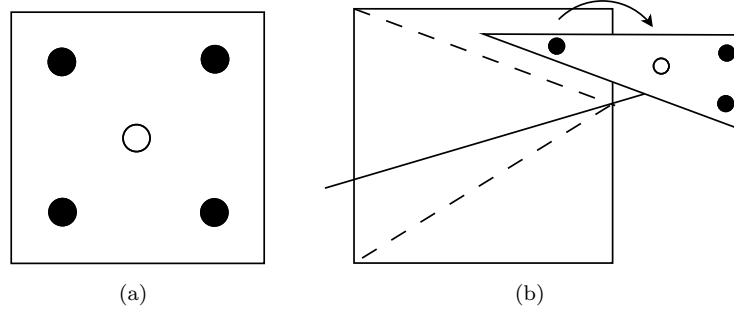


FIGURE 4.19: Integration rule for a regular 4-nodes element: 1 Gauss point for the reduced rule and 4 Gauss points for the complete rule; b) Integration rule for an element crossed by a discontinuity: 1 Gauss point per triangle as a reduced rule and 3 Gauss points per triangle as a complete rule.

Although the extension of this methodology to XFEM is straightforward, it should be noticed that for cracked elements, the  $\mathbf{B}$  matrix contains some extra terms due to the enrichment functions.

#### 4.2.3.2 F-bar method

For problems involving finite deformations, one of the simplest ways of taking advantage of the expansion of the incompressible deformation space, when a reduced integration rule is used, is through the F-bar method [63, 127]. While B-bar is based on the additive decomposition of the  $\mathbf{B}$  matrix, the F-bar is based on the multiplicative decomposition of the deformation gradient [65–67], as described in chapter 2:

$$\mathbf{F} = \mathbf{F}_{dev} \mathbf{F}_{vol} \quad (4.31)$$

where

$$\mathbf{F}_{dev} = (\det \mathbf{F})^{-\frac{1}{3}} \mathbf{F} = J^{-\frac{1}{3}} \mathbf{F} \quad (4.32)$$

$$\mathbf{F}_{vol} = (\det \mathbf{F})^{\frac{1}{3}} \mathbf{I} = J^{\frac{1}{3}} \mathbf{I} \quad (4.33)$$

The F-bar deformation gradient is simply obtained by replacing the regular volumetric part by the volumetric part,  $\mathbf{F}_0$ , calculated at the centroid of the element (for a 4-node quadrilateral or a 8-node hexahedron), reading:

$$\bar{\mathbf{F}} = \mathbf{F}_{dev}(\mathbf{F}_0)_{vol} = \left( \frac{\det \mathbf{F}_0}{\det \mathbf{F}} \right)^{\frac{1}{3}} \mathbf{F} = \left( \frac{J_0}{J} \right)^{\frac{1}{3}} \mathbf{F} \quad (4.34)$$

The application of the F bar method to enriched elements follows the same principle as the B-bar method, hence, constructing the numerical integration rules in a sub triangulation base, for each Gauss point of the complete rule (typically 3 Gauss points per triangle/4 Gauss points per tetrahedron), the volumetric part of the deformation

gradient,  $\mathbf{F}_0$ , will be calculated at the centroid of the respective triangle/tetrahedron (figure 4.19).

As in the B-bar formulation, it should be noticed that the deformation gradient of the elements crossed by discontinuities contains some extra terms associated with the enrichment of the displacements, which is clear when  $\mathbf{F}$  is defined in terms of the displacement field:

$$\mathbf{F} = (\mathbf{I} + \nabla \mathbf{u}) \quad (4.35)$$

Therefore, considering a general enrichment function,  $\psi$ , and respective associated degrees of freedom,  $\boldsymbol{\psi}$ , the deformation gradient can be written as:

$$\mathbf{F} = \mathbf{I} + \sum_{i=1}^n \mathbf{u}_i \otimes \nabla_X N_i + \sum_{j=1}^m \boldsymbol{\psi}_j \otimes \nabla_X N_j \psi \quad (4.36)$$

recalling that  $\nabla_X$  denotes the gradient with respect to the reference configuration, usually implying a coordinate transformation to the isoparametric mapping. Departing from the enriched form of the deformation gradient it is easy to adapt a finite strain code to include XFEM enrichment functions. Readers may consult references [133–135] for details.

The presented extension of the B-bar and F-bar methodologies to XFEM is expected to alleviate locking in fracture problems where the satisfaction of the incompressibility constraint plays a major role. Therefore, the performance of these techniques will be illustrated in the next section with some numerical examples involving linear and non-linear materials.

#### 4.2.4 Numerical examples

In this section, the conclusions regarding the numerical integration strategies and their ability to reproduce incompressible states will be illustrated through some numerical examples, not only focusing on each type of enriched element by itself, but also analysing their influence when inserted in a mesh.

In the examples incompressibility in a XFEM framework is addressed in both small and finite strain problems.

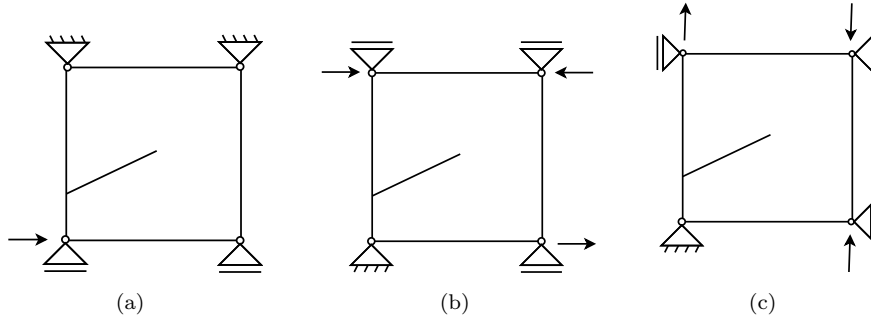


FIGURE 4.20: Test examples for single element containing a crack.

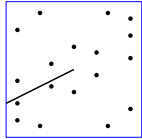
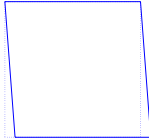
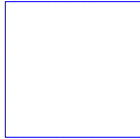
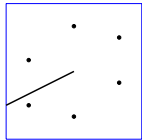
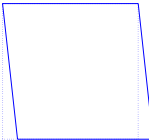
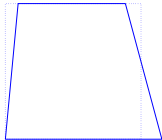
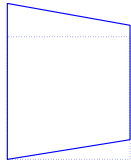
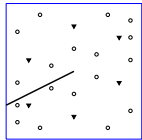
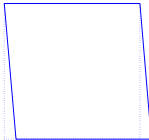
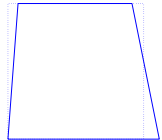
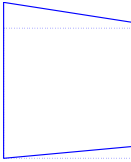
#### 4.2.4.1 Single Element

Analysing table 4.2 from section 4.2.2.1, it is prominent the absence of the deformation modes m6 and m7 for a complete integration rule, while the mode m4 may be reproduced by both complete and reduced integration rules. This fact suggested the single element test illustrated in figure 4.20, where a 4-node element in a plane strain condition is submitted to 3 different loading scenarios. The material considered is linear elastic and the nearly incompressible behavior is obtained setting the value of the Poisson coefficient to  $\nu = 0.499999$ . The Young's Modulus has a value of  $E = 10^3$  and the load is unitary. All the quantities are supposed to be expressed in a consistent unit system. The element contains a crack segment starting at one quarter of an edge and finishing at the element center. The element edges have length 2.

In this analysis, the complete integration rule consists of eighteen integration points placed on six sub-triangles and the reduced integration rule consists of a single integration point per triangle. The B-bar technique is applied for the combination of these two rules as previously described. The tip enrichment is the one as defined in equation 4.8. In the table 4.5 it is possible to observe the deformed configuration obtained as a function of the loading and integration rule used.

As it was expected, using a complete integration rule, the element exhibits volumetric locking for the cases b) and c) in figure 4.20. Differently, both reduced integration and B-bar methodologies are able to reproduce the correct deformations and do not present any locking behaviour. Nevertheless, the reduced integration may encompass some drawbacks when used on a finite element mesh, which will become clearer in the following numerical examples.

TABLE 4.5: Deformed configurations for different integration rules.

| Integration Rule                                                                              | a                                                                                  | Problem<br>b                                                                        | c                                                                                    |
|-----------------------------------------------------------------------------------------------|------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------|
| <br>Complete |   |    |   |
| <br>Reduced  |   |   |   |
| <br>B-bar   |  |  |  |

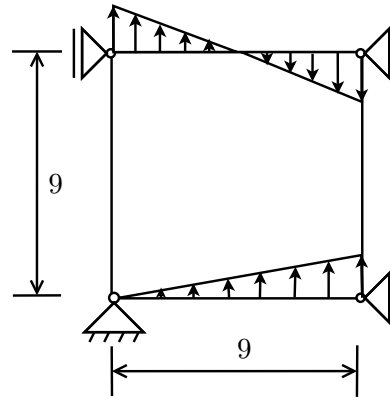


FIGURE 4.21: Cracked plate with respective boundary conditions.

#### 4.2.4.2 Incompressible behavior of XFEM elements in a mesh

The problems presented in this section intend to analyse the influence of enriched elements within a mesh under an incompressibility constraint. A similar example as the previous one is tested with two types of mesh, containing regular and enriched elements as shown in figure 4.21. The material properties are the same as in the previous example. The plate is discretized with a coarse mesh and with a fine mesh containing regular and enriched finite elements, as can be observed in figures 4.21 and 4.22.

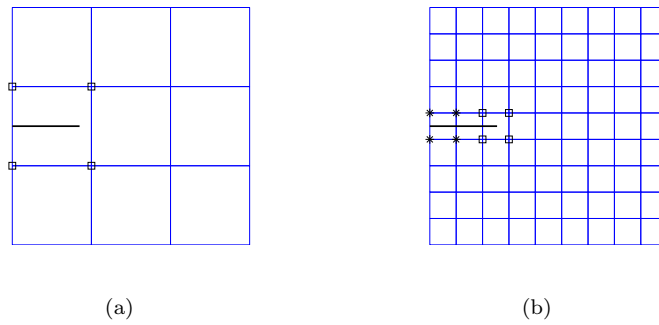


FIGURE 4.22: a) Coarse finite element mesh. b) Fine finite element mesh.

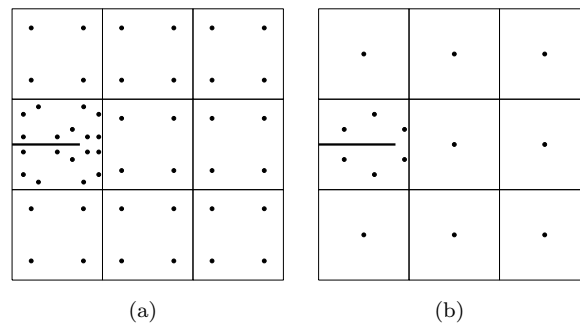


FIGURE 4.23: a) Complete integration rule; b) reduced integration rule.

For each type of element, different integration rules are considered, i. e., a complete integration rule and a reduced integration rule for regular elements consisting of four Gauss points and one Gauss point, respectively. For the enriched element, sub triangulation is applied with three Gauss points per triangle for a complete integration rule and one Gauss point per triangle for a reduced integration rule, as can be observed in figure 4.23.

To investigate the locking effects and the efficiency of the proposed B-bar methodology, four types of integration schemes are tested:

- (a) Complete integration rule for all the elements
- (b) Reduced integration rules for all the elements
- (c) B-bar methodology applied only to the regular finite elements
- (d) B-bar methodology for both regular and enriched finite elements

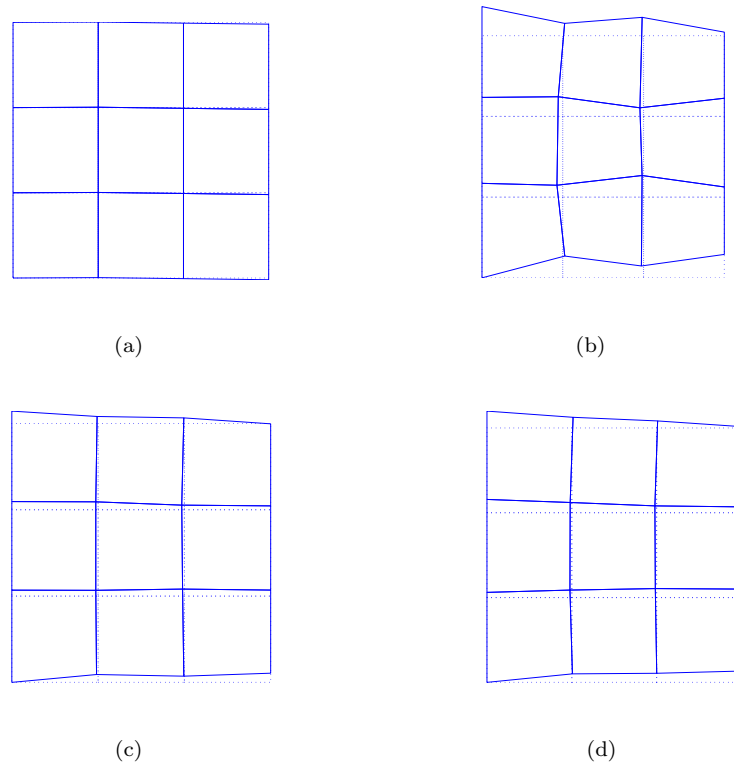


FIGURE 4.24: Deformed configurations for different integration schemes: a) complete integration rule for all the elements; b) reduced integration rules for all the elements; c) B-bar methodology applied only to the regular finite elements; d) B-bar methodology for both regular and enriched finite elements.

Next the results obtained for each integration scheme applied to each one of the meshes are presented and discussed.

**Coarse Mesh** The coarse mesh used (figure 4.22(a)) consists of nine 4-node elements, including one cracked element. The deformed configurations obtained for each integration scheme are represented in figure 4.24 for a certain level of applied load. The third degree tip enrichment function (equation 4.8) is used, although no perceptible differences were detected when using other enrichment  $R$  functions (equations 4.6-4.7).

The volumetric locking problem is evident when a complete integration rule is employed, as the deformed configuration overlaps the initial configuration (figure 4.24(a)). Moreover, using purely reduced integration, a non-physical solution arises as depicted in figure 4.24(b).

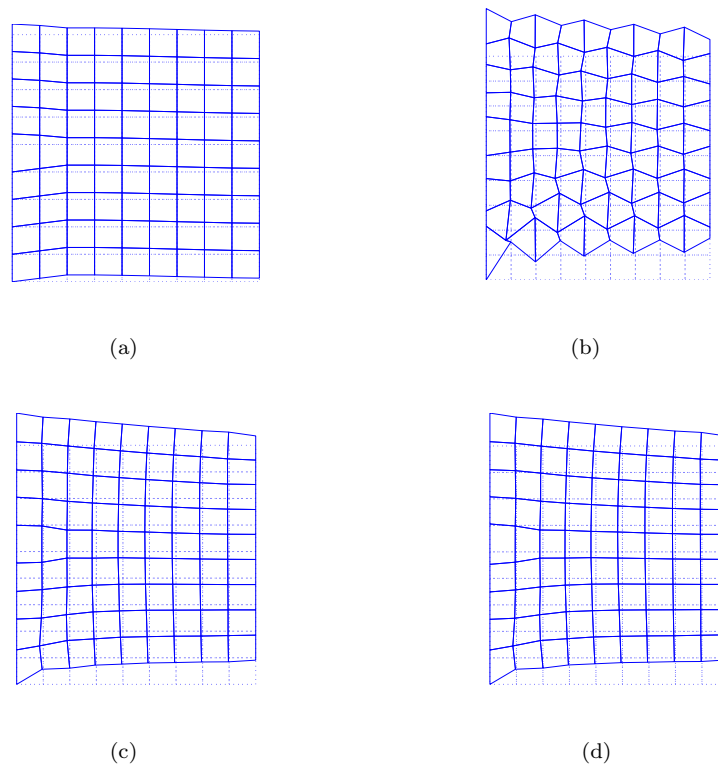


FIGURE 4.25: Deformed configurations for different integration schemes: a) complete integration rule for all the elements; b) reduced integration rules for all the elements; c) B-bar methodology applied only to the regular finite elements; d) B-bar methodology for both regular and enriched finite elements.

Applying the classical B-bar formulation to the regular finite elements (figure 4.24(c)), the locking is attenuated but it only vanishes when the methodology is also used for the enriched element (figure 4.24(d)). In fact, observing figure 4.24(c), it is perceptible that the element containing the crack only undergoes a rigid body motion, while in figure 4.24(d), the element reproduces the expected *bending* mode.

**Fine Mesh** In a general problem involving the XFEM, not only the tip enrichment will be present but also Heaviside enrichment for the elements totally cut by the crack, which is the case when a fine mesh is used.

The results follow the trend of the previously obtained with the coarse mesh, as can be observed in figure 4.25. These images were obtained using the tip enrichment from equation 4.6 and, as referred for the previous example, there are no major differences when using the enrichments from equations 4.6 and 4.7. Once more are clear the volumetric locking caused by the complete integration rule (a) and the *hour-glass* effect

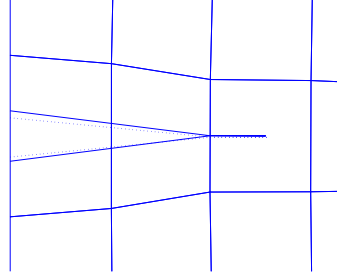


FIGURE 4.26: Crack opening for integration schemes c (line) and d (dashed line).

produced by the reduced rule (b). With the mesh refinement, the necessity of applying the B-bar formulation to both regular and enriched elements is not so obvious, as integration schemes c) and d) result in similar deformation patterns.

Nevertheless, there is still some volumetric locking of the tip element that only becomes evident when the crack opening is computed (figure 4.26). In fact, when B-bar is not applied in the XFEM elements, the element containing the crack tip only undergoes a rigid body motion instead of reproducing the expected *bending* mode. Although the differences in the crack opening are not perceptible for the tip element, the locking behaviour affects the surrounding elements and, as a consequence, the total crack opening diminishes.

The crack opening distance may be crucial for crack propagation and failure predictions, increasing the importance of the presented B-bar methodology.

#### 4.2.4.3 Cook's membrane problem

The following benchmark problem, often referred as Cook's Membrane, is commonly used to assess finite elements under shear and bending, for both linear and non linear analysis [126, 136, 137]. Here it is slightly modified from its original version to include a crack, in line with reference [129].

The problem consists of a trapezoidal panel clamped on one end and subjected to a shearing-load on the other, as displayed in figure 4.27.

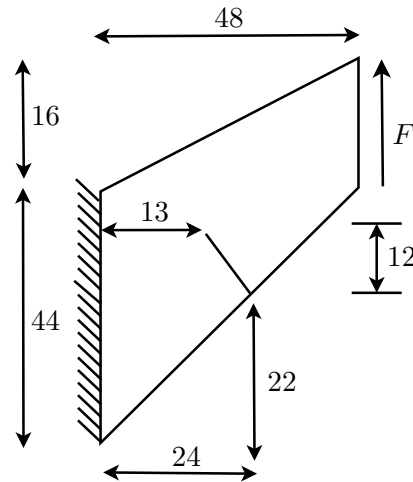


FIGURE 4.27: Cook's membrane problem.

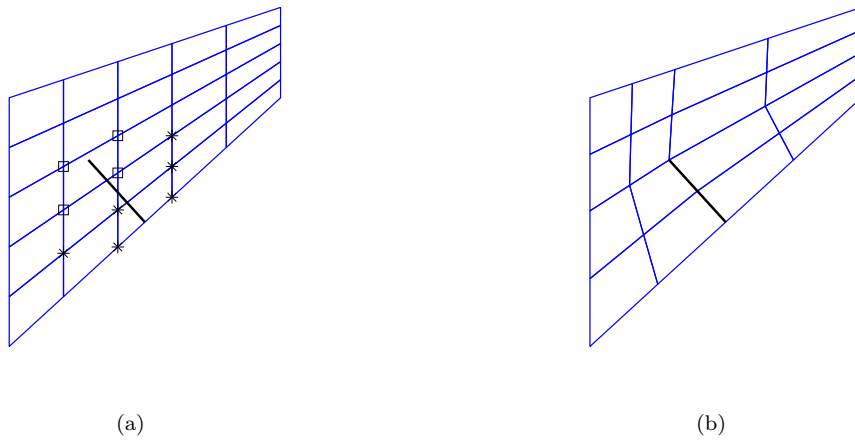


FIGURE 4.28: a) Example of a mesh with the crack modeled through enrichment. b) Example of a mesh containing a crack explicitly modeled.

**Small Strain Analysis** For a small strain analysis, once more we consider a linear elastic material characterized by a Poisson coefficient of  $\nu = 0.49999$  and Young's Modulus of  $E = 240565$  MPa. A distributed load of  $F = 10$  N is applied according to figure 4.27. The crack is modeled using the XFEM enrichment, considering the Heaviside enrichment for elements totally crossed by the crack and the tip enrichment for the elements partially cut.

The analysis of the top right vertical displacement is carried out for increasingly refined meshes and, in order to have a reference solution, the crack is explicitly modeled using traditional finite elements conforming its geometry (figure 4.28).

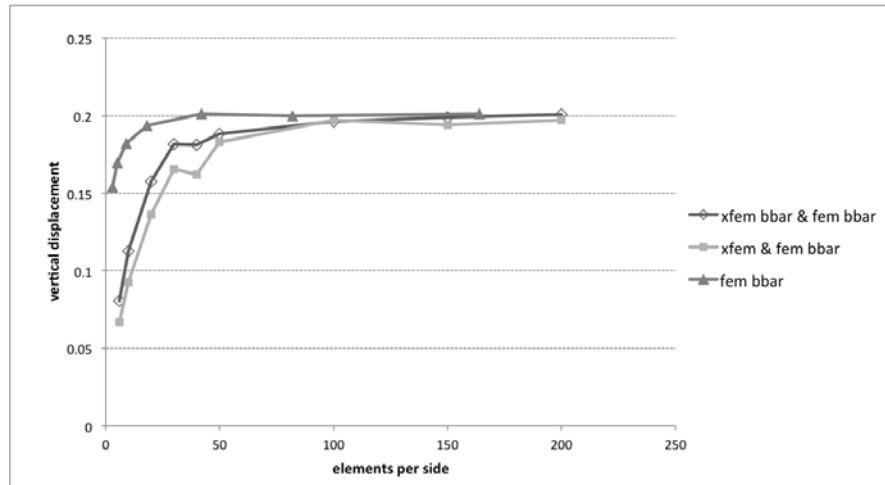


FIGURE 4.29: Vertical displacement of the top right corner node, as a function of the number of elements per side, for the explicitly meshed crack and enriched crack.

Adopting the strategy from the previous examples, two distinct integration schemes are compared:

- (a) B-bar methodology applied only on the regular finite elements (xfem & fem bbar);
- (b) B-bar methodology applied to regular finite elements and to enriched elements (xfem bbar & fem bbar).

In the explicitly meshed crack the B-bar technique is applied in all the finite elements (fem bbar).

In the chart of Figure 4.29 is represented a plot of the top right vertical displacement as a function of the number of elements in the mesh. The tip enrichment employed is the one of a polynomial type as defined in equation 4.8. Figure 4.29 indicates that is advantageous to apply the B-bar formulation to both XFEM and regular finite elements. As expected, the enriched solutions converge a bit slower than the explicitly meshed solution. However, in problems involving crack growth the enriched approach can have other compensating advantages, such as the absence of the necessity of remeshing, straightforward incorporation of cohesive laws and introduction of analytical solutions into the general displacement approximation.

To finalize this study, in figure 4.30 a comparison is made between the different types of tip functions, in which the B-bar methodology was applied to all the finite elements. As can be observed, the lower order tip functions converge slightly faster to the solution.

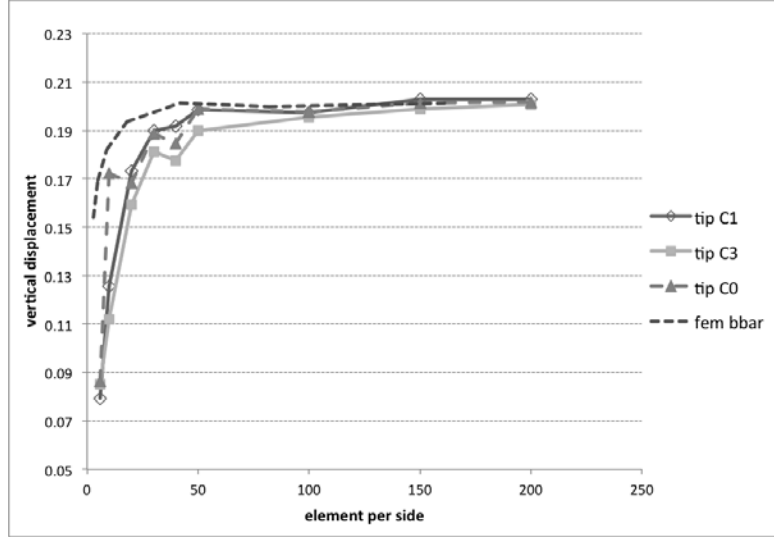


FIGURE 4.30: Comparison of the vertical displacement of the top right corner node, as a function of the number of elements per side, for different tip enrichment functions.

**Finite Strain Analysis** In this section the same example but at finite strains is used to evaluate the performance of the proposed extension of F-bar formulation to XFEM and compare it with the enhanced strain formulation for XFEM proposed by Dolbow et al. [129]. A hyperelastic material response governed by the following stored energy function,  $W$ , is considered:

$$W = \frac{\mu}{2} [J^{-\frac{2}{3}} \text{tr}[\mathbf{C}] - 3] + \frac{\kappa}{2} (J - 1)^2 \quad (4.37)$$

where  $\mu$  represents the shear modulus and  $\kappa$  the bulk modulus. The nearly incompressible behavior is obtained setting the material parameters as  $\kappa = 40.010^4$  Pa and  $\mu = 80.0$  Pa. In this type of constitutive behaviour, the relevant physical quantities can be derived directly from the energy function making it appealing for automatic differentiation and automatic code generation [84, 85]. Therefore, the previously described *AceGen* and *AceFEM* systems will be employed. In particular, for this hyperelastic problem, we will consider the volumetric/deviatoric split of the stored energy function [62, 138, 139], as follows:

$$W = W_{dev} + W_{vol} \quad (4.38)$$

$$W_{dev} = \frac{\mu}{2} [J^{-\frac{2}{3}} \text{tr}[\mathbf{C}] - 3] \quad (4.39)$$

$$W_{vol} = \frac{\kappa}{2} (J - 1)^2 \quad (4.40)$$

As outlined in chapter 3, using a Newton-Raphson procedure, the internal force,  $\mathbf{R}_e$ , may be obtained integrating, over the domain, the derivative of the strain energy in

respect to the displacement field. Consequently, the tangent stiffness matrix,  $\mathbf{K}_T$  is obtained as the derivative, in respect to the displacement field, of the internal force vector:

$$\mathbf{R}_e = \int_{\Omega} \frac{\partial W}{\partial \mathbf{u}} d\Omega \quad (4.41)$$

$$\mathbf{K}_T = \frac{\partial \mathbf{R}_e}{\partial \mathbf{u}} \quad (4.42)$$

Here, the derivative of the strain energy potential is presented in terms of the deviatoric part of second Piola-Kirchhoff tensor,  $\mathbf{S}$ , and the hydrostatic pressure  $p$ :

$$\frac{\partial W}{\partial \mathbf{u}} = \frac{1}{2} \mathbf{S}_{dev} : \frac{\partial \mathbf{C}_{dev}}{\partial \mathbf{u}} - p \frac{\partial J}{\partial \mathbf{u}} \quad (4.43)$$

with

$$\mathbf{S}_{dev} = (2 \frac{\partial W_{dev}}{\partial \mathbf{C}})_{dev} = 2 \frac{\partial W_{dev}}{\partial \mathbf{C}_{dev}} - \frac{2}{3} \text{tr}[\mathbf{C}_{dev} \frac{\partial W_{dev}}{\partial \mathbf{C}_{dev}}] \mathbf{C}_{dev}^{-1} \quad (4.44)$$

and

$$p = - \frac{\partial W_{vol}}{\partial J} \quad (4.45)$$

where  $\mathbf{C}_{dev}$  corresponds to the deviatoric part of the right Cauchy-Green tensor, depending on the deviatoric part of the deformation gradient,  $\bar{\mathbf{F}}$ :

$$\mathbf{C}_{dev} = \bar{\mathbf{F}}_{dev}^T \bar{\mathbf{F}}_{dev} = J^{-\frac{2}{3}} \mathbf{C} \quad (4.46)$$

With the *AceGen* system all the presented derivatives are calculated automatically and optimized. It should be noticed that the global vector of unknowns includes the displacements as well as the extra degrees of freedom introduced by the XFEM. The analysis is performed using *AceFem*.

For the analysis of the finite strain version of the Cook's Membrane, a load of 1 N is applied according to figure 4.27 during 30 load steps. Only the Heaviside enrichment is employed to model the crack. In line with the infinitesimal strain version, the vertical displacement of the top right corner is plotted as a function of the number of finite elements per edge. In addition the incompressibility constraint,  $J = \det \mathbf{F} = 1$ , is checked for all the Gauss points in the mesh.

Initially, in order to evaluate the model implementation in the *AceGen* system, the solution for the example with the explicitly meshed crack, illustrated in figure 4.28(b), is compared with the one obtained in reference [129]. As can be seen in figure 4.31 a

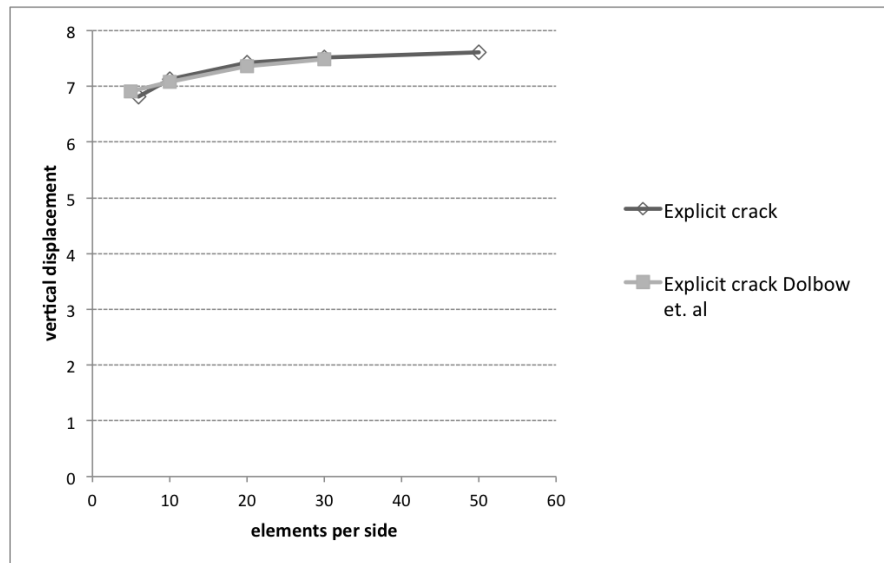


FIGURE 4.31: Vertical displacement of the top right corner node, as a function of the number of elements per side, obtained for the explicitly meshed crack of figure 4.28(b), using the F-bar methodology and the Enhanced strain approach used by Dolbow et al.

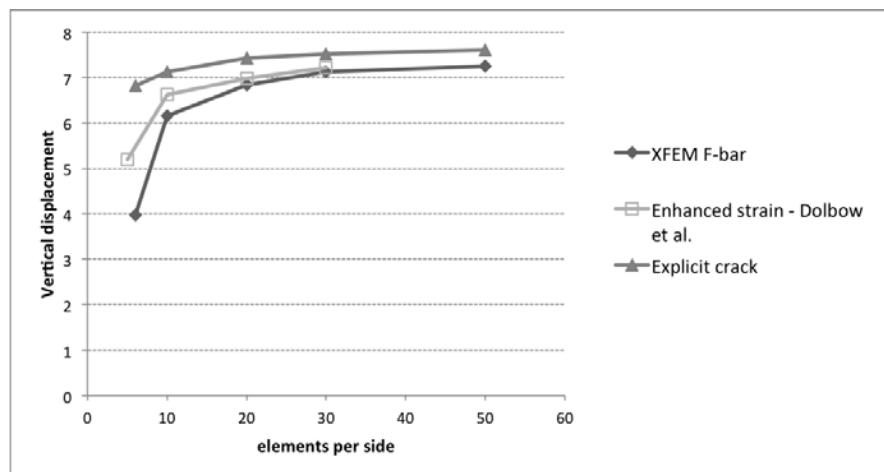


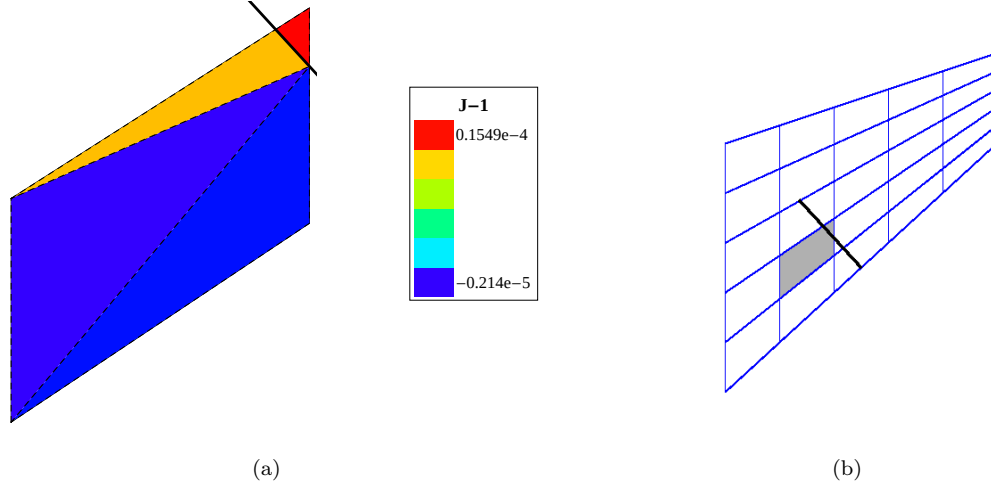
FIGURE 4.32: Comparison of the vertical displacement of the top right corner node, as a function of the number of elements per side, for explicitly meshed and enriched approximations using the F-bar methodology and the Enhanced Strain approach employed by Dolbow et al.

very good correlation is obtained.

Next the F-bar methodology applied to the XFEM is assessed. In figure 4.32 its results are compared with those obtained by Dolbow et al. [129] using the enhanced strain method and having as a reference solution the one with the crack explicitly meshed. Although, as expected, it converges slightly slower than the enhanced strain formulation developed by Dolbow et al., it reproduces better the incompressibility condition as can be observed in table 4.6. The F-bar methodology for XFEM approximates the incompressibility condition better than the Assumed Enhanced Strain approach developed by

TABLE 4.6: Maximum value of the deviation from the incompressibility condition,  $\max |J - 1|$ .

| Elements per side | Explicitly Meshed |                       | Enriched       |                       |
|-------------------|-------------------|-----------------------|----------------|-----------------------|
|                   | F-bar             | Enhanced Dolbow et al | F-bar for XFEM | Enhanced Dolbow et al |
| 5                 | 0.000030          | 0.0004                | 0.00048        | 0.018                 |
| 10                | 0.000047          | 0.0007                | 0.00047        | 0.024                 |
| 20                | 0.000075          | 0.0012                | 0.00046        | 0.025                 |
| 30                | 0.000093          | 0.0016                | 0.00044        | 0.030                 |

FIGURE 4.33: a) Maximum value of the deviation from the incompressibility condition,  $(J - 1)$ , in the element crossed by the crack marked in the mesh b).

Dolbow et al. Nevertheless, the value of  $J$  slightly depends on the mesh, namely, on the size of the triangles obtained during the sub cell division for integration. In general, the higher deviation from  $J = 1$  occurs around the crack tip, in the smaller sub cells, as depicted in figure 4.33.

Besides the good performance exhibited, the F-bar method is relatively simple to implement on computer programs, making the proposed approach for XFEM suitable for simulating crack propagation in problems involving large strains where incompressibility plays a major rule, such as in elasto-plastic materials.

### 4.3 Interaction with non-linear material models

In the previous section, suitable strategies for numerical integration in XFEM elements in the presence of incompressibility constraints were developed. Nevertheless, in a ductile fracture problem the crack path is not defined *a priori* but the discontinuities are

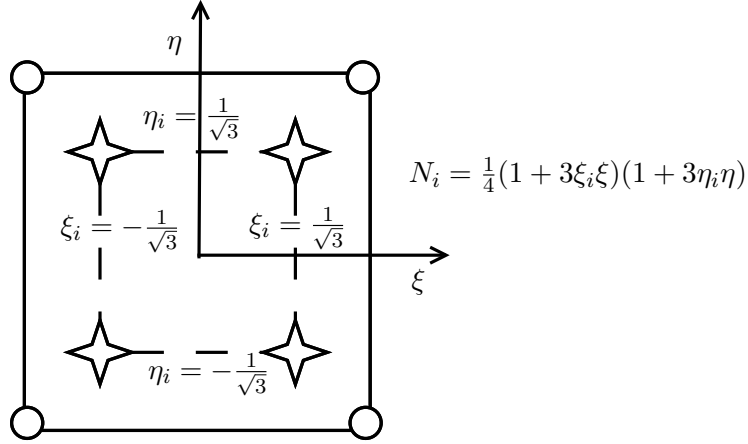


FIGURE 4.34: Definition of interpolatory shape functions used in the variable transfer.

rather introduced at some stage of material degradation. This means that the positions and weights of the Gauss points of a certain finite element may change during the problem analysis. As the Lemaitre model for damage presented in chapter 2 is history dependent, a proper variable transfer strategy has to be defined.

Here a local smoothing technique, consisting of a bilinear extrapolation of the quantities from the existing Gauss points to the new, using shape functions, is employed. This technique is used in reference [80] to transfer quantities stored in the Gauss points to the nodes. Basically, any variable in the new Gauss points,  $\alpha^{new}$ , may be obtained using the following expression:

$$\alpha^{new} = \sum_i^{ngpt} N_i^g \alpha_i \quad (4.47)$$

where  $\alpha_i$  represents the values of the variable  $\alpha$  at each one of the  $ngpt$  old Gauss points. The interpolatory shape functions are defined at the set of old Gauss points according to figure 4.34.

In the particular case of the damage model considered, the variables which reflect the history of the deformation are the plastic multiplier, the strain and the damage. The stresses may be recovered using the return-mapping equations.

It should be noticed that this technique differs from remeshing, as only the quantities stored in Gauss points are transferred inside the same finite element; the mesh, as well as the quantities stored in the nodes, such as the displacements, remain unchanged.

*Remark 4.2. Depending on the particular problem, different strategies to recover equilibrium, after the variable transfer may be required. These strategies are developed and discussed in chapter 5.*

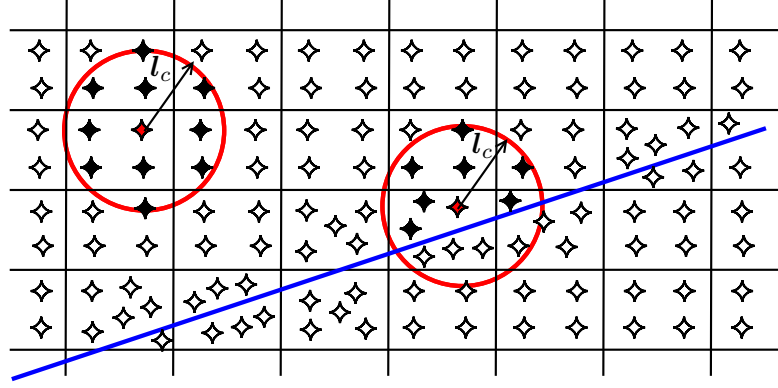


FIGURE 4.35: Group of Gauss points (in black) that influence a particular one. When a Gauss point is located near a discontinuity, only the points in the same side of the discontinuity is selected.

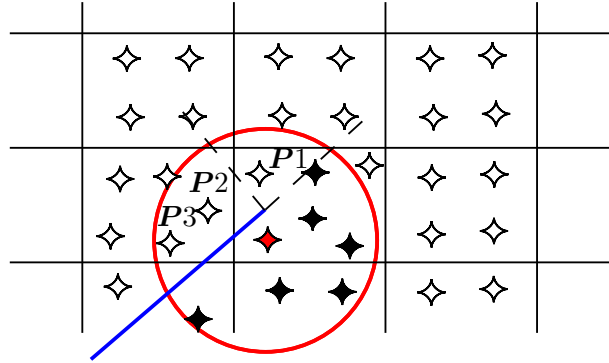


FIGURE 4.36: Group of Gauss points (in black) that influence a particular one, located near a crack tip.

In chapter 2, a non-local formulation to prevent mesh pathologies, when implementing the damage model was also presented. In this methodology, the characteristic length,  $l_c$ , determines which points should influence the history of a particular point  $x$  (figure 4.35). Nevertheless, when a crack is inserted in the mesh, its surfaces no longer interact, especially in the case of a traction-free crack. Therefore, the Gauss points near the interface should only be influenced by other Gauss points laying in the same side of the crack, as illustrated in figure 4.35.

If a point is located close to the crack tip, different selection criteria may be adopted. Considering only a normal level set function, all the points  $P1$ ,  $P2$  and  $P3$ , shown in figure 4.36, are excluded from the group of Gauss points influencing the red point. In the other hand, considering an additional tangent level set function,  $P1$  may be included in the set. Despite the different options, the influence in the results is nearly unnoticeable.

## 4.4 Conclusions

In this chapter the general formulation of the XFEM was presented, focusing in the enrichment functions suitable to describe a ductile fracture process. The basic implementation steps were outlined, followed by a comprehensive study of integration strategies, which is one most relevant parts of this chapter.

While in most of the existing studies on integration rules for XFEM, the accuracy of the integration schemes is based on the ability to reproduce the stress intensity factors in problems featuring known analytical solutions, here we favoured an approach based on the analysis of the underlying sub-space of incompressible modes embedded in the XFEM approximation. Several integration rules were compared in terms of the deformation modes that can actually be captured.

In general, considering the sub division of the elements crossed by a crack it is possible to expand the underlying sub-space of incompressible deformations using a reduced integration rule over each sub cell, when compared with full integration schemes. This fact motivated the extensions of B-bar and F-bar methodologies for XFEM, which somehow rely on the selective integration rules, with encouraging results.

In the final part of the chapter some more features required for the combination of the XFEM with non-linear materials, namely, the variable transfer and the non-local interaction, were also addressed.

All these techniques are useful in the study of the final stage of failure of materials which undergo large strain processes without noticeable volume changes, as it will be described in the following chapters.

## Chapter 5

# Ductile Fracture Model: Traction-Free Cracks

Material failure is often related to the development of micro-defects at the micro-structural level, in particular to damage mechanisms. Damage is characterized by the nucleation growth and coalescence of voids, which results in a loss of mechanical properties and leads to fracture [27].

In the case of ductile metals, the so-called *ductile damage* is strongly related with large plastic straining. The nucleation of voids occurs after a certain threshold of plastic strain and their growth and coalescence are governed by plastic instability, as schematically illustrated in figure 5.1 [27, 69]. This type of metals is usually constituted by second phase particles or inclusions immersed in a matrix (figure 5.1(a)). When sufficient stress is applied, matrix-particle debonding or particle cracking may occur, leading to the nucleation of voids (figure 5.1(b)). Subsequently these voids may grow (figure 5.1(c)) and, after reaching a certain size, they start interacting with the neighbouring voids. Plastic strain tends to concentrate along a preferential direction, causing local necking instabilities (figure 5.1(d)). Finally, voids coalesce and a fracture surface is created (figure 5.1(e)).

The Lemaitre model for ductile damage presented in chapter 2 is able to describe material degradation by the introduction of a damage variable,  $D$ , which accounts for the loss of stiffness due to the presence of voids in an averaging way. Nevertheless, this material model is unable to capture the last failure stage corresponding to crack initiation and propagation.

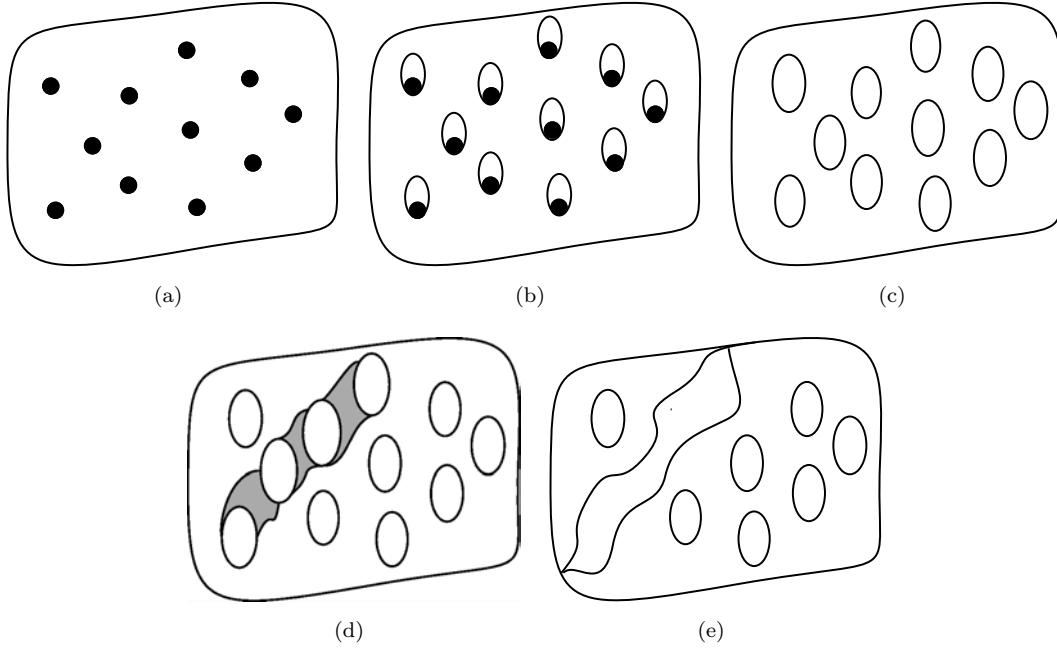


FIGURE 5.1: Ductile fracture process: a) inclusions in a metallic matrix; b) void nucleation; c) void growth; d) strain localization and necking between voids; e) void coalescence and formation of a fracture surface.

A complete ductile failure model may be constructed combining the damage material model with the XFEM discretisation, introduced in chapter 3. The stage illustrated in figure 5.1(d) may be associated to a critical damage value,  $D_c$ , which is determined through the continuous theory. When this damage level is reached, a discontinuity surface may be inserted in the corresponding region using the XFEM.

Therefore, in the first section of this chapter a damage based criterion for transition from damage to fracture is proposed. The same ideas are applied to crack propagation and therefore the two phenomena are dealt with in an unified way. In terms of numerical implementation the continuous-discontinuous model requires some further developments discussed in section 5.2. Next, in sections 5.3 and 5.4, the efficiency of the proposed model is illustrated through various numerical examples. This chapter finalizes with some general conclusions regarding the full ductile fracture model.

## 5.1 Transition criterion from damage to fracture

The transition criterion from Damage to Fracture may be simply stated as *a crack is inserted when critical damage is reached in the corresponding region of the domain*. The

main question is how to determine the crack characteristics, namely the initiation point, direction and length, from the critically damaged area.

In a problem discretised through the FEM, the values of the damage variable are stored in each Gauss point, from which the damage distribution pattern follows directly. This information may be used to determine the characteristics of a crack, but to meet a good accuracy and flexibility an interpolation strategy to calculate the damage value at any point of the domain must be defined.

A simple way to obtain the damage value at an arbitrary point is to use bilinear extrapolation with Lagrange polynomials. The damage value is determined making use of the values at the Gauss points of the element in which the point is contained, similarly to the variable transfer technique described in chapter 4. Nevertheless, to increase the accuracy of the crack definition it is interesting to gather the information of a patch of elements and, alternatively, the approximation based on B-spline functions [140–142] may be employed.

The B-spline basis functions are defined recursively from a set of control points,  $[\xi_1, \xi_2, \dots, \xi_n]$ , using the following recursion formula [143, 144]

$$N_{i,0}(\xi) = \begin{cases} 1 & \text{if } \xi_i \leq \xi \leq \xi_{i+1} \\ 0 & \text{otherwise} \end{cases} \quad (5.1)$$

$$N_{i,p}(\xi) = \frac{\xi - \xi_i}{\xi_{i+p} - \xi_i} N_{i,p-1}(\xi) + \frac{\xi_{i+p+1} - \xi}{\xi_{i+p+1} - \xi_{i+1}} N_{i+1,p-1}(\xi) \quad (5.2)$$

A B-spline curve,  $\mathbf{C}$ , in  $\mathbb{R}^d$  is built as a linear combination of B-spline basis functions as:

$$\mathbf{C}(\xi) = \sum_{i=1}^n N_{i,p} \mathbf{P}_i \quad (5.3)$$

where  $i$  denotes the  $i$ -th control point and not each one of its coordinates. Unlike Lagrange polynomials, functions constructed in this way are monotone and consequently do not introduce new maxima in the distribution. Moreover, a B-spline object of dimension  $d$  is itself a B-spline of dimension  $d - 1$ , which means that a variable at a point at the boundary of a B-spline surface/volume may be interpolated with the same functions as a point lying inside the domain. These properties may bring important advantages in the treatment of a damage distribution, insuring that damage does not grow artificially due to the interpolation technique and allowing an unified treatment of crack initiation

and crack propagation.

Therefore, for the particular case of the damage distribution, a cubic basis will be employed as follows:

$$\begin{aligned} N_1 &= \frac{1}{8}(1 - \xi)^3 \\ N_2 &= \frac{3}{8}(1 - \xi)^2(1 + \xi) \\ N_3 &= \frac{3}{8}(1 - \xi)(1 + \xi)^2 \\ N_4 &= \frac{1}{8}(1 + \xi)^3 \end{aligned} \tag{5.4}$$

The cubic basis ensures a good ratio between the quality of the interpolation and the computational cost [142]. The control points are defined around the element which contains the point where the damage value is to be determined, as illustrated in figure 5.2. Considering a coordinate system,  $(\xi, \eta)$ , originating in the central element of figure 5.2, the B-spline surface may be defined as:

$$\begin{aligned} &\text{for } \xi \leq 0 : \\ &\mathbf{N}_\xi = \left\{ \frac{1}{8}(1 - \xi)^3, \frac{3}{8}(1 - \xi)^2(1 + \xi), \frac{3}{8}(1 - \xi)(1 + \xi)^2, \frac{1}{8}(1 + \xi)^3, 0, 0, 0 \right\} \\ &\text{for } \xi > 0 : \\ &\mathbf{N}_\xi = \left\{ 0, 0, 0, \frac{1}{8}(1 - (\xi - 2))^3, \frac{3}{8}(1 - (\xi - 2))^2(1 + (\xi - 2)), \right. \\ &\quad \left. \frac{3}{8}(1 - (\xi - 2))(1 + (\xi - 2))^2, \frac{1}{8}(1 + (\xi - 2))^3 \right\} \\ &\text{for } \eta \leq 0 : \\ &\mathbf{N}_\eta = \left\{ \frac{1}{8}(1 - \eta)^3, \frac{3}{8}(1 - \eta)^2(1 + \eta), \frac{3}{8}(1 - \eta)(1 + \eta)^2, \frac{1}{8}(1 + \eta)^3, 0, 0, 0 \right\} \\ &\text{for } \eta > 0 : \\ &\mathbf{N}_\eta = \left\{ 0, 0, 0, \frac{1}{8}(1 - (\eta - 2))^3, \frac{3}{8}(1 - (\eta - 2))^2(1 + (\eta - 2)), \right. \\ &\quad \left. \frac{3}{8}(1 - (\eta - 2))(1 + (\eta - 2))^2, \frac{1}{8}(1 + (\eta - 2))^3 \right\} \end{aligned} \tag{5.5}$$

Then, the damage value at a point  $\mathbf{p}$ ,  $D_p$ , may be calculated using the relation:

$$D_p = \mathbf{N}_\xi \mathbf{D}_{\xi\eta} \mathbf{N}_\eta \tag{5.6}$$

where  $\mathbf{D}_{\xi\eta}$  is a matrix containing the damage values in the control points.

In the following sections it will be described how this interpolation technique is used to determine the crack initiation point and growth direction.

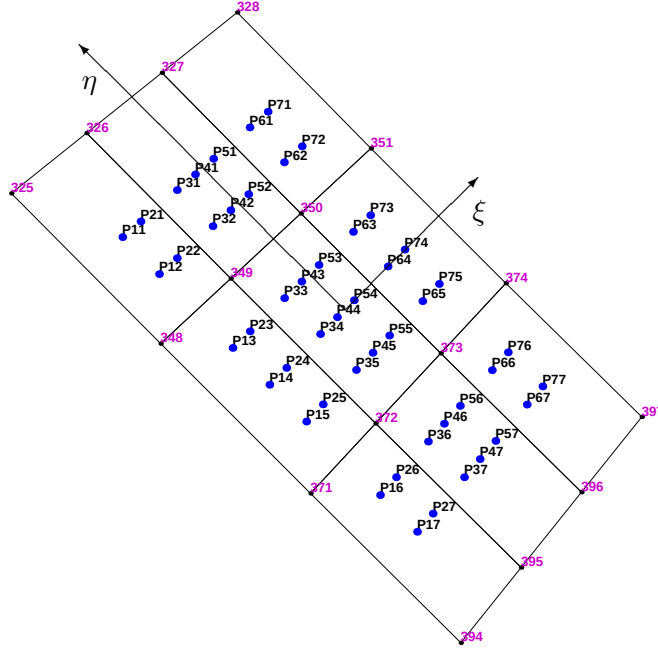


FIGURE 5.2: Set of control points to define the interpolatory B-spline patch of the central element.

### 5.1.1 Crack initiation point

The crack initiation point lies in the region where damage firstly reached the critical value. In a numerical simulation, the elements in which the damage of at least one of the Gauss points is higher than the critical value are selected and grouped into clouds. For each cloud a crack should be inserted, unless it is connected to an existing crack and, in this case, the crack growth algorithm described in the next section will be applied. For the damage clouds without existing cracks two distinct situations may arise, as described in the following paragraphs. It should be noticed that, at this stage, a damage cloud corresponds to a single crack. Therefore, the problems handled with this methodology do not include crack branching.

**Critically damage area connected to the domain boundary** In this situation it is likely that the crack will initiate at the boundary of the domain and, therefore, the search for the initiation point will be performed in the element segments that constitute the domain boundary.

In order to obtain the initiation point, the element with the highest value of damage at the boundary is selected and in particular its boundary segment. Furthermore, to increase the accuracy of the process, the information contained in the surrounding area

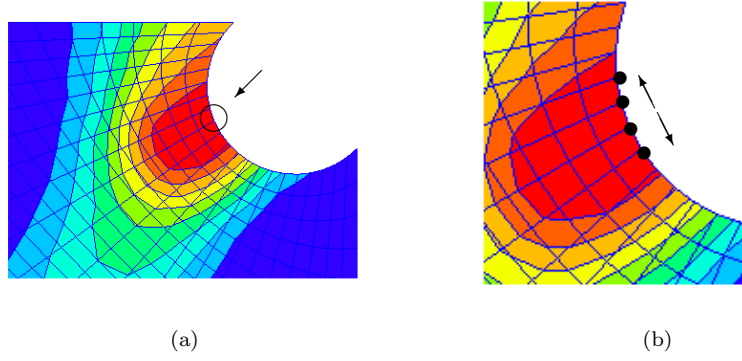


FIGURE 5.3: Search for the point with highest damage at the boundary of the domain: a) Selection of the element with the highest damage value and b) selection of the adjacent segments and respective nodes.

is also considered, selecting the two adjacent segments, as illustrated in figure 5.3.

Using the selected four nodes, it is possible to define a B-spline curve to calculate the value of the damage variable at any point of the boundary, as previously described. The initiation point will then correspond to the point of the boundary with the highest damage value.

After determining the initiation point, the crack direction will be searched 360 degrees around the initiation point, excluding the points lying outside the domain. The technique to calculate the crack growth direction will be described in section 5.1.2.

**Critically damage area inside the domain** When a damage cloud does not touch the boundary of the domain, the initiation point is considered to be in the *damage center*,  $\mathbf{p}$ , obtained using the following expression:

$$\mathbf{p} = \sum_{i=1}^n \frac{\mathbf{x}_i e^{D_i}}{\sum_{j=1}^n e^{D_j}} \quad (5.7)$$

where  $\mathbf{x}_i$  are the coordinates of each Gauss point with  $D \geq D_c$ . The averaging with the exponential of the damage ensures that points with a higher damage have a higher influence in the determination of the damage center.

In this case, the crack direction must be searched 360 degrees around the damage center, and once it is defined, let's say by vector  $\mathbf{v}$ , the furthest point with  $D \geq D_c$  should be searched along the directions defined by  $\mathbf{v}$  and  $-\mathbf{v}$ . This means that the crack will have

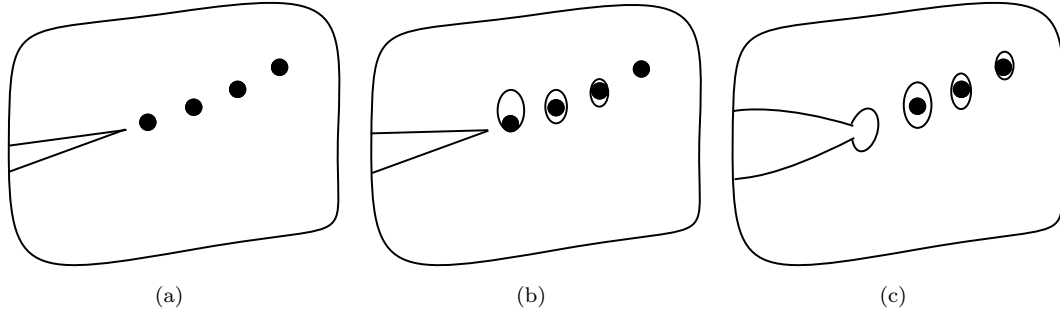


FIGURE 5.4: Ductile crack growth: a) void nucleation ahead of the crack tip; b) void growth; c) voids connect to the main crack causing its propagation.

two active tips, from which it may grow.

### 5.1.2 Crack direction and crack propagation

In this model, crack propagation is also governed by damage. In ductile metals the stress triaxiality ahead of the crack tip may favour the nucleation voids, as schematically illustrated in figure 5.4(a). The voids grow and that eventually connect to the main crack, causing its propagation (figures 5.4(b)-5.4(c)) [27, 69]. As previously referred, the void effect is considered in an averaging way, through the damage variable. Therefore, crack initiation and crack propagation are governed by the advance of critically damaged regions.

In terms of numerical implementation, the crack initiation algorithm is a particular case of the crack propagation algorithm in which the starting point of the crack is unknown. Therefore, during crack propagation, the last crack tip will be the starting point of the new crack segment, while to determine the initial point of a new crack one of the processes described in the previous section must be adopted. In either cases, the crack growth direction and length are to be determined.

To derive the new segment direction a set of points is selected along a circumference, centred at the last crack tip, which contains all the elements where the critical damage value has been reached in at least one Gauss point, according to figure 5.5. As it is unlikely that the crack will snap back, the points behind the previous crack segment are excluded and, subsequently, the point with the highest damage value should be determined.

The damage value at each point of the circumference is calculated using the cubic B-spline previously introduced. The crack direction is then obtained by joining the last

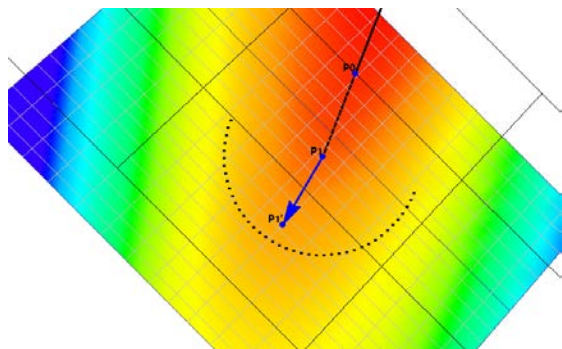


FIGURE 5.5: Selection of points to determine the crack growth direction.

crack tip to the point with the highest damage. Moreover, for a good accuracy two more circumferences, with a slightly higher and slightly smaller radius, are tested and then the three directions are averaged.

To determine the crack length, the furthest point with  $D \geq D_c$  is searched along the crack growth direction, using a mid-point algorithm. In all the points between the old crack tip and the new crack tip damage should be higher than  $D_c$ . The maximum search length is prescribed by the user and it is chosen in such a way that the point located at the maximum search length has a damage value lower than  $D_c$ .

During a simulation, after the critical damage has been reached and the start and end points of the new crack have been defined, a discontinuity should be introduced in the model, which may be done by applying the XFEM, as described in chapter 4. Although apparently simple, the combination of XFEM with the Lemaitre requires some care in terms of numerical implementation, which will be addressed in the next section.

## 5.2 Numerical implementation

The use of XFEM has been mostly confined to brittle materials where its modelling usually does not require the development of special features, as in ductile materials. The main issues concerning the use of XFEM for ductile fracture, such as adequate numerical integration rules, strategies to deal with incompressibility and near incompressibility constraints, variable transfer and equilibrium recovery were covered in chapter 4, which together with chapters 2 and 3 intended to be the preparation for this final fracture model. Therefore, in this section some general overview on the numerical implementation will be presented, focusing on the equilibrium recovery algorithm.

### 5.2.1 General numerical implementation using AceGen/AceFEM

The possibilities offered by the *AceGen* System [83], presented in chapter 3 make it the ideal tool to implement the full failure model. In this work, *AceGen* was used for the development of the finite element equations at high abstract level and generation of the computer code of a finite element with the following characteristics:

- . quadrilateral topology - 2D element with 4 nodes;
- . XFEM formulation to be activated when the fracture criterion is met;
- . Non-local integral Lemaitre material model under finite strain assumption (chapter 2);
- . standard Gaussian quadrature for non-enriched elements and sub division in triangles for enriched elements (chapter 4);
- . F-bar formulation to alleviate locking in the respective standard/XFEM methodology (chapter 4).

We briefly recall that the individual element contribution  $\mathbf{R}_{en+1}$  to the global residual  $\mathbf{R}_{n+1}$  is derived from the virtual work principle as:

$$\mathbf{R}_{en+1} = \int_{\Omega_e} \mathbf{S}_{n+1} \frac{\partial \mathbf{E}_{n+1}}{\partial \mathbf{p}_{en+1}} d\Omega_e \quad (5.8)$$

where  $\mathbf{S}_{n+1}$  and  $\mathbf{E}_{n+1}$  are, respectively, the previously defined Piola-Kirchhoff stress and Green-Lagrange deformation tensor,  $\Omega_e$  is the domain of the element and  $\mathbf{p}$  is the vector of unknowns, in this case consisting of the nodal displacements  $\mathbf{u}_i$  and the extra degrees of freedom associated with the XFEM enrichment,  $\mathbf{a}_j$  and  $\mathbf{b}_k$ . Consequently, the tangent operator,  $\mathbf{K}_{Ten+1}$ , may be automatically derived from the residual as:

$$\mathbf{K}_{Ten+1} = \frac{\partial \mathbf{R}_{en+1}}{\partial \mathbf{p}_{en+1}} \quad (5.9)$$

It should be noticed that due to the non-local nature of the problem, each material point depends on other surrounding points and therefore the system of equations must be sought globally [78, 79]. Moreover, using symbolic derivations, the obtained derivatives are exact, leading to a quadratically convergent Newton iterative scheme.

Although the generated element is consistent, during the analysis phase (performed with *AceFEM* [89]), an element may change from standard to enriched, which means that the number of unknowns may change each time step. Therefore, whenever new elements are enriched a process to recover equilibrium has to be developed, as described in the

following section.

### 5.2.2 Equilibrium recovery algorithm

Regarding numerical implementation, the equilibrium recovery required when new elements are enriched is the most critical part of the model. Each time new elements are enriched due to crack initiation and/or propagation, the number of degrees of freedom increases, as well as the number of Gauss points inside the enriched elements and hence the equilibrium between internal and external forces has to be re-established.

In fact, when an element is enriched the positions and weights of the Gauss points change and consequently the internal variables have to be transferred from the old Gauss points to the new ones, which is done by applying a local smoothing technique as explained in chapter 4. It should be noticed that this process differs from remeshing as only the quantities stored in the Gauss points, namely the plastic strain and the damage variable, are transferred in a process occurring only inside each element; the mesh, as well as the quantities stored in the nodes remain the same. In a second stage, a load increment with null amplitude is performed. However, due to the highly non-linear nature of the problem, this procedure may be inefficient and a more complex algorithm had to be developed, as described in the following paragraphs.

The key feature for equilibrium recovery is the constancy of the nodal quantities. When a discontinuity is introduced in a particular element, the continuous problem should be equivalent to the continuous-discontinuous problem. Even though the approximation function for the element changed from:

$$\mathbf{u}(\mathbf{x}) = \sum_{i=1}^n N_i \mathbf{u}_i \quad (5.10)$$

to

$$\mathbf{u}(\mathbf{x}) = \sum_{i=1}^n N_i \mathbf{u}_i + \sum_{j=1}^{n_{split}} N_j [H(\mathbf{x}) - H(\mathbf{x}_j)] \mathbf{a}_j \quad (5.11)$$

in elements which became totally cut by a crack, or to

$$\mathbf{u}(\mathbf{x}) = \sum_{i=1}^n N_i \mathbf{u}_i + \sum_{j=1}^{n_{tip}} N_j R(\mathbf{x}) [H(\mathbf{x}) - H(\mathbf{x}_j)] \mathbf{b}_j \quad (5.12)$$

in elements, which became tip elements, after solving the system of equations, the nodal displacements should remain the same. Therefore, when an element is about to be enriched, its displacements,  $\mathbf{u}_{nenrich}$ , are stored. Then, after introducing the discontinuity, the problem is solved imposing the stored displacements,  $\mathbf{u}_{nenrich}$ , as prescribed displacements, resulting in a set of residual forces,  $\mathbf{F}_{Res}$ , at the enriched nodes. Subsequently, the nodes are released and the problem is solved for progressively reduced residual forces, according to the scheme in figure 5.6.

To finalize the algorithm description, it should be noticed that, although the crack length step is calculated using the methodology proposed in section 5.1.2, sometimes it is divided in several steps to facilitate equilibrium recovery. Moreover, during the analysis time stepping is usually not constant. When critical damage is reached, the program goes back one time step and continues with a fraction of the first time step according to the scheme in figure 5.7. In this way the crack initiation stage is captured with more detail. As crack propagation in ductile metals is usually stable it may be successfully simulated using a quasi-static formulation.

Now that the fracture model is fully presented, its effectiveness will be illustrated through various numerical examples, presented in the remaining of this chapter.

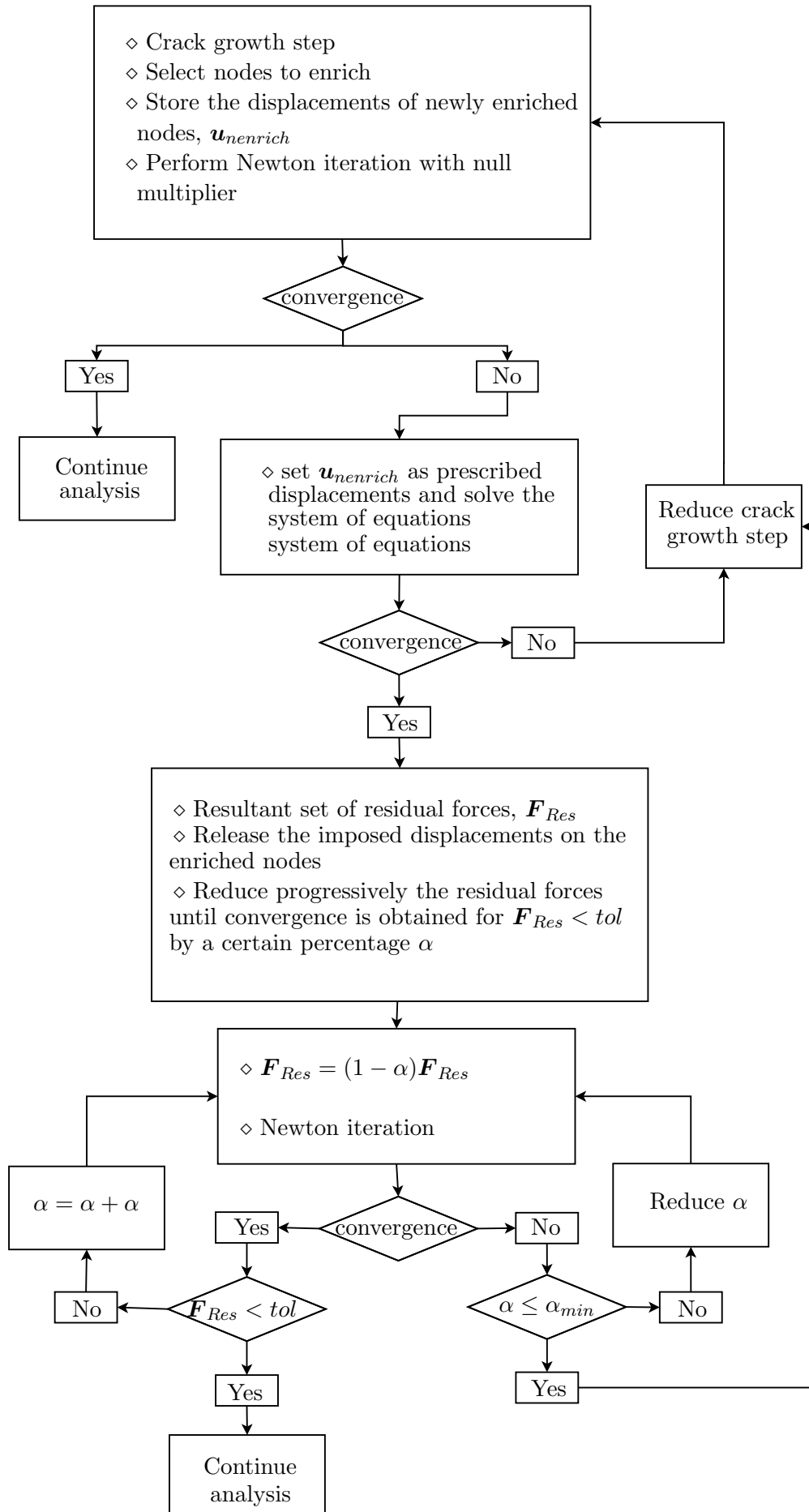


FIGURE 5.6: Iterative scheme for equilibrium recovery during a crack growth step.

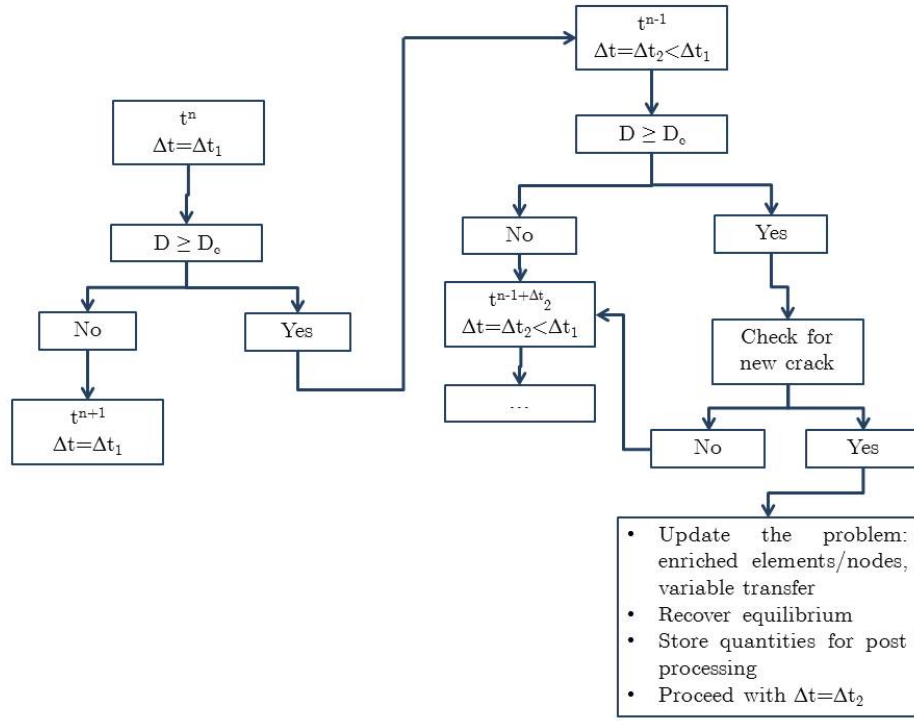


FIGURE 5.7: Time-stepping scheme before and after crack initiation/propagation.

### 5.3 Numerical examples 1: Plate with an initial crack

Before evaluating the total fracture model, involving crack initiation and propagation, a specimen with an initial crack is studied. This numerical example is intended to evaluate the effects of the non-local damage formulation, when applied in conjunction with the XFEM. In a second phase, damage based crack propagation is inspected as well.

Following this line, this example consists of a cracked plate illustrated in figure 6.9. The material properties and dimensions are summarized in table 5.1. Three different FEM meshes are considered, as shown in figure 5.9, under plane strain assumption.

For the analysis, besides the material parameters defined in table 5.1, the proposed model requires a value for the non-local regularization length,  $l_r$ . This parameter cannot be measured directly from experiments but is usually obtained through inverse analysis [77, 79]. As the presented non-local formulation has proven to be able to alleviate pathological mesh dependence,  $l_r$  may be regarded as a numerical regularization parameter to be prescribed by the user. Therefore, three different situations, corresponding to three values of  $l_r$  are analysed:  $l_r = 0$  (the local case),  $l_r = 0.8\text{mm}$  and  $l_r = 1.6\text{mm}$ . The damage contours obtained in each case, for an applied displacement of  $0.05\text{mm}$ , are

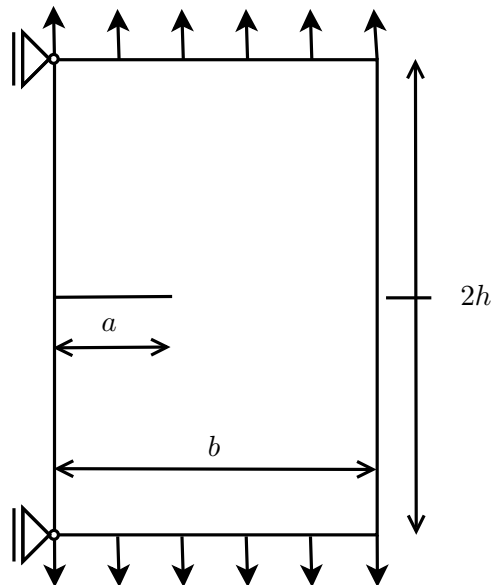


FIGURE 5.8: Pre-cracked plate

TABLE 5.1: Material properties of the plate with an initial crack.

| Property             | Value                                                          |
|----------------------|----------------------------------------------------------------|
| Elastic modulus      | $E = 206.9 \text{ GPa}$                                        |
| Poisson's ratio      | $\nu = 0.29$                                                   |
| Damage exponent      | $s = 1.0$                                                      |
| Damage denominator   | $r = 1.25 \text{ MPa}$                                         |
| Hardening function   | $\tau_y(R) = 450 + 129.24R + 265(1 - e^{-16.93R}) \text{ MPa}$ |
| Dimension            | $h = 15 \text{ mm}$                                            |
| Dimension            | $b = 20 \text{ mm}$                                            |
| Initial crack length | $a = 20/3 \text{ mm}$                                          |

displayed in figures 5.10 - 5.12.

Results demonstrate a clear mesh dependence pathology in the local case. Instead of providing better resolution in the crack tip vicinity, mesh refinement causes spurious damage localization.

As expected, the non-local formulation alleviates the mesh dependence, as can be observed in figures 5.11 and 5.12, where the damage contours do not vary significantly in the different meshes. Nevertheless, for  $l_r = 0.8\text{mm}$ , there is still some excessive damage concentration at the crack tip, which suggests that the larger  $l_r$  is a better choice. In fact, when analysing the crack growth,  $l_r = 0.8\text{mm}$  will prove to be insufficient. As a final note on the use of the Lemaitre model under a non-local formulation with discontinuous cracks, it should be noticed that the maximum damage values region is connected

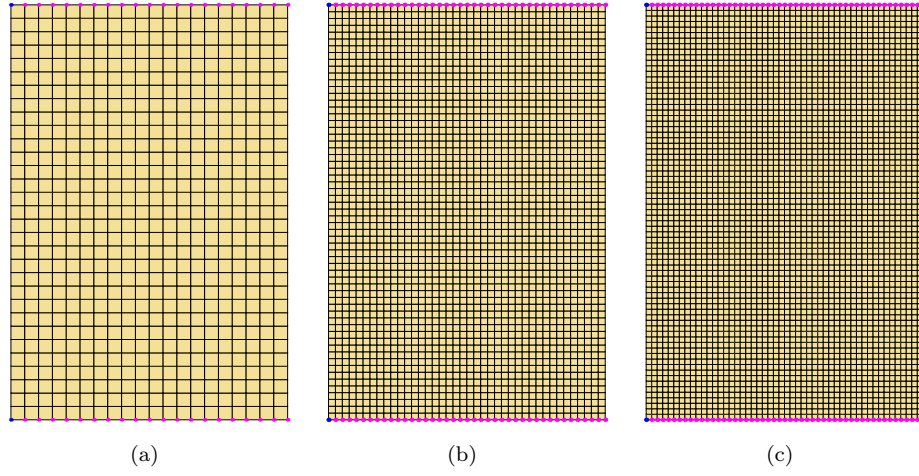


FIGURE 5.9: Mesh refinement for the plate with an initial crack: a)  $20 \times 31$ , b)  $40 \times 61$  and c)  $50 \times 75$  elements.

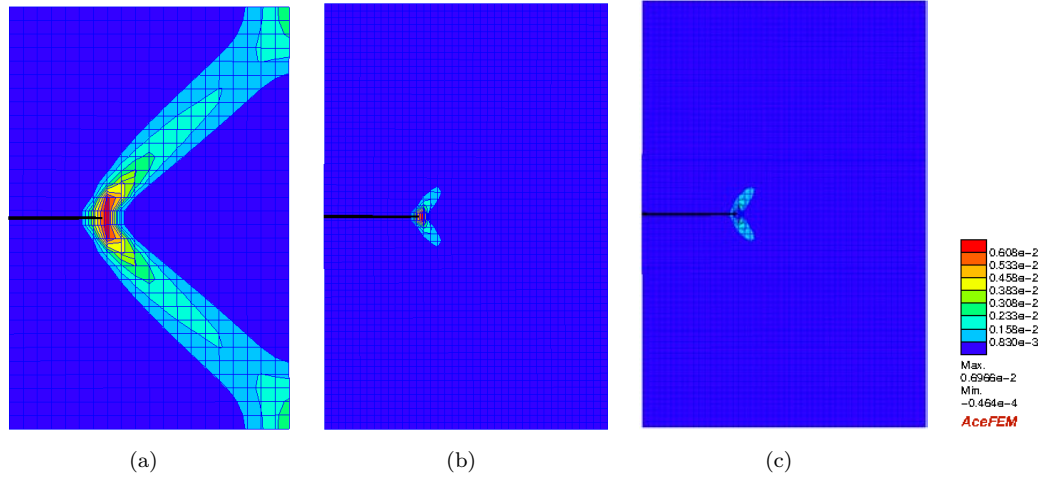


FIGURE 5.10: Damage contours obtained for the local case, for an applied displacement of 0.05mm for three meshes a)  $20 \times 31$ , b)  $40 \times 61$  and c)  $50 \times 75$  elements.

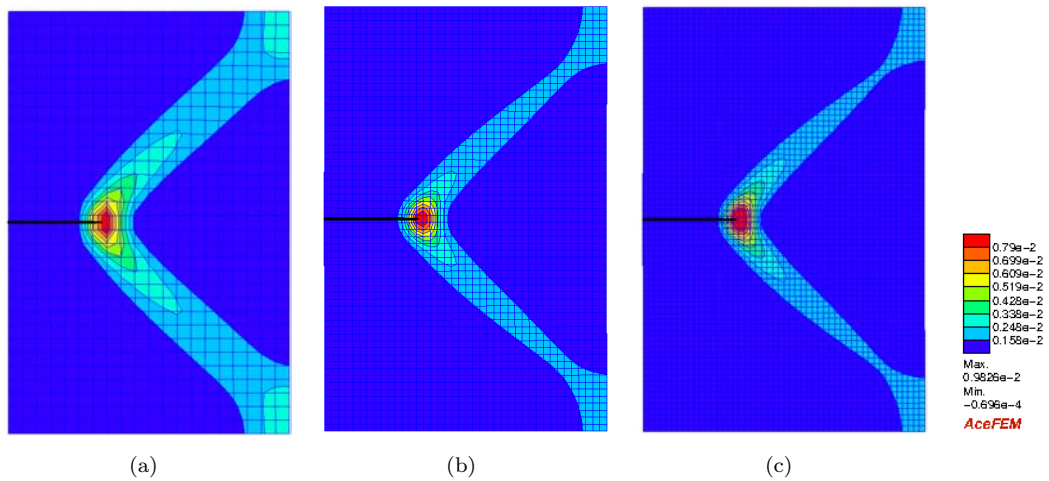


FIGURE 5.11: Damage contours obtained for  $l_r = 0.8\text{mm}$ , for an applied displacement of 0.05mm, for three meshes a)  $20 \times 31$ , b)  $40 \times 61$  and c)  $50 \times 75$  elements.

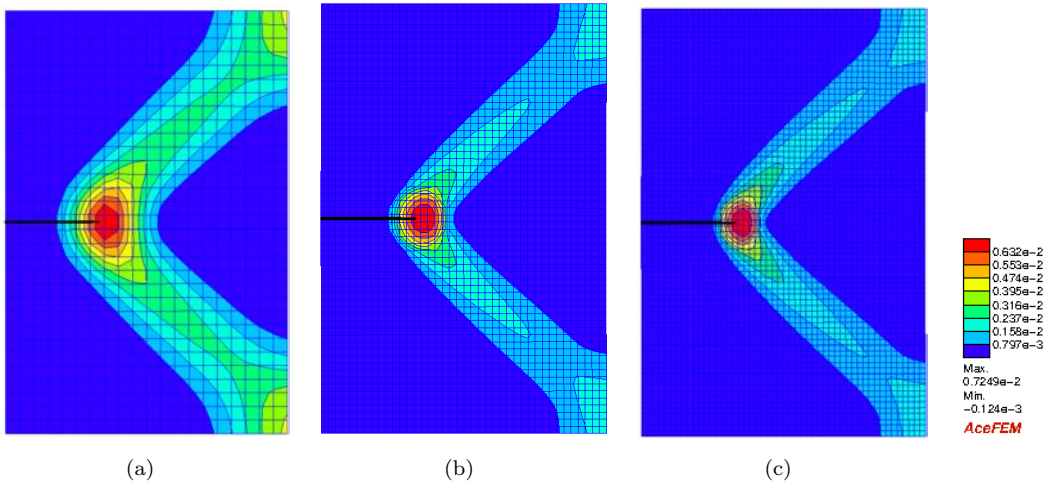


FIGURE 5.12: Damage contours obtained for  $l_r = 1.6\text{mm}$ , for an applied displacement of  $0.05\text{mm}$ , for three meshes a)  $20 \times 31$ , b)  $40 \times 61$  and c)  $50 \times 75$  elements.

with the crack tip, and therefore correlates with micro mechanical approach described previously in this chapter: the triaxiality state at the crack tip favours the nucleation and growth of voids, which eventually connect to the main crack causing its propagation.

**Ductile Crack Growth** The analysis of the damage-based crack growth is now presented. One more model parameter, the critical damage value,  $D_c$ , which triggers the crack advance must be defined. Following the work of Lemaitre [27], in real parts and structures the critical damage value is not 1, which would correspond to theoretical fully damaged material, but is rather located between 0.2 and 0.5. At this stage, the values of 0.2 is employed and further discussion is left for the full model involving crack initiation and propagation.

In this study, the same three meshes and non-local lengths were employed. Results are depicted in figures 5.13 and 5.14, where the final crack paths and damage contours may be observed.

For the regularization length of  $0.8\text{mm}$  there is still some damage localization at the crack tip. In the coarse mesh (figure 5.13(a)) just a few Gauss points in the vicinity of the crack tip reach the critical damage. Consequently the convergence of the iterative scheme is affected during the crack growth simulation. The finer meshes (figures 5.13(b) and 5.13(c)) provide more resolution, however only with the later is possible to simulate the expected crack path. This case illustrates one of the disadvantages of the proposed

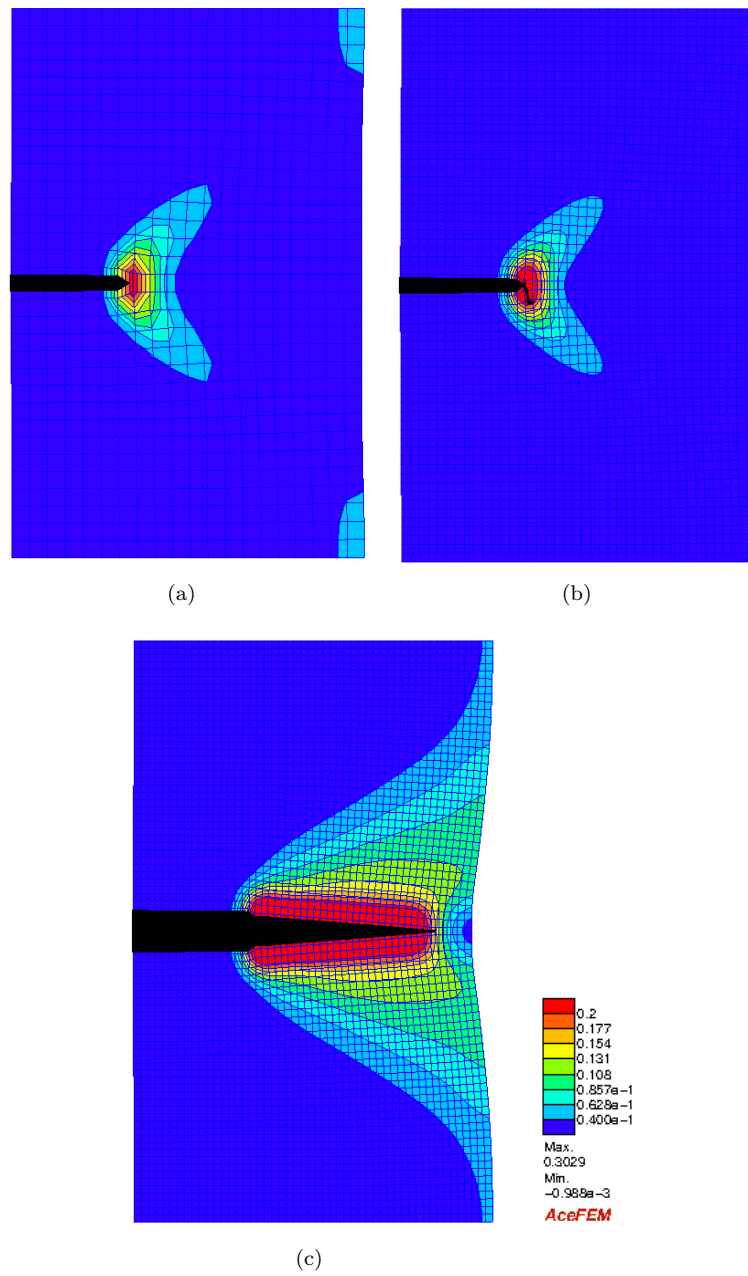


FIGURE 5.13: Crack path obtained using  $l_r = 0.8$  mm, for three meshes a)  $20 \times 31$ , b)  $40 \times 61$  and c)  $50 \times 75$  elements.

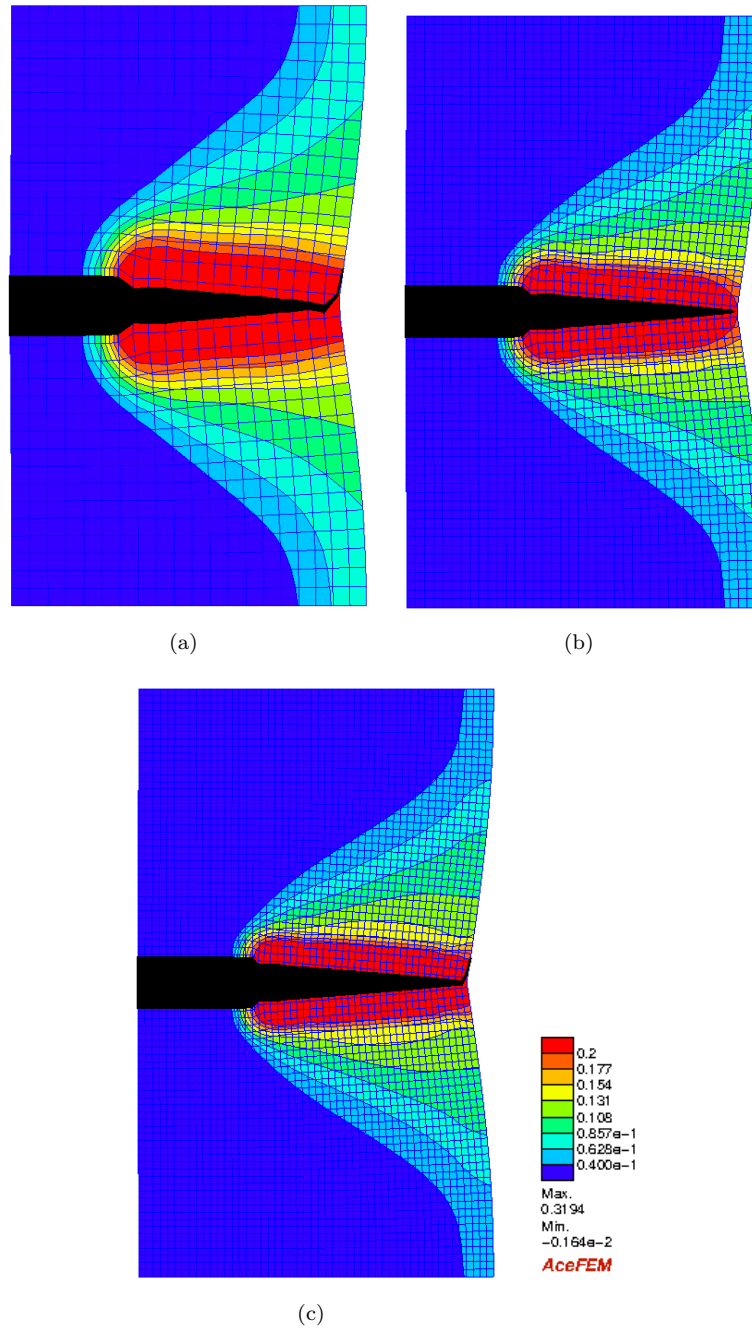


FIGURE 5.14: Crack path obtained using  $l_r = 1.6$  mm, for three meshes a)  $20 \times 31$ , b)  $40 \times 61$  and c)  $50 \times 75$  elements.

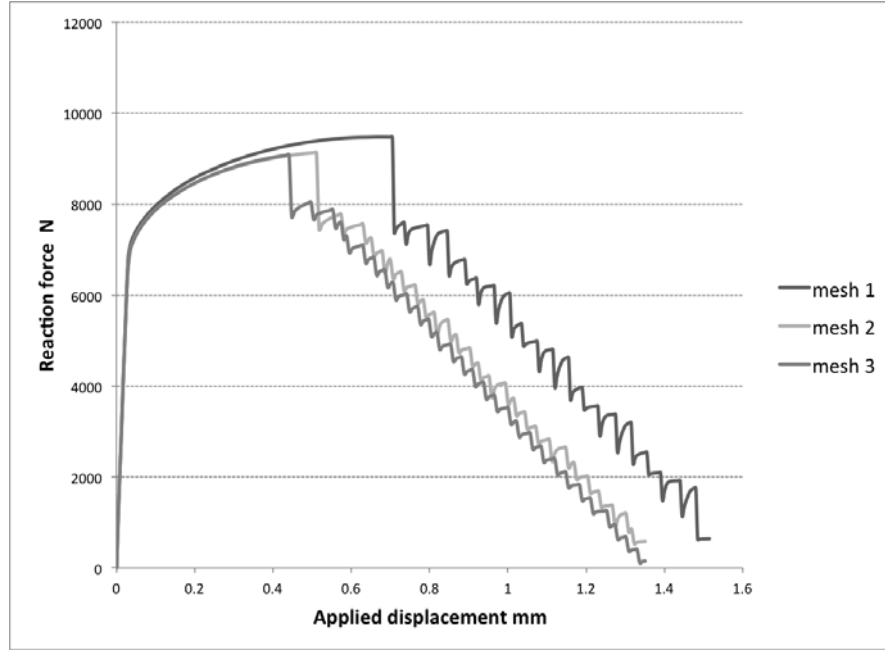


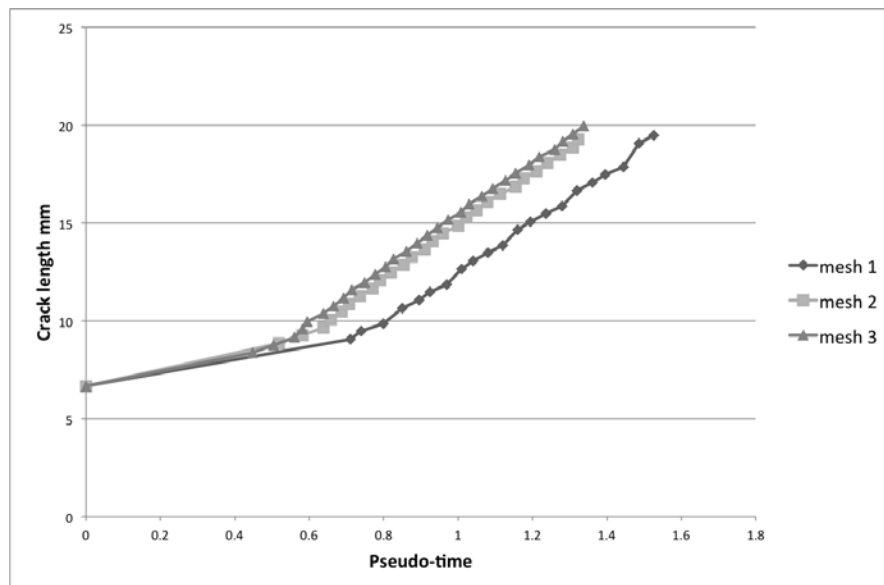
FIGURE 5.15: Reaction force in function of the applied displacement  $l_r = 1.6\text{mm}$ .

damage criterion: due to its geometric nature, an accurate calculation of the crack direction, requires that critical damage is reached in a certain number of Gauss points. Nevertheless, this disadvantage is usually overcome by selecting an adequate non-local length, as it will be demonstrated in the remaining examples.

In particular, for the length of 1.6mm, crack growth can be simulated successfully for all the meshes. Nevertheless, when the specimen is close to complete rupture, some numerical instabilities may arise causing a slight change of the crack direction.

In figure 5.15 the reaction force-applied displacement curves are displayed. The curves are convergent upon mesh refinement, which demonstrates the efficiency of the proposed crack growth criterion, based on damage evolution.

To finalize this example, the crack length evolution is depicted in figure 5.16. The

FIGURE 5.16: Crack length evolution  $l_r = 1.6\text{mm}$ .

crack growth velocity is also convergent. The non-local model ensures similar damage patterns in all the meshes and the mesh refinement provides a better resolution on both the damage pattern and crack growth steps.

## 5.4 Numerical Examples 2: Transition from damage to fracture

The efficiency of the complete model for crack initiation and propagation in ductile metals is evaluated in this section, through some numerical examples.

The Lemaitre model, which is used to describe the constitutive relations is applicable to a wide range of ductile metals such as steel, aluminium or copper [27]. In the following simulations the chosen material is a steel, whose properties are summarized in table 5.2.

TABLE 5.2: Material properties used in the numerical examples.

| Property           | Value                                                          |
|--------------------|----------------------------------------------------------------|
| Elastic modulus    | $E = 206.9 \text{ GPa}$                                        |
| Poisson's ratio    | $\nu = 0.29$                                                   |
| Damage exponent    | $s = 1.0$                                                      |
| Damage denominator | $r = 1.25 \text{ MPa}$                                         |
| Hardening function | $\tau_y(R) = 450 + 129.24R + 265(1 - e^{-16.93R}) \text{ MPa}$ |

### 5.4.1 Notched bar

The first example assessed is an axisymmetric notched bar in tension, whose geometry is represented in figure 5.17. Vertical displacements are applied to the top and bottom edges. The problem is discretized with five different FEM meshes, with 11, 21, 31, 41 and 51 elements per side, some of which are represented in figure 5.18.

Similarly to the previous section, besides the material parameters defined in table 5.2, the proposed model requires a value for the regularization length,  $l_r$ , and for the critical damage,  $D_c$ , that triggers the inclusion of a crack in the model. Therefore, different values of  $l_r$  (1.6 mm and 2.0 mm) are employed to evaluate its influence in crack initiation and propagation, as well as different critical damage values (0.2, 0.5, 0.7).

In the initial analysis the following values are considered:  $l_r = 1.6 \text{ mm}$  and  $D_C = 0.2$ . In figure 5.19 the force-displacement curves obtained are displayed.

All the stages of material behaviour can be clearly identified: elastic, plastic-hardening and softening up to total failure. It can also be observed that results are convergent upon mesh refinement.

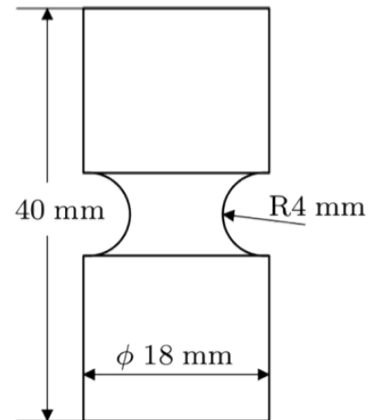


FIGURE 5.17: Axisymmetric Specimen

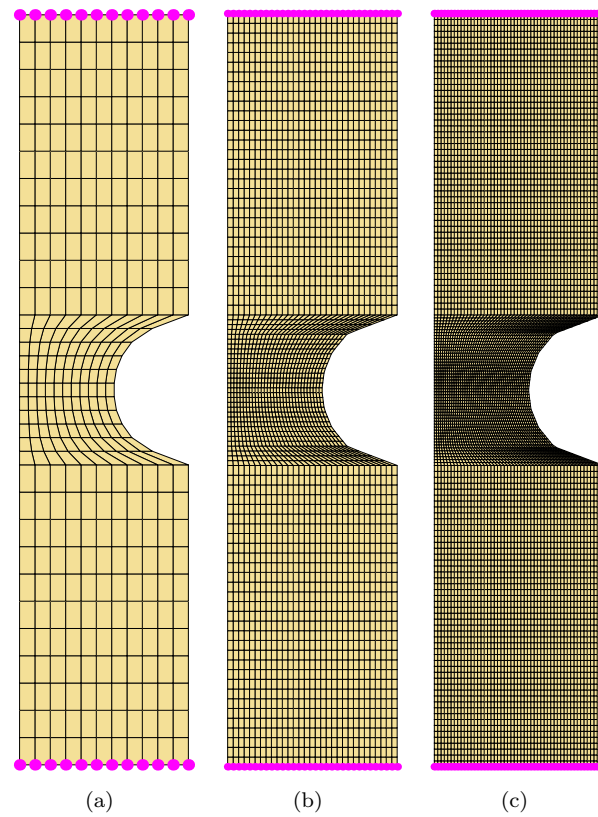


FIGURE 5.18: Mesh refinement for the axisymmetric notched specimen, mesh density of a) 11, b) 31 and c) 51 elements per side.

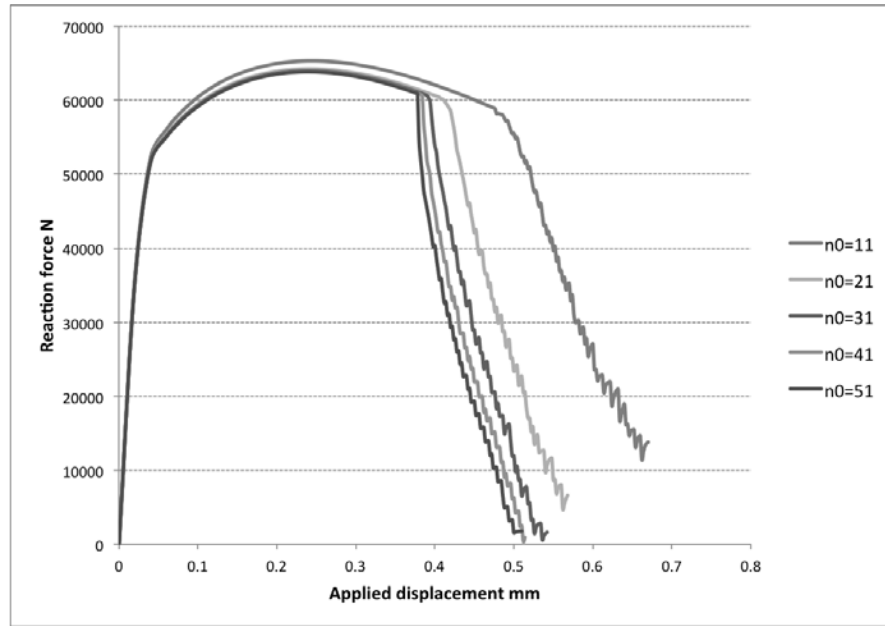


FIGURE 5.19: Relation between the reaction force and the displacement applied to the top edge of the notched specimen for the different meshes, considering  $l_r = 1.6$  mm and  $D_C = 0.2$ .

In the following analysis a higher critical damage value is considered,  $D_C = 0.5$ . In addition two different values for the intrinsic length are applied,  $l_r = 1.6$  mm and  $l_r = 2.0$  mm. The results are displayed in figures 5.20 and 5.21.

As expected, for a higher critical damage, the propagation is slower and smoother.

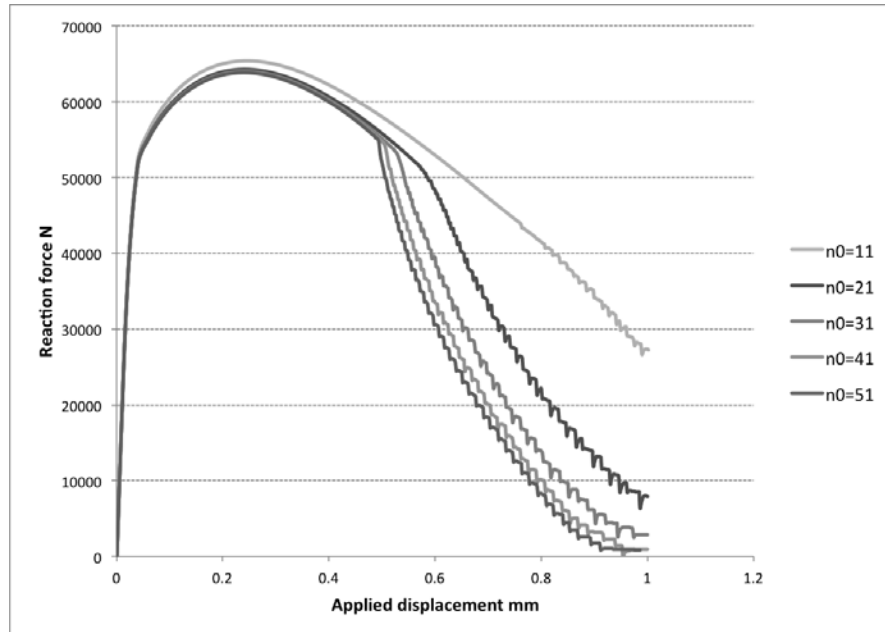


FIGURE 5.20: Relation between the reaction force and the displacement applied to the top edge of the notched specimen for the different meshes, considering  $l_r = 2.0$  mm and  $D_C = 0.5$ .

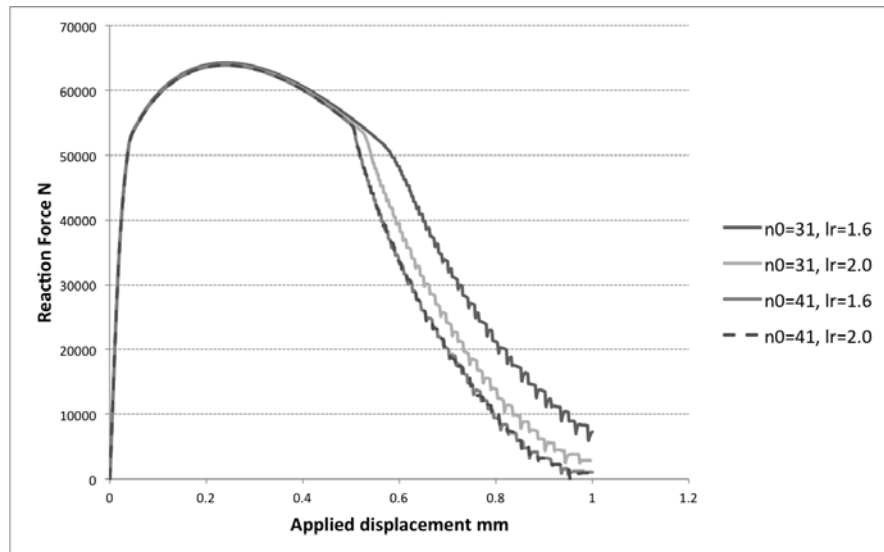


FIGURE 5.21: Comparison between the force-displacement curves obtained for the intrinsic lengths  $l_r = 1.6$  mm and  $l_r = 2.0$  mm. Critical damage has the value  $D_C = 0.5$ .

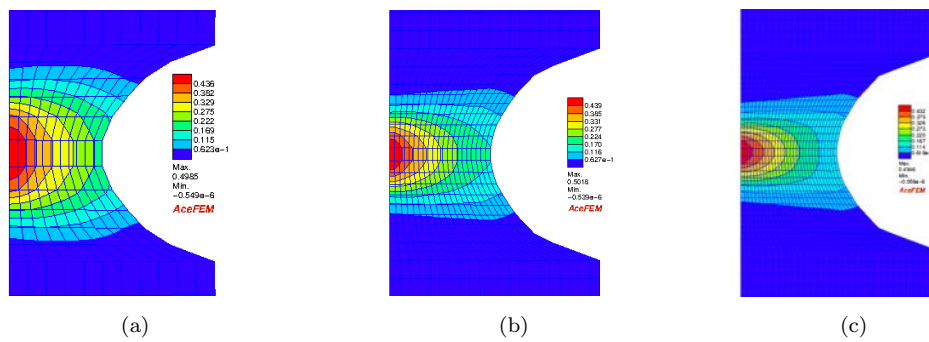


FIGURE 5.22: Damage contour prior to crack insertion for mesh a) 11, b) 21 and c) 31 elements per side.

Again, after a certain mesh refinement, results converge.

In figure 5.21 the effect of the intrinsic length parameter is investigated: for  $l_r = 2.0$  mm the force-displacement curves for mesh densities 31 and 41 are closer than using  $l_r = 1.6$  mm. Although further experimental validation would be required for a more precise choice of this parameter, the results of the damage distribution patterns observed in figures 5.22 and 5.23, prior to crack formation and at the end of the simulation, qualitatively show that it can be conveniently used as a localization limiter. After a certain mesh refinement, the damaged areas become approximately constant and spurious damage localization is considerably attenuated.

The evolution of the crack is illustrated in figure 5.24. In the coarse mesh, crack initiation occurs at a later stage due to the poor resolution offered. This graphic completes the

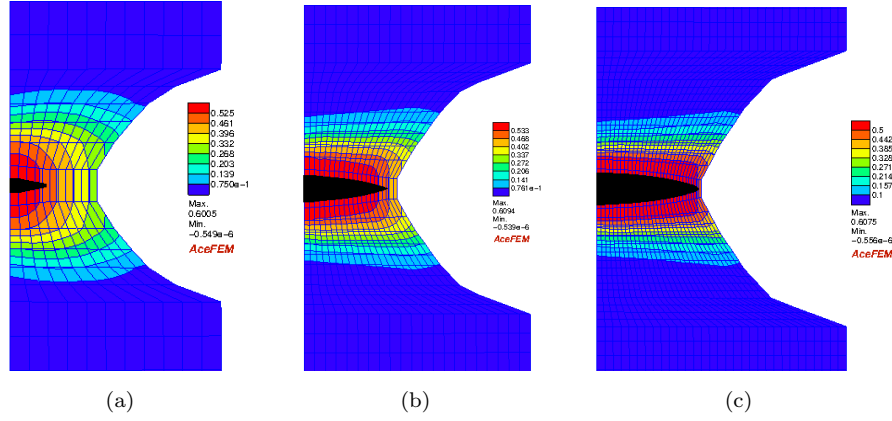


FIGURE 5.23: Damage contour and crack, for an applied displacement of 0.9 mm, for mesh a) 11, b) 21 and c) 31 elements per side.

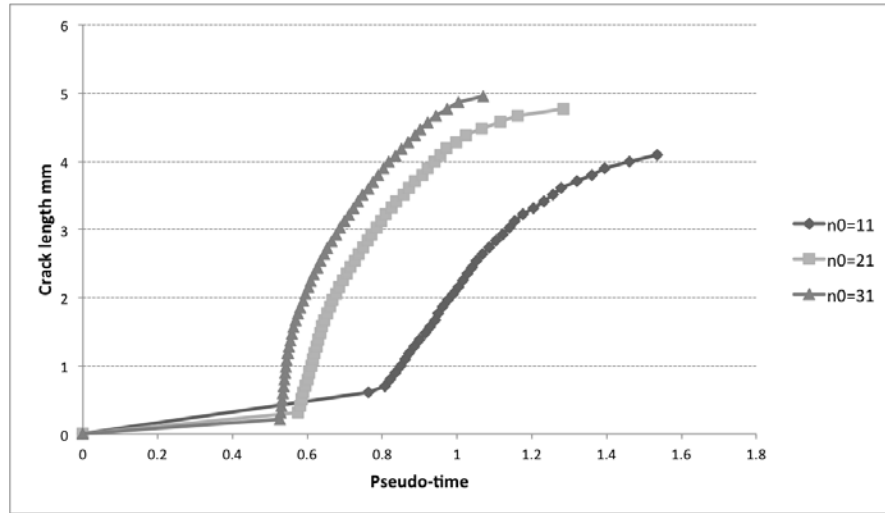


FIGURE 5.24: Crack length evolution considering  $l_r = 2.0$  mm and  $D_C = 0.5$ .

information provided by figure 5.23, as it shows why, at the same time step, the crack length in the first mesh is much smaller than in the others. It can be observed that crack evolution is convergent upon mesh refinement. It is also interesting to compare this graphic with the graphic of figure 5.16. In the case of the plate with an initial crack, the crack speed is approximately constant throughout the simulation, while in the notched specimen the speed varies. This suggests, that in the case of a pre-existing crack, prescribing a constant crack growth increment would be a good approximation, however, accuracy would be lost in the case of the notched specimen.

This study is finalized analysing the effect of different critical damage values in the force-displacement curves. In figure 5.25 the force-displacement curves for the mesh with 31 elements per side, considering  $l_r = 2.0$  mm, are displayed. As expected, increasing  $D_C$ , crack propagation is slower and less catastrophic, indicating once more that the final

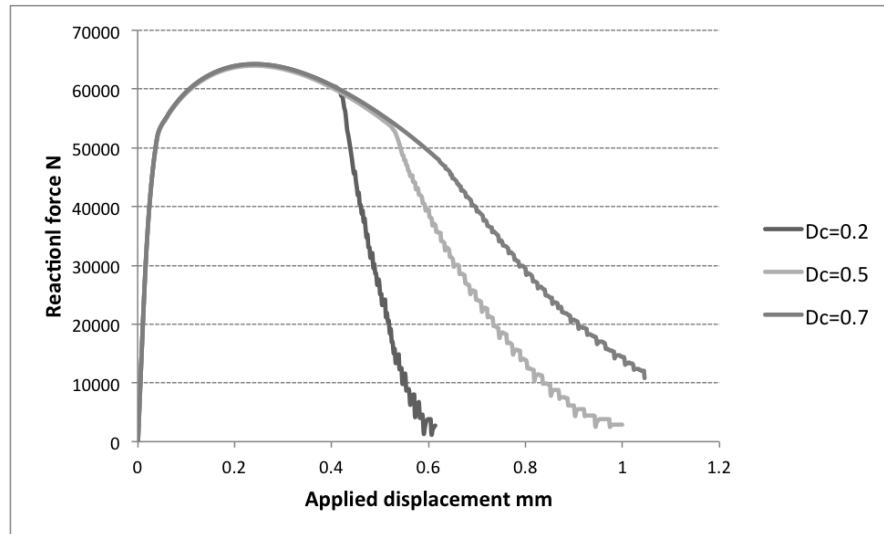


FIGURE 5.25: Relation between the residual force and the displacement applied to the top edge of the notched specimen for the mesh with 31 nodes per side, considering  $l_r = 2.0$  mm and different values for  $D_C$ .

calibration of the proposed methodology is dependent on the characterization of the continuum model parameters, regardless of the good performance exhibited so far.

#### 5.4.2 Plane strain specimen

In this example, the performance of the proposed methodology under the plane strain condition is tested using the specimen depicted in figure 5.26.

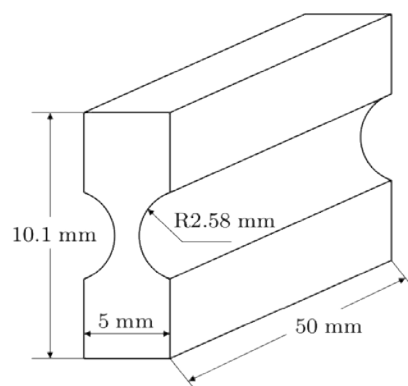


FIGURE 5.26: Plane strain specimen.

For this analysis, the internal length,  $l_r$  has the value of 1.6 mm and the critical damage value is 0.5. The analysis is performed for the four meshes represented in figure 5.27, prescribing adequate symmetry conditions and applying a displacement to the top and

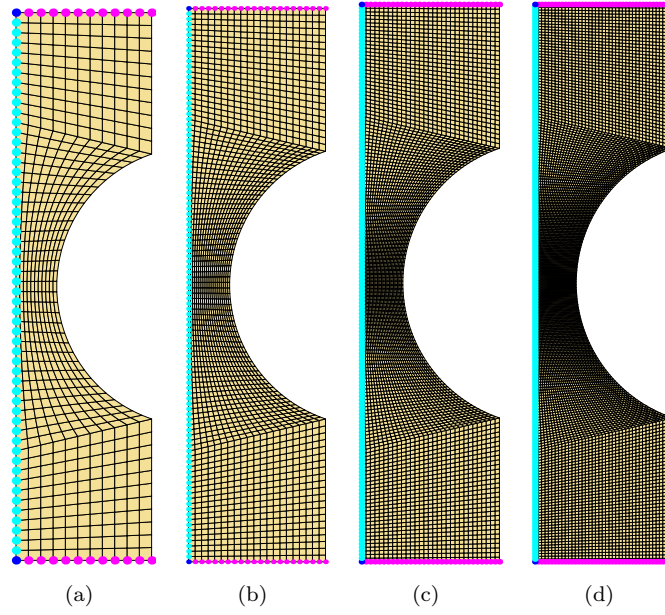


FIGURE 5.27: Mesh refinement for the plane strain specimen, mesh density of a) 11, b) 21, c) 31, d) 41 elements per side.

bottom edges.

In figure 5.28 the reaction force-displacement curves obtained are represented. As in the previous example, all the stages of material behaviour, including hardening and softening up to failure, are clearly represented. Results are also convergent upon mesh refinement.

Under a plane strain condition, the non-local integral model also avoids pathological mesh dependence and spurious damage localization, as may be observed in the damage distribution contours illustrated in figure 5.29.

Finally, in figure 5.30 different crack growth steps for the mesh with 41 elements per side are illustrated, illustrating, once more, the close relation between damage evolution and crack growth in ductile metals.

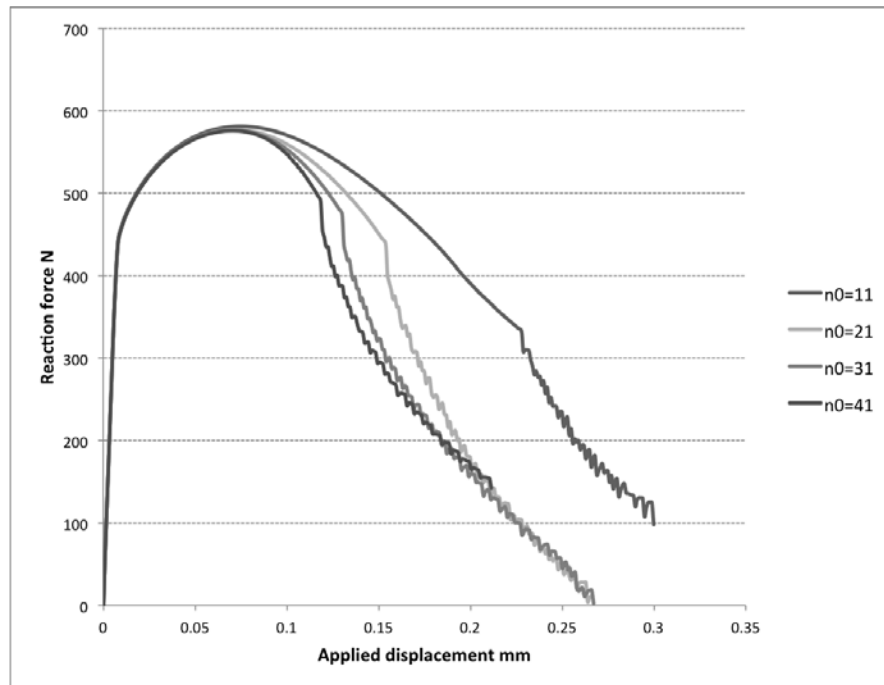


FIGURE 5.28: Reaction force as a function of the applied displacement of the top nodes of the plane strain specimen.

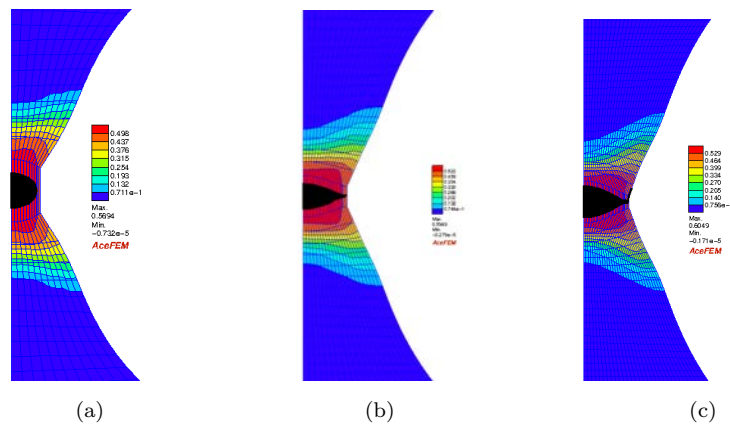


FIGURE 5.29: Damage contour and final crack for mesh a) 11, b) and 21 c) 31 elements per side.

### 5.4.3 Double notched specimen

The main objective of this example is to compare the crack path obtained with different meshes. The previous examples are not fully illustrative, as the crack always progresses in a straight line. For that purpose, a double notched specimen, as represented in figure 5.31, is chosen and is loaded so that a shear-like failure mode would occur. The analysis is performed for the two meshes represented in figure 5.32, considering a critical damage value of 0.5, a regularization length of 1.6 mm and applying a displacement of 1.5 mm.

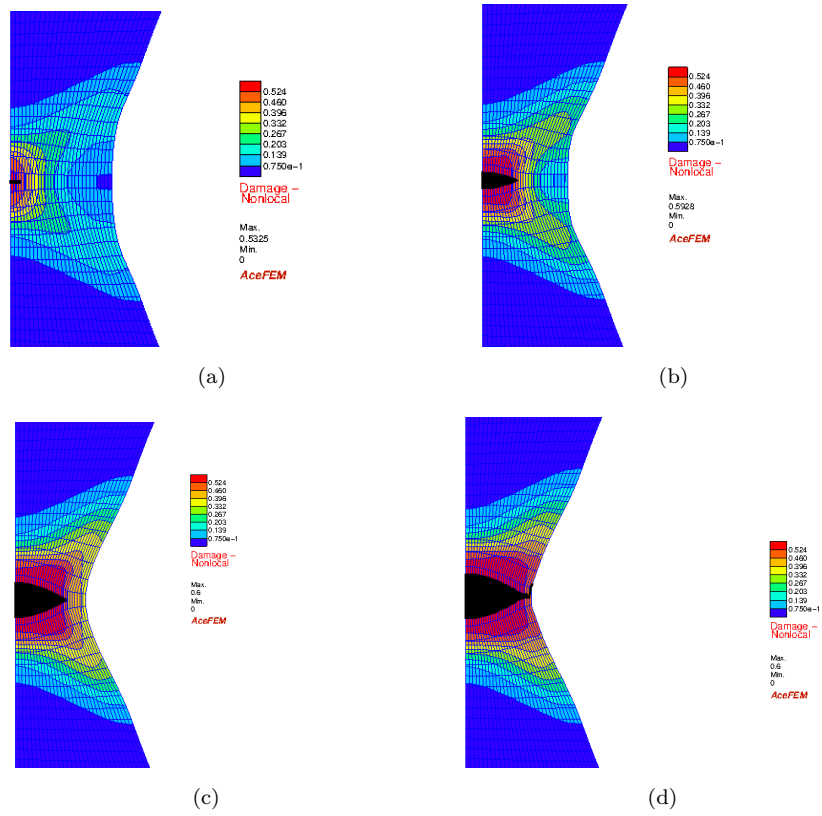


FIGURE 5.30: Different crack growth steps for the mesh with 41 elements per side.

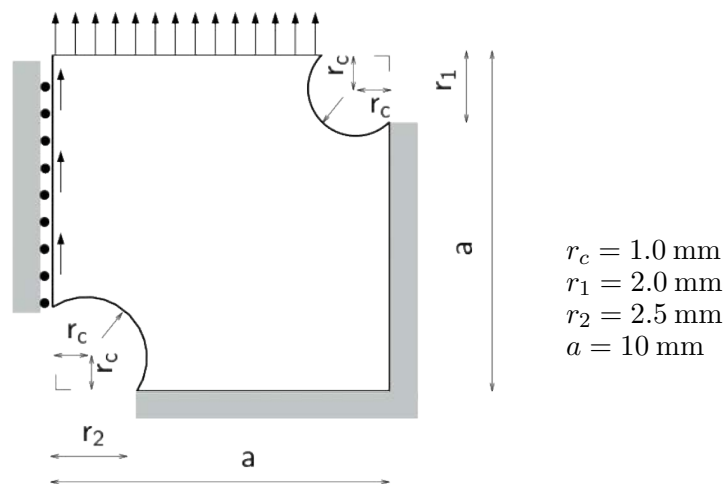


FIGURE 5.31: Shear Specimen

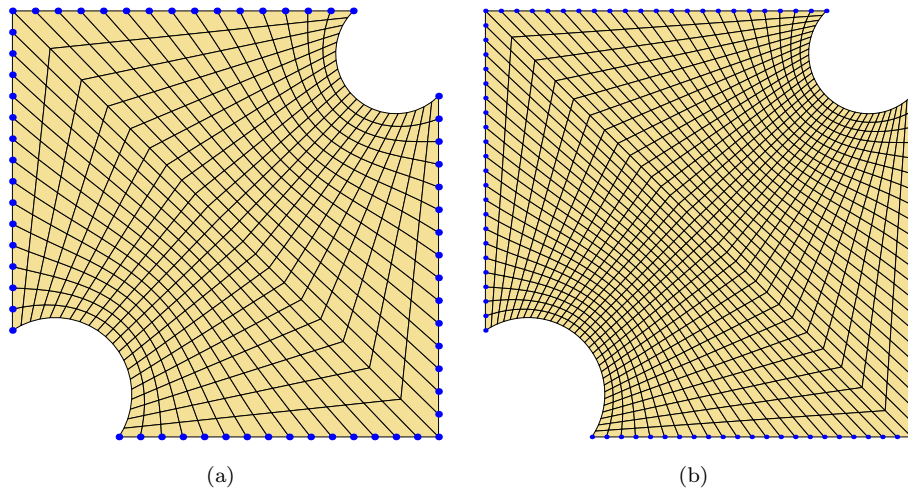


FIGURE 5.32: FEM meshes used in the double notched specimen: a) mesh with 16 nodes per side, b) mesh with 23 nodes per side.

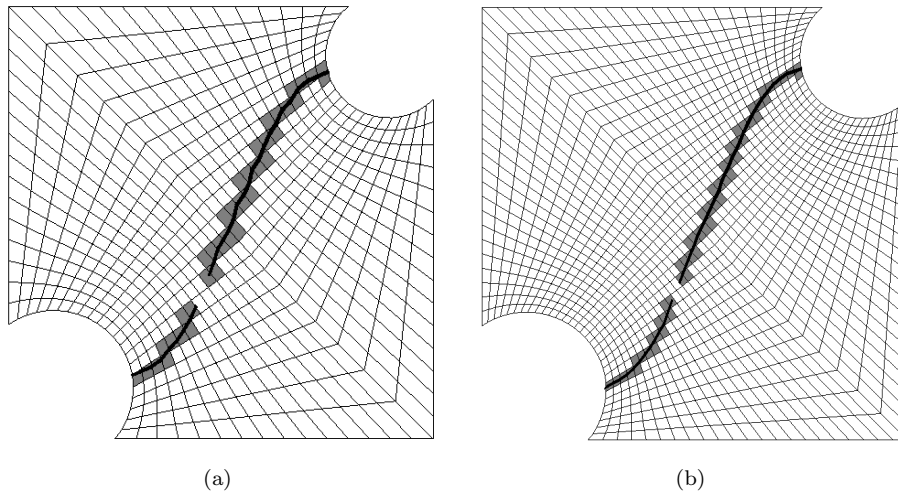


FIGURE 5.33: Crack path obtained for a) mesh a, b) mesh b.

In figure 5.33 the crack paths obtained for the two different meshes are represented. It can be observed that the paths are nearly the same for both cases, that is, the crack path can be considered as mesh independent.

The non-local integral model avoids spurious localization of damage, resulting in similar damaged areas for different mesh refinements (figure 5.34). The subsequent insertion of the crack through the XFEM respects these damage contours independently from the mesh as well, indicating that this methodology is adequate to predict failure in specimens of arbitrary shape.

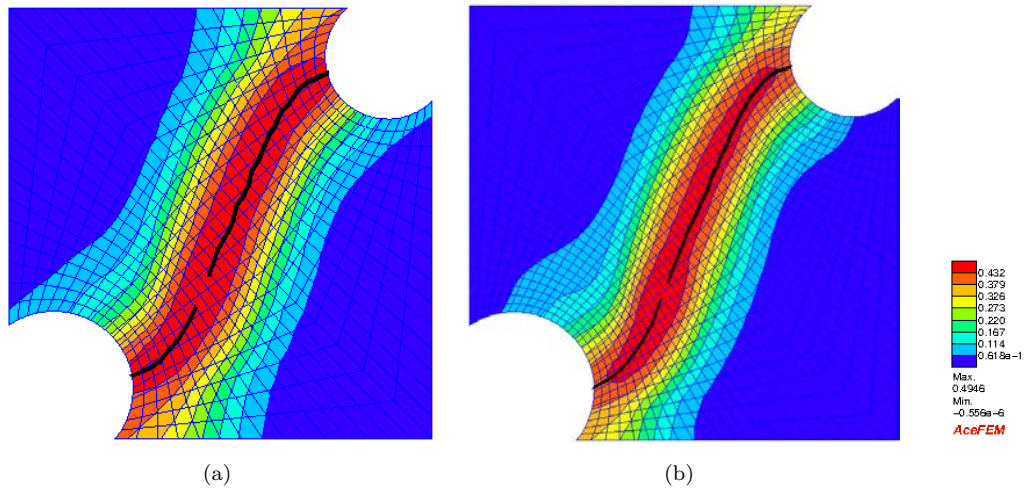


FIGURE 5.34: Damage contour and final crack for mesh a) and mesh b).

## 5.5 Conclusions

Phenomenologically, the initiation of a crack in ductile metals is connected to the evolution of damage, which may be described by a continuum model. Nevertheless, for a complete description of the failure process, a discontinuity should be inserted in the domain, once a critical damage value is met.

In this chapter, a model able to represent all the stages of material behaviour was presented. It was shown that ductile fracture may be successfully dealt with by combining the XFEM with a plastic-damageable material model. Furthermore, the proposed methodology features the following advantages:

- . Crack characteristics are determined directly from the continuous model and therefore there is no need of identifying additional material parameters for fracture. Moreover, crack initiation and propagation are dealt with in an unified way.
- . Crack initiation locus does not need to be known in advance and crack progression is independent of the mesh, saving computational resources when compared with competing approaches such as remeshing.
- . Results are mesh independent upon a certain mesh refinement.
- . The Lemaitre model in its non-local integral formulation ensures similar damage patterns in coarse and fine meshes. Therefore crack advance velocity and crack patterns are also accurately determined, even in coarse meshes.

The possible drawbacks of the proposed methodology are related to parameter identification, such as the non-local intrinsic length and the critical damage value, which may be determined by inverse analysis using a proper combined numerical-experimental approach.

From the theoretical point of view, there is an energy gap when performing a transition from damage to a traction-free crack at damage values lower than 1 and therefore the introduction of a cohesive crack may be regarded as an improvement of the model and will be addressed in the following chapter. Nevertheless, we believe that the approximation developed in this chapter is good enough to describe ductile fracture in a wide range of industrial processes.

## Chapter 6

# Ductile Fracture Model: Cohesive Cracks

In the previous chapter a model for ductile fracture, governed by damage evolution, was presented. When damage reaches a critical value a crack is initiated and subsequently propagates following the damage pattern.

In theory, to ensure thermodynamical consistency in the model in use, the transition from damage to fracture should occur when the material is fully degraded, that is, for  $D_c = 1$ . At this point the damage energy release would be equivalent to the energy necessary to create a crack surface [145]. However, setting the damage value to 1 leads to a singularity in the continuum equations, with its natural numerical consequences.

In the previous chapter it was also outlined that experimentally the critical damage value is, in general, located between 0.2 and 0.5, and therefore there is still an energy gap which should be fulfilled.

One possible solution to this problem is to add a cohesive law to the model. In the previous model it was considered that once a crack is introduced, the newly formed surfaces no longer interact, that is, the cracks were considered traction-free. A cohesive law is a traction-displacement relation which models the interaction between the two surfaces of a crack [12, 13, 22, 146, 147]. From the micro-mechanical point view, it may be interpreted as material which is not fully damaged and, consequently there is still some connection between the two crack surfaces, as schematically illustrated in figure

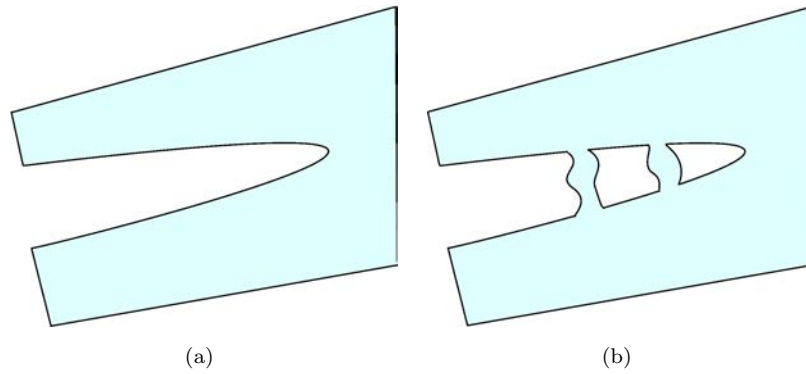


FIGURE 6.1: a) Traction-free crack b) Cohesive crack.

6.1.

In terms of macro-modelling, the transition from damage to fracture for critical damage values lower than one could be compensated by the cohesive law. This concept has been previously applied by Cazes et al. [58, 59], in a formulation that does not require a pre-defined shape for a cohesive law but in which the location of the crack must be known in advance. As additional disadvantage, the model was only fully developed for 1D cases.

In this work, a shape for the cohesive law will be assumed but its parameters will be fitted following energetic considerations. Therefore, this chapter initiates with a brief review of the basic equations and implementation of a cohesive law. Then the influence of the cohesive zone in the model developed in chapter 5 is investigated. Encouraged by the results of this study, a strategy to achieve an energetically consistent transition from damage to fracture is proposed and illustrated through some numerical examples. Finally, the main conclusions of the developed approach are outlined.

## 6.1 Basic equations and implementation of a cohesive law

### 6.1.1 Variational formulation

In a domain containing a cohesive crack, the stress field must be related not only to the external loading but also to the cohesive tractions, which are active in the cohesive zone. An additional condition for the cohesive interface must be satisfied together with the equilibrium equation, as described in the following paragraph.

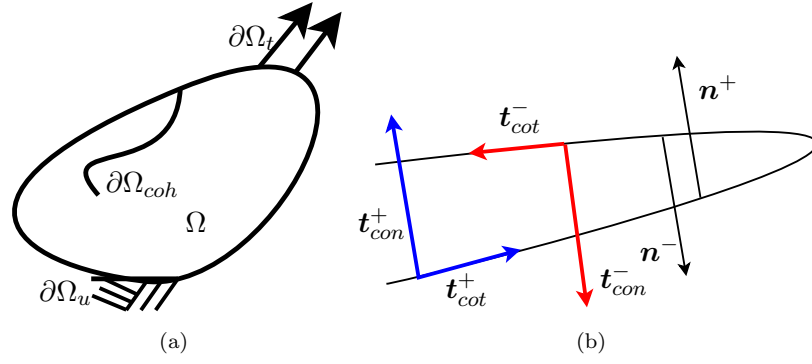


FIGURE 6.2: a) Body containing a cohesive crack. b) Detail of the cohesive crack

Considering the body containing a cohesive crack, represented in figure 6.2, the equilibrium equation for the static case is given by:

$$\text{div}_x \boldsymbol{\sigma} = 0 \text{ in } \Omega \quad (6.1)$$

and the applied tractions,  $\bar{\mathbf{t}}$ , must satisfy

$$\bar{\mathbf{t}} = \boldsymbol{\sigma} \mathbf{n} \text{ at } \partial\Omega_t \quad (6.2)$$

In the cohesive zone, considering normal and tangential interactions as represented in figure 6.2(b), the cohesive tractions,  $\mathbf{t}_{co}^-$  and  $\mathbf{t}_{co}^+$ , are given by:

$$\mathbf{t}_{con}^+ = \boldsymbol{\sigma} \mathbf{n}^+ = -\mathbf{t}_{con}^- = \boldsymbol{\sigma} \mathbf{n}^- \quad (6.3)$$

and

$$\mathbf{t}_{co}^+ = (\mathbf{t}_{con}^+ + \mathbf{t}_{cot}^+) = -\mathbf{t}_{co}^- = -(\mathbf{t}_{con}^- + \mathbf{t}_{cot}^-) \quad (6.4)$$

where  $\mathbf{n}^-$  and  $\mathbf{n}^+$  are the normal vectors to the crack surfaces, as illustrated in figure 6.2(b). The cohesive tractions are considered to be a function of the crack opening,  $\boldsymbol{\omega}$ , defined as:

$$\boldsymbol{\omega} = (\mathbf{u}^- - \mathbf{u}^+) \text{ at } \partial\Omega_n \quad (6.5)$$

Equation 6.5 may be split in a normal component and a tangential component as follows:

$$\begin{aligned} \omega_n &= \boldsymbol{\omega} \cdot \mathbf{n} \\ \omega_t &= \boldsymbol{\omega} \cdot \mathbf{t} \end{aligned} \quad (6.6)$$

where  $\mathbf{t}$  is a vector perpendicular to  $\mathbf{n}$  and, consequently:

$$\begin{aligned} t_{con} &= t_{con}(\omega_n) \\ t_{cot} &= t_{cot}(\omega_t) \end{aligned} \quad (6.7)$$

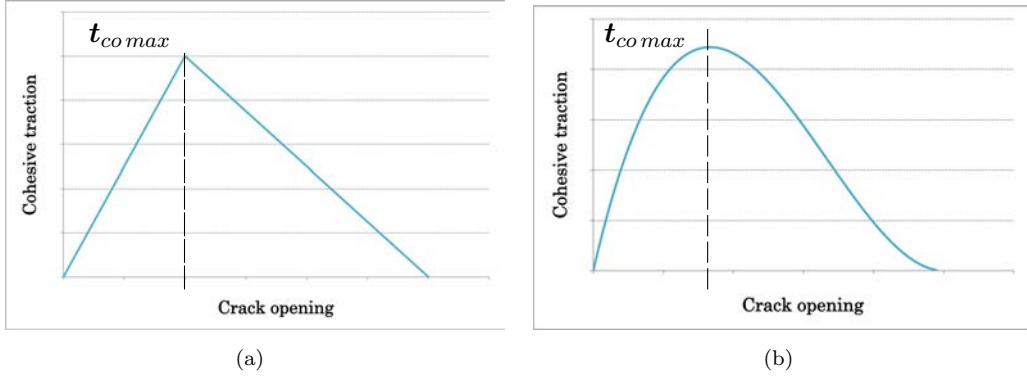


FIGURE 6.3: a) Bilinear cohesive law. b) Polynomial cohesive law.

Finally, due to the additional condition introduced by the cohesive zone interface, the weak form of the equilibrium equation is given by:

$$\int_{\mathcal{X}(\Omega)} \boldsymbol{\sigma} : \nabla_x \boldsymbol{\eta} \, dv + \int_{\mathcal{X}(\partial\Omega_n)} \mathbf{t}_{co} \cdot \boldsymbol{\omega}(\boldsymbol{\eta}) \, da = \int_{\mathcal{X}(\partial\Omega_t)} \bar{\mathbf{t}} \cdot \boldsymbol{\eta} \, da \quad (6.8)$$

for an admissible virtual displacement  $\boldsymbol{\eta}$ .

### 6.1.2 Shape and parameters of the cohesive law

After writing the equilibrium equation, a constitutive law for the cohesive zone should be formally defined.

The shape and parameters of a cohesive law are often related to the micro-mechanical mechanisms happening in the so-called fracture process zone, that is, in the region where fracture is likely to happen. Particle-matrix decohesion, void growth and coalescence or solute segregation are examples of such mechanisms, which subsequently give rise to macro-crack propagation.

In general, when the cohesive zone model is used to describe the complete fracture process, the effect of micro-mechanical processes prior to material separation is described by an increasing traction across the interface. The maximum traction,  $\mathbf{t}_{co\,max}$ , triggers the initiation of material separation and consequently, the traction decreases and eventually vanishes permitting a complete decohesion [22, 146–149]. To accommodate those physical features, the cohesive traction-crack opening relation may be mathematically expressed by a bilinear or a polynomial/exponential type law as represented in figure 6.3 [146, 147, 149]. In the case of homogeneous materials, which is the often the case with

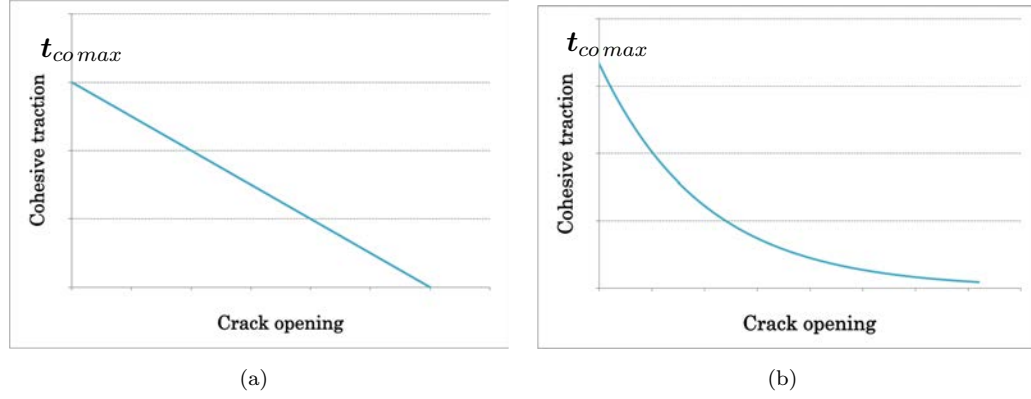


FIGURE 6.4: a) Linear cohesive law. b) Exponential cohesive law.

ductile metals, the shape of the cohesive law is regarded to be of secondary importance [150] and, in terms of a numerical simulation, the effect of linear or exponential laws in the global material response is qualitatively similar.

When the onset of fracture is triggered with some additional criterion, like in this work, where macro-cracks are initiated when damage reaches a critical value, the first part of the cohesive law vanishes. The cohesive law is only used to model the interaction of the two surfaces of a crack until full material separation, prior to crack initiation material behaviour is fully determined by the continuum model. In particular for ductile metals, the linear type and the exponential type of cohesive laws (figure 6.4) are the mostly used [22, 147–150]. In both types of laws, the maximum cohesive traction occurs at the crack tip and its influence decreases away from it. The main difference is that, in the linear case, there is a certain crack opening threshold from which the cohesive law stops acting, while in the exponential case the cohesive law is permanently active (although, after a certain crack opening value its influence is negligible).

An exponential cohesive law may be written in the general form:

$$t_{co} = t_{co\max} e^{-\omega_0 \omega} \quad (6.9)$$

and therefore is characterised by two parameters, the maximum cohesive tension,  $t_{co\max}$ , discussed in the previous paragraphs and the shape factor,  $\omega_0$ . Here, the normal and tangential components of the cohesive tension will be considered as follows:

$$\begin{aligned} t_{con} &= F_n e^{-\omega_{0n} \omega_n} \\ t_{cot} &= F_t e^{-\omega_{0t} \omega_t} \end{aligned} \quad (6.10)$$

where  $F_n$  and  $F_t$  represent the maximum cohesive tension and  $\omega_{0n}$  and  $\omega_{0t}$  are shape factors of the cohesive law for the normal and tangential components, respectively.

*Remark 6.1. Alternatively, an exponential cohesive law may be characterized by the maximum cohesive traction and the associated energy,  $\Gamma$ , which corresponds to the area under the cohesive traction-crack opening curve. However, the two descriptions,  $t_{cmax}-\omega_0$  and  $t_{cmax}-\Gamma$ , are indeed equivalent as  $\Gamma = \int t_{co} d\omega$ .*

*Remark 6.2. In the problems addressed in this thesis the effect of the tangential component of the cohesive traction is not significant and therefore the parameter fitting will focus on the normal component.*

Traditionally the parameters of the cohesive law are considered to be characteristic of a certain material and are often related to the fracture energy,  $G_f$ , defined as the amount of energy dissipated in the creation of a unit traction-free crack. For instance, Alfaiate et al [55] proposed for the normal cohesive tension the following expression:

$$t_n = f_{t0} e^{-\frac{f_{t0}}{G_f} \omega_n} \quad (6.11)$$

where  $f_{t0}$  is the initial tensile strength of the undamaged material. As these parameters, especially  $G_f$  are obtained through LEFM considerations, they may not be adequate for ductile fracture. In fact, even the extensions of LEFM to include plastic effects, such as the J-Integral, fail in describing the fracture process in materials which deform substantially in the plastic regime.

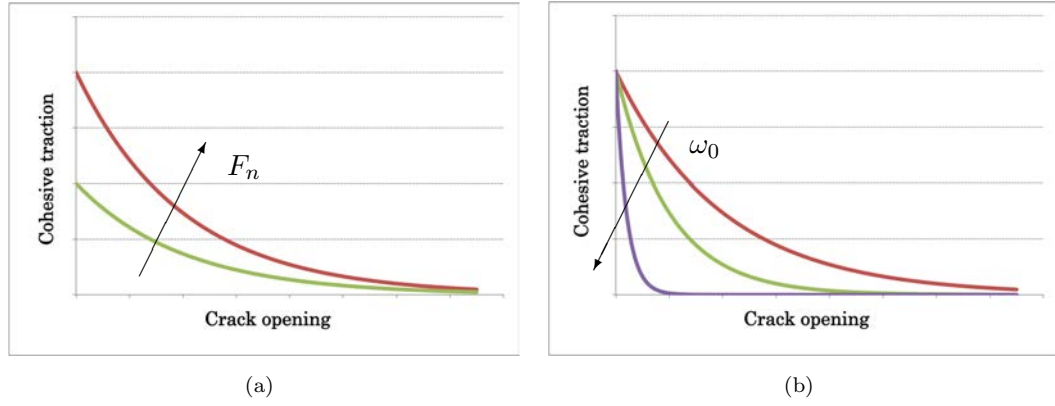
An interesting approach may be found in the work of Tvergaard and Hutchinson [22], who studied ductile fracture using a Gurson-type model. There, it was proposed that the energy necessary to create a macro-crack,  $\Gamma_F$ , is a function the energy required to grow and coalesce the voids in the material,  $\Gamma_0$ , that is

$$\Gamma_F = \Gamma_F(\Gamma_0) \quad (6.12)$$

with

$$\Gamma_0 = \tau_y \frac{D_V}{2} \quad (6.13)$$

In equation 6.13  $\tau_y$  is the yield strength and  $D_V$  is the average void fraction. The authors also observed that the intensive plastic strain in the vicinity of the crack tip accelerates the nucleation of additional voids, which consequently has the potential of significantly lowering the relative crack resistance. The explicit form of the function  $\Gamma_F$  is simultaneously dependent on the plastic strain and on the void fraction, resulting in

FIGURE 6.5: Changes in the cohesive response in function of a)  $F_n$  b)  $\omega_0$ .

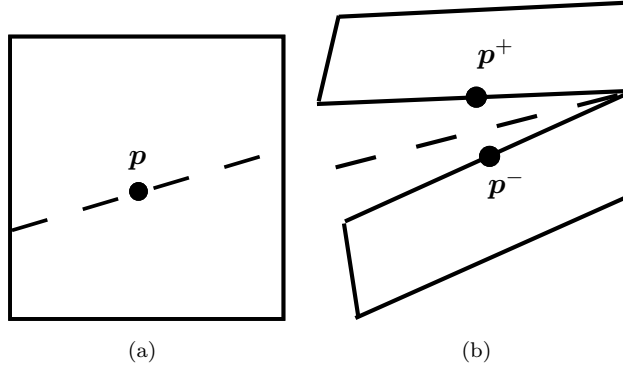
a traction-separation law equally dependent on these phenomena.

Establishing a comparison between the Gurson and the Lemaitre model, it follows that, in the later, the parameters of the cohesive law should somehow be related to the damage variable, as well as to plastic strain. In the model developed in this thesis, the onset of fracture is determined by the critical damage value,  $D_c$ , meaning that for  $D_c < 1$ , the material is not fully degraded and therefore, the cohesive law should simulate the remaining material interaction between the two sides of a crack. Consequently, the parameters of the cohesive law should not be a characteristic of the material but adjusted according to the stage at which transition from damage to fracture is performed. The magnitude of the parameters of the cohesive law may vary widely. Following the above considerations, the following relation will serve as a first estimate for  $F_n$ :

$$F_n \approx (1 - D_c)\tau_y \quad (6.14)$$

where  $\tau_y$  is the maximum yield traction and therefore the cohesive law is related to plastic straining and damage. In terms of  $\omega_0$ , as it influences the shape of the cohesive law, its value should ensure that the effects of the cohesive zone are noticeable in the final response of the component. In figure 6.5, the general influence of the parameters in the cohesive tension-crack opening curve is depicted.

In this work the cohesive law is inserted with the objective of making the transition from damage to fracture energetically consistent. Therefore, to fit the parameters of the cohesive law, an energy equivalence between the model with and without cohesive law should be established. However, before proposing an explicit form for the energy balance, it is worthwhile to analyse the influence of the cohesive law in some of the examples presented in chapter 5. As the insertion of a cohesive law represents an increase

FIGURE 6.6: a) Point  $p$  on the crack surface. b) Images of point  $p$ .

in the strain energy, its effect in the global model is expected to be equivalent to increase the critical damage value.

### 6.1.3 Numerical implementation

In a problem where cracks are modelled with the XFEM, the implementation of a cohesive law is straightforward [151]. A point  $p$ , located exactly on the crack, may be considered to have two images when the crack opens:  $p^+$  on one crack surface and  $p^-$  on the other, as illustrated in figure 6.6. For cracks represented through the XFEM, the difference between  $p^+$  and  $p^-$  lays in the value of the Heaviside function  $H$ , that is:

$$\begin{aligned} H(p^+) &= 1 \\ H(p^-) &= -1 \end{aligned} \quad (6.15)$$

Consequently, the crack opening at point  $p$  is given by:

$$\omega = (u(p^+) - u(p^-)) = 2 \sum_{j=1}^{n_{split}} N_j a_j \quad (6.16)$$

or by

$$\omega = (u(p^+) - u(p^-)) = 2 \sum_{k=1}^{n_{tip}} N_k R b_k \quad (6.17)$$

for  $p$  located in a split or a tip element, respectively.

In terms of numerical integration, two Gauss points per crack segment, per element are employed, as schematically illustrated in figure 6.7.

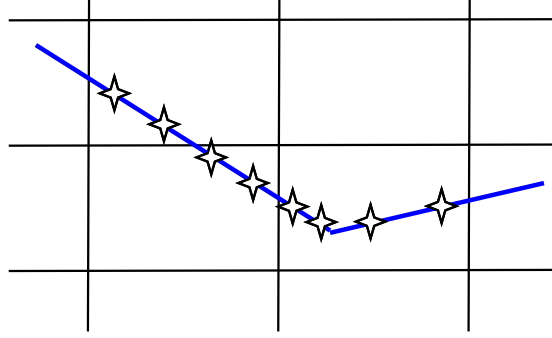


FIGURE 6.7: Gauss points used in the integration of a cohesive law.

## 6.2 Numerical study on the influence of a cohesive law

In this first set of numerical examples it is intended to investigate the influence of a cohesive law in crack initiation and propagation. Therefore, some of the examples presented in chapter 5 are simulated with a formulation enhanced with a cohesive law.

The finite element formulation is prepared to deal simultaneously with a normal and a tangential cohesive laws, however, as in the problems addressed, the influence of the normal cohesive law is dominant, the tangential part will be neglected.

### 6.2.1 Plate with an existing crack

Although the general purpose of this thesis is to address problems with large yielding, the first example is again a plate with an existing crack. In this type of problem it is easier to track the influence of the cohesive law.

The geometry and boundary conditions are represented in figure 6.13, as well as the finite element mesh employed. The material properties are summarized in table 6.1. The analysis is run under plane strain assumption.

As previously mentioned, the cohesive law employed has the following form

$$t_{cn} = F_n e^{-\omega_0 \omega} \quad (6.18)$$

$F_n$  is chosen in such a way  $F_n \approx (1 - D_c)\tau_y$ , which corresponds to  $F_n \approx 225$  MPa. In terms of  $\omega_0$ , as it influences the shape of the cohesive law, its value should ensure

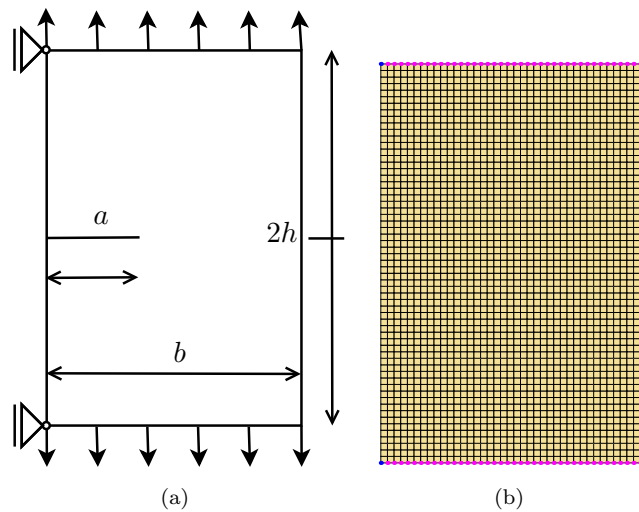


FIGURE 6.8: a) Plate with initial crack b) FEM mesh.

TABLE 6.1: Material properties of the cracked plate.

| Property           | Value                                                       |
|--------------------|-------------------------------------------------------------|
| Elastic modulus    | $E = 206.9 \text{ GPa}$                                     |
| Poisson's ratio    | $\nu = 0.29$                                                |
| Damage exponent    | $s = 1.0$                                                   |
| Damage denominator | $r = 1.25 \text{ MPa}$                                      |
| Hardening function | $t_y(R) = 450 + 129.24R + 265(1 - e^{-16.93R}) \text{ MPa}$ |
| Critical damage    | $D_c = 0.5$                                                 |
| Non-local length   | $l_r = 1.6 \text{ mm}$                                      |

that the effects of the cohesive zone are noticeable in the final response of the component.

The influence of the cohesive law in the reaction force-applied displacement curve of the plate, prior to crack growth is represented in figures 6.9 and 6.10. The model exhibits a higher sensitivity to  $F_n$  than to  $\omega_0$ . As expected, increasing the value of  $F_n$  the strain under the reaction force-applied displacement curve increases significantly. On the other hand, in terms of  $\omega_0$ , the effects of the cohesive law nearly vanish for  $\omega_0 > 1 \text{ mm}^{-1}$ , as from this value the slope of the cohesive law becomes appreciable and, consequently the crack becomes nearly traction-free.

This preliminary study is finalized inspecting the crack growth phase. The effect of the cohesive law in the reaction force-applied displacement curve and in the crack length evolution are displayed in figures 6.11 and 6.12, respectively. It can be observed that the cohesive law delays slightly the propagation of the crack and increases the global strain energy, which suggests that the cohesive law could have the same effect as increasing

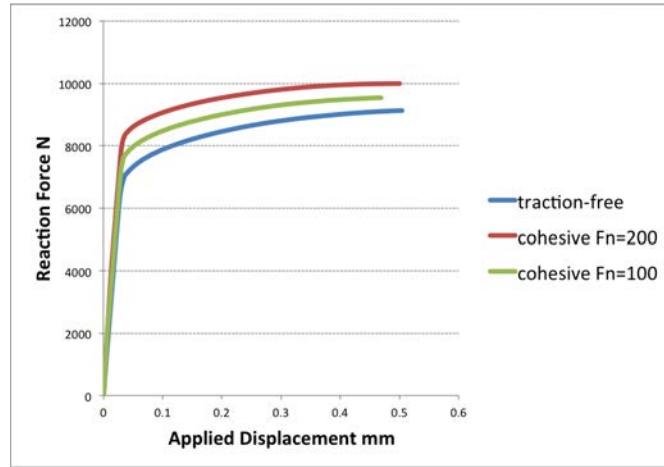
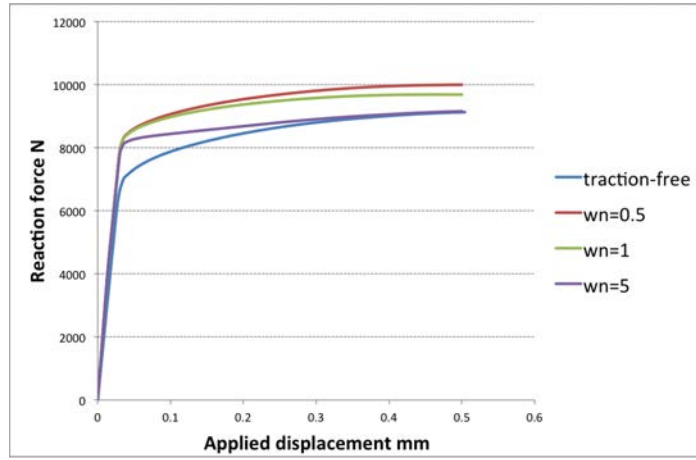
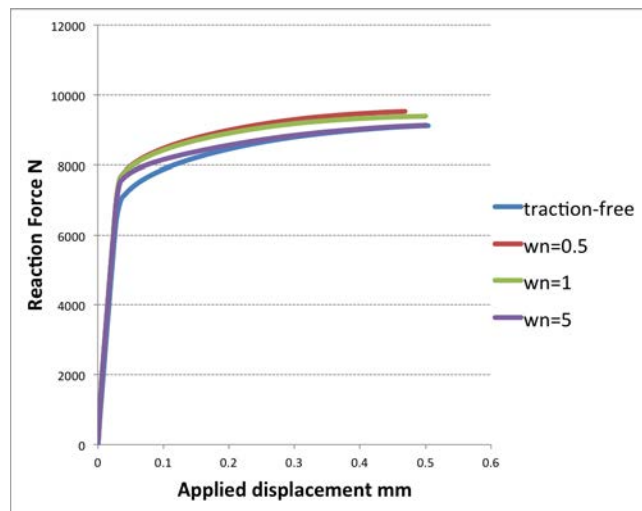


FIGURE 6.9: Influence of  $F_n$  in the response of the cracked plate for constant  $\omega_0 = 0.5 \text{ mm}^{-1}$ .



(a)



(b)

FIGURE 6.10: Influence of  $\omega_0$  in the response of the cracked plate for constant a)  $F_n = 200 \text{ MPa}$  b)  $F_n = 100 \text{ MPa}$ .

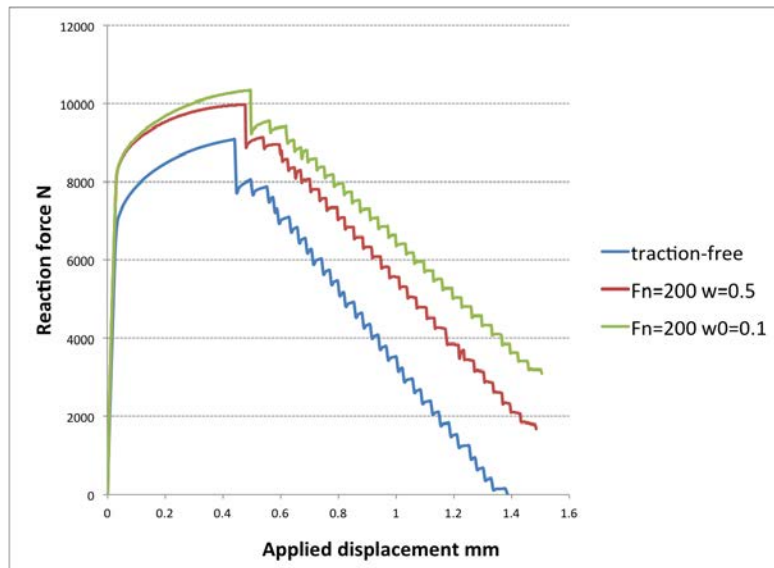


FIGURE 6.11: Influence of a cohesive law in the reaction force during crack propagation.

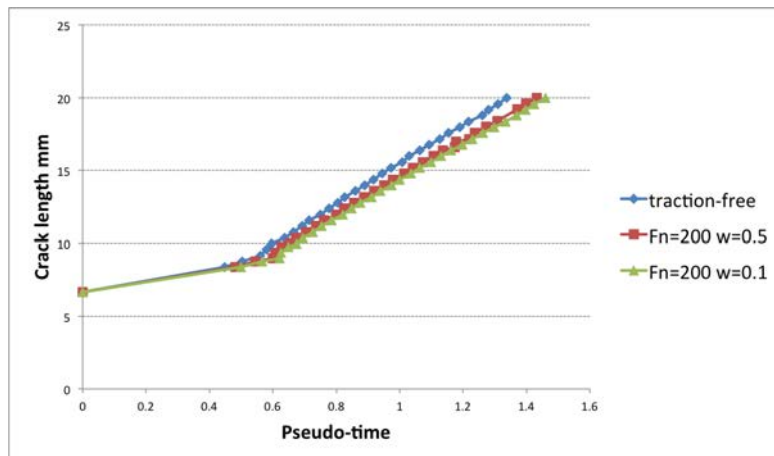


FIGURE 6.12: Influence of a cohesive law in the evolution of the crack length.

the critical damage value.

The main objective of this problem was to check the sensibility of the damage model to the cohesive law before moving to the transition problems. However, the importance given to the magnitude of the cohesive parameters is relative, as in this work they are regarded as numerical parameters, rather than material characteristics.

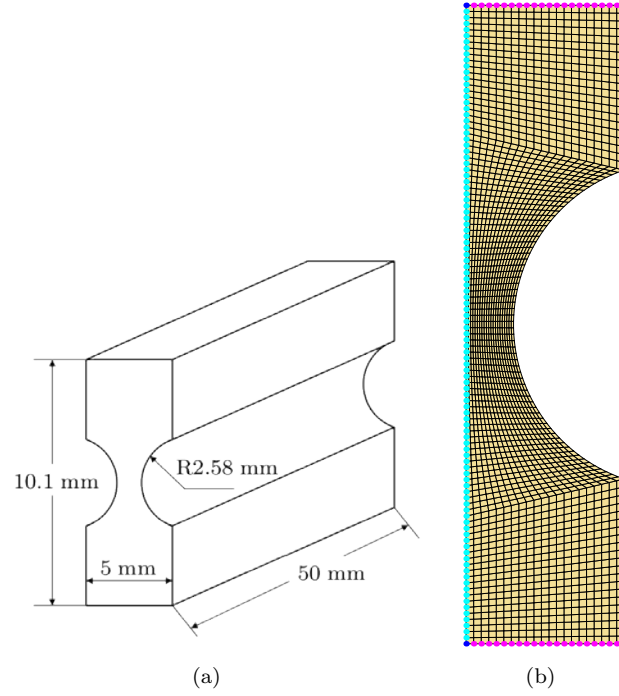


FIGURE 6.13: a) Plane strain specimen b) FEM mesh.

### 6.2.2 Transition from damage to fracture

In the previous example it was possible to get a first estimate of the magnitude of the cohesive law parameters:  $\omega_0 \leq 1 \text{ mm}^{-1}$  and  $F_n \approx (1 - D_c)\tau_y$ . Now an example considering the full model of transition from damage to fracture is inspected. It consists of a plane strain specimen, illustrated in figure 6.13, which was previously analysed in the context of traction-free cracks. In the same figure it is represented the finite element mesh employed, which has a 2205 elements. The material properties are the same used in the previous example, with the exception of the critical damage value and the parameters of the cohesive law.

In the first analysis the critical damage has the value of  $D_c = 0.4$ . The reaction force-applied displacement curve of a traction-free crack is compared with the one of a cohesive crack. The cohesive law parameters are  $F_n = 200 \text{ MPa}$  and  $\omega_0 = 0.5 \text{ mm}^{-1}$ . Results are displayed in figure 6.14.

The cohesive law ensures a smoother transition from damage to fracture and a smoother crack propagation, as a result the strain energy under the reaction force-applied displacement curve increases. Comparing the results with the case of a traction-free crack where  $D_c = 0.5$ , it can be observed in figure 6.15 that the curve corresponding to  $D_c = 0.5$  may

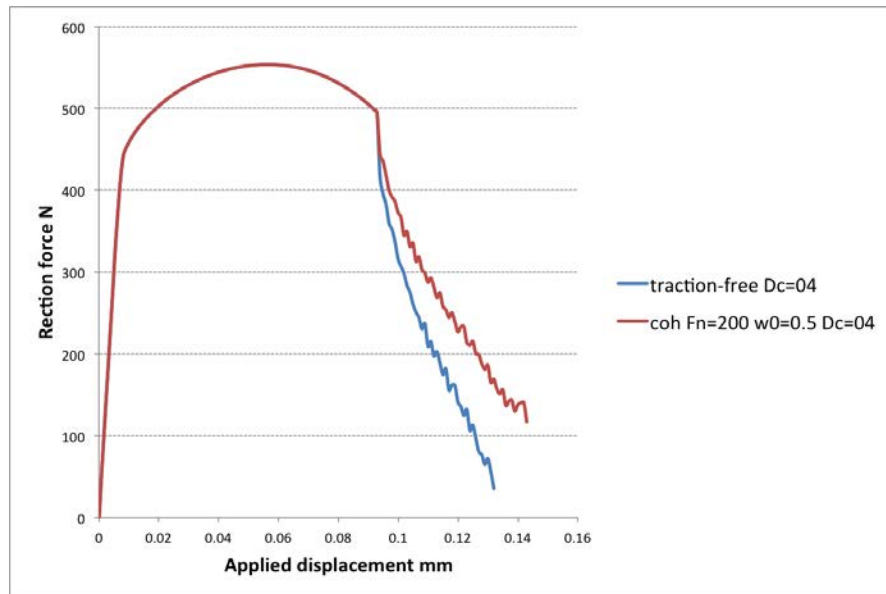


FIGURE 6.14: Reaction force-applied displacement curves.

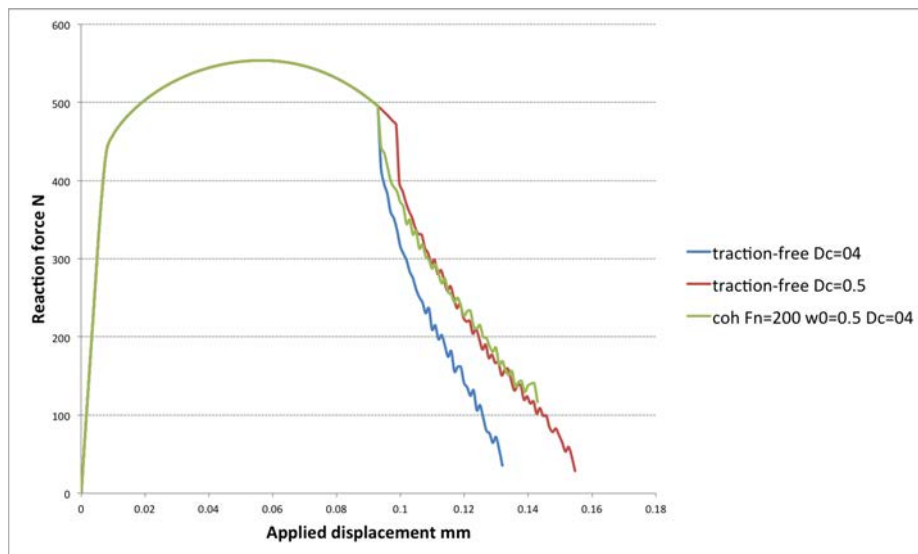


FIGURE 6.15: Reaction force-applied displacement curves and respective influence of the cohesive law.

be approached by the curve  $D_c = 0.4$  enhanced by the cohesive law. This fact suggests that the curve corresponding to the traction free crack  $D_c = 1$  could be approached by setting the cohesive parameters at the right values.

To finalize this example, the crack evolution is illustrated in figure 6.16, however, the effect of the cohesive law is not so significant. The crack growth speed is still higher for  $D_c = 0.4$  combined with the cohesive law than for  $D_c = 0.5$ . Depending on the particular application, it may be more important to have an accurate prediction of the load level/applied displacement at which the failure of the component happens or an

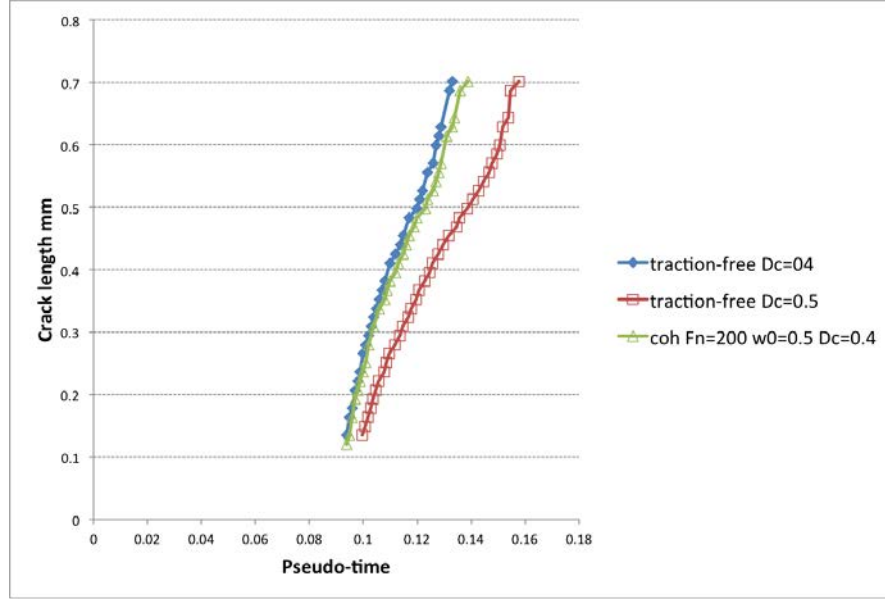


FIGURE 6.16: Influence of the cohesive law in the evolution of the crack length.

accurate prediction of the crack length evolution. The important conclusion is that simulations with high critical damages may be approached by simulations with lower critical damages, combined with a cohesive law. Therefore, in the next section an energy relation between the traction-free model and the cohesive model will be proposed, with the objective of fitting the cohesive law parameters. By setting these parameters to the right values, it will be possible to approach the transition from damage to fracture at  $D_c = 1$ .

### 6.3 Energy balance and calibration of the parameters of the cohesive law

The early crack propagation models, based in LEFM concepts, assume that there is a certain amount of dissipated energy, which is material-specific and is responsible for a certain crack extension. Fracture is triggered by a single parameter such as the Griffith fracture energy or the stress intensity factor. Even extensions of this theories to include crack tip plasticity still rely on a single parameter and consider that the total amount of dissipated energy in a deformation process is used to propagate cracks [147, 152].

In materials which exhibit substantial deformations prior to crack growth at least two energy consuming processes should be considered, one related to plastic deformation and another related to progressive material degradation, that is, related to damage. In this context, Mazars and Pijaudier-Cabot [145] developed the equivalent crack concept,

in which the damage energy release rate is equivalent to the crack surface energy, as follows:

$$\int_V -Y \dot{D} dV = -G_F \dot{A} \quad (6.19)$$

In equation 6.19  $V$  is the overall volume of the structure,  $Y$  is the damage energy release rate (as defined in chapter 2),  $D$  is the damage variable,  $G_F$  is the fracture energy and  $A$  is the area of the crack. One of the main limitations of this approach is that requires the value of the fracture energy, which is a parameter derived from the LEFM and its applicability in a ductile fracture context may be questionable.

Alternatively, Cazes et al. [58, 59], propose a formally identical expression, where  $G_F$  is replaced by the area under the traction curve of a cohesive model. The equivalence of damage to fracture is also performed locally and the model is only fully developed for 1D problems.

The work developed in this chapter is conceptually related to these approaches. In fact, the results presented so far indicate that a cohesive law may actually compensate for a transition from damage to fracture before for critical damage values lower than one. Nevertheless, in opposition to the described models, we believe that the energy balance between damage and fracture should be evaluated in a global way. A local balance may be ambiguous in terms of the elements which should contribute for the energy balance: all the elements which reached critical damage in a certain region, or only the elements which will contain the crack? In addition, the direct energy transfer from the damaged volume to the crack surface admits that the micro-mechanical damage processes in that volume stop evolving and that all the energy stored in the micro-structure is transmitted to the dominant macro-crack, which is not necessarily true.

Here, having in mind that the strain energy may be given by

$$\Gamma = \int_{\mathcal{X}(\Omega)} \boldsymbol{\sigma} : \mathbf{d} dv \quad (6.20)$$

a function,  $\Gamma = \Gamma(D_c)$ , will be constructed for traction-free cracks, in order to approximate the value of  $\Gamma(D_c = 1)$ . Then, departing from a certain value of  $D_c < 1$ , a cohesive law will be added in order to meet the condition:

$$\Gamma(D_c < 1 + \text{cohesive law}) = \Gamma(D_c = 1) \quad (6.21)$$

In the next section, the efficiency of this methodology will be illustrated through some numerical examples.

## 6.4 Numerical examples

### 6.4.1 Plane strain specimen

This section starts by going back to the plane strain specimen of section 6.2.2 and analyse the strain energy involved in each one of the cases presented: traction-free crack with  $D_c = 0.4$ , traction-free crack with  $D_c = 0.5$  and cohesive crack with  $D_c = 0.4$ . The respective values of the strain energy are displayed in table 6.2.

TABLE 6.2: Strain energy for  $D_c = 0.4 - 0.5$ .

| Case                      | Strain energy - J |
|---------------------------|-------------------|
| traction-free $D_c = 0.4$ | 101.4             |
| cohesive $D_c = 0.4$      | 121.7             |
| traction-free $D_c = 0.5$ | 121.8             |

In terms of energy balance, the introduction of a cohesive law is indeed equivalent to rise the critical damage value. To emphasise this fact, the influence of the cohesive law for  $D_c = 0.6$  and  $D_c = 0.7$  is illustrated in figure 6.17. The respective values of the strain energy may be found in table 6.3. Choosing the values  $F_n = 80 \text{ MPa}$  and  $\omega_0 = 1.0 \text{ mm}^{-1}$ , the curve corresponding to a traction-free case with  $D_c = 0.7$  is very well approximated. In terms of energy balance, the choice  $F_n = 150 \text{ MPa}$  and  $\omega_0 = 0.5 \text{ mm}^{-1}$  also produces good results, but the crack propagation phase is over-smoothed, suggesting that approximations using lower values of the strain energy are preferable to approximations using higher values of the strain energy.

TABLE 6.3: Strain energy for  $D_c = 0.6 - 0.7$ .

| Case                                                                              | Strain energy - J |
|-----------------------------------------------------------------------------------|-------------------|
| traction-free $D_c = 0.6$                                                         | 132.4             |
| traction-free $D_c = 0.7$                                                         | 139.6             |
| cohesive $D_c = 0.6$ , $F_n = 80 \text{ MPa}$ , $\omega_0 = 1 \text{ mm}^{-1}$    | 136.4             |
| cohesive $D_c = 0.6$ , $F_n = 150 \text{ MPa}$ , $\omega_0 = 0.5 \text{ mm}^{-1}$ | 140.1             |

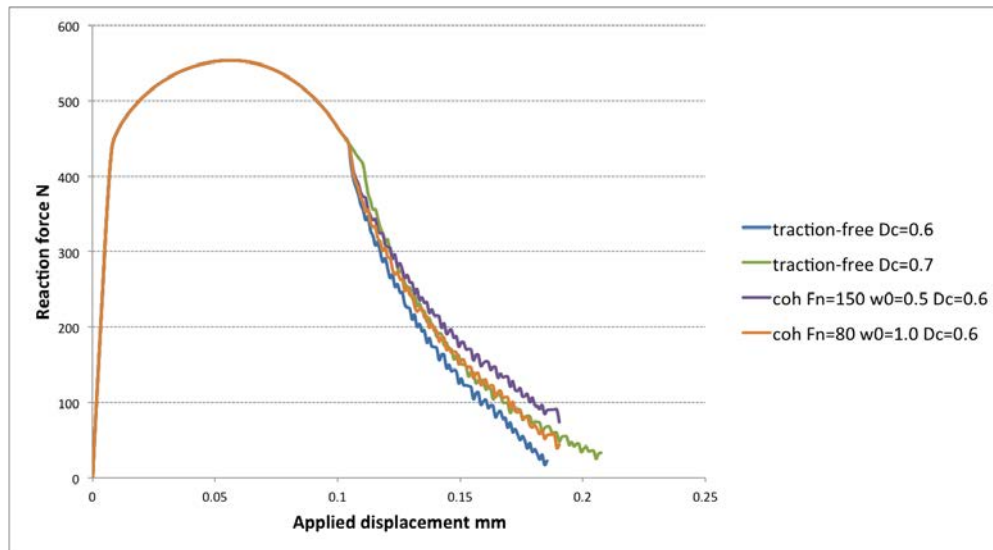


FIGURE 6.17: Reaction force-applied displacement curves and respective influence of the cohesive law.

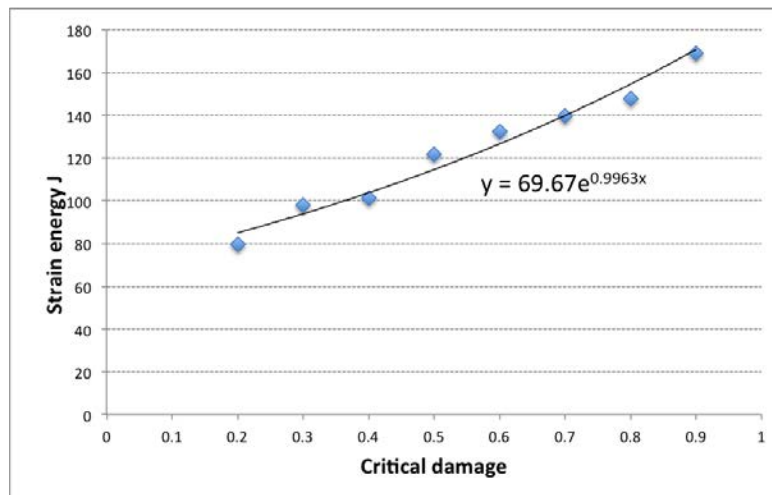


FIGURE 6.18: Strain energy as a function of the critical damage. Correlation factor:  $R^2 = 0.985$ .

To achieve the energetically consistent transition from damage to fracture, one must determine the strain energy for  $D_c = 1$ . In figures 6.18 and 6.19 the strain energy as a function of the critical damage value is represented, together with two alternative fittings: an exponential function of the type  $y = ae^{bx}$  and a polynomial function as  $y = ax^3 + bx^2 + cx + d$ . The coefficients defining each function were determined using the least-squares method. Using the exponential function the strains energy value is  $\Gamma(D_c = 1) = 188.7 \text{ J}$ , while using the polynomial function  $\Gamma(D_c = 1) = 186.4 \text{ J}$ . The proximity of the two values suggests that the real value of  $\Gamma(D_c = 1)$  should be of this order of magnitude. Therefore, departing from a critical damage value of  $D_c = 0.8$ , a cohesive law was added in order to meet  $\Gamma(D_c = 0.8 + \text{cohesivelaw}) \approx 187 \text{ J}$ .

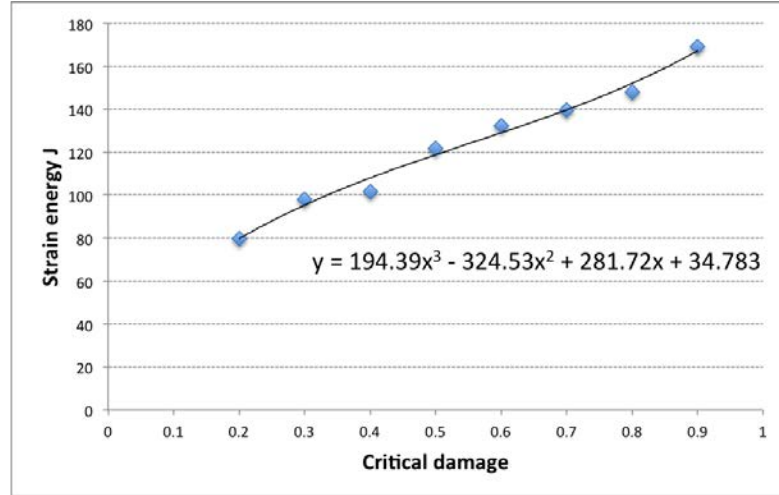


FIGURE 6.19: Strain energy as a function of the critical damage. Correlation factor:  $R^2 = 0.967$ .

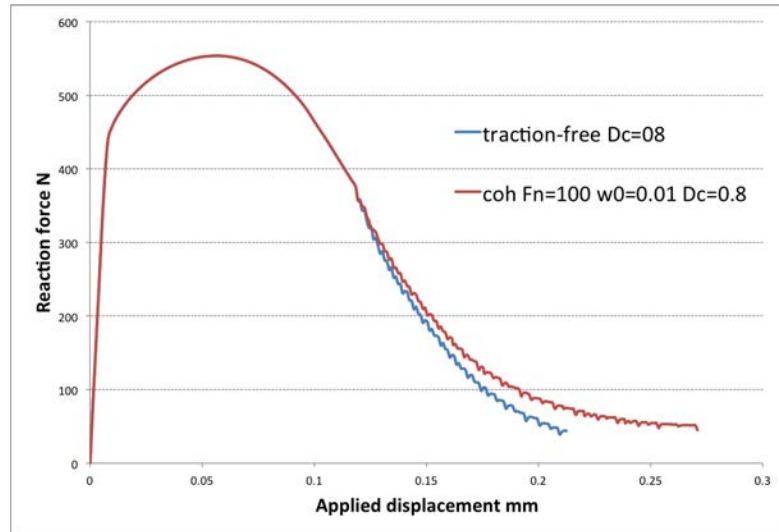


FIGURE 6.20: Reaction force-applied displacement curves and respective influence of the cohesive law.

The best fit is obtained setting the parameters of the cohesive law to  $F_n = 110\text{MPa}$  and  $\omega_0 = 0.01\text{mm}^{-1}$ . The strain energy obtained is  $\Gamma(D_c = 0.8 + \text{cohesivelaw}) = 185.1\text{J}$ , which is quite close to the expected value. In figure 6.20 it is possible to observe the difference between the traction-free and the cohesive reaction force-applied displacement curves.

Throughout this chapter it has been mentioned that a cohesive law increases the total strain energy under the reaction force-applied displacement curve, which has been verified through various numerical examples. However, in the context of this work, the cohesive law parameters are not a characteristic of the material, but numerical parameters which adapt to the critical damage value. Physically they may be interpreted as

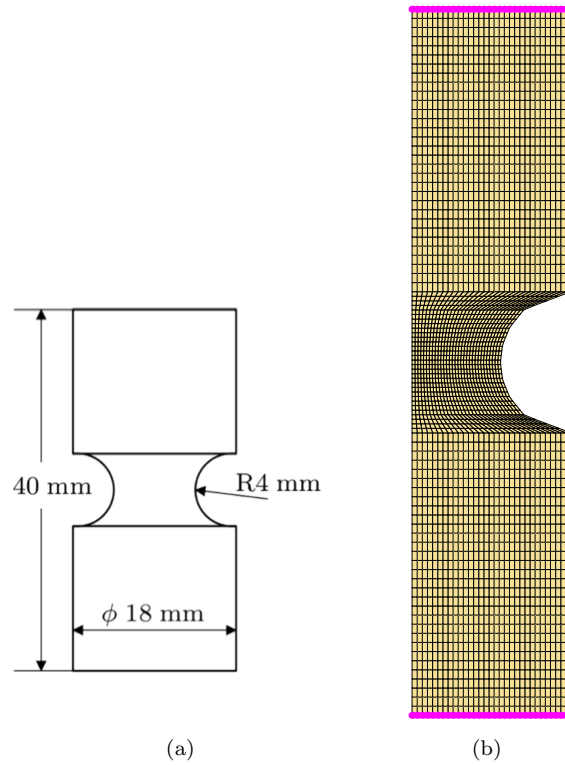


FIGURE 6.21: a) Plane strain specimen b) FEM mesh.

resulting from material which is still interacting between the two surfaces of a crack. Although further studies are necessary for a better calibration of the model, we believe this results constitutes an important step towards energetically transition from damage to fracture.

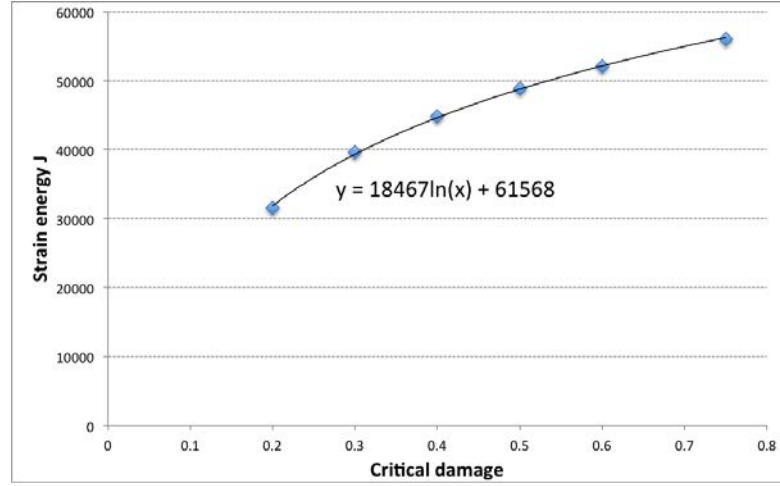
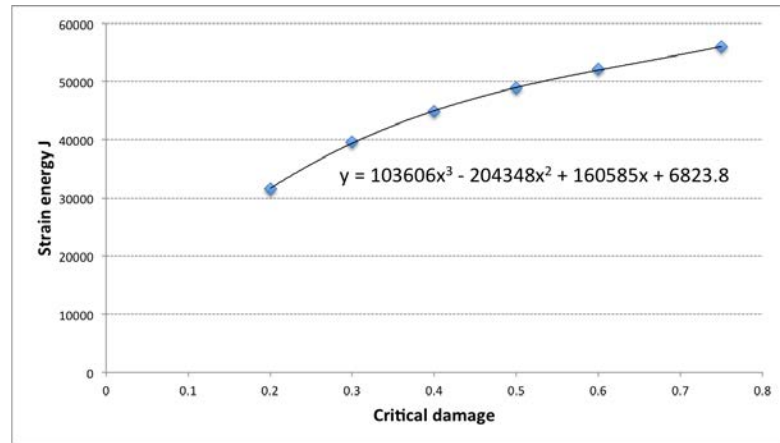
#### 6.4.2 Axisymmetric specimen

The proposed methodology for energetically consistent transition from damage to fracture is now analysed for an axisymmetric example. The specimen is also the same used in chapter 5 and is represented in figure 6.21, along with the corresponding finite element mesh, with 2883 elements. The material properties are summarized in table 6.4.

In this example, the strain energy is also expressed as a function of the critical damage, however, observing the distribution pattern, a logarithmic fitting seems more adequate than the exponential fitting used in the previous example. Therefore, a fitting considering a logarithmic function of the type  $y = a \ln(x) + b$  and a fitting considering a polynomial function as  $y = ax^3 + bx^2 + cx + d$  are respectively displayed in figures 6.22 and 6.22 . Accordingly it follows that  $\Gamma(D_c = 1) = 61568 \text{ J}$  or  $\Gamma(D_c = 1) = 66667 \text{ J}$ .

TABLE 6.4: Material properties of the axisymmetric notched specimen.

| Property           | Value                                                       |
|--------------------|-------------------------------------------------------------|
| Elastic modulus    | $E = 206.9 \text{ GPa}$                                     |
| Poisson's ratio    | $\nu = 0.29$                                                |
| Damage exponent    | $s = 1.0$                                                   |
| Damage denominator | $r = 1.25 \text{ MPa}$                                      |
| Hardening function | $t_y(R) = 450 + 129.24R + 265(1 - e^{-16.93R}) \text{ MPa}$ |
| Non-local length   | $l_r = 2.0 \text{ mm}$                                      |

FIGURE 6.22: Strain energy as a function of the critical damage. Correlation factor:  $R^2 = 0.999$ .FIGURE 6.23: Strain energy as a function of the critical damage. Correlation factor:  $R^2 = 0.999$ .

Once more the two values are relatively close and an attempt to reach  $\Gamma(D_c = 1)$  is depicted in figure 6.24.

Choosing the parameters of the cohesive law as  $F_n = 150 \text{ MPa}$  and  $\omega_0 = 1.0 \text{ mm}^{-1}$ , the strain energy obtained is  $\Gamma(D_c = 0.75 + \text{cohesivelaw}) = 59644.6 \text{ J}$ , which is an

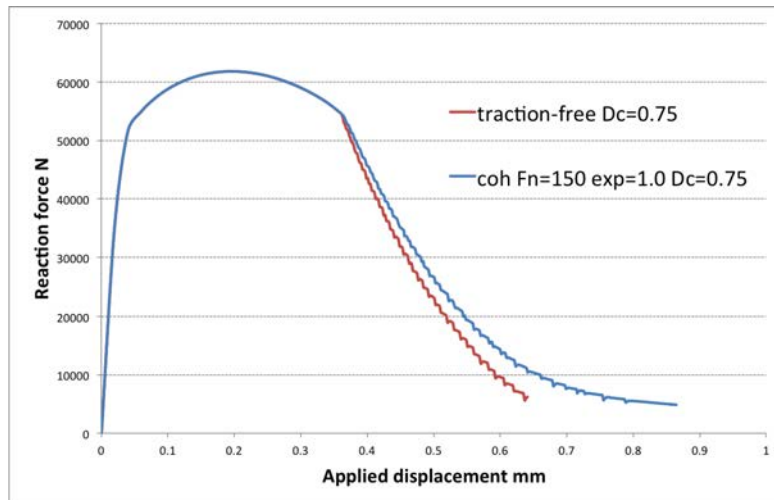


FIGURE 6.24: Reaction force-applied displacement curves and respective influence of the cohesive law.

encouraging result, showing that the proposed methodology is suitable for both plane strain and axisymmetric problems.

Despite the good performance exhibited, these are still preliminary results. The model assumes that the strain energy associated to  $D_c = 1$  follows the trend of the strain energy for  $D_c < 1$  and the target value is determined using approximation techniques, which have a certain error associated. At this stage, experimental data is highly desired to evaluate the real magnitude of the strain energy involved in a ductile fracture process. Additionally, from a numerical point of view, the calculation of the sensitivities associated to the cohesive parameters may provide a better understanding of the effects of the developed approach.

## 6.5 Conclusions

In this chapter a cohesive law of the exponential type was introduced in the model presented in chapter 5, with the objective of making the transition from damage to fracture energetically consistent.

A cohesive law may be viewed as the interaction between the two surfaces of a crack and may be used to model material which is not fully degraded. Therefore an energetically consistent transition from damage to fracture, corresponding to  $D_c = 1$  may be approximated by simulation in which  $D_c < 1$  is enhanced by a cohesive law.

Constructing a function,  $\Gamma(D_c)$ , relating the strain energy with the critical damage value, it was possible to estimate the strain energy associated with  $D_c = 1$ . Subsequently, considering  $D_c < 1$ , the parameters of a cohesive were adjusted in order to meet  $\Gamma(D_c = 1)$ . This means that, in this model the parameters of the cohesive law are not a characteristic of the material, but a numerical parameter associated with  $D_c$ .

There are still open questions related to the determination of the cohesive parameters, especially because one single energetic equivalence is used to fit two parameters. In the future, the proposed methodology may be improved by determining the sensitivity of the full model to the cohesive law parameters. We recall that the proposed ductile fracture model features geometrical and material non-linearity, includes a non-local formulation and a discontinuous formulation, and therefore the calculation of the associated sensitivities is not a simple task. Nonetheless, the model is conceptually successful.



## Chapter 7

# Final Remarks

Ductile fracture has been a key issue within industry, as a considerably large number of materials fail according to this mechanism, in particular ductile metals such as steel or aluminium. Accurate simulations of this phenomenon are essential to produce safer designs and at the same time save resources, from the economical and environmental perspectives.

Modelling ductile fracture is a complex task as it involves geometrical and material non-linearities and propagation of discontinuities. A continuum model is adequate to describe the underlying microscopic mechanisms which trigger fracture initiation. Nevertheless, a discontinuous approach is more suitable to describe the last stage of failure, which involve the propagation of macro-cracks. Therefore, the aim of this work was combine the advantages of both continuous and discontinuous approaches in order to build a model able to handle simultaneously large strains, damage localisation and crack propagation.

In ductile metals, material progressive degradation is strongly associated with large plastic strains. This behaviour may be captured using the Lemaitre damage model, in which the nucleation, growth and coalesce of micro-voids, is considered in an averaging way through the damage variable. Once a critical damage level has been reached, the damage variable distribution may be used to define the size and orientation of a crack, which, in this work, is inserted in the simulation using the XFEM.

The development of the proposed model includes several contributions, which are related to finite element technology or to phenomenological aspects, each of them described in the following paragraphs.

### **Finite element technology**

The use of the XFEM in ductile fracture raised some questions relative to the standard implementation generally followed in the case of brittle fracture problems. One of the key issues is numerical integration, as results produced by regular Gaussian rules are not accurate enough, due to the presence of discontinuous functions. This fact motivated the development of various integration techniques, available in the literature, in which the accuracy is typically measured by the ability of reproducing stress intensity factors. Here, an approach based on the underlying sub-space of incompressible deformation modes was favoured. The aforementioned sub-space gives precious hints on the ability of a particular method to reproduce incompressible deformations, essential in problems where plasticity plays an important role. Moreover, valuable information on how spurious deformation modes may be prevented or on how over integration rules may be avoided are also provided. As a consequence, the conventional formulations of B-bar and F-bar were adapted to include the XFEM enrichment functions.

Still regarding element technology, the interaction of the XFEM with the non-local averaging operator and the issue of variable transfer, when an element changes from standard to enriched, were also addressed.

### **General ductile fracture modelling**

A realistic description of all the stages of material behaviour was achieved by combining the XFEM with the Lemaitre damage model. Furthermore, the non-local damage model clearly alleviates the pathological mesh dependence associated with local continuum formulations. This ensures similar damage patterns in coarse and fine meshes and consequently, similar crack paths and velocity. There is no need of determining additional material parameters related to crack propagation.

The energetic consistency issue during the transition from damage to fracture was also addressed. It was shown that the propagation of a traction-free crack considering a certain critical damage value, could be approximated by a lower critical damage value,

inserting a cohesive law. The parameters of the cohesive law were not regarded as characteristic of the material but were rather fit following global energetic considerations. Furthermore, a numerical strategy to approach the fully degraded material condition was developed.

### **Advantages and drawbacks relative to competing approaches**

The XFEM is a highly flexible method, allowing the representation of arbitrary crack paths within a finite element mesh. In the particular case of this model, crack initiation and crack propagation are handled in a unified way, in an approach closely related to plasticity and damage, suitable to describe large scale yielding problems. Moreover, the location of the cracks does not need to be known in advance allowing the simulation of ductile failure in components of arbitrary shape. All these are aspects which are not well covered by the existing literature on the XFEM.

Although there is a minimal variable transfer, when the location of the Gauss points inside a particular element is changed, the numerical implementation is quite robust. There is no projection outside a particular element, which means that quantities stored at the nodes, such as the displacements, remain constant during crack initiation and propagation. In addition, the XFEM formulation itself together with the automatic generated code, which is highly optimized, ensure a good computational performance - the simulations presented in this work were run in a common laptop in what we believe to be a reasonable time (less than one or two hours). The resulting model is then competitive with remeshing in terms of accuracy, while saving computational resources.

The drawbacks of the proposed approach are more related to the XFEM itself than with the developments presented herein. As an enrichment method, the extra degrees of freedom contribute for a larger stiffness matrix and the implementation in a certain FEM environment requires that the chosen system is prepared to accommodate these extra degrees of freedom. Nevertheless, with the *AceGen* system, the same code may be generated for different platforms, and therefore these problems are easily overcome. The remaining aspects are related to work that has not been developed yet, and not exactly to intrinsic limitations of the model, such as extension to 3D, crack bifurcation and crack joining. Therefore, this thesis finalises with some suggestions for further developments.

## 7.1 Suggestions for future work

### Extension to 3D

During the development of this work some incursions to 3D problems were made, namely in chapter 4 with the study of the incompressible deformation associated to enriched elements.

The main issues regarding the extending the full damage model to 3D are the crack path tracking and the extension of the proposed criterion for the transition from damage to fracture. In terms of the crack description, it may be regarded as a computational geometry problem, as it does not interfere in the phenomenological model itself. The crack initiation and propagation criterion is based on the damage distribution, which was handled with cubic B-splines. A 3D damage distribution may also be handled with a 3D B-spline patch and, consequently, analysing the derivatives of the B-spline, it will also be possible to determine the maximum damage plane and introduce a crack surface.

### Alternative damage/material models

Although the proposed ductile fracture model considers isotropic damage and isotropic hardening, there is no intrinsic limitation regarding these aspects. Therefore, the scalar damage variable may be replaced by a tensor damage variable, which allows, for instance, the modelling of anisotropic materials. In the same way, the isotropic hardening condition may be replaced by a kinematic hardening law.

Another interesting study would be to replace the Lemaitre model by the Gurson model, as both models are suitable for describe the behaviour of ductile metals prior to crack initiation. This would demand an adaptation of the cracking criterion driven by porosity or void volume fraction rather than damage.

### Improvement of the crack initiation criterion

The developed model is able to handle with several cracks in one problem, as long as they are associated to different damage clouds. In order to handle crack bifurcation problems, the analysis of the size and shape of the damage cloud may be coupled with the analysis of additional variables such as stress triaxiality or the Lode angle.

## **Sensitivity analysis**

The aim of sensitivity analysis is to determine the variation of a model response with respect to certain parameters. The response functional may depend on model inputs such as material constants or shape parameters or on intermediate or final results of the analysis such as damage or triaxiality.

Sensitivity analysis would be particularly interesting in the context of the subject of this thesis to analyse, in a first stage, the influence of the critical damage value and, in a second stage, the dependence of the model on the cohesive law parameters. As the sensitivity problem may be obtained from the primal problem by differentiating the response functional and the residual with respect to the design parameters, the potentialities of automatic code generation may be applied to this analysis.

## **Experimental validation**

Although the developed model was able to capture the trend of crack initiation and propagation and to reproduce reaction force-applied displacement curves which are qualitatively correct, more experimental data is required to calibrate the model. In this work, some material constants, such as the non-local regularization length or the critical damage were regarded as numerical parameters and therefore, their experimental identification would be of major importance.

Additional experimental data would permit the evaluation of the real magnitude of the strain energy involved in a ductile fracture process, resulting in a better fitting of the cohesive parameters and efficiency of the global approach.



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