Computational methods for ductile fracture modeling at the microscale

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Abstract This paper is a state-of-the-art review of computational damage and fracture mechanics methods applied to model ductile fracture at the microscale. An emphasis is made on robust and stable methods that can handle heterogeneous structures, large deformations, and cracks initiation and coalescence. Ductile materials' microstructures feature brittle and ductile components whose heterogeneous behavior can give raise to cracks initiation due to stress concentration. Due to large deformations, cracks initiated by brittle components failure transform into large voids. These major voids interact and coalesce by plastic localization within ductile components and lead to final failure. This process can involve minor voids nucleated directly within ductile components at sub-micron scales.
State-of-the-art discontinuous approaches can be applied to discretize accurately brittle components and model their failure, given that large deformations can be handled. For ductile components, continuous approaches are discussed in this review as they can model the homogenized influence of minor voids, hence alleviating the burden and computational cost overhead that an explicit discretization of those voids would require. Close to final failure, when major voids are coalescing, and the influence of minor voids becomes comparable to that of major voids, the transition from a continuous damage process within ductile components to the initiation and propagation of discontinuous cracks within these components has to be modeled. This review ends with a discussion on computational methods that have successfully been applied to model the continuous-discontinuous transition, and that could be coupled to discontinuous approaches in order to model ductile fracture at the microscale in its full three-dimensional complexity.

Keywords ductile fracture; heterogeneous structure; microstructure; computational fracture mechanics; computational damage mechanics

Modesar Shakoor
MINES ParisTech, PSL Research University, CEMEF-Centre de mise en forme des matériaux, CNRS UMR 7635, CS 10207 rue Claude Daunesse, 06904 Sophia Antipolis Cedex, France
E-mail: modesar.shakoor@mines-paristech.fr

Nomenclature

2D	Two-Dimensional
3D	Three-Dimensional
CDM	Continuum Damage Model
CDT	Continuous-Discontinuous Transition
CZM	Cohesive Zone Model
DNS	Direct Numerical Simulation
FE	Finite Element
GFEM	Generalized Finite Element Method
GTN	Gurson-Tvergaard-Needleman
LS	Level-Set
PF	Phase-Field
RVE	Representative Volume Element
X-FEM	eXtended Finite Element Method

1 Introduction

Predicting ductile fracture is of high interest to the metal forming, transport and energy industries among

others. In order to improve the predictive capabilities of existing modeling approaches, it will be necessary to improve the understanding of this phenomenon, but also to propose numerical methods that can model it in its full complexity. For instance, the severe plastic deformation that occurs in ductile materials prior to final failure, as opposed to brittle materials, raises a number of challenges for computational methods.

Plasticity, which is incompressible, leads to well-known locking issues if one does not choose an appropriate discretization. Thus, a robust Finite Element (FE) modeling of ductile fracture first requires a robust FE implementation of plasticity. This can be done by using mixed formulations, which introduce additional pressure degrees of freedom and a higher order displacement discretization (Lorentz et al (2008)) or bubble stabilization terms (Areias et al (2011); El khaoulani and Bouchard (2013)). The latter is also known as MINI or $P1^+/P1$ element formulation. Other options are the F-bar element (Andrade Pires et al (2004)), and selectively reduced integration (Mediavilla et al (2006b)). All these formulations consist in isolating the volumetric parts of the strain and stress tensors and discretizing or integrating them separately. The reader is referred to nonlinear FE textbooks for more details on these methods (Belytschko et al (2013)).

Additionally, ductile fracture is the result of interacting plastic localization and failure mechanisms at different scales (Pineau et al (2016)). There has been a great interest in the recent literature for experimental and computational methods that can be applied at multiple scales. On the experimental side, *in situ* loading machines and X-ray imaging can now provide full three-dimensional (3D) visualization of ductile fracture at the microscale, and be coupled to force sensors and surface images to also acquire macroscopic information (Shakoor et al (2017c)). On the computational side, current and future efforts towards integrated computational materials engineering are motivating the development of multiscale computational methods (Matouš et al (2017)).

As a first step, an attempt can be made at accounting for ductile materials' microstructures and their role during failure. These microstructures are often assumed to be composed of a metallic ductile component, the matrix, in which are embedded brittle components, the particles[1]. Ductile fracture initiates by void nucleation due to particle fragmentation or debonding. The subsequent voids grow and interact by plastic localization, until this void coalescence mechanism becomes dominant and leads to final macroscopic failure (Pineau et al (2016)).

Experimental observations of these micromechanisms are shown in Figure 1. Due to the low particles and voids volume fraction of the material shown in this figure, the influence of the microstructure on the crack propagation path can be observed, but void nucleation micromechanisms cannot be clearly distinguished. A better view of ductile fracture at the microscale is shown in Figure 2. The material shown in this figure has a high nodules volume fraction, which allows to distinguish void nucleation mainly by debonding, with some fragmentation, followed by void growth and coalescence. The initiation and propagation of a macroscopic crack by void sheeting along the shear band can also be observed.

Modeling all these micromechanisms is a computationally challenging problem. Indeed, it raises a number of issues for computational fracture mechanics approaches. While crack modeling techniques that can handle multiple crack initiation sites can be found, it will be shown in this review that there are only a few methods that can also handle large deformations and cracks coalescence. For instance, Antretter and Fischer (1998) have focused on simple two-dimensional (2D) configurations with a single pre-existing crack, and addressed only the influence of particles on crack propagation within the matrix. Simulations with multiple crack initiation sites at arbitrary locations with both particle fragmentation and debonding modeling in 3D can be found in Shakoor et al (2017a). The latter study assumes a brittle fracture of particles and their interfaces, while void growth and coalescence are assumed to be purely plasticity driven.

As pointed out by Tekoğlu et al (2015), recent experimental evidence suggests that for some materials and loading conditions a minor void population nucleates, grows, and coalesces within the matrix. This void population is coined as minor due to its small size compared to voids that nucleate due to particles debonding and fragmentation. As explicitly meshing these voids along with particles and voids of the major population would be computationally extremely demanding, Areias et al (2015) among others have relied on continuous approaches. Continuous approaches are computationally interesting as they can represent very large numbers of voids at low computational cost, and with low implementation burden as opposed for instance to remeshing techniques or the eXtended Finite Element Method (X-FEM). However, continuous approaches require to define a so-called Continuous-Discontinuous Transition (CDT), at which the minor void population

[1] Other variants such as dual phase steels and polycrystals with multiple ductile components are also considered in the present review.

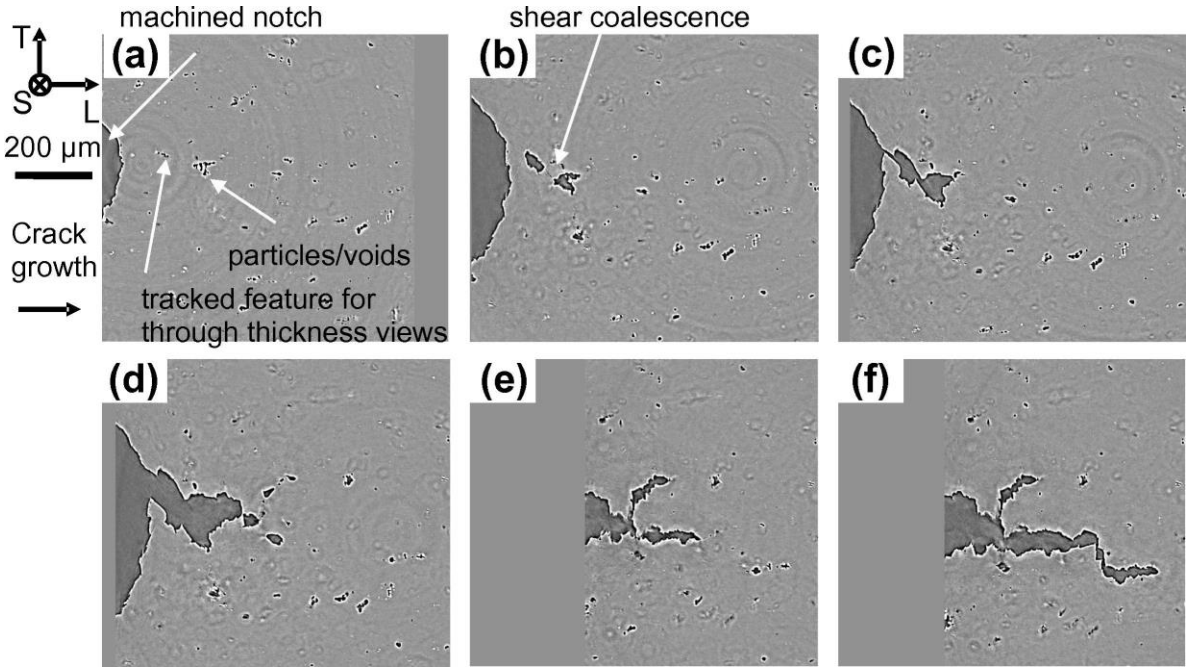

Fig. 1 Cross section from 3D X-ray images of the microstructure of a thick notched specimen under tensile loading at different crack mouth opening displacements: (a) 0 mm, (b) 1.625 mm, (c) 1.875 mm, (d) 2.0625 mm, (e) 2.3125 mm, (f) 2.375 mm. The material, an aluminum alloy with less than 1% initial particles/voids volume fraction, fails by the initiation and propagation of a macroscopic crack in a zig-zag pattern due to the influence of the microstructure. Reprinted from Morgeneyer et al (2011), with permission from Elsevier.

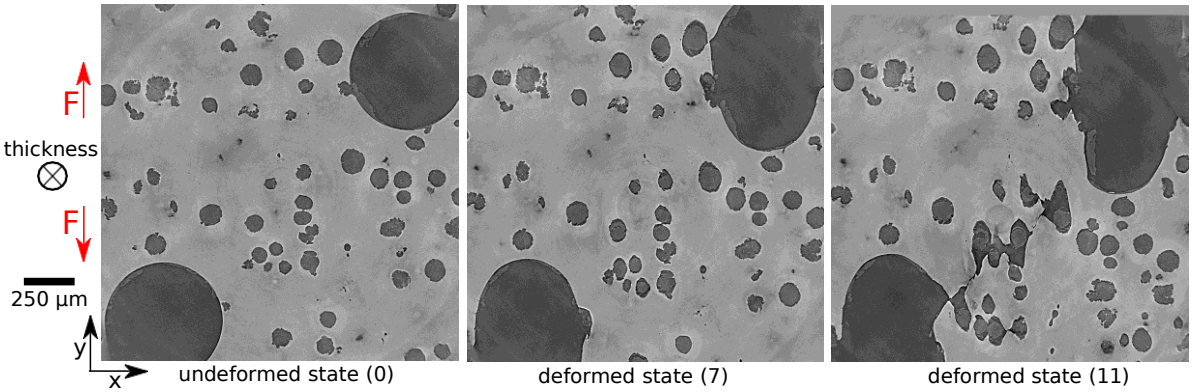

Fig. 2 Cross section from 3D X-ray images of the microstructure of a flat specimen with two machined holes at 45° under tensile loading. The material, nodular cast iron, fails by debonding and fragmentation of the nodules, and then void growth, coalescence and sheeting in the shear band between the two machined holes. Reprinted from Shakoor et al (2017c), with permission from Elsevier.

has grown and coalesced enough so that its size and influence becomes comparable to that of the major void population. At this critical point, one has to consider 3D crack initiation and propagation criteria within the matrix, for instance using the method proposed by Feld-Payet et al (2015).

To follow the emergence of these sophisticated numerical methods, the present review starts in Section 2 by a discussion of numerical methods with a discontinuous modeling of fracture. Here discontinuous implies that the crack is explicitly modeled, with a discontinuous jump of the displacement field across crack faces. These methods have been developed mainly for brittle materials. They can be applied to model the fracture of brittle components of the microstructures of ductile materials, and also the fracture of ductile components if the softening effect due to the minor void population can be neglected.

Then, methods that can model the softening response of ductile materials are reviewed in Section 3. A focus is made on the application of these methods to the

matrix component of these materials' microstructures to account for minor void populations. Additionally, multiscale methods can be seen as continuous methods where the effect of micro-cracks and microstructural damage is modeled using continuous analytic or computational homogenization. This is of particular interest as ductile fracture has to be modeled simultaneously at two or more scales.

Finally, the limitation of continuous methods during the final stage of ductile fracture, where the softening effect becomes predominant over the hardening effect, up to final failure, lead to the CDT problem. This problem can be modeled by coupling continuous models to discontinuous approaches. As detailed in Section 4, this coupling raises other issues that make 3D problems still challenging.

Discussions throughout the paper and in Section 5 should give the reader insights on current and future efforts on micromechanical modeling of ductile fracture. In particular, the authors wish to highlight methods that seem to be the most promising options to handle all difficulties raised by ductile fracture modeling in heterogeneous structures.

2 Discontinuous approaches

If the softening effect before crack initiation and propagation can be neglected, ductile fracture can be modeled using the same numerical methods as brittle fracture. Some differences arise regarding the crack initiation and propagation criteria, as plastic strain and loading path should be accounted for in the ductile case. As this review article does not focus on the criteria but the crack modeling methods, we discard discussions on the criteria. It must however be pointed out that crack propagation criteria are rare for the 3D case, in particular if there are multiple initiation sites as in void nucleation in ductile microstructures. Void nucleation itself is a challenging application for discontinuous approaches, as at the microscale void nucleation can be considered as the brittle failure of particles or particles/matrix interfaces. The main challenge in that case is that these micro-cracks open to a quite large extent before propagating, which restricts the applicability of brittle fracture modeling methods that cannot handle large deformations.

2.1 Element erosion

A simple way to dynamically introduce discontinuities in a FE simulation is to remove elements from the FE mesh and/or the associated contributions from the FE formulation based on an appropriate fracture indicator. This method is often referred to as element deletion, element removal or kill element. The terms element erosion are used to depict the fact that elements are generally removed after *eroding* their load carrying capacity over several load increments to avoid convergence issues (Wulf et al (1996)).

When it comes to ductile fracture, the element erosion method is most often associated to Continuum Damage Models (CDMs, see Subsection 3.1). However, some studies can be found where a failure criterion was used to trigger element deletion or erosion without accounting for the softening effect.

Wulf et al (1996) presented an application of element erosion to a 2D aluminum alloy microstructure. Matrix failure was modeled by progressively setting the stress and stiffness of matrix elements to zero depending on a plastic strain based failure criterion. As pointed out by Wulf et al (1996), a strain based criterion is convenient as it also removes distorted elements that should otherwise be treated with mesh adaption (Subsections 2.4 and 4.4). Another important remark of the authors is that nodes surrounded with eliminated elements must also be eliminated to avoid the discretization of balance equations to be ill-defined.

A plastic strain based criterion was also used by McHugh and Connolly (2003) to trigger a progressive release of stress and stiffness in given elements. It is important to point out that while the progressive relaxation is justified as a numerical technique used to improve convergence by Wulf et al (1996), it is defined as a gradual process comparable to the mechanical process of ductile failure by McHugh and Connolly (2003). Thus, the number of load increments over which element erosion occurs is defined as a material parameter by McHugh and Connolly (2003). The proposed application is the microstructure of a metal alloy, wherein the matrix is modeled using a crystal plasticity FE method coupled to element erosion.

A more advanced empirical criterion accounting for plastic strain and also the stress state was applied to a dual phase steel by Perzyński et al (2017). In particular, 2D and 3D micromechanical simulations accounting for ductile fracture of the ferrite phase were conducted. The ductile fracture indicator was fitted to experimental data giving the plastic strain at failure for ferrite at different stress triaxiality ratios. As shown in Figure 3, promising simulation results of the failure process of dual phase steel microstructures were obtained. These results showed the interaction between brittle fracture in the martensite phase, and ductile failure in the fer-

rite phase.

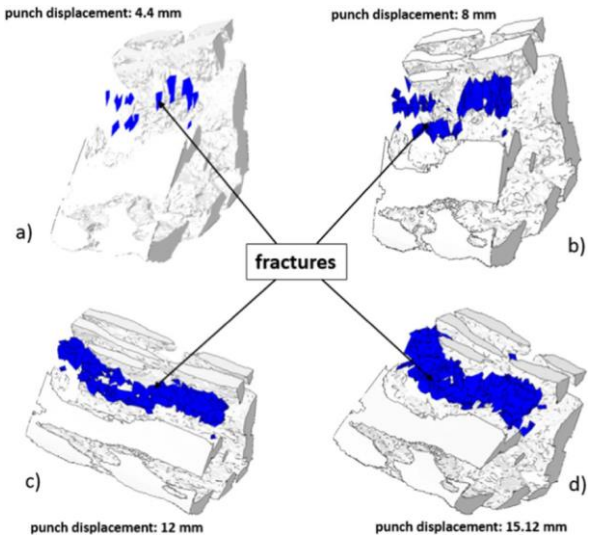

Fig. 3 Micromechanical simulation of a 3D dual phase steel microstructure showing in white the martensite phase, and in blue eroded elements from the ductile ferrite phase. The reader is referred to Perzyński et al (2017) for indications on the relation between punch displacement and boundary conditions at the microscale. Reprinted from Perzyński et al (2017), with permission from Elsevier.

In spite of these interesting applications, element erosion has well-known mass loss, mesh size dependence and element shape dependence issues (Mediavilla et al (2006a)). Computational approaches to ductile fracture at the microscale decades ago (Wulf et al (1996)), at a time where high performance computing capabilities were not as accessible as today, used this method. This is mainly due to its ease of implementation and low computational cost compared to the methods that are discussed in the following. The aim of these methods is to allow the modeling of cracks as new interfaces inserted dynamically during the FE simulation. To avoid the numerical issues raised by the element erosion method, the following methods are designed so that cracks can be initiated at arbitrary locations and propagated along arbitrary directions, independently of the FE mesh.

2.2 Enriched Finite Element methods

2.2.1 Introduction

In order to model discontinuities without element erosion or remeshing, a family of enriched FE methods have been developed and have been documented by different authors (Jirásek (2000); Oliver et al (2006); Fries and Belytschko (2010)). The most popular of these methods is the X-FEM (Moës et al (1999)), which is based on the partition of unity concept (Babuska and Melenk (1995)). The Generalized Finite Element Method (GFEM) is another relevant enriched method (Strouboulis et al (2000)). Initially, in GFEM, all the nodes in the discretization were enriched; later, local enrichment was adopted. The distinction between X-FEM and GFEM has become less clear as the methods have evolved (Fries and Belytschko (2010)). A very attractive feature of these methods is the fact that discontinuities might be modeled independently of the mesh, *i.e.,* conformity is not required. Most of the applications of enriched FE methods have been dedicated to brittle fracture. This subsection discusses some of the works that have dealt with ductile fracture.

2.2.2 Strong discontinuities

Strong discontinuities such as cracks and holes can be modeled with enriched FE methods. The material/void interface is captured thanks to a discontinuous enrichment, typically using the Heaviside function as enrichment function (Moës et al (1999)). To capture the stress singularity in the near crack tip region, an additional enrichment is necessary (Belytschko and Black (1999)). The latter requires careful choice of the enrichment function, and knowledge of the analytic solution. These enrichment techniques are usually implemented locally and not in the whole FE mesh. This constitutes the basis of X-FEM.

Sukumar and Belytschko (2000) showed how the basic methodology can be extended to account for arbitrary branched and intersecting cracks in 2D cases such as a cross or star shaped crack. An extension to 3D of the basic X-FEM methodology was provided by Sukumar et al (2000) by enriching the elements near the crack front with the radial and angular behavior of the 2D asymptotic crack tip displacement field. Analogous development have been made with the GFEM (Duarte et al (2001)). Further flexibility in the description of the crack geometry was introduced by coupling the Level-Set (LS) method (Osher and Sethian (1988)) to the X-FEM: the zero isovalue of a signed distance function gives the position of the crack surface, and its intersection with a second and almost orthogonal signed distance function describes the crack front (Moës et al (2002); Gravouil et al (2002)). The semicircular crack in a Maltese cross modelled by Moës et al (2002), is an example of the more complex and non planar crack geometries that can be studied with this technique.

2.2.3 Weak discontinuities

When the X-FEM is used to model a strong discontinuity, the crack is embedded within some FE elements, that will distort significantly due to the displacement jump. The X-FEM can also be used to define a stress/strain jump with a continuous displacement. This is relevant for the modelling of inclusions in ductile fracture simulations.

Sukumar et al (2001) presented 2D examples of inclusions to show the potential of this approach to represent complex internal boundaries. In the elements containing the matrix/inclusion interface, *i.e.,* the weak discontinuity, the absolute value of an LS function was used as enrichment function. This aspect was further explored by Huynh and Belytschko (2009) with 2D and 3D examples in composite materials. More sophisticated approaches for modeling inclusions with the X-FEM have been developed more recently. Wang et al (2016) proposed an adaptive X-FEM strategy coupling the X-FEM to mesh adaption techniques (Subsection 4.4), and compared its accuracy and computational performance with standard X-FEM.

Some works have applied the capabilities of X-FEM to modelling weak discontinuities along with cracks in ductile materials. Singh et al (2011) studied the effect of the presence of minor cracks, voids and inclusions in the vicinity of a major crack for multiple configurations. Ye et al (2012) analyzed the stress dissipating effect under small strain of reinforcing particles on fatigue close to the crack tip. Metal matrix composites of various particle sizes were investigated. A multiscale approach with the projection method (Loehnert and Belytschko (2007)) was used by Liu et al (2017a) to assess the effect of micro-cracks, inclusions and voids for different relative positions with respect to the tip of a major crack under mode I and mode II loading. These three cited works investigated only 2D configurations.

2.2.4 Discussions

Enriched FE methods provide the capability of modelling weak and strong discontinuities, *i.e.,* interfaces between two material phases (Sukumar et al (2001); Huynh and Belytschko (2009)) and void/material interfaces (Moës et al (1999)), as well as stress singularities (Belytschko and Black (1999)). These methods can handle branching and intersecting cracks (Sukumar and Belytschko (2000); Belytschko et al (2001)), non planar cracks (Moës et al (2002); Gravouil et al (2002)) and complex 2D and 3D geometries (Sukumar et al (2000)). These features are relevant for the study of ductile damage.

Yet, most of the literature is dedicated to brittle fracture. Even in works in which ductile materials are the object of study (Loehnert and Belytschko (2007); Liu et al (2017a)), the focus is on the calculation of stress intensity factors and large deformations are not pursued. The small number of works with enriched FE methods dedicated to ductile fracture might be partially explained by the fact that these methods were conceived precisely to avoid remeshing, which might be necessary if the considerable deformation associated to ductile fracture is to be accounted for, even with an enriched FE formulation.

The practical application of enriched FE formulations is less straightforward than the implementation of its basic techniques; limitations and additional complications arise. Their implementation can be burdensome depending on the structure of the FE code due to the variable number of degrees of freedom that comes with local enrichment (Rabczuk et al (2010)).

Traditional Gauss quadrature is not adequate for enriched elements. There are different strategies to tackle this problem, but the most common one is subpartioning of enriched elements, with higher order integration for crack tip elements (Moës et al (1999)).

In the first X-FEM implementations, topological enrichment was used for the crack tip enrichment, *i.e.,* only those nodes whose support contained the crack tip were enriched. This resulted in a deteriorated order of convergence. To solve this issue, a geometric enrichment was proposed where enrichment is added for all nodes within a distance to the crack tip (Laborde et al (2005)). Although this improves the convergence rate, the conditioning is deteriorated and the problem size increases (Sukumar et al (2015)). Another factor that might affect the order of convergence is the use of approximate enrichment for the crack tip instead of full enrichment (Huynh and Belytschko (2009)).

Ill-conditioning can also arise if an element is cut by an interface such that one of the resulting subvolumes is comparatively very small with respect to the other. To alleviate the conditioning problems associated to X-FEM, ad hoc preconditioners have been proposed, an example of which can be found in Béchet et al (2005). X-FEM related convergence issues are, however, lesser than those that have been found for mixture laws and multiphase elements (Wulf et al (1996)).

An additional obstacle to the application of enriched FE methods to ductile fracture problems is related to their application beyond elastic problems. Even though bimaterial interfaces or void/material interfaces can be handled transparently independently of the behavior of the material, crack tip enrichment functions depend on

material behavior. Although some developments have been made for elasto-plastic materials (Elguedj et al (2006)), their application remains restricted to confined plasticity, and enriching crack tip elements for more advanced material laws remains a considerable challenge.

These drawbacks of X-FEM might deter from its application to ductile fracture problems. Indeed, the number of works that employ it to study ductile fracture is very small with respect to brittle fracture. It should nevertheless not be discarded as it can be applied to model the fracture of brittle components in ductile materials' microstructures. For instance, the failure of ductile dual phase steels has been studied at the microscale by applying the X-FEM to the brittle martensitic phase (Vajragupta et al (2012); Ramazani et al (2013); Perzyński et al (2017)). As shown in Figure 4, remarkable results can be obtained using this approach. However, due to technical limitations, Perzyński et al (2017) used two separate codes for brittle and ductile failure, and enriched elements were considered as deleted in the ductile fracture code.

Void nucleation by fracture of brittle components within ductile materials' microstructures can hence be modeled using the X-FEM. Enriched FE methods are nevertheless not applicable yet to model the growth of these cracks into large voids.

2.3 Cohesive Zone Models

While enriched FE methods solve completely the mass loss, mesh size dependence, and element shape issues raised by the element erosion method, they fall short in modeling the energy dissipation rate. Indeed, once a displacement jump is introduced within an element, its load carrying capacity is instantly lost. In element erosion, the energy dissipation rate could be controlled based on numerical (Wulf et al (1996)) or physical arguments (McHugh and Connolly (2003)) by progressively setting the stress and stiffness to zero. When the crack is defined not by element removal but by an actual interface across which the displacement is defined as discontinuous, Cohesive Zone Models (CZMs) can be introduced to model the energy dissipation rate.

The origins of CZMs date back to the 60's and the concepts were initially introduced by Barenblatt (1962) and latter described by Rice (1968a). The concept of CZM is simple and states that, at the crack tip, there is a finite size region where the material transitions from a fully broken material to a sound material. Figure 5 shows a schematic representation of a fracturing process taking place on a brittle material and its interpretation using a CZM model. This region, called the cohesive region or process zone, corresponds to prospective fracture surfaces ahead of a crack which are permitted to separate under loading. This separation process and crack surface creation process are opposed by atomic or molecular cohesive forces (Rice (1968b)). The energy dissipated by the breakage of the atomic bounds corresponds to the fracture energy required to create the new free surfaces and break the material.

The force opposed to the opening of the new surfaces is called cohesive force and modeled by a phenomenological traction-separation law. There are many traction-separation laws that can be used to model the fracture process.

In comparison with other methods used to model fracture, cohesive elements are independent from mechanical behavior of the bulk material, the extend of the cracks and the size of the plastic zone (Ortiz and Pandolfi (1999)), which represents a very interesting advantage. Within the context of FE models, there are different ways of using CZMs. Enrichment based numerical techniques, such as XFEM or GFEM (Moës et al (1999); Strouboulis et al (2000); Reed and Hill (1973); Aragón and Simone (2017)), will not be discussed in this subsection. These techniques are used by a large part of the community, in particular XFEM approaches which are discussed in Subsection 2.2. Another technique is based in the insertion of "cohesive elements" into the mesh. These cohesive elements, which can be seen as some kind of special surface element, obey a constitutive law that corresponds to the selected traction-separation law.

In practical terms, a cohesive element is inserted at a face separating two bulk elements as it can be seen in Figure 6A. The insertion is simply performed by duplicating the nodes forming the separating face and inserting a new *cohesive element* linking the original nodes to the new duplicated ones (Figure 6C). It is worth mentioning that cohesive elements are initially flat (Figure 6B) and, in contrast to a regular bulk FE, this flatness does not represent any issue regarding the capability of cohesive elements to properly describe the mechanical response of the process zone.

The implementation of CZMs into a FE framework has strong implications on the way cohesive elements can be used to model fracture and, in some cases, can represent a limitation of the method. Some of these limitations are presented here and classified by different topics: insertion methods and crack propagation approaches.

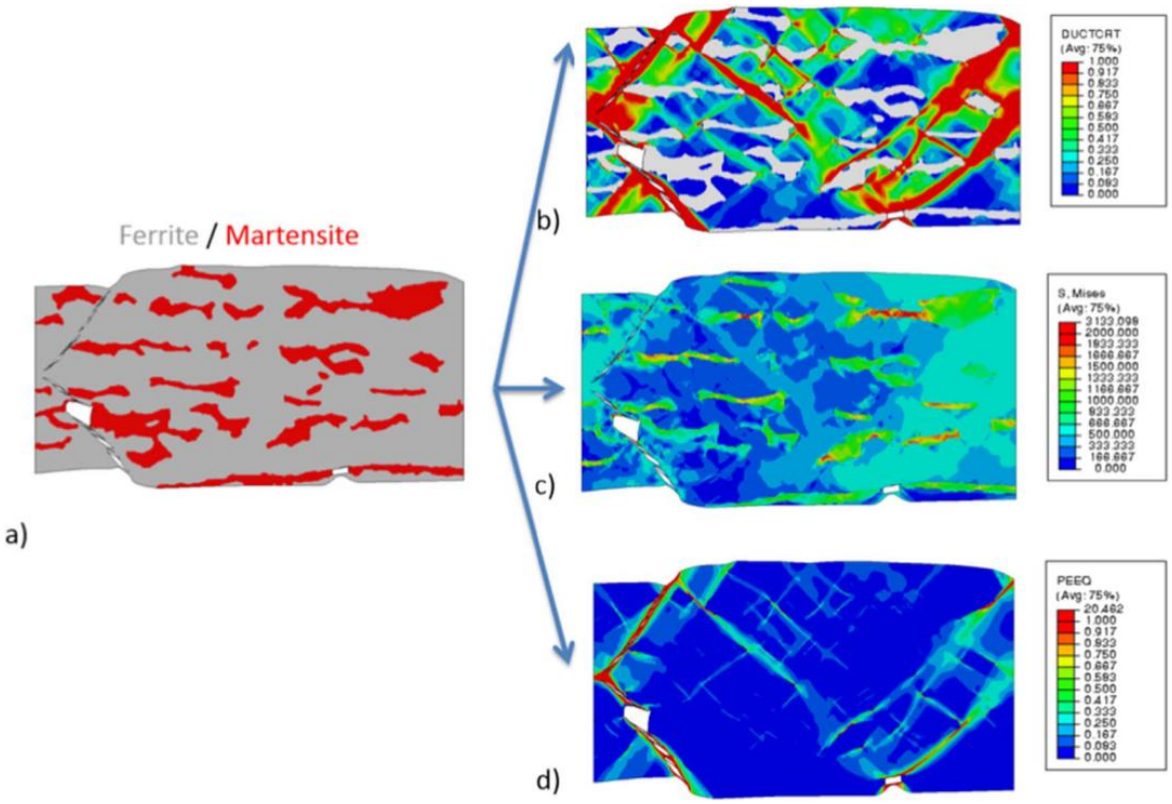

Fig. 4 Micromechanical simulation of a 2D dual phase steel microstructure showing the ductile fracture of the ferrite phase modeled using element deletion and the brittle failure of the martensite phase modeled using X-FEM. (a) Microstructure with ferrite in gray and martensite in red. (b) Damage variable in ferrite phase. (c) Von Mises stress field. (d) Equivalent plastic strain field. Reprinted from Perzyński et al (2017), with permission from Elsevier.

2.3.1 Insertion methods

Intrinsic methods The simplest way of handling cohesive element insertion is to insert these elements since the beginning of the simulation. This approach is very interesting since its implementation in any standard FE code is straightforward and many problems such as particle debonding can be simulated with this approach. However there is a strong drawback: an artificial reduction of the stiffness of the material is induced. In fact, most traction-separation laws have an initial region where the traction increases monotonically from a zero up to a maximum value (in some cases this increase is linear). This increase of the traction level as a function of the opening displacement leads to the introduction of an artificial stiffness into the system that modifies the macroscopic response of the material (Tomar et al (2004)). A way to overcome this problem is to use an infinite cohesive stiffness up to the critical cohesive traction. This can be achieved by introducing Lagrange multipliers in such a way that the opening of the element is only allowed once a critical traction is achieved (Lorentz (2008)). However this solution requires the modification of the standard FE formulation and, in this way, the main advantage of the approach (the use of a standard FE code) is lost.

Extrinsic methods An alternative method to handle the insertion of cohesive elements is to dynamically duplicate the nodes of faces where a given criterion is satisfied and then insert the new cohesive element. This technique is very interesting because it allows to get rid of the artificial modification of the global stiffness of the material but its implementation is not straightforward. The implementation requires the modification of the core features of the FE library, in particular concerning the mesh module, and it is particularly complex within the context of distributed computing (Vocialta et al (2017)). Although this extrinsic approach allows to circumvent spurious stiffness problems, it still suffers from some mesh dependency problems, as discussed in the following.

2.3.2 Crack propagation approaches

Mesh dependency Whether an intrinsic or an extrinsic approach is used, CZMs within the context of FE meth-

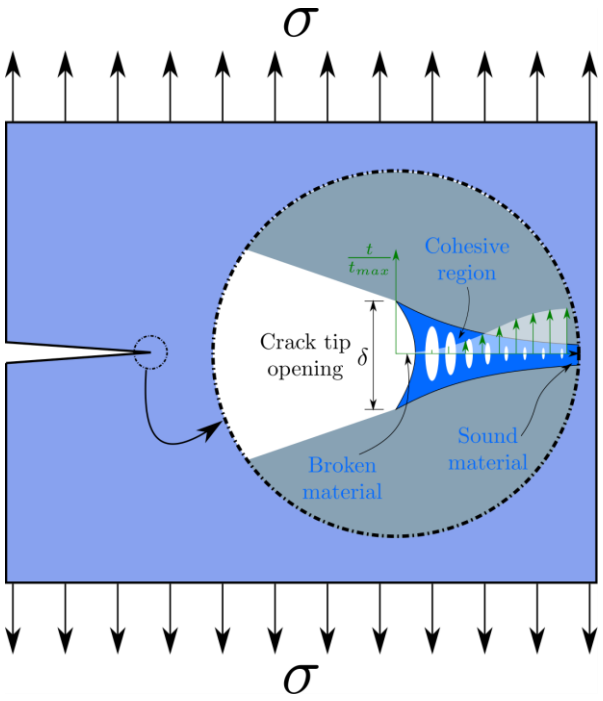

Fig. 5 Schematic representation of the cohesive zone: transition from sound material to broken material. The green arrows represent the distribution of tractions over the cohesive region.

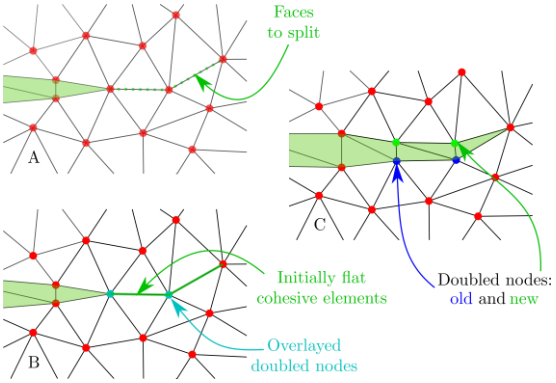

Fig. 6 Schematic representation of the insertion of a cohesive element: A. The green dashed line shows the faces that will be split. B. The cyan dots correspond to the nodes that have been doubled and therefore there are indeed two nodes at the same location. The green line corresponds to a initially flat cohesive element. C. After loading the new inserted cohesive elements open.

ods suffer from mesh dependency. In fact since cracks appear at the faces separating two bulk elements, therefore the crack path depends on the mesh and this is true for simulations involving structured and non structured meshes. The issue is illustrated in Figure 7 where the predicted crack path and the actual one are shown in blue and green, respectively. This means that if the mesh changes, the crack pattern slightly changes too.

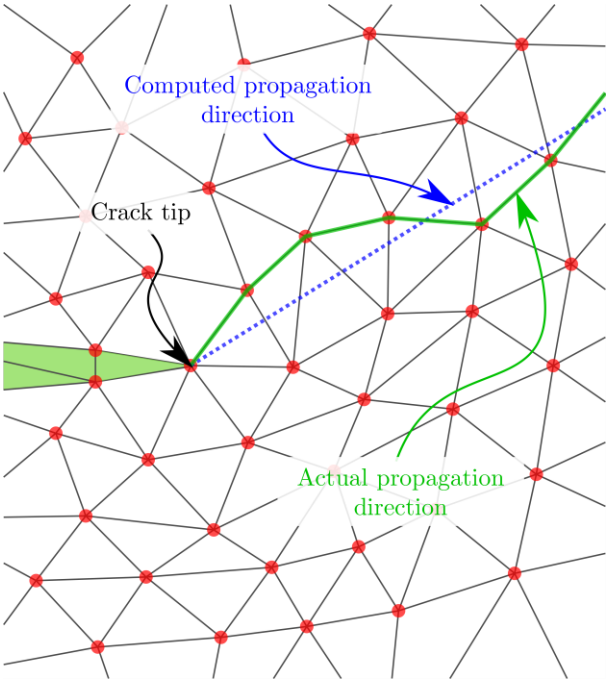

Fig. 7 Prescribed crack path (dashed blue line) and the actual crack path (solid green line) after cohesive elements insertion.

Debonding It is therefore clear that the CZM is very well adapted for problems where the crack path is known in advance. This is the case of problems involving debonding of interface. The literature studying the application of CZM to this kind problems is rather broad (Chandra et al (2002); Turon et al (2007); Li and Ghosh (2004); Turon et al (2010)). In the case of microscopic modeling of materials, the CZM are very well suited to model the debonding that can take place between the inclusions and the matrix of a metallic or composite material.

2.3.3 General remarks

CZM within the context of FEs represent a very interesting tool regarding fracture modeling. The discontinuities of displacement fields that appear during the fracture process are naturally handled by the method. It also allows to introduce interesting physical mechanisms into the fracture model through the use of different kind of traction-separation laws and the energy dissipation rate can be controlled very accurately. These traction-separation laws can include rate effects (Salih et al (2016)), account for stress triaxiality ratio (Banerjee and Manivasagam (2009)) and fatigue effects (Nguyen et al (2001)), among others.

Cohesive elements are widely used in the community for applications involving brittle materials and also within the context of fragmentation where most materials fail in a brittle fashion under violent dynamic load-

ings. Although some traction-separation laws for ductile materials exist (Scheider (2009)), problems arise when ductile materials are subjected to complex non proportional loadings and, in particular, to low stress triaxiality ratio loading. These problems come from the fact that it is still a big challenge to handle contact in problems involving non monotonic loading path that can eventually lead to crack closure and friction.

There are also some drawbacks that often restrict the use of CZM in classical FE codes. The need of handling mesh operations to dynamically insert cohesive elements (extrinsic approach) is extremely important and mesh dependency remains an issue regardless of the insertion approach. Recent approaches as the one introduced by Soghrati et al (2017) tackle mesh dependency issues. Alternatively, mesh dependency issues related to CZMs can be overcome by using advanced crack initiation and propagation techniques (Subsections 2.2 and 2.4).

In spite of the drawbacks discussed previously, CZMs present interesting features that can be used within the context of heterogeneous materials modeling. A brief overview of different works using CZMs to study heterogeneous materials is proposed in the following.

2.3.4 Applications to heterogeneous materials

It is now clear that cohesive elements can be used to study the fracture of heterogeneous materials but it is necessary to use this technique carefully since its drawbacks could lead to non physical results. Taking into account the advantages and drawbacks of CZM presented previously, CZMs have mainly been used for problems involving debonding between inclusions and the matrix (Liang and Sofronis (2003); Meng and Wang (2015); Giang et al (2017)), inclusions failure (Steglich et al (1999); Giang et al (2017)), and problems where the crack paths are prescribed (Giang et al (2017)). The previous cited works will be briefly discussed.

Steglich et al (1999) proposed an interesting and pioneering application of cohesive elements to the modeling of fracture of metal matrix composite materials for which failure is dominated by particle cracking. At the macroscopic level, the damage process for this material was modeled using a Gurson-Tvergaard-Needleman (GTN) model (Section 3). The parameters of this micromechanical CDM model were obtained from *unit cell* computations where the two phases of the material (inclusions and matrix) were meshed. Cohesive elements were initially placed over the equatorial plane of the inclusion and the failure process was modeled by using a classic exponential traction-separation law (Xu and Needleman (1994)). Although inclusion/matrix debonding and matrix failure was neglected in the unit cell computations, the multiscale principle of *fitting* macroscopic failure models from simulations of more advanced mesoscopic models was highlighted. A similar *unit cell* approach modeling the debonding of particles instead of their fragmentation was proposed by Meng and Wang (2015) among others.

Since debonding can be modeled very accurately by using cohesive element approaches, this technique has been widely used within the context of heterogeneous materials. Liang and Sofronis (2003) tackled a very challenging problem that remains a hot topic in the field of metallic materials modeling: hydrogen embrittlement. It is well know that hydrogen induces embrittlement of ductile materials as hydrogen induces debonding at the interface between carbides and the matrix. This debonding was modeled by using a traction-separation law that accounts for the hydrogen concentration in the material. Although the use of cohesive elements to study debonding is logic and simple, the coupling of fracture processes with complex multiphysics phenomena is not. It is indeed very interesting to see how complex multiphysics phenomena, such as hydrogen diffusion, can be coupled to the mechanical response of a material containing cracks.

An interesting contribution to micromechanical modeling using CZMs was proposed recently by Giang et al (2017). Ductile fracture was modeled at the scale of large 3D periodic arrays of inclusions. Cohesive elements with a classic exponential traction-separation law (Xu and Needleman (1994)) were placed at interfaces between particles and matrix, and along a predefined crack propagation path. The latter was mainly used to model matrix micro-cracking, but it also included the equatorial planes of some particles, which enabled to model their fragmentation. This is hence a combination of previous works by Steglich et al (1999); Meng and Wang (2015), with the addition of a matrix micro-cracking model. Examples of results using this approach are shown in Figure 8. These results reveal a competition between particle debonding and fragmentation depending on material properties. Although these results are promising, Giang et al (2017) used an intrinsic method and had to define the crack path *a priori* both for particle fragmentation and matrix micro-cracking.

2.3.5 Conclusion

CZMs are relevant for modeling the initiation and propagation of brittle and ductile cracks. This is done either by inserting cohesive elements along any potential crack initiation and propagation surfaces, or by dynam-

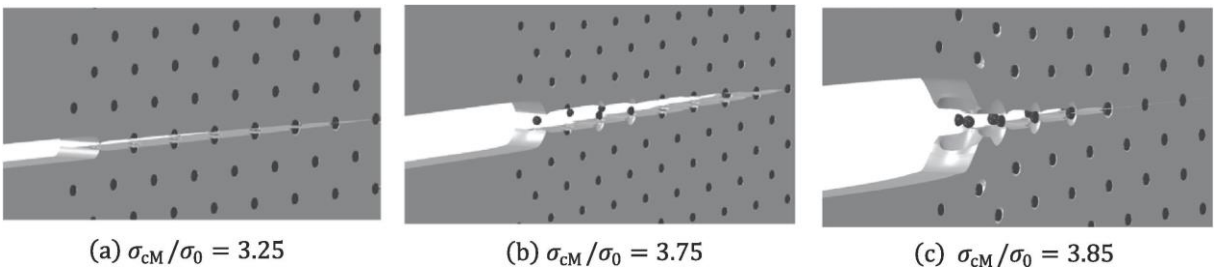

Fig. 8 FE simulation of a ferritic steel microstructure using CZMs at particles/matrix interfaces, and along a predefined crack propagation path through particles and matrix at the midsection of the specimen. The ratio σ_{cM}/σ_0 is the ratio between matrix cohesive strength and matrix yield stress. Reprinted from Giang et al (2017), with permission from Elsevier.

ically inserting cohesive elements during the simulation. These elements have a negligible volume initially, and will progressively open as the crack grows, with an accurate modeling of the energy dissipation rate through a traction-separation law.

The implementation of CZMs for particle debonding modeling is facilitated, as cohesive elements can be inserted initially or dynamically along particles/matrix interfaces. Particle fragmentation and matrix microcracking modeling is less straightforward, as the crack propagation path is generally not known *a priori*. For such arbitrary crack paths, CZMs should be coupled to the methods presented in Subsections 2.2 and 2.4. For instance, Wolf et al (2017) coupled a CZM to the X-FEM in order to model ductile fracture in 2D configurations.

2.4 Mesh modification

2.4.1 Introduction

CZMs can already be seen as a mesh modification, as new elements are inserted to model the discontinuity. If no CZM is considered, the nodes along the crack path can be simply duplicated. As in element erosion approaches, this instantaneous fracture modeling can be smoothed by releasing node tractions progressively over several increments. It must be pointed out that these smoothing techniques are usually expressed as functions of increments or time, while a CZM is expressed as a function of crack opening displacement (Antretter and Fischer (1998); McHugh and Connolly (2003); Ortiz and Pandolfi (1999)). Cohesive elements also use a surface discretization, while traction release is expressed directly at nodes (Antretter and Fischer (1998)).

Antretter and Fischer (1998) considered a 2D problem of a ductile material with two inclusions explicitly meshed. Crack initiation was not modeled as one of the two inclusions was considered as initially fragmented. The propagation of this fragmentation crack within the matrix and towards the second inclusion was modeled by triggering node release along a predefined crack path based on a crack tip opening angle criterion.

For arbitrary crack paths where the crack propagation criterion not only determines the propagation onset, but also the propagation direction, the numerical implementation becomes quite complex. Robust mesh modification operations have to be developed to dynamically discretize new interfaces during the FE simulation, as discussed hereafter.

Note that the terms mesh modification are rarely used. Most authors use the word remeshing, which is a quite ambiguous term as it may encompass full remeshing, local remeshing, or adaptive mesh refinement. The most widely used remeshing technique for large deformations simulations involves a human operator whose role is to correct the initial FE model if element inversion occurs during the simulation. There are automatic procedures to avoid human intervention, although they are often restricted to tetrahedral elements. Automatic remeshing can simply mean moving some nodes to avoid element inversion. This can be combined or replaced by automatic mesh topology changes (*e.g.*, by edge or face swapping). Alternatively, remeshing can mean regenerating the whole mesh from some representation of the current geometry whenever there is a risk of element inversion.

Adaptive mesh refinement, or local mesh refinement, is often presented as a type of remeshing technique, although it only consists in splitting edges, faces, and elements to refine the mesh. Mesh adaption seems to be less ambiguous as it usually means that mesh size is being varied spatially and sometimes also in time to automatically adapt the FE mesh to the solution's variations. This can be done dynamically and automatically throughout the FE simulation, which requires proper transfer operators to map variables between old mesh and new mesh after the FE mesh has been modified. It can also be done after the whole FE simulation has been conducted, to restart with a new mesh.

To summarize, we will use the word remeshing whenever a mesh modification is operated to avoid element inversion or modify the model geometry. This modification can be a change to the positions of some or all nodes, and/or a change to the topology of some or all FEs. Full remeshing will mean that the whole FE mesh is being regenerated from some representation of the domain geometry, and in particular of its boundaries (including the crack geometry).

Mesh adaption will refer to mesh modifications operated to adapt the FE mesh to the FE solution's variations and reduce some estimated error. This may be done solely using local mesh refinement, or accompanied by node position and element topology changes.

In all cases, we only refer in the following to automatic mesh modifications that do not require human intervention and can be applied dynamically during the FE simulation, as the crack path is not known *a priori*.

2.4.2 Methods and their applications

Mediavilla et al (2006a) used an *uncoupled* non local integral damage indicator as crack initiation and propagation criterion [2]. This criterion was used to introduce a new crack geometry, which was itself used as input to a full remeshing algorithm. A similar approach was proposed earlier by Bouchard et al (2000), using a stress based crack initiation and propagation criterion. At each load increment, the crack was advanced by a given length, which was considered a purely numerical parameter. The numerical approach proposed by Mediavilla et al (2006a) consisted in first introducing the new crack segment in the FE mesh, without opening it. Then, an appropriate transfer operator was applied for history variables, before duplicating the nodes along the new crack segment and recomputing strain and stress fields for the new geometry.

While the full remeshing based crack modeling and history variables transfer process used by Mediavilla et al (2006a) may seem quite complex, each step is necessary to ensure consistent mechanical equilibrium throughout crack propagation. Transfer operators are very strongly related to remeshing algorithms, as all mesh modifications, except hierarchical mesh refinement, lead to artificial energy diffusion (Mediavilla et al (2006a); Shakoor et al (2015)). For ductile fracture problems a robust transfer operator to conserve plasticity history variables is of high interest, in particular if the crack propagation criterion depends on plastic strain (Mediavilla et al (2006a); Shakoor et al (2015)). A simple solution is to solve mechanical balance equations after each crack initiation or modeling step (Mediavilla et al (2006a); Shakoor et al (2015, 2017a)). An important remark of Shakoor et al (2017a) is that, although a weak (or explicit) coupling between crack modeling and mechanical solution was used, crack initiation and propagation was modeled before mechanical solution. This is a relevant choice for micromechanical analysis using computational homogenization, as it ensures that all quantities of interest are consistent with the geometry. To further improve energy conservation during remeshing, higher order interpolation techniques are interesting as they reduce the diffusion induced by the interpolation step between old mesh and adapted mesh (Mediavilla et al (2006a)).

Both artificial energy diffusion and the accuracy of the crack propagation criterion can be improved using mesh adaption. A first *a priori* error minimization approach is to refine the mesh close to crack faces and especially crack tips (Bouchard et al (2000); Mediavilla et al (2006a)). More mathematically sound *a priori* and *a posteriori* error estimators based on the representation of the geometry [3] have been proposed in the literature. In particular, for a first order FE scheme, the geometric error can be expressed as a function of the principal curvatures of geometric boundaries, which can be estimated using distance functions and their second derivatives (Roux et al (2013); Shakoor et al (2015)). Since at least one of the principal curvatures is infinite at crack tips, a minimum mesh size parameter is usually defined to limit mesh refinement in crack tips regions, while mesh size varies smoothly depending on the local principal curvatures in the whole FE domain (Roux et al (2014)). Because principal curvatures are generally different in distinct directions (similarly to principal stresses), anisotropic elements can be used to refine the mesh only in given directions (Roux et al (2013)). These elements are however not recommended for large deformation simulations as they raise a higher risk of element inversion (Shakoor et al (2017b,a)).

Both remeshing and mesh adaption were used for micromechanical ductile fracture modeling by Roux et al (2014), although the proposed approach can be seen as an element deletion, or region deletion method. It consisted in using an LS function and error estimator based anisotropic mesh adaption method to define the crack geometry. Then, instead of introducing a new crack sur-

[2] The word *uncoupled* means that in this work the softening effect was not modeled, as opposed to coupled damage models discussed in Subsection 3.1. A non local regularization was nevertheless judged necessary by Mediavilla et al (2006a) to "reduce the influence of local damage variations which are a result of the discretization".

[3] Error estimators can also be based on mechanical variables as discussed in Paragraph 4.4.1.

face, a region of small thickness was introduced and modeled with a very low stiffness to simulate an actual void. The proposed method enabled void nucleation, growth and coalescence simulations of 2D microstructures of complex morphology, which required a robust remeshing technique to handle very large deformations (Roux et al (2013)). Stress based criteria were used to predict particle fragmentation and debonding.

A limitation of the method proposed by Roux et al (2014) was that the interface between the void region and the other material components (matrix and inclusions) was not meshed explicitly. Thus, material interfaces could cross arbitrarily through some mesh elements, whose behavior was defined using mixture laws. Although these laws can be relevant for multiphase fluid flow modeling (see *e.g.,* Hirt and Nichols (1981)), they cannot define the mixture of an elastic inclusion with an elasto-plastic matrix. An extension to this region deletion method was proposed by Shakoor et al (2015). To avoid mixture laws[4], remeshing operations were extended to dynamically construct an explicit interface discretization. This method was first applied to model void coalescence by matrix micro-cracking in 2D using an uncoupled Lemaitre damage indicator by Shakoor et al (2015), and later extended to model particle fragmentation and debonding in 3D by Shakoor et al (2017b) for academic test cases.

This region deletion method avoided the mesh shape dependence issue of the element deletion method, as LS functions were used to define any arbitrary shape for the region to be deleted. LS functions are signed distance functions to the interface computed at FE mesh nodes, with an arbitrary sign convention that distinguishes mesh nodes inside a given component of the material from outer nodes (Osher and Sethian (1988)). For LS functions to be well-defined, the mesh had to be fine enough (or the region thickness large enough) so that some nodes would be located within the region to be deleted (and thus have a different sign from other nodes of the FE mesh). Although in ductile fracture cracks grow up to become large interacting voids, this requirement on mesh size raised computational cost issues (Roux et al (2014)), even if interfaces were explicitly meshed (Shakoor et al (2015, 2017b)). This limitation was removed by Shakoor et al (2017a), where the authors proposed to use multiple LS functions to capture the crack geometry, as proposed by Sukumar et al (2001) in the context of the X-FEM. Two LS functions were used to define the two faces of the deleted region (the two crack faces), while a third LS function was used to delimit its extent (the crack tip). The thickness of the deleted region could then be reduced to at least one order below mesh size. This framework was applied to model crack initiation in 3D using stress based particle fragmentation and debonding criteria by Shakoor et al (2017a). As shown in Figure 9, this framework is promising as the large deformation of nucleated voids can be tracked up to the void coalescence phase. Results at 50% of applied strain in Figure 9 illustrate well these capabilities provided by remeshing methods.

[4] Element enrichment approaches such as the X-FEM can also be used (Subsection 2.2).

2.4.3 Discussions

Remeshing and mesh adaption based crack modeling methods are summarized in Figure 10. An advantage of the methods proposed by Roux et al (2014); Shakoor et al (2015, 2017a) over those proposed by Bouchard et al (2000); Mediavilla et al (2006a), is that they used a local mesh modification algorithm (Gruau and Coupez (2005); Shakoor et al (2017b)), instead of regenerating the whole mesh at each initiation or propagation step (*i.e.,* full remeshing). This is relevant for:

- conservation of history variables, because numerical diffusion is only introduced close to the crack tip, where the mesh is finer,
- computational cost, as mesh modification operations are restricted to a small region,
- distributed computing, as independent and spatially local operations are easier to distribute among multiple processors.

It can be observed in Figure 10 that the methods developed by Shakoor et al (2015, 2017a) place FEs within the crack or deleted region. Since crack faces are explicitly meshed in these methods, one could consider removing these elements. However, the mesh motion and adaption method proposed by Shakoor et al (2017b) uses these elements within the crack or void to model its growth and linkage with neighboring voids.

The main limitation of remeshing and mesh adaption based crack modeling is the high technicality of mesh modification operations and the difficulty to implement them, especially in 3D, in comparison to element erosion for instance. Additionally, the difficulty is severely increased if the mesh comprises elements of different types and higher order. Mediavilla et al (2006a) developed an algorithm for quadrangle elements in the 2D case, but linear tetrahedra are systematically used in 3D to avoid the difficulty in adapting meshes with hexahedral or higher order elements. Shakoor et al (2017a) alleviated the difficulty of updating crack geometry by using LS functions, but no 3D crack propagation criterion was proposed. Crack propagation techniques introduced earlier by Carter et al (2000) could complete

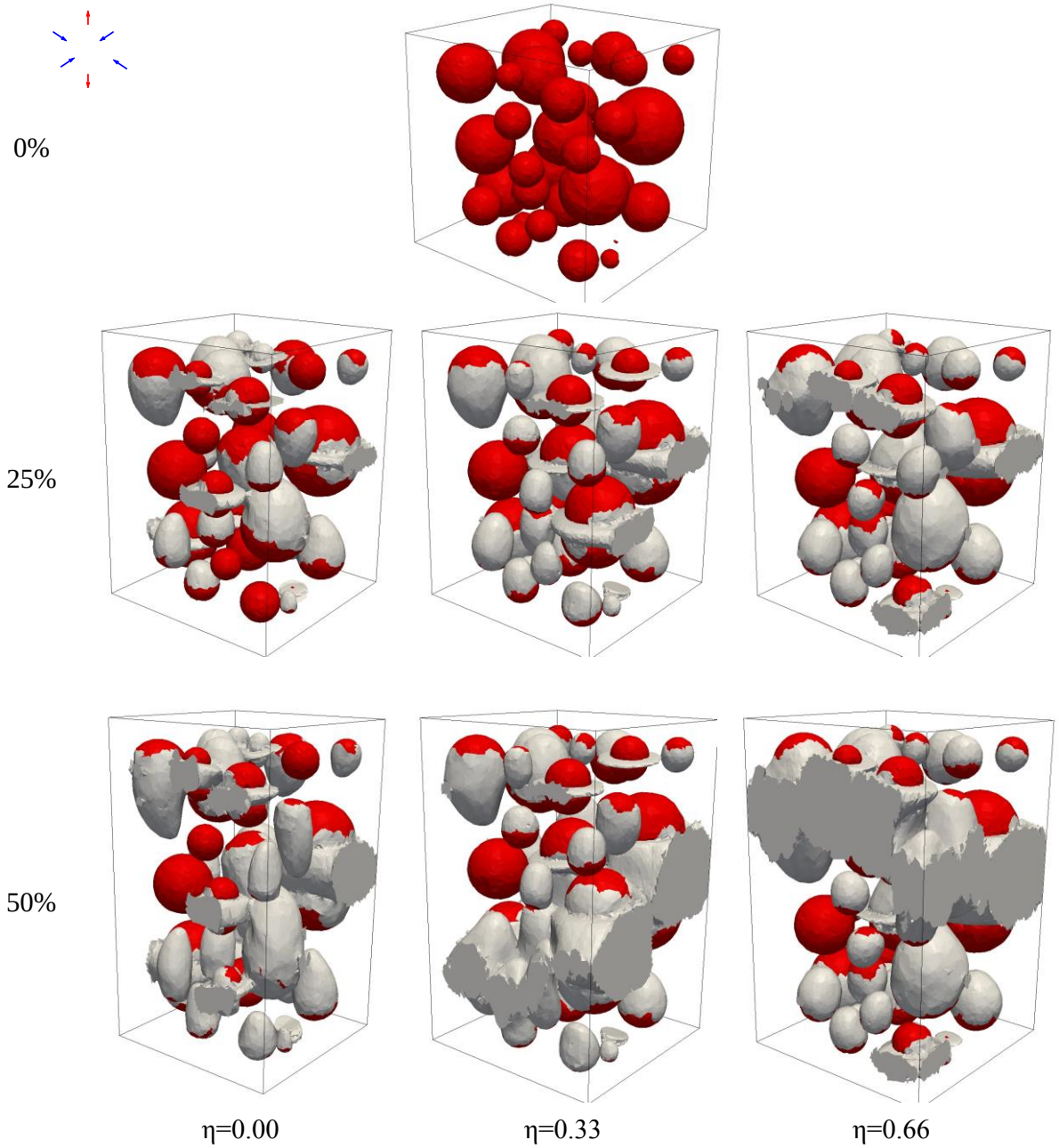

Fig. 9 Micromechanical simulations of a metal matrix composite microstructure showing remeshing based modeling of void nucleation by particle debonding and fragmentation followed by void growth and coalescence. Voids are shown in light gray, particles in red, and η refers to the stress triaxiality ratio. Reprinted from Shakoor et al (2017a), with permission from Elsevier.

the method of Shakoor et al (2017a). The latter only focused on void nucleation for a high particle volume fraction metal matrix composite for which matrix microcracking was neglected and void coalescence was assumed to be purely plasticity driven.

As a conclusion, discontinuous approaches to ductile fracture where crack initiation and propagation are modeled using mesh modifications have been developed in the two last decades. In particular, these methods have extensively been applied to model the brittle fracture micromechanisms of particle fragmentation and debonding which play a major role in ductile fracture. The use of remeshing in these developments is justified by a large deformation of crack faces and a significant void growth before final failure. Remarkable results have been obtained regarding crack initiation in 2D and 3D, but crack propagation modeling is for the moment restricted to 2D. This limitation does not seem to be linked to the crack modeling methods, as has already

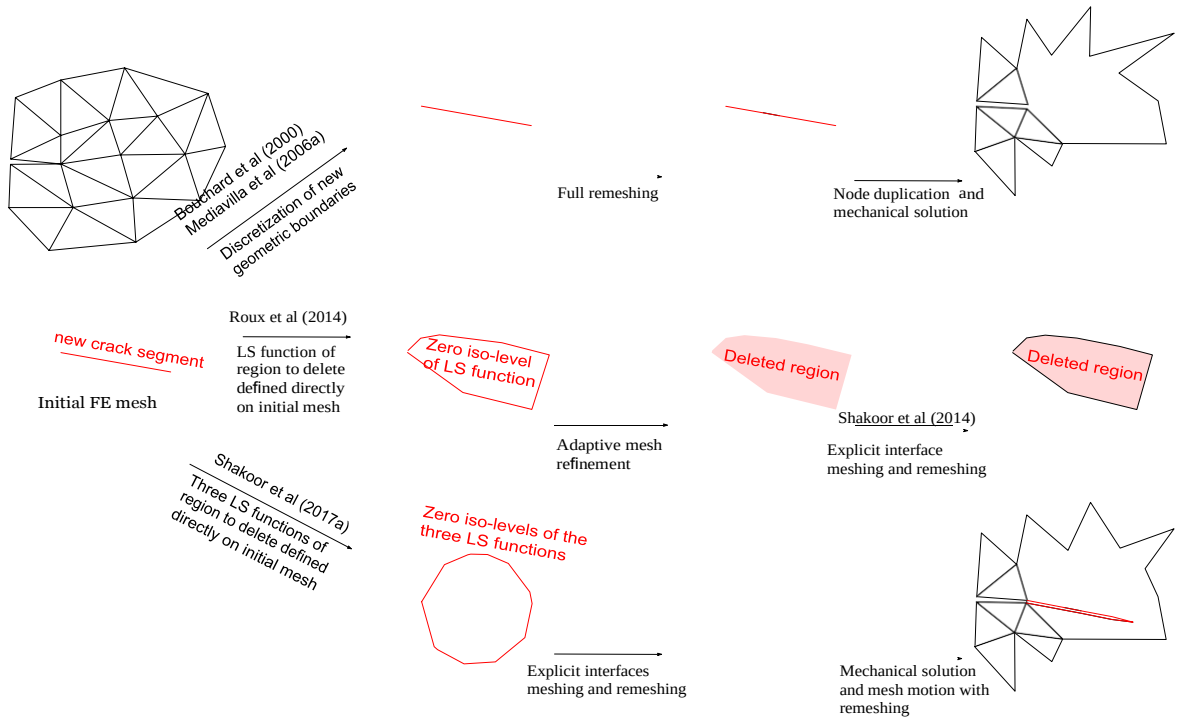

Fig. 10 Summary of remeshing and mesh adaption based discontinuous approaches. In the first line, crack meshing and node splitting as proposed by Bouchard et al (2000); Mediavilla et al (2006a). In the second line, region deletion with an LS function as proposed by Roux et al (2014), possibly with an additional explicit interface meshing step as proposed by Shakoor et al (2015, 2017b). In the third line, crack meshing and node splitting using three LS functions as proposed by Shakoor et al (2017a). Mesh modifications are systematically followed by the transfer of history variables.

been observed in Subsection 2.2, but to the absence of 3D crack propagation criteria that can handle multiple crack initiation sites.

2.5 Conclusion

While they cannot account for the influence of a minor void population within the matrix, the computational methodologies reviewed in this first section already reveal the complexity of ductile fracture modeling at the microscale. The features of interest for discontinuous approaches are mesh independence, energy dissipation rate modeling, compatibility with large deformations, and ease of implementation.

Removing any elements that are too distorted or have satisfied some fracture criterion is the most straightforward discontinuous approach. It is easy to implement, and solves any element inversion issues in large deformations. It can be completed with a progressive release of stress and stiffness tensors to control the energy dissipation rate. However, it raises mesh size and mesh element shape dependence issues as the crack can only propagate from element to element. Removing elements also leads to a loss of mass.

As a consequence, there is a need for methods that can model cracks as new interfaces dynamically and arbitrarily inserted and modified during the FE simulation, depending on some crack initiation and propagation criteria. The first option to reach such end is enriched FE methods, and in particular the X-FEM. This method enables to define interfaces independently of the FE discretization, as cracks can cross mesh elements and crack tips can be embedded within elements. The implementation of the X-FEM requires some modifications to the FE code as additional degrees of freedom are added, and some numerical issues have to be handled. Apart from these difficulties, it seems a perfect candidate to model the failure of brittle components of ductile materials' microstructures. However, it has been applied mostly to brittle materials. This is due mainly to the impossibility of modifying enriched FEs and thus ensuring these elements keep a good shape throughout the deformation process. There is hence a need for improved versions of these enriched FE methods so that large deformations can be handled.

The second option for initiating and propagating arbitrary cracks without any mesh dependence is through remeshing. The latter can naturally handle large deformations as distorted FEs can be eliminated by topological operations. However, remeshing has some conse-

quences that require a special care. First, it can induce unbalance and significant diffusion if a proper transfer operator is not implemented. Second, its implementation is quite complex especially in a distributed computing context, although this difficulty is alleviated if local remeshing is used instead of full remeshing. Recent FE simulations of ductile fracture at the microscale show that remeshing based techniques are a promising discontinuous approach. These remarkable simulations show void nucleation by failure of brittle components or their debonding, and the growth of these voids up to large sizes where they start interacting by plastic localization. There is no example of a similar result obtained with enriched FE methods.

Neither the X-FEM nor remeshing based techniques have a built-in model for the energy dissipation rate. The latter can be modeled using CZMs. Indeed, while CZMs alone have limiting mesh dependence issues, developments coupling CZMs to the X-FEM have shown that this limitation can be overcome. There is however no study showing the compatibility of CZMs with remeshing, especially in the large deformations case.

Finally, both enriched FE methods and remeshing based techniques require appropriate crack initiation and propagation criteria. While 3D particle debonding and fragmentation criteria have been mentioned in this section, there is still much work to be done regarding 3D crack propagation. The capabilities of existing 3D crack propagation methods have not been demonstrated for problems with multiple crack initiation sites and large deformations yet. It is a main limitation of discontinuous approaches that can be overcome by using continuous approaches to model crack propagation within the matrix material.

3 Continuous approaches

As stated in Section 2, robust and stable discontinuous approaches have been proposed and applied in the literature to model the brittle failure of particles and their interfaces. The energy dissipation rate can be modeled using CZMs. Mesh independence can be achieved using the X-FEM or remeshing based techniques. The latter have also been proven interesting capabilities in handling large deformations and purely plasticity driven void coalescence within the matrix.

In this section, a more complete model accounting for the nucleation, growth and coalescence of submicron sized voids within the matrix material is thought through. While discontinuous approaches could theoretically be used once again, this would lead to an extremely high computational cost. For instance, O'Keeffe et al (2015) report that for the studied aluminum alloy, a small volume containing on the order of 10^2 particles would contain on the order of 10^7 minor voids. To avoid this prohibitive computational cost, continuous approaches have been considered in the literature. These approaches have initially been proposed to model the influence of the major void population on material behavior at the macroscale. There are herein considered to model the influence of the minor void population on matrix behavior at the microscale.

Continuous approaches consist in modeling the influence of minor voids as a homogenized effect leading to a continuous material degradation process. An advantage of continuous approaches is that damaged regions can naturally grow, branch, coalesce without any numerical difficulty. Full material degradation and the initiation and propagation of cracks within damaged regions require a proper CDT model. CDT modeling, including Phase-Field (PF) models, is not discussed in the present section but in Section 4, as well as applications of continuous approaches beyond the void coalescence phase.

3.1 Continuum Damage Models

CDMs are certainly the most active and widely used modeling approaches to ductile fracture in the recent literature. This is in part due to their implementation in commercial codes, and the ease of implementing new ones as user subroutines. Some of these codes also include regularization techniques, which will be discussed hereafter.

3.1.1 Models

On the one hand, when it comes to fracture problems at room temperature, the Lemaitre model seems to be adopted by most researchers (Vaz and Owen (2001); Andrade Pires et al (2004); César de Sá et al (2006); Bouchard et al (2011); Seabra et al (2013)), for instance to model cold metal forming processes. It can be coupled to the Johnson-Cook elasto-viscoplastic model to address rate dependent problems (Broumand and Khoei (2015)). The Lemaitre model is based on a damage variable D and an effective stress definition $\sigma_{eff} = \frac{\sigma}{1-D}$, first proposed by Kachanov (1958), which corrects the conventional stress tensor σ to account for the presence of voids. This definition of σ_{eff} requires D to be comprised between 0 (defect free material) and 1 (fully degraded material). Many authors use empirical evolution laws for D (Borouchaki et al (2005); Mediavilla et al (2006b); Areias et al (2011)). The work

of Lemaitre consisted in deriving a phenomenological model with a sound theory with respect to the principles of thermodynamics (Lemaitre and Chaboche (1978); Ibijola (2002)). For instance, D cannot decrease.

On the other hand, the work of Gurson (1977) motivated researchers to look into more micromechanical approaches to model the softening effect in ductile fracture. This led to the development of micromechanical models such as the GTN model (Tvergaard and Needleman (1984)) and the Rousselier model (Rousselier (1987)). These models introduce a micromechanical porosity variable which can be related to the physical porosity in ductile materials, as they are originally based on the analytic[5] micromechanical analysis of a void within a perfectly plastic material (Gurson (1977)). Consequently, these models rely on a new yield criterion depending explicitly on the porosity, where the latter does not affect the elastic part, as opposed to most CDMs (see Andrade Pires et al (2004) for a modification of the Lemaitre model decoupling the elastic part).

Micromechanical models share multiple deficiencies with the Lemaitre model and other CDMs, in that they often require empirical or phenomenological modifications in order to yield accurate predictions for real industrial problems. For instance, an additive split of tension and compression stresses is often applied to the Lemaitre model to improve predictions in problems featuring both stress states (Andrade Pires et al (2004); César de Sá et al (2006); Bouchard et al (2011)). The GTN model in its original formulation has well-known issues when applied to shear dominant problems, for which phenomenological corrections have been proposed Nahshon and Hutchinson (2008); Xue (2008). Both the GTN model and the Rousselier model rely on a phenomenological split between porosity evolution due to void growth and that due to void nucleation (Tvergaard and Needleman (1984); Samal et al (2008)). Additionally, anisotropic versions, where the damage or porosity variable is a tensor field, can be found both for empirical or phenomenological CDMs and micromechanical models (Gologanu et al (1993); Lemaitre et al (2000); Scheyvaerts et al (2011)). The reader is referred to Besson (2010) for a recent review on all these models and their variants.

Therefore, in the following, empirical or phenomenological CDMs and micromechanical models are all addressed within the same discussion and are all abusively referred to as *CDM* s. The phrasing *damage variable* in the following will thus indifferently refer to an empirical or phenomenological damage variable, or a micromechanical or phenomenological void volume fraction or porosity variable. It will be seen that all CDMs lead to the same difficulties regarding the numerical implementation, and choice of discretization for the damage variable. Additionally, any of these CDMs can be used at the microscale to model minor void populations leading to damage in the ductile components of the microstructure, or directly at the macroscale to model the major (or unique) void population.

[5] See Subsection 3.2 for comments on the relations between multiscale methods and micromechanical models.

3.1.2 Elasto-plasticity and damage coupling

The first choice for the numerical implementation of a CDM is the choice of coupling. A strong coupling consists in considering the damage variable as an internal variable together with the equivalent plastic strain or any other variables indicating the plastic strain state. All these variables are defined at integration points inside FEs, while displacements are defined at FE mesh nodes. Material integration leads to a multidimensional problem implicitly relating damage and plasticity internal variables which must be solved simultaneously, as done for instance by Vaz and Owen (2001). A weak coupling consists in updating the damage variable using an explicit relation only at the end of each load increment, which avoids any changes to conventional implicit return mapping schemes for plasticity (El khaoulani and Bouchard (2013)). This can be quite time saving as empirical modifications of CDMs for applications to industrial problems require a trial-and-error process that becomes quite long if a new tangent modulus has to be derived at every single step. As shown by El khaoulani and Bouchard (2013), the counterpart is that smaller time steps must be used with a weak coupling compared to a strong one.

Independently of the choice of coupling, and even if locking issues linked to plasticity are properly handled, a pathological damage localization problem can be revealed. It can be shown that damage will always localize in a single layer of elements, which leads to a dependence of mechanical response on mesh size, with a dissipated energy converging to zero with mesh refinement (Bažant and Jirásek (2002)). For instance, Borouchaki et al (2005); Drabek and Böhm (2005) present results of FE simulations with pathological mesh dependence. In the following paragraphs, existing solutions to this problem are reviewed.

3.1.3 Non local integral formulations

A first solution to mesh dependence is to average some state variable r around each integration point. This state variable can be related to plasticity or directly

the damage variable (Bažant and Jirásek (2002)). Then, damage evolution in each integration point will be diffused to the surrounding neighborhood, avoiding any pathological localization. Mathematically, the non local variable $\bar{r}$ is defined within the FE domain Ω by

$$\bar{r}(x) = \int_{B(x)} w(x-y) r(y) \mathrm{d}y, \quad \forall x \in \Omega, \int_{B(x)} w(x-y) dy = 1, \quad B(x) = \{y \in \Omega, ||x-y|| < l_c\}. \tag{1}$$

The size of the averaging window $B(x)$ is often referred to as characteristic length l_c, and this type of regularization as non local integral averaging (Jackiewicz and Kuna (2003); Drabek and Böhm (2005); Seabra et al (2013)). A generally nonlinear weight function w, or kernel function, can be defined to decrease the weights of each integration points' neighbors y depending on their distance $||x-y||$ from it. The result of the averaging operation is called non local variable $\bar{r}$, and replaces its local equivalent r in all constitutive equations (Bažant and Jirásek (2002)).

Depending on whether a weak or strong coupling is used for the damage evolution equation, the averaging operation itself is respectively done at the end of each load increment or inserted within the FE discretization matrix. The latter option has the consequence of increasing the bandwidth of the FE discretization matrix depending on the averaging length, which in turn increases both computational cost and memory consumption (Bažant and Jirásek (2002)). A larger matrix bandwidth is also an issue for distributed computing, as well as the search of each integration point's neighbors.

From a numerical point of view, the averaged variable in non local integral models can be considered as an additional degree of freedom carried at integration points. Its discretization depends purely on the kernel function, the positions of the integration points, and the characteristic length l_c. In particular, it does not depend explicitly on the FE mesh and its topology. This conclusion has led some researchers to exploit mesh-free discretizations where all variables are carried by points, or particles, and interactions between these particles are constructed thanks to non local averaging and given choices of kernel functions (Liu et al (1999); Simonsen and Li (2004)). These methods share the same computational cost issues as non local integral models with strong coupling. However, the numerical implementation becomes more straightforward as non local regularization is built-in and no FE mesh is needed, which is also convenient for large deformation problems where FEs might invert.

3.1.4 Non local implicit gradient formulations

To reduce the computational cost overhead due to neighbors search and averaging in non local integral formulations, the latter can be approximated. If the weighting function $\bar{w}$ is chosen as a Gaussian function, it can be shown by a first order Taylor series expansion that the non local variable $\bar{r}$ can be approximated by solving a partial differential equation instead of integral averaging. As first introduced by Peerlings et al (1996), this equation is

$$\bar{r} - l_c^2 \Delta \bar{r} = r, \text{ in } \Omega. \tag{2}$$

This type of regularization is referred to as non local implicit gradient regularization, as the gradient of $\bar{r}$, which appears in the Taylor series expansion, is not explicitly computed but implicitly appears through the Laplacian operator Δ.

First, boundary conditions are voluntarily omitted in Equation 2 as they are still an open research question, in particular if this equation is to be used at the microscale for the matrix component of a ductile material. Most authors impose $\nabla \bar{r}$ to be orthogonal to the domain boundary $\partial\Omega$ (Peerlings et al (1996); Samal et al (2008); El khaoulani and Bouchard (2013)), but it is unclear whether this should be the case if the FE domain is a microstructure with particles or multiple ductile components (see Paragraph 3.1.7).

Second, the non local implicit gradient regularization suffers from a similar computational cost and memory consumption increase as its integral origin, although the bandwidth does not depend on l_c due to the first order approximation (Samal et al (2008)). Another advantage of the gradient version of the non local integral regularization technique is that, as long as a weak coupling is used, it can rely on the same FE discretization techniques as that used for balance equations.

3.1.5 Strain gradient plasticity formulations

Another type of non local formulation that has gained interest in recent literature is strain gradient plasticity formulations. These formulations are quite similar to non local implicit gradient damage, as they rely on the gradient of an internal variable, with similar implications on the numerical implementation with additional degrees of freedoms. The difference is that in strain gradient plasticity, the gradient terms are explicitly added within the principle of virtual work, leading to higher order stresses. Any localization of plasticity or damage leads to an increase of the gradient of these variables and, equivalently, of higher order stresses, which

are penalized in the principle of virtual work. Thus, localization is limited and a non local effect is obtained (Lorentz et al (2008)).

There are also versions of strain gradient plasticity where gradient terms are not added directly to the principle of virtual work but into the definition of the yield stress (Chen and Yuan (2002)), which avoids the introduction of higher order stresses. In all cases, boundary conditions in strain gradient plasticity models raise the same questions as for non local implicit gradient damage models (Chen and Yuan (2002)). Additionally, due to the explicit presence of gradient terms in the principle of virtual work or the definition of the yield stress, strain gradient plasticity requires a fully coupled discretization with additional degrees of freedom (Lorentz et al (2008)). This increases the bandwidth of the FE discretization matrix, leading to an increase of computational cost and memory consumption, as well as increased complexity for distributed implementations.

3.1.6 Thick Level-Set method

A last option for limiting damage localization that has been proposed in recent literature is the thick LS method (Moës et al (2011)). This method borrows the idea of limiting the damage gradient over a given length that is at the core of non local models. The main difference is that instead of defining a persistent non local variable throughout the whole damage process and the whole FE domain, the damage gradient is limited only in localization regions. In particular, any initiation and growth of damage that does not lead to high gradients is not affected by the regularization process. The numerical implementation of the method consists in a distance computation technique where damage values are ramped linearly over the characteristic length. This operation can be implemented efficiently using *e.g.,* a fast marching algorithm (Moës et al (2011)).

Although we do not know of any application of the thick LS method to ductile materials yet, it is included in the present review as it includes a promising modeling approach to the CDT. Indeed, a key aspect that was voluntarily omitted in this Subsection is what happens when the damage variable reaches large and unrealistic values. For instance if it comes close to 1. This problem is addressed in Section 4.

3.1.7 Discussions

To summarize, all regularization techniques introduce a characteristic length parameter. Damage localization is limited either by averaging a chosen state variable, or controlling its gradient. Non local integral formulations have a significant computational cost overhead and increased complexity for distributed computing implementations. Thus, non local implicit gradient formulations have been proposed. For a weak coupling strategy where the damage variable is only updated explicitly at the end of each load increment, these methods only require the solution of an additional partial differential equation at each load increment. For a strong coupling strategy where damage and elasto-plasticity are solved simultaneously, additional degrees of freedom must be added with the consequence of increasing the bandwidth of the FE discretization matrix. The formulation is then quite similar to that of strain gradient plasticity. The computational cost overhead is nevertheless not as significant as with the integral version.

The non local integral formulation in Equation (1) can be implemented efficiently within a mesh-free discretization, with the added advantage of avoiding element inversion issues in large deformations. For FE implementations, the non local implicit gradient formulation with weak coupling is computationally effective as it avoids neighbors search, and can rely on existing distributed FE solvers to approximate Equation (2).

In all non local formulations, an important requirement is that mesh size should be smaller than the characteristic length l_c. Although mesh adaption techniques can be used to locally refine the mesh only in damage localization regions (Paragraph 4.4.1), this requirement increases the computational cost significantly. It also raises the question of the definition of the characteristic length l_c.

Drabek and Böhm (2005); Hu and Ghosh (2008); Areias et al (2011) have applied non local regularization techniques to micromechanical problems involving 2D arrangements of inclusions or fibers. Although l_c was defined as a material parameter, the authors did not explain how to determine it. For macroscale applications, l_c is usually related to microstructural aspects such as the average distance between particles (Bažant and Jirásek (2002)). As a consequence, for microscale applications, it would be related to the average distance between voids of the minor void population.

Added to the definition of the characteristic length, which may require very refined meshes, non local implicit gradient and strain gradient theories raise the issue of boundary conditions. This is of high importance if the method is used at the microscale where a ductile component might share boundaries with particles, voids, and possibly other ductile components. Peerlings et al (1996) recognized that imposing $\nabla \bar{r}$ to be orthog-

onal to domain boundaries was an arbitrary choice. For microscale applications, Equation (1) should consider only integration points within the matrix material. Similarly, Equation (2) should be solved only within the matrix, as plasticity and damage are not defined in brittle components where linear elasticity and discontinuous approaches are employed. Boundary conditions for $\bar{r}$ should hence be defined at the boundaries of the matrix phase. Forest (2009) proved this result using mathematical arguments.

Physical aspects of these boundary conditions remain to be discussed, in particular if the microstructure features multiple ductile components of different composition. In the context of strain gradient plasticity, Hutchinson (2012) described different conditions to be imposed for each boundary depending on whether it separates two plastic components or an elastic and a plastic component. To the authors knowledge, there is no study conducting the same analysis for non local implicit gradient damage in a heterogeneous structure featuring both brittle and ductile components.

Last but not least, physical aspects of the models themselves are being discussed in the literature. Following the work of Gurson (1977), a number of micromechanical approaches to ductile fracture modeling have been considered, including the well-known GTN model. Ductile components of the microstructure could hence be modeled with advanced material laws accounting for the shape and distribution of minor voids and inclusions. For an even more accurate description, computational multiscale theories are being developed.

3.2 Multiscale methods

The aim of the present review is to provide insights on computational methods that could handle the full complexity of ductile fracture at the microscale and the associated micromechanisms. The application of these methods at the scale of industrial parts could theoretically be done by modeling the whole microstructure of these parts. This so-called Direct Numerical Simulation (DNS) approach is practically unfeasible. For instance, a centimeter-scale part of a material with a particle volume fraction of 0.5% and particles of average diameter 10 μm would contain millions of particles. Recent 3D DNS results using distributed computing can only account for hundreds of particles (Matouš et al (2017); Shakoor et al (2017c)).

To reduce computational costs, an option is to model the microstructure only in a limited region of interest, and to assume a homogeneous material for the rest of the macroscale model. This technique has been used by Tian et al (2010); Hosokawa et al (2013). In particular, Tian et al (2010) compared their FE simulation results to experimental data obtained using a destructive 3D imaging technique. The material outside the region of interest was assumed to be linear elastic. Shakoor et al (2017c) recently showed that this technique underestimates damage, even if more advanced constitutive models are considered outside the region of interest. Shakoor et al (2017c) considered an alternative avoiding the challenge of finding a suitable constitutive model for the outer material. This alternative consisted in relying on *in situ* tests with 3D X-ray imaging and digital volume correlation to measure boundary conditions for the same region of interest throughout deformation. These measured boundary conditions were applied directly as applied displacements to the boundaries of the meshed microstructure within the region of interest. The analysis was thus limited to the region of interest and the problem of finding an appropriate homogenized behavior for the surrounding material was circumvented.

For larger specimens and industrial parts where there could be multiple regions of interests, and for which 3D imaging is not possible, more general methods are necessary. In order to model microstructural effects at the industrial scale, and also to model the influence of minor voids on matrix behavior at the microscale, alternatives to DNS are investigated in the following. As opposed to phenomenological CDMs, Gurson (1977) proposed a micromechanical approach where the behavior of a simple idealization of the microstructure was computed analytically with a suitable choice of boundary conditions, and used as yield criterion at the macroscale. For less idealist and more realist microstructures, this micromechanical problem cannot be solved analytically.

Boundary conditions and numerical approaches to transfer information between two scales are discussed in the following. For the sake of generality, the two scales are named coarse scale, and fine scale. If the coarse scale problem is an industrial part or specimen, it is solved using conventional FE technology for homogeneous materials, while the fine scale problems are solved using the computational methods discussed in this review for heterogeneous materials. Multiscale methods can also be used at the microscale to model minor voids in the matrix material. In this case, the coarse scale problem is the heterogeneous microstructure but assuming a homogeneous matrix, while the fine scale problems feature the minor voids in the matrix.

3.2.1 Principles

The appeal of multiscale methods relies on the fact that DNS are prohibitively time consuming. Put simply, the objective of multiscale methods is to obtain a coarse scale response from fine scale calculations. This grants the possibility of decreasing considerably the problem size and thus tackling more complex problems. In this way, materials engineering and design applications become more feasible (Panchal et al (2013)). This is a very active field of research and the scope of the following paragraphs is merely to highlight aspects relevant to ductile failure. The reader is referred to recent reviews by Geers et al (2010); Nguyen et al (2011); Matouš et al (2017) for a more complete discussion on the topic.

Two categories of homogenization may be distinguished: analytic homogenization, and computational homogenization. Analytic homogenization is restricted in terms of the geometrical and material behavior complexity that it can handle (Gurson (1977)). Phenomenological parameters are usually added to analytic homogenization results in order to correct predictions (Tvergaard and Needleman (1984)). These parameters can be identified using experimental results or numerical simulations of more representative fine scale structures and loading conditions, called Representative Volume Elements (RVEs). Analytic homogenization and these identification techniques have been instrumental in the development of more advanced and physical CDMs (see, for example, Allen and Searcy (2001) or Jain and Ghosh (2009)). One advantage of this methodology is that, after proper calibration, the model may be readily used in complex simulations. However, the validity of the model is limited to the conditions it was calibrated for and cannot account for complex fine scale changes that its *a priori* assumed analytic form does not describe.

The second and more versatile homogenization category is computational homogenization. In this approach, coarse and fine scales are solved simultaneously. The coarse scale provides the boundary conditions for the fine scale problems, and the results of these fine scale problems, solved in RVEs, are upscaled to provide the homogenized response to be used in the coarse scale problem. Fine scale problems can be solved using fast Fourier transform methods (Lebensohn et al (2013)), mean field methods (Östlund et al (2016)), Voronoï cell FE methods (Moorthy and Ghosh (1998)), or reduced order modeling (Liu et al (2017b)). In the present review, a focus is made on FE methods, in which case computational homogenization is often referred to as FE^2 method. Although costlier than its analytic version, computational homogenization allows the user to obtain a coarse scale behavior under any given loading present in the simulation that adapts to complex fine scale changes. To achieve this, two important ingredients are necessary: an appropriate homogenization scheme and a robust and pertinent fine scale model.

3.2.2 Ductile fracture modeling

In the use of multiscale approaches to model ductile failure, two important difficulties arise. The first one is successfully transitioning scales under coarse scale strain localization and the second one is choosing appropriate boundary conditions for the fine scale problems. These difficulties are added to the challenge of adequately modelling the fine scale changes inherent to ductile damage, that are the object of this review. Another aspect of fine scale problems is RVE size. It has to be large enough so that the fine scale model accounts for the variability and distribution of fine scale features. Mathematically, the RVE should contain enough features (particles if the fine scale is the microscale) so that different realizations of the same statistical features distribution do not affect the homogenized material response significantly.

Once RVE size has been determined, different options are possible for boundary conditions. In the context of first order homogenization, which is the most popular approximation (Geers et al (2010)), strains can be assumed to be homogeneous at RVE boundaries, or periodic. Homogeneous stress boundary conditions can also be applied, or mixed boundary conditions where parts of RVE boundaries are subjected to homogeneous strains and other parts to homogeneous stresses (Böhm (2004)).

The large gradients associated to coarse scale strain localization represent a very important limitation of first order computational homogenization schemes (Matsui et al (2004); Yuan and Fish (2008)). In first order schemes with homogeneous or periodic strain boundary conditions, the information received by the fine scale model is limited to the first gradient of the coarse scale displacement field. First order approaches cannot account for size effects, as the homogenized response does not depend on any length scale parameter (RVE or particles size). They do not account for the non local effects discussed in Subsection 3.1.

Second order homogenization schemes with periodic strain boundary conditions (Geers et al (2001)) introduce size effects by defining RVE size as a length scale parameter (Kouznetsova et al (2004)). Although this size must still be large enough for the RVE to be statistically representative, it has to be small enough not to exceed the length scale that characterizes linear varia-

tions of the coarse scale strain field (or quadratic variations of the coarse scale displacement field). This allows for a better treatment of strain localization than first order schemes if strain gradients are moderate.

Ductile fracture often produces intense strain localization and second order homogenization schemes prove insufficient. Applying periodic boundary conditions is also limiting as cracks may not necessarily be orthogonal to RVE boundaries. Svenning et al (2017) proposed to use different boundary conditions for parts of RVE boundaries intersected by cracks, while weakly periodic boundary conditions were used in other parts. The latter are relevant for remeshing, which can be overconstrained when periodic meshes have to be maintained.

For general configurations where the crack propagation path at the coarse scale is unknown, advanced computational methods have to be designed. Localization in fine scale problems must be automatically detected and a propagation criterion has to be deducted for coarse scale cracks from RVE solutions. This problem is quite similar to that of handling large damage values in CDMs. Indeed, there is a critical onset where high damage values in CDMs and significant localization and damage in RVEs in computational homogenization require the introduction of discontinuities in the coarse scale discretization. Different options for modeling this CDT are discussed in Subsection 4.3. The added difficulty regarding computational homogenization methods is that a consistent relation must be maintained between coarse and fine scale problems.

3.3 Conclusion

As summarized in Figure 11, different options are available for modeling the continuous material degradation process at the macroscale in ductile materials or at the microscale in ductile components of the microstructure. In the later case, the aim is to model the influence of minor voids and their growth on the behavior of the matrix in ductile materials' microstructures. The most widely used approaches are CDMs, but recent efforts towards more predictive material modeling tools for materials engineering and design have led to the development of more advanced multiscale methods.

The first class of CDMs is based on Kachanov theory and empirical or phenomenological damage evolution laws. A damage variable is introduced and its local evolution is written as a function of stress state and loading history. This damage variable explicitly appears in the definition of stresses.

The second class of CDMs is based on Gurson theory and micromechanical or phenomenological yield criteria and porosity evolution laws. A porosity variable is introduced and its local evolution is computed by solving a micromechanical problem involving idealized microstructures and loading conditions. The solution of the micromechanical model includes a yield criterion explicitly accounting for the non linear effect of porosity. For improving predictions in general loading conditions, phenomenological parameters are generally added to both the porosity evolution law and the yield criterion.

CDMs (Figure 11a) systematically require special care regarding numerical implementation. Regularization techniques must be used to avoid pathological mesh dependence issues. These techniques can rely on averaging, which can naturally be implemented using meshfree methods, or on gradient terms, which can naturally be implemented using the FE method. For ease of implementation and model modification, a weak coupling seems preferable as long as the time step is small enough.

Regularization techniques involving gradient terms require the definition of boundary conditions that are not well understood. This is particularly problematic for boundaries between brittle and ductile components or between two different ductile components of a same microstructure.

Both averaging and gradient based regularization techniques involve a length scale parameter which is often related the distance between particles when it is used at the macroscale. If these techniques are applied to ductile components of the microstructure, then it may be related to the distance between minor voids. Physical arguments have not yet been discussed in the literature to defend such assumption.

Last but not least, computational homogenization techniques are worth considering (Figure 11e). Instead of correcting the limitations of analytic Gurson-like models by adding phenomenological parameters, computational methods can be used to solve the micromechanical problems numerically. In the context of ductile fracture, the computational methods discussed in the present review should be used. These methods would be used to solve sub-micron scale problems featuring the minor voids in the matrix, while at the microscale the microstructure would feature a homogeneous matrix. Material laws for this homogeneous matrix would be computed using computational homogenization of the response of sub-micron scale RVEs. Solving coarse scale and fine scale problems concurrently avoids the huge ex-

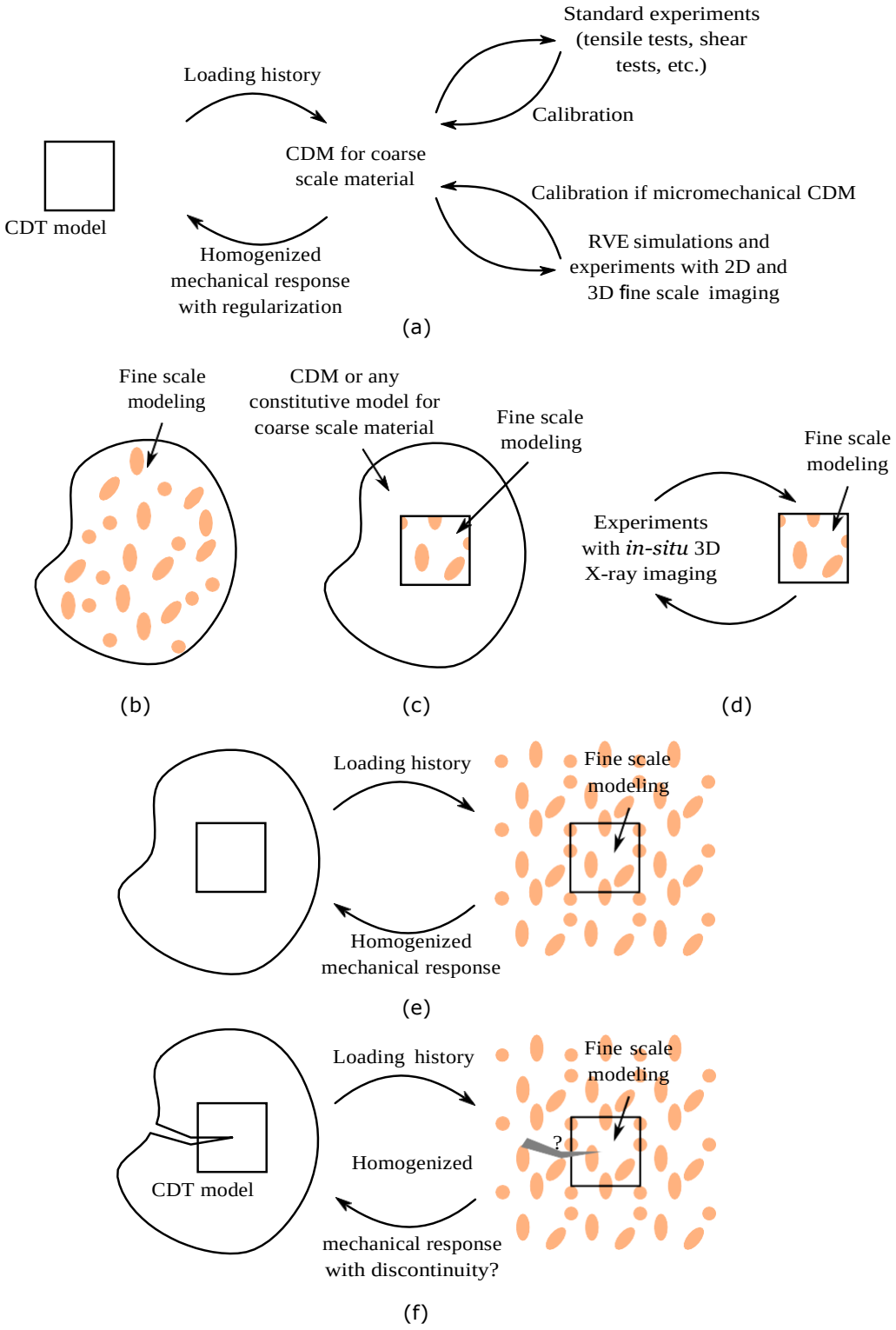

Fig. 11 Summary of continuous approaches: (a) Empirical, phenomenological or micromechanical CDMs; (b) DNS using fine scale models; (c) DNS using fine scale models only in a region of interest, using a CDM elsewhere; (d) DNS using fine scale models only in region of interest and measured boundary conditions based on *in situ* 3D X-ray data; (e) Computational homogenization using periodic boundary conditions; (f) Computational homogenization with CDT modeling.

perimental or computational cost that DNS schemes in Figures 11b-d would require.

Computational homogenization can be implemented using various choices of boundary conditions, which define how information is transferred from the microscale to the sub-micron scale. The main issues appear in the presence of strain localization within sub-micron scale RVEs or at the microscale. In such conditions, second order homogenization schemes have been considered. The latter do not enable ductile fracture modeling after the onset of void coalescence, close to the CDT.

The CDT is a key problem both for CDMs and computational homogenization approaches. In the case of CDMs, cracks must be initiated and propagated in damage localization regions to prevent the damage or porosity variable from reaching unrealistic values (Figure 11a). In the case of computational homogenization, cracks must be initiated and propagated in the matrix at the microscale to regularize RVE problems at the sub-micron scale (Figure 11f).

4 Continuous-Discontinuous transition

As mentioned in Paragraph 3.1.1, the most widely used CDMs assume that the damage or porosity variable remains small. For instance, Lemaitre and Chaboche (1978) pointed out that values of D higher than 0.5 are not realistic. A common correction to the Lemaitre model is to introduce a cutoff value for D, usually between 0.2 and 0.5, at which the element is considered as fully damaged with a complete loss of load carrying capacity. This value of 0.2 is similar to the value at which void coalescence was assumed to be the dominating damage mechanism by Tvergaard and Needleman (1984), although damage and porosity are two different concepts. Therefore, the GTN model includes a correction of Gurson's porosity evolution law to accelerate the load carrying capacity drop for high porosity values, up to final failure. The same correction was used for the Rousselier model by Samal et al (2008).

CDMs can hence model softening only up to a certain point, at which element erosion is necessary. Numerical issues arise if elements with very low stiffness and in particular nodes surrounded by such elements are kept in the FE mesh, which is another reason for using element erosion. An alternative is to initiate and propagate a crack within the damage localization region, with the consequence of relaxing stresses and preventing the damage variable from reaching unrealistic values. These different options to model the CDT are reviewed in the following. These techniques can also involve alternative paradigms to CDMs, such as multiscale methods or PF methods.

4.1 Element erosion

Element erosion is usually the default method for handling the CDT using CDMs. It is for instance the method used by Tvergaard and Needleman (1984) in their initial version of the GTN model, as well in their later studies (Mathur et al (1994)). It consists in deleting from the FE mesh any element that reaches a given critical (or cutoff) porosity threshold, and any node that is surrounded only by deleted elements. This GTN model with element erosion has been used by Nègre et al (2003), while Jackiewicz and Kuna (2003) added regularization by non local integral averaging. Similarly, Samal et al (2008) used element erosion with a non local implicit gradient formulation of the Rousselier model. Drabek and Böhm (2005) also used the Rousselier model with element erosion, but using non local integral averaging. Drabek and Böhm (2005) proposed applications to random 2D fibers arrangements.

An important remark is that here erosion is not an arbitrary progressive linear degradation of material stiffness over several load increments to avoid numerical issues as in Subsection 2.1. Instead, it is built within the CDM.

For phenomenological CDMs, elements are generally deleted whenever the damage variable reaches a given critical damage threshold (César de Sá et al (2006)). Vaz and Owen (2001) discussed alternatives. They conducted an analysis of the damage field close to the crack tip. Although the damage variable is relevant for defining the point at which material degradation can be considered as excessive, Vaz and Owen (2001) pointed out that the total damage work shows higher variations and localized distribution close to the crack tip. Thus, they considered that an element erosion criterion based on a total damage work threshold is more relevant. This approach has also been used by Andrade Pires et al (2004), with the argument that one must ensure that elements with high total damage work must be removed from the FE mesh to avoid non physical fracture patterns close to the crack tip.

Vaz and Owen (2001); Andrade Pires et al (2004); Borouchaki et al (2005); Areias et al (2015); El khaoulani and Bouchard (2012, 2013) proposed to couple element erosion to mesh adaption in order to reduce mass loss issues raised by the deletion of elements. These adaptive element erosion methods are reviewed in Subsection 4.4.

Although the use of element erosion with regularized CDMs may seem attractive as regularization ensures a

mesh independent damage localization, deficiencies of the element erosion method are still present. For instance, the removal of a triangular element from the FE mesh induces spurious damage localization due to the shape of the removed element. This could be avoided if the removed region was of smooth contour, as in PF methods.

4.2 Phase-Field methods

So far it has been shown that ductile failure modeling is of high complexity. It is expected that numerical frameworks should be able to properly reproduce and predict the main features of ductile fracture. Therefore, the numerical framework should account for non proportional stress states, possibly topologically complex damage patterns, crack initiation, propagation and branching. On top of that the mechanical response of the material should, of course, also be in agreement with the force-displacement experimental measurements.

Discontinuous approaches have been proven to be relevant for modeling void nucleation micromechanisms in Section 2, but they have not yet been proven capable of propagating 3D cracks initiated at multiple initiation sites. CDMs, as such presented in Paragraph 3.1.1, are appropriate to model damage initiation and growth, up to fracture. These approaches suffer from spurious numerical effects induced by the decrease of the load carrying capacity of the material that leads to strain and damage localization. To tackle this issue, non local and gradient based models have been developed (see Paragraph 3.1.3). These models introduce a material length scale that allows to capture material size effects (Ambati et al (2015)).

A derivation of these CDMs is the PF method, which can be seen as an optimization problem where the potential energy is minimized (Borden et al (2016); Francfort and Marigo (1998)). Similar to CDMs, in PF approaches damage is described by a bulk variable φ ranging in the interval [0, 1]. In this way, sharp interfaces that are created by cracks are weakly described through the continuous PF variable φ. This powerful idea allows to drop the requirement of remeshing or front tracking methods needed to follow the evolution of discontinuities since the evolution of the the PF variable φ itself completely describes the crack and the damaged regions of the material.

4.2.1 Brittle failure modeling

In the case of brittle materials, the most basic minimization functional (Π^{Br}) is given by:

$$\Pi^{\mathrm{Br}}(\mathbf{u},\varphi) = \underbrace{\int_\Omega g(\varphi)\Psi_e(\varepsilon(\mathbf{u}))\,dV}_{\text{elastic potential energy}} + \underbrace{\int_\Omega G_c H(\varphi) dV}_{\text{fracture energy}} \tag{3}$$

where $\Psi_e(\varepsilon(\mathbf{u}))$ is the elastic energy density function, function $g(\varphi)$ couples the PF variable to the elastic energy, G_c is the critical fracture energy and $H(\varphi)$ is called the crack density functional. Typically, the latter is given by:

$$H(\varphi) = \frac{1}{4l_c}\cdot(1-\varphi)^2 + 4l_c^2\,\|\nabla\varphi\|^2 \tag{4}$$

where l_c is the material length scale. Furthermore, it has been noticed in Paragraph 3.1.1 that damaged materials lose their load carrying capacity but only when they are submitted to tension. Which means that a damaged material should still be able to withstand compressive loads. To this end, the elastic potential energy in Equation 3 is often modified so that tension and compression are dissociated. This is achieved by decomposing the energy into two terms as follows:

$$\Pi^{\mathrm{Br}}(\mathbf{u},\varphi) = \int_\Omega \underbrace{g(\varphi)\,\Psi^+(\varepsilon(\mathbf{u}))}_{\text{tension}} + \underbrace{\Psi^-(\varepsilon(\mathbf{u}))}_{\text{compression}}\,dV + \underbrace{\int_\Omega G_c H(\varphi) dV}_{\text{fracture energy}} \tag{5}$$

where $\Psi_e^+(\varepsilon(\mathbf{u}))$ and $\Psi_e^-(\varepsilon(\mathbf{u}))$ are the portions of the elastic energy density that correspond to tension and compression, respectively. These elastic energy densities are often computed by using deviatoric/volumetric decomposition or by using a spectral decomposition of the strain tensor (see Ambati et al (2015); Borden et al (2016); Miehe et al (2010b); McAuliffe and Waisman (2016) for more details). In this way, the load carrying capacity of the material is not affected by damage when the material is submitted only to compression.

The PF potential is then used to deduce the constitutive equations of the problem using the second law of thermodynamics (Clausius-Duhem inequality). This leads to two equations that allow to compute the stress and the evolution of the PF variable. An important point here is that the irreversibility of the damage process should be enforced. In fact, using the potential presented in Equation 5, the PF variable could decrease

(and therefore induce healing) if the elastic energy decreases. This unphysical behavior is corrected by introducing a history functional into the PF variable evolution equation, see Miehe et al (2010a) for further details.

Finally, the expression of the function that couples the PF variable to the elastic energy $g(\varphi)$ can be different depending on the choice of PF model. Its most simple expression is given by:

$$g(\varphi) = \varphi^2 + \eta \tag{6}$$

where η is an artificial residual stiffness ($0 < \eta \ll 1$) that plays a role over the regions that have been completely damaged ($\varphi = 0$) so that the numerical scheme remains stable. This artificial stiffness is not used in all models (Borden et al (2016)).

4.2.2 Ductile failure modeling

It is important to mention that even though PF models have mainly been used within the context of brittle fracture (Francfort and Marigo (1998); Bourdin et al (2000); Amor et al (2009); Miehe et al (2010b) among many others), some extensions to ductile materials have also been proposed. This extension is not straightforward, as difficulties arise due to the complexity of the damage process in ductile materials. In fact, as pointed out by Ambati et al (2015), there is no variational theory describing ductile damage in its full complexity. To overcome this problem, all existing PF ductile failure models *mimic* the regularized behavior of the potential used for brittle fracture (Equation 5). Although it is possible to find small differences on how the ductile plastic behavior is introduced and how it is coupled to the existing elastic and fracture terms, all existing PF ductile models enhance the brittle potential (Equation 5) by adding a plastic term. In general the ductile PF potential functional (Π^{Duc}) takes the form:

$$\begin{aligned}\Pi^{\text{Duc}}(\mathbf{u}, \varphi) = &\int_\Omega \Big[g(\varphi)\Psi^+(\varepsilon^e(\mathbf{u})) + \Psi^-(\varepsilon^e(\mathbf{u})) \Big] dV \\ &+ \underbrace{\int_\Omega g_p(\varphi)\Psi_p(\alpha_i) dV}_{\text{plastic potential energy}} \\ &+ \int_\Omega G_c H(\varphi) dV\end{aligned} \tag{7}$$

where $\Psi_p(\alpha_i)$ corresponds to the plastic potential density function, α_i is a set of internal variables related to plasticity (*e.g.*, isotropic and kinematic hardening). The function $g_p(\alpha)$ couples the PF variable to the plastic energy. In most PF models $g_p(\varphi) \equiv 1$, which means that the plastic behaviour of the material is not modified by the failure process. The consequence of this choice is that the yielding surface of the material remains unchanged, and at some point plastic deformation saturates leading to a process dominated by elastic strains (Borden et al (2016)). Borden et al (2016) tested different expressions for $g_p(\varphi)$ so that the yielding surface evolves as damage takes place.

An important feature of PF methods is that they allow to naturally drive the evolution of damage. This could be seen as an advantage since no *ad hoc* criteria are needed to model complex ductile damage processes. Nevertheless, it comes at a cost, and it is precisely related to the difficulty of controling the onset of damage. This was very well illustrated by Borden et al (2016) by studying the impact of using Equation 6 for a ductile material. In fact, it was shown that no matter the material parameters used, the PF variable will reach high values before the critical stress is achieved, which is a non physical consequence of the choice of the coupling function $g(\varphi)$.

It is clear then that the choice of the coupling function $g(\varphi)$ is extremely important since it will directly impact the kinetics of damage. Furthermore, it can also affect the stress evolution up to the critical stress. Therefore, quantitative evaluations of force-displacement curves could become complicated and model dependent. Different choices of coupling function taking this into account can be found in the literature.

Ambati et al (2015, 2016); Ambati and De Lorenzis (2016) introduced a dependency to the plastic internal variables into the coupling function $g(\varphi)$. The function $g(\varphi, \alpha_i)$ then accounts for the plastic internal variables. This is done in such a way that the nucleation of damage is delayed by the plastic deformation. A simple expression for $g(\varphi, \alpha_i)$ is given by:

$$g(\varphi, \alpha_i) = \varphi^{2p(\alpha_i)} + \eta \tag{8}$$

where $p(\alpha_i)$ is a function of the cumulative plastic strain which, for a simple isotropic plastic hardening material, is an internal variable of the plastic model. The consequence of this choice is that the damage onset is delayed and, more importantly, the evolution of damage (the PF variable φ) will mainly be driven by the plastic energy term $\Psi_p(\alpha_i)$.

Another approach is to replace the quadratic form of the coupling function (Equation 6) by a higher order function with no coupling to the plastic variables. The main goal is to trigger the damage process at a later stage of the deformation. However this leads to higher

critical stress and therefore the corresponding material length scale has to be corrected (Borden et al (2016)).

It is nevertheless possible to model complex ductile failure phenomena by using PF approaches. Some of these approaches will be discussed in the next section in particular regarding heterogeneous materials.

4.2.3 Applications to heterogeneous materials

PF methods became very popular in the last few years and not only in the field of fracture mechanics. The mathematical beauty of the method combined with the ease of implementation, make of PF a very appealing numerical technique. Regarding fracture mechanics, applications to brittle materials are extensive. On the other hand, applications and PF methods themselves for ductile materials are not that widespread. A very challenging problem that has successfully been tackled by using a PF approach is related to brittle-ductile transition of materials submitted to dynamic loading. The latter type of loading condition has not been discussed in this section, but PF methods can be used for dynamic and quasi-static problems in the same way. Brittle-ductile transition is observed in materials whose failure mechanisms evolve during loading. Thermal softening comes into play and competes with plastic hardening. This thermal softening mechanism leads to the formation of shear bands that localize deformation and induce a fast loss of load-carrying capacity for the material (Arriaga et al (2015)). The interesting feature of this brittle-ductile transition phenomenon is that the amount of energy dissipated by ductile failure is much higher than the one dissipated by brittle fracture, and the transition can take place due to slight variations of the loading velocity (McAuliffe and Waisman (2016)).

McAuliffe and Waisman (2016) used a PF method to study the brittle-ductile transition on a notched plate impacted on one side of the notch on a direction parallel to the notch. Under low velocity impacts, loading induces brittle failure of the material and the crack propagates at an oblique angle with respect to the initial notch orientation. As the impact velocity is increased, plasticity takes place at a faster rate and therefore a fraction of the plastic energy is transformed into heat. This heat locally increases the temperature of the material and leads to thermal softening. This complex failure mechanism can be recovered by the PF approach proposed by the authors. To this end, a thermal term was included into the ductile PF functional (Π^{Duc}). The proposed approach, which also included a finite strain formulation, allowed to successfully reproduce experimental observations. Fracture patterns of materials under dynamic loading are extremely difficult to predict even in a qualitative way.

It would be very interesting to check if the set of numerical parameters identified by McAuliffe and Waisman (2016), is able to be predictive when loading conditions or sample geometry are changed. In fact, there are studies, on brittle fracture though, that show that a single set of numerical parameters within the context of a non local CDM does not allow to simultaneously predict the crack propagation speed and a qualitatively realistic crack pattern. This issue has been reported by Wolff et al (2015).

The unified numerical framework proposed by PF models allows to account for different physics that might take place during ductile failure. However, it is mainly well suited for homogeneous materials. This means that it is complex to propose a PF potential functional that simultaneously takes into account failure mechanisms that are of different nature such as brittle particle fracture, matrix/inclusion debonding and ductile damage of the matrix. Unfortunately, this is necessary for ductile fracture modeling at the microscale since microstructures are very heterogeneous and each of their components might fail according to completely different mechanisms.

A way to try to account for these heterogeneities at the microscale is to use a regular ductile PF potential functional enhanced with a very accurate plasticity model. Shanthraj et al (2016) proposed a numerical model where crystal plasticity was used at the microscale. This crystal plasticity model allowed to reproduce the highly anisotropic behavior observed in polycrystalline metallic materials. Material texture evolutions could be reproduced, as well as a progressive development of material anisotropy. For this application, even though the material was heterogeneous (*e.g.,* crystallographic orientations varied between grains), the failure mechanism was homogeneous. Failure was defined as a consequence of plasticity and its coupling on the PF potential functional.

Figure 12 shows the simulated microstructure at different time steps. It can be seen (Figure 12a) how damage nucleates at a triple junction as a consequence of the stress (and therefore plastic strain) induced by the change of crystallographic orientations between grains. Furthermore, the anisotropic behavior of the material might lead to the nucleation of secondary cracks, resulting from strain localization on some other grain boundaries. Nevertheless, it can be observed that damage is a consequence of plasticity, and other than stress concentration sites, grain boundaries do not represent regions

along which cracks would propagate, at least not in a direct way.

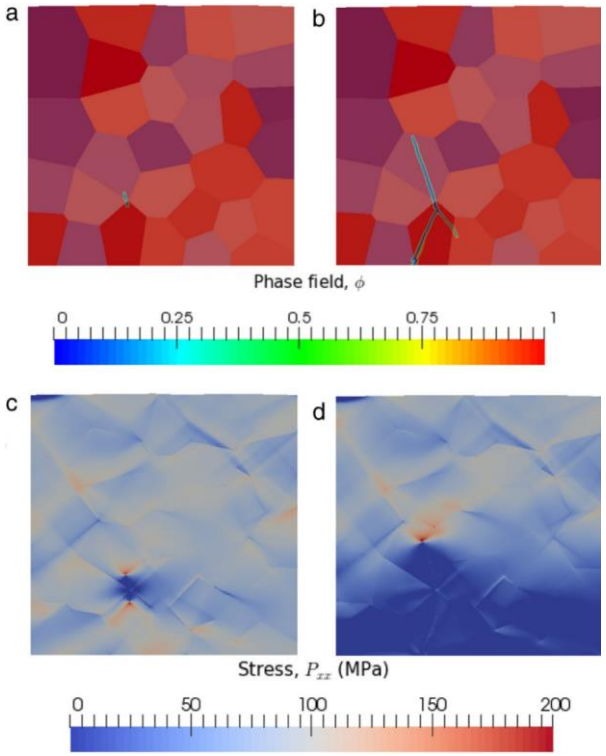

Fig. 12 Evolution of the damage PF variable (φ) and stress in a polycrystalline patch loaded in the horizontal direction at an applied tensile strain of: (a, c) 1.16%, (b, d) 1.21%. Reproduced from Shanthraj et al (2016), with permission from Elsevier.

4.2.4 Conclusion

PF methods are very well established to model fracture of brittle materials. The mathematical foundations of the approach make of PF a very robust and reliable numerical framework to account for the discontinuities inherent to damage and fracture both in 2D and 3D. In general, PF methods are very well suited to study materials at the macroscale where their mechanical behavior can be considered as homogeneous. Nevertheless, the mathematical rigor of the approach makes it difficult to enhance in order to account for more complex physical mechanisms that might be pertinent at the onset of fracture.

For instance, the extension of the well established brittle PF approaches to ductile failure modeling is not straightforward. In fact, the coupling between the different terms of the PF potential functional is done through the introduction of multiple coupling functions. The results as well as the kinetics of the evolution of damage processes is very sensitive to the choice of coupling function. As for CDMs, different options have been proposed in the literature for this coupling function. In particular, it is complicated to *design* a coupling function to obtain a specific feature of the failure when it is related to the physics or the kinematics of the damage process.

Regarding failure modeling of heterogeneous materials at the microscale, it seems rather complicated to include failure mechanisms of different nature into a single PF potential functional. Therefore, PF methods are not very well suited for this kind of applications. For instance, PF methods have been used to model crack initiation and propagation in a polycrystal, proving that they could be applicable to modeling particles fragmentation and matrix micro-cracking. In a more general sense, everything indicates that PF methods could be used to model the damage and fracture of brittle and ductile components of ductile materials' microstructures, given that appropriate PF potential functionals are defined for each of these components. However, PF methods do not seem to be capable of modeling debonding mechanisms.

4.3 Enriched Finite Element methods

There has been a lot of interest in the literature for CDT modeling using enriched FE methods, and in particular the X-FEM. Three different approaches can be distinguished. First, as mentioned in Paragraph 3.1.6, the TLS method includes both damage regularization and CDT modeling. Second, conventional non local integral or gradient regularization techniques can be coupled to crack initiation and propagation criteria to prevent the damage variable from reaching high values. Third, these criteria can also be used with multiscale methods, given that information is properly exchanged between coarse scale cracks and fine scale damage.

4.3.1 Thick Level-Set method

A way of handling the CDT was proposed by Moës et al (2011) with the thick LS approach. As in the PF approach, a transition zone of a given length l_c exists between the fully damaged material and the undamaged material. This transition zone is imposed by defining an LS function to capture the contour of the damaged material, and smoothing the damage variable D linearly from 0 at the contour, to 1 at a distance l_c to the contour. As discussed in Paragraph 3.1.6, this has the consequence of regularizing the damage variable.

It also has the consequence of modeling the CDT. Indeed, the LS function captures the $D = 1$ contour,

which delimits the region of fully damaged material. In other words, as the damaged material front evolves, it is followed, at a distance l_c, by the fully damaged material front. Since the fully damaged region geometry is defined by the LS function, its shape is arbitrary and does not depend on the FE mesh. The discontinuity within elements crossed by the $D = 1$ contour is modeled using the X-FEM. Branching and coalescence of damaged material regions are handled naturally in this approach thanks to the use of a CDM and an LS function.

Apart from its original regularization technique, the TLS method is very similar to PF approaches. Interesting features of PF approaches regarding regularity and CDT modeling are preserved by the TLS method, but these features are coupled to a CDM, which avoids the definition of PF potential functionals. In particular, micromechanical damage models can be used. The CDT modeling approach in the TLS method can be seen as a region deletion method, where a region with a smooth contour represents the fully damaged material, thus avoiding element shape dependence issues inherent to the element erosion method. This can be compared to the remeshing based discontinuous approach developed by Roux et al (2014) and discussed in Subsection 2.4. It will be interesting to follow future developments regarding the TLS method, as it has not been applied to ductile fracture modeling at the microscale yet.

4.3.2 Continuum Damage Models

The combination of CDM or micromechanical models and enriched FE methods provides another way of dealing with the CDT. Pourmodheji and Mashayekhi (2012) combined the Lemaitre damage model and the X-FEM to study ductile damage evolution in a steel alloy. A critical damage crack initiation criterion was proposed. The crack initiation direction was determined as the direction of the first principal stress. Once a crack was inserted in an element, it propagated to neighboring elements whose damage was beyond the critical damage threshold. In this way, the CDM provided the X-FEM with a natural crack initiation criterion. The critical damage value was determined based on the local plastic strain at the moment of macroscopic crack initiation. In the same study, the Lemaitre model was calibrated and a comparison between experimental and numerical results for compact tension and three-point bending tests was carried out with promising results.

Seabra et al (2013) proposed a similar approach with a non local integral Lemaitre model. Crack initiation was also determined with a critical damage criterion. Although the crack initiation criterion was similar to the one proposed by Pourmodheji and Mashayekhi (2012), a more elaborate geometrical crack propagation criterion was used. A radial search for the direction of maximum damage determined the propagation direction, and the propagation length was determined by the maximum length in the chosen direction in which damage was beyond the critical threshold. Figure 13 shows the damage and crack evolution in a plane strain specimen all the way from crack initiation up to final failure. Mesh independence was observed after a certain level of mesh refinement.

Mesh independence is also confirmed by Broumand and Khoei (2015), who used a similar technique with a non local gradient damage model. Broumand and Khoei (2015) tested their method on 2D configurations with holes, which are close to the void growth and coalescence problems that are targeted in the present review. Their results are promising for future developments regarding matrix micro-cracking, given that these crack initiation and propagation criteria can be extended to 3D. The results presented by Pourmodheji and Mashayekhi (2012) and Seabra et al (2012) are also restricted to 2D.

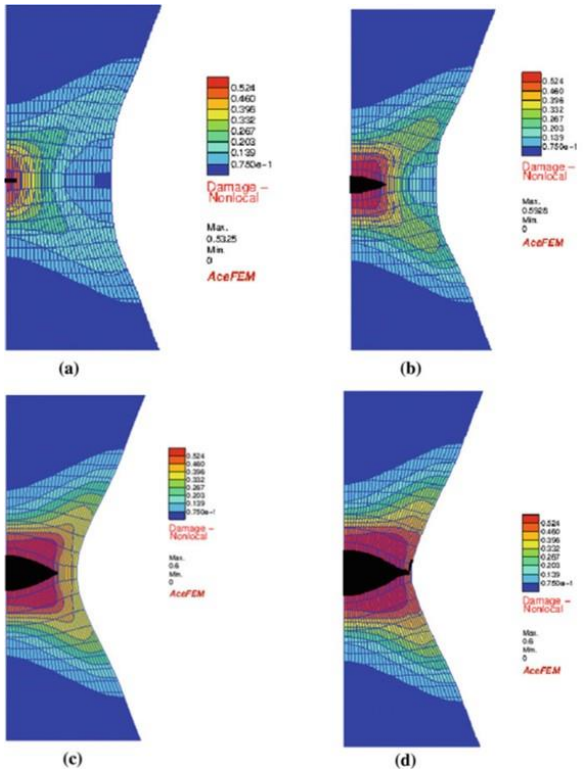

Fig. 13 Damage and crack evolution in a plane strain specimen from crack initiation up to final failure. Reprinted from Seabra et al (2013), with permission of Springer.

These techniques coupling a CDM to the X-FEM are compatible with micromechanical models, as shown

by Crété et al (2014), who used a modified Gurson-based model. An averaging procedure in front of the crack tip was carried out to avoid mesh dependence of crack propagation, which was considered to be the consequence of void coalescence induced strain localization. The propagation direction was thus determined by finding the strain localization plane ahead of the crack tip. After determining the crack propagation direction, a stored energy based criterion was evaluated in a half circle shaped patch. If the criterion was satisfied, the crack was propagated in one element, and the procedure restarted until the criterion was no longer satisfied. A mesh sensitivity analysis in different 2D configurations was carried out for the proposed method, and also for an element erosion technique based on the porosity fraction. The proposed methodology exhibited convergence in terms of mesh dependence as opposed to the element erosion technique.

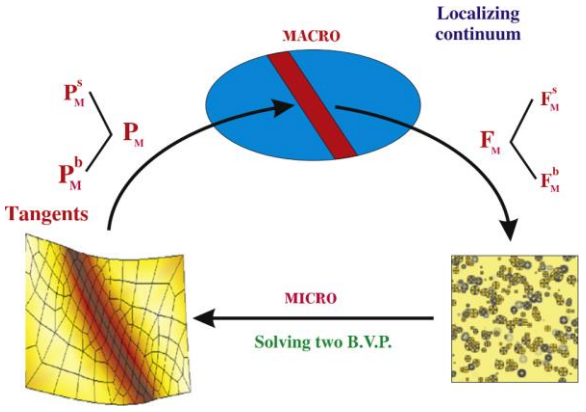

Fig. 14 Continuous-discontinuous homogenization scheme. A deformation gradient for the unloading material (F^s_M) and one for the localization band (F^b_M) is transferred from the macroscopic model to two different microscopic models. The microscopic models produce the homogenized responses represented here by two tangent moduli and two first Piola-Kirchhoff stress tensors for the respective zones. Reprinted from Geers et al (2010), with permission from Elsevier.

4.3.3 Multiscale methods

In PF and TLS methods, the PF or damage field determine the fully damaged material region where a discontinuity is inserted. In techniques coupling a CDM to the X-FEM, a crack initiation and propagation criterion must be defined to initiate cracks at damage localization sites, and propagate them along the directions of highest damage. In multiscale methods, the added difficulty is that a coarse scale discontinuity must be related to the fine scale.

Embedded localization band approaches (Massart et al (2007)) provide an interesting solution to problems induced by strain localization at both the coarse and fine scales. This solution is schematized in Figure 14. When a coarse scale strain localization band is detected, two boundary value problems at the fine scale are solved, one inside the localization band and one in the unloading material. Two sets of homogenized properties are hence provided for use in their corresponding coarse scale zones. A usual simplifying hypothesis in this continuous-discontinuous homogenization scheme is that the width of the localization bands remains constant (Geers et al (2010)). Although Massart et al (2007) did not use an enriched FE method for the coarse scale problem, the authors acknowledged that it would be necessary to guarantee consistent coarse scale results.

An alternative methodology for introducing discontinuities in a multiscale approach is the so-called multiscale aggregating discontinuities method (Belytschko et al (2008)). In this methodology, when a material instability is detected within a fine scale RVE problem, the zone containing the instability is excluded from the averaging procedure. For this reason, these RVEs are called perforated RVEs. An analysis to separate the bulk deformation from the deformation associated to material failure, follows. The result of this analysis is an equivalent discontinuity that represents the potentially multiple discontinuities in the RVE. This equivalent discontinuity is then inserted in the coarse scale analysis using the X-FEM. One limitation of this method is that it requires the fine scale domain to correspond to the size of the coarse scale element. An advantage is that this method includes a criterion to determinate the coarse scale crack propagation direction from fine scale problems.

It must be pointed out that Massart et al (2007) did not propose applications to ductile materials or 3D examples, and neither did most studies on this topic (Loehnert and Belytschko (2007); Toro et al (2016)). Belytschko et al (2008) proposed an application to a ductile material where particle debonding and matrix micro-cracking were modeled in fine scale 2D RVE problems and related to a coarse scale 2D crack propagating in a zig-zag pattern due to the microstructure's influence. An application of a similar method to void growth and coalescence has been proposed by Bosco et al (2015). These results are promising as the presence of the coarse scale crack induces localization at

the fine scale, where void growth and coalescence in the localization band determine crack opening at the coarse scale.

To summarize, all these extensions of multiscale methods to localization problems are based on a decomposition of fine scale problems responses into continuous and discontinuous parts that are homogenized separately. The continuous parts follow conventional homogenization schemes, while the discontinuous parts are related to discontinuities embedded into the coarse scale problem using an enriched FE method. This relationship between coarse scale discontinuities and fine scale localization bands is very close to the concept of traction-separation laws described in Subsection 2.3, although it is not phenomenological but based on a multiscale theory.

4.3.4 Conclusion

While the TLS method has not been applied to ductile materials yet, methods coupling a CDM to an X-FEM based discontinuous approach to model the CDT have been successfully applied to ductile materials. These methods enable the modeling of crack initiation at multiple sites based on the damage field, while crack propagation occurs along directions of maximum damage. This has only been demonstrated for 2D configurations.

This restriction to 2D is also true for multiscale methods. The latter add an additional difficulty, since the coarse scale crack has to be related to fine scale problems. This is done by splitting the homogenization process into two parts, a continuous one and a discontinuous one. The latter accounts for the localization band at the RVE level, and homogenizes it as a traction-separation law for the coarse scale crack, which is modeled using element enrichment.

For future work, it will be interesting to see if these techniques can be extended and demonstrated for 3D configurations. The large deformation of complex 3D microstructures might lead to issues that have not been considered yet.

4.4 Mesh modification

There are multiple differences and particularities in CDT modeling using mesh modifications, as opposed to purely discontinuous approaches discussed in Subsection 2.4. Even before the CDT, mesh adaption[6] can be used to improve the quality of the discretization. The use of a regularization technique is mandatory (Subsection 3.1), as the behavior of a mesh dependent model used with a spatially and temporally varying mesh size is unpredictable. In spite of this undefined behavior, some studies of mesh adaption with a CDM but no regularization can be found in the literature (Vaz and Owen (2001); Andrade Pires et al (2004); Borouchaki et al (2005)).

With mesh adaption, the CDT can be modeled simply with the element erosion method. The main advantage is that a finer mesh size in the localization region will reduce mass loss. Another option is to use similar remeshing based crack initiation and propagation techniques as presented in Subsection 2.4.

These different options are discussed in the following.

4.4.1 Mesh adaption in the continuous regime

The most widely used approach to estimating the approximation error in computational solid mechanics was introduced by Zienkiewicz and Zhu (1987). This well-known ZZ estimator relies on estimating the error on any variable based on the difference between this variable's FE approximation and a reconstructed higher order approximation of this variable. The higher order approximation is usually reconstructed using the first order Superconvergent Patch Recovery technique initially proposed by Zienkiewicz and Zhu (1987) and later on improved to the second order by Zhang and Naga (2005).

The ZZ estimator requires an initial FE approximation of the variable. The most common choice is to use the solution for the current load increment and the associated error estimate to adapt the mesh for the next increment (Vaz and Owen (2001); Andrade Pires et al (2004)). For this prediction to be accurate and account for the future evolution of the damage field, a common choice of variables for error estimation are the damage rate, the energy release rate, or combinations of these (Vaz and Owen (2001); Andrade Pires et al (2004)).

The mesh size field for the current FE mesh is corrected so that the estimated error matches a user-prescribed tolerance equally on the whole FE domain. For a linear FE method, this means scaling mesh size by a local factor depending on the local error estimate. Then, a mesh adaption algorithm is used to conduct node position and element topology changes and bring edge lengths as close as possible to the prescribed mesh size field, while at the same time guaranteeing optimal element shapes to avoid element inversion (Gruau and Coupez

[6] We refer the reader back to Subsection 2.4 for the definition of mesh adaption, as opposed to remeshing or full remeshing.

(2005); Shakoor et al (2017b)).

The definition of optimal element shape can be modified to consider anisotropic elements. Although stretched elements may not seem appropriate for large deformation problems with element inversion issues, they are interesting in terms of computational cost compared to isotropic elements. This was shown by El khaoulani and Bouchard (2012) using a non local implicit gradient Lemaitre damage model. This study was not based on the ZZ theory but on a relation between the approximation error and the interpolation error known as Cea's lemma (El khaoulani and Bouchard (2012)). For a first order FE interpolation, the interpolation error is given by the Hessian matrix. Therefore, El khaoulani and Bouchard (2012) reconstructed Hessian matrices of both the damage variable and its rate and used them to build an anisotropic mesh size field, also known as metric tensor. This tensor was given as input to an anisotropic mesh adaption algorithm developed by Gruau and Coupez (2005). An example of an adapted FE mesh produced by this technique is shown in Figure 15a.

In spite of its interesting properties in terms of computational cost, anisotropic mesh adaption is rarely used for ductile fracture problems. This is most probably due to the risk of element inversion, as reported by Shakoor et al (2017b). Isotropic mesh adaption is hence the most popular solution, especially for use with non local CDMs where the mesh can be refined in localization bands.

Alternatively to the ZZ error estimator or the Hessian matrix based estimator, some authors have simply chosen to refine the mesh in regions with high damage (Borouchaki et al (2005); Areias et al (2015)). Independently of the chosen method, local mesh refinement is particularly interesting to satisfy the constraint on mesh size imposed by non local models, as mesh size cannot be higher than the characteristic length in the localization region (Peerlings et al (1996); Bažant and Jirásek (2002)). It is also relevant for modeling the CDT, as discussed in the following paragraph.

4.4.2 Remeshing based continuous-discontinuous transition modeling

Mesh adaption reduces the artificial loss of mass due to element erosion because elements within damage localization regions are automatically refined prior to deletion (El khaoulani and Bouchard (2012)). Element erosion is hence the most straightforward method to use in combination with both isotropic and anisotropic mesh adaption based on the damage variable, its rate, or the

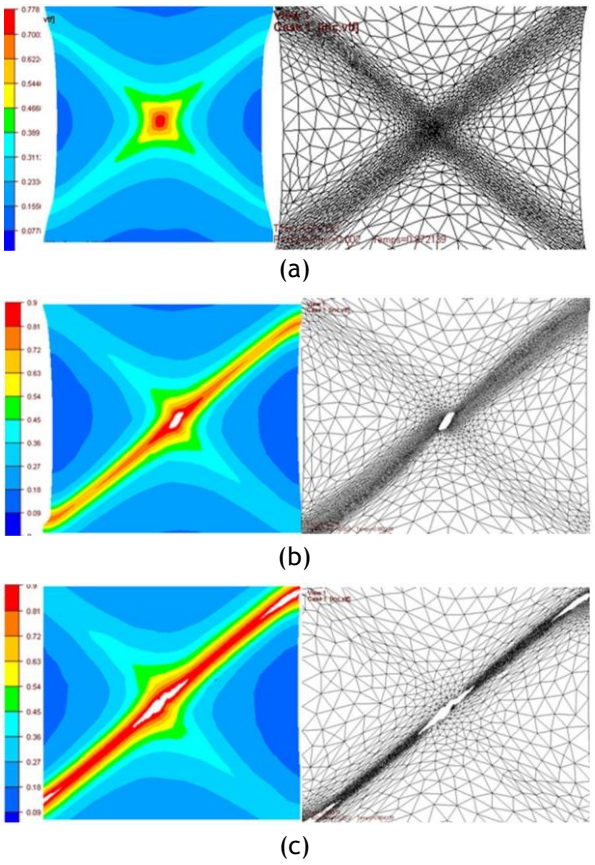

Fig. 15 Cross sections of a 3D tension test simulation using ductile fracture modeling by element erosion and anisotropic mesh adaption at an engineering tensile strain of: (a) 21.80%, (b) 22.05%, (c) 22.10%. Damage distribution is shown on the left, and the adapted FE mesh on the right. Reprinted from El khaoulani and Bouchard (2013), with permission from Elsevier.

energy release rate. This option was chosen by Vaz and Owen (2001); Andrade Pires et al (2004); Borouchaki et al (2005); Areias et al (2015) with no regularization and by El khaoulani and Bouchard (2012, 2013) using non local implicit gradient theory. An example of simulation result with anisotropic mesh adaption and element erosion is shown in Figure 15. Damage localization within a single shear band occurs once the first elements get eroded. Due to mesh anisotropy, eroded elements are elongated along the shear band.

A more technically complex option to model the CDT is to initiate and propagate an explicitly meshed crack through remeshing operations. One of the first results using such method was obtained by Mediavilla et al (2006b). This study is similar to a previous work (Mediavilla et al (2006a)), where the same authors used an uncoupled non local integral damage model as crack initiation and propagation criterion. For details on the method, the reader is referred back to (Subsection 2.4),

with the novelty of Mediavilla et al (2006b) being that the damage model was coupled to constitutive equations using non local implicit gradient regularization and Kachanov theory. Both works were restricted to 2D crack modeling.

An interesting remark by Mediavilla et al (2006b) was that when the damage variable is coupled to constitutive equations, some convergence issues due to large energy dissipation in the discontinuous case are avoided. This is due to softening of the mechanical response and progressive energy dissipation within mesh elements before they are reached by the crack. Feld-Payet et al (2015) made the same remark and added that the crack must remain within the damage localization region to avoid convergence issues.

The remeshing based CDT modeling approach proposed by Feld-Payet et al (2015) is quite similar to that of Mediavilla et al (2006b). The authors show the ability of their method to model crack initiation and propagation in 3D for flat specimens. The novelty of the method is a 3D discretization of the crack, which can be used to localize the crack within the FE domain, and compute the propagation criterion. At each loading step, the 3D discretization can be updated and full remeshing used to adapt the mesh to the new geometry.

An important point is that the approaches proposed by Mediavilla et al (2006b) and Feld-Payet et al (2015) both rely on full remeshing. Discontinuous crack modeling methods based on mesh adaption and local remeshing have been mentioned in Subsection 2.4, with interesting features regarding computational cost, distributed computing and conservation of history variables. A local mesh modification procedure has been proposed for 2D triangular meshes by Areias et al (2009). The authors developed a method to split mesh elements arbitrarily in order to allow for the crack to propagate along any direction depending on some chosen criterion. This edge and node splitting method is followed by a node re-positioning algorithm to restore the quality of the modified elements.

The method proposed by Areias et al (2009) was coupled to an empirical CDM with non local integral regularization by Areias et al (2011). It was later on used by Areias et al (2013) with a Rousselier model and no regularization. Areias et al (2013) based their crack propagation criterion on a critical damage value for the propagation threshold and linear elastic fracture mechanics for the direction. A similar approach was used by Areias et al (2011), with an additional crack initiation criterion based on the maximum principal strain.

The last option for mesh modification based CDT modeling is the mesh-free paradigm. As mentioned in Paragraph 3.1.4, mesh-free approaches have been proposed in the literature as a discretization method with built-in non local integral regularization. As reaching the CDT requires a robust large deformation modeling method, mesh-free methods are particularly interesting since the element inversion issue is avoided. As discussed by Andrade Pires et al (2004); Simonsen and Li (2004), these methods can be seen as an alternative to automatic remeshing algorithms.

The damage variable in mesh-free approaches is not discretized at integration points but at particles. A CDT modeling technique for the 2D case has been proposed by Simonsen and Li (2004) using the GTN model, and by Simkins and Li (2006) using the Johnson-Cook damage model. The proposed crack propagation algorithm can be seen as an element erosion method, only there are no elements but only particles in a mesh-free discretization. Thus, there is no loss of mass. However, Simkins and Li (2006) acknowledged that, due to the propagation of the crack only from particle to particle, the method is particle distribution sensitive. This is quite similar to FE methods where the crack propagates along edges by node splitting.

An interesting feature proposed by Ren et al (2011) using the same 2D particle splitting method with mesh-free discretization is the modeling of crack or void coalescence. Areias et al (2009) obtained similar results also in 2D but using an FE discretization. These developments are particularly relevant for ductile fracture modeling at the microscale, where multiple crack initiation sites lead to multiple cracks and coalescence events. The mesh-free method proposed by Ren et al (2011) to model void coalescence is nevertheless particle distribution sensitive.

To summarize this presentation of mesh modification based CDT modeling methods, the studies have focused mostly on 2D. While mesh-free methods do not allow for arbitrary crack propagation paths, this is possible in the frame of the FE method. Full remeshing based methods consist in modifying the geometry when the damage variable reaches a given threshold, and generating a new mesh adapted to the new geometry. Local remeshing methods have also been proposed to modify the mesh only in the crack tip region. Although the propagation threshold is always damage-based, different models have been proposed for predicting the propagation direction, including searching for the direction of maximum damage, or using techniques borrowed from linear elastic fracture mechanics. In the following, applications of these models are discussed.

4.4.3 Applications and discussions

A commonly used test case in the studies reviewed in the previous paragraphs is the double notched specimen model where two cracks initiate (one at each notch) and then propagate towards each other. This 2D model features a plastic localization band with high shear components, which drives damage localization and then cracks propagation. It has been used by Mediavilla et al (2006b) and Feld-Payet et al (2015) for both crack initiation and propagation modeling, with two crack tips.

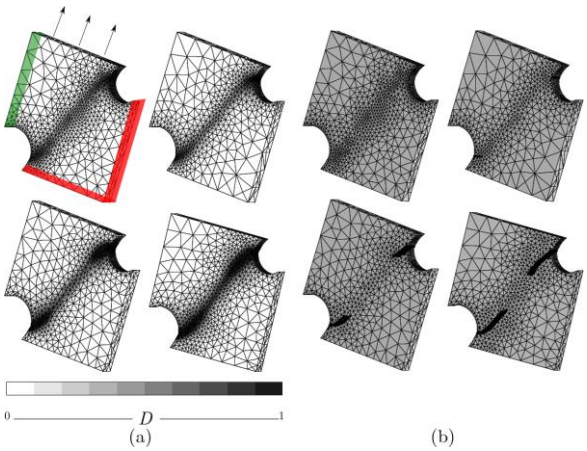

Fig. 16 Double notched 3D specimen test case result at four load increments. Arrows point out the loading direction. Red faces are fixed. Green face is sliding along the loading direction. (a) View of the continuous damage field D. (b) View of the two cracks. Reprinted from Feld-Payet (2010).

The 3D version of the double notched specimen test that was studied by Feld-Payet (2010) is shown in Figure 16. Crack propagation was modeled using a 3D discretization of the crack surface where the propagation direction could theoretically be chosen independently for each segment discretizing the crack tip. In practice, technical difficulties required Feld-Payet (2010) to force the crack to remain flat. The FE mesh used in the model was also quite coarse in the thickness direction (only 5 elements).

Areias et al (2011) proposed a 2D micromechanical application of their remeshing based CDT modeling method. The model accounted for interactions between matrix cracking and particle debonding. However, as shown in Figure 17, matrix cracks and debonding cracks did not coalesce. Cracks coalescence was also not accounted for by Feld-Payet (2010), as shown in Figure 16.

Limitations in the remeshing techniques will hence have to be overcome before 3D cracks can be initiated and propagated using remeshing based CDT modeling. The work of Feld-Payet et al (2015) is however promising, as it theoretically overcomes the limitations regarding 3D crack propagation criteria mentioned in Subsection 2.4. This is done by using a shape analysis technique that defines the crack as the topological skeleton of the damage field (Feld-Payet et al (2015)). This definition is close to that used to model the CDT in Moës et al (2011) within the thick LS framework.

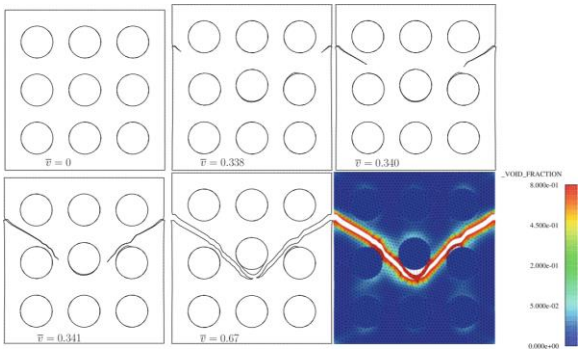

Fig. 17 FE simulation of a 2D inclusions array using remeshing based cracks initiation and propagation. Results are shown at various applied displacement $\overline{v}$. Reprinted from Areias et al (2011), with permission of Springer.

For application to the microstructure of ductile materials, one could use the 3D crack initiation and propagation algorithm introduced by Feld-Payet et al (2015) to model matrix cracking and couple it to the approach proposed by Shakoor et al (2017a) to model particle fragmentation and debonding (Subsection 2.4). The method proposed by Shakoor et al (2017a) could also be used to model cracks coalescence, as illustrated in Figure 18. There is hence a lot of interest for these remeshing methods, as they can be applied both to the brittle and ductile components of the microstructure. An added advantage is that remeshing can also be used to avoid element inversion and model large deformations. It is certain that micromechanical simulations with remeshing based modeling of cracks initiation, propagation, and coalescence in both brittle and ductile components will soon be possible in full 3D and for large deformations.

4.5 Conclusion

CDT modeling is certainly one of the most active research topic discussed in the present review. Computational methods proposed in the literature to handle the CDT can be classified into two categories. The first category of methods embed a damage model, a regularization technique, and a CDT model within the same theory. This is the case for PF methods and the thick LS method. The second category of methods allow different combinations of CDMs or multiscale methods and

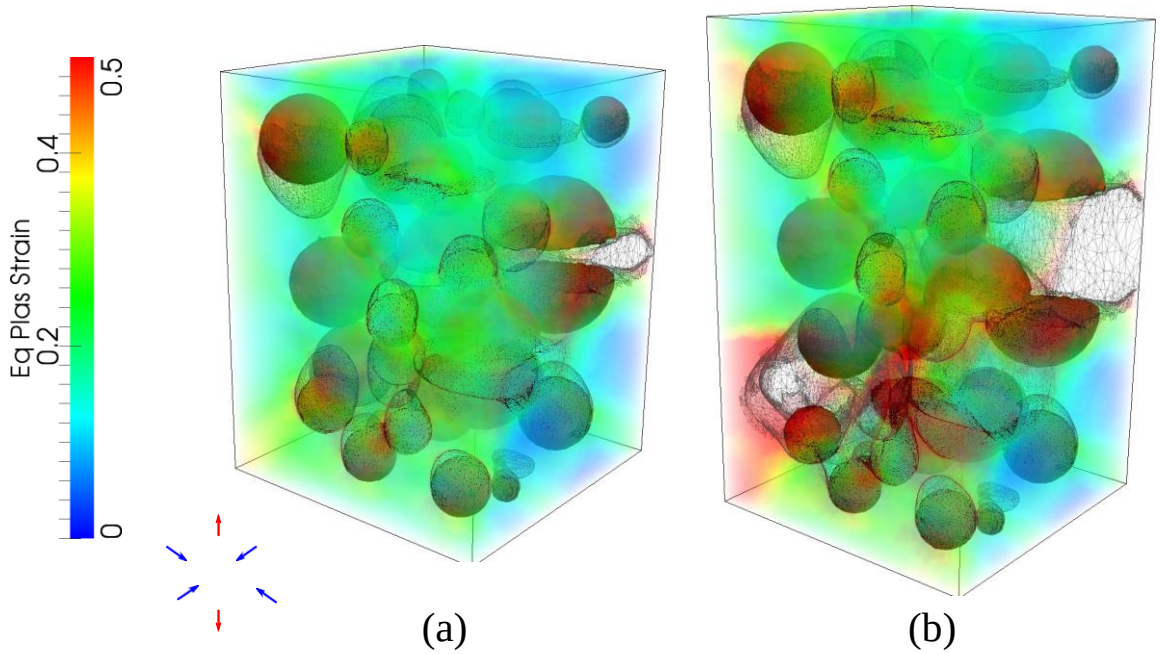

Fig. 18 Micromechanical simulation of a metal matrix composite microstructure showing void nucleation by particles debonding and fragmentation, growth and coalescence modeled using remeshing at an applied tensile strain of: (a) 25 % and (b) 50%. Particles are shown in red and the color code in the matrix is associated to the equivalent plastic strain. Reprinted from Shakoor et al (2017a), with permission from Elsevier.

regularization techniques, coupled to a discontinuous approach for modeling the CDT.

In all these methods, the crack, or fully damaged material region, is defined as the topological skeleton of the damaged material region. The goal is to relieve damaged material regions from any load. This is done by defining a discontinuity at a given contour of the damage field (*e.g.*, $D = 1$) in PF methods and the thick LS method. In discontinuous approaches based on the X-FEM or remeshing, a crack must be initiated and propagated along the topological skeleton of the damaged material region. This is done by initiating cracks at local damage localization points, and incrementally propagating these cracks along the directions of highest damage. This becomes technically more difficult in 3D or with multiples branching or coalescing cracks.

An additional difficulty is also raised by multiscale methods, as they require the discontinuity at the coarse scale to be related to the fine scale problems. This has been done by multiple authors using an enriched FE method at the coarse scale, and multiscale methods extended to localization problems at the fine scale. These methods have not been applied to complex 3D ductile fracture problems yet.

5 Conclusion

Modeling ductile fracture at the microscale requires computational methods that can handle heterogeneous three-dimensional (3D) structures, large plastic deformations, and the initiation and propagation of multiple cracks along arbitrary paths. Microstructures of ductile materials are heterogeneous as they feature multiple ductile and brittle components of complex morphology. Without loss of generality, this microstructure can be assumed to be composed of brittle particles and a ductile matrix. Once this heterogeneity is modeled, crack initiation and propagation must be considered. Cracks initiate mainly by debonding and fragmentation of particles, although they can also nucleate directly within the matrix. These cracks then propagate along particles/matrix interfaces and within the matrix, and may coalesce. Simultaneously to their propagation, cracks open and grow to become large microscopic voids. This process is joined by large plastic strains that may localize and lead to interaction micromechanisms between cracks/voids, favoring their coalescence. The latter may itself be favored by matrix softening due to potential sub-micron sized voids. The accumulation of coalescence events leads to final macroscopic failure.

All these micromechanisms can easily be modeled using the Finite Element (FE) method with element

erosion, but at the price of mass loss and mesh dependence issues. In order to avoid these issues, more advanced computational methods must be considered. Both the eXtended Finite Element Method (X-FEM) and remeshing based discontinuous approaches have been proven to enable the modeling of the initiation, propagation and coalescence of multiple 3D cracks (see *e.g.,* Figure 4 for the X-FEM, and Figures 9 and 18 for remeshing). Large deformations, however, seem to be accessible only through remeshing, although mesh-free techniques could also be employed. Independently of whether the X-FEM or remeshing are used, CZMs (Cohesive Zone Models) should be considered to model the energy dissipation rate (see *e.g.,* Figure 8 for a use of CZMs at predefined locations). Although methods coupling the X-FEM and CZMs can be found, there is no result showing the compatibility of CZMs with remeshing and large deformations.

Discontinuous approaches such as the X-FEM or remeshing based techniques cannot model matrix softening. Physically, matrix softening is related to the presence of sub-micron sized voids that must be modeled in a homogenized sense either using Continuum Damage Models (CDMs), which can be empirical, phenomenological, or micromechanical, or using multiscale methods. Multiscale methods can also be employed to consider the influence of ductile fracture micromechanisms on the macroscale. Independently of the scale at which they are used, CDMs and multiscale methods require regularization through averaging or the introduction of gradient terms, and a Continuous-Discontinuous Transition (CDT) model. At the microscale, the CDT is the transition from a continuous damage process to the initiation and propagation of micro-cracks within the matrix.

On the one hand, methods embedding altogether a damage model, a regularization technique, and a CDT model have been proposed. Phase-Field (PF) methods and the thick Level-Set (LS) method are examples of those. The applicability of these methods to ductile fracture modeling at the microscale, with severe plastic deformation, has not been demonstrated yet.

On the other hand, CDMs with non local integral or gradient based regularization have been coupled to the element erosion method. Although this approach inherits the deficiencies of the element erosion method, mass loss can be alleviated using adaptive mesh refinement in the localized damage regions (see *e.g.,* Figure 15). Adaptive mesh refinement also enables to satisfy mesh size constraints raised by regularization techniques with a reduced computational cost.

To completely avoid the issues raised by the element erosion method, discontinuous approaches based on the enriched FE methods or remeshing can be considered to model the CDT. Enriched FE methods, in particular, have been proven to be compatible with multiscale methods. These CDT models based on discontinuous approaches all consist in detecting damage localization regions from the considered CDM or multiscale method, and then model the initiation and propagation of cracks along the directions of higher damage. While this has been demonstrated to be possible in 2D by multiple authors (see *e.g.,* Figure 13 for a CDM with X-FEM based CDT modeling, and Figure 17 for a CDM with remeshing based CDT modeling), 3D results are not so common (see *e.g.,* Figure 16).

As a conclusion, no simulation modeling ductile fracture at the microscale with all its complexity has been conducted yet, but there is a wide extent of literature on the topic. There are hence opportunities for future research in computational damage and fracture mechanics. Furthermore, due to the prolific literature on this research problem and the large number of research groups working on it, solutions should soon be available for integrated computational materials engineering. These solutions would also be applicable to heterogeneous structures in general.

In the near future, the most promising solution would consist in combining existing approaches, as shown in Figure 19. Both enriched FE methods and remeshing based techniques can definitely be applied to model void nucleation by particle debonding and fragmentation, while the energy dissipation rate can be modeled using CZMs. Enriched FE methods can be coupled to CZMs, but they should be improved in order to handle large deformations. Remeshing techniques can handle large deformations, but have not been coupled to CZMs yet. CDMs and multiscale methods can both model the continuous damage process leading to matrix softening. The regularization of these methods can be done efficiently by relying on adaptive mesh refinement in localization regions. These regions should be detected accurately in order to model the CDT, which should be possible in 3D with multiple crack fronts soon.

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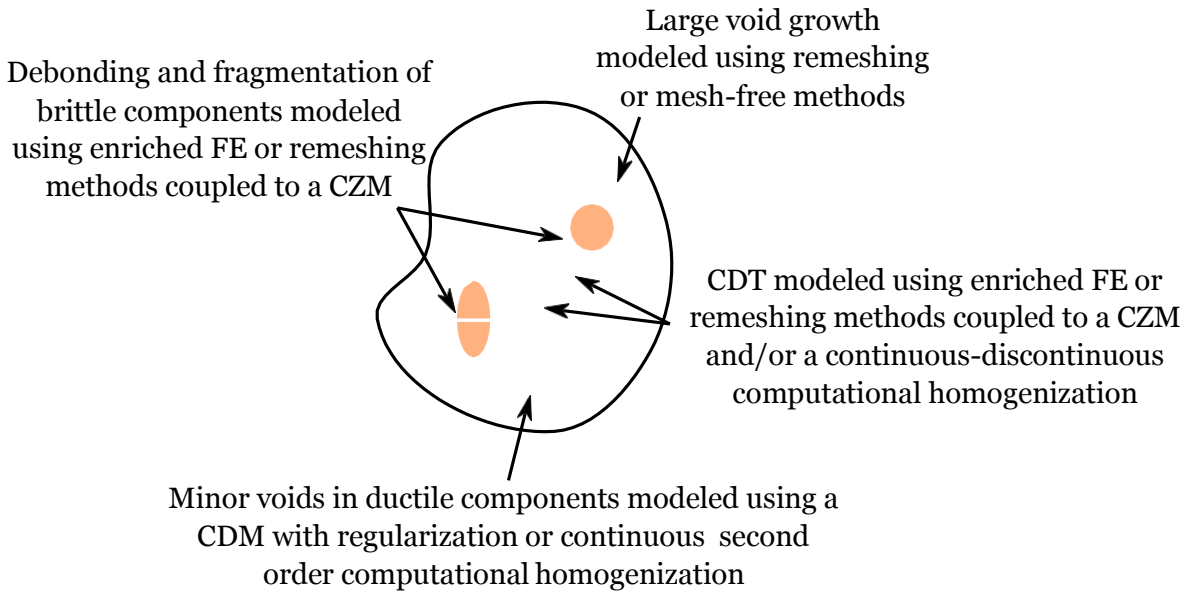

Fig. 19 Main approaches retained in the present review for numerical modeling of ductile fracture at the microscale.

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