

UNIVERSIDAD POLITÉCNICA DE MADRID
Escuela Técnica Superior de Ingenieros de Caminos, Canales y
Puertos



Microscale Fracture Modeling using Phase-Field and FFT-based Homogenization.

DOCTORAL THESIS

Submitted for the degree of Doctor by:

Pedro Miguel Aranda Acuña

Master of Science in Engineering, Major in Mechanical Engineering.

Madrid, 2025



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*Now this is not the end. It is not even the beginning of the end. But it is, perhaps, the end of
the beginning.*

-Winston Churchill

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Abstract

In materials engineering, understanding fracture processes at the microscale is essential for predicting and improving the mechanical performance of materials. To this aim, the development of physically based, robust, and efficient computational tools becomes fundamental. This work proposes a general implementation of the Phase-Field Fracture (PFF) model within a numerical homogenization framework based on the Fast Fourier Transform (FFT) to explore this phenomenon at the microscale. The main objective is to investigate the representation of micromechanical fracture mechanisms, particularly under conditions of unstable crack propagation, and to analyze their influence on macroscopic fracture-related properties.

The original PFF model for elastic brittle materials is considered first, and a staggered FFT solver is proposed which combines a Fourier Galerkin approach to solve the mechanical problem with a pre-conditioned Krylov solver for the Helmholtz damage equation. Subsequently, a load control strategy is introduced in which the dissipated fracture energy (proportional to crack length) is employed to drive the simulations. This method adapts the applied stress during the fracture process to fulfill Griffith's criterion during all the crack propagation, resolving all the snap-backs and leading to stable crack propagation. To validate the control scheme proposed, results are compared against both a classical PFF implementation and Finite Element Method (FEM) simulations incorporating similar control strategies.

With the numerical tools developed, an estimate of the effective toughness as a function of the microstructure is proposed for heterogeneous elastic brittle materials. The estimate is based on propagating in a stable manner an initial crack on an RVE of the material microstructure. The effective toughness of the RVE is then defined as the total energy consumed (easily quantified thanks to the control technique) divided by the RVE length. In this form, crack deflections and the crack crossing through tougher areas are the microscopic toughening mechanisms.

This approach enables the study of how localized fracture events influence global material performance. The approach proposed is used to obtain estimates of the effective toughness in various types of heterogeneous media, including laminates, composites, and polycrystals with cleavage. It is found that the heterogeneity of both the local toughness and local stiffness leads to an increase in the energy needed to extend a macroscopic crack. As in the homogenization of other material properties, the effective toughness is affected by phase properties (here stiffness and toughness) and microstructure. It is also found that the effect of local phase property contrast saturates in many cases, and further changes of phase response do not increase the overall toughness.

Finally, the microscopic fracture approach is extended to study the elasto-plastic fracture of polycrystals, using in this case crystal plasticity as a constitutive equation. The resulting method is able to predict crack deflection and plastic localization. Notable differences are observed between FFT and FEM implementations for coarse discretizations. To reduce the differences, crack tip enrichment techniques are adapted to FFT and it is shown that these discrepancies decrease. Moreover, convergence is observed between both approaches when sufficiently fine discretizations are used, even in complex microstructural configurations.

Resumen

En ciencia de materiales, comprender procesos de fractura en materiales a nivel de microescala es esencial para predecir y mejorar el comportamiento mecánico en dichos materiales. Este trabajo presenta la implementación de un modelo general de "*Phase-Field Fracture*" (PFF, por sus siglas en inglés) dentro de un marco de homogeneización numérica basado en la Transformada Rápida de Fourier (FFT, por sus siglas en inglés) para explorar este fenómeno a nivel microscópico. El principal objetivo de esta implementación es investigar la representación de la evolución de la fractura particularmente bajo condiciones de propagación inestable de grietas, y analizar su influencia en propiedades macroscópicas relacionadas con la fractura, como la tenacidad.

El modelo PFF se formula inicialmente en un marco variacional clásico para materiales frágiles, donde tanto la energía elástica como la energía de disipación por fractura están acopladas mediante campos escalares de daño que describen la evolución de la grieta. Esta formulación está diseñada para ser flexible y aplicable a diversos materiales, caracterizados por distintas microestructuras y distintos comportamientos constitutivos. Se introduce una estrategia de control numérico donde la energía disipada por fractura se utiliza para controlar el avance de las simulaciones. Esto permite recuperar la respuesta mecánica completa durante el proceso de fractura y facilita la homogeneización de propiedades macroscópicas efectivas. Con este esquema se ponen a prueba materiales con dominios microestructurales complejos, evaluando el desarrollo exacto de la grieta y la resistencia a la fractura del medio.

Un aspecto clave de este trabajo radica en la exploración de estrategias de homogeneización para materiales con distintas microestructuras. Se analiza en detalle el potencial del esquema de control por disipación para calcular propiedades homogeneizadas directamente dentro del marco basado en FFT, ofreciendo un medio para conectar los fenómenos de fractura a microescala con el comportamiento mecánico macroscópico. Este enfoque permite estudiar cómo los eventos de fractura localizados influyen en el rendimiento global del material.

Los resultados numéricos demuestran que el esquema propuesto proporciona un marco computacional robusto y eficiente para simular el comportamiento frente a fractura. Se muestra que el método captura con precisión la respuesta mecánica completa durante la propagación de grietas y ofrece estimaciones confiables de la tenacidad efectiva, en concordancia con el comportamiento de dicha propiedad reportado en la literatura. Para validar la eficacia del esquema, los resultados se comparan con una implementación clásica de PFF y simulaciones por el Método de Elementos Finitos (FEM), incorporando estrategias de control similares.

Además, las capacidades del modelo se evalúan más a fondo mediante comparaciones detalladas con simulaciones FEM de modelos basados en Plasticidad Cristalina, con el fin de probar la implementación en materiales con comportamientos complejos. Aunque surgen diferencias notables debido a las estrategias de discretización contrastantes entre FFT y FEM, se demuestra que estas discrepancias pueden mitigarse mediante técnicas de enriquecimiento PFF, acercando ambos esquemas a una concordancia numérica. Asimismo, se observa convergencia entre ambos enfoques cuando se utilizan discretizaciones lo suficientemente finas, incluso en configuraciones microestructurales de alta complejidad.

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Abbreviations and acronyms

2D Two-Dimensional.

3D Three-Dimensional.

FEM Finite Element Method.

FFT Fast Fourier Transform.

PFF Phase-Field Fracture.

RVE Representative Volume Element.

CP Crystal Plasticity model.

ν Poisson's ratio.

MPC Multi-Point Constrains.

PFE Phase-Field Enrichment.

CTE Crack tip Enrichment.

CPFE Complete Phase-Field Enrichment.

Chapter 1

Introduction

There is a growing need in the design and fabrication of materials intended for specific applications. In this process, it becomes fundamental the use of models able to provide a fast estimation of the response of these materials as a function of their microstructure and environmental conditions, allowing reducing the number of experimental tests and accelerating their industrial incorporation. Nowadays, the need for high accuracy and predictive capacity has made fundamental the use of computational-based models relying on efficient numerical methods. In addition, the huge advance in computational capacity has been decisive for the incorporation of computational models as a major tool in materials virtual testing and design.

Focusing on structural materials, an example of this class of tools is micromechanics-based models, which provide the macroscopic response accounting for the complex deformation mechanics at the microscale, linking in this form microstructure and mechanical performance. These models represent a significant advantage since it has been demonstrated that such microscopic effects control the macroscale mechanical response in materials. However, despite the aforementioned computational advances, the computational cost of these models is very high, and simulations require very long times and/or strong simplifications.

One of the aspects that has more interest in (but not only) structural materials is the study of their structural integrity, e.g. the prediction of the material failure or fracture under some particular loading conditions. Mechanical degradation is a complex phenomenon, driven by mechanics (localization of deformation), but influenced by many environmental factors such as temperature, corrosion, etc. Moreover, fracture is a typical multiscale problem. It depends on the nucleation of damage or cracks at the nano-microscale, which are strongly affected by the nature of the material and microstructure, and on their propagation at the macroscale driven by macroscopic stress states. This complexity implies coupling several effects occurring in parallel and usually requires complex predictive models to describe it, which in turn need to be solved with computational models.

Most of the computational tools available to predict fracture are focused on the macroscopic level and show in many cases very good prediction capacity. However, these models rely on some macroscopic material parameters, which define the fracture toughness, that depend on the microstructure and have to be obtained from experiments. Moreover, there is not a

unique set of parameters for a material, and the processing conditions or treatment drastically change the material behavior.

It is well known that microstructural effects have an important influence on the macroscopic fracture, specially if the material exhibits heterogeneous and anisotropic microstructure such as metallic alloys and composite materials. The former group often exhibits microstructures with granular arrangements (polycrystals), and it has been shown that the macroscopic fracture process is highly influenced by the geometric distribution of the grains (Benzerga et al., 2016). The combination of geometry, orientation, elastoplastic behavior, and local fracture resistance of individual grains controls the generation of microcracks that eventually result in the macroscopic failure of the material. In composite materials, where the microstructure includes phases with laminar, fibrous or particulate configurations, the micromechanical problem is similar. The geometry, orientation and mechanical response of the reinforcement phase control the nucleation of a crack and its extension to the macroscale. In addition, reinforcement decohesion usually plays a fundamental role here.

Numerous studies can be found focusing on the simulation of the microscopic fracture in various heterogeneous materials, including concrete (Huang et al., 2021; H. Zhang et al., 2020), biological materials (Abdel-Wahab et al., 2012; Gustafsson et al., 2019), composite materials (Mishnaevsky and Brøndsted, 2009; Segurado and LLorca, 2004), metallic composites (LLorca and Segurado, 2004; Shakoor et al., 2018), porous materials (Weck et al., 2007; Zymbell et al., 2014), and polycrystalline materials (Crocker et al., 2005; Ma and Sun, 2021). Many of these studies rely on the numerical solution of a problem that includes the microstructure in Representative Volume Elements (RVEs), in which only a statistically representative segment of the microstructure with periodic physical conditions is modeled, allowing one to observe representative behavior of any microstructural space in the material. In addition to reducing the computational cost of the simulations, this approach has the advantage of being able to be included in multi-scale frameworks (Arunachala et al., 2023; Oliver et al., 2017), which establishes links between different scales for a comprehensive view of the material's mechanical behavior. This alternative offers complex and detailed solutions, making the aforementioned studies of micromechanical modeling correspond to single material points and allowing them to be actively included in macroscopic behavior.

Computational models of fracture at the microscale aim at (1) describing the fracture process and the sequence of microscopic events which lead to macroscopic crack formation and (2) providing estimates of macroscopic fracture parameters. In case (1) the objective is to represent explicitly the microscopic deformation mechanisms which control fracture and their interaction in a loading process. Typical mechanisms include phase decohesion, microcrack/damage nucleation, and complex constitutive behavior. Macroscopic failure needs to be understood as the result of the interaction of these mechanisms, and microscopic models can help to clarify their role. An example is the description of the elasto-plastic fracture of metals, which at the microscale combines the non-linear deformation of the grains (modeled by crystal plasticity) and its incompatibility between grains with dissipation mechanisms related to fracture such as cleavage, micro-void formation and growth, crack nucleation, etc. Coupling such behaviors has implications in the formulation of macroscopic fracture models, and their study is also a current topic of actual research.

The use of micro-models to obtain estimates for macroscopic parameters (case 2) is a very interesting and practical use of damage in micromechanics, which is indeed a research hot topic in homogenization. Depending on the material, different types of models describe the fracture/damage at the macroscale, requiring different material parameters to be used. Typical fracture responses range from linear elastic fracture mechanics for brittle materials to continuous ductile damage models for ductile metals, and including also cohesive crack theories for quasibrittle material. Although each model incorporates different parameters, a common one in all these descriptions is the energy needed to create new surfaces (cohesive energy, or energy release rate) . The use of computational models to obtain some effective macroscopic parameters defining the toughness allows quantifying the influence of the material internal structure on a macro-fracture process. Indeed, perspective (2) is just an **homogenization** strategy in which a macroscopic parameter (e.g. energy release rate) is obtained from the properties of the present phases and interfaces and geometrical descriptors of the microstructure. Although homogenization is a very well-established topic to obtain effective parameters of standard constitutive equations (e.g. stiffness terms, diffusivity, conductivity), the definition of an effective fracture toughness is elusive. There is no consensus on whether microstructure and fracture properties of the phases can themselves provide an effective measure of toughness (M. Schneider, 2020) or if homogenization should also involve the mechanical parameters since fracture relies on local stress and stress fields (Hossain et al., 2014).

In any of the cases, modeling material behavior with fracture at the microscopic or mesoscopic level results in computationally expensive models due to the need of using a very large discretization of the RVE with phase behavior modeled using complex non-linear constitutive models. There is great interest in developing computational fracture models together with robust and fast computational tools to efficiently and optimally model the fracture of heterogeneous materials from a microscale perspective. These developments are the motivation for this doctoral work. In particular, it is planned the extension of a high efficiency solution framework for micromechanical problems, FFT-based solvers, to fracture processes. The computational models developed will consider different materials ranging from linear elastic fracturing materials (homogeneous and brittle) to materials with high complexity such as heterogeneous/anisotropic microstructures or constitutively complex materials. The problem of homogenizing properties related to fracture phenomena will be also discussed, and the possibility of including such estimations in the developed scheme is addressed. The following sub-sections deepen in the above-mentioned topics that will be important to establish the guidelines of this work.

1.1 Fracture Models

Fracture models available in the literature have been developed to address different aspects of the fracture process in materials under various conditions and scales. One of the first approaches to fracture modeling originated in the works of Griffith, 1921, where the fracture of elastic and brittle materials was studied. This model proposes that the conditions necessary for crack propagation are related to the rate of variation of elastic energy produced by crack growth, whose geometric shape is modeled as a zero-thickness fissure with a known length and

a specific mathematical impact on the energy functional (Anderson, 2008). Crack propagation occurs when this energy release rate exceeds a limit defined by the energy required to create new fracture surfaces, which is a material property related to fracture toughness. This model presents some of the elements that would later be used in modern models, such as coupling material degradation to a specific energy functional, the geometric definition of the crack, and the definition of an energy limit associated with the material's resistance to fracture. Its extension to elastoplastic materials, like in the work of Irwin, 1957 that incorporates the plastic energy dissipated near the crack tip into the fracture toughness, demonstrated the versatility of the method and introduced fracture toughness measurement tools applicable to elastic and elastoplastic materials, such as stress intensity factors K or the J -integral (Anderson, 2008).

Subsequently, other types of models were also developed, which can be classified by their different approaches to incorporate material degradation or their specific way to model defects and couple mechanical behavior with fracture. An example is those known as discontinuous fracture models that can model cracks, interstitial defects, or interfaces in microstructures as discontinuous functions, allowing great precision in representing these defects with the advantage of coupling their specific evolution to the mechanical response. Examples of discontinuous models include the Cohesive Zone Model (CZM) (Remmers et al., 2003; Segurado and LLorca, 2004), X-FEM (Gustafsson et al., 2019), or the Strong Embedded Discontinuity Model (SEDM) (Oliver et al., 2017; Sanz et al., 2018). The mentioned models are specifically designed to be used with the Finite Element Method (FEM). The CZM allows the modeling of cracks and laminar interfaces by introducing special finite elements that emulate the separation of two surfaces. This enables the modeling of crack opening and decohesion between microstructural phases. The other two models define defects using discontinuous functions to enrich the displacement fields in the vicinity of a finite element, indirectly simulating the existence of the defect. A disadvantage is that since these models are strongly tied to the FEM, either using the connection between elements or special-purpose elements, their extension to other numerical frameworks is not straightforward. In addition, the location of the defect must be known in advance.

Another approach to modeling mechanical degradation and failure in materials is the use of Continuous Damage Mechanics (CDM) models. Among the most widely used models in this group are the Gurson model for ductile fracture (Gurson, 1977; Reusch et al., 2008; Tvergaard and Needleman, 1984) and the Lemaitre model (Lemaitre, 1985; Magri et al., 2021), which have been extensively applied to many situations. CDM models allow the representation of material degradation through the concept of damage, which is defined as a continuous scalar field variable that evolves along with some internal variable of the considered model. Damage can be understood as a parameter that homogenizes and quantifies the volumetric amount of microvoids/microcracks forming at a local point in the material (Lemaitre, 1985). In Lemaitre's model, this evolution is defined by material-specific evolution laws (Thakkar and Pandey, 2007), while in the Gurson model it is governed by plasticity laws specifically designed to emulate the phenomena of growth, nucleation, and coalescence of the forming microvoids in ductile metals. In both cases, the local increase in damage results in a reduction of stresses and stiffness at the local level, which enables the representation of material softening and deterioration at both local and global scales.

By employing the concept of damage field, CDM models do not explicitly account for crack discontinuities, unlike discrete fracture models do, nor do they consider the influence of crack geometry on the thermodynamics of the problem, as Griffith's model does. While this is a limitation in the precise representation of real cracks, it also provides the advantage of representing the nucleation of damaged zones without the need to predefine the position and shape of a crack, as in discontinuous models or Griffith's model. Another advantage of these models is that they are not dependent on the numerical scheme employed, as they use continuous scalar fields that can be discretized using any numerical method. Despite this, CDM models face the issue of becoming strongly discretization-dependent and prone to the artificial localization of damage in zero-thickness bands (Jirasek, 2007). This occurs because of the loss of ellipticity of the governing PDE in the material softening stage due to damage (Magri et al., 2021). To avoid this well-known pathological dependency, non-local versions of CDM models are commonly used, which allow for the regularization of a damaged region by introducing a characteristic length that controls the interaction radius over which damage has effect.

The most widely adopted approach for these models is known as gradient damage models (Peerlings et al., 2001; Pham et al., 2011), which enable the formulation of the problem in a variational manner by establishing governing equations through the minimization of the material total energy. The energy is usually defined with subdivisions of different functionals, which formulation depends on the constitutive nature of the material. Some of that subdivision can be defined as dependent on the damage variable and its spatial gradient (Marigo et al., 2016) in order to couple the damaging phenomena to the mechanical part of the energy. In addition to eliminating mesh dependency, the inclusion of the damage gradient allows one to control the size of damage bands, providing numerical flexibility and offering multiple options for representing damaged zones. However, these models still consider damaged regions rather than explicitly including cracks, which remain the main difference between this method and discrete models.

The Phase-Field Fracture model

An alternative approach that shares characteristics with the two previously discussed methods is the *Phase-Field Fracture* model (PFF), which has become a significant advancement in the simulation of linear elastic fracture, providing a robust framework to capture complex phenomena associated with crack propagation.

The method has its origins in the seminal work of Francfort and Marigo, 1998, and was developed using the theoretical foundation established by authors such as Ambrosio and Tortorelli, 1990, to address problems with abrupt discontinuities. The model was further refined and analyzed by authors like Bourdin et al., 2008, culminating in modern versions of the model in the works of Miehe et al., 2010a. This model is directly based on the energetic approach of Griffith's model and is formulated variationally using energy functionals for elastic and fracture dissipation energies influenced by scalar damage fields, similar to CDM models. Moreover, the PFF model specifically shares many similarities with gradient CDM models as both are designed to represent the propagation of damaged zones to pristine materials. Indeed, the mathematical formulation of the energy functionals is analogous in both PFF

and gradient CDM, as both use a characteristic length to regularize damage and incorporate the gradients of the damage field (De Borst and Verhoosel, 2016). Nevertheless, PFF models also share some aspects with discontinuous fracture models. In PFF, the crack geometry is well-defined, as required in the Griffith approach on which the model is based. This geometry is defined by the smooth damage field, and its value is obtained from a crack functional depending on the damage field and the characteristic length. Moreover, fully-formed cracks can be predefined prior to deformation processes using these functionals (Singh et al., 2016), as in discontinuous models, allowing for subsequent analysis of crack propagation from them. The Phase-field description of a crack can even be extended to cohesive models (L. Chen and De Borst, 2021; C. V. Verhoosel and De Borst, 2013), establishing a numerical foundation to define the interface between phases of any geometrical arrangement defined for a domain, through regularized functionals.

The specific formulation of PFF crack functionals relies on the definition of damage profiles with non-singular behavior, resulting in smooth and highly concentrated fields around the location of an actual crack. It has been demonstrated that the specific form of this damage distribution exhibits Γ -convergence to an actual discontinuity (Bourdin et al., 2008), validating its ability to effectively represent the presence of cracks in elastic materials. The crack propagation and evolution depend directly on the elastic energy available at the local level, which in turn depends on the constitutive model and the heterogeneity of the domain. This enables the model to compute, with low discretization dependence, multiple fracture patterns that can exhibit high topological complexity (Farrell and Maurini, 2017; Oñate et al., 2017).

Although the PFF model was initially developed for isotropic elastic and brittle materials (Ambati et al., 2015a; Miehe et al., 2010a), different implementations have been developed for diverse types of materials in the last decade. For instance, the model has been extended to anisotropic elastic materials and elastic polycrystals, where the crack functional and constitutive model are influenced by the orientation of the lattices present in the material. The anisotropic fracture functional coupled with the anisotropic constitutive law has been successfully implemented to represent cracks primarily caused by cleavage (Clayton and Knap, 2016; Clayton and Knap, 2015; Ma and Sun, 2021; Teichtmeister et al., 2017). This extension provided a solid basis for developing the model in elastoplastic crystals, however the model was first implemented using classical models of isotropic plasticity. Such implementation implies incorporating Griffith’s energetic principles into the modeling of cracks under small and large strain scenarios with plasticity and was first made focusing on J-2 plasticity models (Ambati et al., 2015b; M. Borden et al., 2018; Fang et al., 2020; Miehe et al., 2016). This incorporation in the model is not evident since the classical formulation of the PFF model, based on Griffith’s model, is inherently governed by elastic functionals which can adequately represent brittle fracture. However, ductile fracture is phenomenologically different, and further study has been required to incorporate it into the PFF model. A comprehensive review by Alessi et al., 2018 highlights different models integrating isotropic plasticity into PFF, with particular emphasis on models leveraging hardening-related and plastic dissipation-related functionals.

The development of the PFF model within Crystal Plasticity models (CP) marked a significant advancement in ductile fracture modeling. At the microscopic level, Crystal Plasticity models

have been widely employed to describe the anisotropic plastic response of single crystals and are the basic tool for modeling the elastic-plastic response of polycrystals at the mesoscale. The extension of the PFF model to CP was initially introduced in the works of De Lorenzis et al., 2016 and Diehl et al., 2017, focusing on the analysis of crack growth in single-crystal media with various types of discontinuities. Furthermore, recent works also develop similar schemes (Cui et al., 2023; Lucarini et al., 2023) and it has been successfully implemented for the analysis of intragranular or intergranular fracture in quasi-brittle polycrystals, where fracture highly depends on lattice orientations (Na and Sun, 2018).

1.2 Effective toughness estimates from micromechanical simulations

As mentioned in the beginning of this work, macroscopic fracture simulation studies are often thought to study material reliability in a particular loading condition for a given geometry. In these simulations, a critical point is the material parameters used in the fracture model adopted, which control the fracture toughness of the material at the macroscale. Early definitions of a single parameter defining the fracture toughness of a material go back to linear fracture mechanics (LEFM). In the local approach of LEFM, this property is given as a critical stress intensity factor K_c , that characterizes the local stress concentration at the crack tip at which fracture occurs. Alternatively, in the global approach introduced in the Griffith fracture model, this property is defined with the critical energy release liberation due to fracture G_c , at the point in which crack propagation is irreversible. Toughness can also be defined with line integral calculations, e.g. J – *integral* (Rice, 1968), that account for the influence of local discontinuities on the energy field. Several studies have demonstrated that these three parameters can be related to each other (Zhu and Joyce, 2012) and their use is still in force in numerous studies.

In order to measure toughness experimentally, several procedures can be found in the literature, which rely on some of the above mentioned analytical definitions to formulate the toughness of specific specimens. The most common tests are designed to directly obtain an estimation of K_c based on analytical solutions of the macroscopic stress field for the cracked specimen shape considered (Gross et al., 2020; Gupta et al., 2020; S. Li et al., 2020; Shokrieh and Zeinedini, 2014; Wang et al., 2004; C. Zhang et al., 2022), and generally on pure mode-I. Nevertheless, some fracture modes are difficult to replicate experimentally (e.g. pure mode II opening) to obtain a clear measure. In these cases, the combination of a more simple experiment with computational modeling of the fracture process can be used to identify the corresponding fracture parameters in complex scenarios as e.g. T-stresses in mixed mode fracture cases (Mousavi et al., 2020; Wei et al., 2021) or Roesler’s constant for spherical indentation tests (Marimuthu et al., 2016). The mentioned works are purely macroscopic and the toughness estimated from the tests, even when combined with simulations, characterizes the macroscopic material fracture response for the particular microstructure of the material tested.

Also at the macroscale, some materials have a mesostructure with a characteristic length similar to the specimen size, for example composite laminates, sedimentary rocks, parts fabricated by lattice structures, foams, etc. In these cases, experimental measures of the

toughness strongly depend on specimen size and alternatively numerical approaches are used to estimate the toughness of an effective equivalent material based on some fracture parameters of the constituents (bars, lamina, interfaces, etc). For example in lattice materials with modular arrangement, K_c was estimated using a beam elements approach in Choi and Sankar, 2005; Christodoulou and Tan, 2013. Similar studies use J-integrals toughness estimations (Tiwari et al., 2020) to determine macroscopic toughening of heterogeneous laminates using a cohesive zone model in FEM. In the case of sedimentary rocks, in Na et al., 2017 a PFF model was used to compute energetic fracture dissipation as an indirect estimation of the rock toughness, considering two constituents including the stiff and soft layers with the same toughness but different elastic moduli.

The mentioned works demonstrate the strong influence of the mesostructure on the fracture toughness of macroscopically heterogeneous materials. However, there is much experimental evidence that shows that the material toughness is also influenced by its internal structure at lower scales. It is well known that parameters like K_c for macroscopic cracks are strongly dependent on the presence of microcracks (Rose, 1986) or variations of micro-mechanical properties (Gao, 1991). This microstructure dependency of the toughness cannot be derived from experiments performed at macroscale.

Considering the effect of the microscopic heterogeneity, the macroscopic toughness measured can be considered as an *effective toughness* for the particular microstructure, which will depend on the toughness of the present phases, their arrangement at the microscale and the presence of microvoids or microcracks. From a theoretical perspective, the work of Gao, 1991 and later studies (Papanastasiou, 1999; Roux et al., 2003) proposed the term *effective toughness* as the overall/macroscopic value of the fracture parameter which provides the same fracture resistance as the one obtained (analytically or numerically) considering the heterogeneous microstructure. Specifically, in the work of Roux et al., 2003, an analytic equivalent toughness K_c is obtained by averaging the crack advance over a medium with heterogeneous toughness, and in the work of Papanastasiou, 1999, the increase of the effective toughness from a defined micro-toughness formulation in hydraulic fracture is studied using a finite element cohesive zone crack model and J-integral calculations.

Other studies as Y. Li and Zhou, 2013 and Hossain et al., 2014 perform direct FEM simulations with fracture on RVEs considering different microstructures, including heterogeneities in toughness or stiffness, and link the simulation results with the effective fracture energy G_c by computing the J-integral on the full RVE considered. Those works pointed out that both heterogeneities in G_c and stiffness are in fact toughening mechanisms. This leads to formulate definitions of effective toughness such as the one of Y. Li and Zhou, 2013 where a time-averaged value of the macroscopic J-integral (when fracture stabilizes) is taken as effective, considering that an averaged value would characterize better the process. Other definition is the one of Hossain et al., 2014 where the value of the maximum macro-J-integral is taken as effective, under the argument that micro-cracks have to overcome that value at some point in order to complete the fracture process.

It must be noted that in the last work mentioned, and later related works as Na et al., 2017, a constitutive framework based on Phase Field Fracture was used, implemented in a FEM scheme (FEM-PFF). As mentioned in section 1.1, the PFF model has gained strong acceptance

in matters of fracture simulations, being developed primarily for elastic/brittle materials with an energetic variational approach that also allows defining fracture dissipation energy functionals. This perspective offers advantages for estimating effective fracture toughness, since the elastic energy and fracture dissipation functionals of the material can be computed directly during a fracture process (Hossain et al., 2014; Na et al., 2017) requiring microscopic G_c values as an input that facilitates the definition of local fracture toughness. Furthermore, since this model defines crack-growth driving force as energy functionals dependent on local strain states, complex and heterogeneous microstructures with differences in stiffness and local G_c have a major influence on microcrack path, which can be estimated to obtain macroscopic estimates of G_c (Hossain et al., 2014).

The vast majority of studies mentioned at this point have been performed primarily using FEM schemes for their robustness and versatility, but a few works can be found that use alternative numerical schemes for solving PFF. In the work of Lebihain et al., 2020 and Lebihain et al., 2021, a stochastic/perturbative method based on LEFM is applied in particle reinforced composite materials to obtain a statistical, but physically based, fracture representation that considers weighted states of interaction between particles and the matrix with high local toughness contrast between them. Despite the lack of material constitutive consideration, it is a very efficient scheme allowing for the resolution of a crack over thousands of particles. With the crack path within microstructure phases, it is possible to define another criterion for effective toughness formulated as the spatial average of the local toughness along the crack surface. This is defined under the argument that the crack only perceives and overcomes the local resistance of the zones through which it is passing, so that only these zones can contribute to the effective value. Other important works in the matter of effective toughness estimations have been done with Fast Fourier Transform (FFT) based solvers, which are specially designed for homogenization strategies that fit perfectly in this topic. These models form a major part of the present work and are therefore described in the following subsection.

1.3 Fast Fourier Transform based solvers in fracture simulations

The PFF model formulates its governing equations and crack representation through analytical scalar fields, similar to CDM models as mentioned earlier. This allows for the implementation of the PFF model with any numerical Partial Differential Equations (PDE) solver, some of which offer advantages not present in FEM schemes. In particular, homogenization-based numerical schemes based on the Fast Fourier Transform (FFT) (Lucarini et al., 2021; Moulinec and Suquet, 1994) have gained prominence in recent years, especially in studies where micromechanical effects are significant, as in the case of fracture modeling.

Both FEM and FFT solvers offer unique advantages, making them suitable for different contexts. FFT techniques in particular, provide significant computational efficiency advantages when periodic domains are simulated. Many studies have shown that the computational cost of the method concerning the number of degrees of freedom n is approximately $n \log(n)$. This scalability allows FFT solvers to handle much more complex RVEs within practical computational times, as observed in Fig.1.1, making them especially well-suited for microstructural

studies.

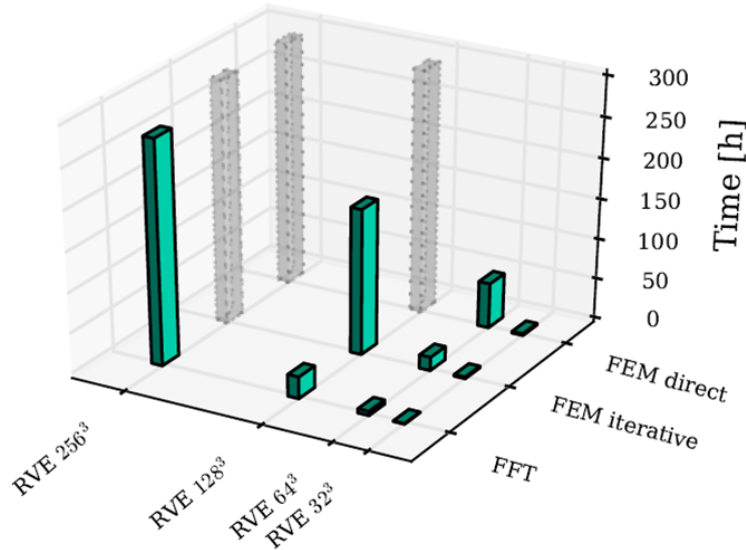


Figure 1.1: Comparison of the efficiency of FEM and FFT numerical schemes concerning the number of discretized elements in a model. Estimations reported in the work of Lucarini and Segurado, 2019b.

FFT solvers operate on a voxel-based discretization, similar to finite differences, instead of the FEM mesh arrangements. While this feature limits their ability to locally refine the discretization or adapt the modeling of complex geometries, it simplifies computational processing by avoiding reliance on nodes and elements arrangements and simplifies data handling by having all scalar and tensor variables in one position. Moreover, periodic boundary conditions are inherent in FFT schemes, which is advantageous for micromechanical simulations to reduce the effect of boundary layers and reach a statistically representative RVE size earlier. The mathematical structure by which both methods construct the solution is also different. FFT solutions are formed by the combination of trigonometrical polynomials with support on the full RVE domain. Alternatively, FEM solutions are defined by the combination of shape functions with a local support.

Despite their limitations, due to their superior computational efficiency and the preferential use of periodic boundary conditions in computational homogenization, FFT methods have gained wide acceptance for computational micromechanical simulations. Complex microstructures encapsulated in RVEs with very fine discretizations can be modeled, obtaining highly accurate results even using particularly complex constitutive models such as crystal plasticity (Hu et al., 2021; Zecevic et al., 2022), microstructure damage in polycrystals (Pokharel et al., 2012) and damage generation due to microscopic degradation (Cocke et al., 2023). Extensive reviews of the method and its applications can be found in the works of Lucarini et al., 2021; M. Schneider, 2021.

FFT schemes have a wide potential to solve problems related to fracture and damage at the microscale. In particular, the implementation of the PFF model in FFT solvers provides the opportunity to study micromechanical fracture processes in detail, leveraging the

computational efficiency and robustness of the method. Indeed, pioneering implementations of PFF-FFT have been made, being initially focused on brittle fracture. Some examples of this are studies focusing on the implementation of memory-efficient implicit schemes to solve for the elastic micro-fracture problem (Y. Chen et al., 2019; Ernesti et al., 2020), or studies that extended PFF-FFT approaches to cleavage-dominated fracture in strongly anisotropic materials (Ma and Sun, 2021), or the study of chemical diffusion influenced mechanical fracture in materials for batteries (Zarzoso et al., 2025). Regarding elasto-plastic constitutive materials, the PFF method combined with CP has been recently implemented in FFT, allowing for the inclusion of crystal orientation and anisotropy in different evolving crack scenarios, encompassing quasi-static fracture (Cui et al., 2023) and fatigue (Lucarini et al., 2023).

Also in the context of fracture, FFT based approaches have been used in the homogenization of microstructural effective toughness, M. Schneider, 2020, Ernesti and Schneider, 2021 and Ernesti and Schneider, 2022. In these works, a variational framework is proposed to obtain the effective fracture energy as the result of a minimization of the fracture energy dissipated, based on a primal-dual method and an alternating direction method of multipliers, and implemented using FFT solvers. This approach considers full scale separation and assumes homogeneous elastic fields at the microscale (Braides et al., 1996). This variational procedure has proven to be very efficient thanks to the resolution approximation and use of FFT solvers and is oriented to make calculations over ensembles of large RVEs.

Despite the growing number of papers dealing with PFF in spectral solvers, there are still many unsolved problems in these implementations, many of which motivate this work. These issues will be discussed in detail in the next section.

1.4 Challenges in Phase-Field fracture

Regardless of the discretization scheme, the typical computational resolution procedure employed in PFF models involves iterative procedures controlled with a defined variable which can be an applied displacement/force at the boundary or a component of the macroscopic strain, that is monotonically increased. This type of control is particularly useful in stable fracture situations (Carpinteri and Accornero, 2018), where this kind of variable is strictly increasing with crack growth. However, in many cases, fracture exhibits unstable behavior appearing in many macroscopic scenarios but being much more common at the microscale. In this regime, crack propagates rapidly without allowing the material to redistribute stresses or dissipate energy effectively, and it cannot be assured that displacement or strain type variables are strictly increasing concerning crack growth. Furthermore, the use of monolithic schemes is not possible due to the non-convexity of the minimization problem presented by the PFF model (Gerasimov and De Lorenzis, 2016; Svolos et al., 2023). Most studies using this model employ **staggered schemes** (Ambati et al., 2015b; Miehe et al., 2010a) in which PFF governing equations are solved independently within a self-consistent numerical scheme, since such equations are convex with respect to their objective fields (Gerasimov and De Lorenzis, 2016). Staggered strategies do not allow finding equilibrium when the crack propagates unstably, meaning the propagation occurs in metastable regimes causing

jumps in the material response (Carpinteri and Accornero, 2018) as is depicted in the blue curve of Fig.1.2. The numerical resolution of the instability is challenging, and reaching the next stable state of the crack using staggered solvers requires significant computational time. An alternative to this strategy consists in actually obtaining the solution during unstable crack growth, which requires capturing a mechanical snap-back behavior (Carpinteri and Colombo, 1989), which is also depicted in Fig.1.2 with the black curve. This constitutive trajectory allows overcoming numerical jumps and enables the implementation of monolithic schemes, where the displacement-type and force-type variables evolve as a function of a third monotonically increasing variable. According to thermodynamics, fracture is an irreversible process that therefore involves a monotonically increasing energy dissipation (M. Borden et al., 2018). Using this principle, an ideal experiment can be designed where dissipation is imposed to adjust the previously mentioned boundary conditions.

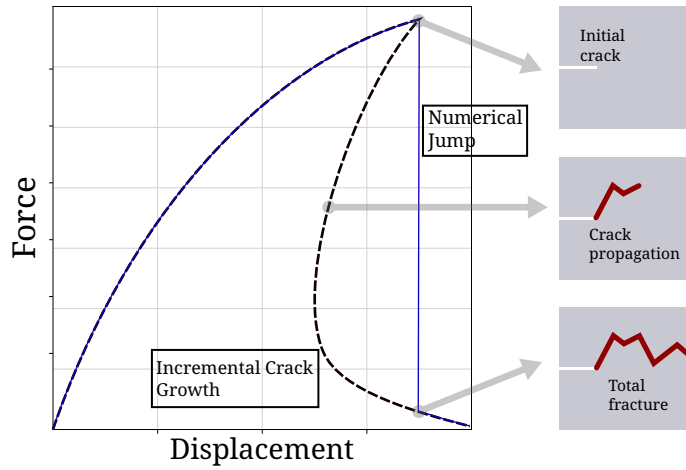


Figure 1.2: Representative scheme of mechanical response during crack growth in a numerical scheme with displacement control (blue) and dissipative control (black).

Approaches with this strategy exist mainly in FEM schemes and were developed in the context of CDM models (Gutiérrez, 2004) and gradient damage models (C. Verhoosel et al., 2009), using arc-length methods and defining control functionals dependent on local forces. These arc-length methods have subsequently been extended to PFF-FEM schemes at macroscale, with the work of Singh et al., 2016 being one of the first studies to utilize it in a PFF method, using its own crack functional as a control parameter. This idea was later exploited in other studies (Bharali et al., 2022; Zambrano et al., 2023) of which the majority have been conducted with FEM schemes and mainly for macroscopic fracture, and there are no microstructural approaches to this technique in the literature in other schemes such as FFT-based solvers. Implementations on simulation control methodologies for micro-fracture problems are few but demonstrate to be useful also in obtaining homogenized material properties. The advantage of these strategies is the obtention of the complete time evolution of crack and some microscale influenced parameters, e.g. toughness, which can be significantly affected by the irregularity of crack paths due to microstructure. This is not possible with classic schemes in unstable crack propagation. An example of this is the micro-fracturing study of Hossain et al., 2014 in which the so-called Surfing boundary conditions are implemented in order to emulate the passage of a macroscopic crack through a microstructure, imposing a time dependent displacement

field on the contour that allows to obtain a very complete evolution of the micro-crack in order to calculate effective toughness. This one and similar procedures implemented in FEM schemes (Y. Li and Zhou, 2013) usually consider material constitutive evolution as a secondary result, and on the contrary, most of FEM dissipation control methods are usually made to get detailed mechanical response behaviors, but its use to estimate effective toughness as a result of energetic optimizations is not exploited. Regarding FFT procedures for effective toughness estimations (as the one of M. Schneider, 2020), they rely on a purely dissipation optimization approach and do not consider the material mechanical behavior.

Indeed, dissipation control methods could be used to define an effective toughness estimation since they allow computing with precision the macroscopic energy spent in fracture, which is related to an overall estimation of fracture resistance. It could be used in specific microstructures without requiring J-integrals that can be path-dependent for heterogeneous RVEs. This proposal, taking elements of the already mentioned procedures for effective toughness (Hossain et al., 2014; M. Schneider, 2020), can be extended to the PFF model in a FFT framework providing a more accurate and efficient way of obtaining the effective toughness. Nevertheless, current approaches in PFF-FFT use external strain control in which this strategy has not been accurately tested.

Summarizing, the implementation of a PFF fracture model in a FFT solver with a dissipated energy control, that has not been addressed yet, presents an enormous potential. This type of control in PFF-FFT would present the advantage of obtaining efficiently both the complete representation of crack propagation under unstable regimes and of making effective toughness estimations on different microstructures. Nevertheless, a clear procedure for toughness homogenization using PFF-FFT and dissipation control has to be defined and numerically validated, against standard PFF-FFT implementations in stable growth cases or against dissipation control in PFF-FEM.

This comparison between FFT and FEM simulation of microscopic fracture using PFF is the last of the challenges identified. Comparison between FEM and FFT for various mechanical problems can be found in the literature (Liu et al., 2010; Lucarini and Segurado, 2019b; Zarzoso et al., 2025; Zeman et al., 2017) to validate new procedures or algorithms. However, no studies have been made comparing both methods in fracture simulations using the PFF model. The large number of studies in PFF-FEM has generated extensive knowledge about its computational aspects, but most of these aspects in FFT-PFF models are unexplored. Although both solvers should theoretically converge to equivalent responses, their natural differences imply that result convergence would occur for very fine discretizations depending on the problem considered. Moreover, PFF-FEM schemes have been shown to have inaccuracies in physically representing crack lengths (Miehe et al., 2010a) and fracture resistance limits (Bourdin et al., 2008) due to FEM discretization. This discretization effect on the length and fracture resistance is unexplored in FFT and can be very different due to the different nature of interpolating functions. Additionally, the Arc-length approaches aforementioned for PFF-FEM schemes Bharali et al., 2022; De Borst and Verhoosel, 2016; Singh et al., 2016; C. Verhoosel et al., 2009; Vignollet et al., 2014; Zambrano et al., 2023 rely on stiffness matrix factorization, which cannot be easily adapted to FFT methods that are usually based on iterative approaches (either fixed-point iterations or Krylov-based solvers).

Therefore, a comparative study between both schemes would be useful in validating the use of FFT schemes with PFF models against a robust and widely used method as FEM will allow verifying under which conditions they produce acceptably similar results. Moreover, this comparison should go beyond elastic brittle fracture since in a realistic microstructure even having a nearly linear response until fracture at the macroscale, local phase response can reach a non-linear regime by developing, for example, microplasticity. In this way, the study of elasto-plastic polycrystals could constitute a great extension to the aforementioned cases of brittle fracture, allowing us to analyze the differences between FEM and FFT solvers in a large strain non-linear history dependent framework. The extension of the PFF method to a complex plasticity model such as crystal plasticity in FEM and FFT will improve the proposed scheme, and being developed in the context of finite strains, it will emphasize the differences between the two schemes allowing a more accurate framework to search for the equivalence of the two models.

1.5 Motivation and Objectives of the Work

According to the discussion in the previous section, Phase-Field Fracture models have shown to be a reliable fracture approach with many applications in the literature; however, their applicability has been mainly reduced to macroscopic fracture, using FEM schemes and displacement simulation control strategies.

Regarding toughness estimations, various numerical frameworks have been proposed to obtain homogenized estimations of fracture resistance. However, some of these estimates neglect the mechanical response of the material at the microscale M. Schneider, [2020](#), and others Hossain et al., [2014](#) based on PFF-FEM do not fulfill a clear scale separation.

These evidences suggest that the implementation of a Phase-Field Fracture model in a numerical scheme based on the FFT and considering a crack-length/dissipation control constitutes an unexplored framework offering several clear advantages for micro-fracture simulations. Such a scheme could constitute a general framework to model efficiently microscopic material fracture, allowing one to obtain the complete mechanical response during crack propagation. Moreover, this framework would allow defining clear estimates of the effective toughness under clear scale separation and considering the cross play between microscopic strain fields and fracture. The development of this framework constitutes the main motivation of this work.

In addition, an exhaustive comparison of the PFF-FFT technique with a more established method such as FEM is missing. This analysis is a necessary step to further validate the framework proposed and critically assess the results obtained.

The general objective of this work is to **develop a general framework for *Phase-Field Fracture* simulations at the micro/mesoscale and its numerical implementation using FFT based solvers to homogenize the fracture behavior of heterogeneous materials.**

Specific objectives include:

- ◊ Development of a robust implementation of the PFF model in an FFT-based scheme,

including an energy dissipation control method to simulate unstable crack propagation in heterogeneous media.

- ◊ Propose an estimate of the effective fracture toughness to link the microstructure and microscopic phase properties of heterogeneous materials with the macroscopic fracture response.
- ◊ Extend the PFF framework at the microscale to elasto-plastic fracture by coupling the model with crystal plasticity and perform a comparative study between the FFT implementation and a typical FEM scheme.

Scope of the Work

This thesis has been carried out within the framework of the ANID agency's PhD abroad scholarship program, with funding from the scholarship ANID-BECAS CHILE 2020-72210273. The work primarily focuses on implementing computational solvers for simulating microfracture processes using the proposed PFF model, applied to cases of elasticity (both isotropic and anisotropic) and crystal plasticity in 2D and 3D. Validation is carried out through comparisons with more robust numerical schemes, as previously mentioned.

This thesis is divided into chapters that cover, in the first place, the introduction of the study that presents the advances of numerical fracture models and their computational solution, together with its main problems focusing particularly on the Phase-Field fracture model (PFF). Chapter 2 presents a state of the art in which the mathematical and physical details of the fracture study are deepened and the advances of the literature on these topics are detailed. Then, the advances of the PFF model developed in this work are presented, which are divided in 3 parts to be treated in Chapters 3, 4 and 5, focusing mainly on the implementation and validation of the dissipative simulation control (Chapter 3), the proposal and comparison of the effective toughness procedure of this work (Chapter 4) and the comparison of the PFF scheme in complex material behavior (CP models) with respect to an implementation made in FEM (Chapter 5). All the mathematical formulations, the numerical implementation, the validation tests and the results of the cases simulated with the developed scheme are detailed in each chapter. Finally, in Chapter 6 the conclusions of the work are presented together with the topics to be considered for future work.

Chapter 2

State of art

This chapter presents an overview of a recent bibliographic review of the theory behind the models treated in this work and similar computational implementations on which the proposed models are based. Since this work mainly focuses on the implementation of a fracture model, it begins with a short review of the fundamental theory of linear fracture mechanics and the mathematical tools that will later be used for the proposed Phase Field Fracture model. Then, the foundations of the PFF model are described, contemplating its basic definitions and connections with the concepts described in chapter 1, ranging from mathematical aspects of the PFF basic scheme with displacement control to its extensions to classical plasticity models. Also, some models boarded in this work require the finite strain theory, e.g. crystal plasticity models, which will also be introduced in this chapter. Regarding the applications of the models, all the proposed toughness estimations and finite element comparisons will be described in the body of the thesis. However, other existing estimation procedures in the literature are selected and summarized in this chapter.

From a numerical point of view, the computational implementation of models like the PFF elastic brittle fracture with strain control and the PFF model with crystal plasticity will be depicted in the main body of the work, despite its implementation already existing in the literature in order to provide a better description of the modifications made on it. However, this implementation requires the description of the numerical aspects of a FFT-based solver, so the foundations of this framework are summarized as well as the specific versions employed for the implementation in the proposed PFF model.

2.1 Homogenization in micromechanical problems

There are a number of techniques that focus on solving problems at the macroscale taking into account the effects of the microscale, which is referred to as multiscale methods. Despite both scales can separately be described by e.g. continuum mechanics at macroscale or stochastic atomic behavior of discrete particles for the microscale, the objective of multiscale modeling is linking these distinct scales Kochmann, 2018. Depending on the problem and the context, distinct discretization methods may be required for each scale, including methods like finite element (FEM) or FFT based solvers. Ideally, calculations in those frameworks would use

segments of the material volume, referred to as unit cells, to capture material's representative behavior. In order to completely describe material's behavior, infinitely large unit cells would be required, but in practice, this is not feasible. Instead, finite-size domains called Representative Volume Elements (RVEs) are chosen to approximate the infinite space limit as closely as necessary. The RVE should be as large as needed for accuracy, yet as small as possible for efficiency.

A common assumption for RVEs is defining their geometry having statistical homogeneity (see Fig.2.1a), meaning the material's microstructural properties remain uniform across the macroscale (Kochmann, 2018). This assumption leads to homogenization techniques, in which an effective description of the behavior of a material with heterogeneous microstructure is obtained from microscopic simulations. This is achieved by replacing the response of the complex microscopic medium by an equivalent one with homogenized properties that is valid on a larger scale (as in Fig.2.1c). In mechanical problems, RVEs of volume Ω are used to determine stress $\boldsymbol{\sigma}$ and strain $\boldsymbol{\varepsilon}$ at larger scales. It's generally accepted that the volume averages of the stress and strain across the domain represent the homogenized versions of these variables $\boldsymbol{\Sigma}_M$ and $\boldsymbol{E}_M$ that define the constitutive behavior of the RVE at macroscale,

$$\boldsymbol{E}_M = \frac{1}{\Omega} \int_{\Omega} \boldsymbol{\varepsilon} d\Omega \quad ; \quad \boldsymbol{\Sigma}_M = \frac{1}{\Omega} \int_{\Omega} \boldsymbol{\sigma} d\Omega \quad (2.1)$$

This approach constitutes what is known as averaging theorems, and in Eq.(2.1) has been depicted for a small strain framework. At finite strains, the deformation gradient tensor $\mathbf{F} = \nabla \vec{\varphi}$ characterizes the deformation process, which describes the transformation from a reference-undeformed configuration with $\vec{X}$ material coordinate system to an actual-deformed configuration with a coordinate system $\vec{x} = \vec{\varphi}(\vec{X})$, where $\vec{\varphi}$ is a deformation mapping defining the movement of all material points corresponding with the actual deformation process. The resulting averaging theorems can be further manipulated using the divergence theorem to represent the macroscopic values as surface integrals, being $\delta\Omega$ the domain's boundary,

$$\boldsymbol{F}_M = \frac{1}{\Omega} \int_{\Omega} \mathbf{F} d\Omega = \frac{1}{\Omega} \int_{\delta\Omega} \vec{\varphi} \otimes \vec{N} dS \quad ; \quad \boldsymbol{P}_M = \frac{1}{\Omega} \int_{\Omega} \mathbf{P} d\Omega = \frac{1}{\Omega} \int_{\delta\Omega} \vec{T} \otimes \vec{X} dS \quad (2.2)$$

and where $\mathbf{P}$ is the first Piola-Kirchhoff stress tensor characterizing the stress field at the undeformed configuration, $\vec{T}$ are traction forces present on the boundary, and $\vec{N}$ is the normal vector to the boundary (both in Fig.2.1c). In order to define an inter-scale transition for stress/strain relations, the principle of energy conservation ensures that in a conservative system, the strain energy stored at microscale is equivalent to the one stored in a local material point on the macroscale. This implies that,

$$\boldsymbol{E}_M : \boldsymbol{\Sigma}_M = \frac{1}{\Omega} \int_{\Omega} \boldsymbol{\sigma} : \boldsymbol{\varepsilon} d\Omega \quad ; \quad \boldsymbol{P}_M : \delta \boldsymbol{F}_M = \frac{1}{\Omega} \int_{\Omega} \mathbf{P} : \delta \mathbf{F} d\Omega, \quad (2.3)$$

where $\boldsymbol{P}_M$ and $\boldsymbol{F}_M$ are the macroscopic local Piola stress and local macroscopic deformation gradient tensors, respectively. This definition for both small and large deformation schemes is known as the Hill-Mandel conditions (Hill, 1963; Lucarini et al., 2021; Mandel, 1973). These conditions have proved to be fulfilled with several boundary conditions applied over the RVE. The boundary conditions are important in the determination of the homogenized response in

the material and allow for adequately representing the behavior of the material under specific load situations. The following options exist,

- ◇ Affine displacement: enforce Dirichlet boundary conditions on $\delta\Omega$ with a given constant $\mathbf{F}_o$ or $\boldsymbol{\varepsilon}_o$ as,

$$\vec{x} = \mathbf{F}_o \vec{X} \quad \text{or} \quad \vec{u} = \boldsymbol{\varepsilon}_o \vec{x}, \quad (2.4)$$

where $\vec{u}$ is the displacement field over $\delta\Omega$.

- ◇ Uniform traction: enforce Neumann boundary conditions on $\delta\Omega$ with a given constant tensor $\mathbf{P}_o$ or $\boldsymbol{\sigma}_o$ as,

$$\vec{T} = \mathbf{P}_o \vec{N} \quad \text{or} \quad \vec{t} = \boldsymbol{\sigma}_o \vec{n}, \quad (2.5)$$

where $\vec{n}$ is also a normal to the boundary.

- ◇ Periodic BCs: enforce field continuity on $\delta\Omega$ displacements and a consistent equilibrium at the boundary faces tractions (antiperiodic condition) as,

$$\vec{x}^+ = \vec{x}^- + \mathbf{F}_o(\vec{X}^+ - \vec{X}^-) \quad \text{and} \quad \vec{T}^+ = -\vec{T}^- \quad (2.6a)$$

$$\vec{u}^+ = \vec{u}^- + \boldsymbol{\varepsilon}_o(\vec{x}^+ - \vec{x}^-) \quad \text{and} \quad \vec{t}^+ = -\vec{t}^-, \quad (2.6b)$$

where the positive/negative superscript are described at Fig.2.1b.

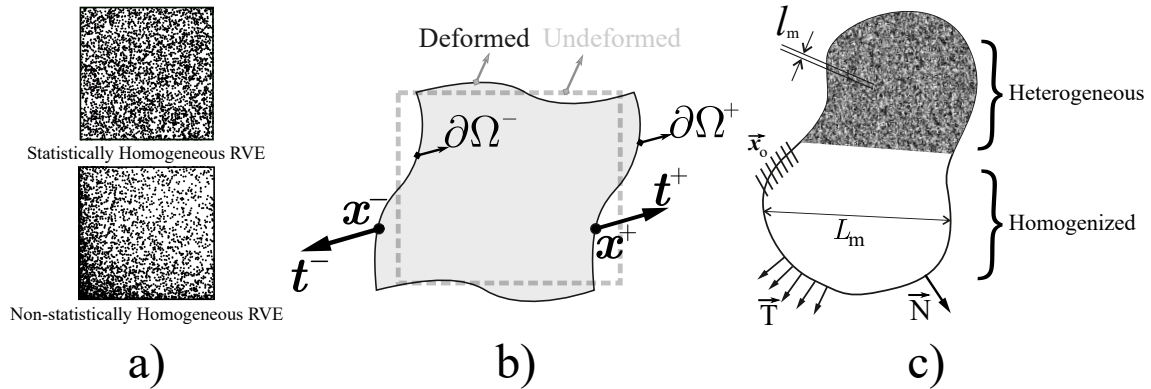


Figure 2.1: Schematization of homogenization features (obtained from (Kochmann, 2018)): (a) Statistically homogeneous RVE. (b) Periodic boundary conditions. (c) Characteristic lengths (l_m and L_m) comparison.

Computational homogenization addresses how microscale variations lead to effective macroscale behavior. Consider a heterogeneous material where properties vary across phases. In a generic elastic problem at the microscale fulfilling mechanical equilibrium, the problem can be stated as in the work of Lucarini et al., 2021 for periodic RVEs and periodic boundary conditions, as follows,

$$\left\{ \begin{array}{l} \nabla \cdot \boldsymbol{\sigma} = 0 \\ \text{with } \mathbf{E}_M = \frac{1}{\Omega} \int_{\Omega} \boldsymbol{\varepsilon}(\vec{x}) d\Omega \\ \vec{u} \text{ Periodic.} \\ \boldsymbol{\sigma} \cdot \vec{n} \text{ Antiperiodic.} \end{array} \right. , \quad (2.7a)$$

The same formulation can be stated for finite strains also as in the work of Lucarini et al., 2021 where the equilibrium is defined over the reference configurations through the operation $\nabla_{\vec{X}}$.

$$\left\{ \begin{array}{l} \nabla_{\vec{X}} \cdot \mathbf{P} = 0 \\ \text{with } \mathbf{F}_M = \frac{1}{\Omega} \int_{\partial\Omega} \vec{\varphi} \otimes \vec{N} dS \\ \mathbf{F}(\vec{X}), \vec{u} \text{ Periodic.} \\ \mathbf{P} \cdot \vec{N} \text{ Antiperiodic.} \end{array} \right. \quad (2.8a)$$

The resolution of the Eq.(2.8) allows determining the fields that exhibit periodicity within the RVE due to the imposed boundary conditions. Moreover, defining the macroscopic variables as the volumetric averages of the corresponding solution fields ensures a consistent relationship between both scales, regardless of fluctuations in the microscopic field caused by the heterogeneity of the medium. Normally, this approach is used when there is a clear difference between the dimensions of the microscale and macroscale, and the effects of the microscale don't influence the response perceived at the macroscale.

Considering the scheme in Fig.2.1c, this can be quantified by defining a characteristic length scale l_m in which variations of the strain/stress fields due to microstructure are important, in comparison with an equivalent length in which L_m where macroscopic features and load conditions exist. If the dimensions of the problem satisfy $l_m/L_m \ll 1$, then a scale separation is achieved, where the effective smooth macroscopic behavior of the material can be separated from the highly oscillatory behavior at smaller scales. Considering this, the fields of interest can be defined to have two clear components corresponding to the field's average (equal to the microscopic local variable) and the complement part that contains all fluctuations over the average. With this, in a small strains framework the strain field can be defined as follows (Lucarini et al., 2021),

$$\boldsymbol{\varepsilon}(\vec{x}) = \tilde{\boldsymbol{\varepsilon}}(\vec{x}) + \bar{\boldsymbol{\varepsilon}}, \quad (2.9)$$

and for finite strains formulation, the deformation gradient can also be defined as,

$$\mathbf{F}(\vec{X}) = \widetilde{\mathbf{F}}(\vec{X}) + \bar{\mathbf{F}}. \quad (2.10)$$

By definition, the fluctuating parts represented by the $\sim$ symbol have zero mean value, which implies that although they exist at the microscale, they have no influence at the macroscale. This can be demonstrated since, using the Hill-Mandel conditions, it can be shown that $\int_{\Omega} \tilde{\boldsymbol{\sigma}} : \tilde{\boldsymbol{\varepsilon}} d\Omega = (\int_{\Omega} \tilde{\boldsymbol{\sigma}} d\Omega) : (\int_{\Omega} \tilde{\boldsymbol{\varepsilon}} d\Omega) = 0$.

This micromechanical formulation is performed only considering the classical mechanical problem of elasticity applied to microstructures with any kind of heterogeneity. In later sections, the coupling of these schemes with PFF fracture models will be performed.

2.2 Fundamentals of Fracture Mechanics

As previously mentioned, the model implemented in this work is closely related to fracture models based on energy equilibrium. This approach was developed in the work of Griffith, 1921, where it was defined that the evolution of a crack is determined by the minimization

of the total energy of the material. In this model, considering elasticity and excluding microstructural effects, the total energy Π is thermodynamically associated with the internal elastic potential energy stored in the material, Ψ , and the total energy dissipation due to fracture, D . The formulation of this energy considers the existence and evolution of a defect in the system, that also alters the value of Ψ at any time. If the defined crack has a known length a and the system is subjected to prescribed displacements u , the variation of $\Psi(u, a)$ due to an incremental crack area growth da is given by Eq.(2.11),

$$\frac{\delta \Pi}{\delta a} = \frac{\delta \Psi}{\delta a}(u, a) + \frac{\delta D}{\delta a}(a), \quad (2.11)$$

The dissipation term $D(a)$ can be related to the work required to break the material, generating two new surfaces, and its variation with respect to the crack length reflects the energy needed to create two surfaces of length da . Under the previous assumptions, this energy requirement can only come from elastic potential energy, which can be computed as $\Psi = \int \psi dV$, where ψ represents the stored strain energy density.

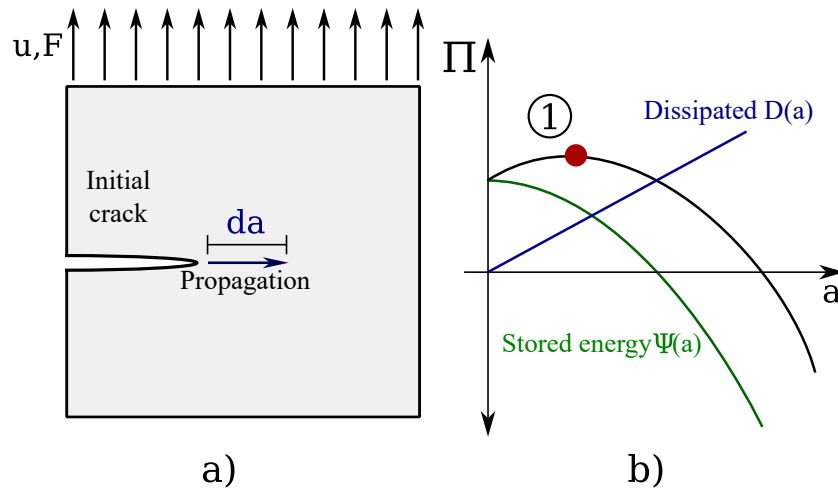


Figure 2.2: Schematic representation of Griffith's model. a) Elliptical representation of the crack and its propagation direction. b) Energy functionals scheme of the model.

Griffith's postulate states that crack growth and propagation in the material occur when the system reaches a state where, upon a virtual increase of the crack da , the total energy decreases. This happens at point 1 in Fig.2.2, where

$$\frac{\delta \Pi}{\delta a} = 0 \rightarrow -\frac{\delta \Psi}{\delta a}(u, a) = \frac{\delta D}{\delta a}(a), \quad (2.12)$$

implying that crack propagation occurs when the energy release rate $G = -\delta \Psi / \delta a$ matches or exceeds the energy rate required to create surfaces $G_c = \delta D / \delta a$. This critical value represents the critical point of fracture propagation and is considered a material property associated with fracture toughness.

The purely energetic approach of Griffith was later extended to more complex scenarios in the context of Linear Elastic Fracture Mechanics (LEFM). In the work of Irwin, 1957, the introduction of the stress intensity factor K defines a local parameter at which a crack propagates, allowing us to include the effect of crack geometry and its specific impact on Ψ . For instance, a crack can be modeled with an elliptical geometry, enabling the crack tip to be defined using the axes of the ellipse (Inglis, 1913) and affecting stress concentration within the material. The influence on crack geometry is used in further related models, like the one treated in this work.

Another important aspect of fracture behavior is its stability. Depending on loading conditions (displacement or force) or domain geometry, the crack may propagate in a controlled manner (stable propagation) or abruptly and instantaneously (unstable propagation). This behavior depends on the evolution of the functionals G and G_c once the crack propagates. Considering the derivative of the rates with respect to crack length, the stable crack growth condition is described by Eq.(2.13), which, if not satisfied, will make crack growth unstable. Although many materials exhibit a variable G_c behavior, an invariant value has been considered for Eq.(2.13) due to the nature of the models in this work.

$$\frac{\delta G}{\delta a} \leq 0. \quad (2.13)$$

These concepts are crucial for predicting crack propagation and describing its behavior. However, they require analytical expressions of G , which may not be feasible in complex cases such as plasticity or anisotropy. However, this work aims to find numerical responses represented through field discretizations, and approximations of the energy functionals depicted here can be obtained. This allows studying fracture-related properties in the material such as toughness. Implementations with this will be developed in chapter 4. Another alternative is the numerical adaptation of contour integrals. In particular, the integral developed by Rice, 1968, known as the J -integral, is useful for measuring energy dissipation rates in nonlinear materials. For elastic materials, it holds that $J = G$, and its definition for any path l_J as in Fig.2.3 is given by Eq.(2.14).

$$J = \int_{l_J} \left(W \delta_{1j} - \sigma_{ij} \frac{\partial u_i}{\partial x_1} \right) n_j dl. \quad (2.14)$$

Being W is the strain energy density, σ is the stress field, u is the displacement field, and x_1 is the horizontal direction described in the figure. This work employs specific numerical versions of this integral, which are described in Chapter 3.

2.3 Phase-Field Fracture Model

As described in Chapter 1, the Phase Field Fracture model emerges as an alternative to the discrete and continuous fracture models, having aspects of both groups and a strong resemblance to the gradient damage models. It has been widely developed in the literature (Ambati et al., 2015b; Miehe et al., 2010a; Oñate et al., 2017), and tested by many authors for a diverse group of materials and constituent models. Those studies deepen the mathematical

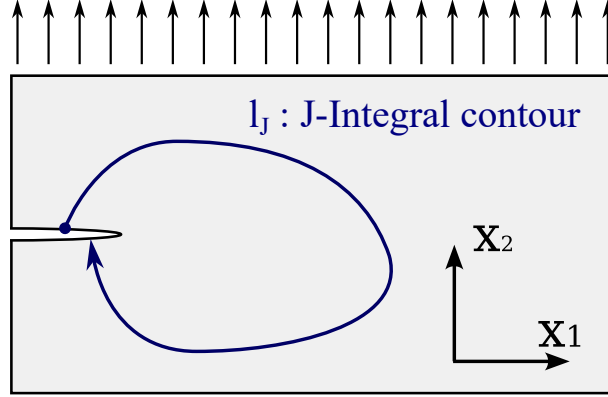


Figure 2.3: Schematic of the path required by the J -integral to calculate the dissipation rate.

and geometrical features of crack representation and the mechanical response of the material. The model aims at modeling crack growth following an energy criterion, where the crack is represented by a continuous scalar field called damage (ϕ), which varies between 0 (undamaged material) and 1 (fully damaged material). This *Phase Field* allows representing the crack in a smooth way, as it is shown in Fig.2.4, evolving spatially and temporally depending on the domain geometry and the material model to which it is coupled.

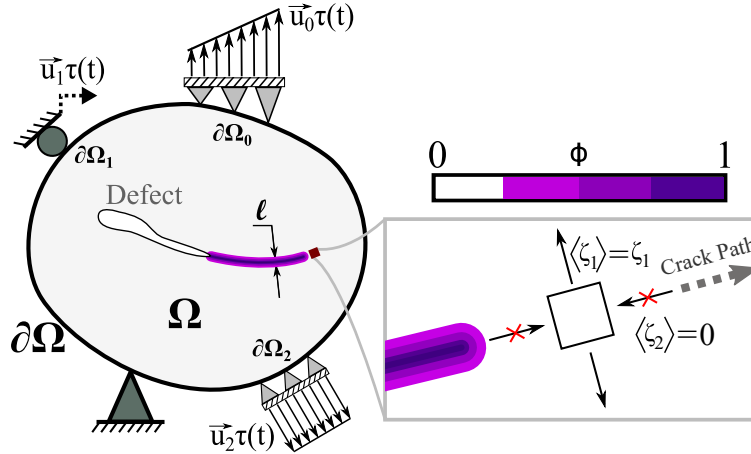


Figure 2.4: Damage Phase Field representation of the crack.

The problem of the PFF in an elastic media can be stated as a variational problem that can involve the displacement field $\vec{u} : \Omega \rightarrow \mathbb{R}^3$ and the damage field $\phi : \Omega \rightarrow \mathbb{R}$ from the principle of virtual power (Gurtin et al., 2010; Miehe et al., 2010b)

$$\dot{\Pi}_I(\vec{u}, \phi) = \dot{\Pi}_M \Rightarrow \dot{E}_{mec}(\vec{u}, \phi) + \dot{D}(\phi) - \dot{\Pi}_M = 0, \quad (2.15)$$

where the functional Π_I represents the internal energy and is composed of the free energy E_{mec} and a fracture dissipation functional D similar to the one in the last section, which are balanced by the power of external loads Π_M . The free energy considers the elastic energy of the damaging material, defined as the sum of the elastic energy density ψ_e as

$$E_{mec} = \int_{\Omega} \psi_e d\Omega = \int_{\Omega} g(\phi) \psi_{o1} + \psi_{o2} d\Omega, \quad (2.16)$$

where the density is often decomposed into different parts in order to couple specific energetic components of the mechanical behavior to the PFF fracture dissipation through a damage dependent function called $g(\phi)$. Usually, such a decomposition allows the model to describe the progress of a crack taking into account the strain state of the material. Many alternatives have been developed in the literature (Kuhn and Müller, 2010; D. Schneider et al., 2016) considering the total energy of the material where the elastic density is described as

$$\psi_{o1} = \frac{1}{2} \lambda \text{tr}^2(\boldsymbol{\varepsilon}) + \mu \boldsymbol{\varepsilon} : \boldsymbol{\varepsilon} \quad (2.17a)$$

$$\psi_{o2} = 0, \quad (2.17b)$$

where $\boldsymbol{\varepsilon} = \text{sym}(\nabla \vec{u})$ is the strain tensor, λ and μ are the Lamé elastic constants of the material. This alternative has the advantage of not introducing residual stresses near the crack and being easy to implement for any scheme. Nevertheless, for fracture cases that do not correspond with a mode I fracture situation, errors are induced due to the generation of cracks in compressive components of the local strain state. Some alternatives to this formulation can be found in literature, relying on decompositions of the strain tensor to define ψ_{o1} and ψ_{o2} . For instance, in the work of Amor et al., 2009 or the work of Ma and Sun, 2021, the strain decomposition into its hydrostatic $\boldsymbol{\varepsilon}_h$ and deviatoric $\boldsymbol{\varepsilon}_{dev}$ parts is used to define the energy as

$$\psi_{o1} = \frac{1}{2} \lambda \langle \text{tr}(\boldsymbol{\varepsilon}) \rangle_+^2 + \mu \boldsymbol{\varepsilon}_{dev} : \boldsymbol{\varepsilon}_{dev} \quad (2.18a)$$

$$\psi_{o2} = \frac{1}{2} \lambda \langle \text{tr}(\boldsymbol{\varepsilon}) \rangle_-^2 \quad (2.18b)$$

$$\text{where } \boldsymbol{\varepsilon}_{dev} = \boldsymbol{\varepsilon} - \boldsymbol{\varepsilon}_h ; \quad \boldsymbol{\varepsilon}_h = \frac{1}{3} \text{tr}(\boldsymbol{\varepsilon}) \mathbf{I}, \quad (2.18c)$$

where the function $\langle \bullet \rangle_{\pm} = (\bullet \pm |\bullet|)/2$ represents the positive and negative Heaviside brackets. This alternative successfully biases many of the cases of compressive crack propagation since it depends on the trace of the strain state that exalts in ψ_{o1} when positive hydrostatic components are dominant. Another alternative is the one used in the work of Miehe et al., 2010a, or the one by Ambati et al., 2015a, that depends on the positive and negative parts of the strain tensor obtained from its spectral decomposition

$$\psi_{o1} = \frac{1}{2} \lambda \langle \text{tr}(\boldsymbol{\varepsilon}) \rangle_+^2 + \mu \boldsymbol{\varepsilon}^+ : \boldsymbol{\varepsilon}^+ \quad (2.19a)$$

$$\psi_{o2} = \frac{1}{2} \lambda \langle \text{tr}(\boldsymbol{\varepsilon}) \rangle_-^2 + \mu \boldsymbol{\varepsilon}^- : \boldsymbol{\varepsilon}^- \quad (2.19b)$$

$$\text{where } \boldsymbol{\varepsilon}^{\pm} = \langle \zeta_1 \rangle_{\pm} \vec{e}_1 \otimes \vec{e}_1 + \langle \zeta_2 \rangle_{\pm} \vec{e}_2 \otimes \vec{e}_2 + \langle \zeta_3 \rangle_{\pm} \vec{e}_3 \otimes \vec{e}_3, \quad (2.19c)$$

being $\zeta_i, \vec{e}_i$ the eigenvalues and eigenvectors of the strain. Only the ψ_{o1} functional is degraded to avoid crack growth in the compressive principal strain directions as is represented in Fig.2.4, which makes this functional highly non-linear regardless of the decomposition employed. The degradation function $g(\phi)$ usually has a scalar definition that locally affects energy depending on the position of the crack. The specific definition of this function can affect the rate of energy loss by fracture, which directly affects the growing rate of the crack. Also, many definitions have been employed to define degradation, being the most usual the quadratic

definition (M. Borden et al., 2018; Y. Chen et al., 2019; Gerasimov and De Lorenzis, 2016; Miehe et al., 2010b),

$$g(\phi) = (1 - \phi)^2 - k, \quad (2.20)$$

where k is a numerical constant that allows us to avoid numerical problems when damage is fully developed (Miehe et al., 2010a). Other works, like the one by M. J. Borden et al., 2016, use cubic definitions to better control the formulation derivatives in a variational scheme,

$$g(\phi) = (1 - \phi)^2(1 + \phi(2 - k)). \quad (2.21)$$

Also, alternatives in which highly non-linear degradation functions can be defined to overcome numerical aspects of the model and a more controlled softening response after fracture propagation (Alessi et al., 2015),

$$g(\phi) = \frac{(1 - \phi)^2}{k - (k - 1)(1 - \phi)^2}. \quad (2.22)$$

Regardless of the choice, the functional $g(\phi)\psi_o^+$ represents the total elastic energy density available in the system for the crack to grow, and also contributes to the non-linear behavior of this functional.

With regards to the dissipation functional D in Eq.(2.15) and considering brittle fracture modeling in elastic materials, dissipation can be only attributed to fracture processes and is defined by a critical energy release rate G_c and the crack density functional $\gamma_f(\phi)$. The development of such functionals was proposed in the work of Ambrosio and Tortorelli, 1990, from a reinterpretation of Griffith's problem that leads to a Mumford-Shah energy functional that can be approximated by the PFF formulation in the mentioned work and in the one of Ambrosio, 1992. This functional allows us to represent the geometrical features of the crack and whose integral in the domain defines the total crack surface in 3D or the crack length in 2D as depicted in Eq.(2.23) and Eq.(2.24). Generally, there are two versions of this crack density functional that stand out, known as the AT2 quadratic formulation (Ambrosio, 1992),

$$\Gamma = \int_{\Omega} \gamma_f d\Omega = \int_{\Omega} \frac{1}{2\ell} \phi^2 + \frac{\ell}{2} \nabla \phi \cdot \nabla \phi d\Omega, \quad (2.23)$$

where ℓ is the PFF characteristic length that defines the width of the continuous crack, as depicted in Fig.2.4, and the AT1 linear formulation (Bourdin et al., 2014)

$$\Gamma = \int_{\Omega} \gamma_f d\Omega = \int_{\Omega} \frac{3}{8\ell} \phi + \frac{3\ell}{8} \nabla \phi \cdot \nabla \phi d\Omega. \quad (2.24)$$

Any of these functionals in conjunction with the critical energy release rate constitutes the functional $D = G_c \Gamma$, that represents the total energy dissipated due to fracture if G_c is homogeneous in the domain.

The functionals defined in this section allow us to form a PFF model for elastic materials, being able to choose those with suitable structural properties for many situations. Extensions to other types of materials are described in later sections. From now on, for all the schemes used in this work, a quadratic degradation function (Eq.(2.20)) and an AT2 model (Eq.(2.23)) are chosen to represent the crack.

2.3.1 Classical Phase-Field Fracture scheme

With free energy and dissipation functionals defined, differentiation with respect to time and the application of integration by parts allow us to derive the strong form of the governing equations of the problem from Eq.(2.15). The following section describes this derivation considering the formulation of classical control methods in PFF models, for a homogeneous material that considers a spectral decomposition for the elastic energy density will be performed (Miehe et al., 2010b).

The domain Ω can be subjected to a set of prescribed tractions or displacement restrictions on the boundary. Focusing only on applied displacements $\vec{u}_i$, a set of surface subdomains $\partial\Omega_i$ can be used to impose these displacements as a function of time as in Fig.2.4. The function $\tau(t)$ in this figure, often called the load factor, is used as parametric control to drive the numerical simulation, enforcing proportionality between each $\vec{u}_i$ (Bharali et al., 2022; Singh et al., 2016). Considering again the power balance in Eq.(2.15), the external energy is defined as the work of the traction forces $\vec{t}$ on the boundary as a result of the applied displacement, $\Pi_M = \int_{\partial\Omega} \vec{t} \cdot \vec{u} d\partial\Omega$. The following relation can be established:

$$\int_{\Omega} \dot{\psi} + G_c \dot{\gamma}_f d\Omega = \int_{\partial\Omega} \vec{t} \cdot \dot{\vec{u}} d\partial\Omega. \quad (2.25)$$

It is important to note that for the definition of Π_M , all body forces and inertial forces will be considered negligible in this work. Using the definitions of the last section, we obtain,

$$\int_{\partial\Omega} \vec{t} \cdot \dot{\vec{u}} d\partial\Omega = \int_{\Omega} \left(g \frac{\partial \psi_o^+}{\partial \epsilon} + \frac{\partial \psi_o^-}{\partial \epsilon} \right) : \dot{\epsilon} + \frac{dg}{d\phi} \psi_o^+ \dot{\phi} + G_c \frac{d\gamma_f}{d\phi} \dot{\phi} d\Omega. \quad (2.26)$$

The stress field σ can be defined as the derivative of the energy density (Ambati et al., 2015a), which leads to the definition in Eq.(2.27) in which integration by parts is used to obtain a definition in terms of $\vec{u}$,

$$\int_{\Omega} \left(g \frac{\partial \psi_o^+}{\partial \epsilon} + \frac{\partial \psi_o^-}{\partial \epsilon} \right) : \dot{\epsilon} d\Omega = \int_{\Omega} \sigma : \dot{\epsilon} d\Omega = \int_{\Omega} -\nabla \cdot \sigma \cdot \dot{\vec{u}} d\Omega + \int_{\partial\Omega} \sigma \cdot \vec{n} \dot{\vec{u}} d\partial\Omega. \quad (2.27)$$

Replacing this result in Eq.(2.26), we obtain:

$$\int_{\Omega} -\nabla \cdot \sigma \cdot \dot{\vec{u}} + (g' \psi_o^+ + G_c \gamma_f') \dot{\phi} d\Omega = \int_{\partial\Omega} (\vec{t} - \sigma \cdot \vec{n}) \cdot \dot{\vec{u}} d\partial\Omega, \quad (2.28)$$

where $\gamma_f' = \partial\gamma_f/\partial\phi$ and $g' = \partial g/\partial\phi$. Thus, Eq.(2.28) leads to the system of governing equations (2.29), under the assumption that $\dot{\vec{u}} \neq 0$ and $\dot{\phi} \neq 0$.

$$\nabla \cdot \left(g \frac{\partial \psi_o^+}{\partial \epsilon} + \frac{\partial \psi_o^-}{\partial \epsilon} \right) = \nabla \cdot (g \sigma_o^+ + \sigma^-) = \nabla \cdot \sigma = 0 \quad (2.29a)$$

$$g' \psi_o^+ + G_c \gamma_f' = 0 \quad (2.29b)$$

$$\vec{u} = \vec{u}_i \tau(t) \text{ on } \partial\Omega_i ; i = 1, 2, 3... \quad (2.29c)$$

where the derivative of the crack functional γ_f' with respect to ϕ is

$$\gamma_f'(\phi) = \frac{1}{\ell} \phi - \ell \nabla^2 \phi. \quad (2.30)$$

The Eq.(2.29a) represents the mechanical equilibrium at every point, and Eq.(2.29c) is a condition equation fulfilling equilibrium at the boundary. Since the traction forces $\vec{t}$ correspond to the displacements $\vec{u}_i$, the right-hand side of Eq.(2.28) can be fulfilled with the condition in Eq.(2.29c), implying that displacements imposed with τ are in equilibrium with the tensions at the boundary.

The Eq.(2.29b) is a Helmholtz type equation that represents the energy balance that exists between the potential energy and the energy dissipated in fracture that allows calculating ϕ using ψ_o^+ as a driving force. Note that, although different phases can be considered, ϕ is defined here in all the domain assuming standard continuity conditions in the displacement and damage fields and jump conditions on their gradients. This assumption allows the damage field to penetrate the interfaces without any restriction depending on the heterogeneity defined for G_c or stiffness. However, it is possible to emulate Neumann free boundary conditions of the fracture field in interfaces between two phases using heterogeneous values of ℓ between phases (Magri et al., 2021).

In micromechanical simulations, which are the cases usually represented in FFT homogenization schemes, the domain can be modeled as a RVE of the microstructure. The deformation process within is dictated by the macroscopic strain $\mathbf{E}_M$, which relates with the microscopic strains through their average $\bar{\boldsymbol{\varepsilon}} = \mathbf{E}_M$. Following Eq.(2.9) the decomposition $\boldsymbol{\varepsilon}(\vec{x}) = \tilde{\boldsymbol{\varepsilon}}(\vec{x}) + \bar{\boldsymbol{\varepsilon}}$ holds, being $\tilde{\boldsymbol{\varepsilon}}$ the strain fluctuation field, which average in the RVE vanishes. The external work of Eq.(2.15) for this situation can be expressed as $\Pi_M = \mathbf{E}_M : \boldsymbol{\Sigma}_M$ where the macroscopic strain $\mathbf{E}_M$ and macroscopic stress $\boldsymbol{\Sigma}_M$ are defined as volume averages of their microscopic counterparts. The macroscopic energy should be equal to the microscopic one, following Hill-Mandel conditions expressed in section 2.1, and therefore the restriction in Eq.(2.29c) can be modified. Considering full strain control conditions, the corresponding PDEs and constraints for the phase-field micromechanical problem are given by Eq.(2.31).

$$\nabla \cdot \boldsymbol{\sigma} = 0 \quad (2.31a)$$

$$g'\mathcal{H} + G_c\gamma_f'(\phi) = 0 \quad (2.31b)$$

$$\mathbf{E}_M = \frac{1}{\Omega} \int_{\Omega} \boldsymbol{\varepsilon} d\Omega = \tau(t). \quad (2.31c)$$

This allows us to use the macroscopic strain as a control variable in the solution scheme, by establishing $\tau(t)$ as a linear ramp with respect to the time. Schemes that impose macroscopic deformation, such as the one in Eq.(2.31), are often used in mechanical studies at the microscale (Y. Chen et al., 2019). Note that Eq.(2.29b) could lead to a healing effect of the crack for some damage configurations if the energy ψ_o^+ decreases with time. This can be overcome by imposing the damage driving force with the function $\mathcal{H}$ as in Eq.(2.31b), which represents a history function over ψ_o^+ (Miehe et al., 2010b) where the local driving force will only be considered to be the maximum of the local energy density in all the fracturing processes,

$$\mathcal{H}(t) = \max(\psi, \mathcal{H}(t_a)) \quad ; \quad t_a \in [0, t], \quad (2.32)$$

which allows us to enforce the crack propagation to be an irreversible process. The resolution of the system in Eq.(2.31) can be done by many numerical procedures, some of the most relevant depicted in Chapter 3.

2.3.2 Phase-Field Fracture model extension to crack-length control methods

The classical PFF schemes described in the last section (controlled with E_M and u_i) have proven to be reliable procedures in many studies. However, they present the problems described in Chapter 1 in representing fracture propagation in unstable regimes, which can be addressed by crack-length related control methods.

Following Griffith's theory, the condition for crack propagation in Eq.(2.13) adapted to the PFF functionals corresponds to

$$\left. \frac{-\delta E_{mec}}{\delta a} \right|_u = G_c, \quad (2.33)$$

where E_{mec} is the elastic energy of the RVE and a is the crack surface (length), then a crack of a given shape and size will continue growing in a stable manner if

$$\frac{\delta}{\delta a} \left(\left. \frac{-\delta E_{mec}}{\delta a} \right|_u \right) \leq 0. \quad (2.34)$$

In Phase Field fracture, the term a has a direct equivalence with the crack area functional (Eq.(2.23)) and E_{mec} is defined in Eq.(2.16). If at a time t Eq.(2.34) is not fulfilled, in order to maintain the fracture condition in Eq.(2.33), the displacement or macroscopic strain control variables should be reduced and therefore $\tau(t)$ function of Eq.(2.29c) should decrease with time. As a consequence, the control approaches of the last section, in which $\tau(t)$ is imposed as a monotonic function (e.g. a ramp), will result in uncontrolled crack growth, leading to the problems described in the introduction chapter.

To overpass this problem, any function or variable related with the crack growth can be prescribed as a function of time, to derive an algorithm to control micromechanical simulations by crack-length and find the fields ϵ and ϕ fields depending on the control. This is convenient because the definition of the PFF model with history variables ensures the irreversible nature of the crack growth, making it strictly increasing. Examples of variables that fit this definition are local displacement at the crack mouth such as Crack Mouth Opening Displacement, CMOD (Carpinteri and Colombo, 1989), or Crack Mouth Sliding Displacement, CMSD (Rots and De Borst, 1987), and also the energy dissipation functionals (Singh et al., 2016) which in a PFF model can be represented with $G_c \Gamma$ from Eq.(2.23).

As a consequence, any displacement at the boundary $\vec{u}\tau$ in Eq.(2.29c) or macroscopic strain $E_M(\tau)$ in Eq.(2.31c), which could have been used as control in the classical model, becomes an unknown in this technique, where τ remains the load factor associated with it. In literature, these schemes for PFF models are normally performed in FEM schemes with implementations of the arc-length method, in which the relations between external nodal forces $\vec{f}_{ext}$ or displacement (such as mentioned above) can be related to the governing equations in the system of Eq.(2.29) and calculations are controlled by constant increases of these variables by means of an imposed variable $\Delta\tau_c$. Solving this relations, depicted in Eq.(2.35), implies to find $[\vec{u}, \phi, \tau]$ that make governing equation null, which is often solved by mean of linearizations and iterative schemes (like Newton-Raphson). A general system can be formulated using a set of

external loads $\vec{f}_{ext}$ and internal forces, with its corresponding linearization, as

$$\begin{aligned} F_{\vec{u}} &= \vec{f}_{ext}(\vec{u}, \tau) - \nabla \cdot \boldsymbol{\sigma} = 0 \\ F_{\phi} &= g'(\phi)\psi_o^+ + G_c\gamma_f'(\phi) = 0 \\ F_{con}(\vec{u}, \phi, \tau, \Delta\tau_c) &= 0 \end{aligned} \Rightarrow \begin{pmatrix} \frac{\partial F_{\vec{u}}}{\partial \vec{u}} & \frac{\partial F_{\vec{u}}}{\partial \phi} & \frac{\partial F_{\vec{u}}}{\partial \tau} \\ \frac{\partial F_{\phi}}{\partial \vec{u}} & \frac{\partial F_{\phi}}{\partial \phi} & \frac{\partial F_{\phi}}{\partial \tau} \\ \frac{\partial F_{con}}{\partial \vec{u}} & \frac{\partial F_{con}}{\partial \phi} & \frac{\partial F_{con}}{\partial \tau} \end{pmatrix} \begin{bmatrix} \partial \vec{u} \\ \partial \phi \\ \partial \tau \end{bmatrix} = - \begin{bmatrix} F_{\vec{u}} \\ F_{\phi} \\ F_{con} \end{bmatrix} \quad (2.35)$$

where F compose the set of governing equations and F_{con} correspond with the control equation in which the earlier discusses strategies can be implemented. Following this scheme, many studies in literature has proposed their own definition for this equation enhanced by set of constrains that allows to define the problem. Examples of this are the study of De Borst and Verhoosel, 2016 in which punctual forces are constrained to be proportional with the load factor τ and the control equation is defined to impose a constant external power rate

$$\begin{pmatrix} \frac{\partial F_{\vec{u}}}{\partial \vec{u}} & \frac{\partial F_{\vec{u}}}{\partial \phi} & -\vec{f}_{ext} \\ \frac{\partial F_{\phi}}{\partial \vec{u}} & \frac{\partial F_{\phi}}{\partial \phi} & 0 \\ \frac{\partial F_{con}}{\partial \vec{u}} & 0 & 0 \end{pmatrix} \begin{bmatrix} \partial \vec{u} \\ \partial \phi \\ \partial \tau \end{bmatrix} = - \begin{bmatrix} \nabla \cdot \boldsymbol{\sigma} - \tau \vec{f}_{ext} \\ F_{\phi} \\ F_{con} \end{bmatrix} ; \quad F_{con} = \frac{1}{2} \vec{f}_{ext} \cdot (\tau \Delta \vec{u} - \Delta \tau \vec{u}) - \Delta \tau_c. \quad (2.36)$$

Another example can be found in the work of Bharali et al., 2022, also in the framework of a PFF model, where the problem constraint is made over local displacements in the actin punctually in the load areas. There, displacement are an addition of free unknown displacements $\vec{u}_o$, prescribed displacement $\vec{u}_p$ and the unit vector $\vec{u}_i$ as $\vec{u} = \boldsymbol{c}\vec{u}_o + \vec{u}_p + \tau \vec{u}_i$, with $\boldsymbol{c}$ a constraint matrix. This affects the equations system by chain rule as depicted in Eq.(2.37) and the control equation is defined over a variation of the dissipation functional $G_c\Gamma'$ defined for the AT1 model of Eq.(2.24) and AT2 model of Eq.(2.23), impose a constant energy release rate with an invariable value of $\Delta\tau_c$

$$\begin{pmatrix} \frac{\partial F_{\vec{u}}}{\partial \vec{u}} & \frac{\partial F_{\vec{u}}}{\partial \phi} & \frac{\partial F_{\vec{u}}}{\partial \tau} \cdot \vec{u}_i \\ \frac{\partial F_{\phi}}{\partial \vec{u}} & \frac{\partial F_{\phi}}{\partial \phi} & \frac{\partial F_{\phi}}{\partial \tau} \cdot \vec{u}_i \\ 0 & \frac{\partial F_{con}}{\partial \phi} & 0 \end{pmatrix} \begin{bmatrix} \partial \vec{u} \\ \partial \phi \\ \partial \tau \end{bmatrix} = - \begin{bmatrix} \nabla \cdot \boldsymbol{\sigma} \\ F_{\phi} \\ F_{con} \end{bmatrix} ; \quad F_{con} = G_c \int_{\Omega} \gamma_f' d\Omega - \Delta \tau_c. \quad (2.37)$$

A similar scheme is defined in the work of Singh et al., 2016, where the load factor is implicit at the displacement field and only the crack surface is used as control. In that work, the control equation is imposed in a non-variational way in order to always fulfill it, maintaining a constant crack growth as

$$\begin{pmatrix} \frac{\partial F_{\vec{u}}}{\partial \vec{u}} & \frac{\partial F_{\vec{u}}}{\partial \phi} & 0 \\ \frac{\partial F_{\phi}}{\partial \vec{u}} & \frac{\partial F_{\phi}}{\partial \phi} & 0 \\ 0 & \int_{\Omega} \gamma_f' d\Omega & 0 \end{pmatrix} \begin{bmatrix} \partial \vec{u} \\ \partial \phi \\ \partial \tau \end{bmatrix} = - \begin{bmatrix} \nabla \cdot \boldsymbol{\sigma} \\ F_{\phi} \\ \Delta \tau_c \end{bmatrix} ; \quad F_{con} = \Delta \Gamma - \Delta \tau_c. \quad (2.38)$$

In this form, the control equation is also known as the trajectory tracking constraint and if $\Delta\tau_c$ is a constant for all time steps, this constraint imposes a constant crack growth rate. All these approaches can be solved with direct strategies, which have efficiency and performance

advantages. However, for the different definitions of Eq.(2.35), some derivatives result null by the definition of the governing equation set, leading to ill-conditioning and asymmetry in the system. This often requires alternative solution strategies to solve the problem in this form. Despite this fact, these solutions show a great approach in representing fracture. From a microstructural point of view, imposing local controls or punctual load factors is difficult, since such schemes are often resolved with macroscopic/averaged constraint. For this reason the adaptation of a similar procedure involving this microstructural perspective for a FFT solver will be developed in chapter 3. Also, a FEM scheme similar to those described in this section will be developed for comparison with the resulting formulation in the FFT solver.

2.3.3 Phase-Field Fracture model extension to classical plasticity

Extensions of the PFF model to plastic constitutive materials have been done in the literature, considering J2 type models (Oñate et al., 2017) and crystal plasticity models (De Lorenzis et al., 2016). The implementation of the crystal plasticity model with PFF proposed in this work shares a similar deduction to those mentioned. For this reason, the PFF extension to J2 models is summarized here as an introduction to the implementation in chapter 5. Such an extension requires certain considerations, since the original formulation of the PFF model was developed for brittle materials where most of the micromechanical processes in the problem occur with elastic energy as the primary source. Elastoplastic materials account for effects such as strain hardening and plastic dissipation, which must be included in the energy formulation. A modified version of Eq.(2.15) is shown below, considering a spectral decomposition of the energy density ψ ,

$$\begin{aligned} \Pi_{int}(\boldsymbol{\varepsilon}_e, \boldsymbol{\varepsilon}_p, \gamma, \phi) = \int_{\Omega} \underbrace{g(\phi)\psi_{eo}^+(\boldsymbol{\varepsilon}_e) + \psi_{eo}^-(\boldsymbol{\varepsilon}_e) + g_p(\phi)\psi_p(\gamma)}_{\psi} + \\ \underbrace{G_c\gamma_f(\phi) + g_d(\phi)D_p(\gamma)}_{D_t} d\Omega = \Pi_{ext}, \end{aligned} \quad (2.39)$$

where the plastic part of the free energy ψ_p represents the energy accumulated by the material due to hardening, which could be associated with recrystallization processes and the rearrangement of dislocations in the material. The additional independent variables correspond to the plastic strain $\boldsymbol{\varepsilon}_p$ and an internal variable γ associated with material internal plastic strain and hardening. Additionally, the total energy dissipation in the material D_t consists of the previously mentioned fracture dissipation and the plastic dissipation density D_p . Additionally, this formulation allows us to affect both the plastic energy associated with hardening and the plastic dissipation with degradation functions, g_p and g_d respectively, which enable us to incorporate plastic effects in the fracture evolution (Oñate et al., 2017).

Considering a small strain framework, an additive decomposition of the elastic and plastic strains $\boldsymbol{\varepsilon} = \boldsymbol{\varepsilon}_e + \boldsymbol{\varepsilon}_p$ is assumed. Also, combining the local versions of the principle of virtual work and the Clausius-Duhem inequality, the local free energy balance $\dot{\psi} + \dot{D}_t = \boldsymbol{\sigma} : \dot{\boldsymbol{\varepsilon}}$ (Gurtin et al., 2010) can be used similarly as Eq.(2.25). The integrand of Eq.(2.39) must fulfill this

relation, and considering the additive strain decomposition, we obtain

$$\begin{aligned} \left(g(\phi) \frac{\partial \psi_{eo}^+}{\partial \boldsymbol{\varepsilon}_e} + \frac{\partial \psi_{eo}^-}{\partial \boldsymbol{\varepsilon}_e} \right) : \dot{\boldsymbol{\varepsilon}}_e + g' \psi_{eo}^+ \dot{\phi} + g_p \frac{\partial \psi_p}{\partial \gamma} \dot{\gamma} + g'_p \psi_p \dot{\phi} = \\ \boldsymbol{\sigma} : \dot{\boldsymbol{\varepsilon}}_e + \boldsymbol{\sigma} : \dot{\boldsymbol{\varepsilon}}_p - G_c \gamma'_f \dot{\phi} - g_d \dot{D}_p - g'_d D_p \dot{\phi}. \end{aligned} \quad (2.40)$$

It can be demonstrated that for J_2 plasticity models and crystal plasticity models in general, any definition of $\boldsymbol{\varepsilon}_p$ is deviatoric (Gurtin et al., 2010). In the former models, this makes it convenient to employ the relation $\boldsymbol{\sigma} : \dot{\boldsymbol{\varepsilon}}_p = \mathbf{s} : \dot{\boldsymbol{\varepsilon}}_p$, where $\mathbf{s}$ is the deviatoric part of the stress. Based on these definitions, three formulations are established, from the relations obtained in section 2.3.1, to satisfy Eq.(2.40):

- ◇ The total stress in the system is defined based on the elastic strain field, just as in Eq.(2.26) of the elastic model in section 2.3:

$$g(\phi) \frac{\partial \psi_{eo}^+}{\partial \boldsymbol{\varepsilon}_e} + \frac{\partial \psi_{eo}^-}{\partial \boldsymbol{\varepsilon}_e} = \boldsymbol{\sigma}. \quad (2.41)$$

- ◇ A Helmholtz equation similar to that of section 2.3.1 is formulated here with functionals related to $\dot{\phi}$. This definition includes the material hardening functional and the plastic dissipation:

$$g' \psi_{eo}^+ + g'_p \psi_p + g'_d D_p + G_c \gamma'_f = 0. \quad (2.42)$$

- ◇ With the previous definitions, a relationship between the plastic dissipation rate $\dot{D}_p$ and the material hardening functional can be inferred through the stress. This result matches definitions established in works like the one of Wulfinghoff and Böhlke, 2012:

$$g_d(\phi) \dot{D}_p = \mathbf{s} : \dot{\boldsymbol{\varepsilon}}_p - g_p \frac{\partial \psi_p}{\partial \gamma} \dot{\gamma} \quad (2.43)$$

Note that in a 1-D Von Mises plasticity model, where $\dot{\boldsymbol{\varepsilon}}_p = \dot{\gamma} \frac{\mathbf{s}}{\|\mathbf{s}\|}$, this formulation relates with the classical definition of plastic dissipation $\dot{D}_p = f_y \dot{\gamma}$, where f_y is the yield stress function and $g_d = 1$.

With definitions in equations Eq.(2.42) and Eq.(2.41), the governing equations of the problem can be derived from the minimization of the energy functional in Eq.(2.39) by taking its time derivative, $\frac{\partial \Pi}{\partial t} = 0$. Considering that the power of external loads can be defined as in Eq.(2.25) in section 2.3.1 we obtain,

$$\int_{\partial\Omega} \vec{t} \cdot \vec{u} d\partial\Omega = \int_{\Omega} \boldsymbol{\sigma} : \dot{\boldsymbol{\varepsilon}}_e + \mathbf{s} : \dot{\boldsymbol{\varepsilon}}_p + [g' \psi_{eo}^+ + g'_p \psi_p + g'_d D_p + G_c \gamma'_f] \dot{\phi}, \quad (2.44)$$

where considering that $\dot{\phi} \neq 0$ and $\dot{\boldsymbol{\varepsilon}} = \dot{\boldsymbol{\varepsilon}}_e + \dot{\boldsymbol{\varepsilon}}_p \neq 0$, Eq.(2.44) leads to the system:

$$\nabla \cdot \boldsymbol{\sigma} = 0 \quad (2.45a)$$

$$-2(1 - \phi)\mathcal{H} + G_c \left(\frac{1}{\ell} \phi - \ell \nabla^2 \phi \right) = 0 \quad (2.45b)$$

$$\vec{u} = \vec{u}_i \tau(t) \text{ en } \partial\Omega_i ; \quad i = 1, 2, 3... \quad (2.45c)$$

where σ includes plastic effects in its constitutive definition, and g has been redefined as in Eq.(2.20). The history variable in Eq.(2.45b) includes the hardening energy:

$$\mathcal{H}(t) = \max \left(\psi_{eo}^+ + \frac{g_p'}{g'} \psi_p + \frac{g_d'}{g'} D_p, \mathcal{H}(t_a) \right) ; \quad t_a \in [0, t[, \quad (2.46)$$

which results in a damage-independent definition if the functions $g_p(\phi)$ and $g_d(\phi)$ are defined proportionally to the function $g(\phi)$, leading to constant values for g_p'/g' and g_d'/g' . One of the challenges in extending the PFF model to plasticity lies in the nature of material failure and how to represent such failure. As mentioned at the beginning of this section, the PFF model was initially developed to represent brittle fracture in elastic materials. Experimental observations show that in brittle elastic materials the existence and propagation of cracks is the natural failure mechanism, which allows a good representation of them by using formulations of LEFM or PFF models.

However, elastoplastic materials often fail in ductile ways, and crack propagation may occur in conjunction with other phenomena. While there are elastoplastic materials, e.g. among metallic alloys where crack propagation is important, their evolution is influenced by plasticity, and modeling fracture solely based on an elastic source is not always representative. For this reason, the mathematical inclusion of plasticity functionals in the PFF model formulation determines its applicability to ductile failure modes. Although there is no consensus on how to include them, studies such as Alessi et al., 2018 have compiled several PFF models incorporating J2 plasticity, distinguishing two main ways in which plasticity influences fracture: modifying the function $g(\phi)$ so that it evolves based on plastic internal variables, and the inclusion of the already mentioned functions $g_p(\phi)$ and $g_d(\phi)$.

An example of the first case is developed in Ambati et al., 2015a, where the following degradation function is defined:

$$g(\phi, \gamma) = (1 - \phi)^{2 \frac{\gamma}{\gamma_{crit}}}, \quad (2.47)$$

with $g_p = g_d = 0$. This implies that fracture will occur in regions of high elastic strain, but will occur faster if those regions develop plastic strains. This can be controlled by the definition of the parameter γ_{crit} that alters the exponent of the degradation function if γ is high. Since plastic strains are typically much larger than elastic, fracture will progress slowly before the crack propagation, which causes a high accumulation of strain around the crack tip, resembling blunting, and then a high accumulation of damage resulting in the crack propagation.

Examples of the second case can be found in M. J. Borden et al., 2016, where different types of degradation functions $g(\phi)$ (mostly cubic) are defined, but always satisfying the equality:

$$g(\phi) = g_p(\phi) = g_d(\phi). \quad (2.48)$$

This choice affects Eq.(2.45b), meaning that cracks will not only form in regions of high elastic strain but also in regions with significant plastic deformation. This doesn't result in particularly slow fracture development, however, the wider distribution of plastic strain fields leads to blunter cracks. This allows us to emulate better the blunting effect observed in most ductile materials, making fracture behavior more ductile-like.

An important implementation for the present work is the approach developed by Duda et al., 2015, where a quadratic degradation function is defined, with null plastic and dissipation degradation functions,

$$g_p(\phi) = g_d(\phi) = 1. \quad (2.49)$$

This approach allows the study of crack propagation in materials which exhibit a propagation closer to that in brittle materials but also exhibiting plasticity, such as gray cast iron or some martensitic steels. A similar modeling will be done in this work in chapter 5 but with implementing the formulation of this section in a finite strains scheme.

2.4 Crystal plasticity model

The PFF models described in the last section, implemented in a small strain framework, are useful as references for the proposed models in this work made to represent brittle fracture processes. Nevertheless, crystal plasticity models (CP) and their implementation in a PFF model are also addressed in this work, to establish the model for complex constitutive relations and validate the model against a similar FEM scheme. Although implementations of CP with PFF models already exist in the literature for FEM (De Lorenzis et al., 2016) and FFT solvers (Lucarini et al., 2023), the derivation and implementation of the specific model of this work are described in chapter 5 for better continuity in the comparison of both computational schemes.

This section offers an introduction to the CP models without fracture, presenting the essential constitutive and kinematic formulation for the model in the framework of Continuum Mechanics and finite strains. With these models, the deformation process is characterized by the deformation gradient tensor $\mathbf{F}$, which describes the transformation from a reference-undeformed configuration with $\vec{X}$ material coordinate system in a volume Ω_o to an actual-deformed configuration with $\vec{x}$ coordinate system in a volume Ω . This transformation is defined through a multiplicative decomposition, as illustrated in Eq.(2.50)

$$\mathbf{F} = \frac{\partial \vec{x}}{\partial \vec{X}} = \mathbf{F}_e \mathbf{F}_p, \quad (2.50)$$

where $\mathbf{F}^e$ represents the elastic component of the deformation gradient, while $\mathbf{F}^p$ corresponds to the plastic contribution. For this reason, an intermediate configuration with volume Ω_I is considered, where only plastic strains are present, as depicted in Fig.2.5.

The kinematics of the deformation process are governed by the elasto-plastic counterparts, $\mathbf{F}_e$ and $\mathbf{F}_p$. Nevertheless, for processes involving detailed microstructural descriptions and time-dependent effects, it is essential to account for the rate of deformation. The spatial velocity gradient defined by the displacement vector $\vec{u}$ as $\mathbf{L} = \nabla_x \dot{\vec{u}}$ can also be expressed as in Eq.(2.51) in terms of $\mathbf{F}$ considering the relation $\mathbf{F}^{-1} = \mathbf{I} - \nabla_x \vec{u}$ in the absence of rigid translations or rotations.

$$\mathbf{L} = \dot{\mathbf{F}}\mathbf{F}^{-1} = \mathbf{L}_e + \mathbf{F}_e \mathbf{L}_p \mathbf{F}_e^{-1} ; \text{ where } \mathbf{L}_e = \dot{\mathbf{F}}_e \mathbf{F}_e^{-1} \text{ and } \mathbf{L}_p = \dot{\mathbf{F}}_p \mathbf{F}_p^{-1}. \quad (2.51)$$

The tensors $\mathbf{L}_e$ and $\mathbf{L}_p$ represent the elastic and plastic contributions to the spatial velocity gradient, respectively. On the other hand, the elastic strain between the intermediate and

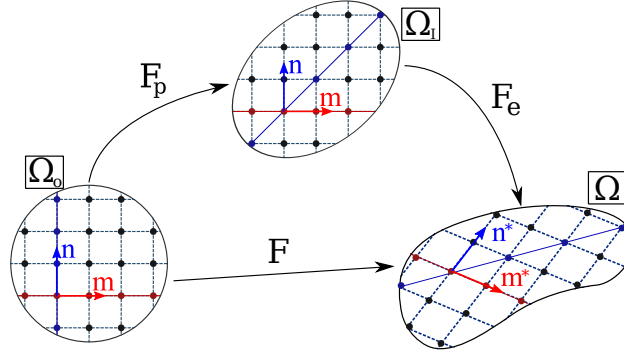


Figure 2.5: Scheme of the elasto-plastic deformation process.

the deformed configurations can be measured by means of the Green-Lagrange tensor $\mathbf{E}_e$, defined in terms of the elastic component of the deformation gradient as shown in Eq.(2.52). Consequently, the time derivative of $\mathbf{E}_e$ can be associated with the elastic stretching tensor $\mathbf{D}_e$, defined through the elastic part of the velocity gradient $\mathbf{D}_e = \text{sym}(\mathbf{L}_e)$:

$$\mathbf{E}_e = \frac{1}{2} (\mathbf{F}_e^T \mathbf{F}_e - \mathbf{I}) \quad \Rightarrow \quad \dot{\mathbf{E}}_e = \mathbf{F}_e^T \mathbf{D}_e \mathbf{F}_e. \quad (2.52)$$

Considering the Cauchy stress tensor $\boldsymbol{\sigma}$ defined in the current configuration, an alternative version of the second Piola-Kirchhoff stress tensor $\mathbf{S}$ is defined in the intermediate configuration rather than the reference configuration. Also, the first Piola-Kirchhoff stress tensor $\mathbf{P}$ in the reference configuration can be expressed as

$$\mathbf{S} = J \mathbf{F}_e^{-1} \boldsymbol{\sigma} \mathbf{F}_e^{-T} \quad (2.53a)$$

$$\mathbf{P} = \mathbf{F}_e \mathbf{S} \mathbf{F}_e^T \mathbf{F}^{-T}. \quad (2.53b)$$

An elastic constitutive formulation can be derived by considering the free energy in the material Ψ . The specific form of this functional varies depending on the chosen formulation (Gurtin et al., 2010), but its dependencies in the intermediate configuration are:

$$\Psi = \int_{\Omega_I} \psi_e(\mathbf{E}_e) + \psi_p(\gamma^\alpha) d\Omega_I \quad \Rightarrow \quad \mathbf{S} = \frac{\partial \psi}{\partial \mathbf{E}_e} = \frac{\partial \psi_e}{\partial \mathbf{E}_e} \quad (2.54)$$

Here, ψ_e and ψ_p represent the elastic and plastic parts of the local energy density. The functional ψ_p accounts for the plastic-hardening contribution of the strain energy and depends on γ^α , which denotes the microscopic shear strain along a specific slip system α defined by the lattice of the material in Fig.2.5. The evolution of γ^α is governed by the crystal plasticity model, which captures the plastic deformation through dislocation motion across all active slip systems α . In this work, the general structure of the crystal plasticity model follows the formulation outlined in Segurado et al., 2018.

Given an initial orientation of the material slip systems, the model can calculate and incorporate their subsequent kinematics to accurately describe the evolution of γ^α . Each slip system is characterized by the slip direction vector $\vec{m}$ and the normal to the slip plane $\vec{n}$ (see Fig.2.5), both defined in the reference configuration and assumed to maintain their orientations in

the intermediate configuration. Using these orientations, the stress internal conjugate of γ^α , known as the resolved shear stress τ^α , is kinematically formulated as a projection of the macroscopic stress tensor $\mathbf{S}$ in the intermediate configuration (Segurado et al., 2018),

$$\tau^\alpha = \mathbf{F}_e^T \mathbf{F}_e \mathbf{S} : \mathbf{Z}^\alpha \approx \mathbf{S} : \mathbf{Z}^\alpha \quad ; \text{ with } \quad \mathbf{Z}^\alpha = \sum_{\alpha} \mathbf{m}^\alpha \otimes \mathbf{n}^\alpha. \quad (2.55)$$

Here, $\mathbf{Z}^\alpha$ is the Schmidt tensor associated with the α slip system. This tensor establishes a link between variables at the microscale and macroscale, incorporating the lattice orientation influence into the formulation of the material behavior. With the resolved stress τ^α , a constitutive relation for the plastic slip rate $\dot{\gamma}^\alpha$ can be expressed at the microscale by means of a power-law formulation:

$$\dot{\gamma}^\alpha(\tau^\alpha, s^\alpha) = \dot{\gamma}_o \left(\frac{\tau^\alpha}{s^\alpha} \right)^{1/m} \text{sgn}(\tau^\alpha). \quad (2.56)$$

This visco-plastic definition captures the shear strain rate within each independent slip system α . The $\dot{\gamma}_o$ represents the initial plastic slip rate and m is the power-law exponent that dictates the level of rate sensitivity in the system response. The term s^α , known as the critical resolved shear stress (CRSS), represents the stress limit at which a particular slip system α becomes active. The evolution of the CRSS is typically determined incrementally:

$$\dot{s}^\alpha = \sum_{\beta} H_{\alpha\beta} |\dot{\gamma}^\beta|. \quad (2.57)$$

The evolution of this variable is primarily attributed to the accumulation of dislocations within the microstructure of the material, and its macroscopic consequence is the increase in the yield strength (Wulfinghoff and Böhlke, 2012), which is related to the hardening of the material captured in Eq.(2.57) through $H_{\alpha\beta}$. This second-order tensor denotes the hardening modulus of the material across all slip systems, encompassing the effect of self-hardening within each individual slip system α and latent hardening effects arising from interactions among different slip systems β :

$$H_{\alpha\beta} = h (q + (1 - q)\delta_{\alpha\beta}). \quad (2.58)$$

Here, the scalar variable q represents the latent hardening and h denotes the evolution of hardening as a function of accumulated plastic strain. For this study, the Voce-Tomé model Tome et al., 1984 is employed, which denotes an exponential behavior for hardening.

$$h(\Upsilon) = h_s \left[1 - \exp \left(\frac{-h_o \Upsilon}{\tau_s - \tau_o} \right) \right] + (\tau_s - \tau_o + h_s \Upsilon) \frac{h_o}{\tau_s - \tau_o} \exp \left(\frac{-h_o \Upsilon}{\tau_s - \tau_o} \right), \quad (2.59)$$

where Υ represents the macroscopic projection of the accumulated shear strain γ^α of all slip systems:

$$\Upsilon = \sum_{\alpha} \int_t |\dot{\gamma}^\alpha| dt \quad (2.60)$$

This definition provides a measure of the macroscopic plastic strain, which can also be used to formulate an alternative definition of the plastic strain rate tensor $\mathbf{L}_p$ from Eq.(2.51), as the microscopic measure of the plastic rate, capturing the evolution of plastic deformation within each slip system:

$$\mathbf{L}_p = \sum_{\alpha} \dot{\gamma}^\alpha \mathbf{Z}^\alpha = \sum_{\alpha} \dot{\gamma}^\alpha \mathbf{m}^\alpha \otimes \mathbf{n}^\alpha \quad (2.61)$$

2.5 Homogenization solvers based in the Fast Fourier Transform

2.5.1 Classical Lippmann–Schwinger approaches

As mentioned in previous sections, solvers for boundary value problems using FFT-based techniques have become a very popular alternative to the FEM method for micromechanical problems, especially for solutions involving computational homogenization. This framework aims to solve a boundary value problem at small scales to obtain the mechanical response of a section of the material, usually corresponding to its microstructure, under the imposition of local macroscopic loads over periodic RVEs. Effective mechanical behavior of the material and its influence on macroscopic scales can be obtained. FFT-based homogenization solves the boundary value problem by replacing the governing differential operators of the problem with their Fourier space equivalents, which provide the aforementioned advantages in terms of computational performance. This section presents some basic characteristics of the method, which has been extensively studied in the literature, as can be seen in reviews such as the one of Lucarini et al., 2021.

FFT-based homogenization was first proposed by Moulinec and Suquet, 1994 for solving the Lippmann-Schwinger equation using fixed-point algorithms in composite materials. Different approaches have been proposed for this resolution (Eyre and Milton, 1999; Monchiet and Bonnet, 2012), but all based on principles of the work of Moulinec and Suquet. The most basic scheme requires the properties of a reference medium imposed directly in the mechanical equilibrium, $\nabla \cdot \boldsymbol{\sigma} = 0$, which in an elastic material correspond with the definition of a reference stiffness $\mathbb{C}^o$. Considering the decomposition in Eq.(2.9) as $\boldsymbol{\varepsilon} = \nabla^s \tilde{\mathbf{u}} = \nabla^s \tilde{\mathbf{u}} + \bar{\boldsymbol{\varepsilon}}$, the mechanical equilibrium can be established as:

$$\nabla \cdot \boldsymbol{\sigma} = 0 \quad \Rightarrow \quad \nabla \cdot (\mathbb{C}^o : \nabla \tilde{\mathbf{u}} + \boldsymbol{\tau}^{prox}) = 0 \quad \Rightarrow \quad \nabla \cdot (\mathbb{C}^o : \nabla \tilde{\mathbf{u}}) = -\nabla \cdot \boldsymbol{\tau}^{prox}, \quad (2.62)$$

where $\boldsymbol{\tau}^{prox} = [\mathbb{C} - \mathbb{C}^o] : \boldsymbol{\varepsilon}$ is a polarization tensor that acts as a source term for Eq.(2.62) and appears as a consequence of introducing $\mathbb{C}^o$. This boundary value problem can be solved by means of a particularization of the Green's function method (Lucarini et al., 2021) which allows us to establish a formulation for the vector field $\tilde{\mathbf{u}}$ caused by the imposition of any body force, as the convolution of the body force with a second order tensor $\mathbf{G}$ which is an explicit version of Green's operator (Lucarini et al., 2021). Using the polarization tensor as a body force, it can be established that

$$\tilde{\mathbf{u}} = -\mathbf{G} * \boldsymbol{\tau}^{prox} \quad \rightarrow \quad \tilde{\boldsymbol{\varepsilon}} = \nabla \tilde{\mathbf{u}} = -\mathbb{F} * \boldsymbol{\tau}^{prox}, \quad (2.63)$$

where $\mathbb{F}$ corresponds to the spatial derivative of the Green function, which is a fourth-order projection operator conformed with $\mathbf{G}$ and defined in Fourier space as $\hat{\mathbb{F}}_{ijkl}(\vec{\xi}) = \xi_i \xi_j \hat{\mathbf{G}}_{ki}$. Further details of this deduction and the proper definition of $\mathbb{F}$ can be found in the work of Moulinec and Suquet, 1994 and in the work of Lucarini et al., 2021. A linear operator for the strain field can be defined from Eq.(2.63), using Fourier space and Eq.(2.9):

$$\hat{\boldsymbol{\varepsilon}}(\vec{\xi}) = \bar{\boldsymbol{\varepsilon}} - \hat{\mathbb{F}} : \hat{\boldsymbol{\tau}}(\boldsymbol{\varepsilon}), \quad (2.64)$$

where $\vec{\xi}$ represents the frequency vector in three-dimensional Fourier space. Eq.(2.64) represents a system of equations whose resolution is highly efficient with FFT. In general, classical schemes are usually solved using iterative approaches, where the external load is typically introduced by imposing macroscopic strain to compute the effects of microscopic stress and strain. The macroscopic stress tensor or some of its components can also be imposed in a mixed control scheme, which requires more iterations for resolution. The approach proposed in the work of Kabel et al., 2016 introduces projection tensors to account for load control and solve the problem with Krylov iterative schemes. This optimizes the method but still requires defining a reference medium, which can influence the convergence rate of the solution.

2.5.2 Fourier-Galerkin Method

A different approach to FFT homogenization is the so-called Fourier-Galerkin method, which was mainly developed in the works of Vondřejc et al., 2014; Zeman et al., 2017. The method does not require a reference medium as the basic Lippmann–Schwinger scheme of the last section and can directly use the corresponding tangents of the material behavior to solve a mechanical problem. Consider a domain represented by a periodic RVE with elastic-heterogeneous properties in a small strain scheme. For a total strain control in which the macroscopic loading path is given, the objective is to find the microscopic fluctuant strain field $\tilde{\epsilon}$, following Eq.(2.9). Considering the mechanical elastic problem of Eq.(2.31a), the method can be stated using the weak formulation of the problem depicted in Eq.(2.65), considering a set of strain-like test functions $\Delta\epsilon$ (as in FEM), which could be derived in the variational resolution of the mechanical problem.

$$\int_{\Omega} \sigma : \Delta\epsilon \partial\Omega = 0 \Rightarrow \int_{\Omega} \sigma : [\mathbb{G} * \zeta] \partial\Omega = 0. \quad (2.65)$$

Here, the strain set $\Delta\epsilon$ has to be a compatible strain tensor. To enforce this compatibility in the method, a projection operator $\mathbb{G}$ convoluted with a general non-compatible second-order tensor ζ is introduced in the weak form as also depicted in the right part of Eq.(2.65) (Lucarini et al., 2021; Zeman et al., 2017). Using the properties of the convolution, $*$, the resulting form of the weak formulation is expressed in Eq.(2.66).

$$\int_{\Omega} \sigma : [\mathbb{G} * \zeta] \partial\Omega = \int_{\Omega} \zeta : [\mathbb{G} * \sigma] \partial\Omega. \quad (2.66)$$

Note that this problem formulation does not specify the need for the domain to be homogeneous. After proper discretization of the space and using the Fourier space, the fields involved in the problem are defined by trigonometric polynomials formulated with a set of frequencies $\vec{\xi}_i$, with i representing the points of the grid. Since equilibrium must be fulfilled locally, the test functions ζ can be eliminated, leading to a discrete linear system of equations of the local stress field σ_i (Vondřejc et al., 2014) as,

$$\mathbb{G} * \sigma_i = \mathcal{F}^{-1} \left\{ \hat{\mathbb{G}}(\vec{\xi}_i) : \mathcal{F} \{ \sigma_i \} \right\} = 0. \quad (2.67)$$

The use of the FFT in this equation is convenient since the formulation of the convolution operation can be defined as the corresponding product in the dimension of the functionals

being operated, which in this case is the contraction of both fields. However, the fourth-order projector used in the method must be expressed in the Fourier space $\widehat{\mathbb{G}}$, which formulation has been derived in the work of Vondřejc et al., 2014 for total strain control as

$$\widehat{\mathbb{G}} = 0 \text{ for } \vec{\xi} = \vec{0} ; \quad \widehat{\mathbb{G}}_{ijkl}(\vec{\xi}) = \delta_{ik} \frac{\xi_j \xi_l}{\vec{\xi} \cdot \vec{\xi}} \text{ for } \vec{\xi} \neq \vec{0}, \quad (2.68)$$

and has also been derived for a mixed control, which is defined in a way that allows filtering the mean part of the components that are imposed as macroscopic strain and computing the mean part of the components defined for macroscopic stress. This version of the projection operator needs an additional definition to properly manage the filtering. To distinguish between strain- and stress-controlled components, the tensor $\mathbf{c}$ is introduced, being 0 for strain-controlled components and 1 for the stress-controlled ones, as follows

$$\widehat{\mathbb{G}}_{ijkl} = \begin{cases} \delta_{ik} \delta_{lj} & \text{for } \vec{\xi} = \vec{0} \text{ and } ij \text{ where } \mathbf{c}_{ij} = 1 \\ 0 & \text{for } \vec{\xi} = \vec{0} \text{ and } ij \text{ where } \mathbf{c}_{ij} = 0. \end{cases} \quad (2.69)$$

It should be noted that the arrangement of this formulation allows its resolution with any numerical method, with Krylov solvers being a very common choice. The solution procedure will depend on the constitutive definition of $\boldsymbol{\sigma}$, since Eq.(2.67) has to be treated in order to elect a proper numerical resolution scheme, which is often done extending the definition of the stress. The non-linearity that an elastoplastic behavior or the influence of the PFF damage as described in section 2.3 could bring to the stress field will also affect the resolution of the problem.

Taking the example of an isotropic elastic material in a micromechanical domain with a given macroscopical strain (Lucarini et al., 2021). Using Eq.(2.9) and $\boldsymbol{\sigma} = \mathbb{C} : \boldsymbol{\varepsilon}$ as the definition of stress, the following system can be established from Eq.(2.67):

$$\mathcal{F}^{-1} \left\{ \widehat{\mathbb{G}} : \mathcal{F} \{ \mathbb{C} : \tilde{\boldsymbol{\varepsilon}}_i \} \right\} = -\mathcal{F}^{-1} \left\{ \widehat{\mathbb{G}} : \mathcal{F} \{ \mathbb{C} : \mathbf{E}_M \} \right\}, \quad (2.70)$$

which correspond to a closed system that could be solved with any Krylov-type scheme. Specific definitions for the cases in the following chapters will be defined depending on the material used and implemented together with the appropriate solution method in the body of the work.

2.6 Numerical estimations of effective toughness

As it was discussed in Chapter 1, one application of homogenization schemes is the estimation of effective fracture toughness G_c in heterogeneous media. The idea behind this concept is to calculate a geometrically and constitutively adequate value, G_{Ceff} , that represents the homogenized fracture resistance of the media. In this case, in which microstructural homogenization is studied, this value will represent the resistance of a domain at microscale that is equivalent to the toughness at a local point at the macroscopic scale. For this reason, this value must be determined from simulations including microstructure fracture and possibly heterogeneous or anisotropic constitutive properties.

As summarized in the introduction, two kinds of estimations of the effective toughness can be mentioned. The first one, proposed by Hossain et al., 2014 the J-integral is used on a RVE domain in which the microstructure is explicitly modeled and special boundary conditions are introduced which represent the displacement field of the mode I surface separation (Zehnder, 2012) corresponding to the macro-crack advance in a particular direction oriented with the RVE. In this case, the toughness estimate can be obtained by means of a J-integral (Eq.(2.14)) surrounding this domain, which is considered an estimation of the energy release rate G on the macroscopic scale that directly captures the influence of the microstructure (Brach et al., 2019). This influence depends directly on the propagation of a microcrack that can be arrested or deflected by differences in stiffness and local toughness. Such microcrack propagation is modeled with a PFF model and its changes in direction and phase crossing can be perceived by the J-integral. In that work, the maximum value over time t of the J-integral is defined as the effective toughness estimate of the microstructure, arguing that the maximum G is a rate of energy that is necessary to overpass at some point to fracture the microstructure.

$$G_{CeH} = \max_t J(t). \quad (2.71)$$

This metric considers the influence of the microstructure both due to heterogeneity in stiffness and toughness. However, the use of path integrals is not clear when the microstructure is heterogeneous, which has the disadvantage of having to resort to special materials at the boundary to perform the integral.

Other alternative for effective toughness definition is the one developed by M. Schneider, 2020 with a variational basis, where it is stated that the fracture dissipation functional is independent of the mechanical microfields, idea postulated in Braides et al., 1996.

$$\Psi = \int_{\Omega} \frac{1}{2} \varepsilon : \mathbb{C}_{eff} : \varepsilon d\Omega + \int_{S_{\phi}} G_{CeS}(\vec{t}_c) dS_{\phi}, \quad (2.72)$$

with G_{CeS} the effective toughness, $\mathbb{C}_{eff}$ the effective stiffness, S_{ϕ} the geometrical surface where the crack is located, and $\vec{t}_c$ a vector defining the normal to the macroscopic crack.

The independence of the functional from local strain or stress fields allows us to state a minimization problem to find a crack path that represents the minimum fracture energy over microstructures with heterogeneous local toughness fields. As a result, non-planar crack paths corresponding to a minimal energy state are obtained, and the effective toughness is directly linked with the energy spent on that particular crack path. The definition of this effective energy release rate corresponds to Eq.(2.73),

$$G_{CeS}(\vec{t}_c) = \lim_{L \rightarrow \infty} \inf_{S_{\phi} \subseteq Q_L} \frac{1}{|Q_L|} \int_{Q_L} G_c \left\| \vec{t}_c + \nabla \Phi \right\| d\Omega. \quad (2.73)$$

Here Φ is a smooth scalar function characterizing the crack (similar to ϕ in the PFF model) and Q_L is the RVE volume with size L in which the minimization is performed. The fact that this procedure includes the limit of $L \rightarrow \infty$ indicates that an adequate estimation of effective toughness has to be made over scales much larger than the microstructure and the geometries that could be modeled in it, which is also reported in other works like Lebihain et al., 2020, 2021. In the work of M. Schneider, 2020 the size of Q_L was studied for a fiber

reinforced composite and convergence was found, allowing us to obtain results for relatively small RVE sizes.

Some differences can be highlighted between the calculation mentioned (Hossain et al., 2014; M. Schneider, 2020). The one in the former is an estimation of the energy release rate, since it includes the complete crack and the volume of the RVE in its final state, contrary to the estimation in the latter one that is defined as an instantaneous rate. This method is limited in the application of the J-integral, meanwhile the method of M. Schneider, 2020 is a direct energy method that doesn't have this issue and is able to make highly optimized calculations. However, the procedure of Hossain et al., 2014 includes an adequate boundary condition that represents the passage of a crack at macroscale and actually includes microstructural effects from the strain/stress distributions, contrary to the method of M. Schneider, 2020 where the assumption that the microstructure forms the crack of minimal energy in a periodic RVE without influence of the constitutive behavior is assumed, and the connection with the macroscale relies on a direction vector that doesn't relate to any principle of fracture mechanics.

One of the purposes of this work is to propose a procedure to estimate the effective toughness from the fracture model developed, which allows considering the material characteristics at microscale to define the homogenized toughness. The proposed method is detailed in chapter 4 taking aspects of both methodologies mentioned and being tested for a set of different microstructures.

Chapter 3

Crack dissipation control scheme in a PFF-FFT framework

As seen in previous chapters, classical PFF implementations typically use a monotonic displacement or strain increase to perform the calculations within efficient monolithic solvers. This is not directly possible in unstable fracture due to the non-convexity of a Phase-Field formulation (Gerasimov and De Lorenzis, 2016; Svolos et al., 2023). Despite several solutions have been proposed to obtain solutions in staggered schemes (Ambati et al., 2015b; Miehe et al., 2010a) or in extensions to use modified monolithic algorithms that could involve line search (Gerasimov and De Lorenzis, 2016) or quasi-Newton BFGS schemes (Kristensen and Martínez-Pañeda, 2020), the use of any of these options leads to the numerical jump behavior described in chapter 1.

One of the major contributions of this chapter is the implementation of a dissipative control scheme in a FFT homogenization solver. The proposal consists of the application of this control to obtaining the snap-back behavior mentioned in chapter 1, allowing the macroscopic stress and strain variables to be non-monotonous and leading to the complete fracture material behavior for analysis. Early approaches to this kind of strategy were developed in FEM schemes and consisted in using constraint equations involving local displacements rather than global constraints. As examples of this, in the seminal work of Carpinteri and Colombo, 1989 a Crack Mouth Opening Displacement (CMOD) control scheme is introduced with a cohesive crack model to study catastrophic softening in elastic bending simulations. In the works by De Borst, 1987 and of Rots and De Borst, 1987 a modified arc-length method is used to study the snap-back behavior in concrete structures for highly localized failure modes using indirect displacement control or the Crack Mouth Sliding Displacement (CMSD) as constraint respectively. More recently, energy dissipation control was introduced to follow snap-back response in the context of CDM and also gradient damage models, such as the works of Gutiérrez, 2004 and C. Verhoosel et al., 2009 who develop arc-length methods on local external forces or displacements associating them with energy dissipation functionals. An alternative approach was proposed to resolve instabilities in micromechanical problems in composites by Segurado and LLorca, 2004, setting the total CMOD of a set of predefined cracks as the control parameter. Arc-length based methods have been subsequently extended to capture

the snap-back behavior in PFF-FEM at the macroscopic level (De Borst and Verhoosel, 2016; Vignollet et al., 2014). One of the first works to use the PFF crack dissipation energy in an arc-length scheme was the work of Singh et al., 2016, who implemented a model with the PFF regularization of the crack as a control parameter. This idea was also exploited later in the work of Bharali et al., 2022 where monolithic arc-length schemes are compared with local displacement control models in FEM, or in the work of Zambrano et al., 2023 where a modified staggered scheme on PFF-FEM with arc-length model is proposed to study the snap-back behavior in brittle fracture.

One of the main objectives of this work is the implementation of an energy dissipation control scheme based on the PFF model for its use in fracture studies at the microscopic level. The strategy proposed relies on a monolithic solver in which the fracture variable, the micro-strain field, and its corresponding macro-strain are the problem unknowns. As has been advanced in previous chapters, this implementation in FFT-based solvers has very few precedents and could have advantages when performing homogenization of effective properties. Differences between the proposed model in FFT and the models of the works mentioned for FEM are also expected, so under the assumption that for high-resolution discretization both schemes have to converge, a comparative study between the FFT proposal and one made in FEM with crack-length control is conducted in order to validate the FFT results. Implementations of the PFF-FFT model are commonly boarded in literature with strain control schemes, as depicted in chapter 2. Despite this approach having already been studied, its use as a reference for dissipation-controlled simulations in stable crack propagation regimes can be made in order to verify the control implication on the response obtained. The numerical implications of the adaptation of the PFF model in FFT are also studied, since FEM-PFF models have demonstrated to have numerical issues (Bourdin et al., 2008; Miehe et al., 2010b) that will be important in toughness measures of chapter 4

3.1 Numerical implementation

3.1.1 Strain-controlled PFF scheme in FFT

The numerical scheme depicted here corresponds to the procedure to solve the classical fracture PFF problem represented in the governing equations system from Eq.(2.31) at section 2.3.1. The implementation has been performed in the FFT based solver FFTMAD (Lucarini and Segurado, 2019a; Lucarini et al., 2021). Consider an RVE in a 3D domain Ω of size L_1, L_2, L_3 and discretized in a grid of n_x, n_y, n_z voxels, referred to as an orthonormal basis x, y, z . Using the Fourier space, the fields involved in the problem can be discretized by trigonometric polynomials defined with a set of frequencies ξ and the values of the points of the grid in real space.

The proposal for solving the problem is similar to the implicit-staggered scheme described in the works of Miehe et al., 2010a and Gerasimov and De Lorenzis, 2016, that can be adapted to find the fields $\tilde{\epsilon}$ and ϕ . The problem is split in two, solving first Eq.(2.31a) considering a constant damage field (micromechanical sub-problem) and then Eq.(2.31b) considering a constant strain field (Damage sub-problem). Both sub-problems are solved sequentially at

each stagger iteration s , conforming a self-consistent procedure that continues until both objective fields converge. Then, values of $\tilde{\epsilon}$ and ϕ obtained are kept as the result of the time step n .

Within the stagger cycle, the Fourier-Galerkin method (Vondřejc et al., 2014; Zeman et al., 2017) is used to solve the micromechanical sub-problem, and a Krylov approach is used to solve the damage sub-problem. For the former, Eq.(2.67) is used to formulate the equilibrium, and a similar procedure to the one exposed in section 2.5.2 can be followed. Nevertheless, the damage coupling makes the mechanical sub-problem non-linear, so an iterative Newton-Raphson scheme (NR) is proposed. From this perspective, Eq.(2.70) is replaced by one formulated with a linearization of stress in order to find increments of the strain field, $\Delta\epsilon$, instead of the field itself (Ma and Sun, 2021). Defining i as the subindex of an actual NR iteration, the linearization on the left of Eq.(3.1) leads to the weak form of mechanical equilibrium at the right of the same equation,

$$\sigma \approx \mathbb{C}_i : \Delta\epsilon + \sigma_i \Rightarrow \mathbb{G} * [\mathbb{C}_i : \Delta\epsilon + \sigma_i] = 0, \quad (3.1)$$

where $\mathbb{C}_i$ is the mechanical elastic tangent including damage, σ_i the stress of the actual iteration and $\Delta\epsilon$ is the unknown strain increment estimated for every NR iteration. The right part of Eq.(3.1) corresponds to a linear system of equations in which the convolution of the stress with the projection $\mathbb{G}$ can be obtained by transformation to Fourier space as

$$\mathcal{F}^{-1} \left\{ \hat{\mathbb{G}} : \mathcal{F} \{ \mathbb{C}_i : \Delta\tilde{\epsilon} \} \right\} = -\mathcal{F}^{-1} \left\{ \hat{\mathbb{G}} : \mathcal{F} \{ \sigma_i \} \right\}, \quad (3.2)$$

where $\mathcal{F}()$ and $\mathcal{F}^{-1}()$ correspond to the discrete Fourier and inverse Fourier transforms, $\hat{\square}$ represents a field in Fourier space and the expression for $\mathbb{G}$ is the same in Eq.(2.68) or Eq.(2.69). In the case of high phase stiffness contrast, as it happens in the presence of a crack, numerical noise might appear. In the present case, to mitigate this noise we use a discrete projection operator based on finite differentiation (in particular the rotated scheme proposed by Willot Willot, 2015) which is included using modified frequencies in the Fourier expression of $\mathbb{G}$ (Eq.(2.68))

Note that in Eq.(3.2) $\Delta\tilde{\epsilon}$ is placed instead $\Delta\epsilon$ since in the definition of $\mathbb{G}$ null values are imposed for $\vec{\xi} = \vec{0}$ allowing to filter the average fields. Eq.(3.2) can be solved using the conjugate gradient method, in which the left-hand side of the equation is a linear operator acting on the discrete field $\Delta\tilde{\epsilon}$. The key point for the efficiency of the method is that the coefficient matrix does not need to be formed and stored for the iterative process, but only the action of the linear operator on the current value of the strain. With this, ϵ is obtained by accumulation of $\Delta\tilde{\epsilon}$ in the last iteration, as stated in Eq.(3.3a), which considers the prescribed mean strain. At the end of each Newton iteration, the stress and the elastic stiffness for the new update $i + 1$ are defined in Eq.(3.3b):

$$\epsilon_{i+1} = fE + \sum_{k=0}^{i+1} \Delta\tilde{\epsilon}_k \quad (3.3a)$$

$$\sigma_{i+1} = \sigma(\epsilon_{i+1}, \phi_s) \ ; \ \mathbb{C}_{i+1} = \left. \frac{\partial \sigma}{\partial \epsilon} \right|_{\epsilon_{i+1}} \quad (3.3b)$$

where the subindex s stands for the last converged stagger iteration and is considered constant at this stage.

The second sub-problem, called here the Helmholtz problem, is solved from Eq.(2.31b) with a constant strain field, implying a constant energy field. To prevent the healing of an already developed crack, the energy field ψ_o^+ in Eq.(2.31b) is usually replaced by some history variable $\mathcal{H}$ (Miehe et al., 2010a), leading to

$$g'\mathcal{H} + G_c\gamma'_f(\phi) = 0 \rightarrow \left(\frac{G_c}{\ell} + 2\mathcal{H}\right)\phi + G_c\ell\nabla^2\phi = 2\mathcal{H}. \quad (3.4)$$

A common choice for the history is the maximum local positive energy of the complete mechanical process,

$$\mathcal{H} = \max(\psi_{o_{i+1}}^+, \mathcal{H}^{n-1}), \quad (3.5)$$

where $\mathcal{H}_{n-1}$ stands for the history value obtained in the last converged time step and $\psi_{o_{i+1}}^+$ is the energy field obtained in the last converged mechanical problem of the actual stagger iteration.

To solve the problem, the linear differential operator on the left hand side of Eq.(2.31b) is replaced by a discrete linear operator in which the Laplacian is computed based on Fourier derivatives. Note that in the Fourier transform of the Helmholtz equation, standard frequencies are used, contrary to the mechanical case where the rotated scheme is used (Willot, 2015). The resulting linear system of equations to be solved corresponds to

$$\mathcal{A}(\phi) = 2\mathcal{H} \quad ; \quad \text{being } \mathcal{A}(\phi) = \left(\frac{G_c}{\ell} + 2\mathcal{H}\right)\phi - G_c\ell\mathcal{F}^{-1}[\vec{\xi} \cdot \vec{\xi}\hat{\phi}] = 2\mathcal{H}. \quad (3.6)$$

The left hand side of this linear equation has been defined as a linear operator, $\mathcal{A}(\phi)$, and the equation can be solved by the conjugate gradient method with the discrete ϕ field as the unknown, obtaining the field ϕ_{s+1} to be used in Eq.(3.3b) in the next stagger iteration. Nevertheless, the resolution of this system can be highly improved by including a preconditioner, A_p , defined in Eq.(3.7) (proposed by Magri et al., 2021), for the application of the conjugate gradient. Thus, the actual system to be solved to obtain the damage field is the following:

$$A_p(\phi)\mathcal{A}(\phi) = 2A_p(\phi)\mathcal{H} \quad ; \quad A_p(\phi) = \mathcal{F}^{-1}\left[\frac{1}{\left(\frac{G_c}{\ell} + 2\mathcal{H}\right) - G_c\ell\vec{\xi} \cdot \vec{\xi}}\hat{\phi}\right]. \quad (3.7)$$

Both equations Eq.(3.2) and Eq.(3.6) are solved at each stagger step s of the implicit staggered scheme, which is depicted in algorithm 1. Once the staggered scheme converges and both fields, $\tilde{\epsilon}$ and ϕ , are obtained for the current time step, the modulus of the macroscopic strain E (control variable) is increased for the next time step. The convergence of each sub-problem and the staggered scheme is determined in relative terms of the unknowns. The mechanical problem error of Eq.(3.8a) is defined as the maximum strain increment with respect to the field norm and the Helmholtz problem has the characteristic absolute residual of a conjugate gradient method. The stagger error is based on relative errors of the variables $\tilde{\epsilon}$ and ϕ as in

Eq.(3.8b):

$$err_{Mech} = \frac{\max(|\Delta\tilde{\epsilon}|)}{\|\tilde{\epsilon}_i\|} \quad (3.8a)$$

$$err_{sta} = \max\left(\frac{\|\epsilon_s - \epsilon_{s-1}\|}{\|\epsilon_s\|}, \frac{\|\phi_s - \phi_{s-1}\|}{\|\phi_s\|}\right), \quad (3.8b)$$

where i corresponds to a NR iteration, s corresponds to a Stagger iteration, ϕ_{s-1} corresponds with the last iterated field in the CG problem, $|\bullet|$ is the absolute value at every point of a field, and $\|\bullet\|$ is the Euclidean norm of a vector or tensor field.

Regarding the algorithm 1, every variable has three indices where the upper-right accounts for time, the upper-left accounts for the stagger iterations, and the bottom-right accounts for the mechanical NR iterations.

Algorithm 1 : Implicit staggered scheme with strain control

```

1: Initial data:  $\tilde{\epsilon}^0 = 0, E^0 = 0, \phi^0 = 0, \mathcal{H}^0 = 0$ 
2: Control variable  $\Delta E$  fixed
3: Time index:  $n = 0$ 
4: while  $t^{n+1} < t_{final}$  do
5:   Initiate Stagger fields:  ${}^0\epsilon = \epsilon^n + \Delta E$  ;  ${}^0\phi = \phi^n$ 
6:   Evaluate constitutive equation: find  ${}^0\sigma = \sigma({}^0\epsilon, {}^0\phi)$  and  ${}^0\mathbb{C} = \frac{\partial\sigma}{\partial\epsilon}|_{{}^0\epsilon}$ 
7:   Stagger index:  $s = 0$ 
8:   while  $Err_{sta} \geq tol_{sta}$  do
9:     Initialize mechanical fields:  $\epsilon_0 = {}^s\epsilon$  ;  $\sigma_0 = {}^s\sigma$  ;  $\mathbb{C}_0 = {}^s\mathbb{C}$ 
10:    Newton index:  $i = 0$ 
11:    while  $Err_{Mech} \geq tol_{Mech}$  do
12:      Mech. solver FFT: find  $\Delta\tilde{\epsilon}(\sigma_i, \mathbb{C}_i)$  that fulfills Eq.(3.2)
13:      Update strain:  $\epsilon_{i+1} = \epsilon_i + \Delta\tilde{\epsilon}$ 
14:      Evaluate constitutive equation: find  $\sigma, \psi_o^+$  and  $\mathbb{C}$  such:
15:         $\sigma_{i+1} = \sigma(\epsilon_{i+1}, {}^s\phi)$  ;  $\mathbb{C}_{i+1} = \frac{\partial\sigma}{\partial\epsilon}|_{\epsilon_{i+1}}$  ;  $\psi_o^+{}_{i+1} = \psi_o^+(\epsilon_{i+1})$ 
16:    end while( $i = i + 1$ )
17:    Update fields:  ${}^{s+1}\epsilon = \epsilon_{i+1}$  ;  ${}^{s+1}\sigma = \sigma_{i+1}$  ;  ${}^{s+1}\mathbb{C} = \mathbb{C}_{i+1}$ 
18:    Update History:  $\mathcal{H}^{n+1} = \max(\psi_o^+{}_{i+1}, \mathcal{H}^n)$ 
19:    Helm. solver FFT: find  ${}^{s+1}\phi = \phi(\mathcal{H}^{n+1})$  that fulfills Eq.(3.6)
20:  end while( $s = s + 1$ )
21:  Update strain and damage:  $\phi^{n+1} = {}^{s+1}\phi$  ;  $\epsilon^{n+1} = {}^{s+1}\epsilon$ 
22: end while( $n = n + 1$ )

```

3.1.2 Dissipation controlled PFF scheme in FFT

As seen in chapter 2, an alternative control strategy can be applied to the PFF model that consists of defining a control method depending on crack length development or the associated energy dissipation. This type of control allows resolving all the macroscopic stress and strain states during stable crack propagation, avoiding numerical jumps in the response of the classical control scheme and resolving the snap-backs that allow us to use a monolithic solver

with better convergence (Khalil et al., 2022). Several approaches with this technique have been developed for FEM/macroscopic calculations, as depicted in section 2.3.2. In this section, the proposed adaptation of the arc-length procedure developed for the FFT-PFF microscale framework is made.

The models presented in chapter 2 rely on similar governing equations as those presented here and in section 3.1.1, but for the dissipation-based models, the control equation has to be related to crack growth and one of the variables has to be formulated as a load factor. In this work, we propose this variable to be related to macroscopic strain $\mathbf{E}_M$ and the control equation to be defined with a similar formulation to the one in the work of Bharali et al., 2022 or the one in Singh et al., 2016, but defining the dissipation energy as an absolute value and not defining its rate. The scheme proposed uses the PFF model with an AT2 crack functional, a spectral decomposition of the strain to define the energetic driving force of damage, and an isotropic elastic homogeneous material for constitutive modeling.

Let the macroscopic strain be written as $\mathbf{E}_M = \mathbf{f}E$, being E its scalar modulus, that can be understood as the load factor, and $\mathbf{f}$ a dimensionless tensor that allows to define the proportionality between components of the mean strain tensor. Then, E is now considered an unknown that defines the mean field of $\boldsymbol{\varepsilon}$, which is equal to the tensor $\mathbf{E}_M$. Alternative mixed boundary conditions could be introduced by using E as the only macroscopic strain controlled component, letting the other components be determined by macroscopic stress conditions (Lucarini et al., 2021). The new unknown in the system is compensated by adding a new constraint equation, which replaces the one in the control equation Eq.(2.31c) defined in section 2.3.1. A new system of governing equations is defined in Eq.(3.9) as,

$$\nabla \cdot (\mathbb{C} : \tilde{\boldsymbol{\varepsilon}} + \mathbb{C} : \mathbf{f}E) = 0 \quad (3.9a)$$

$$g'(\phi)\mathcal{H} + G_c\gamma_f'(\phi) = 0 \quad (3.9b)$$

$$G_c \int_{\Omega} \gamma_f(\phi) d\Omega = \tau(t). \quad (3.9c)$$

Note that in the equilibrium equation depicted in Eq.(3.9a) the stress is replaced by the derivative of the elastic energy density, $\boldsymbol{\sigma} = \mathbb{C} : (\tilde{\boldsymbol{\varepsilon}} + \mathbf{f}E)$. Here the fourth-order tensor $\mathbb{C}$ represents the actual elastic stiffness of the material and is calculated based on the positive/negative definition of the energy in Eq.(2.19) in a similar way to the stress in Eq.(2.29a) (Gerasimov and De Lorenzis, 2016),

$$\mathbb{C} = g(\phi) \frac{\partial^2 \psi_o^+}{\partial \boldsymbol{\varepsilon}^2} + \frac{\partial^2 \psi_o^-}{\partial \boldsymbol{\varepsilon}^2}. \quad (3.10)$$

The function $\tau(t)$ in Eq.(3.9c) is established as a linear ramp with respect to the time, which implies a constant dissipation increase. This is equivalent to the constant crack growth rate imposed through a constant $\Delta\tau_c$ in Eq.(2.37) from the work of Bharali et al., 2022. As in the strain control scheme, to avoid that Eq.(3.9b) drives to crack healing, the definition of the history $\mathcal{H}$ is included in its formulation following the same definition as in Eq.(3.5). With this, the technique aims to find at each time step the macroscopic strain modulus E as well as the fields $\tilde{\boldsymbol{\varepsilon}}$ and ϕ for a prescribed value of $\int_{\Omega} G_c \gamma_f d\Omega$.

The system of governing equations in Eq.(3.9) can be linearized in order to establish a Newton-Raphson scheme (NR) similar to the one established for the mechanical problem in

the last section. Let $F(q)$ be the non-linear residual of the NR procedure, where q is the set of unknowns $q = \{\tilde{\epsilon}, \phi, E\}$, and which can be split into three different terms as,

$$\begin{aligned} F_1(\tilde{\epsilon}, \phi, E) &= \mathbb{G} * \boldsymbol{\sigma}(\tilde{\epsilon}, \phi, E) = \mathcal{F}^{-1} \left\{ \widehat{\mathbb{G}} : \mathcal{F} [\mathbb{C} : \tilde{\epsilon} + \mathbb{C} : \mathbf{f}E] \right\} \\ F_2(\tilde{\epsilon}, \phi, E) &= \left(\frac{G_c}{\ell} + 2\mathcal{H} \right) \phi - G_c \ell \mathcal{F}^{-1} \left[\vec{\xi} \cdot \vec{\xi} \widehat{\Delta \phi} \right] - 2\mathcal{H} \\ F_3(\tilde{\epsilon}, \phi, E) &= G_c \int_{\Omega} \gamma_f(\phi) d\Omega - \tau(t), \end{aligned} \quad (3.11)$$

where F_1 corresponds to the residual of the equilibrium equation written following the Fourier-Galerkin form in Eq.(2.67), similar to the operator in Eq.(3.2) and with the stiffness defined in Eq.(3.10). F_2 corresponds to the residual in the Helmholtz equation (Eq.(3.6)) with the Laplacian computed as the Fourier transform of the inner product of the gradients of γ_f . F_3 is the residual which defines the difference between the actual crack area/length and the prescribed one, $\tau(t)$, being the term $\gamma_f(\phi)$ computed using Fourier transforms as

$$\gamma_f = \frac{1}{2\ell} \phi^2 + \frac{\ell}{2} \mathcal{F}^{-1} \left(\vec{\xi} \widehat{\phi} \right) \cdot \mathcal{F}^{-1} \left(\vec{\xi} \widehat{\phi} \right). \quad (3.12)$$

The Newton-Raphson method linearizes the system with respect to q considering the corresponding infinitesimal variations of the unknowns $\Delta q = \{\Delta \tilde{\epsilon}, \Delta \phi, \Delta E\}$ (Farrell and Maurini, 2017; Gerasimov and De Lorenzis, 2016),

$$\begin{pmatrix} \Delta F_1 \\ \Delta F_2 \\ \Delta F_3 \end{pmatrix} = \begin{pmatrix} \frac{\partial F_1}{\partial \tilde{\epsilon}} \Delta \tilde{\epsilon} + \frac{\partial F_1}{\partial \phi} \Delta \phi + \frac{\partial F_1}{\partial E} \Delta E \\ \frac{\partial F_2}{\partial \tilde{\epsilon}} \Delta \tilde{\epsilon} + \frac{\partial F_2}{\partial \phi} \Delta \phi + \frac{\partial F_2}{\partial E} \Delta E \\ \frac{\partial F_3}{\partial \phi} \Delta \phi \end{pmatrix}. \quad (3.13)$$

The result of this derivative corresponds with the NR Jacobian, which defines a linear system in $\mathbb{R}^{7(n_x n_y n_z)+1}$ given by the set of equations of Eq.(3.14)

$$\begin{aligned} \Delta F_1(q, \Delta q) &= \mathcal{F}^{-1} \left\{ \widehat{\mathbb{G}} : \mathcal{F} \left[\mathbb{C} : \Delta \tilde{\epsilon} - 2(1 - \phi) \frac{\partial \psi_o^+}{\partial \epsilon} \Delta \phi + \mathbb{C} : \mathbf{f} \Delta E \right] \right\} \\ \Delta F_2(q, \Delta q) &= -2(1 - \phi) \frac{\partial \mathcal{H}}{\partial \epsilon} : (\Delta \tilde{\epsilon} + \mathbf{f} \Delta E) + \left(\frac{G_c}{\ell} + 2\mathcal{H} \right) \Delta \phi - G_c \ell \mathcal{F}^{-1} \left[\vec{\xi} \cdot \vec{\xi} \widehat{\Delta \phi} \right] \\ \Delta F_3(q, \Delta q) &= G_c \int_{\Omega} \frac{1}{\ell} \phi \Delta \phi - \ell \mathcal{F}^{-1} \left[\vec{\xi} \cdot \vec{\xi} \widehat{\Delta \phi} \right] \Delta \phi d\Omega. \end{aligned} \quad (3.14)$$

In ΔF_2 of Eq.(3.14) the derivative of the history with respect to damage is included. This definition is fundamental to include the history in the monolithic scheme. Since the history is defined with the function maximum, as is stated in Eq.(3.5), its derivative is by definition a piecewise function.

$$\frac{\partial \mathcal{H}}{\partial \epsilon} = \begin{cases} 0 & \text{if } \psi_o^+ \leq \mathcal{H} \\ \frac{\partial \psi_o^+}{\partial \epsilon} & \text{if } \psi_o^+ > \mathcal{H}, \end{cases} \quad (3.15)$$

where $\partial \psi_o^+ / \partial \epsilon$ can be understood as the undamaged positive part of the stress tensor field $\boldsymbol{\sigma}^+$, mentioned in Eq.(2.29) and defined in the work of Miehe et al., 2010a.

It is observed that the introduction of E as unknown in the system in Eq.(3.14) together with the restriction in F_3 makes the system non-symmetric. Therefore, a Krylov method valid for this type of system has to be used. In our study, we rely on the Bi-conjugate gradient stabilized method for providing an optimal compromise in robustness and efficiency. If i is the iteration number in the Newton-Raphson scheme, the resulting equation to be solved at each iteration is

$$[\Delta F(q_{i-1}, \Delta q)] = -\{F(q_{i-1}, \tau)\}, \quad (3.16)$$

where the unknown is Δq and the set q_{i-1} of the last iteration is obtained from the successive accumulation of the set Δq , allowing to calculate the new NR set as $q_i = \Delta q + q_{i-1}$. In Eq.(3.16) the value of τ parameter is set as a function of time, so it doesn't depend on i . The convergence criterion is similar to Eq.(3.8b), where the maximum of the errors defined in each equation F for every unknown in q is calculated as in Eq.(3.17):

$$err = \max \left(\frac{\Delta E_i}{\|\epsilon_i\|}, \frac{\|\Delta \phi_i\|}{\|\phi_i\|}, \frac{G_c \Gamma_i - \tau}{\tau} \right). \quad (3.17)$$

In the resulting equations, the definitions of $\mathbb{C}$, $\mathbb{G}$ and ψ_o^+ are the ones given in the strain control method of section 3.1.1. Additionally, a successive over-relaxation parameter α can be defined as it's shown in algorithm 2, since it has been found that for highly developed cracks the use of $\alpha < 1$ improves convergence. The resulting algorithm is given in algorithm 2 where the complete sequence of resolution is described.

Algorithm 2 : Monolithic scheme with crack-length control

- 1: Initial data: $\tilde{\epsilon}^0 = 0, E^0 = 0, \phi^0 = 0, \mathcal{H}^0 = 0$
- 2: Control variable τ fixed
- 3: Time index $n = 0$
- 4: **while** $t^{n+1} < t_{final}$ **do**
- 5: Initiate NR scheme fields: $\epsilon_0 = \epsilon^n$; $\phi_0 = \phi^n$
- 6: Evaluate constitutive equation: find $\sigma_0 = \sigma(\epsilon_0, \phi_0)$ and $\mathbb{C}_0 = \frac{\partial \sigma}{\partial \epsilon} \big|_{\epsilon_0}$
- 7: Time index $i = 0$
- 8: **while** $Err \geq tol$ **do**
- 9: Solver FFT: find $\Delta q(\sigma_i, \mathbb{C}_i, \mathcal{H}^n)$ that fulfills Eq.(3.16)
- 10: Update variables^a : $\epsilon_{i+1} = \epsilon_i + \alpha \Delta \tilde{\epsilon} + \alpha f \Delta E$; $\phi_{i+1} = \phi_i + \alpha \Delta \phi$
- 11: Constitutive equation: find σ, ψ_o^+ and $\mathbb{C}$ such
- 12: $\sigma_{i+1} = \sigma(\epsilon_i, \phi_i)$; $\mathbb{C}_{i+1} = \frac{\partial \sigma_{i+1}}{\partial \epsilon_i}$; $\psi_{o\ i+1}^+ = \psi_o^+(\epsilon_i)$
- 13: Update History: $\mathcal{H}^{n+1} = \max(\psi_{o\ i+1}^+, \mathcal{H}^n)$
- 14: **end while**($i = i + 1$)
- 15: Update variables: $\epsilon^{n+1} = \epsilon_{i+1}$; $\phi^{n+1} = \phi_{i+1}$
- 16: **end while**($n = n + 1$)

^aParameter α stands for the relaxation parameter in case of successive over-relaxation is used.

3.1.3 FEM implementation of crack-length control

In order to validate the proposed FFT-PFF procedure, the implementation of a similar formulation for the crack-length control technique is implemented in a FEM code, in this case

FENICS (Alnæs et al., 2014; Baratta et al., 2023), in which the same functionals defined in section 3.1.2 are used. In this work, an implementation based on Lagrange multipliers is adopted to take into account the restrictions in boundary conditions, but sharing similitude with cases proposed in works previously mentioned (Bharali et al., 2022; Singh et al., 2016) in the definition of the control restriction.

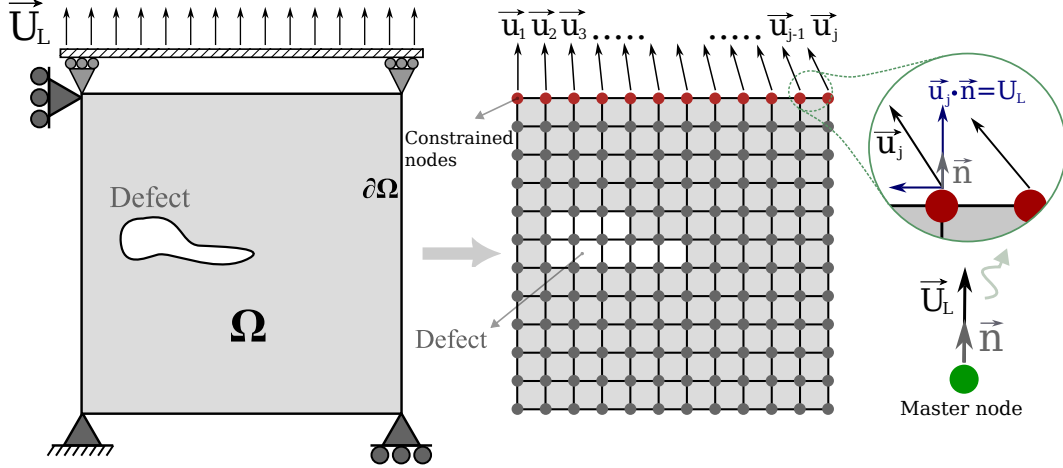


Figure 3.1: FEM discretization representation and the boundary conditions associated.

Consider the case on the left of Fig.3.1 of a two-dimensional domain Ω with boundary $\partial\Omega$ discretized in a regular mesh of triangular elements. To set Dirichlet displacements on any boundary in a similar way that in Fig.2.4 using a proportional factor as in Eq.(2.29c), the displacement of the nodes involved should be linked by multi-point constraints (MPC). Following the scheme developed in the work of Segurado and LLorca, 2004, a master node L with imposed displacement $\vec{U}_L = U_L \vec{n}$ is defined as shown in Fig.3.1, where $\vec{n}$ is a unit vector in the direction of the applied load. Then, the projection of the displacement in the direction of $\vec{n}$ of the nodes in the moving boundary (constrained nodes in Fig.3.1) is set equal to the displacement U_L of the master node, making vector $\vec{n}$ act similarly to the tensor $\mathbf{f}$ in the FFT scheme. This multi-point constraint is imposed by adding one Lagrange multiplier ϑ_j for each node j in Fig.3.1.

The crack-length restriction of Eq.(3.9c) in FEM is implemented in a slightly different manner with respect to FFT. The function $\tau(t)$ is also defined as the control parameter but, in order to improve convergence in the absence of an initial crack field, this value sets a weighted sum of the crack length and the master node displacement U_L ,

$$\tau(t) = w_a \int_{\Omega} \gamma_f(\phi) d\Omega + w_l U_L \quad (3.18)$$

being w_a and w_L the constant weights. Thus, the problem can be solved with crack-length control ($w_l = 0$), with standard displacement control ($w_a = 0$) or with a combination of both. With this restriction and non-zero weights, at the beginning of the simulation (when the field ϕ is very small) the value of $\tau(t)$ corresponds almost entirely to the displacement U_L . When a crack forms, the crack-length control part will become dominant, allowing decreasing values of U_L . It will be shown in the numerical results that this combined control leads to the

same results as the simple crack length prescription, allowing us to represent the snap-back behavior properly.

To impose the above described control, the FEM scheme developed by Segurado and LLorca, 2004 is adapted to a PFF formulation. The idea behind Eq.(3.18) is to introduce a crack-length control linked to a representative displacement, such as U_L , to emulate the FFT scheme in which the formulation is linked to the macroscopic strain. This leads the formulation to be naturally represented by a non-symmetric system. To represent the MPC condition described earlier and the Eq.(3.18), a Lagrange multipliers formulation is used. The new system is similar to the one obtained by Gerasimov and De Lorenzis, 2016 and is defined by a weak form of a non-linear residual equation F_{fem} , which has to be zero for a set of test functions $\Delta q = \{\Delta \vec{u}, \Delta \phi, \Delta U_L, \Delta \lambda, \Delta \vartheta_j\}$. Similar to the FFT scheme of the last section, this weak form of the residual can be split into the following three terms,

$$\begin{aligned} F_{1fem}(q, \Delta q) &= \int_{\Omega} \boldsymbol{\sigma}(\vec{u}) : \boldsymbol{\varepsilon}(\Delta \vec{u}) + g'(\phi) \psi_o^+(\vec{u}) \Delta \phi + G_c \gamma_f'(\phi) \Delta \phi d\Omega \\ F_{2fem}(q, \Delta q) &= - \sum_j [\vartheta_j (\Delta U_L - \Delta \vec{u}_j \cdot \vec{n}) + \Delta \vartheta_j (U_L - \vec{u}_j \cdot \vec{n})] - w_l \lambda \Delta U_L \\ F_{3fem}(q, \Delta q) &= - \Delta \lambda \left(w_a \int_{\Omega} \gamma_f(\phi) d\Omega + w_l U_L - \tau(t) \right). \end{aligned} \quad (3.19)$$

F_{1fem} contains the Mechanical/Helmholtz problem, F_{2fem} includes the MPC for displacement on the boundary and a last term that connects U_L with F_{3fem} , which corresponds to the control functional where Eq.(3.18) is imposed. The set Δq relates to the set of unknowns $q = \{\vec{u}, \phi, U_L, \lambda, \vartheta_j\}$, where $\vec{u}$, ϕ are the displacement and the damage fields respectively, and ϑ_j is the set of MPCs Lagrange multipliers. The test function $\Delta \lambda$ is used to introduce the control in the formulation (Eq.(3.18)) and the test function ΔU_L appears as a consequence of introducing U_L as an extra variable, similar to the FFT scheme where the control equation is a consequence of introducing the macroscopic strain as an unknown. In this work, the mixed function space of $\vec{u}$ and ϕ in Ω is discretized using triangular elements with bi-linear interpolation and full integration. For ϑ_j and λ , single valued elements are introduced.

A monolithic Newton scheme is used to solve the weak form of the residual $\mathcal{F}_{fem} = F_{1fem} + F_{2fem} + F_{3fem}$, finding the set of functions q that makes $\mathcal{F}_{fem} = 0$ for any suitable function Δq and for a prescribed value of τ . To solve this non-linear problem in the Newton-Raphson scheme, the $\mathcal{F}_{fem}$ needs to be linearized to a bilinear form. For this purpose, another set of trial functions Δq_t are defined similarly to the test functions Δq and used to obtain the Gateaux derivative of the functional of Eq.(3.19), $\Delta \mathcal{F}_{fem}$. For a Newton iteration i , being q_i the current value of the fields, the linear problem to be solved consists in finding the fields Δq_t which fulfill

$$[\Delta \mathcal{F}_{fem}(q_i, \Delta q, \Delta q_t)] = -\{\mathcal{F}_{fem}(q_i, \Delta q)\}, \quad (3.20)$$

for every possible test function Δq , leading to the next iteration defining $q_{i+1} = q_i + \Delta q_t$. As in the FFT implementation, the resulting linear system of Eq.(3.20) is non-symmetric and is solved using a direct LU solver from the UMFPACK library. Note that in the variational problem, additional Dirichlet boundary conditions can be imposed. The particular conditions depend on the problem and are specified in section 3.3.

3.2 Numerical estimations of fracture toughness

As mentioned previously, crack-length control methods have been used to obtain detailed responses of the fracture process in the numerical simulations. The results obtained using these schemes assume a specific loading path and provide its characteristic energetic evolution. The evolution of the energy is closely linked to the effective toughness of the material and, in the case of a homogeneous material where the toughness is an input, this evolution can be used to evaluate the accuracy of the PFF simulation, as will be discussed in section 3.3.3. In this section, relevant procedures to take into account in the obtention of this property are described.

3.2.1 Numerical correction to the critical energy release rate

In the seminal work of Bourdin et al., 2008, the energy functional in the presence of a PFF crack is analyzed, including its Γ -convergence to a real crack and the effect of the FEM projections in this convergence. One conclusion of this work is the existence of an effective numerical toughness G_{Ceffo} , defined as the input value G_c in the PFF mode multiplied by a factor A_{fem} that depends on the regularization parameter ℓ and the size of the FEM element h in the discretization as,

$$G_{Ceffo} = G_c \left(1 + \frac{h}{2\ell} \right) = G_c A_{fem}. \quad (3.21)$$

This relation is further validated in many works (Costa et al., 2023; Hossain et al., 2014; Tanné et al., 2018) for FEM-PFF discretizations. Nevertheless, this relation does not hold in the present FFT implementation, considering h as the voxel size. For this reason, a numerical study of the energy functional needs to be performed to check if the FFT implementation converges to the discontinuous result in the same way as in FEM. For this purpose, the difference between the discrete crack surface functional, $\int_{\Omega} \gamma_f d\Omega$ considering Eq.(2.23), depending on h and ℓ , and the actual value of the crack surface obtained analytically is examined.

From a similar procedure to the one presented by Alberti, 2000, we consider a 3D square plate of side L and thickness b , with an already existent PFF crack as in Fig.3.2c. For a one-dimensional trajectory in the domain, parameterized with the variable $x \in \mathbb{R}$ and crossing the crack perpendicularly as depicted in Fig.3.2c, the damage distribution on x can be defined as the optimal minimizer of the PFF problem considered by Miehe et al., 2010a, $\phi_m(x) = e^{-\frac{|x-a|}{\ell}}$, where a is the position of the center of the crack in a trajectory. The trajectory x is defined to span the periodic length of the domain L , which defines a one-dimensional slice of the crack with a surface defined as,

$$\Gamma_x(\phi) = \int_{\Omega} \gamma_x(\phi) d\Omega = Lb \int_0^L \frac{1}{2\ell} \phi^2(x) + \frac{\ell}{2} \left(\frac{d\phi}{dx}(x) \right)^2 dx. \quad (3.22)$$

Here, it can be shown that assuming $L \gg \ell$ the value for $\Gamma_x(\phi_m)$ is approximately equal to the cross-sectional area Lb (becoming identical for $L \rightarrow \infty$).

The projection of the optimal damage function in the trigonometrical polynomial space using a discretization of N points/frequencies is defined by means of a Fourier series approximation

with coefficients $\hat{\phi}_k$ as

$$\phi(x) \approx \sum_{k=-N/2}^{N/2} \frac{\hat{\phi}_k}{N} e^{\frac{i2\pi k}{L}x}, \quad (3.23)$$

where $k = \left[-\frac{N}{2}, \dots, 0, \dots, \frac{N}{2}\right]$ represents the discrete Fourier frequency set. The definition of Γ_x in Eq.(3.22) includes the derivative of damage, which definition in the trigonometrical function space is,

$$\frac{d\phi}{dx}(x) \approx \sum_{k=-N/2}^{N/2} \frac{\hat{\phi}_k}{N} \frac{i2\pi k}{L} e^{\frac{i2\pi k}{L}x}. \quad (3.24)$$

Replacing these definitions in Eq.(3.22) we obtain the following approximation by Fourier series of the crack integral,

$$\Gamma_x \approx \frac{Lb}{2\ell} \int_0^L \sum_{k=-\frac{N}{2}}^{\frac{N}{2}} \sum_{j=-\frac{N}{2}}^{\frac{N}{2}} \frac{\hat{\phi}_k \hat{\phi}_j}{N^2} \left[1 + \left(\frac{i2\pi k j \ell}{L} \right)^2 \right] e^{\frac{i2\pi}{L}(k+j)x} dx, \quad (3.25)$$

where k and j represent two independent and equivalent frequency sets. The exponential part of the functional is the only one depending on x , which implies that it is the only integrand in equation 3.25:

$$\Gamma_x \approx \frac{Lb}{2\ell} \sum_{k=-\frac{N}{2}}^{\frac{N}{2}} \sum_{j=-\frac{N}{2}}^{\frac{N}{2}} \frac{\hat{\phi}_k \hat{\phi}_j}{N^2} \left[1 + \left(\frac{i2\pi k j \ell}{L} \right)^2 \right] \int_0^L e^{\frac{i2\pi}{L}(k+j)x} dx, \quad (3.26)$$

In order to express this integral correctly, all the combinations that fulfill $k + j = 0$ are separated from the sum and expressed as 1. Thanks to the orthogonality of trigonometric polynomials, the value of the integral for every discrete frequency fulfilling $k + j \neq 0$ is zero and the expression of Eq.(3.26) results in:

$$\Gamma_x \approx \frac{Lb}{2\ell} \sum_{k=-\frac{N}{2}}^{\frac{N}{2}} \frac{\hat{\phi}_k \hat{\phi}_{-k}}{N^2} \left[1 + \left(\frac{i2\pi k j \ell}{L} \right)^2 \right]. \quad (3.27)$$

This expression allows us to calculate the integral of Eq.(3.22) for any Fourier projection of $\phi(x)$, where the definition of the discretization through N defines the voxel size h_v . It's clear from Eq.(3.27) that even replacing the damage distribution for the optimal ϕ , the value of the crack surface approximated with this particular projection is not the analytical value Lb . Similarly to Eq.(3.21), a toughness amplification factor for FFT can be defined as the ratio $A_{fft} = \Gamma_x / Lb$ for a given h_v and ℓ .

$$A_{fft} = \frac{1}{2\ell} \sum_{k=-\frac{N}{2}}^{\frac{N}{2}} \frac{\hat{\phi}_k \hat{\phi}_{-k}}{N^2} \left[1 + \left(\frac{i2\pi k j \ell}{L} \right)^2 \right]. \quad (3.28)$$

Considering the Fourier discretization of the optimal distribution ϕ_m and its derivative, examples considering $N = 65$ and $N = 257$ are depicted in Fig.3.2a and Fig.3.2b. It can be

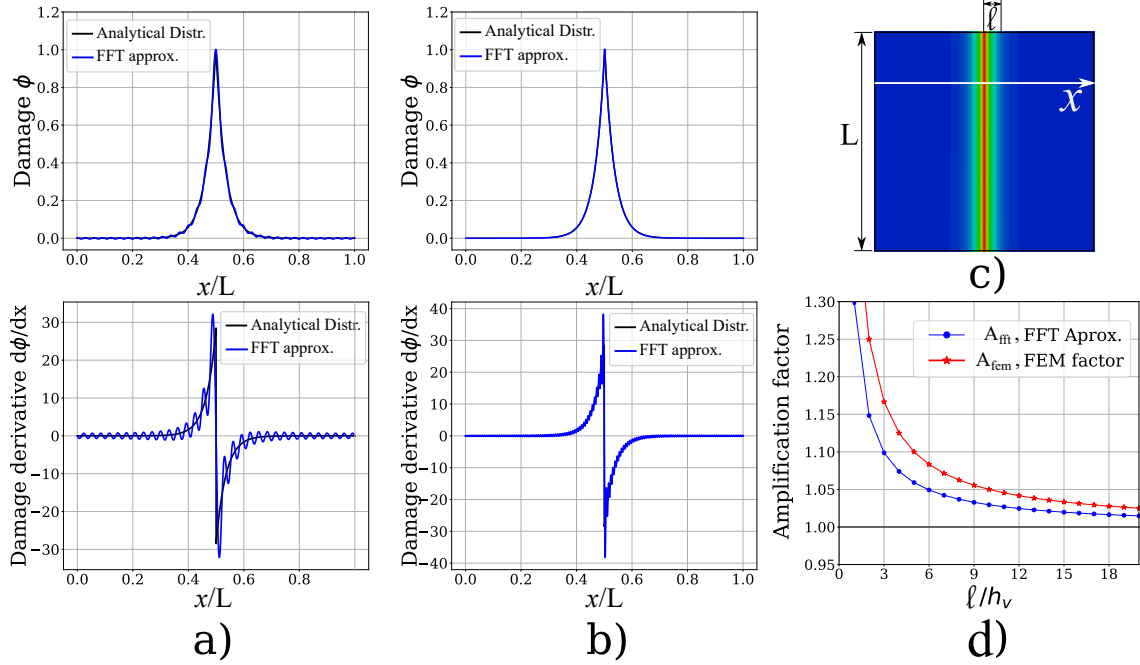


Figure 3.2: (a) FFT approximation of damage distributions for a number of $N = 65$ points, (b) FFT approximation of damage distributions for $N = 257$, (c) Domain and crack path of the example and (d) FFT and FEM deviations from imposed toughness.

seen how the Fourier approximation converges to the analytic distribution of ϕ_m . Also, the evolution of the factor A_{fft} for $N = 257$ and a varying ℓ is shown in Fig.3.2d and compared with the FEM factor of Eq.(3.21). It can be seen that the behavior is similar for both formulations, where the amplification factor approximates to 1 when the ratio ℓ/h_v grows. It can also be seen that this occurs faster in FFT than in FEM. This can be due to the fact that in FFT the derivative of damage has a better approximation in the proximity of the center of the crack, despite the oscillatory behavior observed. In this work, this numerical value of the amplification factor is used to estimate G_{Ceffo} .

3.2.2 Energy release rate measures with J -integral

The definition of the numerical effective toughness in the previous section has consequences in the representation of fracture. For example, it may alter the mechanical stress/strain response since the perceived toughness is higher. In this thesis, a crack-length control method has been proposed, representing a loading path in which the crack growth is constant. In this context, it's interesting to verify the evolution of the energy release rate compared to the effective one of section 3.2.1. The J -integral can be used to calculate toughness evolution during a stable crack growth process.

Many works have developed numerical versions of the J -integral (Costa et al., 2023; Y. Li and Zhou, 2013; Sicsic and Marigo, 2013), all based on the original proposal of Rice, 1968, also depicted in Eq.(2.14). In the work by Hossain et al., 2014, toughness measures have been made with this technique in PFF models, using the definition of the Energy-Momentum

Eshelby tensor Λ and following the definition,

$$J = \vec{t}_j \cdot \int_{l_j} \Lambda \cdot \vec{n} \, dl \quad ; \text{ where } \Lambda = \psi \mathbf{I} - \nabla \vec{u}^T \boldsymbol{\sigma}, \quad (3.29)$$

where $\mathbf{I}$ is the identity tensor, $\vec{t}_j$ is a vector representing the crack propagation direction (green line in Fig.3.3), $\vec{n}$ is a vector normal to the integral trajectory l_j (Fig.3.3) and ψ is the elastic energy density in Eq.(2.16) (note that Hossain's work does not use an energy decomposition in the PFF model). In Hossain et al., 2014 it is shown that the numerical evaluation of this measure in a PFF-FE framework provides an accurate value of the fracture toughness. Later, more specific expressions have been developed specifically for the PFF model, such as the one proposed in the work of Ballarini and Royer-Carfagni, 2016, also used in the study by Costa et al., 2023. This version of J relies on a definition of the Energy-Momentum tensor defined with the total power density π as,

$$J = \vec{t}_j \cdot \int_{l_j} \left(\pi \mathbf{I} - \nabla \vec{u}^T \boldsymbol{\sigma} - G_c \ell \nabla \phi \otimes \nabla \phi \right) \cdot \vec{n} \, dl \quad ; \quad \pi = \int_t \boldsymbol{\sigma} : \dot{\boldsymbol{\epsilon}} dt, \quad (3.30)$$

where the term $G_c \ell \nabla \phi \otimes \nabla \phi$ is a correction factor proposed for PFF models in order to account for smeared cracks in the Energy-Momentum tensor. This term can be neglected if the ℓ value is small with respect to the domain considered and the path l_j intersects the crack at 90° at a far location from the crack tip (Sicsic and Marigo, 2013) which is ensured by the configurations of this work depicted in Fig.3.3.

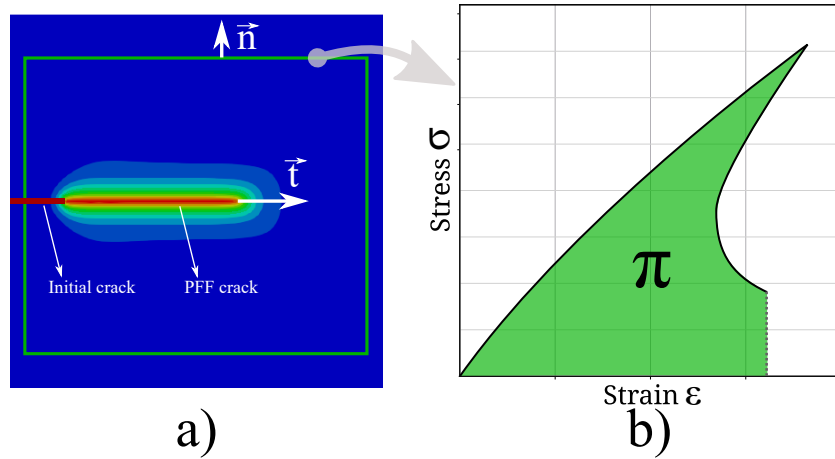


Figure 3.3: J -integral schematization for the measurements in this work. (a) Approximate position of the integral path respect the initial crack. (b) Local energy history π in a local point used in Eq.(3.33).

The extension of either of the previous expressions to FFT-based solvers implies a proper definition of a displacement field $\vec{u}$, which is not computed in the Fourier-Galerkin approach followed here. Following the formulation in the work of Lucarini and Segurado, 2019a, the gradient of the displacement field $\nabla \vec{u}$ can be inferred in the Fourier space using the frequencies in that space and electing certain components of the strain, since all of them fulfill compatibility between them. Since an infinite number of displacement configurations

are compatible with a given strain field, this result is complete, including the effect of field rotations. Nevertheless, the expression for the gradient without this effect, and for a frequency vector with non-zero components, is,

$$\widehat{\nabla \vec{u}} = \begin{pmatrix} \hat{\varepsilon}_{11} & \frac{\xi_2}{\xi_1} \hat{\varepsilon}_{11} & \frac{\xi_2}{\xi_1} \hat{\varepsilon}_{11} \\ \frac{\xi_2}{\xi_1} \hat{\varepsilon}_{22} & \hat{\varepsilon}_{22} & \frac{\xi_2}{\xi_1} \hat{\varepsilon}_{22} \\ \frac{\xi_2}{\xi_1} \hat{\varepsilon}_{33} & \frac{\xi_2}{\xi_1} \hat{\varepsilon}_{33} & \hat{\varepsilon}_{33} \end{pmatrix} ; \text{ if } \xi_1, \xi_2, \xi_3 \neq 0. \quad (3.31)$$

For a null component of the frequency vector, the formulation changes depending on the component, as,

$$\begin{aligned} \widehat{\nabla \vec{u}} &= \begin{pmatrix} \hat{\varepsilon}_{11} & 2\hat{\varepsilon}_{12} & 2\hat{\varepsilon}_{13} \\ 0 & \hat{\varepsilon}_{22} & \frac{\xi_2}{\xi_1} \hat{\varepsilon}_{22} \\ 0 & \frac{\xi_2}{\xi_1} \hat{\varepsilon}_{33} & \hat{\varepsilon}_{33} \end{pmatrix} \text{ if } \xi_1 = 0 ; \quad \widehat{\nabla \vec{u}} = \begin{pmatrix} \hat{\varepsilon}_{11} & 0 & \frac{\xi_3}{\xi_1} \hat{\varepsilon}_{11} \\ 2\hat{\varepsilon}_{12} & \hat{\varepsilon}_{22} & 2\hat{\varepsilon}_{23} \\ \frac{\xi_3}{\xi_1} \hat{\varepsilon}_{33} & 0 & \hat{\varepsilon}_{33} \end{pmatrix} \text{ if } \xi_2 = 0; \\ \widehat{\nabla \vec{u}} &= \begin{pmatrix} \hat{\varepsilon}_{11} & \frac{\xi_2}{\xi_1} \hat{\varepsilon}_{11} & 0 \\ \frac{\xi_1}{\xi_2} \hat{\varepsilon}_{22} & \hat{\varepsilon}_{22} & 0 \\ 2\hat{\varepsilon}_{13} & 2\hat{\varepsilon}_{23} & \hat{\varepsilon}_{33} \end{pmatrix} \text{ if } \xi_3 = 0. \end{aligned} \quad (3.32)$$

Considering Eq.(3.31) and Eq.(3.32), is possible to compute the transpose of the gradient in real space. Therefore, neglecting the term $G_c \ell \nabla \phi \otimes \nabla \phi$, the formulation of the J -integral in this work is

$$J = \vec{t} \cdot \int_{l_j} (\pi \mathbf{I} - \nabla \vec{u}^T \boldsymbol{\sigma}) \cdot \vec{n} \, dl, \quad (3.33)$$

where the local energy expenditure π has to be obtained in every point in l_j and is depicted in Fig.3.3b, where the mechanical in any point in the framework of the proposed crack-controlled model could have the snap-back behavior discussed in Fig.1.2 and depicted in Fig.3.3. With such information, the value of π can be estimated numerically for all points in l_j using, for example, Simpson's rule.

In the works of Costa et al., 2023 and in the one by Hossain et al., 2014, is reported that J -integral measurements should converge to the Bourdin et al., 2008 approximation for a sufficiently precise FEM discretization. This will be tested in section 3.3.2 for the FFT scheme cases presented in this work.

3.3 Validation and comparison with FEM

The control schemes developed are used here to perform the set of simulations described from section 3.3.1 onward. The former will include a comparison of FFT and FEM simulations, in order to validate the equivalence of the control method proposed for both frameworks and to analyze the differences between the two types of solvers. The next subsection will analyze the consequences of the crack-length control developed in terms of Griffith postulates, as well as the equivalence of the predicted crack paths obtained using crack control or a standard staggered solver.

For this purpose, macroscopic tensile cases are mainly used, and the corresponding control variables are specified in Eq.(3.34). Three linear elastic materials are used in simulations,

named as matrix, flexible material, and rigid inclusion, and their properties are given in table 3.1. In addition, a material representing the empty space is used for the cases including voids.

$$\mathbf{f} = \underbrace{\begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix}}_{\text{for Dissipative control}} ; \quad \mathbf{E}_M = \underbrace{\begin{pmatrix} 0 & 0 & 0 \\ 0 & \tau(t) & 0 \\ 0 & 0 & 0 \end{pmatrix}}_{\text{for Strain control.}} \quad (3.34)$$

This condition can also be replicated for a case with imposed macroscopic shear strain, as

$$\mathbf{f} = \underbrace{\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}}_{\text{for Dissipative control}} ; \quad \mathbf{E}_M = \underbrace{\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & \tau(t) \\ 0 & \tau(t) & 0 \end{pmatrix}}_{\text{for Strain control.}} \quad (3.35)$$

	Matrix	Void	Flexible material	Rigid Inclusion
$E_{Young}[GPa]$	20.8	1e-8	10.4	104
ν	0.3	0.4	0.3	0.3
$G_c[J/m^2]$	2700	-	-	-

Table 3.1: Mechanical and PFF properties of materials.

Regarding the PFF properties, all cases were simulated with a fracture resistance parameter of $G_c = 2700 J/m^2$. The characteristic length ℓ was selected depending on the discretization of each case in order to have a sufficient representation of ϕ fields around the cracks. Its value is set as two times the distance between FFT voxels and it's used in both FEM and FFT simulations. This election is made considering a geometrical similarity between a voxel and an element, since this value is reported by Miehe et al., 2010a for PFF-FEM problems as the minimum required for Γ functional match the crack length. In FEM simulations, the weights in Eq.(3.18) are set as $w_l = w_a = 1$, and in FFT simulations, no relaxation parameter is used ($\alpha = 1$ in Algorithm 2).

3.3.1 FFT-FEM comparison

FEM and FFT simulations of the same problem using crack-length control are performed using the boundary conditions represented in Fig.3.4. In the case of FFT, 3D models with a single voxel in the Z-direction are used, while a two-dimensional plane strain condition is used in 2D FEM models.

The FEM model in Fig.3.4b presents two symmetry boundary conditions applied in axis Y and X, on the bottom and left edges, respectively. A free strain boundary condition is used for the right edge, and a displacement restriction for all points in the Z direction is applied to represent a plain strain state. The upper boundary, with nodes whose displacement is assigned to be the same as the master node U_L described in section 3.1.3, is remarked in

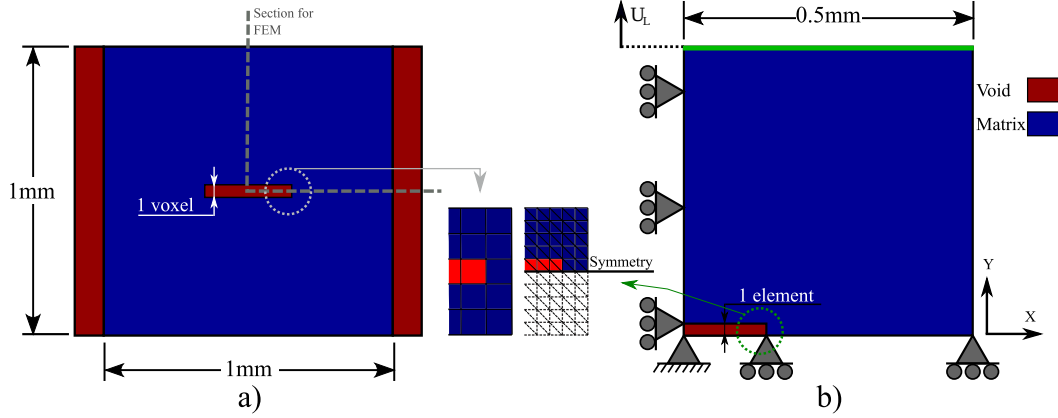


Figure 3.4: FEM and FFT geometry models.

green in Fig.3.4b. The initial crack is emulated with the region indicated in the same figure with the properties of the void material of table 3.1.

In the FFT model of Fig.3.4a, no symmetry is applied and periodic boundary conditions are used in the full simulation domain. To represent the free boundary condition in FFT, two bands of void material are placed in the left and right edges of the geometry. Considering the load direction $\mathbf{f}$ selected, this representation of the free boundary resembles the plane strain conditions used in the 2D FEM simulations.

The thickness of the initial crack in the FFT model is one voxel, so to fit the symmetry condition in FEM with the same ℓ , the number of elements is the same number of voxels but in half of the space (See comparison in Fig.3.4). Cases with 39x39 voxels, 77x77, and 155x155 voxels and their equivalent cases in FEM are solved to demonstrate the equivalence of the control technique in both numerical frameworks. The mechanical response for all cases is described in Fig.3.5 and the damage and stress fields are depicted in Fig.3.6 for the case of 155x155 voxels simulation and its equivalent in FEM for the step ② of Fig.3.5.

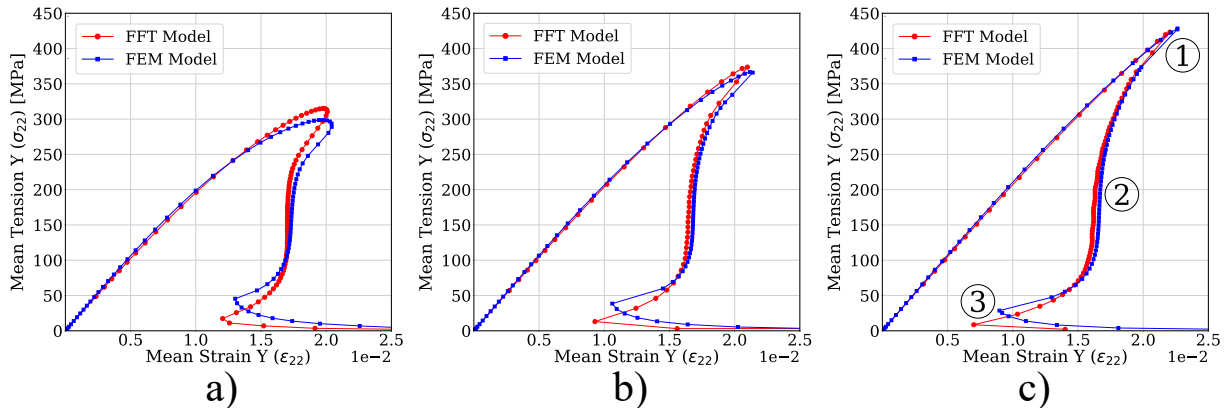


Figure 3.5: FEM/FFT comparison curves for 3 different discretizations, on the left 39x39 voxels, center 77x77 and on the right 155x155

As described in Carpinteri and Accornero, 2018, the fracture process follows three steps, that are stated with numbers in Fig.3.5c (case of 155x155 voxels). In step ① crack growth

starts and the snap-back response is observed after the high stress concentration observed in Fig.3.6. During step ②, this stress concentration is kept at the crack tip as is also observed in Fig.3.6a. Step ③ represents the end of the fracture process.

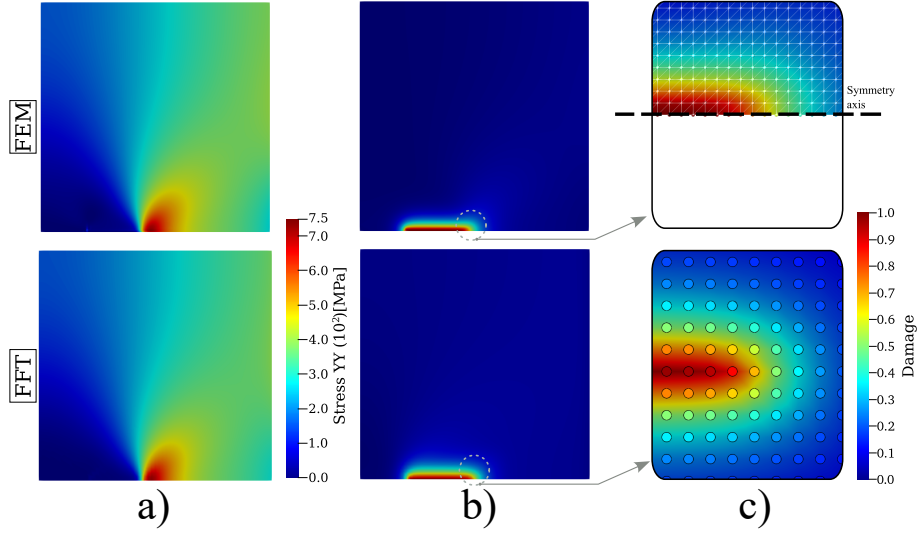


Figure 3.6: Damage/stress fields for 155x155 voxels case in the second step of Fig.3.5 .

The difference between FEM and FFT results when the number of elements in the FEM model is chosen to be equivalent to the number of FFT voxels can be due to the dissimilar approximations of both techniques, for example in the representation of the fields and integration. Nevertheless, it can be observed in Fig.3.5 that convergence with discretization is reached for both FEM and FFT for relatively coarse meshes. In the case with the finest discretization, 155x155 voxels, step ① and ② are essentially superposed, and only very small differences can be observed in the response for the step ③. This small deviation in the final stage, when the crack is almost fully developed, can be due to the differences in the particularities of the control technique in both numerical approaches.

3.3.2 Fracture stability study: Strain and crack control comparison

As shown in the previous section, a complete and stable representation of the cases that would have an unstable fracture in deformation control has been obtained with crack-length control. To further analyze the conditions during propagation, simulations of a Griffith panel with initial crack length a and different width B are performed (Fig.3.7d). In Fig.3.7a, the stress-strain response for three a/B ratios on simulations of 257x257 voxels is shown. It can be seen that all curves follow the same stress-strain path once the crack starts, so this path corresponds to the limit in which the crack propagates, independently of the original crack length. In the classic Griffith fracture theory, these states correspond to the limit in which the elastic energy G release rate reaches the critical energy release rate of the material G_c (Eq.(2.33)).

To validate the fulfillment of Griffith condition during propagation, two graphs are represented in Fig.3.7b and Fig.3.7c. The first one shows the available potential energy of the material Ψ^+

in continuous lines with points, and the energy dissipation due to crack D using discontinuous lines, both with respect to the crack length. It can be seen that, for the same crack length, cases with an initial crack have the same available potential energy as cases in which the crack is already growing. Also, it can be observed the similarity of slopes between dissipation and energy curves, which implies the rates are the same, as dictated by the minimization of the total energy. Nevertheless, to obtain a more accurate measure of G , the J-integral of section 3.2.2 is computed. The trajectory followed to compute the line integral corresponds with the outer contour of the matrix material, as depicted in Fig.3.7d, and the measure of the energy release rate is shown in Fig.3.7c for all cases.

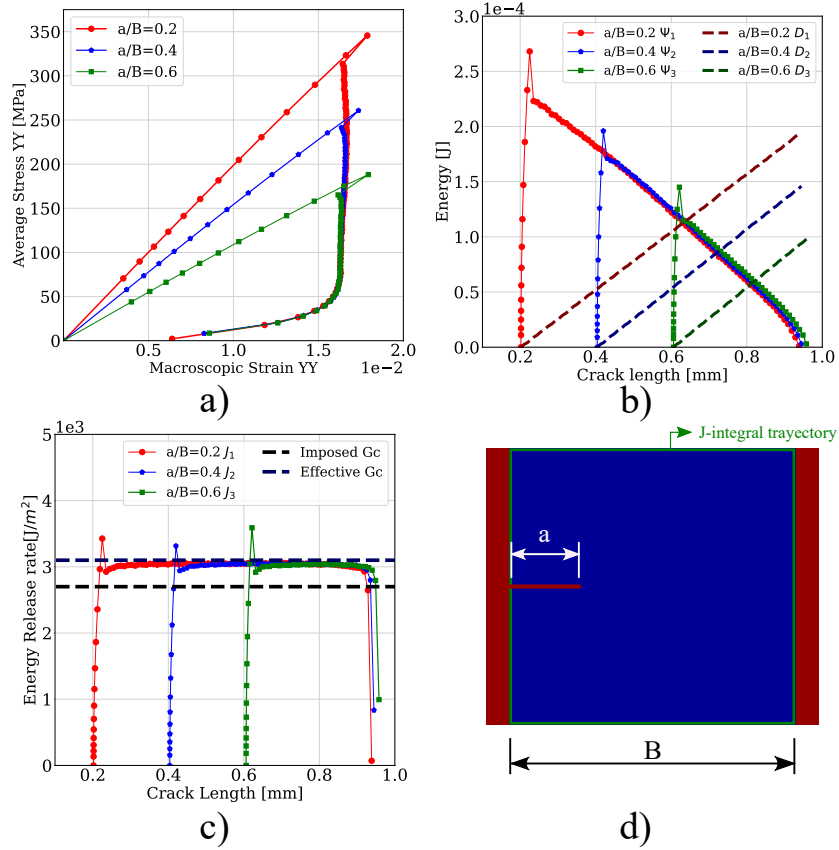


Figure 3.7: FFT study on the stability of the crack growth in a Griffith panel. a) stress-strain curves, b) Elastic energy degradation as function of crack length, c) J-integral measurements, d) Geometry of the Griffith panel

As explained in section 3.2.1, it can be observed that the value of the fracture energy obtained is slightly higher than the critical energy release rate used as input data, G_c . The numerical effective toughness G_{Ceffo} has been quantified for FFT in section 3.2.1 showing an increase with respect to G_c of approximately 14.8%. The input energy release rate limit and the corresponding effective limit are marked with dashed lines in Fig.3.7c. It is observed that the value of G obtained with J-integral is very accurate with G_{Ceffo} , showing also a constant behavior which is consistent with the idea that this simulation condition represents a stable fracture process. This value of G is only slightly different from G_{Ceffo} at the beginning of the process and at the end. The loss of energy release rate shown at the end of the process

is an artifact in the measure of J , because at that stage the crack reaches the integral path. The excess of energy and G that is observed in Fig.3.7b and Fig.3.7c at the beginning of the crack propagation is similar to what has been reported by Hossain et al., 2014 and by Singh et al., 2016. The reason for this peak may be related to the energy needed to nucleate a phase field crack from a notch or mesh discontinuity. This feature can be released using crack tip enrichment techniques (Singh et al., 2016; Zambrano et al., 2023) in the definition of the initial crack geometry, but since in the homogeneous simulations observed this effect is only relevant in the first point of propagation, standard representations of initial cracks are kept for clarity in this study. Despite the foregoing, this peak in the J integral has a negligible contribution to the dissipated energy (area under the curve in Fig.3.7a) for the geometries tested.

This study shows that under this control method the fracture is an energetically stable process, which fracture resistance energy can be quantified. Despite results showing great agreement with the corrected fracture resistance G_{Ceffo} for cases with 257×257 voxels, this quantification also depends on the ratio between ℓ and the voxel size h_v . This dependence can be tested using the same geometry depicted in Fig.3.7d for different discretizations, maintaining the width B constant to modify h_v , but modifying the value of ℓ to match the ℓ/h_v values depicted in Fig.3.8b. Since measures of J in Fig.3.7c show no dependency on the initial crack length, all cases here are tested preserving the ratio $B/a = 0.2$.

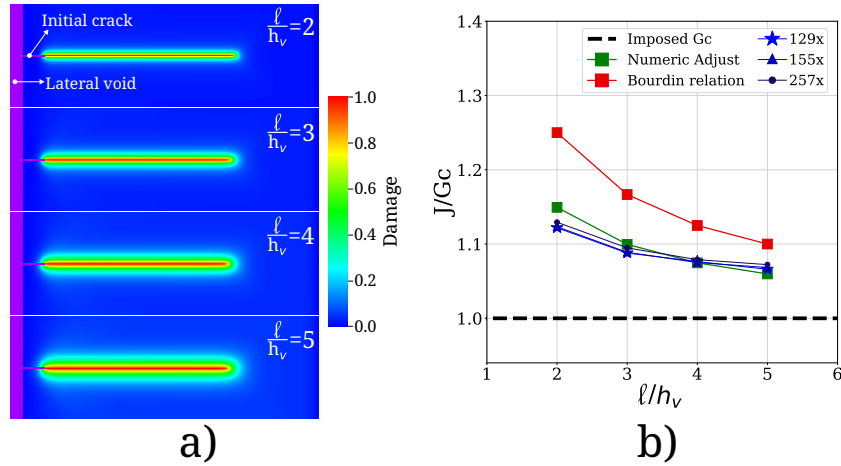


Figure 3.8: Comparison between the approximation of the FFT amplification factor with J-integral measures of G_{Ceffo} . a) Damage fields obtained. b) Simulation responses with 129×129 , 155×155 and 257×257 voxels.

All J-integral measures show similar behavior to that in Fig.3.7c, showing an excess of energy rate at the beginning and maintaining a constant value from there. This constant value has been extracted from every case to compose the curves in Fig.3.8b, which are compared to the numerical estimations of Bourdin's increase factor for FEM and FFT described in section 3.2.1 and depicted in Fig.3.2d. It can be seen a good agreement with the numerical estimation for FFT, but this comparison shows a certain deviation at $\ell/h_v = 5$, that can be attributed to PFF history variable $\mathcal{H}$ that was not considered in the analysis of section 3.2.1, and for high values in ℓ/h_v could lead to damage distributions that affect this estimation. The fact that

toughness estimations get close to FFT G_{Ceffo} approximation and similar values are obtained for different discretizations and ℓ values proves that Bourdin's postulate is also valid in FFT discretizations. Also, Fig.3.8a shows the crack representation of a group of cases with the same discretization (257x257) but different ℓ/h_v (which implies variations in ℓ), as a reference to the distributions of the cases represented in the estimations in Fig.3.8b.

3.3.3 Comparison of strain control and crack-length control

Since the stress-strain path for the crack-length controlled simulations has proven to be stable, a similar path is expected to be obtained in strain controlled cases where propagation is always stable. This comparison further validates the crack control technique by observing how a strain stable fracture response is represented identically by both models.

The case studied corresponds to the same plate in Fig.3.9d, with the conditions described in the beginning of section 3.3 and solved with crack-length control and strain control models. Since this case has demonstrated to be unstable for strain control in section 3.3.1, the ratio A/B of Fig.3.9d is modified to fit cases of $A/B = 1$, $A/B = 0.5$ and $A/B = 0.3$ with 1x243x243, 1x121x243 and 1x81x243 voxels correspondingly.

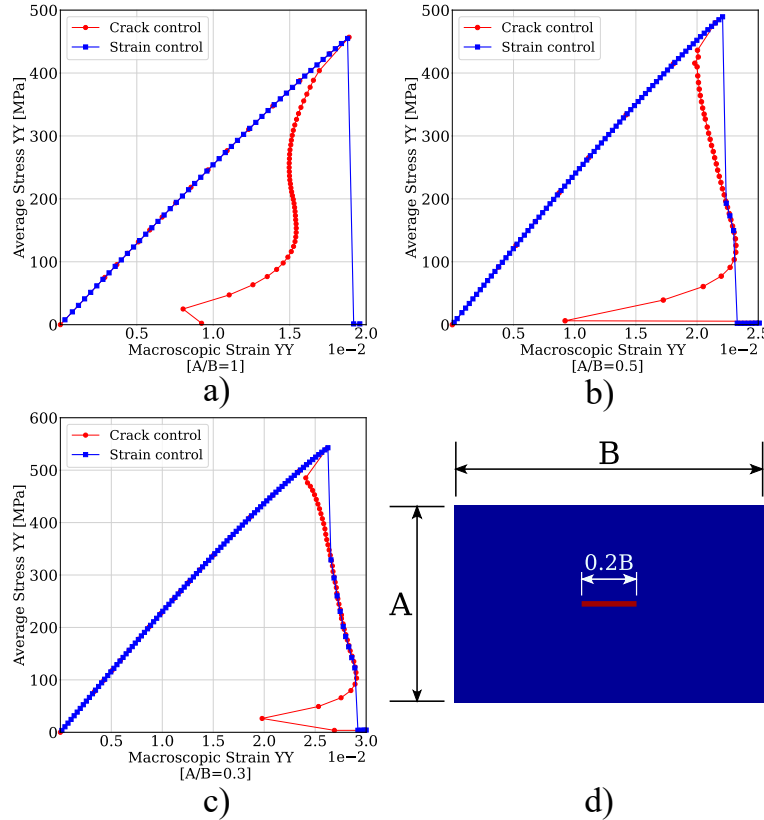


Figure 3.9: Comparison of Strain/crack-length control for different geometries of Griffith panel, using curves of average strain/stress in direction Y for: a) $A/B = 1$ case, b) $A/B = 0.5$ case and $A/B = 0.3$ case, with dimensions reference in d).

It can be shown using simple linear elastic fracture mechanics that the reduction of the

Griffith panel height A reduces the release energy for a differential crack extension leading eventually to a stable regime. Also, since flat displacement on the upper surfaces is equivalent to periodicity for this geometry, this simulation is equivalent to an infinite array of cracks aligned vertically. In this case, reducing the A/B ratio increases the density of periodic fissures with respect to the total volume, allowing redistributing the available elastic energy of the volume in more fracture processes, causing the rate of dissipation in each fissure to decrease and making each one more stable. This has been demonstrated by Rooke and Cartwright, 1976, where it is explained that the influence of an arrangement of parallel cracks in the perpendicular direction to the crack leads to a decrease of the stress intensity factor in each crack, which implies a generalized decrease of the evolution of the energy release rate. The results obtained are shown in Fig.3.9.

It is observed that both types of control lead to the same stress-strain curves during the stable propagation stages. Moreover, the curves obtained using crack control can be used to determine the range of crack lengths in which growth is stable for a given geometry. Another interesting result is that, in this case, if the staggered approach is used with a very restrictive tolerance, it results in a crack shape equal to the one obtained under crack-length control, validating the *metastable* propagation of the crack during the staggered iterations.

The growth under mixed mode, as noted in the beginning of section 3.3, is also analyzed by simulating propagation under a macroscopic shear stress. Pure shear cases have boundary conditions with difficult representation in FFT, so the conditions in Eq.(3.35) are used. The simulation is performed using a full periodic domain with a crack in the middle, and in this case, periodicity is fulfilled in the two directions, as depicted in Fig.3.10. The geometry of Fig.3.9d is used with $A/B = 1$, an initial crack length of $0.2B$, and a discretization of 243×243 voxels is used.

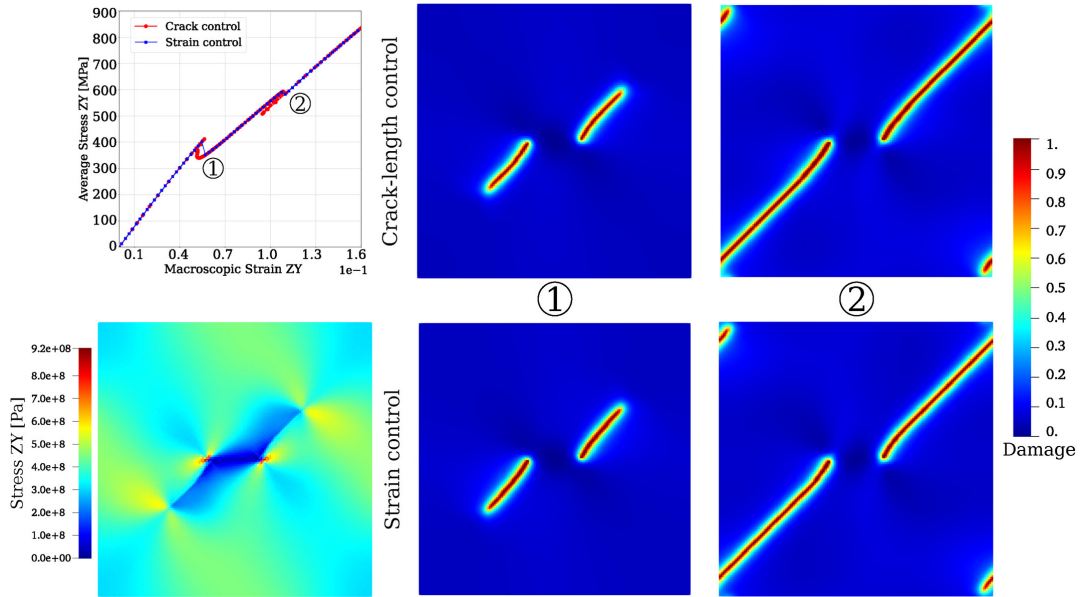


Figure 3.10: Comparison between Crack-length and strain control models in 2D Shear simulation.

The similarity between both schemes is similar to those in Fig.3.9 for the tensile cases. It

must be noted that snap-back in this configuration is much smaller, demonstrating stable propagation for the majority of the simulation time.

3.4 Numerical examples

In this section, simulations of crack propagation in heterogeneous microstructures are presented to show the potential of the technique developed. Two types of materials will be studied: composites and a porous material.

3.4.1 Fracture of composite materials

The following simulations correspond to the fracture of a RVE of a laminate and a fiber reinforced material under a macroscopic uniaxial tensile case (see Eq.(3.34)). Both cases have been discretized in a grid of 121x243 voxels with the same elastic matrix (see table 3.1). In all cases, an initial crack modeling similar to that of previous sections is performed, and no over-relaxation is used in Newton-Raphson. The geometries employed, modeled as 2D plates, are indeed 2D sections of 3D microstructures under plane strain, whose representation is adequate due to RVE periodicity.

The first case consists of a laminate with regularly distributed flexible sheets (see table 3.1) of equal thickness and perpendicular to the initial crack that represent an area fraction of 27.1%. The domain is shown in Fig.3.11a and is loaded by a macroscopic strain in the Y direction, parallel to the laminate. All materials are perfectly bonded and no heterogeneous crack resistance is considered in the domain, so the fracture propagation is only driven by the heterogeneity of strain microfields due to the stiffness difference between the phases. A unique fracture field is chosen for the whole domain and no additional condition on the fracture field is imposed in the internal interfaces. This means that cracks are allowed, if energetically favored, to penetrate either phase without any restrictions. Results on this case are shown in Fig.3.11.

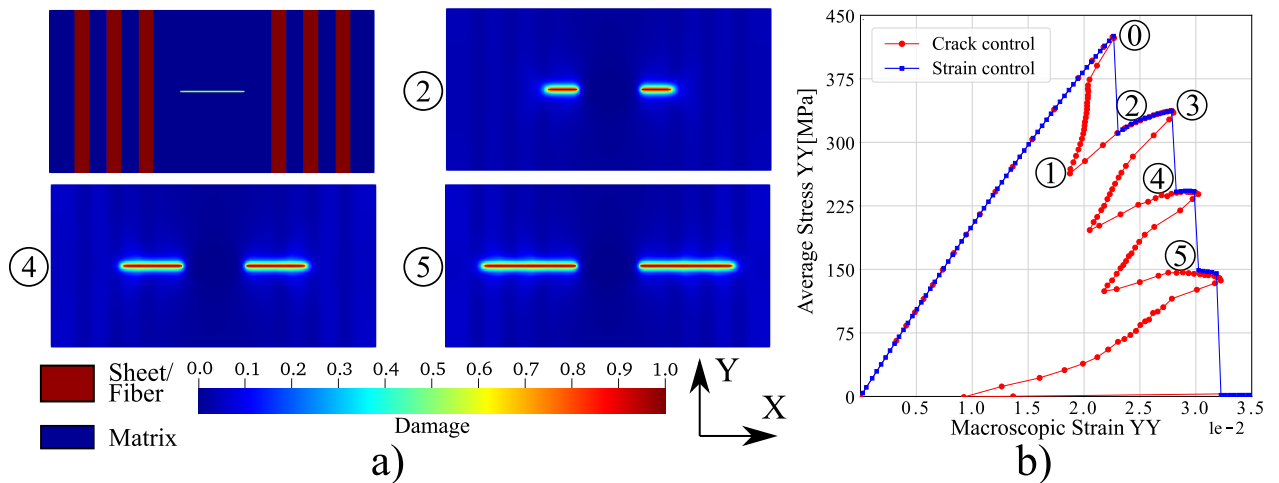


Figure 3.11: Fracture of a laminate material, (a) crack evolution and (b) stress-strain curve.

The curve of Fig.3.11b shows the stress-strain behavior obtained for the layered composite under the two types of controls presented. The curve obtained using crack control presents a saw-tooth shape in which each snap back corresponds with the fracture of a different layer of the geometry. The curve obtained under strain control presents several jumps, which correspond to the regions of unstable growth. Different stages have been marked with numbers that correspond with the damage fields in Fig.3.11a. By the parallel disposition of the layers, the matrix tends to accumulate more potential energy than the flexible sheets due to the difference in stiffness.

When the crack starts at ① in Fig.3.11b, the matrix is the first to be broken. The local strain caused by the crack allows the near sheet to accumulate potential energy, but this accumulation is lower than the loss of energy in the matrix, so a similar fracture process to the example of Fig.3.9a occurs between points ① and ② of Fig.3.11b, where the macroscopic strain and stress decrease. Then, the fissure enters the first sheet where the crack can grow stably because the next section of the matrix accumulates more energy than is lost in the sheet. This allows the macroscopic strain and stress between points ② and ③ of Fig.3.11b to increase. The stable crack growth allows capturing the process in the strain-controlled simulation between points ② and ③ of Fig.3.11b, validating the results obtained during the staggered iterations. Similar processes occur for the other two ramifications, and the damage state of points ②, ④, and ⑤ of Fig.3.11b is shown in Fig.3.11a, where it can be seen that the crack is in the middle of each flexible sheet.

The second case tested in this section corresponds to the fracture in the transverse section of a long fiber reinforced composite, with randomly distributed rigid fibers (see table 3.1) of circular cross section, representing an area fraction of 38.5%. Similar to laminates, the domain is loaded in the Y direction, a homogeneous crack resistance field is considered, and perfectly bonded interfaces are assumed with no additional condition on the damage field therein (penetration is allowed).

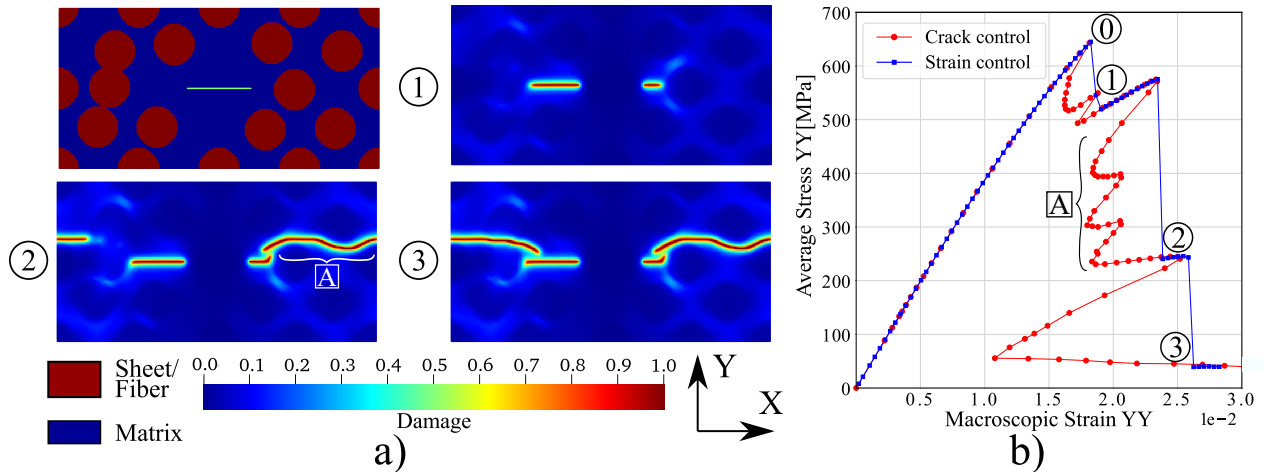


Figure 3.12: Fracture of the cross section of a long fiber reinforced composite (c) crack evolution and (d) stress-strain curve.

The mechanical response observed at Fig.3.12b is similar to that of laminates, but due to

the random distribution of the fibers, the ramifications are less symmetric. After point ① the fracture only occurs at the matrix, so the behavior is similar to that in Fig.3.9a, but one of the crack tips propagates sooner than the other, leading to asymmetric crack growth characterized by the two snap backs before point ②, where both cracks get arrested by the fibers. This causes that in the section following this point, stable propagation occurs while the crack begins to deflect. This deviation effect occurs because the fibers are several times stiffer than the matrix and they are not able to get enough strain to accumulate the necessary energy to create cracks. This forces the crack to develop mostly in the areas of the matrix close to a fiber, being the crack unable to penetrate them.

It can be seen in Fig.3.12a how the crack follows a path that avoids the position of the fibers, which occurs mostly in an unstable crack propagation between points ① and ② of Fig.3.12b. The crack-length controlled simulation is able to capture the behavior between these two points, which is marked as [A] in Fig.3.12b and in Fig.3.12a at point ②. Here, it is shown that crack deflection can also generate a saw-tooth shape behavior in the response, similar to that originated by crack penetration in multi-phase domains such as the case of the laminate in Fig.3.11. Then, as it is shown in Fig.3.12a for the point ②, the only resisting material is a joint group of fibers. Only at this point, the crack enters the fiber to end the fracture process between points ② and ③ of Fig.3.12b. The behavior in the response at this segment is larger and sharper snapback than the others, which is due to the penetration of the crack into a stiffer phase that makes the snapback similar to that observed in the laminates of Fig.3.11b.

Similar effects between the crack-length and strain controlled simulations are observed in both simulations. It can also be remarked that crack paths and stress-strain curves coincide with the ones obtained in a staggered approach if a very restrictive tolerance is used. In this case, several hundred iterations are needed to resolve the unstable stages. On the contrary, if the staggered solver is used with a less restrictive tolerance to improve convergence, differences are found both in the stress-strain curve and crack shapes after instability.

3.4.2 3D cases: Circumferential fissure and porous material

In order to show the validity and efficiency of the method proposed, full three-dimensional microstructures are simulated. Two cases are studied. The first one corresponds to a homogeneous elastic matrix with a rectangular crack in the center. The second case is a porous material, represented as a matrix with an array of 8 randomly distributed spherical voids (material properties in table 3.1) with a void fraction of 20%. The RVE is discretized in $105 \times 105 \times 105$ voxels. The boundary conditions described in Eq.(3.34) at the beginning of section 3.3 are used here. Simulations are performed using the crack dissipation control, and the non-linear resolution of the system in Eq.(3.9) includes here a relaxation parameter of $\alpha = 0.8$, since it was found that this value improved the convergence. Simulation results are shown in Fig.3.13.

Two stages can be identified in Fig.3.13a for the first case, where the first stage covers points ① to ③ and the second stage covers points ③ to ⑤. Their damage states are shown in Fig.3.13b, where thanks to the symmetry only half of the domain is presented to show the middle YX plane for a better understanding. From ① to ③, the snap-back behavior is

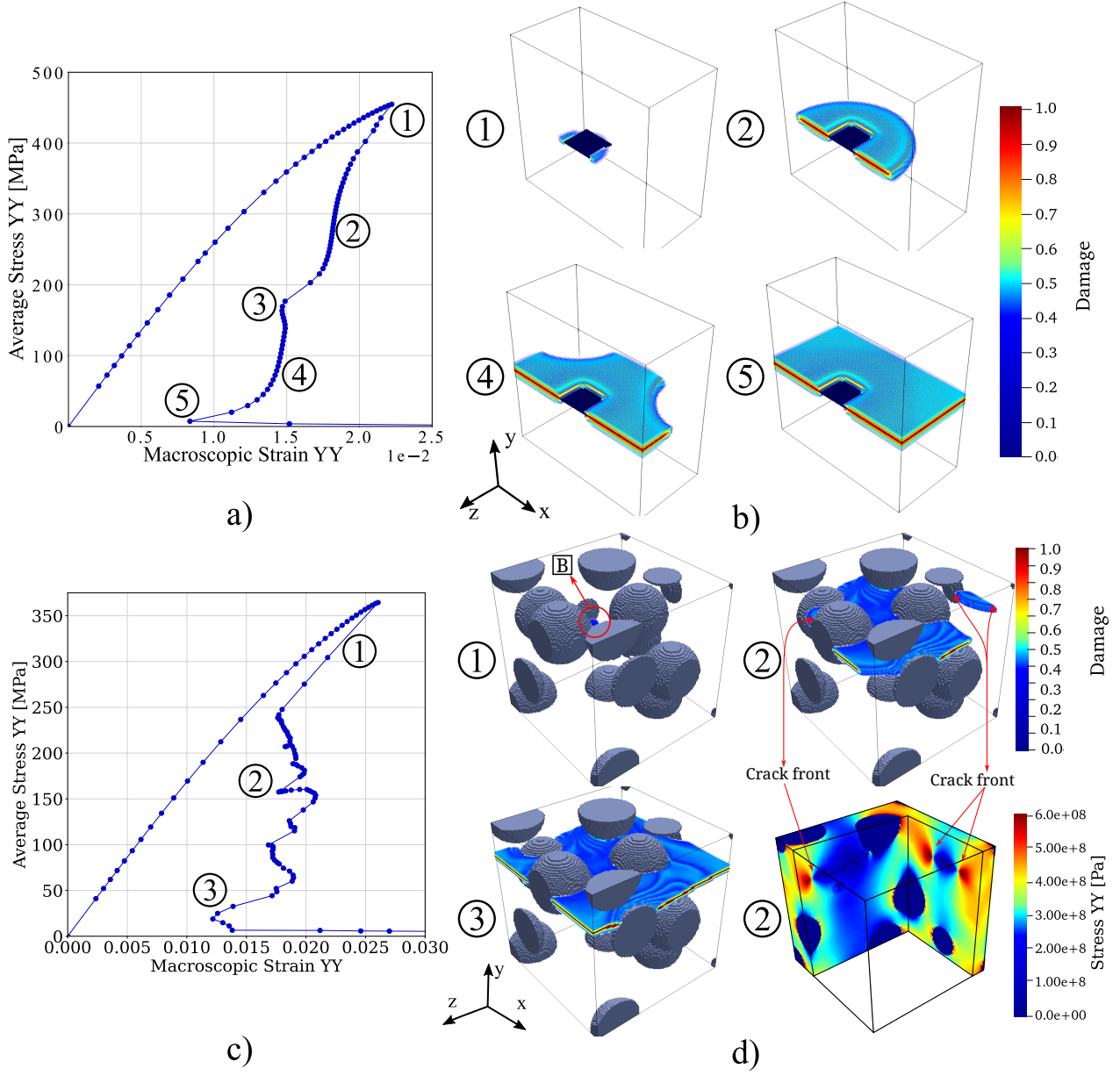


Figure 3.13: Simulations of two 3D cases with Crack-length control. Top: homogeneous material with a single rectangular initial crack, (a) Stress-strain curve, (b) crack evolution. Bottom: Porous material with randomly distributed spherical pores, (c) Stress-strain curve, (d) crack evolution.

similar to that of the previous sections, but the crack propagates in the two directions of the plane, transforming from a square crack to an ellipsoidal one, as observed in Fig.3.13b for the point ②. After point ②, crack growth becomes anisotropic and accelerates in the areas near the periodic boundaries due to the interaction with the periodic cracks. Point ③ in Fig.3.13a represents the coalescence of the crack, which alters the stress-strain path due to the abrupt change in stiffness that occurs in the matrix before both crack fronts encounter. The fracture process up to this point shows an identical snapback behavior to that observed in the 2D homogeneous domain of Fig.3.9a, where the mechanical behavior also presents the abrupt recoil observed at the end caused by an equivalent coalescence mechanism. In the second stage, the rest of the remaining material is fractured in a similar process until the point ⑤ where the fracture is complete.

In the case of the porous material, the stress-strain response is shown in Fig.3.13c with damage and stress states shown in Fig.3.13d for the points marked in the graphic. It has to be noted that no initial sharp fissure was introduced, and the crack propagates from the initial voids. The initial crack propagation (point ①) occurs due to the finite value of ℓ , and no crack would appear for $\ell \rightarrow \infty$ since linear elastic fracture mechanics just considers propagation from initial sharp discontinuities. The position at which the crack nucleates (point ① of the stress-strain curve) is marked with the [B] at Fig.3.13d, where the damage field is represented. Then, the crack grows following a similar process to those studied in previous sections, where the snap backs observed in Fig.3.13c are similar to those observed in Fig.3.12a for the segment [A], and are caused by crack deflections shown in Fig.3.13d for the points ② and ③. These deflections in turn are caused by a heterogeneous energetic driving force in the domain, due to the presence of pores that cause stress concentrations, which are shown in the stress field in Y direction presented for the point ② in Fig.3.13d, in a plane that allows to show 3 different crack fronts. It can be seen that the stress concentration fields around the crack are similar to those presented in Fig.3.6 for 2D cases and are dominant with respect to the ones formed around pores, but still influenced by its presence.

Chapter 4

Effective toughness estimations in a FFT-PFF model implementation

The use of homogenization in problems involving fracture or softening is controversial since damage and crack evolution at the macroscale is a localized phenomenon. In these cases, the stress-strain response of a single RVE is only representative of the macroscopic response until localization, e.g. the maximum of the stress-strain curve. After that point, some regions concentrate the deformation and damage while the rest of the material unloads. Therefore, computational homogenization can only be used to define the stress-strain response in the context of multiscale problems, using a different RVE simulation for each macroscopic point (Arunachala et al., 2023; Oliver et al., 2017). Nevertheless, computational homogenization is still extremely useful in the context of fracture as a tool to estimate *Effective* properties of heterogeneous media that represent the homogenization of that property to be included at macroscale calculations.

As reviewed in chapter 1, the estimation of effective fracture response presents differences to the homogenization of the elastic properties. In this context, computational microscopic models can be used with special boundary conditions to model the damaging region with a clear connection between macroscale and microscale (Hossain et al., 2014; Y. Li and Zhou, 2013). Alternatively, standard homogenization boundary conditions can be used, assuming a clear scale separation, to obtain homogenized fracture energies M. Schneider, 2020. In this last case, the use of periodic cells with periodic boundary conditions becomes an advantage to minimize cell boundary effects.

The numerical procedures developed by Hossain et al., 2014 and by M. Schneider, 2020 to obtain estimations of the effective fracture have been described in chapter 2 (section 2.6). Both methods provide interesting estimates of the fracture toughness of heterogeneous media, but present some differences between them and show some limitations. The first one uses a PFF model with special boundary conditions, but is limited to the path dependence of the J-integral Hossain et al., 2014 and proposes an arguable estimate of macroscopic toughness for clear scale separation. The other approach (M. Schneider, 2020) is based on an FFT-based approach and is specifically oriented to microscale simulations, but doesn't consider the effect

of stiffness heterogeneity at the microscale.

A clear challenge in homogenization is establishing a procedure for estimating the effective fracture energy (called from here effective toughness) based on RVE simulations and clear scale separation which considers the effect of both heterogeneity of the elastic response and fracture toughness at the microscale. The objective of this work is to propose such a procedure relying on the proposed PFF-FFT model with crack length control of chapter 3

The technique developed in chapter 1 allows us to compute the energy dissipation in general models, independently of their variational basis. Moreover, in chapter 3 the technique was used to analyze the fracture energy in simple cases, using the J-integral, opening the possibility of establishing a definition of the effective toughness based on the energy computed. In this chapter, a rigorous and general estimate of the effective toughness will be proposed, based on computing the fracture energy through the dissipation energy control. This estimate will consider any type of microstructure with heterogeneity in the elastic response and fracture energy, and phases potentially having elastic anisotropic mechanical behavior and anisotropic fracture response (cleavage). This framework will then be used to analyze the effective fracture toughness of composite materials and elastic polycrystals as a function of the stiffness and local toughness ratios of their constituents.

4.1 A new estimate of the effective toughness for heterogeneous media

A novel procedure is proposed for the determination of an effective toughness. The approaches proposed by Hossain et al., 2014 and by M. Schneider, 2020, described in section 2.6 are taken as a reference to the one proposed here, which takes elements from both approaches and aims at overcoming some of their limitations.

Let be a macroscopic crack on a heterogeneous material, Fig.4.1. The objective is to derive the propagation conditions considering the microstructure and properties of the phases.

Assuming separation of scales, the response of each macroscopic point (characterized by Σ_M and E_M) can be interpreted as the homogenized response of the microstructure. This microstructure is represented with an RVE, with heterogeneous microscopic stress and strain fields, and potentially the propagation of microcracks.

A differential of crack propagation at the macroscale would require the total rupture of the RVE by coalescence of microcracks. Therefore, from an energetic viewpoint, the condition for macroscopic propagation is that the total work of macroscopic stress on the RVE equals the dissipated energy in the coalescence of new microscopic crack surfaces (as proposed in M. Schneider, 2020). Focusing on a particular quasistatic macroscopic loading process, defined by the tensor $\mathbf{f}$ (section 3.1.2) $E_M = \mathbf{f}E$, the total work Π_M is defined as the integral of the internal power (product of Σ_M and $\dot{E}_M$). In the context of fracture, Eq.(2.15) establishes that the dissipated energy after the full rupture ($E_{mec} = 0$) of the RVE equals the integral of the internal power.

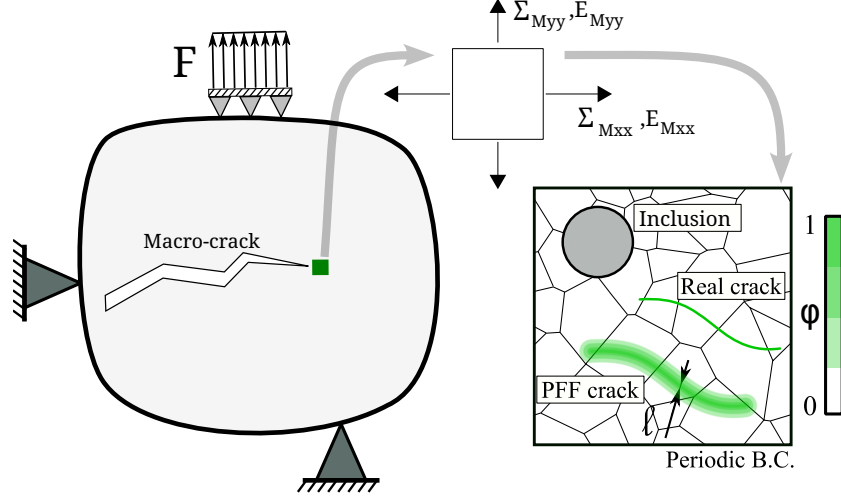


Figure 4.1: Damage Phase Field representation of the crack.

$$D = \Pi_M \quad (4.1)$$

Then, the local microscopic fracture energy integrated along the microscopic crack surfaces on the RVE can be used to define the effective toughness (M. Schneider, 2020).

In order to replace the heterogeneous material with an equivalent homogeneous one, the total dissipation D computed on the RVE by a microscopic tortuous crack can be associated with the effective toughness G_{Ceff} multiplied by the area A_g of a straight crack crossing the RVE (a length L_g in 2D cases). Therefore, the estimate proposed here for the effective fracture toughness is

$$G_{Ceff}(\mathbf{f}) = \frac{D}{A_g}. \quad (4.2)$$

The fact that G_{Ceff} depends on $\mathbf{f}$ highlights the dependency of energy dissipation with loading direction, similar to the dependency of the toughness with the macroscopic crack direction $\vec{t}_c$ in Eq.(2.73) (M. Schneider, 2020).

In a variational PFF framework, the dissipation in the RVE after fracture D can be obtained by evaluating directly the fracture energy in Eq.(3.9c). However, in most cases, the PFF approach introduces some non-variational elements such as the history term defined in Eq.(3.5) or the use of hybrid approaches (Ambati et al., 2015b), in which these expressions do not coincide exactly with the dissipation. In a totally general case, the dissipated energy at the final fracture stage can be rigorously evaluated using Eq.(4.1), if the external work on the RVE is adequately obtained. This is precisely the advantage of the control method proposed in chapter 3, where this external energy can be obtained as the integration of the external power over a process that is always in equilibrium. The valuation of Eq.(4.1) will coincide with the dissipation functional in pure variational PFF, but will include other dissipation sources in general cases. Moreover, even for a variational PFF model, under unstable propagation, the uniqueness of the crack path obtained using a staggered scheme is not guaranteed. Therefore, also in this case, the integration of Eq.(4.1) over a stable load path using the model in chapter

3 provides a clearer result from the microscopic viewpoint.

Finally, it is important to note that the estimate proposed introduces a dependence on the initial crack introduced in the RVE. It has been observed that the influence of its size is negligible, since this value drives the stress at which the crack propagates, but not the energy needed for propagation. On the contrary, there is a non-negligible effect on the crack position which controls the initiation of the crack and therefore introduces a bias in the optimal crack path. To overcome this effect, sampling on different crack positions could be done for the same RVE, defining the estimate as the minimum toughness.

Non-uniqueness of crack paths in staggered schemes

The PFF-FFT scheme of the previous chapter allows us to calculate the complete *snap-back* response, which makes it possible to compute the total external energy even in cases with unstable fracture. The adequate obtention of the external energy in fracture simulations is highlighted as an advantage of the dissipation control scheme; however, it is not the only option. Potentially, this value could be obtained in a PFF simulation under strain control as the value of the fracture functional at the final fracture stage using Eq.(3.9c), as proposed by Na et al., 2017.

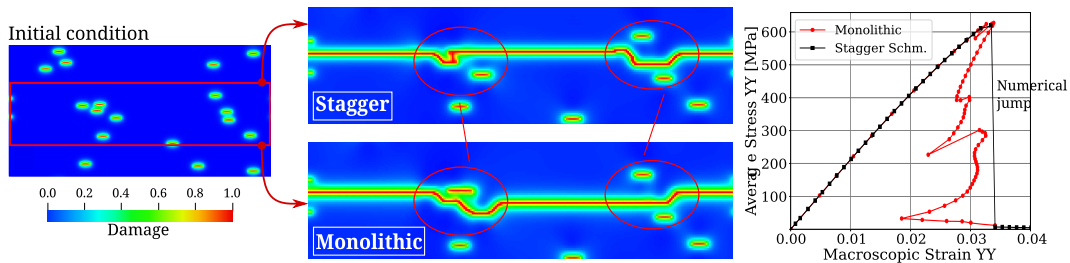


Figure 4.2: Staggered strain control Vs Monolithic dissipation control methods for multi-crack initial condition.

However, the unstable crack propagation is normally surpassed by the use of staggered algorithms, which makes uncertain the uniqueness of the final crack obtained. Moreover, despite model comparisons between dissipation control and strain controlled simulations in chapter 3 that match their responses adequately, comparisons only consider highly stable fracture or homogeneous domains. In a case where fracture is highly unstable, the solution obtained using a staggered approach might differ from one obtained following a stable dissipation load path. This can be demonstrated by employing both schemes to calculate the fracture response in a domain with complex conditions, e.g. multiple initial cracks, which could have many final configurations satisfying the conditions of the problem in staggered schemes, as shown in Fig.4.2.

Both final cracks obtained have the same length, but present different paths. In the case of the staggered simulation, various equivalent responses (which depend on the algorithm choices) might be obtained during the metastable growth in which irreversibility is not imposed. On the contrary, in the proposed control technique, every step represents an irreversible process

due to history. Since the objective is to study complex microscopic domains and general (non-pure variational) PFF models, the dissipation control method is a more accurate and robust option.

4.2 Phase Field fracture model with heterogeneous fracture energy

The FFT-PFF model implementation in Chapter 3 represents the fracture in stiffness-heterogeneous materials. Focusing on Eq.(3.9), such heterogeneities are primarily governed by the equilibrium equation in Eq.(3.9a). However, heterogeneous microstructures may also exhibit phase-dependent variations in fracture energy limit, referred to from here as local toughness. The PFF model of the previous chapter can be easily extended to capture this heterogeneity by introducing a spatially dependent G_c , modifying the damage equation (Eq.(3.9b)) and altering the energy dissipation formulation, which can no longer be expressed as $D = G_c \Gamma$, but as an area integral. To consider this change, the total surface of the actual crack Γ is defined with Eq.(2.23) and the dissipation functional, defined with an AT2 dissipation density, is modified to consider a non-constant local toughness field,

$$D(\phi, \ell, G_c) = \int_{\Omega} G_c(x) \left(\frac{1}{2\ell} \phi^2 + \frac{\ell}{2} \nabla \phi \cdot \nabla \phi \right) d\Omega. \quad (4.3)$$

From Fig.4.1, the external energy associated with the local macroscopic state relates with microscopic variables as described by Eq.(2.15) as $\dot{\Pi}_M = \dot{E}_{mec} + \dot{D}$. In chapter 3, the elastic free energy E_{mec} described in Eq.(2.16) is formulated using the spectral decomposition (Eq.(2.19)). Since the toughness estimation provided by Eq.(4.2) assumes that all mechanical energy is dissipated through fracture, it is expected that the macroscopic stress of the material approaches zero at the end of the fracture process. Nevertheless, this is not always observed, as shown in the simulations presented in Fig.3.10, Fig.3.13, and Fig.3.12. This deviation is present in cases where the crack path deviates, and it can be attributed to residual stress transfer in localized regions. Such effects arise when the spectral decomposition approach is employed to define the PFF driving force.

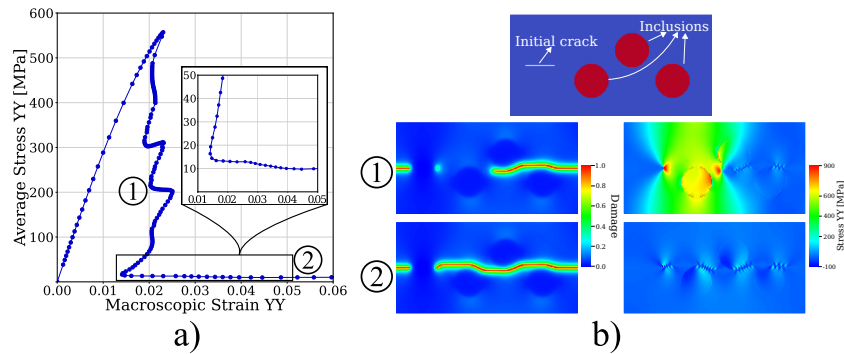


Figure 4.3: Residual stresses with the model proposed in chapter 3. (a) Stress/strain response. (b) Domain selected and σ_Y fields (Deformed representation)

A representative example of these residual stresses is shown in the tensile test simulation including rigid inclusions of Fig.4.3, where the residual stress levels depicted in Fig.4.3b remain non-negligible after fracture. This residual stress may introduce minor inaccuracies in the estimation of the effective toughness. A straightforward strategy to mitigate this issue involves subtracting the energy contribution associated with the residual stresses from the total energy measurement. However, for the sake of simplicity, the present chapter opts to use a simple the driving force formulation given by Eq.(2.17). Although this approach may lead to a less realistic representation of crack evolution, it significantly reduces the residual stress, thereby facilitating a more direct and consistent toughness estimation. Considering this, the value of E_{mec} in Eq.(2.15) is taken as,

$$E_{mec} = \int_{\Omega} \psi(\boldsymbol{\varepsilon}, \phi) d\Omega = \int_{\Omega} g(\phi) \psi_o(\boldsymbol{\varepsilon}) d\Omega = \int_{\Omega} g(\phi) \frac{1}{2} \mathbb{C}_o(x) : \boldsymbol{\varepsilon} : \boldsymbol{\varepsilon} d\Omega. \quad (4.4)$$

Here, ψ_o corresponds to the undamaged density energy, $\mathbb{C}_0$ corresponds to the pristine fourth order isotropic stiffness tensor that can vary in space and $g(\phi)$ is taken as quadratic. With these modifications, the damage equation of the governing equations (in strong form) is redefined as in Eq.(4.5b), which replaced the derivative of the dissipation density defined in Eq.(2.30),

$$\nabla \cdot \boldsymbol{\sigma} = \nabla \cdot [g(\phi) \mathbb{C}_o : \tilde{\boldsymbol{\varepsilon}} + g(\phi) \mathbb{C}_o : \mathbf{f}E] = 0 \quad (4.5a)$$

$$g' \mathcal{H} + \frac{G_c}{\ell} \phi - \nabla \cdot [\ell G_c \nabla \phi] = 0 \quad (4.5b)$$

$$\int_{\Omega} G_c \gamma_f d\Omega = \tau(t) \quad (4.5c)$$

where the history function $\mathcal{H}$ is equivalent to the one defined by Eq.(2.32).

4.2.1 Phase Field Fracture extension to anisotropic materials

Heterogeneity in the material response at the microscale can also arise due to the presence of an anisotropic material with different local orientations, as it happens, for example, in polycrystalline materials. To this aim, the functionals defining the elastic and fracture energies can be modified to include anisotropic elastic energy and anisotropic fracture energy densities.

Focusing on the elastic energy density, the definition of the elastic stiffness in Eq.(4.4) can be directly redefined to represent a material with cubic anisotropy,

$$E_{mec} = \int_{\Omega} g(\phi) \psi_o(\boldsymbol{\varepsilon}) d\Omega = \int_{\Omega} g(\phi) \frac{1}{2} \mathbb{C}_o^r : \boldsymbol{\varepsilon} : \boldsymbol{\varepsilon} d\Omega, \quad (4.6)$$

where $\mathbb{C}^r$ is the stiffness tensor after a rotation to its actual orientation. This rotation is represented by the tensor $\mathbf{R}$, and the resulting stiffness in global axis is given by Eq.(4.7):

$$\frac{\partial^2 \psi}{\partial \boldsymbol{\varepsilon}^2} = g(\phi) \mathbb{C}_0^r = g(\phi) R_{im} R_{jn} R_{kp} R_{lq} C_{mnpqo} \quad (4.7)$$

where $\mathbb{C}_0^r$ is the pristine stiffness tensor in lattice axes, which for cubic anisotropy, depends on three independent parameters C_{1111} , C_{1122} , C_{1212} .

In addition to the mechanical response, anisotropy can appear in the damage fields, due to the presence of brittle crystallographic planes that make it necessary to modify the dissipation functional in Eq.(3.9b) to account for the influence of such planes. These ideas have been applied in many PFF implementations, as in the case of representing crack orientation in single directional planes (Clayton and Knap, 2015), or to define systems of crack orientations in orthotropic, cubic and transverse isotropy cases (Teichtmeister et al., 2017), or to consider preferential crack propagation planes in multi-PFF models (Ma and Sun, 2020; Na and Sun, 2018). These models are conceived to represent fracture processes similar to cleavage and aim to generate weakening in the damage field at specific orientations by defining a second-order anisotropy tensor $\mathbf{A}_f$. Based on this, the dissipation density can be modified to emulate PFF-cleavage directions as proposed by Clayton and Knap, 2015 and later formally implemented in a PFF model by Na and Sun, 2018 and Ma and Sun, 2020:

$$D(\phi, G_c, \mathbf{A}_f) = \int_{\Omega} \gamma_f(\phi, G_c, \mathbf{A}_f) d\Omega = \int_{\Omega} \frac{G_c}{2\ell} \phi^2 + \frac{G_c \ell}{2} \mathbf{A}_f : (\nabla \phi \otimes \nabla \phi) d\Omega, \quad (4.8)$$

where we assume a potential case in which G_c could be heterogeneous if this were the case. Also, the crack surface (length) functional can be defined as

$$\Gamma(\phi, \mathbf{A}_f) = \int_{\Omega} \frac{1}{2\ell} \phi^2 + \frac{\ell}{2} \mathbf{A}_f : (\nabla \phi \otimes \nabla \phi) d\Omega, \quad (4.9)$$

Also The tensor $\mathbf{A}_f$ is defined using the vector $\vec{n}$ which corresponds to the normal of a weak plane, typically a cubic direction for cubic symmetry. In the case of 2D domains, the projection of the crack vector onto the domain plane $\vec{n}_{pl}$ is used and the anisotropy tensor is defined as

$$\mathbf{A}_f = \mathbf{I} + \beta(\mathbf{I} - \vec{n}_{pl} \otimes \vec{n}_{pl}) \quad (4.10)$$

where $\mathbf{I}$ is the second order identity and β a weight parameter that allows setting the level of anisotropy in the crack. Damage isotropy can be recovered by making $\beta = 0$. With these definitions, a new system of governing equations can be defined including modifications to the energy functionals:

$$\nabla \cdot \boldsymbol{\sigma} = \nabla \cdot [g(\phi) \mathbb{C}_o^r : \tilde{\boldsymbol{\varepsilon}} + g(\phi) \mathbb{C}_o^r : \mathbf{f} E] = 0 \quad (4.11a)$$

$$g' \mathcal{H} + \gamma'_f(\phi, G_c, \mathbf{A}_f) = 0 \quad (4.11b)$$

$$\int_{\Omega} \gamma_f(\phi, G_c, \mathbf{A}_f) d\Omega = \tau(t). \quad (4.11c)$$

where the derivatives with respect to ϕ of the dissipation density are

$$\gamma'_f(\phi, G_c, \mathbf{A}_f) = \frac{G_c}{\ell} \phi - \nabla \cdot (G_c \ell \mathbf{A}_f \cdot \nabla \phi). \quad (4.12)$$

Since the energy driving force of Eq.(4.6) is a scalar field, the same definition over the history parameter $\mathcal{H}$ defined in Eq.(3.5) can be used in Eq.(4.11b).

4.3 Numerical framework

4.3.1 FFT based implementation of PFF model

In this section, the FFT implementation of the PFF model is described considering the general case of a material that could present heterogeneity in stiffness and toughness, as well as anisotropic phases in both elastic response and fracture energy (cleavage). Since the scheme is equivalent to the one in section 3.1.2, only major changes will be exposed.

Focusing on the governing equations system in Eq.(4.11), the objective of the scheme is to find, at each time step (denoted by the superscript n) the values of the set $q = \{\tilde{\epsilon}, \phi, E\}$ that fulfill the governing equations for a given value of the macroscopic fracture energy D^n at Eq.(4.8). To this aim, a Newton-Raphson scheme (NR) similar to the one at section 3.1.2 is implemented, where its residual $R(q)$ is obtained from the system in Eq.(4.11). For each Newton iteration i , the linearization of this residual around the current value of the set q_i provides a Jacobian bi-linear form $J(q_i, \Delta q)$ which depends on the variation of the unknown variable set $\Delta q = \{\Delta \tilde{\epsilon}, \Delta \phi, \Delta E\}$. The linearized expression of the residual is then set to 0 to replicate the equations system in Eq.(3.16)

$$R = 0 \Rightarrow R(q_i + \delta q) \approx R(q_i) + [J(q_i, \Delta q)] = 0, \quad (4.13)$$

where the increment Δq is the unknown to be found at each NR iteration. Similar to the residual $F(q)$ in Eq.(3.11) for the model in section 3.1.2 was obtained from the equation system in Eq.(3.9), the residual $R(q)$ is obtained from Eq.(4.11) considering the heterogeneous/anisotropic PFF model as,

$$\begin{aligned} R_1(q_i) &= \mathcal{F}^{-1} \left\{ \hat{\mathbb{G}} : \mathcal{F} [\mathbb{C}_i^r : \tilde{\epsilon}_i + \mathbb{C}_i^r : \mathbf{f} E_i] \right\} \\ R_2(q_i) &= g'(\phi_i) \mathcal{H}_i + \frac{G_c}{\ell} \phi_i - \mathcal{F}^{-1} \left[\vec{\xi} \cdot \mathcal{F} \left[G_c \ell \mathbf{A} \cdot \mathcal{F}^{-1} [\vec{\xi} \hat{\phi}_i] \right] \right] \\ R_3(q_i) &= \int_{\Omega} G_c \left[\frac{1}{2\ell} \phi_i^2 + \frac{\ell}{2} \mathbf{A} : \left(\mathcal{F}^{-1} [\vec{\xi} \hat{\phi}_i] \otimes \mathcal{F}^{-1} [\vec{\xi} \hat{\phi}_i] \right) \right] d\Omega - \tau^n, \end{aligned} \quad (4.14)$$

where $\mathcal{F}$, $\mathcal{F}^{-1}$ and $\vec{\xi}$ account for the Fourier operation, inverse Fourier operation, and the complex frequency vector as in the previous chapter. The functions R_1 , R_2 and R_3 correspond respectively to the residual of equilibrium, the residual of the damage equation, and the control equation residual. Similarly, the Jacobian is defined in Eq.(4.15) as

$$\begin{aligned} J_1(q_i, \Delta q_{i+1}) &= \mathcal{F}^{-1} \left\{ \hat{\mathbb{G}} : \mathcal{F} \left[\mathbb{C}_i^r : \Delta \epsilon_{i+1} + g'(\phi_i) \frac{\partial \psi_{oi}}{\partial \epsilon_i} \Delta \phi_{i+1} \right] \right\} \\ J_2(q_i, \Delta q_{i+1}) &= g'(\phi_i) \frac{\partial \mathcal{H}_i}{\partial \epsilon_i} : \Delta \epsilon_{i+1} + \left(\frac{G_c}{\ell} + 2\mathcal{H}_i \right) \Delta \phi_{i+1} - \mathcal{F}^{-1} \left[\vec{\xi} \cdot \mathcal{F} \left[G_c \ell \mathbf{A} \cdot \mathcal{F}^{-1} [\vec{\xi} \widehat{\Delta \phi}_{i+1}] \right] \right] \\ J_3(q_i, \Delta q_{i+1}) &= \int_{\Omega} \frac{G_c}{\ell} \phi_i \Delta \phi_{i+1} - G_c \ell \mathcal{F}^{-1} \left[\vec{\xi} \cdot \mathcal{F} \left[\mathbf{A} \cdot \mathcal{F}^{-1} [\vec{\xi} \hat{\phi}_i] \right] \right] \Delta \phi_{i+1} d\Omega, \end{aligned} \quad (4.15)$$

where $\Delta \epsilon_{i+1} = \Delta \tilde{\epsilon}_{i+1} + \mathbf{f} \Delta E_{i+1}$. The expression of the projection operator $\hat{\mathbb{G}}$ in Fourier space is given by Eq.(2.68) and the history variable and its derivative are similar to the ones in Eq.(3.5) and Eq.(3.15), but modified to account for the anisotropic energy density at Eq.(4.6)

as,

$$\mathcal{H}_i = \max(\psi_{oi}, \mathcal{H}^n) ; \quad \frac{\partial \mathcal{H}_i}{\partial \varepsilon_i} = \begin{cases} 0 & \text{if } \psi_{oi} \leq \mathcal{H}_i \\ \sigma_{oi} & \text{if } \psi_{oi} > \mathcal{H}_i. \end{cases} \quad (4.16)$$

With $J(q, \Delta q)$ and $R(q)$, at each time step and NR iteration the linear system with $7(n_x \cdot n_y \cdot n_z) + 1$ unknowns given in Eq.(4.13) is solved to find Δq . Since this system is non-symmetric, the bi-conjugate gradient stabilized method is used as in section 3.1.2. Then, the new value of the unknown set, q_{i+1} is determined by adding the increment Δq_{i+1} to the current q_i , leading to

$$q_{i+1} = q_i + \Delta q \quad ; \quad q_0 = q^n, \quad (4.17)$$

where q^n corresponds to the converged value on the previous time step. After computing the new q_{i+1} , the fields depending on q are also updated using equations in section 4.2,

$$\sigma_{i+1} = \sigma(q_{i+1}) ; \quad \mathbb{C}_{i+1} = \mathbb{C}(q_{i+1}) ; \quad \psi_{oi+1} = \psi_o(q_{i+1}) ; \quad \mathcal{H}_{i+1} = \max(\psi_{oi+1}, \mathcal{H}^n), \quad (4.18)$$

where $\mathcal{H}^n$ is the history of the last converged time. The criteria to stop iterating in the NR scheme is defined with the error in Eq.(3.17) with respect to a defined tolerance. If the Newton iterative process converges, the resulting set of unknowns is updated in time as $q^{n+1} = q_{i+1}$ together with the history as $\mathcal{H}^{n+1} = \mathcal{H}_{i+1}$.

The convergence of the Newton-Raphson (NR) method can be enhanced by employing the successive relaxation strategy described in section 3.1.2. In this approach, the parameter α penalizes each computed increment Δq during NR iterations, effectively damping the solution to improve stability. Given the increased complexity of the simulations in this chapter, an adaptive under-relaxation strategy is adopted (Bharali et al., 2022; Storkvik et al., 2021), ensuring a more robust convergence. Here, the parameter α is dynamically updated at each time step as a function of the maximum macroscopic stress from previous time steps,

$$\alpha^n = \max\left(\theta, \frac{\Sigma_{max}}{\Sigma^{n-1}}\right) ; \quad \Sigma_{max} = \max([0, \Sigma^{n-1}]), \quad (4.19)$$

where θ is the minimum relaxation parameter allowed. With this definition, the value of α_n will be 1 until propagation occurs, and then it will decrease as it approaches coalescence. As said before, the procedure depicted here resembles the one in section 3.1.2, so details of the procedure can be reviewed in algorithm 2.

4.3.2 Computation of effective toughness

The effective toughness estimate proposed in Eq.(4.2) requires the evaluation of the work of external stresses over the RVE, Π_M , in Eq.(4.1). This energy can be computed under an equilibrium loading path by the integration of the internal power. The external energy introduced in the full RVE can be obtained from the integration of the internal power based on the macroscopic Σ_M and $\mathbf{E}_M$, as depicted in Fig.4.4. In this figure, the lower area is related to the elastic energy E_{mec} stored at a given point of the fracture process, Eq.(4.4). By thermodynamic equilibrium, the upper part of the area must correspond to the energy density of the dissipative processes, which for elastic materials should only be attributed to fracture

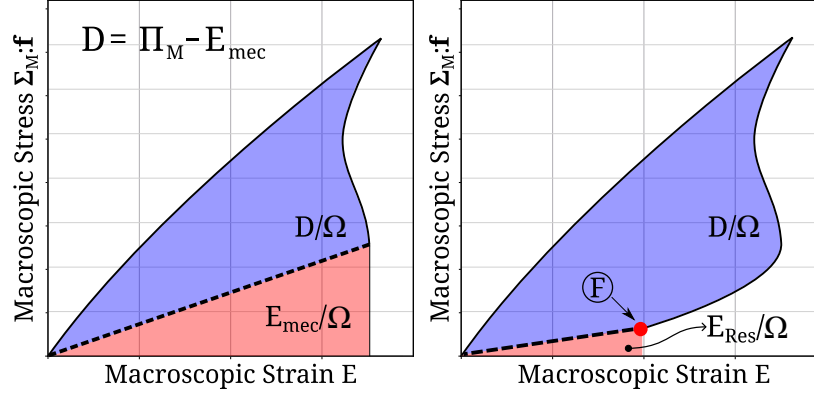


Figure 4.4: External power Π_M , stored energy E_{mec} and dissipation D represented by areas under the curve of a snap-back/fracture behavior of an RVE of volume Ω .

dissipation also represented by Eq.(4.3). However, as previously stated, the introduction of a local history might influence this statement as it will be analyzed later.

Using the PFF-FFT model with dissipation control of section 4.2 allows us to obtain the exact fracture point of the full RVE, providing the energy that corresponds to the complete fracture process. Beyond that point, the (small) elastic energy remaining in Eq.(4.4) becomes the value E_{res} depicted at the right in Fig.4.4, attributed to the residual stiffness of the cracked area. The fracture point, marked as (F) at this figure, is reported as the moment when the coalescence of PFF cracks occurs either with the domain boundary (Zambrano et al., 2023) or with other PFF cracks and usually corresponds to a strain lower than the maximum, typical in cases with unstable crack growth, so it is not always possible to find (F) in a controlled strain/displacement scheme (Singh et al., 2016).

The definition of the effective toughness is made according to Eq.(4.2) using the integration of the external power,

$$G_{Ceff}(\mathbf{f}) = \frac{\Omega}{A_g} \left(\int_{E=0}^{E=E_f} \Sigma_M : \mathbf{f} dE - E_{res} \right), \quad (4.20)$$

where Ω is the volume of the RVE, E_f is the value of the strain E at the crack coalescence point (F). In this expression, the value of the integral at Eq.(4.20) has to be numerically inferred from the calculated macroscopic strain-stress curve. To this aim, Simpson's rule is used to compute the area under the curve until the fracture point, from which the residual energy must be removed:

$$\int_0^{E_f} \Sigma_M : \mathbf{f} dE - E_{res} = T^f - \frac{1}{2} \Sigma^f E^f \quad ; \quad T^f = \sum_{j=1}^f \frac{1}{2} (\Sigma^j + \Sigma^{j-1})(E^j - E^{j-1}), \quad (4.21)$$

where T is the total area under the curve and the super-index $n = f$ in every variable represents a value of the iterative procedure in section 4.3 at the step time n in which crack coalescence occurs (at (F) in Fig.4.4). It should be noted that for any other time-step $n \neq f$, the value obtained from Eq.(4.21) corresponds to the actual fracture energy part of the area under the curve, allowing us to study the evolution of the dissipation energy.

In comparison with the work of Hossain et al., 2014, it is important to remark that Eq.(4.20) corresponds to the full process, while in the mentioned work the fracture energy is defined based on the instantaneous values of the energy release rate at every time as in Eq.(2.71). In order to compare the results, our model also allows us to obtain estimations of the instantaneous energy release rate based on Eq.(2.33) by computing the variation of the dissipation with respect to the variation of the total crack surface. This can be calculated with the numerical derivative $\partial T^n / \partial \Gamma$ as,

$$G = \frac{-\delta E_{mec}}{\delta \Gamma} = \frac{\Omega(T^n - T^{n-1})}{\Gamma^n - \Gamma^{n-1}} \quad ; \quad T^n = \sum_{j=1}^n \frac{1}{2}(\Sigma^j + \Sigma^{j-1})(E^j - E^{j-1}), \quad (4.22)$$

where the value of the crack surface (length) a has been replaced by its PFF equivalent in Eq.(2.23) or Eq.(4.9). This value has an equivalence to the one obtained with the procedure of Eq.(2.71) and also with calculations with J-integral in the case of a homogeneous material in chapter 3. Despite a great agreement with theoretical values discussed in that section being achieved with J-integral calculations, in complex microstructures, the path dependency of this procedure is not clear, which is not the case for the formulation proposed at Eq.(4.22), that will be tested in the section 4.4.1.1.

Regarding the definition of the effective toughness in the work of M. Schneider, 2020, Eq.(2.73) corresponds to the total energy dissipation weighed on a specific volume, so it should be equivalent to the value of the functionals in Eq.(4.3) or Eq.(4.8) over the same volume, which for variational PFF coincides with the area under the curve described above. For this reason, both this method (M. Schneider, 2020) and our approach should converge to the same value for a given crack path.

However, notable differences with our method have also to be highlighted. Since an adequate interpretation of the classic elastic PFF model (Miehe et al., 2010b) cannot consider crack nucleation, so an initial crack should be included in the RVE. This controls the position of fracture initiation, making it so that the studied PFF crack doesn't correspond to the minimal energy crack in the RVE as in the mentioned work. Another difference is that no macroscopic crack direction is explicitly imposed, but arises as a result of the loading direction dictated by $\mathbf{f}$. This macroscopic strain direction influences the toughness estimation consequently with the influence that the macroscopic strain at a point would have on the crack resistance assuming scale separation. Finally, another important difference is that in our approach the heterogeneity of elastic properties at the microscale is considered and might affect the toughness estimated by Eq.(4.2). This effect will be analyzed in section 4.4.

4.3.3 Modeling pre-existing cracks

The PFF model for brittle fracture requires a pre-existing crack to propagate fracture. The most rigorous and efficient method to introduce this crack is still an open issue. Often, notches or sharp contours are used to emulate a crack (Ambati et al., 2015b; Miehe et al., 2010a; G. Zhang et al., 2019), especially in FEM where adaptive meshes can be used. Other strategies consist of using boundary conditions, e.g., unconnected FEM nodes on a symmetry boundary (Segurado and LLorca, 2004), or to emulate the presence of a crack indirectly with local conditions, e.g. localized crack opening (M. Borden et al., 2018).

Alternatively, a notch can also be modeled by introducing regions with negligible stiffness as in (Y. Chen et al., 2019), which is very convenient for grid methods such as FFT solvers. Nevertheless, this procedure has certain limitations. First, the minimum crack thickness corresponds to one voxel, which makes the crack sharpness mesh-dependent. Also, the severe phase contrast might induce noise and convergence problems in FFT solvers (Ma and Sun, 2020).

Any of these approaches imply that no pre-existing damage field is present in the domain and, before a PFF crack propagates, a large amount of relatively dispersed damage is generated near the concentrator due to elastic energy accumulation. This effect emulates a nucleation phenomenon and could be understood as the nucleation of a PFF crack. However, there is no clarity in this respect and while some studies claim that nucleation of a PFF crack is possible and well represented (Tanné et al., 2018), more recent studies claim that this process does not correspond to a real physical process (Lopez-Pamies et al., 2025). Additionally, the numerical effects of this disperse damage have been reported (Singh et al., 2016; Zambrano et al., 2023), showing that this process requires additional energy and alters the crack propagation point.

For these reasons and in order to be able to provide accurate estimations of toughness using the mechanical response, this issue must be contained. The strategy followed here is the use of Phase Field enrichment strategies in which the domain includes specific distributions of an initial damage field to emulate pre-existing fissures, allowing us to avoid the phenomenon of PFF nucleation (Singh et al., 2016). Furthermore, since in the model a propagating crack is defined with a PF damage distribution, it is more adequate to model an initial crack similarly. Several works in the literature follow these strategies, highlighting the Crack Tip Enrichment procedure (CTE) (Singh et al., 2016; Zambrano et al., 2023) in which equations equivalent to Eq.(3.9b) are used to generate disperse damage fields from spatial discrete functions in the crack tip. The same strategy can be used to enrich an entire discrete notch (Ambati et al., 2015b; Hossain et al., 2014). Other smoothing equations can be used, e.g. in the work of M. J. Borden et al., 2012 where linear distributions of damage are used to enrich the complete contour of an initial crack. Finally, other studies propose the use of penalization methods, which directly intervene in the damage equation at Eq.(4.11b) to introduce penalized zones imposing damage as Dirichlet boundary conditions (Ma and Sun, 2020). The last work proves that this implementation is also well suited for FFT solvers, where it was effectively applied to model pores and holes.

In this work, different crack tip enrichment (CTE) approximations and a complete Phase Field Enrichment (PFE), in which the complete initial crack is embedded in an initial damage field, will be tested in order to determine a minimal condition in our FFT approach in which the PFF nucleation does not affect effective toughness estimations. The basis of all the approximations tested is the generation of a non-localized continuum damage distribution ϕ_o from a prescribed discrete damage field ϕ_{disc} (representing the sharp crack or its boundary). To this aim, the formulation proposed by Magri et al., 2021 for obtaining non-local damage fields is used throughout Eq.(4.23)

$$\phi_o - \ell \nabla^2 \phi_o = \phi_{disc} \rightarrow \phi_{ini} = \phi_M \frac{\phi_o}{\max(\phi_o)}, \quad (4.23)$$

where ℓ is taken equal to the characteristic length in the PFF model. The continuous

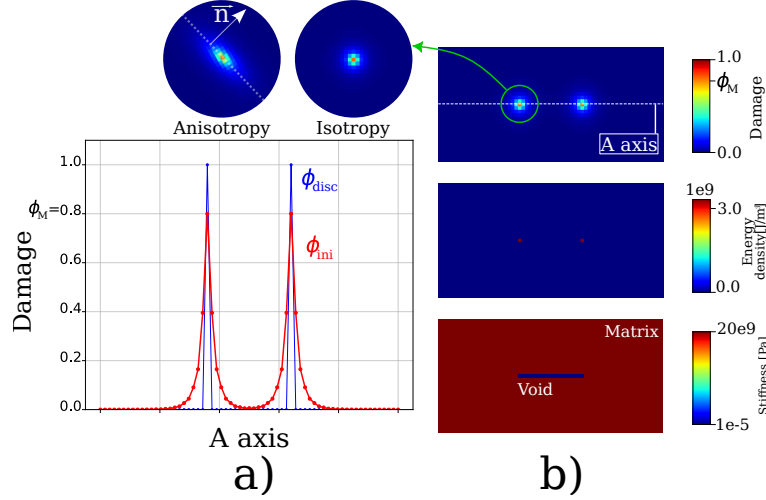


Figure 4.5: CTE condition for a straight crack. a) Sharp damage field and its corresponding smooth counterpart using Eq.(4.23). b) Representation of the spatial distribution of initial damage fields, initial energy density and phases distributions.

distribution resulting from Eq.(4.23) preserves the average of the sharp field ϕ_{disc} , therefore having a maximum of ϕ_o smaller than the maximum of the discrete distribution. For this reason, the resulting distribution is re-scaled, as shown on the right side of Eq.(4.23), ϕ_M being a parameter to control the maximum of the initial damage distribution ϕ_{ini} .

The smooth damage fields obtained using this process are represented in Fig.4.5a. In this example, the crack is defined as a row of voxels with negligible stiffness, and the sharp damage distribution, ϕ_{disc} , is chosen to be zero everywhere with the exception of two points representing the crack tip in 2D, where $\phi_{disc} = 1$. The formulation in Eq.(4.23) will result in an isotropic distribution for ϕ_{ini} and does not consider the anisotropic tensor defined for the cleavage formulation in section 4.2.1. For this reason, the modified formulation of this equation used in the work of Teichtmeister et al., 2017 is made for this kind of material.

$$\phi_o - \ell \nabla \cdot (\mathbf{A} \nabla \phi_o) = \phi_{disc} \rightarrow \phi_{ini} = \phi_M \frac{\phi_o}{\max(\phi_o)}, \quad (4.24)$$

In addition to the definition of the initial damage distribution, the history variable $\mathcal{H}$ from Eq.(4.16) has to be modified accordingly to prevent the initial damage introduced from disappearing during the loading. A similar procedure to the one proposed by Ma and Sun, 2020 or by M. J. Borden et al., 2012 is defined here to include ϕ_{ini} in the history. The energetic conjugate of ϕ_{ini} is defined considering Eq.(3.9b) or Eq.(4.11b), and the initial value of the history is set to that value. This initial energy is inferred from the ϕ_{ini} field using Eq.(4.25a) or Eq.(4.25b) for heterogeneous or anisotropic material, respectively.

$$\psi_{ini} = \frac{G_c}{g'(\phi)\ell} \phi - \frac{\ell}{g'(\phi)} \nabla \cdot [G_c \nabla \phi] = 0 \quad (4.25a)$$

$$\psi_{ini} = -\frac{1}{g'(\phi)\ell} \gamma'_f(\phi, G_c, \mathbf{A}_f), \quad (4.25b)$$

where the expression for γ'_f is the one in Eq.(4.12). Finally, to include this initial energy distribution in the history $\mathcal{H}$, Eq.(4.16) is modified to the definition in Eq.(4.26).

$$\mathcal{H}_i = \max(\psi_{oi} + \psi_{ini}, \mathcal{H}^n). \quad (4.26)$$

Including the conjugate energy additively ensures that new values of damage are calculated based on the initial distribution.

An alternative to the CTE described, which singular points correspond with the crack tip of the initial crack (Singh et al., 2016), the full surrounding area of the initial crack can be introduced as initial damage as proposed by Hossain et al., 2014, defining $\phi_{disc} = 1$ in all voxels representing the sharp crack with negligible stiffness. This procedure is called here Complete Phase Field Enrichment (CPFE) and will be compared with the CTE in section 4.4.1.1.

4.4 Results: effective toughness estimations

In this section the proposed models will be applied in different scenarios. First, the model will be used in homogeneous materials to fit the effective toughness estimates with the imposed PFF toughness as reference and also to test the influence of the initial crack approach considered. Secondly, the method will be applied to 2D laminates in which the effective toughness can be evaluated analytically or with reference to other works (Hossain et al., 2014; M. Schneider, 2020), in order to verify the accuracy of the procedure and to test the effect of stiffness and local toughness heterogeneity in the estimation. Finally, the procedure developed will be used to obtain effective toughness in heterogeneous fiber composites and anisotropic elastic polycrystals.

All cases of homogeneous material or composites will use the material properties in the table 4.1 as matrix, being the properties of inclusions changed and specified for each different case. A unique macroscopic loading condition will be imposed for all cases, which corresponds to uniaxial macroscopic strain described in Eq.(3.34). Two kinds of periodic RVEs will be used in 3D to resemble 2D conditions. The first kind will be rectangular plates, validated in chapter 3 as a less expensive case that is also less prone to unstable fracture, with dimension $L = [L_x, L_y, L_z] = [L_o, L_o/2, L_o/n_x]$, being $L_o = 500\mu\text{m}$ a value fixed in all cases and being n_x the amount of voxels in the X direction to make L_z to be represented by a single voxel. The second geometry will be quadrilateral plates with dimensions $L = [L_o, L_o, L_o/n_x]$. Note that in table 4.1 the value of ℓ in the matrix material is defined with a factor f_f and L_o , to be dependent on the case discretization that will be specified for each case considered. Regarding the numerical under-relaxation formulation, a minimum relaxation of $\theta = 0.3$ is used in every case.

E_{Young} [Pa]	ν	G_c [J/m ²]	ℓ
20e9	0.25	2e3	$f_f L_o / n_x$

Table 4.1: Mechanical and PFF properties of matrix material.

4.4.1 Validation of toughness estimations

4.4.1.1 Homogeneous material validation and crack tip enrichment analysis

The proposed estimate of effective toughness in section 4.1 will be applied here to homogeneous materials. A rectangular RVE with $185 \times 93 \times 1$ voxels is used, considering only the matrix material defined in Table 4.1, with a characteristic length of two voxels, $f_f = 2$ (as Miehe et al., 2010b). The use of the proposed methodology for a case with a homogeneous material should recover the material toughness used in the PFF model; however, it is known that the simulation resistance actually converges to the discretization-dependent numerical toughness used in FEM from the proposal of Bourdin et al., 2008 and in FFT from the estimations of section 3.2.1. Moreover, the effective toughness estimates predicted with our approach would also be affected by the *nucleation*, so a set of simulations has been performed considering a panel with different approximations for the initial crack, including a discrete crack of 1 voxel thickness to different smoothed cracks, and the results are represented in Fig.4.6.

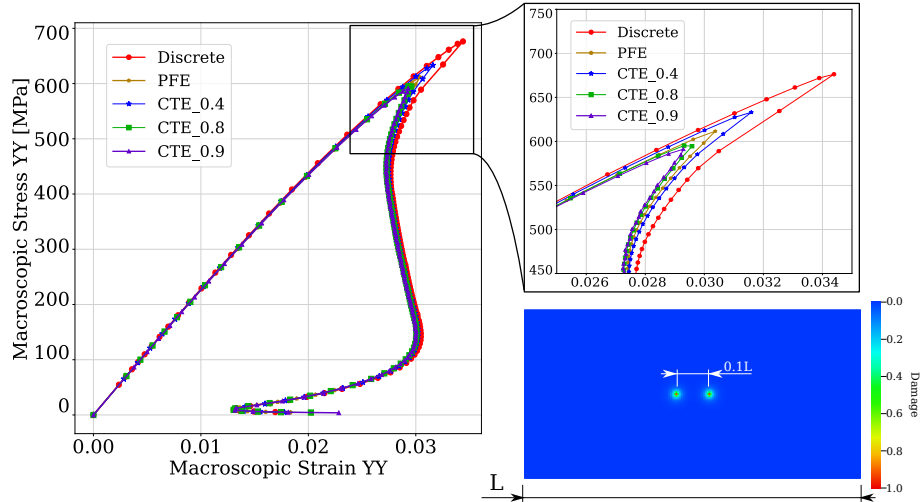


Figure 4.6: Stress/Strain curves for simulations of initial condition, where each curve is: Simulation with no initial damage(Red), CPFE simulation and $\phi_M = 0.98$ (Brown), CTE simulation and $\phi_M = 0.4$ (Blue), CTE simulation and $\phi_M = 0.8$ (Green), CTE simulation and $\phi_M = 0.95$ (Purple).

It can be seen that all the curves converge to the same result at the beginning of the loading process and after crack propagation, but the case in which no initial diffuse crack leads to higher stress and strain than others at the crack propagation point. As expected, this implies a larger area under the curve for this case, which also implies a higher perceived crack dissipation. This area is reduced when some initial damage field around the crack is introduced. A full damage around the crack, CPFE, alleviates this problem, but CTE cases with $\phi_M = 0.8$ and $\phi_M = 0.95$ further improve this result with similar results. Values for the effective toughness estimates in these simulations are depicted in table 4.2. It is observed that using CTE with values higher than $\phi_M = 0.8$ produces results with errors below 1%, being the best option CTE with $\phi_M = 0.95$.

The effect of the characteristic length is then analyzed, exploring the results for $\ell = 2L_o/n_x$,

	Imposed PFF (Corrected)	Discrete initial condition	CPTE $\phi_M = 0.2$	CTE $\phi_M = 0.4$	CTE $\phi_M = 0.8$	CTE $\phi_M = 0.95$
Toughness [J/m^2]	2296.6	2425.74	2317.6	2353.4	2309.9	2302.1
Percent difference	—	5.65%	0.94%	2.50%	0.61%	0.23%

Table 4.2: Effective toughness estimates for homogeneous materials.

$\ell = 3L_o/n_x$ and $\ell = 4L_o/n_x$ considering a CTE with $\phi_M = 0.80$ and $\phi_M = 0.95$. The results are shown in Table 4.3, using as reference the material toughness with the discretization correction also shown in Fig.3.8 of section 3.3.2 for these characteristic lengths.

	$\ell = 2L_o/n_x$		$\ell = 3L_o/n_x$		$\ell = 4L_o/n_x$	
	Toughness [J/m^2]	Percent difference	Toughness [J/m^2]	Percent difference	Toughness [J/m^2]	Percent difference
Imposed PFF (Corr.)	2296.6	—	2197.2	—	2147.8	—
CTE $\phi_M = 0.80$	2309.9	0.58%	2247.2	2.28%	2222.1	3.46%
CTE $\phi_M = 0.95$	2302.1	0.23%	2226.6	1.33%	2200.1	2.44%

Table 4.3: effective toughness estimates for homogeneous materials with different definitions for f_f .

It can be seen that the values obtained have good agreement with the reference values corrected as in Fig.3.8 and obtained with J-integral calculations, which serves as a first validation of the proposed procedure. Also, CTE with $\phi_M = 0.95$ is the best option again for the three lengths, but differences in the results between $\phi_M = 0.8$ and 0.95 are below 1%. Since using CTE values with higher ϕ_M is computationally more demanding in the first time steps, the rest of the calculations of this work will be made with the CTE and $\phi_M = 0.8$.

This accurate result is obtained with the proposed procedure for effective toughness, based on the integration of the loading curve, Eq.(4.20). The equivalence between the proposed procedure and the one obtained using PFF dissipation functional of Eq.(4.3), which can be used at any step of a simulation to obtain the total fracture energy, is analyzed. The effective toughness estimated with the dissipation functional in a simulation with $\ell = 2L_o/n_x$ and initial CTE crack with $\phi_M = 0.80$ gives a value of $G_{Ceff} = 2399.4[J/m^2]$ which implies a difference of 4.6% with respect to the reference value of table 4.3. This small inconsistency when using the dissipation potential directly is mainly due to the formulation of the history variable in the PFF model. This standard definition of history implies that the historical variable $\mathcal{H}$ is used to define the fracture in Eq.(4.11b) but the actual elastic energy ψ is the one controlling the stress in Eq.(4.11a), so the resulting model is not variationally consistent (Gerasimov and De Lorenzis, 2019). If a PFF model without history (and therefore fully variational) is used, the effective toughness obtained using our proposal of integration of the curve Eq.(4.11b) and the value obtained using the dissipation potential become identical. Nevertheless, using a PFF framework without history dependence can lead to negative local dissipation and healing problems in complex cases. Therefore, we will proceed with the proposed estimation, including the history variable to force irreversibility, to define effective toughness in the rest of the chapter.

4.4.1.2 Validation in orthogonal laminates

To further validate the present proposal for heterogeneous materials, microstructural configurations of orthogonal laminae with an initial crack are studied. This type of microstructure was also studied in the work of M. Schneider, 2020 and the one of Hossain et al., 2014, to consider the effect of both local toughness and stiffness heterogeneity. In the former research, it was established that for the geometries depicted in Fig.4.7b, the effective toughness for a crack perpendicular to the laminates is equivalent to the volumetric average of the local toughness, while, by construction, stiffness heterogeneity played no role. In the latter research, effective toughness is defined with the maximum instantaneous energy release rate, and it is reported that in the case of stiffness heterogeneity the effective toughness increase is similar to the stiffness contrast between sheets, and in the case of toughness heterogeneity the effective metric is equal to the maximum local toughness in the domain. The methods in the mentioned works are used as references and have been summarized in section 2.6

The tests have been performed with characteristic length defined by $f_f = 2$ and correspond to a rectangular RVE of 185x93x1 voxels and an initial crack modeled with CTE and $0.1L_x$ of initial length. Three cases are studied: two bi-laminates, two bi-laminates where the first has heterogeneity in toughness and the second local stiffness heterogeneity, and the third case is a tri-laminate with local toughness heterogeneity. Cases with toughness heterogeneity are defined with constant stiffness and cases with stiffness heterogeneity have a constant local toughness, these constant values being defined with the material of the matrix in table 4.1. Details of the properties used in each case are depicted in table 4.4, where the material reference is indicated in Fig.4.7b. In Fig.4.7c results of the instantaneous dissipated energy defined in Eq.(4.21) are depicted similarly as in Fig.4.7d where values of energy release rate are defined in Eq.(4.22).

	Bi-laminate C heter.		Bi-laminate G_c heter.		Tri-laminate G_c heter.	
	Local Toughness [J/m^2]	Local Stiffness [Pa]	Local Toughness [J/m^2]	Local Stiffness [Pa]	Local Toughness [J/m^2]	Local Stiffness [Pa]
Material ①	2000	matrix	matrix	20e9	2000	matrix
Material ②	10000	matrix	matrix	100e9	12000	matrix
Material ③	—	—	—	—	6000	matrix

Table 4.4: Material properties employed in cases of laminates. Material numbers are depicted in Fig.4.7.

It can be seen in Fig.4.7a that several snap-backs are observed in all cases, which correspond to the crack passage between two phases. In Fig.4.7c the estimations of the proposed procedure obtained with the numerical integration in Eq.(4.21) are shown with respect to the crack surface developed in every time step. In the case with heterogeneous stiffness but the same toughness, the evolution of dissipated energy is completely linear, an expected result since the proposed estimation is similar to the one proposed by M. Schneider, 2020, and for this configuration where a straight crack is developed, dissipation is independent of the stiffness of the laminae. This behavior, which is the same as expected in a homogeneous material, can also be observed in Fig.4.7d, where a constant evolution of the energy release rate is obtained. A similar behavior is also observed in the energy release rate obtained with the J-integral at Fig.3.7c for homogeneous materials, which is consistent with the last idea.

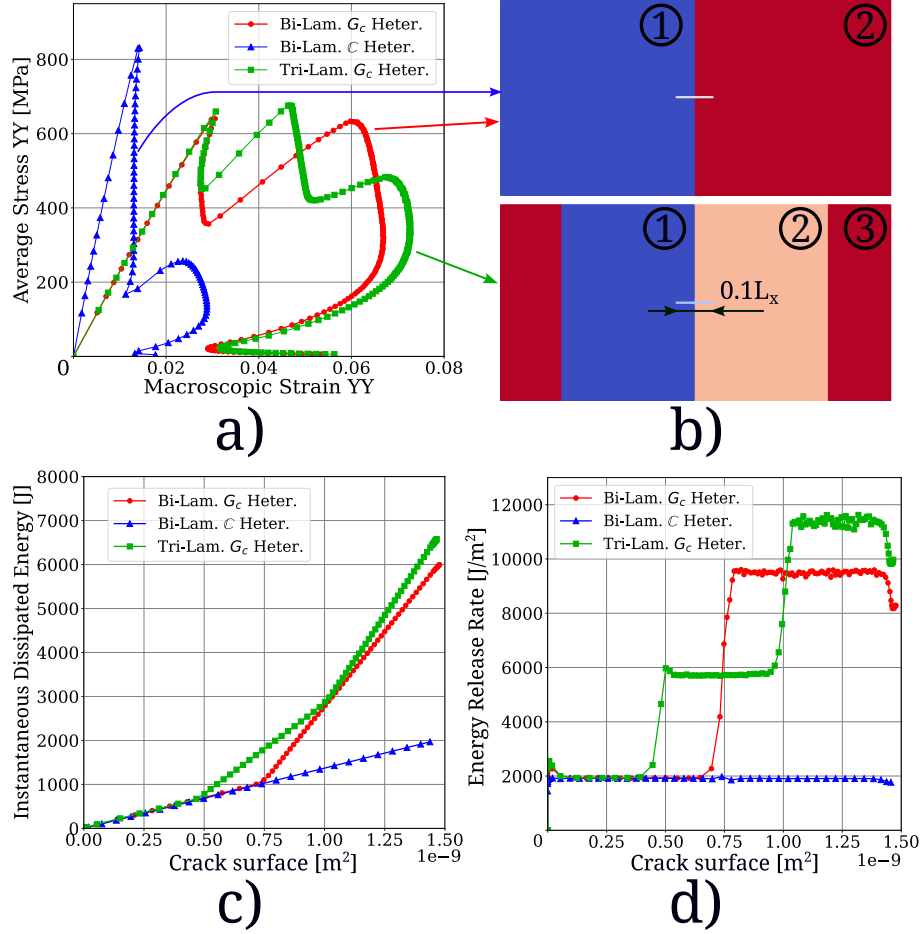


Figure 4.7: Orthogonal laminates test, for verification of the proposed effective toughness estimate: a) Stress/Strain curves for the three cases in study. b) Schematic of the microstructures analyzed. c) Instantaneous estimations of the effective toughness. d) Energy release rate calculations.

In the case where components are heterogeneous in toughness, a piecewise linear evolution is observed, with a slope change every time that surpasses a new phase. This change of slope is due to a higher rate of energy consumption when the crack advances in a tougher material. These changes in the rate of dissipated energy are also reflected in Fig.4.7d, where it can be seen that the energy release rate is constant inside every phase, converging to the local toughness with an error below 5% and presenting jumps when crossing an interface.

In table 4.5 a comparison of the results obtained with our approach with the values obtained with the criteria proposed in the reference works (Hossain et al., 2014; M. Schneider, 2020) in equivalent cases is made. Note that, as discussed in the previous section, the results of toughness obtained with the present method in table 4.5 include the correction of the discretization defined in section 3.2.1.

A very close agreement with the proposition of M. Schneider, 2020 is observed in all cases, with differences below 1%. On the contrary, the comparison with the results obtained with the metric established by Hossain et al., 2014 presents large differences. Regarding heterogeneous

	Eff. toughness (M. Schneider, 2020)	Eff. toughness (Hossain et al., 2014)	Eff. toughness Proposed
Bi-Laminate (G_c het.)	6000.0	10000	6040.1
Bi-Laminate (C het.)	2000.0	~ 10000	2007.4
Tri-Laminate (G_c het.)	6680.6	12000	6630.9

Table 4.5: effective toughness estimates for homogeneous materials. All toughness values in $[J/m^2]$.

stiffness, our procedure gives results very similar to the homogeneous case, which means effective toughness is not affected in this case by the heterogeneity in stiffness, even being formulated with the area under the curve of the stress/strain behavior. Since the crack path obtained is straight, no additional toughening mechanism exists in the case of heterogeneous stiffness, so the estimation resembles the one of M. Schneider, 2020. On the contrary, using the metric by Hossain et al., 2014, based on the maximum of the instantaneous release rate, results in an increase in the effective toughness even for a straight crack. Regarding heterogeneous fracture energy cases, both approaches in the literature predict an effect of local toughness on the effective value. Again, since the crack path predicted is straight, our estimate results identical to the one of M. Schneider, 2020, while the value using the definition of Hossain et al., 2014 would provide an effective toughness equal to the lamina with maximum fracture energy.

4.4.2 Effective toughness estimates in composites

4.4.2.1 Single fiber: stiffness vs toughness heterogeneity effect

A 2D periodic RVE with a single fiber embedded in a homogeneous matrix is studied here aiming at understanding the effect of interfaces non-orthogonal to the crack path. The proposed RVE is shown in Fig.4.8a. Different values of fiber stiffness and local toughness are selected, having a ratio with respect to the corresponding property in the matrix of f_C and f_G respectively.

The simulations consider an initial crack of $0.3L_x$ with the CTE defined in section 4.4.1.1 and spanning the factors defining matrix properties over the ranges $0.5 \leq f_C \leq 5$ and $1 \leq f_G \leq 10$. The obtained stress/strain curves are depicted in Figs.4.8b and Fig.4.8c, together with selected plots of damage distributions in Fig.4.8a.

Two extreme cases are analyzed first, materials having only heterogeneity in toughness and materials presenting only stiffness heterogeneity. In Fig.4.8b, the stress-strain curves obtained for the first case are presented, microscopic homogeneous elastic properties $f_C = 1$ and different values of the ratio between toughness of the phases. All curves are coincident with the homogeneous case (in black dashed line) until the crack reaches the fiber, where the behavior spreads depending on the level of heterogeneity. If f_G is low, the crack has the tendency to cross the interphase and the effective toughness increases with the local toughness contrast between the fiber and the matrix. This is reflected in the stress-strain curve as an increase in its area under the curve, Fig.4.8b. This increase in toughness is gradual, starting to a lesser extent for $f_G = 2.50$, where a diffuse damage around the fiber starts to appear that

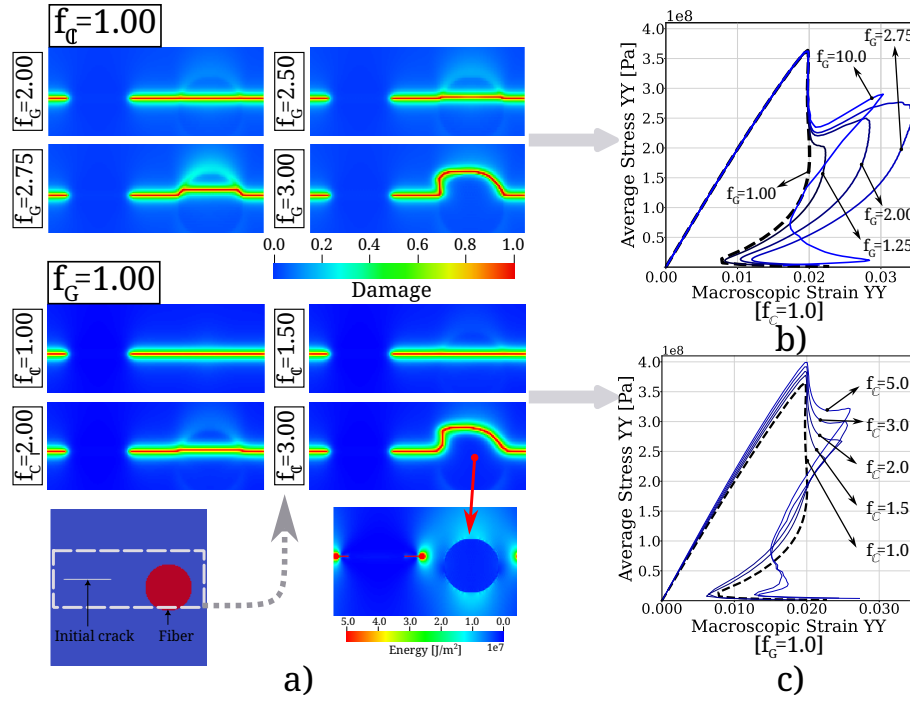


Figure 4.8: Single fiber simulations: a) Damage fields for different f_G and f_C . b) Stress/strain curves evolution for $f_C = 1$. c) Stress/strain curves evolution for $f_G = 1$.

grows until it drives the crack to avoid the fiber. For ratios larger than $f_G = 3.0$, the crack fully deflects and bypasses the fiber as depicted in Fig.4.8a because it becomes energetically more convenient to cross a longer path on a less tough material. This crack behavior agrees with the proposal of M. Schneider, 2020, since a gradual change from crossing to bypassing the fiber is observed for increases in toughness ratio. Results reported by Hossain et al., 2014 on effective toughness also account for this effect.

The other case of interest is materials with homogeneous fracture energy, $f_G = 1.0$, and different local stiffness. In Fig.4.8a it can be observed that for small values of f_C the crack penetrates the fiber following a straight path, cases in which no increase in energy (area behind the curve) or effective toughness is found. For higher values of f_C , the strain concentrates around the fiber due to the difference in stiffness, and the energy inside the fiber becomes insufficient to generate any damage, as seen at the bottom of Fig.4.8a, which leads the crack to bypass the fiber. This case illustrates how, despite the microscopic strain fields do not influence the energy dissipated, their heterogeneous distribution can lead to a crack deflection making stiffness heterogeneity a toughening mechanism. This effect is also reported by Hossain et al., 2014 where the effect of crack deflection due to stiffness local contrast is also observed. On the contrary, the definition of effective toughness of M. Schneider, 2020 does not account for this toughening mechanism since a uniform effective elastic response is assumed at the microscale. The stiffness heterogeneity has an effect on the stress-strain curves, as shown in Fig.4.8c, which deviate from the homogeneous case. In cases where the crack penetrates the fibers, the curve alternates between increasing and decreasing areas, compensating for the total energy consumed, which results almost equivalent to the homogeneous case. On the

contrary, when the fiber deflects the crack, there is a net increase in total area under the curve indicating more consumed energy and therefore higher effective toughness.

The evolution of effective toughness as a function of the heterogeneity level between fiber and matrix is represented in Fig.4.9a and Fig.4.9b for the different cases of stiffness and local toughness heterogeneities mentioned above, which behavior is consistent with the above results. In the former case, effective toughness does not become significant until f_C is big enough to make the crack bypass the fiber. In the latter case, effective toughness grows linearly until f_G reaches the limit of crack deflection, from which it becomes constant.

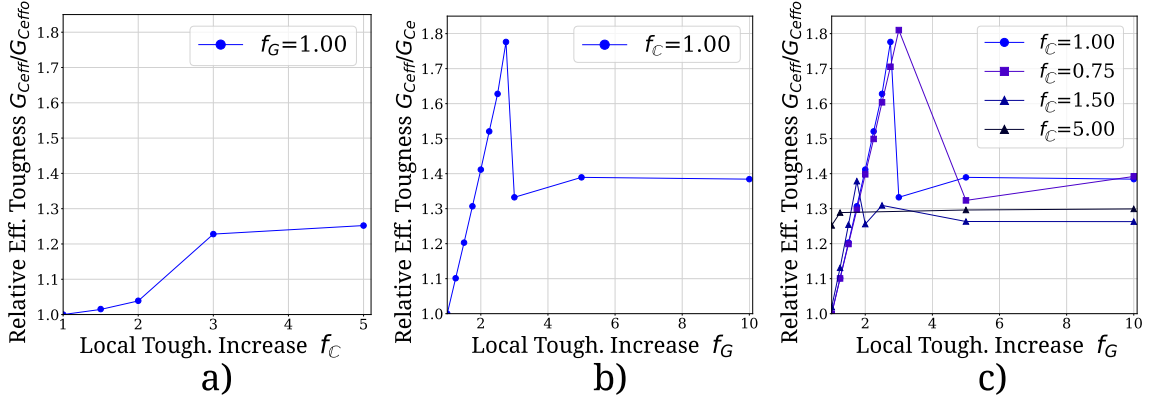


Figure 4.9: Single fiber simulations: a) effective toughness estimate for all cases with $f_G = 1$. b) effective toughness estimate for all cases with $f_C = 1$. c) Effective toughness estimates for all cases depicted.

Finally, the combined effect of having both stiffness and toughness heterogeneity is represented in Fig.4.9c (including the case in Fig.4.9b for comparison). If the fiber is stiffer than the matrix, $f_C > 1$, the bypassing mechanism appears for a smaller ratio in local toughness. The toughening for sufficiently large ratios of f_G and $f_C > 1$ is in the order of the one reached for a homogeneous elastic composite (between 30-40% increase with respect to the matrix) without a clear tendency. Finally, if the fiber is more compliant than the matrix, the opposite effect is observed, making it easier for the crack to penetrate into the fiber and slightly increasing the maximum toughening reachable.

4.4.2.2 Fiber composites microstructures

The cross section of composites with random arrays of monodisperse cylindrical fibers is analyzed in this section. The RVEs used are rectangular and contain a constant number of 20 fibers generated with the Random Sequential Adsorption method (RSA) proposed in Segurado and Llorca, 2002, representing volume fractions $Fvf = [0\%, 15\%, 30\%, 45\%]$. A CTE initial crack of $0.1L_x$ of length is used in all the simulations. As in the previous section, both stiffness and toughness heterogeneity between the fibers and the matrix will be considered, characterized again with the ratios f_G and f_C respectively. The results obtained are represented in Fig.4.10.

First, composites with homogeneous stiffness but heterogeneous toughness are considered, with $f_G = 4$ and $f_G = 2$. These values are selected motivated by the results obtained for the

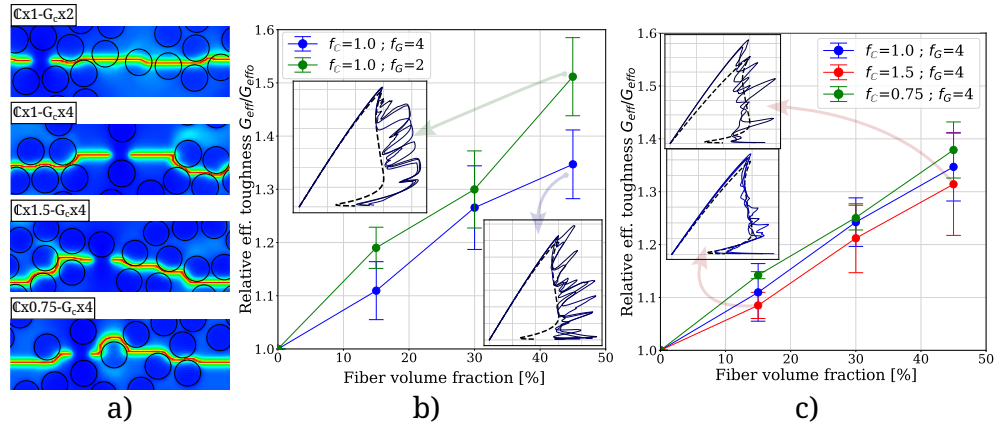


Figure 4.10: Fiber composite simulations: a) Crack path for different study groups. b) Effective toughness estimates in cases with constant (non-enhanced) local stiffness. c) Effective toughness estimates in cases with constant local toughness (enhanced x4)

single fiber, in which the phenomenon of fiber penetration or crack deflection was observed respectively for ratios below and above $f_G = 2.75$ for $f_c = 1$. To capture statistical effects, for each volume fraction 7 individual cases have been simulated. In Fig.4.10b the average effective toughness obtained including the standard deviation bars is represented as a function of the volume fraction. The results are normalized with the effective toughness of the homogeneous material. In the two cases, a monotonic increase of the effective toughness is obtained, obtaining for $Fvf = 45\%$ increases close to 30% for $f_G = 4$ and close to 50% for $f_G = 2$. Similar standard deviations for every case are observed, below 8%. The toughness reached for $f_G = 2$ is higher than for $f_G = 4$ in all the cases, as was also observed for the single fiber. The origin of this tougher behavior is the change of toughening mechanism from fiber crossing, where toughness is increased by the higher energy released within fibers, to fiber bypass, where toughening occurs by the increase of crack length through the matrix. In Fig.4.10a both mechanisms are observed for $f_G = 2$ while for $f_G = 4$ no penetration is observed. These mechanisms are also reflected in the resulting stress-strain curves, represented in Fig.4.10b for two cases with $Fvf = 45\%$. Crack deflection is perceived in those curves with localized sharp peaks for every change of direction. On the contrary, when crack penetration occurs the peaks are less sharp and produce a higher increase of the consumed energy, effect that can only be observed for $f_G = 2$.

The second group of simulations corresponds to a material with a fixed toughness heterogeneity and three levels of stiffness heterogeneity in the range $f_c = [0.75, 1.5]$. An effective toughness increase with volume fraction is also observed (Fig.4.10c), where the three materials present a very similar tendency due to the equivalence of toughening mechanisms, fiber bypass in all the cases. The microscopic crack configurations reached, represented in the last two damage maps of Fig.4.10a, clearly show this unique mechanism. Among the different stiffness ratios, a small increase of the effective toughening is observed with the fiber compliance. As in the case with a single fiber, this can be explained by the strain distribution around the fibers, causing less fiber penetration in the case of high stiffness and more penetration in cases with less stiffness. Regarding stress-strain curves, peak shape observed corresponds to fiber bypass,

where the peaks formed in the case with 15% volume fraction of fiber are smaller than for 40%, due to the smaller radius of the fibers.

4.4.3 Toughening in elastic polycrystals

In this section, the effective toughness of 2D elastic polycrystals will be analyzed. Parallel to the case of composites, the material used in this section is formulated considering two types of anisotropy, in stiffness and in the energy release rate. The anisotropy in stiffness considers cubic materials, with three independent elastic properties, and is controlled by the Zener ratio, z , as

$$z = \frac{2C_{1212}}{C_{1111} - C_{1122}} \quad (4.27)$$

where $z = 1$ corresponds to an isotropic Hookean material. The anisotropy in the fracture energy limit is set to resemble cleavage, considering a single weak crystal direction tensor, characterized by the tensor $\mathbf{A}$ of Eq.(4.10), which is controlled with the parameter β in the same equation. The toughening mechanism in a polycrystal is crack deflection, which will depend on the anisotropy parameters already mentioned. Regarding the effect of microstructure, texture or local misorientation will also control the deflection and therefore the toughening, but these effects are not considered in this study and random orientations are assumed. It is noted that the absolute grain size should not affect the results since our approach is based on homogenization and scale separation (Ernesti and Schneider, 2022; M. Schneider, 2020).

The domain used is a rectangular RVE in which grains are modeled using a weighted Voronoi tessellation, resulting in a log-normal grain size distribution (Lucarini et al., 2021), using for this study a standard deviation of 0.25% of the average grain size and an average of 25 grains in every RVE (unless otherwise stated). Grain orientations are chosen randomly in three dimensions (3 Euler angles) and stiffness is rotated accordingly. In the case of the anisotropy tensor for cleavage, $\mathbf{A}$, it is obtained by rotation and the projection of the normal of the weak fracture plane on the RVE cross section $\vec{n}_{pl}$. Initial cracks are introduced with the same CTE definition of previous sections and the stiffness tensor constants required for defining the unrotated state $\mathbb{C}_o$ in Eq.(4.7) are corresponding with the matrix material of table 4.1, being $C_{1111} = 24$ GPa, $C_{1122} = 8$ GPa, while C_{1212} is obtained as a function of the Zener ratio z following Eq.(4.27).

4.4.3.1 Effect of elastic anisotropy

The first case analyzed is the toughening due to elastic anisotropy, which is controlled by the Zener ratio (Eq.(4.27)). The reference case is a homogeneous and isotropic material ($z = 1$ and $\beta = 0$) in which polycrystal geometry has no effect, and the other cases correspond to Zener values $z = 2, 4, 6, 8$, each case including a set of different simulations that vary the grain distribution and keeping the number of grains as a constant for all cases. The results of the effective toughness as a function of z are represented in Fig.4.11a. Examples of the resulting crack paths obtained for each Zener ratio are represented in Fig.4.11b. Finally, Fig.4.11c shows the average stress/strain curves obtained and used to compute the effective toughness.

The results show an increase in the effective toughness with the level of anisotropy. This

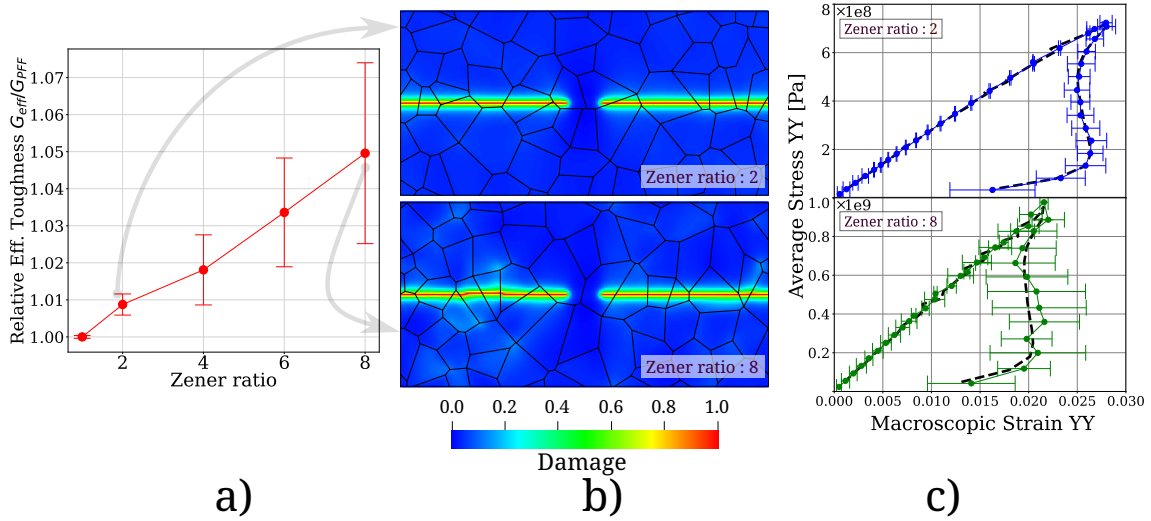


Figure 4.11: Zener ratio parametric study over polycrystal RVEs: a) Effective toughness estimates for various values of z . b) Examples of crack path for the groups with $z = 2$ (above) and $z = 8$ (below), both with average grain size $30\mu m$ and $\beta = 0$. c) Stress/strain average curves for all groups with $z = 2$ and $z = 8$.)

increase reaches 5% for the highest Zener ratio, while toughening for smaller values of this parameter, typical of standard alloys (e.g. very anisotropic crystals as Ni have $z = 2.5$ Rösler et al., 2007), will be below 2%. The toughening mechanism associated with this increase, crack deflection, is clearly observed in Fig.4.11b. These deflections are caused by heterogeneous accumulations of elastic energy in the domain caused by the strain incompatibility between grains. These results are similar to those obtained for local stiffness variations in fiber composites, where strain accumulation was also the origin of crack deflection and toughness increase. It's clear from Fig.4.11b that low heterogeneity, as in the case of $z = 2$, causes low crack deflection and almost no toughening, which emphasizes the idea that differences in local rigidity do not increase toughness unless it generates a significant crack deflection. Also, dispersed damage is observed all over the domain, due to the strain energy concentration around grain boundaries.

In Fig.4.11c, the stress/strain curves of each polycrystal are represented together with the results of an equivalent homogeneous material. The effective stiffness of the equivalent material is obtained, for each Zener ratio, using Fourier-Galerkin homogenization and RVEs with a very large number of grains. The effective toughness is the same as that of the crystals since this case assumes a homogeneous fracture energy.

Effect of anisotropy in toughness

The second case considered is the analysis of the effect of the fracture energy anisotropy. The same polycrystalline RVEs as in the previous section are tested, setting here the Zener ratio at $z = 1$ and varying β in the range $[1, 10]$. The reference toughness is the homogeneous case, which corresponds to $\beta = 0$. The resulting effective toughness as a function of β is shown in Fig.4.12a, crack paths in Fig.4.12b and the stress/strain curves in Fig.4.12c.

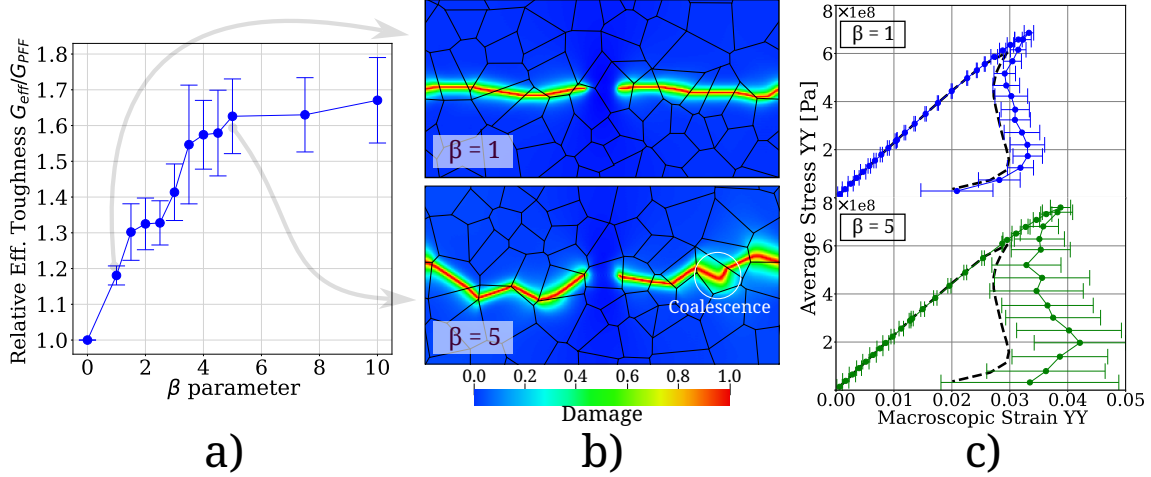


Figure 4.12: Damage anisotropy parametric study over polycrystal RVEs: a) effective toughness estimates (corrected) for various values of β . b) Examples of crack path for the groups with $\beta = 1$ (above) and $\beta = 5$ (below). c) Average stress/strain curves for the entire groups $\beta = 1$ (above) and $\beta = 5$ (below) compared to the behavior in homogeneous case

The effective toughness obtained as a function of β (Fig.4.12a) is highly affected by the level of anisotropy in the crystal toughness. The effective value shows a steep increase until reaching $\beta \approx 4$, where the effective response saturates. The toughening obtained is high compared with the one observed as a result of the elastic anisotropy, reaching here up to 60%. It is interesting to note that the toughness behavior obtained using the proposed approach is very similar to the one obtained by Ernesti and Schneider, 2022, using the definition of effective toughness of M. Schneider, 2020, reaching a saturation of the effective toughness similar to the one obtained here.

The microscopic toughening mechanism is the increment of crack length resulting from the constant change of direction of the crack paths. This effect can be observed in Fig.4.12b where crack paths show a clear cleavage behavior and the crack propagates in a completely transgranular way, changing its direction sharply every time the crack enters a new grain. This effect is higher with the increase of β , for $\beta = 1$ the crack still propagates horizontally in many grains independently of their orientation, while for $\beta = 5$ the crack deviates in each grain to the cleavage plane. The stress/strain behavior of all the polycrystals is identical before crack propagation. After propagation, the stress-strain curves of every case follow a path that is always above the homogeneous behavior. The error bars in the case of $\beta = 5$ are also higher than in the case of $\beta = 1$, reflecting the effect of toughening on the area under the curve in the mechanical responses.

Effect of the RVE size

In order to analyze the effect of RVE size (number of grains) statistical RVEs containing ensembles of 5, 8, 18, 30, 60, 140, 460, 1360, 1690, and 2160 grains are analyzed. In this study, the elastic response is chosen as isotropic, $z = 1$, and damage anisotropy corresponds to a value of $\beta = 1$. A constant value of ℓ is chosen, which might introduce a small effect of

the absolute grain size. This effect, which is purely numerical and should not exist in LEFM when $\ell \rightarrow 0$, is minimized here by choosing an ℓ sufficiently small with respect to grain size in all the cases considered.

The results of the effective toughness as a function of the average number of grains per unit length (proportional to the square root of the total number of grains) are represented in Fig.4.13a. On the same figure, the crack paths for 3 RVE sizes are represented in Fig.4.13b, and the average stress/strain behavior for the RVEs with 18 and 460 grains are represented in Fig.4.13c, including statistical dispersion.

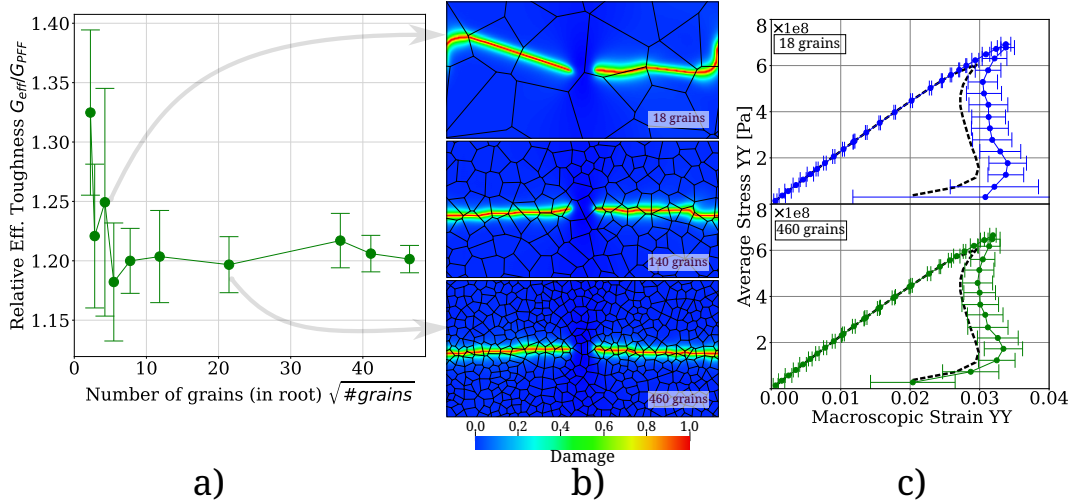


Figure 4.13: Parametric study on grain average number over polycrystal RVE volume: a) effective toughness estimates for various grain average number. b) Examples of crack path for the groups with grain average number of 18 (above), 140 (middle) and 460 (below) grains. c) Stress/strain curves for the entire groups of grain average number of 18 (above) and 460 (below).

In Fig.4.13a it is observed that the effective toughness shows an increase of 20% to 35% for all the RVE sizes considered and that this value seems to converge for a high number of grains, as also reported Ernesti and Schneider, 2022. As expected, standard deviation also decreases with RVE size, as it happens when homogenizing, for example, the mechanical response. Regarding the toughening mechanism, as expected, it is independent of the RVE size and always corresponds to crack path changes. Looking at the average stress-strain curves (Fig.4.13c) it can be observed that the qualitative average response of the polycrystal with respect to the homogeneous material is very similar to that of the study of β in the last subsection. Only when the number of grains is very small does the coalescence part of the stress-strain curve change with respect to the homogeneous materials. This effect is due to the periodicity and becomes negligible for sufficiently large RVEs.

Chapter 5

Comparison between PFF in FEM and FFT-based solvers: application to elastic and elastoplastic polycrystals

This chapter has two main objectives. The first is to extend the Phase-Field Fracture (PFF) model, in its classical strain-controlled version, to plasticity models within a finite strain framework, using the FFT-based solver introduced in previous chapters. The second objective is to compare the resulting implementation in the FFT solver with an equivalent one based on the Finite Element Method (FEM). This comparative study is essential to validate the mechanical response of the implementation against a more established numerical scheme, and to further analyze the numerical differences between both approaches. The mechanical response is evaluated in a complex scenario involving plasticity and fracture of polycrystalline microstructures, including the study of brittle elastic fracture in such materials.

The microstructure of polycrystalline metals consists of an aggregate of single crystal grains, with specific size, shape, and orientation. This structure plays a key role in their elastic, plastic, and fracture behavior. For fracture, especially in early crack growth, models that resolve microstructure explicitly are crucial, as fracture is a localized phenomenon. In brittle fracture, where plasticity is mostly confined near the crack tip, fracture mechanics-based models are preferred. PFF provides a robust framework for simulating crack growth, but as mentioned previously, it does not rigorously account for nucleation (Lopez-Pamies et al., 2025). An initial crack must be introduced to maintain predictive accuracy (Singh et al., 2016; Zambrano et al., 2023), and this chapter emphasizes proper crack initialization.

PFF has been used to model fracture in various heterogeneous, anisotropic materials, as discussed in chapter 4. Its first extensions to elastic-plastic materials focused on J2 plasticity (Alessi et al., 2018), while Crystal Plasticity models (reviewed in chapter 2) have been widely applied to polycrystals, and its coupling with PFF models was initially proposed by De Lorenzis et al., 2016 and by Diehl et al., 2017. Most of the implementations of this model since use FEM due to its flexibility with complex geometries. However, as noted in chapter 1, FFT-based solvers have gained interest for micromechanical fracture, and works including a

combination of PFF and crystal plasticity models on FFT-based solvers have also been made (Cui et al., 2023; Lucarini et al., 2023).

Of the two goals of this chapter, the comparison with FEM is especially relevant. While FEM-based PFF implementations are well studied, FFT-based approaches remain newer and less explored. Although both should ideally yield similar microstructural responses, their inherent differences require careful quantitative comparison—especially in how initial cracks are represented. As noted in chapter 1, prior FEM-FFT comparisons (Liu et al., 2010; Lucarini et al., 2023; Zarzoso et al., 2025; Zeman et al., 2017) do not cover PFF models, not even for elastic cases. This chapter addresses that gap by incorporating elasto-plastic fracture simulations.

5.1 PFF model extension to crystal plasticity

The PFF model adopted in this study follows the variational hybrid scheme proposed by Ambati et al., 2015b, which employs spectral-separated energy functionals and introduces the presence of a crack through isotropic damage fields. In order to extend the model to crystal plasticity in a finite strain scheme, the extension procedure to the J2 plasticity model at section 2.3.3 is followed, and the theory of CP models summarized in section 2.4 is considered.

Same elements of the PFF at small strain are considered, where ℓ is the characteristic length scale parameter, Γ will consider the AT2 functional in Eq.(2.23), being γ_f the crack density functional. With this, and Eq.(2.54), the material internal energy functional can be derived from the power-dissipation imbalance at the first part of Eq.(5.1), as discussed by Gurtin et al., 2010, which also resembles the energy balance at Eq.(2.15) but captures both the fracture and plastic contributions. The definition of the internal energy functional considering plasticity has been developed for a small strain scheme in Eq.(2.39), but for elastoplastic materials in a finite strain scheme, it must consider the correct spatial configurations at Fig.2.5

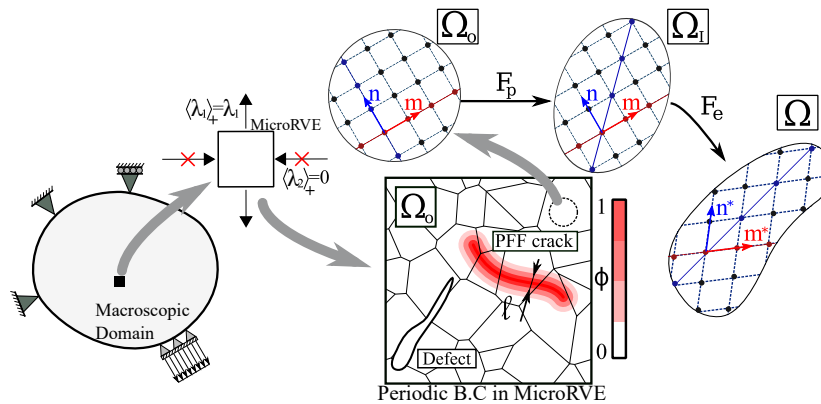


Figure 5.1: Phase-field crack representation and field scheme.

Therefore, the representation of fracture can be stated in a micromechanical media at the reference configuration (Fig.2.5), in which the microstructure volume Ω_o is the material start point as represented in Fig.5.1. The functional at Eq.(2.39) accounts for the total dissipation

$\mathcal{D}_t$, which includes both fracture and plastic dissipation. Rewriting this relation considering the spatial large strain configurations, we get

$$\begin{aligned} \dot{\Pi}_{int} - \int_{\Omega_I} \dot{\psi}(\mathbf{E}_e, \gamma^\alpha, \phi) d\Omega_I &= \int_{\Omega_o} \mathcal{D}_p + \mathcal{D}_f d\Omega_o \geq 0 \\ \Rightarrow \dot{\Pi}_{int} &= \int_{\Omega} \left(\dot{\psi}(\mathbf{E}_e, \gamma^\alpha, \phi) + G_c \dot{\gamma}_f(\phi) + \mathcal{D}_p \right) J^{-1} d\Omega. \end{aligned} \quad (5.1)$$

Here, $\mathcal{D}_p = \dot{D}_p$ is the rate of the equivalent plastic dissipation functional D_p at Eq.(2.39) of the small strain scheme, and represents the dissipation power associated with plastic processes defined in the reference configuration (Gurtin et al., 2010). The fracture contribution is defined at Ω_o through the rate of the fracture dissipation functional of Eq.(3.9), called here D_f , as $\mathcal{D}_f = \dot{D}_f = G_c \dot{\gamma}_f$, where $\dot{\gamma}_f$ is the rate of crack growth (Ambati et al., 2016; M. Borden et al., 2018). The right hand side of Eq.(5.1) has sense since the equivalence $J^{-1} d\Omega = d\Omega_o = d\Omega_I$ with $J = \det \mathbf{F} = \det \mathbf{F}_e$ representing the volume change factor, allows us to define any energy density functional in the intermediate configuration and the reference configuration without any mathematical inconsistency, which will be done from now on. Furthermore, it is evident that the functional ψ now depends on both ϕ and γ^α , which couples the mechanical behavior with the evolution of fracture and with plasticity. As with the model of previous chapters, the minimization of Eq.(5.1) leads to the set of governing equations that describe crack propagation alongside the respective mechanical fields.

However, in addition to the definition of internal power in Eq.(5.1), this functional can be derived from a stress balance perspective, considering both the elastic and plastic microscopic stress fields (De Lorenzis et al., 2016; Gurtin et al., 2010), while neglecting the effects of the strain gradient theory. In combination with Eq.(5.1), the following equation must hold,

$$\dot{\Pi}_{int} = \int_{\Omega_o} \mathbf{S} : \dot{\mathbf{E}}_e + \sum_{\alpha} \tau^\alpha \dot{\gamma}^\alpha d\Omega_o = \int_{\Omega_o} \dot{\psi} + G_c \dot{\gamma}_f + \mathcal{D}_p d\Omega_o. \quad (5.2)$$

From Eq.(5.2), it is evident that a precise definition of the energy functionals is necessary. As stated at the beginning of this section, the effect of the PFF damage on the material behavior is reflected through the anisotropic degradation of the free energy functional, which can be decomposed into its elastic and plastic counterparts, with the elastic energy further decomposed into positive and negative parts:

$$\psi(\mathbf{E}_e, \gamma^\alpha, \phi) = \psi_e(\mathbf{E}_e, \phi) + \psi_p(\gamma^\alpha, \phi) = g(\phi)\psi_{eo}^+ + \psi_e^- + g_p(\phi)\psi_p. \quad (5.3)$$

From the energy density expression on a CP model in Eq.(2.54), ψ_e and ψ_p represent the elastic and plastic contributions to the stored energy density, which must be defined within the framework of the PFF model. To express the formulation in the deformed configuration, with the Green-Lagrange deformation defined in the intermediate one, it is necessary to include the volume change factor J . As also is described at section 2.3.3, coupling the materials behavior to fracture is achieved with degradation functions $g(\phi)$, $g_d(\phi)$ and $g_p(\phi)$ at Eq.(2.39). Specifically, we consider $g(\phi) = (1 - \phi)^2 + k$, where k is a small numerical parameter, and $g_p(\phi) = g_d(\phi) = 1$ to ensure that the material's hardening remains unaffected by damage, following the approach by Duda et al., 2015. This election is significant, as mentioned in section 2.3.3, since the representation of ductile crack propagation can be emulated just by

the inclusion of plastic energetic functionals (Alessi et al., 2018). By neglecting the plastic degradation functions, the fracture behavior tends to be brittle, despite the presence of plasticity in the material, as in the model of Duda et al., 2015. While this approach might not fully represent the material's response in scenarios involving large deformations, where plastic effects dominate leading to purely ductile fracture, it is well-suited for cases where materials exhibit appreciable plasticity but ultimately fracture in a brittle manner.

The positive and negative decomposition of the elastic energy density in Eq.(5.3) is defined by the spectrally decomposed positive and negative counterparts of the Green-Lagrange tensor (Gurtin et al., 2010), similar to the spectral decomposition of Eq.(2.19) in section 2.3. Specifically, the positive and negative components of the Green-Lagrange strain tensor are given by $\mathbf{E}_e^\pm = \sum_i < \zeta_i >_\pm \vec{e}_{vi} \otimes \vec{e}_{vi}$ where ζ_i and $\vec{e}_{vi}$ are correspondingly the eigenvalues and eigenvectors of $\mathbf{E}_e$, and the operator $< \bullet >_\pm$ corresponds to the positive and negative Macaulay brackets. Despite Eq.(2.19) having a clear separation of the positive and negative parts of the density that can be achieved due to the elastic definition of the material behavior, the general decomposition of Eq.(5.4) needs to be assumed for an elastoplastic one,

$$\psi_{eo}^+ = \frac{1}{2} \mathbb{C}_o : \mathbf{E}_e^+ : \mathbf{E}_e^+ \quad (5.4a)$$

$$\psi_e^- = \mathbb{C}_o : \mathbf{E}_e^+ : \mathbf{E}_e^- + \frac{1}{2} \mathbb{C}_o : \mathbf{E}_e^- : \mathbf{E}_e^-, \quad (5.4b)$$

where $\mathbb{C}_o$ represents the undamaged elastic stiffness. This formulation ensures that the negative components of deformation don't contribute to the damage evolution, as depicted in Fig.5.1 and specified in Eq.(5.3) where the negative part of energy is not affected by $g(\phi)$. Considering that $\mathcal{D}_f(\phi) = \int G_c \gamma_f' \dot{\phi} d\Omega_o$, where γ_f' denotes the scalar derivative with respect to ϕ at Eq.(2.30), the formulation of Eq.(5.2) can be extended to:

$$\int_{\Omega_o} \mathbf{S} : \dot{\mathbf{E}}_e + \sum_\alpha \tau^\alpha \dot{\gamma}^\alpha - \left(g(\phi) \frac{\partial \psi_{eo}^+}{\partial \mathbf{E}_e} - \frac{\partial \psi_e^-}{\partial \mathbf{E}_e} \right) : \dot{\mathbf{E}}_e - \sum_\alpha \frac{\partial \psi_p}{\partial \gamma^\alpha} \dot{\gamma}^\alpha - g'(\phi) \psi_{eo}^+ \dot{\phi} d\Omega_o = \int_{\Omega_o} \mathcal{D}_p + \mathcal{D}_f d\Omega_o \quad (5.5)$$

From this expression and following the same procedure at section 2.3.3, three key inferences can be drawn:

- Motivated by Eqs. (2.54) and (5.3), the intermediate second Piola-Kirchhoff stress tensor, $\mathbf{S}$, is defined based on the the elastic energy as follows:

$$\mathbf{S} = g(\phi) \frac{\partial \psi_{eo}^+}{\partial \mathbf{E}_e} + \frac{\partial \psi_e^-}{\partial \mathbf{E}_e} \quad (5.6)$$

- Considering the time derivative of the plastic energy density in Eq.(5.5), the definition of the plastic dissipation can be inferred:

$$\int_{\Omega_o} \sum_\alpha \tau^\alpha \dot{\gamma}^\alpha - \sum_\alpha \frac{\partial \psi_p}{\partial \gamma^\alpha} \dot{\gamma}^\alpha d\Omega_o = \int_{\Omega_o} \mathcal{D}_p d\Omega_o \geq 0 \quad (5.7)$$

- Using Eqs. (5.5)-(5.7), we obtain the following expression, with the energy density ψ_{eo}^+ reasonably written in the reference configuration:

$$\int_{\Omega_o} G_c \gamma_f' \dot{\phi} + g'(\phi) \psi_{eo}^+ \dot{\phi} d\Omega_o = 0 \Rightarrow \left[\frac{G_c}{\ell} + 2\psi_{eo}^+ \right] \phi - G_c \ell \nabla^2 \phi = 2\psi_{eo}^+ \quad (5.8)$$

Finally, this approach yields the balance equations that govern both the mechanical and damage evolution in the material, linking the deformation and fracture processes. In Eq.(5.8) a Helmholtz-type constitutive equation for ϕ is formulated, derived by neglecting $\dot{\phi}$ under the assumption that it is always positive. Finally, the mechanical governing equation is obtained from the principle of virtual power, where the internal power of Eq.(5.2) is now defined in the deformed configuration. The external power is computed while neglecting the effects of strain gradient theory, as well as any body and inertial forces, ensuring the focus remains on the macroscopic deformation and fracture behavior:

$$\underbrace{\int_{\Omega} \boldsymbol{\sigma} : \mathbf{L}_e + J^{-1} \sum_{\alpha} \tau^{\alpha} \dot{\gamma}^{\alpha} d\Omega}_{P_{\text{int}}} = \underbrace{\int_{\partial\Omega} \vec{t} \cdot \dot{\vec{u}} d\partial\Omega}_{P_{\text{ext}}} \quad (5.9)$$

where $\mathbf{L}_e$ is the power conjugate of the Cauchy stress, defined in Eq.(2.51) and $\vec{t}$ the external boundary traction, fulfilling anti-periodicity in the contour in the case of periodicity. Using the definition of the resolved shear stress from Eq.(2.55) and the definition of the plastic velocity gradient from Eq.(2.61), we derive the first part of Eq.(5.10). Next, by employing Eqs. (2.53a) and leveraging the properties of the double contraction operator, we obtain the second part of Eq.(5.10). Finally, by considering the formulation of $\mathbf{L}$ in Eq.(2.51), we derive the third part of Eq.(5.10), which becomes the last part through the kinematical definition of $\mathbf{L}$:

$$\int_{\Omega} \boldsymbol{\sigma} : \mathbf{L}_e + J^{-1} \mathbf{F}_e^T \mathbf{F}_e \mathbf{S} : \mathbf{L}_p d\Omega = \int_{\Omega} \boldsymbol{\sigma} : (\mathbf{L}_e + \mathbf{F}_e \mathbf{L}_p \mathbf{F}_e^{-1}) d\Omega = \int_{\Omega} \boldsymbol{\sigma} : \mathbf{L} d\Omega = \int_{\Omega} \boldsymbol{\sigma} : \nabla_x \dot{\vec{u}} d\Omega, \quad (5.10)$$

where the reader should note that the divergence operator is realized in the current configuration. To set up the problem, we apply integration by parts to the final term in Eq.(5.10) and substitute it into Eq.(5.9). By separating integrals into those defined over the volume and the boundaries, and under the assumption that for an accurate physical representation $\dot{\mathbf{u}}$ is never null, we obtain the expressions for mechanical equilibrium at the domain and in the boundaries respectively:

$$\nabla_x \cdot \boldsymbol{\sigma} = 0 \quad (5.11a)$$

$$\int_{\partial\Omega} \boldsymbol{\sigma} \hat{n} \cdot \dot{\vec{u}} d\partial\Omega = \int_{\partial\Omega} \vec{t} \cdot \dot{\vec{u}} d\partial\Omega. \quad (5.11b)$$

It is important to note that Eq.(5.11a) is formulated entirely in the current configuration. An equivalent formulation in the reference configuration related to the first Piola-Kirchhoff stress $\mathbf{P}$ can be obtained by means of $\mathbf{S}$, following Eq.(2.53a) and Eq.(2.53b) (De Souza Neto et al., 2008). Both stress measures are affected by damage, but to implement the hybrid method where the stress is obtained from an isotropically-affected elastic energy functional (Ambati et al., 2015b), Eq.(5.6) must be approximated as follows:

$$\mathbf{S} \approx g(\phi) \frac{\partial(\psi_{eo}^+ + \psi_e^-)}{\partial \mathbf{E}_e} = g(\phi) \mathbf{S}_o \quad (5.12a)$$

$$\mathbf{P} = g(\phi) J \mathbf{F}_e \mathbf{S}_o \mathbf{F}_e^T \mathbf{F}_e^{-T} = g(\phi) \mathbf{P}_o, \quad (5.12b)$$

The terms $\mathbf{P}_o$ and $\mathbf{S}_o$ represent the non-damaged versions of the respective hybrid stress tensor. The positive/negative separation of the energy, established in Eq.(5.4), is specifically used to

define the damage field from the Helmholtz relation in Eq.(5.8), where the undamaged positive elastic contribution of the free energy serves as the driving force. As previously mentioned, it must be ensured that the condition $\dot{\phi} \geq 0$ holds, so the history variable of Eq.(3.5) is used. By transitioning the system plotted in Eq.(5.11a) to the reference configuration and by incorporating this history variable, the final system of governing equations is obtained. This system, which includes Eq.(5.12b) along with the history-dependent term, forms the complete set of equations to be solved:

$$\nabla_X \cdot g(\mathcal{H})\mathbf{P}_o = 0 \quad (5.13a)$$

$$\left[\frac{G_c}{\ell} + 2\mathcal{H} \right] \phi - G_c \ell \nabla^2 \phi = 2\mathcal{H}. \quad (5.13b)$$

5.2 Numerical implementation

The following section presents the numerical schemes developed to introduce the PFF model. This implementation encompasses both the (i) FFT (section 5.2.1) and (ii) FEM (section 5.2.2) formulations.

5.2.1 FFT-based numerical scheme

The implementation of the PFF-FFT scheme is made in the same FFT-based homogenization code FFTMAD (Lucarini and Segurado, 2019a; Lucarini et al., 2021). The three-dimensional domain Ω_o is discretized into a set of Fourier integration points (voxels) referred to an orthonormal basis. Using the Fourier space, functions and fields are represented as trigonometric polynomials, which are defined by the discrete values of these fields at the spatial points.

Since the system from Eq.(5.13b) is only convex with respect to ϕ and Eq.(5.13a) only with respect to $\mathbf{F}$ (Gerasimov and De Lorenzis, 2016), the problem is decoupled into the same staggered sequential sub-problems defined in section 3.1.1 for the elastic problem, with one sub-problem solving the mechanical equilibrium (Eq.(5.13a)), considering a constant damage field and the second addressing the damage evolution equation (Eq.(5.13b)), assuming a constant deformation gradient. The full system in Eq.(5.13) is solved at each time step n by a fixed-point implicit scheme (Miehe et al., 2010a).

This time, the equilibrium problem requires calculating the stress state $\mathbf{P}(\mathbf{F}, \beta, \phi)$ constitutively. Due to the elasto-plastic nature of the material and the spectral energy decomposition, this problem is highly non-linear and needs to be linearised. This linearization is achieved by decomposing the deformation gradient into its fluctuating and average components $\mathbf{F} = \widetilde{\mathbf{F}} + \overline{\mathbf{F}}$ as in Eq.(2.10). The average part can be directly related to the macroscopic deformation gradient, which is specified as an input in the numerical scheme in every time-step. To focus the solution process on the fluctuating component, the problem in Eq.(5.13a) is reformulated by means of a Fourier-Galerkin scheme (Vondřejc et al., 2014) with a mixed-control scheme (Lucarini et al., 2021), which implies that some components of $\overline{\mathbf{F}}$ are not given but are determined as functions of the imposed macroscopic Piola-Kirchoff stress $\overline{\mathbf{P}}$. A direct outcome of this weak form formulation is the derivation of the following integral equation, similar to

the one at Eq.(2.66):

$$\int_{\Omega} \boldsymbol{\zeta}(\mathbf{x}) : (\mathbb{G} * \mathbf{P}(\mathbf{F}, \beta, \phi) - \bar{\mathbf{P}}) d\Omega = 0, \quad (5.14)$$

where $\boldsymbol{\zeta}$ are arbitrary test functions and $\mathbb{G}$ is the Galerkin operator defined in Eq.(2.68) that includes mixed conditions as depicted in Eq.(2.69). In this study, the parameter $\bar{\mathbf{P}}$ at Eq.(5.14) is set to be zero, which implies that the stress-controlled components will emulate free displacement conditions. Then, the following formulation is equivalent to the one in Eq.(3.2):

$$\mathcal{F}^{-1} \left\{ \hat{\mathbb{G}} : \mathcal{F} \{ \mathbf{P}(\mathbf{F}, \beta, \phi) \} \right\} = \mathbf{0}. \quad (5.15)$$

The $\mathbb{G}$ projection operator used is described at Eq.(2.69) for applying mixed conditions. This version of the projector is designed to filter out the average part of a field during a convolution like the one shown at Eq.(2.69) for the strain-controlled components identified with the inclusion of the control tensor called $\mathbf{c}$ in Eq.(2.69). With this formulation, the non-linear transformation of the stress tensor at Eq.(5.15) can be defined as the operator $\mathcal{G}(\mathbf{F}_i, \beta, \phi_i)$ in $\mathbb{R}^{6n_x n_y n_z}$, where $\mathcal{G}(\bullet) = \mathcal{F}^{-1} \left\{ \hat{\mathbb{G}} : \mathcal{F} \{ \bullet \} \right\}$. In the above-mentioned staggered scheme, where i denotes the current number of increments, the increment of the deformation gradient $\Delta \mathbf{F}_i$ and the last iterated value of the deformation gradient $\mathbf{F}_i = \bar{\mathbf{F}} + \sum_{j=1}^{i-1} \Delta \mathbf{F}_j$ are used to construct the following linearization of the first Piola-Kirchhoff stress tensor, which is similar to the one at Eq.(3.1).

$$\begin{aligned} \mathbf{P}(\mathbf{F}_i + \Delta \mathbf{F}, \beta, \phi_i) &\approx \mathbf{P}(\mathbf{F}_i, \beta, \phi_i) + \mathbb{K}_i(\mathbf{F}_i, \beta, \phi_i) : \Delta \mathbf{F} \\ \text{being } \mathbb{K}_i(\mathbf{F}_i, \beta, \phi_i) &= \frac{\partial \mathbf{P}(\mathbf{F}_i, \beta, \phi_i)}{\partial \mathbf{F}_i}, \end{aligned} \quad (5.16)$$

where the last iterated damage ϕ_i is constant for the resolution of this equation and an additional set needs to be defined for the plastic internal variables, as $\beta = [\mathbf{F}_p, s^\alpha, \gamma^\alpha]$. Combining Eqs. (5.15) and (5.16), the system of linear equations in Eq.(5.17) is defined as:

$$\mathcal{G} [\mathbb{K}_i(\mathbf{F}_i, \beta, \phi_i) : \Delta \mathbf{F}] = -\mathcal{G} [\mathbf{P}(\mathbf{F}_i, \beta, \phi_i)]. \quad (5.17)$$

This system can be solved iteratively, which allows us to solve for $\Delta \mathbf{F}$ without assembling the matrix $\mathbb{K}$ explicitly. In this work, a conjugate gradient method is used over the operator defined with the left-hand side of Eq.(5.17) respect to $\Delta \mathbf{F}$ and the vector defined by the right-hand side of Eq.(5.17). This is possible since the stress field $\mathbf{P}_i$ and the instantaneous tangent $\mathbb{K}_i$ are given in every iteration i by the constitutive relations defined in sections 2.4 and 5.1. Once $\Delta \mathbf{F}$ is obtained, it is used to update the deformation gradient as $\mathbf{F}_{i+1} = \bar{\mathbf{F}} + \sum_{j=1}^i \Delta \mathbf{F}_j$, which is used in the next iteration. This procedure is repeated until $\mathbf{F}_{i+1}$ fulfills Eq.(5.15).

For the damage calculation part of the scheme at Eq.(5.13b), the problem is exactly the same as the one treated at section 3.1.1, considering the history variable $\mathcal{H}$ and the conjugate gradient solution with preconditioning (with α as preconditioner). An equivalent algorithm is also used, but adapted to the finite strains scheme. This adaptation is depicted at algorithm 3 with a similar structure to the algorithm 1, where both stagger and time cycles are identified with the sub-index $\square_i$ and the superscript $\square^n$ respectively. The numerical over-relaxation parameter α is also used here to address numerical instabilities, but its evolution fits the definition of the adaptive over-relaxation parameter defined for the monolithic scheme of

Eq.(4.19) in section 4.3.1. Both stagger sub-problems are solved sequentially, using an error definition similar to the one at Eq.(3.8b), where $\|\bullet\|$ is the Euclidean norm of a vector or tensor field.

$$err_{sta} = max \left(\frac{\|\mathbf{F}_{i+1} - \mathbf{F}_i\|}{\|\mathbf{F}_{i+1}\|}, \frac{\|\phi_{i+1} - \phi_i\|}{\|\phi_{i+1}\|} \right). \quad (5.18)$$

Algorithm 3 : FFT implicit staggered scheme with deformation gradient control

```

1: initial data:  $\widetilde{\mathbf{F}}^0 = 0, \mathbf{F}^0 = 0, \phi^0 = 0, \mathcal{H}^0 = 0, \beta^0 = 0$ 
2: Control variable  $\Delta \widetilde{\mathbf{F}}$  fixed
3: Time index:  $n = 0$ 
4: while  $t^{n+1} < t_{final}$  do
5:   Initiate stagger fields:  $\mathbf{F}_0 = \mathbf{F}^n + \Delta \widetilde{\mathbf{F}}$  ;  $\phi_0 = \phi^n$ 
6:   Evaluate constitutive equation  $\Rightarrow$  find  $\mathbf{P}_0 = \mathbf{P}(\mathbf{F}_0, \beta^0, \phi_0)$  and  $\mathbb{K}_0 = \frac{\partial \mathbf{P}}{\partial \mathbf{F}} \Big|_{\mathbf{F}_0}$ 
7:   Stagger solver index:  $i = 0$ 
8:   while  $err_{sta} \geq tol_{sta}$  do
9:     Mech. solver FFT: find  $\Delta \widetilde{\mathbf{F}}(\mathbf{P}_i, \mathbb{K}_i, \phi_i)$  that fulfills Eq.(5.17)
10:    Update strain:  $\mathbf{F}_{i+1} = \mathbf{F}_i + \alpha \Delta \widetilde{\mathbf{F}}$ 
11:    Helm. solver FFT: find  $\phi_{i+1} = \phi(\mathcal{H}^n)$  that fulfills Eq.(3.7)
12:    Evaluate constitutive equation: find  $\mathbf{P}, \psi_o^+$  and  $\mathbb{K}$  such that:
13:       $\mathbf{P}_{i+1} = \mathbf{P}(\mathbf{F}_{i+1}, \beta^n, \phi_{i+1})$  ;  $\mathbb{K}_{i+1} = \frac{\partial \mathbf{P}}{\partial \mathbf{F}} \Big|_{\mathbf{F}_{i+1}}$  ;  $\psi_{o+1}^+ = \psi_o^+(\mathbf{F}_{i+1})$  ;  $\beta_{i+1} = \beta(\mathbf{F}_{i+1}, \beta^n)$ 
14:      Update History:  $\mathcal{H}^{n+1} = max(\psi_{o+1}^+, \mathcal{H}^n)$ 
15:      Stagger index update:  $i = i + 1$ 
16:   end while
17:   Update strain and damage:  $\phi^{n+1} = \phi_{i+1}$  ;  $\mathbf{F}^{n+1} = \mathbf{F}_{i+1}$  ;  $\beta^{n+1} = \beta_{i+1}$ 
18:   Time index update:  $n = n + 1$ 
19: end while

```

5.2.2 FEM-based numerical scheme

This section introduces the PFF-FEM formulation approach for elasto-plastic polycrystals used for comparison in this chapter. For this, the domain is discretised in a mesh of quadrilateral elements using the commercial software ABAQUS. There, both the displacement field and the phase-field parameter are interpolated in terms of their nodal contributions, averaged by the matrix operator $\mathbf{N}(\vec{\varrho}_c)$ which collects the standard linear shape functions at the element level. There, the vector $\vec{\varrho}_c = \{\varrho_{c1}, \varrho_{c2}, \varrho_{c3}\}$ represents natural coordinates for each element in the 3D case. In addition to this, we also consider the matrix $\mathbf{B}$ which contains the derivative of the shape functions for the 3D setting,

$$\mathbf{B}_a = \begin{bmatrix} N_{a,1} \\ N_{a,2} \\ N_{a,3} \end{bmatrix} \quad (5.19)$$

where the notation $\square_{a,J}$ is used to express the derivative of a variable $\square$ with respect to $\vec{X}_J$ associated with node a .

Analog to section 5.2.1, we solve the equilibrium at Eq.(5.13a) and the phase-field damage at Eq.(5.13b) equations separately following an implicit staggered scheme over both sub-problems. With these considerations, the weak form of the nonlinear equations after the insertion of these interpolation schemes is given by

$$\delta\Pi_u = (\delta\bar{u})^T \int_{\Omega_0} \mathbf{B}^T g(\phi) \mathbf{P} \, dV = 0 \quad (5.20a)$$

$$\delta\Pi_\phi = (\delta\bar{\phi})^T \int_{\Omega_0} \bar{\mathbf{N}}^T \left(g'(\phi) \mathcal{H} + \frac{G_c}{\ell} \phi \right) dV + (\delta\bar{\phi})^T \int_{\Omega_0} G_c \ell \bar{\mathbf{B}}^T \bar{\mathbf{B}} \bar{\phi} \, dV = 0. \quad (5.20b)$$

The residuals that are required for the nonlinear Newton-Raphson solution scheme of the corresponding FEM problem take the form:

$$\mathbf{r}_u^i = - \int_{\Omega_0} \mathbf{B}^T g(\phi) \mathbf{P} \, dV = 0 \quad (5.21a)$$

$$\mathbf{r}_\phi^i = \int_{\Omega_0} \left[\bar{\mathbf{N}}^T \left(g'(\phi) \mathcal{H} + \frac{G_c}{\ell} \phi \right) + G_c \ell \bar{\mathbf{B}}^T \bar{\mathbf{B}} \bar{\phi} \right] dV = 0 \quad (5.21b)$$

From a numerical perspective, the FEM formulation is implemented within the implicit framework of the **ABAQUS** package using the user-defined **UEL** (User Element) and the **UMAT** (User Material) capabilities. Specifically, the staggered solution method employed to solve the discretized system of equations follows the approach outlined in the work of Molnár and Gravouil, 2017. In this method, at each time step, the current displacement is calculated using the phase-field value from the previous step, while the current phase-field is determined based on the energy history as in steps 9 and 11 at algorithm 3. Consequently, the weak form of the displacement problem at time step $n + 1$ is expressed as,

$$\mathbf{r}_u^i = - \int_{\Omega_0} \mathbf{B}^T g(\phi^n) \mathbf{P} dV = 0 \quad (5.22)$$

This equation is solved for $\vec{u}$, assuming ϕ^n known from the previous time step. The phase-field problem is analogously written as,

$$\mathbf{r}_\phi^i = - \int_{\Omega_0} \left[\bar{\mathbf{N}}^T \left(g'(\phi) \mathcal{H}^{n+1} + \frac{G_c}{\ell} \phi \right) + G_c \ell \bar{\mathbf{B}}^T \bar{\mathbf{B}} \bar{\phi} \right] dV = 0 \quad (5.23)$$

where the history variable in the step $n + 1$ is defined equivalently as in Eq.(3.5). Finally, the consistent tangent matrix is computed by performing the consistent linearization of the residual equations as in previous chapters. Consequently, the global system of equations is expressed as,

$$\begin{bmatrix} \mathbf{K}^{uu} & \mathbf{0} \\ \mathbf{0} & \mathbf{K}^{\phi\phi} \end{bmatrix} \begin{bmatrix} \Delta\bar{u} \\ \Delta\bar{\phi} \end{bmatrix} = \begin{bmatrix} \mathbf{r}_u \\ \mathbf{r}_\phi \end{bmatrix}. \quad (5.24)$$

The resolution process over this system is summarized in algorithm 4, following a similar sub-index structure than other algorithms in this work, where variables corresponding to the stagger and time schemes are again identified by the super-index $\square^n$ for time and the sub-index $\square_i$ for stagger iterations. When comparing the convergence criterion with the FFT

method, the expression for error in the FEM follows the average criterion used for ABAQUS problems.

$$err_{sta} = \max(||\mathbf{F}_{i+1}||, ||\phi_{i+1}||). \quad (5.25)$$

Hence, just the Euclidean norm of the residuals is followed for the convergence of the increments, thus following a less strict criterion for the FEM method.

Algorithm 4 : Implicit staggered FEM scheme with displacement control

```

1: initial data:  $\mathbf{u}^0 = 0, \phi^0 = 0, \mathcal{H}^0 = 0, \beta^0 = 0$ 
2: Control variable  $\Delta \mathbf{u}$  fixed
3: Time index:  $n = 0$ 
4: while  $t^{n+1} < t_{final}$  do
5:   Initiate staggered fields:  $\vec{u}_0 = \vec{u}^n + \Delta \vec{u}$  ;  $\phi_0 = \phi^n$ 
6:   Evaluate constitutive equation: find  $\mathbf{P}_0 = \mathbf{P}(\mathbf{F}_0, \beta^0, \phi_0)$  and  $\mathbb{K}_0 = \frac{\partial \mathbf{P}}{\partial \mathbf{F}} \Big|_{\mathbf{F}_0}$ 
7:   Stagger index:  $i = 0$ 
8:   while  $err_{sta} \geq tol_{sta}$  do
9:     Mech. solver FFM: find  $\Delta \vec{u}(\mathbf{P}_i, \mathbb{K}_i, \phi_i)$  that fulfills Eq.(5.22).
10:    Update displacement:  $\vec{u}_{i+1} = \vec{u}_i + \Delta \vec{u}$ 
11:    Helm. solver FEM: find  $\phi_{i+1} = \phi(\mathcal{H}^n)$  that fulfills Eq.(5.23).
12:    Evaluate constitutive equation: find  $\mathbf{P}, \psi_o^+, \beta$  and  $\mathbb{K}$  such:
13:       $\mathbf{P}_{i+1} = \mathbf{P}(\mathbf{F}_{i+1}, \phi_{i+1})$  ;  $\mathbb{K}_{i+1} = \frac{\partial \mathbf{P}}{\partial \mathbf{F}} \Big|_{\mathbf{F}_{i+1}}$  ;  $\psi_{o+1}^+ = \psi_o^+(\mathbf{F}_{i+1})$  ;  $\beta_{i+1} =$ 
       $\beta(\mathbf{F}_{i+1}, \beta^n)$ 
14:    Update History:  $\mathcal{H}^{n+1} = \max(\psi_{o+1}^+, \mathcal{H}^n)$ 
15:    Stagger index update:  $i = i + 1$ 
16:   end while
17:   Update displacement and damage:  $\phi^{n+1} = \phi_{i+1}$  ;  $\vec{u}^{n+1} = \vec{u}_{i+1}$  ;  $\beta^{n+1} = \beta_{i+1}$ 
18:   Time index update:  $n = n + 1$ 
19: end while

```

5.2.3 The problem of prescribed initial cracks

As stated in section 4.3.3, PFF models are able to represent crack propagation, but their representation of crack nucleation is not ensured, and the modeling of a pre-crack is an open matter. For such modeling, several approaches have been mentioned in section 4.3.3, being a common choice to model notches with volumetric zones of negligible stiffness to emulate voids (Y. Chen et al., 2019), an approach that adequately fits for both FEM and FFT schemes. Since the objective of the chapter is to compare both schemes, this aspect makes it convenient to perform it.

In FEM, a crack modeled in this manner will have two nodes at the crack front, as depicted in Fig.5.2a. Once the crack propagates, this configuration results in a constant damage distribution between the rows corresponding to these two nodes (Bourdin et al., 2008). This process leads to a symmetrical accumulation of damage around the initial crack, with the maximum damage of the PFF crack being located between the two rows of nodes. A similar behavior is observed in FFT, where the crack is modeled as being one voxel thick, as shown

in Fig.5.2. As the crack propagates, the maximum damage is localized within a single voxel at the center, leading to a great resemblance between both schemes if the element size in FEM is the same as the voxel size (Fig.5.2) as adopted by Lucarini and Segurado, 2019b.

However, a full equivalence between two initial cracks modeled in this way in FEM and FFT is not trivial due to the inherent differences in discretization between FEM and FFT, as mentioned at chapter 1. FEM employs a mesh-based structure with local support interpolation on the elements while FFT relies on a regular grid and global support interpolation based on trigonometrical polynomials and values at the center of the voxels. The position of the fields and computed variables in FFT is defined in the center of each voxel. Conversely, in FEM, variables such as $\vec{u}$ and ϕ are interpolated from their values at the nodal points, while σ and ε are obtained in the integration points inside the element.

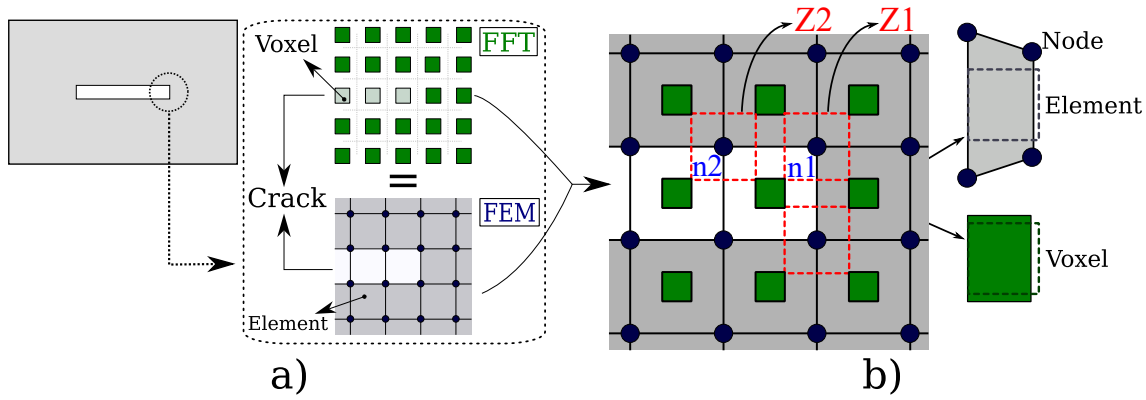


Figure 5.2: Discretization differences between FEM and FFT schemes when modeling discrete cracks.

If cracks are modeled as surfaces with void material and one element/voxel of thickness, as in Fig.5.2a, nodes adjacent to the initial crack can be highly influenced by the void material, as shown in Fig.5.2b for FEM. Specifically, the node labeled $n1$, whose zone of influence is marked as $z1$, is affected by three elements with the matrix material and one with void. On the other hand, the node marked as $n2$ perceives two elements of each material. This arrangement results in a gradient of strain within the finite element (Fig.5.2b), contrary to what happens in FFT where the solution at the voxel is homogeneous. Moreover, mesh/grid refinement will not eliminate the differences since the crack tip produces a singularity in stresses, and the way this singularity is represented in FEM and FFT is different.

An alternative option for modeling initial cracks is to use the Phase-Field enrichment strategies (CPFE), as the ones used at section 4.3.3, in which previous damage fields are used to model initial cracks. This approach improves the representation of initial cracks in PFF models by avoiding issues like energy singularities and critical point instabilities (Singh et al., 2016; Zambrano et al., 2023). Damage distributions are typically applied to enrich specific points at the crack tip (CTE in section 4.3.3) or to enrich the entire notch (CPFE in section 4.3.3). From this second option, this strategy can also be implemented around void material regions, ensuring compatibility with both FEM and FFT methods. In cases where FEM simulations show a higher local energy release rate, introducing a prescribed damage in FFT can make its response closer to the FEM results, due to the stiffness reduction in damaged voxels, which

increases the local energy release rate. Section 5.3 presents the numerical evidence of this issue.

For the application of the CPFE modeling in this chapter, a similar procedure to the one developed in section 4.3.3 is used, where the non-local regularization equation of Magri et al., 2021 is applied to obtain a smooth damage field ϕ_{ini} from a discrete one ϕ_0 ,

$$\phi_{ini} + \ell_0 \nabla^2 \phi_{ini} = \phi_0, \quad (5.26)$$

where ℓ_0 is the length of the initial regularization, defined to control the spatial influence of the CPFE modeling in order to resemble the initial crack influence present in the FEM model. In chapter 4 the objective was to include a CTE condition to eliminate the PFF nucleation energy, and the initial damage field was regularized only by means of a normalization. Nevertheless, this time the objective is to approach the FEM modeling of the crack, so a different procedure is proposed.

As illustrated in Fig.5.3a, the initial discrete distribution ϕ_0 is zero at all points, except for a single row of voxels of length L , where the distribution is constant and equal to ϕ_{0max} . Since ϕ_0 is discrete, the length L corresponds to a certain number of voxels, but the final damage distribution length must be measured with the crack surface functional defined in Eq.(2.23) as $\Gamma(\ell_0)$ (adjusted with the factor of section 3.2.1 to avoid length discrepancies). A property of Eq.(5.26) is that the resulting distribution ϕ_{ini} preserves the volume average of the ϕ_0 . Since the volume where ϕ_0 is non-zero is small compared to the RVE, this leads the maximum of ϕ_{ini} to be significantly smaller than the maximum of ϕ_0 . To define ϕ_{ini} in the range $[0, 1]$, it is convenient to allow ϕ_{0max} to exceed 1 to ensure that the final damage distribution ϕ_{ini} spans the entire range.

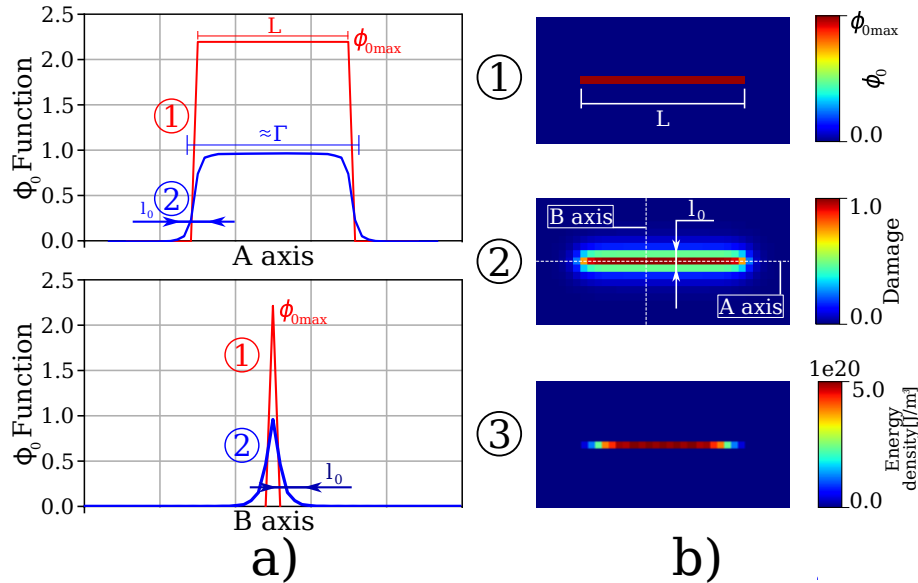


Figure 5.3: Crack tip enrichment initial condition generation for single point application on the material crack zone. a) Distribution of ϕ_0 function and the prescribed CPFE condition distribution. b) Steps of damage field generation and the corresponding energy field.

Parameters ϕ_{0max} , ℓ_0 , L , and Γ are selected following specific criteria. First, Γ and ℓ_0 are

chosen to match the length and the width (one element/voxel) of the elements row defining the crack at the FEM model to ensure the FFT distribution is aligned with FEM, but implying that the crack will be fixed to the discretization in both schemes. Despite ℓ_0 being derived from these criteria, simulation can still use the defined ℓ to solve the problem. Then, an iterative process is employed to find the value of ϕ_{0max} that minimizes L , limiting the search to the distribution of ϕ_{ini} being in the range $[0, 1]$. In addition, a row of voxels with void material corresponding to the length L is placed over this distribution, preventing highly damaged voxels from continuing to increase their values, which alleviates convergence in the first simulation steps. The outcome is a notch with an enriched surrounding damage field that affects the strain field, as is shown in Fig.5.3b.

Up to this point, only an initial damage distribution has been computed. In order to preserve the initial damage distribution in the subsequent iterations, the same formulation of Eq.(4.25) is used to obtain the conjugate energy distribution ψ_{ini} using Eq.(5.13b). This energy is added to the history driving force $\mathcal{H} = \max(\mathcal{H}_{-1}, \psi_{eo}^+ + \psi_{ini})$ as in section 4.3.3 (and as M. J. Borden et al., 2012). This new initial energy distribution is illustrated in Fig.5.3b. Evidence that the CPFE condition is necessary is shown in section 5.3.2 for elastic simulations without the PFF model, providing a comparison of the effects in FFT simulations with FEM, particularly in modeling the initial crack using zones of negligible stiffness.

5.3 Results and comparison

5.3.1 Simulation features

In the following section, a comparative analysis of the FEM and FFT schemes is made. Focusing on micromechanical fracture in heterogeneous domains, a RVE is defined in both schemes. The domain Ω_o is represented by sets of 3D cuboidal geometries with dimensions (L_x, L_y, L_z) along an orthonormal basis, discretized into a grid of (n_x, n_y, n_z) voxels/elements. All cases have been implemented to emulate 2D scenarios by imposing a unit thickness of one element/voxel along the $n_x = 1$ direction, with the lengths set as $L_x = L_y/10 = L_z/10$, effectively modeling the RVE as a 3D periodic plate, as shown in Fig.5.4a. To ensure consistency between the FEM and FFT models, equivalent displacement boundary conditions and macroscopic deformation have been implemented. The boundary conditions resemble plane strain conditions in a periodic medium under a tensile load applied in the Y direction.

In the FEM scheme, macroscopic boundary conditions are applied through nodes positioned at the corners of the plate, as depicted in Fig.5.4a. These master nodes enforce nodal displacements $(\mathbf{u}_x, \mathbf{u}_y, \mathbf{u}_z)$, with corresponding nodal restrictions (c_x, c_y, c_z) (where 0 denotes a free degree of freedom and 1 denotes an imposed displacement component), as depicted in Fig.5.4a. This setup facilitates the imposition of plane strain conditions, as illustrated in Fig.5.4b for the face containing the system origin. Periodic boundary conditions at the faces of the RVE ensure that the movement of the master nodes is mirrored across the boundaries marked in red and blue via multipoint constraints, as described in Fig.5.4b.

The parameters exemplified in Fig.5.4 are used in all FFT/FEM simulations resembling 2D geometry, and for the FEM scheme indicate that the Y -displacement component of the master

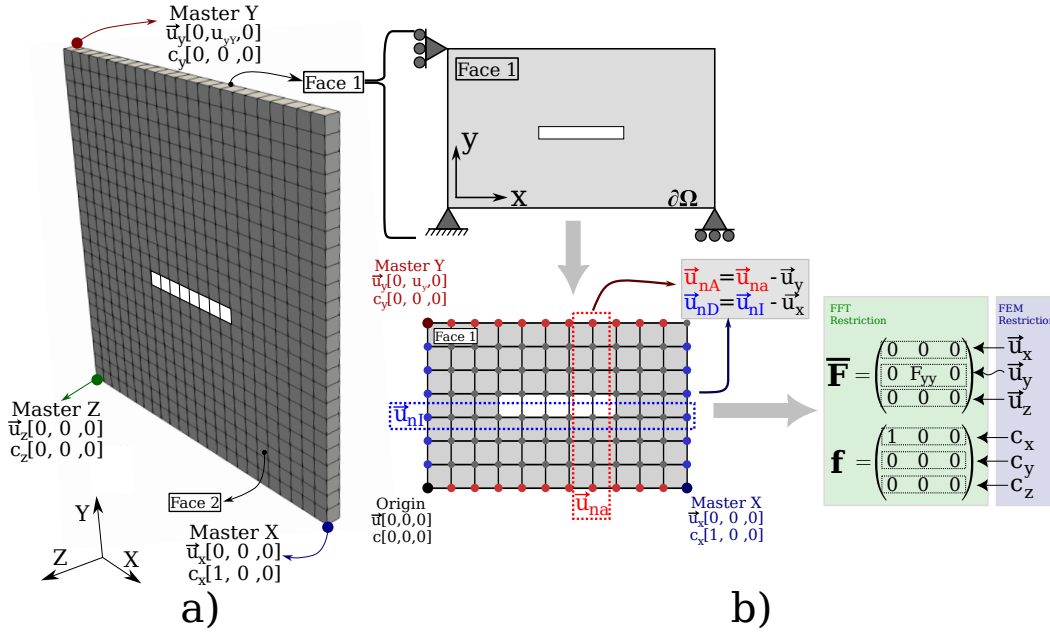


Figure 5.4: Simulation features and boundary condition scheme for simulations. a) 3D representation of the modeled plate. b) Representation of the simulation conditions.

node Y, u_{yY} , is the sole parameter governing the external load. This displacement component is defined as the simulation control variable, evolving with the value of $\Delta \vec{u}$ in algorithm 4. The same restrictions are imposed for the FFT scheme, using the $\vec{F}$ tensor described in section 5.2.1 and the $\vec{c}$ tensor at Eq.(2.69). Both tensors are also illustrated in Fig.5.4b, where the F_{yy} component of $\vec{F}$ serves as the time-dependent control variable. To ensure equivalence between both schemes, the relationship between F_{yy} in FFT and u_{yY} in FEM is given by the relation $F_{yy} = 1 + \frac{u_{yY}}{L_y}$, from equation $\vec{F} = \vec{I} + \frac{\partial \vec{u}}{\partial \vec{X}}$ being $\vec{I}$ the identity tensor and L_y the size of the RVE in the Y direction on the reference configuration. Also, as shown in Fig.5.4b, each master node displacement and restriction is associated with one row of $\vec{F}$ and $\vec{c}$ respectively.

The material in this study is modeled using the elastoplastic formulation outlined in section 5.1 to model single-crystals and polycrystals. In these models, the lattice orientation of each grain sub-domain must be computed locally, as these orientations also influence the elastic stiffness $\mathbb{C}$, defined in Eq.(5.4a), which is defined with cubic anisotropy. Additionally, as shown in Fig.5.4, the simulations include the prescribed cracks detailed in section 5.2.3. The crack zones are modeled with material possessing lattice orientation aligning with the reference system and with a stiffness various orders of magnitude lower than the actual material. The elastic and plastic properties used in the simulations are listed in Table 5.1, where m , $\dot{\gamma}_o$ are referred to Eq.(2.56), while h_o , h_s , τ_o , τ_s are linked back to Eq.(2.59).

Regarding the velocity parameters in Table 5.1, the objective force F_{yyf} corresponds to the maximum value of F_{yy} of Fig.5.4b. This value increases at each time step with a rate of $\dot{F}_{yy}$, being the size of each time step defined by Δt . The same rate is applied to u_{yY} in the FEM scheme, ensuring consistency with F_{yy} . These parameters are important due to the rate-dependent nature of the CP model in section 2.4. Finally, the PFF constants, ℓ and G_c employed in every simulation will be defined for each case.

Elastic properties		Visco-Plastic properties		Hardening properties		Rate parameters	
C11	259.6[GPa]	$\dot{\gamma}_o$	2.42D-3	τ_o	465.5[MPa]	F_{yuf}	2
C12	179.0[GPa]			τ_s	598.5[MPa]		
C44	109.6[GPa]	m	0.1	h_o	6000[MPa]	$\dot{F}_{yy}$	0.2[1/s]
				h_s	300[MPa]	Δt	0.005[s]

Table 5.1: Mechanical and PFF properties of materials.

5.3.2 Validation of the models

To verify the implemented elastoplastic model coupled with PFF, a set of simulations was conducted using both FEM and FFT solvers. The aim of this section is to validate the independent performance of both models across the two numerical schemes and ensure their compatibility. First, simulations without the PFF model were performed on a polycrystal with 12 randomly oriented grains, generated similarly as in section 4.4.3. The boundary conditions outlined in section 5.3.1 were applied to the RVE described in the same section, measuring 0.1×0.1 m and consisting of 85×85 voxels/elements, with the characteristic length scale defined as $\ell = 0.0025$ m. For FFT simulations, the initial crack has been modeled in two distinct ways: (i) using the discrete definition of section 5.2.3 (referred to as the FFT scheme) with a stiffness 10^{10} times lower than that of the surrounding material, and (ii) using the CPFE initial condition described in section 5.2.3 (referred to as the FFT-CPFE scheme). For this case, both FFT simulations are compared with the FEM equivalent in Fig.5.5 to assess equivalence.

The average Cauchy stress component in the tensile direction σ_{yy} is extracted and presented in Fig.5.5a as a function of the corresponding average deformation gradient component F_{yy} . Additionally, the σ_{yy} field and the accumulated plastic strain field Υ , as defined in Eq.(2.60), are extracted from the FEM and FFT simulations in a time step corresponding to an average deformation gradient of $F_{yy} = 1.2$ (indicated by the green arrow in Fig.5.5a) and are compared in Fig.5.5b. The results of the FFT-CPFE simulation yield a very similar field to that of the FFT simulation, so only those of this scheme are shown.

The simulated microstructure, depicted in Fig.5.5b alongside the compared fields, provides a geometric reference for the analysis. Both the FEM and FFT solvers produced similar results in terms of distribution and range of values for the studied fields. The microstructure had a significant influence in both fields, with the initial fissure being the main driver for plastic heterogeneities, particularly at the initial crack tip. Grain boundaries also contributed secondarily but notably to the plastic heterogeneity for both models. While the FEM solution appeared cleaner, the FFT solution displayed negligible oscillations due to FFT frequencies, which minimally affected the field distribution.

High stress values were observed in both the average curves and fields due to the plane strain conditions described in the previous section, which introduced volumetric stresses unaffected by plastic dissipation and the damage field. Additionally, the properties listed in Table 5.1 defined a high deformation rate $\dot{F}_{yy}$, which, in combination with the visco-plastic properties defined in the same table, resulted in high stresses. Overall, both models adequately captured

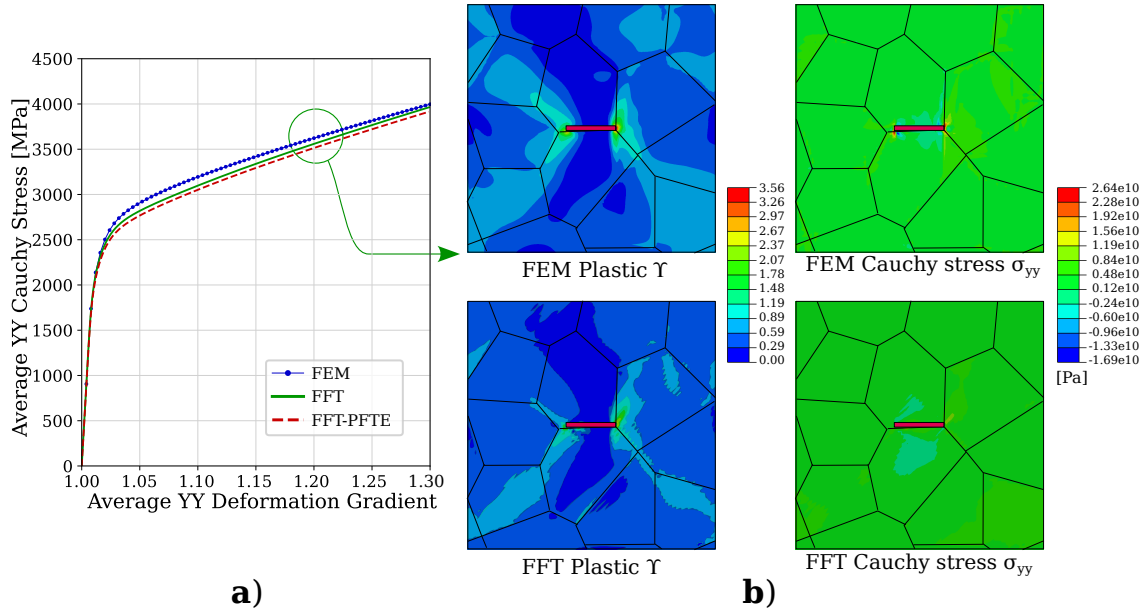


Figure 5.5: 2D polycrystal simulations in FFT and FEM with a non PFF pure elastoplastic model.

the elastoplastic behavior of the material. Despite minor differences between the three curves of Fig.5.5a at the beginning of the plastic regime, similar behavior was observed in the elastic zone and the later stages of plastic deformation, where the slopes of the curves are comparable. Quantitatively, using the Normalized Root Mean Square (NRMS) with the largest stress span available in the strain range of Fig.5.5a as a normalization reference, the FEM and FFT simulations exhibited a 1.8% difference, while the FEM and FFT-CPFE simulations showed a slightly higher difference of 2.9%.

Next, a series of elastic simulations were conducted to evaluate the model performance independently of plasticity. The first one, depicted in Fig.5.6, is a single-crystal configuration without PFF, executed using FFT with both discrete and CPFE initial cracks, as well as FEM, including the features described in section 5.2.3. The main objective of this simulation is to investigate the energy and deformation gradient responses in calculations including those initial crack models, in order to understand the damage driving force behavior for subsequent simulations. Later on, the polycrystal elastic simulation of Fig.5.7 examines the effectiveness of the implemented PFF model in a heterogeneous geometry.

In the single-crystal simulation, three specific points of Fig.5.6a have been selected to analyze the evolution of the local energy density. The corresponding energy curves for these points are displayed in Fig.5.6c. Additionally, the line labeled as T in Fig.5.6a, defined from the crack tip to the boundary of the RVE, is defined to examine the profile of the F_{yy} component of the deformation gradient, which is depicted in Fig.5.6b. Note that for the energy evolution analysis, the voxels corresponding to points ①, ②, and ③ were aligned with their respective nodes, as shown in Fig.5.6a, by applying the *Shift Theorem* to the aforementioned discrete fields in the Fourier space. Similarly, the line T in FEM was defined over a row of nodes depicted in Fig.5.6a in red points, while for the FFT scheme, the voxels along this line were moved with the Shift Theorem to align them in the middle of every two FEM nodes, as shown

in Fig.5.6a in green points.

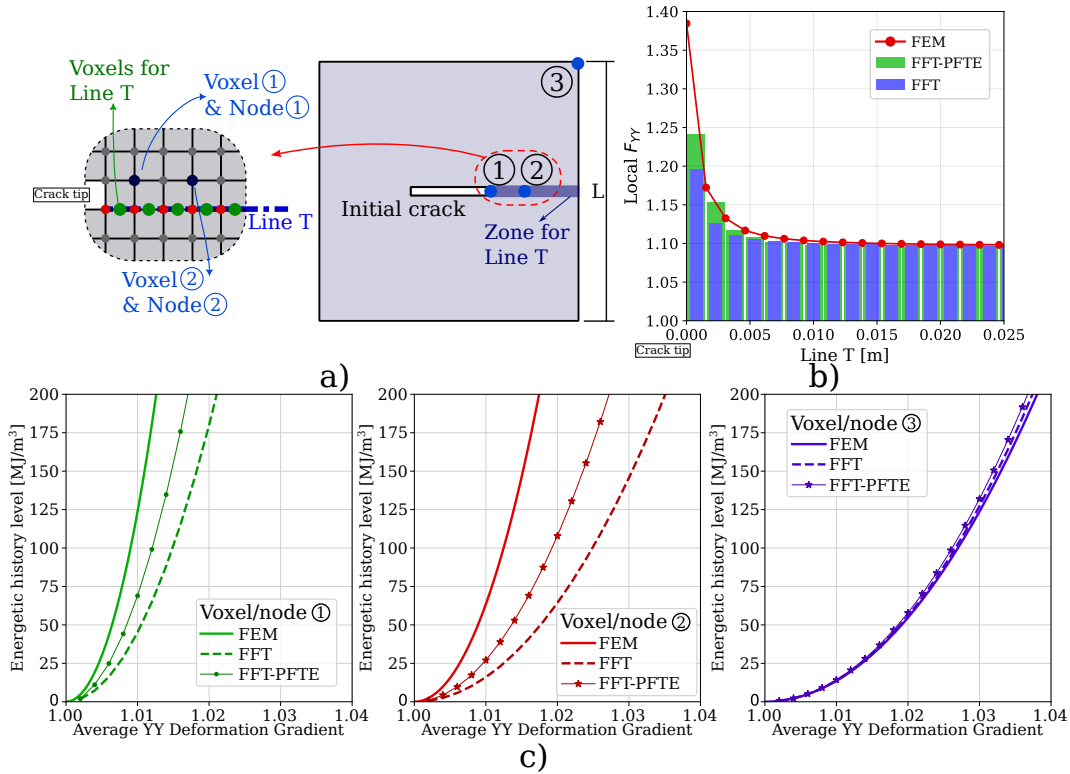


Figure 5.6: 2D elastic simulation with no damage for test CPFE initial condition. a) Schematic features of the simulation. b) Component y_y of the local deformation gradient in line T framed in a) for FEM, FFT and FFT-CPFE simulations over Line T. c) Local evolution of energy in points framed in a).

In Fig.5.6b, it is evident that the distribution of F_{yy} converges to a similar value far from the crack tip but diverges significantly near it. Specifically, the FEM simulation shows larger strain values than the FFT simulation in a highly localized region close to the crack tip. This localized increase in strain is expected to amplify the strain-energy driving force in the PFF model for the FEM simulation, potentially causing the crack to propagate earlier. As discussed in section 5.2.3, this difference may arise due to discretization effects, where the void material zone used to model the crack has more impact in the FEM simulation. In particular, the first FEM node, located closer to the crack tip, is more affected than the first FFT voxel. However, the FFT-CPFE simulation compensates for this difference, as can be seen in Fig.5.6b. This can also be observed in Fig.5.6c for the evolution of energy, where for points ① and ② the FFT-CPFE solution approaches the FEM solution. Despite this improvement, the far field does not require the CPFE condition, as demonstrated by the agreement among all three curves at point ③. These curves indicate that the CPFE condition defined in this work enhances the approximation of fracture behavior in PFF simulations but does not entirely match the FEM definition.

Then, to validate the PFF formulation, the polycrystal elastic simulation plotted in Fig.5.7 focuses on fracture behavior by ignoring large strains and plasticity for a clearer comparison

of FEM, FFT, and FFT-CPFE cases. An RVE with 18 randomly oriented grains, $G_c = 3 \times 10^6 \text{ J/m}^2$, and no over-relaxation parameter is used. From these simulations, the damage fields and the P_{yy} vs F_{yy} curves are extracted for comparison in Fig.5.7. A good agreement is observed between the response curves before crack propagation. However, the FFT-CPFE simulation exhibits a similar stress deviation from the FFT solution, similar to that in Fig.5.5. Considering only the data before the crack propagation in the FEM simulation, a NRMS of 0.3% between FEM and FFT is obtained, but an 1.7% is obtained between FEM and FFT-CPFE. Despite this, the critical point of the FFT-CPFE calculation aligns better with the FEM simulation, due to differences in energy accumulation described in Fig.5.6. For this reason, a higher value of critical strain was expected in the FFT scheme, since its rate of dissipated energy is slower. The critical point descent in the FFT-CPFE simulation is attributed to the presence of a pre-existing crack (Singh et al., 2016; Zambrano et al., 2023), which eliminates the need for nucleation and allows the critical point to be reached with lower strain. Despite this mechanism having such an effect, a better agreement with FEM simulations is expected for the CPFE modeling due to the local effect described in section 5.2.3.

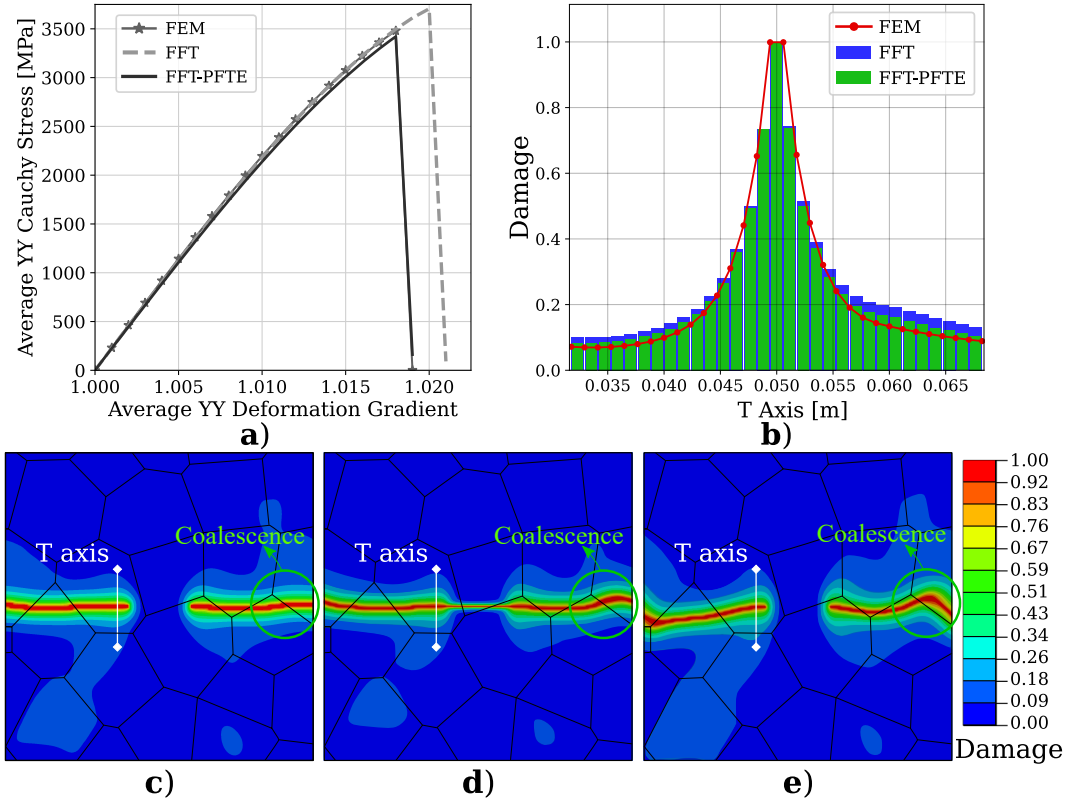


Figure 5.7: 2D polycrystal simulations in elastic PFF-FFT and PFF-FEM with $G_c = 3e6$. a) Comparison of P_{yy} vs F_{yy} curves . b) Damage profile over the axis T (voxels in bars and nodes in points). c) Damage field obtained from the FEM simulation. d) Damage field obtained from the FFT-CPFE simulation. e) Damage field obtained from the FFT simulation.

From Fig.5.7c to Fig.5.7e it is shown that for all simulations the crack paths are principally

originated from the initial prescribed cracks but are significantly influenced by the microstructure. They follow curvilinear trajectories that not always follow grain boundaries, resulting in predominantly transgranular cracking. This occurs because the damage energetic driving force can concentrate within grains, enabling crack propagation, as already seen in section 4.4.3. Consequently, smeared damage zones emerge in regions far from the crack center, where strain energy was insufficient to nucleate a crack but high enough to sustain damage due to the historical formulation of the energy. Minor differences in the damage fields between schemes can be observed in these smeared zones, due to variations in crack regularization and discretization. The FEM crack path in Fig.5.7c shows a straighter trajectory compared to the FFT simulation in Fig.5.7e, reflecting the local discretization differences inherent to each scheme. However, the crack path in the FFT-CPFE simulation, as shown in Fig.5.7d, closely resembles more the FEM trajectory than the FFT path. Later, when the FFT-CPFE crack coalesces, its final position aligns closely with the FEM crack. The coalescence occurs at the edge marked in green, where some discrepancies between FEM and FFT-CPFE are observed. Despite these minor differences caused by discretization, the FFT-CPFE crack trajectory exhibits greater similarity to the FEM result, further validating the effectiveness of the CPFE condition in approximating FEM behavior.

To further examine the damage fields, the regularized damage profile was extracted to characterize the geometrical aspects of the PFF crack and compare its discretization in both solvers. Damage values were extracted from a fictitious line segment, labeled as axis T from Fig.5.7c to Fig.5.7d. For the FEM geometry, axis T coincides with a column of nodes, while for FFT it aligns with the voxels corresponding to the elements of those nodes. These values were extracted after crack propagation and the resulting profile comparison is presented in Fig.5.7b, where the damage profile is eccentric due to the heterogeneity of the damage field. Despite greater diffusion of damage in the FFT simulations, the distribution is similar between FFT and FEM, particularly at the crack center. However, the FFT-CPFE simulation is better aligned with the FEM distribution compared to the standard FFT simulation, due to the higher energy accumulation at the crack tip. This can be quantified using the NRMS metric over FFT data and on FEM points obtained by simple interpolation at Fig.5.7b, in which a 3.9% is obtained between FEM and FFT and a 2.1% is obtained between FEM and FFT-CPFE.

The models tested in this section exhibit strong agreement in their global responses for cases involving no-damage elasticity and elasto-plasticity, even when considering heterogeneous geometries and anisotropy. However, localized behavior of energy at the crack tip reveals differences, with the FFT-CPFE scheme providing a closer approximation to the FEM model with respect to the FFT scheme. This improved accuracy at the crack tip comes at the cost of a slight deviation in the constitutive elasto-plastic behavior relative to the FFT scheme. These localized differences influence the response in simulations incorporating the PFF model, where the FFT-CPFE scheme more accurately approximates the FEM results for the crack propagation point and damage profile. This proves that the modeling of the initial crack has an important effect in the FFT simulation for fracture within the PFF scheme. Despite these observed differences, they remain relatively small, with deviations between FEM and FFT models being less *5%* in terms of mechanical behavior and field approximation.

5.3.3 Phase-Field fracture model on a 2D single-crystal geometry

In the following simulations, the complete elasto-plastic PFF model is evaluated for single-crystal cases. To assess the model's performance under different discretizations, simulations are conducted using 65x65 and 105x105 voxels/elements, incorporating the initial crack modeling described in section 5.2.3. These include discrete cracks with a thickness of one voxel/element and the corresponding CPFE cracks. Additionally, the response of the model to the variation of the fracture limit, defined by the material toughness G_c , is analyzed. Also, it is of particular interest to evaluate the performance of the model in scenarios involving higher fracture limits, which requires increasing the material toughness. For such calculations, cases with $G_c = 2 \times 10^6 \frac{J}{m^2}$ and $G_c = 3 \times 10^6 \frac{J}{m^2}$ are performed for both discretizations mentioned earlier.

In Fig.5.8a, the damage field after crack propagation is depicted for the FEM and FFT-CPFE cases with $G_c = 2 \times 10^6 \frac{J}{m^2}$. For clarity's sake, only one half of the 2D plate is displayed with the corresponding dimensions illustrated in Fig.5.8c. The responses across all cases demonstrate a consistent trend across the different schemes with the variation of discretization and fracture toughness. For the cases shown in Fig.5.8b, the plastic zone is clearly observed with the selected G_c , while the elastic zone still occupies an important part of the solution range. This range increases similarly across all cases in the curves of Fig.5.8c for both discretizations, where the elasto-plastic response progresses into the plastic zone. The constitutive behavior of all simulations aligns closely prior to the critical points, akin to the agreement observed in the no-PFF cases shown in Fig.5.5. This consistency highlights the robustness of the models in capturing the material response under varying fracture limits and discretizations.

As anticipated, all fracture points occur within the plastic zone and exhibit unstable behavior, since it occurs in a single computational step. Despite this phenomenon being common for the PFF model in brittle fracture (Ambati et al., 2015b; Miehe et al., 2010b), the stress-strain curves exhibit a small decrease in stresses near the fracture point and a higher damage accumulation around the crack tip before crack propagation. This effect is common in materials with ductile behavior where crack-tip blunting occurs. The critical points in the stress-strain curves for FEM and FFT-CPFE simulations increase with finer discretizations. Conversely, the FFT simulations with discrete initial cracks tend to exhibit a decrease in this point. This is again indicative of the similarity between the FEM and FFT-CPFE simulations at the onset of crack propagation and may indicate that both schemes are converging to a point between these and the FFT calculations.

When comparing the curves between both discretizations for a specific G_c , significant differences are consistently observed between FFT and FEM, due to the disrepair local energy rate at the crack-tip depicted in Fig.5.6. Since FFT simulations exhibit a much lower rate of damage accumulation, a delay in its crack propagation point was expected. While this effect was already observed in Fig.5.7, here it becomes substantially more pronounced because the damage driving force $\mathcal{H}$ is purely elastic. Since the material is elastoplastic, the elastic evolution reduces its rate of evolution in the plastic zone, which causes the history to have a slower behavior than in a purely elastic material and to present more deformation prior to failure. For this reason, even small differences in G_c lead to significant variations in the

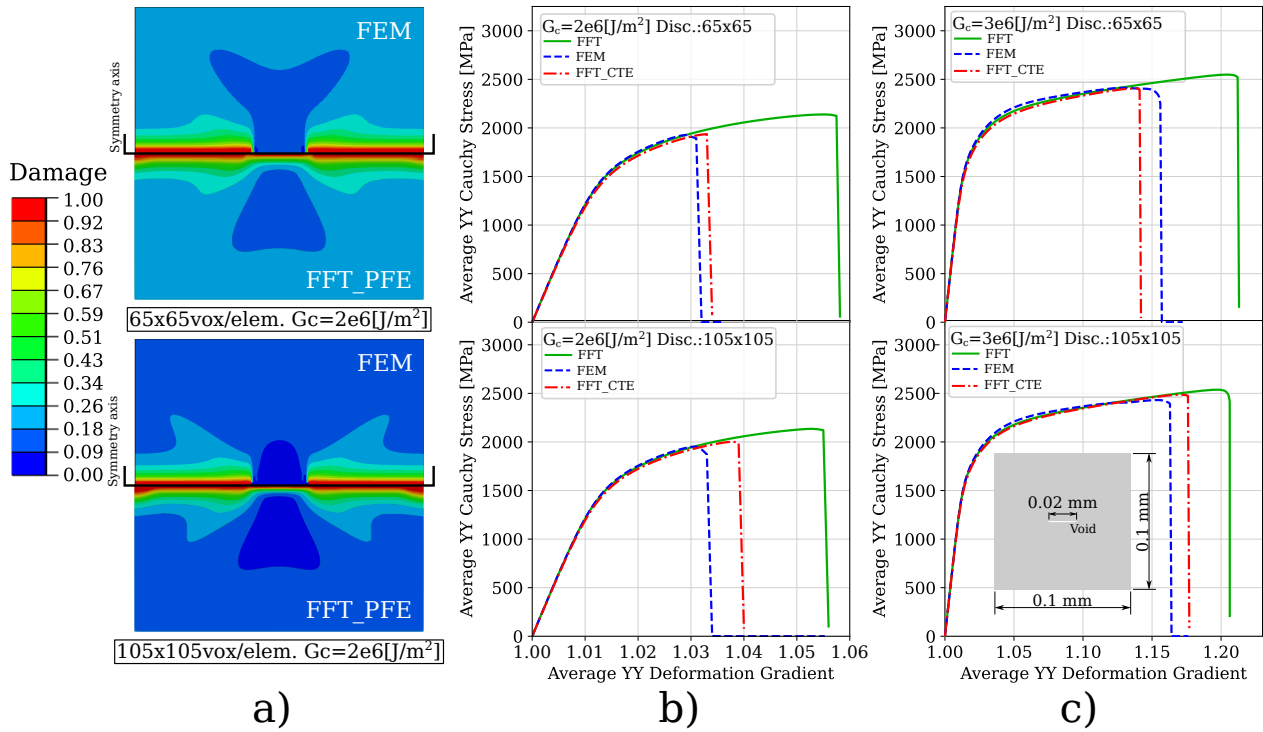


Figure 5.8: 2D single-crystal simulations in FFT and FEM schemes. a) Damage fields for FEM and FFT-CPFE simulations with $G_c = 2 \times 10^6 \frac{J}{m^2}$. b) Average stress v/s strain curves in tensile direction for FEM, FFT and FFT-CPFE simulations of both discretizations and $G_c = 2 \times 10^6 \frac{J}{m^2}$. c) Average stress v/s strain curves in tensile direction for FEM, FFT and FFT-CPFE simulations of both discretizations and $G_c = 3 \times 10^6 \frac{J}{m^2}$.

predicted critical point, and small discrepancies between FFT and FEM simulations in an elastic material are amplified in an elastoplastic one. However, as illustrated in Fig.5.6, the FFT-CPFE scheme mitigates this issue by enhancing the rate of $\mathcal{H}$ and, as a consequence, the FFT-CPFE simulations become more approximate to the FEM ones. This resemblance is further supported by the damage fields shown in Fig.5.8a. In the 65x65 voxel/element discretization, the contours are nearly identical. However, minor discrepancies can be seen in the 105x105 simulations, which are directly linked to the differences in the critical points observed in the curves for 105x105 simulations in Fig.5.8b. This is a consequence of the sensitivity of the local energy rate to discretization.

5.3.4 Phase-Field fracture model on a 2D polycrystal geometry

This section extends the analysis to a 2D polycrystal simulated with the complete PFF model, using the material properties from Table 5.1. A comparative study of numerical accuracy between FEM, FFT, and FFT-CPFE schemes is conducted through three sets of simulations with $G_c = 2 \times 10^6 \frac{J}{m^2}$ on the same 12-grain microstructure from section 5.3.2, shown in Fig.5.9c. The first set uses the original 85x85 voxel/element discretization of the microstructure. For the second and third sets, as shown in Fig.5.9c, the microstructure is refined by dividing each voxel and element into 2x2 and 3x3 subdivisions along the X and Y axes. With this, the

geometry of the second set of simulations results in a 171x171 discretization (one row and column is added to preserve an odd number of voxels in FFT) and the third set of simulations uses a 255x255 discretization.

Although the resulting microstructure features unrealistic grain boundaries, using these geometries enables a focused study of numerical differences among the three cases, minimizing the influence of a refined and smoothed microstructure on the damage and strain fields. The initial crack in all cases remains 1 voxel/element wide, as shown in Fig.5.9c, and the value of ℓ is kept constant, corresponding to the minimum crack size possible in FEM for the 85x85 discretization. Additionally, a numerical over-relaxation parameter of $\alpha = 0.5$ is applied in FFT simulations from the step at which the crack first propagates, improving convergence and in Fig.5.9b, the ϕ and Υ fields are displayed for comparison.

In Fig.5.9b, a crack path similar to that observed in the simulation of elastic fracture at Fig.5.7 is obtained, with predominantly transgranular cracking, but exhibiting deviations due to grain orientations that modify the energy field, making the damage field heterogeneous. At this figure, the comparison focuses only between FEM and FFT-CPFE solutions in the 255x255 discretization, since very similar damage and plastic deformation fields were obtained between FFT and FFT-CPFE. While damage remains similarly concentrated around the original crack and along grain boundaries in both solvers, FFT-CPFE (and FFT) exhibits a noticeably broader dispersion of plastic deformation and damage compared to FEM. This feature may derive from a higher influence of the microstructure on the ϕ and Υ fields. Such an effect is also reflected in the crack path of the FFT-CPFE simulation in Fig.5.9b, which deviates from the FEM crack trajectory. Such discrepancies are also observed in simulations for elastic behavior in Fig.5.7. In that case, the FFT-CPFE simulation closely approximated FEM by adding localized energy adjustments near the crack tip. However, in this scenario, the microstructure introduces variations, even in regions far from the initial crack. Such major influence from the microstructure could be attributed to the initial crack aligning with a grain boundary at Fig.5.9. Another potential explanation lies in the material behavior: In simulations of Fig.5.7, an elastic model was tested, where due to the large deformation scheme, elastic anisotropy was less influential in the strain and damage fields than plastic anisotropy. In contrast, the current study incorporates elasto-plastic behavior, where plastic anisotropy plays a more significant role.

The influence of the microstructure is evident from the curves plotted in Fig.5.9a, where a significant distinction between this case and those of previous sections is present. Unlike prior cases, the case shows a stable fracture for all simulations and discretizations. This stability occurs due to a misalignment of the lattice in a specific grain, marked with the symbol $\boxtimes$ in Fig.5.9b and Fig.5.9c. This grain exhibits less diffusion of damage and Υ compared to others, causing the crack to stop temporarily within it. Consequently, the solvers reach equilibrium during the fracture process, allowing the crack and the strain to grow slowly until the crack becomes unstable again upon exiting the $\boxtimes$ grain. This behavior aligns with findings by Hossain et al., 2014, which reports that cracks in heterogeneous materials with stiffness variations tend to be trapped near compliant phases, enabling solvers to maintain equilibrium temporarily. In Fig.5.9a, such a phenomenon can be seen in the fracture behavior, where the curve collapse happens in two steps. The process is detailed for the 255x255 FFT simulation in

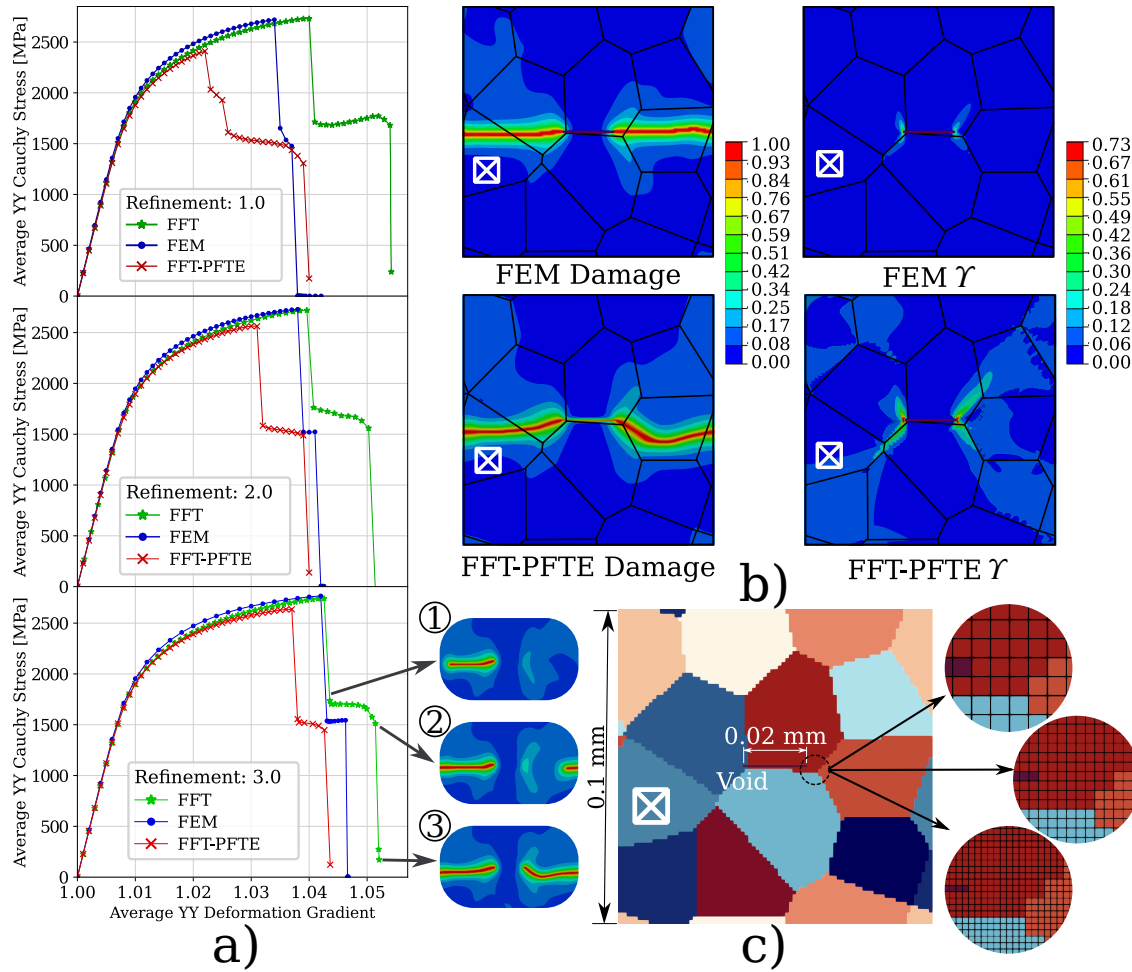


Figure 5.9: 2D polycrystal simulations in FEM, FFT and FFT-CPFE solvers with elastoplastic material with PFF: a) Mechanical response of every simulation set. b) FEM/FFT-CPFE field comparison of damage and accumulated plastic deformation γ . c) Microstructure geometry and refinements.

three steps, marked with numbers at the bottom of Fig.5.9a, with the corresponding damage fields. Point ① shows the halt of the crack inside the $\boxtimes$ grain. Between ① and ②, the crack grows stably, reaching the grain boundary. Finally, from ② to ③, the crack propagates unstably outside the grain. The main differences between FEM and FFT emerge at this last stage, where the FFT crack displays greater curvature. This deviation originates at point ①, where the crack tip in FFT and FFT-CPFE schemes initially deviates to a lower position with respect to FEM. This deviation amplifies during the coalescence at point ③. As noted earlier, the position of the initial crack along a grain boundary and the amplified influence of the microstructure (due to the plastic anisotropy) contribute to this difference. These two effects diminish the CPFE correction, leading to differences with respect to what is reported in previous sections between the FEM and FFT.

Concerning the mechanical responses plotted in Fig.5.9a, the results for the three discretizations (85x85 at the top, 171x171 in the middle, and 255x255 at the bottom) are presented. Before

the first crack propagation, FEM, FFT, and FFT-CPFE curves align across all discretizations. Similar to the observations in section 5.3.3, FEM and FFT simulations exhibit minor variations with refinement, especially the FFT scheme. Such changes occur in the same direction as in the single-crystal cases. In contrast, the FFT-CPFE simulations in this case are highly influenced by refinement. Unlike in single-crystal simulations, here FFT and the FEM simulations align closely, while the FFT-CPFE simulation is far from FEM up to this point. Despite FFT's slower energy dissipation rate at the crack tip compared to FFT-CPFE, FFT simulations display similar crack paths to FFT-CPFE due to the influence of the microstructure affecting both. Notably, after the first crack propagation, both FFT simulations exhibit a plateau stage longer than the FEM simulation, likely due to the $\boxtimes$ grain, which has less impact in FEM. This issue decreases with higher refinement, as the plateau length shortens in FFT samples and extends in FEM simulations, leading FFT-CPFE to a better approximation of FEM's second critical point across all discretizations. Ultimately, all simulations always converge when the geometry is completely fractured. An important observation from Fig.5.9a is the general trend toward convergence in mechanical responses with higher refinements. Although microstructure effects lead to crack deviations in FFT simulations, finer refinements reduce them by matching energetic rates and resolving the local strain heterogeneities.

Chapter 6

Conclusions, future work and contributions

6.1 Conclusions

A general, robust, and computationally efficient *Phase-Field Fracture* (PFF) simulation framework has been developed for problems at the micro/meso scale, using FFT-based solvers and aiming at homogenizing the fracture behavior of heterogeneous materials.

The first objective was developing and implementing a dissipation/crack length control technique in the PFF-FFT framework. The algorithm proposed has been validated against FEM simulations with the same control. The method developed has proven to be robust and efficient, being able to overcome the non-convexity of the problem using a monolithic scheme. Numerical examples have shown the potential of the technique in complex two- and three-dimensional heterogeneous microstructures. The technique proposed allows us to obtain the overall fracture behavior (snap-back) during the entire crack growth process, showing the stable and unstable crack growth stages in the complex fracture process at the microscale. Moreover, the algorithm proposed allows us to overcome important numerical issues present in staggered implementations of PFF, such as numerical jumps in the stress-strain response, and also improves convergence.

A deeper comparison between results under strain control (using a staggered solver) and dissipation control has shown full agreement during stable phases of propagation, both in the stress reduction and crack paths followed. On the contrary, when damage propagation is mainly unstable and several cracks might potentially grow, stress evolution coincides in both approaches, but the crack paths formed might differ. In the case of the dissipation control, the resulting crack paths are unique and dictated by the condition of the loading process (constant dissipation rate) but when using a staggered solver, these paths are controlled by the algorithm during unstable growth since equilibrium is not satisfied.

Secondly, an estimate of the effective toughness of heterogeneous brittle media has been proposed, together with a methodology to compute it from micromechanical simulations with dissipation control. In this methodology, to minimize the difference between PFF numerical

results and LEFM, enrichment strategies are considered. In particular, crack-tip enrichment (Singh et al., 2016) is used since it provides accurate results with a reasonable numerical efficiency.

It is demonstrated that the effective toughness estimate proposed accounts for the effect of both toughness and elasticity heterogeneity at the microscale considering isotropic or anisotropic constitutive models. The method has been used to estimate the effective toughness of composites and elastic polycrystals considering cleavage, showing agreement in cases with analytical solutions. The estimate proposed shows common features with the variational approach developed by M. Schneider, 2020 and the PFF-based approach proposed by Hossain et al., 2014. As in M. Schneider, 2020, effective toughness is given by the energy dissipated by an RVE crossing crack, and not by time-averaged or peaks in the energy release rate during propagation as in Hossain et al., 2014. In our estimate, toughening comes only from crack tortuosity and due to the cross of tougher areas (as in M. Schneider, 2020) but, contrary to Schneider’s approach, and in agreement with Hossain et al., 2014, crack paths are affected by local stiffness differences. It is found also that the heterogeneity of both the local toughness and local stiffness leads to an increase in the energy needed to extend a macroscopic crack. As in the homogenization of other material properties, the effective toughness is affected by the phase properties and microstructure. It is also found that the effect of phase property contrast saturates in many cases, and further changes of phase response do not increase the overall toughness.

The third objective was extending PFF-FFT formulations to simulate the elasto-plastic fracture of polycrystals at the microscale, in order to make a comparative study between PFF-FFT and PFF-FEM schemes. In this case, Crystal Plasticity (CP) is used as a constitutive equation and elastic energy is considered as the driving force for crack nucleation. Here, a staggered solution scheme is proposed, due to the natural dissipation produced by plasticity, which stabilizes the growth and does not require special control techniques. It was found that the use of a highly non-linear constitutive equation as CP in PF enhances the differences between numerical schemes, and convergence between FE and FFT results requires much finer meshes than when considering problems with crystal plasticity or fracture separately.

Differences between FEM and FFT primarily emerged in the damage field due to the differences in the localization of the energy density around the crack-tip. These differences were more pronounced under large plastic deformations, affecting crack path predictions and the location of critical fracture points. A key discrepancy between FEM and FFT was linked to the modeling of initial cracks. To address this, a Phase-Field enrichment technique was implemented in FFT, similar to the one used to improve fracture toughness estimations. This enrichment highly improved the agreement with FEM results in single-crystals (elastic and elasto-plastic cases), as well as in elastic anisotropic polycrystals. However, for elasto-plastic polycrystals, the Phase-Field enrichment method had limited effectiveness. A possible reason for this is that plastic localization near grain boundaries has a stronger effect on crack path than the stress concentration around the initial crack, and this localization is influenced by the numerical method used. Nonetheless, at higher resolutions, FFT and FEM results also converge both in critical fracture behavior and crack paths.

6.2 Future work

Further extensions of the work performed in the thesis are proposed,

- ✧ The dissipation control scheme implemented for elastic brittle fracture can be extended to the elastoplastic fracture model of chapter 5. Considering such scheme is not trivial, since an adequate definition of hardening needs to be taken account and because dissipation here occurs by both crack growth and plasticity.
- ✧ Study of the effective toughness in alternative microstructures, laminates with orientation or polycrystals accounting grain boundaries. Also three-dimensional microstructures can be used, which would allow to extend the study to other crack modes.
- ✧ The effective toughness estimation use an isotropic PFF model, considering all the elastic energy as fracture driving force . In the future, some energy decomposition, as the one based on strain spectral decomposition, could be tested to explore the behavior of residual stresses in cases with significant crack deviation.
- ✧ The effective toughness estimation procedure proposed has been implemented modeling initial crack to avoid the nucleation of a PFF crack. An extension of the methodology to include some phenomenological nucleation model would eliminate the effect of initial crack position.
- ✧ In the calculations with PFF-CP, the initial crack modeling with Phase-Field enrichment techniques has proven to shorten the gap respect simulations in FEM. Nevertheless an accurate representation is still a challenge. Solutions with different element type in FEM or FFT model with modified discrete frequencies (such as the Willot, [2015](#) scheme) could also be tested in the future to explore the differences between both schemes.
- ✧ Regarding how to model an initial crack modeling, a deeper exploration of initial damage fields could be performed in order to explore optimal forms to represent an initial crack in FFT.

6.3 Scientific contributions of the work

From the thesis work presented, different contributions have been developed, which are listed as follows:

JRC indexed papers

- * Aranda, P., & Segurado, J. (2025). A Crack-Length Control Technique for Phase-Field Fracture in FFT Homogenization. *International Journal for Numerical Methods in Engineering*, 126(2), e7664. DOI: <https://doi.org/10.1002/nme.7664>
- * Aranda, P., & Segurado, J. (2025). Effective toughness estimation by FFT based phase field fracture: application to composites and polycrystals. *Mechanics Research Communications*. **(Under review)**
- * Aranda, P., & Segurado, J. (2025). Analysis of FEM and FFT implementations of Phase-field fracture in elastic-plastic polycrystals. **(Under review)**

Conferences proceedings

- * Aranda, P., Zarzoso, G. & Segurado, J. (2022). Implementación de un esquema FFT para un modelo de 'Phase-Field Fracture': Aplicación a metales policristalinos. *Sociedad Española de Integridad Estructural. Grupo Español de Fractura*, pp77-82, Vol.3.
- * Aranda, P., & Segurado, J. (2024). Implementación de una técnica de control por longitud de grieta en problemas micromecánicos de fractura con un modelo de Campo de Fase. *Sociedad Española de Integridad Estructural. Grupo Español de Fractura*, pp161-166, Vol.7.

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