

# Contributions to multiscale modelling of quasi-brittle damage in heterogeneous materials

Thi Hai Nhu Nguyen

# ▶ To cite this version:

Thi Hai Nhu Nguyen. Contributions to multiscale modelling of quasi-brittle damage in heterogeneous materials. Solid mechanics [physics.class-ph]. Université Paris-Est, 2019. English. NNT: 2019PESC2090. tel-03391685

# HAL Id: tel-03391685 https://theses.hal.science/tel-03391685

Submitted on 21 Oct 2021

**HAL** is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers. L'archive ouverte pluridisciplinaire **HAL**, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d'enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.



## UNIVERSITÉ PARIS-EST

ÉCOLE DOCTORALE SCIENCE INGÉNIERIE ET ENVIRONNEMENT

# THÈSE

présentée pour l'obtention du diplôme docteur de

## L'UNIVERSITÉ PARIS-EST

Spécialité: Mécanique des Matériaux et des Structures

 $\operatorname{par}$ 

### Thi Hai Nhu NGUYEN

Sujet de la thèse :

Contributions to multiscale modelling of quasi-brittle damage in heterogeneous materials

### Version préliminaire

Thèse soutenue le 19 April 2019 devant le jury composé de :

Djimedo KONDO	Professeur	Rapporteur
	Paris Sorbonne Université	
Ludovic NOËLS	Professeur	Rapporteur
	Université de Liège	
Pierre-Olivier BOUCHARD	Professeur	Examinateur
	Ecole des Mines ParisTech	
Julien YVONNET	Professeur	Directeur de thèse
	Université Paris-Est Marne-la-Vallée	

#### Acknowledgement

I would like to express my sincere gratitude to my supervisor Julien YVONNET for having guided me during the past three years. The conferences he suggested and supported me to participate have given chances to present my work, meet researchers and broaden my knowledge. My gratitude is also for his encouragement in work and for his sympathy then having facilitated my family's visiting. I am grateful to the 911 program which funded me so that I can come to France and also my colleagues in NUCE for having supported and facilitated procedures which have given me conveniences to do this research. Next, I would like to thank all my Vietnamese friends from MSME Laboratory for sharing a social life with me during this period. Thanks to Minh Xu who has shared her Ph.D. experiences and helped me in my abroad life. I also want to say thanks to Thanh Tung for having replied many of my questions which helped me a lot in my first steps of my thesis work.

To my family: I want to thank my husband for having supported, sympathized and took care of our daughter in my absence time. Great gratitude is for my parents in law. Without you, Soc could not be looked after so carefully. Finally, this thesis is dedicated to Mum and my beloved daughter, who was my motivation to go abroad. And Dad, I know you would be happy if you saw this work.

> Champs sur Marne, April 2019 Nhu NGUYEN

#### Abstract

In this work, contributions to numerical multiscale methods for modeling fracture in heterogeneous quasi-brittle materials are proposed. We first develop a two-scale approach in the case of separated scales, where the fracture occurs at the microscale. The local damage is modeled by the phase field method, which is fully adapted to model initiation, propagation, and merging of complex, multiple cracks such as occurring in heterogeneous media. We propose an original algorithm based on a staggered scheme combined with strain gradient regularization, which offers the following advantages: (a) it removes mesh-dependence and convergence issues which occur by direct application of classical  $FE^2$  schemes in presence of damage at the microscale; (b) it does not require  $C^1$  approximation at the macroscopic scale. The method has been applied to porous and composite materials, and it has been shown that such an approach is able to capture an anisotropic behavior fully induced by the microstructure. We then introduce a simple method to construct a homogenized fracture model in heterogeneous media by directly identifying an anisotropic phase field model at the macro scale whose coefficients are identified by performing preliminary simulations on fully meshed and detailed heterogeneous structures. The main advantage of such technique is that once identified, the model can be used at the macro scale without new RVE calculations and can be used in a context of non-separated scales. Finally, to alleviate the computational costs related to the coupled multiscale analysis, a tentative surrogate approach based on neural networks is then proposed. The technique builds a numerical input-output response model by learning from a collection of RVE data, for several states of macroscopic strains and damage history. The surrogate model allows in some situations capturing with reasonable accuracy the damage response of the RVE in view of multiscale analysis.

**Keywords**: Phase field method; Computational homogenization; Crack propagation; Quasibrittle materials; Surrogate model.

#### Résumé

Dans ce travail, nous proposons des contributions à la modélisation numérique multi échelle dans le cadre des matériaux hétérogènes quasi-fragiles. Nous développons dans une première partie une méthode à deux échelles dans un cadre d'échelles séparées, où la fissuration est modélisée à l'échelle microscopique. L'endommagement local est modélisé par la méthode de champ de phase, bien adaptée pour modéliser l'initiation, la propagation et la coalescence de réseaux complexes de micro fissures pour des microstructures hétérogènes. Nous proposons un algorithme original basé sur des calculs étagés combiné avec une approche à gradient d'endommagement, qui offre les avantages suivants : (a) l'indépendance au maillage et la suppression des problèmes de convergences par rapport au maillage bien connus dans les simulations de l'endommagement; (b) l'approche ne nécessite pas d'approximation de continuité supérieure. La méthode est appliquée à des matériaux poreux et composites. Celle-ci permet de modéliser un endommagement anisotrope complètement induit par la microstructure. Nous introduisons une méthode simplifiée pour la construction d'un modèle de rupture homogénéisé en identifiant directement un modèle de champ de phase anisotrope à l'échelle macro, à partir de calculs préliminaires sur des structures hétérogènes complètement détaillées à l'échelle des hétérogénéités. L'avantage principal est que dans ce cas, il n'est plus nécessaire une fois le modèle identifié, de faire de nouveaux calculs de VER et cela permet de traiter les cas d'échelles non séparées. Finalement, en vue d'alléger les coûts de calcul liés aux calculs couplés multi échelle, une tentative de construction de modèle de remplacement basé sur des réseaux de neurones est proposée. La technique construit un système entrées-sorties purement numérique à partir de calculs préliminaires sur le VER pour différents états de chargement et d'histoire d'endommagement. Le modèle construit permet dans certaines situations de capturer avec une qualité raisonnable et des coûts de calculs réduits la réponse du VER endommageable en vue de calculs multi échelles.

**Mots-clés**: Méthode de champ de phase; Homogénéisation numérique; Propagation de fissures; Matériaux quasi-fragiles; Meta-modèles.

# List of Figures

1.1	a) Microstructure of lightweight plaster [27]; b)Microcracks in porous media [151]	1
1.2	Schematic representation of a cohesive zone [47]	2
1.3	a) Bilinear traction-separation law; b)Exponential law	3
1.4	Enriched nodes in XFEM method for tracking crack	4
1.5	The double-edge-notched (DEN) specimen tested by Nooru-Mohamed (1992) $$	6
1.6	Influence of mesh type and element size [71] on the crack band trajectory in	
	the test for damage models (a) Rankine type definition of equivalent strain, (b)	
	modified von Mises definition of equivalent strain and (c) micro plane damage	
	model (anisotropic damage model).	7
1.7	A test to investigate the convergence w.r.t the mesh [85]: three-point bending	
	test of a concrete beam, corresponding to the results presented in Fig. 1.8	7
1.8	Convergence w.r.t the mesh for: local damage model (a) and nonlocal damage	
	models(b), showing the mesh dependency issue [85]	7
1.9	Smeared representation of a free discontinuity: (a) diffuse representation of crack	
	in 1D case: The crack density function (1.19) gives $d = e^{(- x /l)}$ in the red	
	lines while (1.33) gives $d = e^{(- 2x /l)(1+ 2x /l)}$ in blue lines [195]. Black thick line	
	represents a sharp crack at $x = 0$ ; (b) Diffuse representation of crack in 2D case	
	(using (1.19))	11
1.10	Direct simulation of crack in in a realistic sample concrete for different unit	
	cells comprising: (a) 0.5 million elements; (b) 5 million elements; (c) 9 million	
	elements; (d) 17 million elements and (e) 30 million elements [141]	16
1.11	(a) Linear homogenization scheme; (b) Nonlinear homogenization (FE <sup>2</sup> scheme).	17
1.12	Multiscale modelling of the cohesive crack [144]: the homogenization is related	
	to the traction separation laws whereas the position of crack is known a priori at	
1 10		17
1.13	Continuum multiscale model [146]: (a) failure cell with inclusions and cohesive	10
	bands; (b) geometrical characterization of the failure mode at the microscale.	19
1.14	An L-shaped panel test using adaptive multiscale phase field [152].	19
1.15	Crack propagation in multiscale modelling with phase field method using adaptive	20
	$mesh [152]. \ldots \ldots$	20
2.1	Examples of distributed cracks giving rise to a macroscopic diffuse damage: (a)	
	experimental results in a compression test [164]; (b) simulation results obtained	
	by the phase field method.	22

2.2	Schematic of the $FE^2$ method: the macroscopic behavior is provided by the local	
	mechanical state of an RVE associated which each Gauss point of the macroscopic $% \mathcal{A}$	
	mesh associated with the structure.	23
2.3	(a) solid containing a sharp crack; (b) solid containing a regularized description	
	of the crack	24
2.4	Regularized representation of a crack: one dimensional case: (a) sharp crack model, taking unitary value of $d(x)$ at $x = x_{\Gamma} = L/2$ (crack); (b) regularized	
	representation through phase field [143]	25
2.5	a) Gauss distribution with $l = 0.2$ see (1.10) and b) Shape bell distribution with	
	$R = 0.2 (1.11) \dots $	33
2.6	The traction test to clarify the convergence of the regularised strain before a sharp crack tip: at the bottom, displacements are locked in both the direction X, and Y; at the upper, the displacement along X axis equals zero while a prescribed in $\delta u = 0.01$ is applied in Y axis. The regularised length $\ell = 0.05$ mm	40
2.7	Evolution of the component $\varepsilon_{22}$ strain field with the mesh refinement in four cases:(a)- no regularization treatment ;(b)- convolution regularization with Gauss distribution ; (c) - gradient isotropic regularization (IR);(d) - gradient anisotropic regularization (AR)	41
2.8	Algorithm: proposed 2-scale nonlocal staggered damage model.	42
2.9	a) Geometry of a plate with a sharp crack in the traction test, b) Mesh 1: $h = 2 \text{ mm} (302 \text{ elements}), c)$ Mesh 2: $h = 1 \text{ mm} (738 \text{ elements}), d)$ Mesh 3: $h = 0.5$	
	mm (1430 elements). $\ldots$	43
2.10	Three sizes of RVE: a) one unit cell, b) two unit cells, c) four unit cells	43
2.11	F-u curves for the plate with sharp crack gradient regularisation (isotropic). $\ $ .	44
2.12	Test MS2: geometry of the three-point bending beam	44
2.13	Three refined meshes in the vicinity of the crack path: a) $H1 = 5 \text{ mm} (630 \text{ elements})$ , b) $H2 = 2.5 \text{ mm} (1290 \text{ elements})$ , c) $H3 = 1 \text{ mm} (2762 \text{ elements})$ , d)	
	$H4 = 0.5 \text{ mm (5080 elements)} \dots \dots$	45
2.14	F-u curves for 3 different RVE sizes	46
2.15	Comparison of F-u curves with respect to the four mesh sizes H1, H2, H3 and	
	H4 using isotropic gradient regularization: (a) isotropic regularization (IR) and (b) anisotropic regularization (AR).	46
2.16	Comparison of damage profiles w.r.t the four mesh sizes H1 (a), H2 (b), H3 (c), H4 (d) (Fig. 2.13) using isotropic gradient regularization IR (plotted at the end	
	of the simulation).	47

2.17	Comparison of damage profile w.r.t the four mesh sizes H1 (a), H2 (b), H3 (c), $$	
	H4 (d) in Fig. 2.13 using anisotropic gradient regularization AR (plotted at the $$	
	end of the simulation). $\ldots$	47
2.18	Left: evolution of damage using isotropic regularization (IR); Right: anisotropic	
	regularization (AR) (the mesh H3 in Fig. 2.13 is employed)	47
2.19	L-shaped structure: (a) macrostructure geometry of the L-shape test with di-	
	mensions $L = H = 500$ mm, $d = 30$ mm; (b) mesh involving 2650 elements,	
	$h_{min} \approx 3.5 \text{ mm.} \dots \dots$	48
2.20	Evolution of damage of the L-shaped test using isotropic regularization ( first	
	row) and anisotropic regularization ( second row). $\ldots \ldots \ldots \ldots \ldots \ldots$	49
2.21	Force-displacement curves for the L-shape test.	49
2.22	Composite RVE layers orientation of $45^{\circ}$	49
2.23	a) Geometry of the macro structure of the test in sec. 2.5.4; b) Macro mesh for the	
	porous microstructure using 1296 elements with refinement is in the damage zone	
	h = 2 mm, c) Macro for the composite layered microstructure with refinement is	
	in the damage zone $h = 2$ mm	50
2.24	Damage profiles in case 1 of the plate with a hole (sec. 2.5.4) at the point A	
	( $\Delta u = 0.202 \text{ mm}$ ), B ( $\Delta u = 0.206 \text{ mm}$ ), C ( $\Delta u = 0.208 \text{ mm}$ ), D ( $\Delta u = 0.214$	
	mm) in Fig.2.25 are depicted in (a) (b) (c) (d), respectively. $\ldots \ldots \ldots \ldots$	51
2.25	The force-displacement curve and damage images of the underlying microstruc-	
	ture at the gauss point (center) of the element M in Fig. 2.23 $\ldots$	51
2.26	Damage profiles in case 2 of the plate with a hole (sec. $2.5.4$ ) at load steps A	
	(u = 0.1120  mm), B (u = 0.1200  mm), C (u = 0.1400  mm), D (u = 0.1600  mm)	
	in Fig.2.27 are depicted in (a) (b) (c) (d), respectively	52
2.27	Force-displacement curve in case 2 and damage profiles for an RVE at point M	
	in Fig. 2.23	52
2.28	Cracked square plate: a) Geometry at macroscale; b) Mesh 1: $h\approx 1mm$ (3098	
	elements); c) Mesh 2: $h \approx 1mm$ (3393 elements)	53
2.29	Damage profiles for the cracked square plate in traction for case 1 (porous RVE) $$	
	at $u = 0.63 \text{ mm}$ (a1), $u = 0.70 \text{ mm}$ (b1), $u = 0.80 \text{ mm}$ (c1), $u = 1 \text{ mm}$ (d1); and	
	for case 2 (laminated RVE): $u = 0.2300 \text{ mm} u = 0.2390 \text{ mm}, u = 0.2490 \text{ mm},$	
	u = 0.2590 mm. The IR has been used.	54
2.30	Force-prescribed displacement curves in two case of microstructure	54
2.31	Evolution of damage using isotropic regularization (first row) and anisotropic	
	regularization (second row) in the shear test with the porous RVE	55
2.32	Evolution of damage using isotropic regularization (first row) and anisotropic	
	regularization (second row) in the shear test with composite RVE. $\ldots$ .	55

2.33	Force-prescribed displacement curves of the square plate in the shear test using isotropic regularization (IR case) and anisotropic regularization (AR case): a)	
	with the porous RVE ; b) with the composite RVE	56
2.34	Geometry and the mesh: $H \times L = 80 \times 40$ mm, H1 = 30 mm, R = 5 mm; the	
	mesh size $h_{size} \approx 1$ mm, 2914 elements;	57
2.35	Damage profile of the plate with two asymmetric semicircular notches (a) $u =$	
	0.224 mm, (b) $u = 0.230$ mm, (c) $u = 0.240$ mm, (d) $u = 0.250$ mm which	
	correspond the point A,B,C,D in Fig.2.37 (a)	57
2.36	Damage profile of the plate two asymmetric semicircular notches; (a) $u = 0.3150$	
	mm, (b) $u = 0.3250$ mm, (c) $u = 0.3500$ mm, (d) $u = 0.4000$ mm which corre-	
	spond the points A,B,C,D in Fig.2.37 (b).	58
2.37	Force-prescribed displacement curves in two case of microstructure	58
2.38	Algorithm for the SEN beam test.	59
2.39	Single edge notch beam: the dimension is in mm; a) Load and displacement	
	boundary conditions and b) Mesh and geometry. $\ldots$ . $\ldots$ . $\ldots$ . $\ldots$	60
2.40	Damage profile at the end of simulation	60
2.41	Force-displacement response where displacements are reported at point B	61
3.1	Three favourable orientations of crack in the periodical porous media (a); the porous media is replaced by homogeneous one with there preferential directions	
	where $\mathbf{n}_1, \mathbf{n}_2, \mathbf{n}_3$ are normal vectors (c)	69
3.2	The polar plot of $G_s(\theta)$ w.r.t $\ell$ when $\beta = 50$ : anisotropic effect is clear in three	
	cases of $\ell$ when the number of preferential direction $n = 1, \ldots, \ldots, \ldots$	70
3.3	The polar plot of $G_s(\theta)$ with respect to $\beta$ and $\ell$ : when $\beta = 50$ , the convexity is	
	clear in case $\ell = 0.01$ (b) while it is not obvious in case $\ell = 0.005(a)$ .	71
3.4	Identification procedure for constructing the equivalent homogeneous medium	72
3.5	Periodic hexagonal lattice of circular inclusions or pores $\ldots \ldots \ldots \ldots \ldots$	73
3.6	Test (T1) used to identify the parameters of the homogeneous crack propagation	
	model: heterogeneous media (left) and homogeneous media (right)	74
3.7	$Comparison \ between \ reference \ solution, "ref" \ (heterogeneous \ medium) \ and \ equiv-$	
	alent homogeneous medium, "homo": (a) Force - displacement curve and (b)	
	Energy- displacement curve for the traction test (T1)	76
3.8	Crack networks for the traction test (T1): comparison between the reference	
	solution (heterogeneous medium) and the equivalent homogeneous medium	77
3.9	Validation tests of periodic composite structure with hard inclusions: a shear	
	test $(V1)$ and a double crack test $(V2)$ .	78

3.10	Comparison between the response of homogeneous media ("homo") and het-	
	erogeneous media ("ref") using equivalent parameters in the Table 1: Force -	
	displacement (first column) and Energy- displacement (second column) in the	
	validation shear test (V1)	80
3.11	Comparison of F-u curves and E-u curves of the heterogeneous media and homo-	
	geneous media in the double cracks test (V2) with various regularized length	81
3.12	Comparison of phase field distribution of the heterogeneous media and the ho-	
	mogeneous media in shear test (V1) with various regularized length. $\ldots$ .	82
3.13	Comparison of phase field distribution of the heterogeneous media and homoge-	
	neous media in the double cracks test (V2) with various regularized length	82
3.14	Porous media with $\ell/r = 2.5$ : comparison of F -u relations and crack profiles in	
	three tests: $T1,V1,V2$	83
3.15	Comparison between (a) the total energy and (b) the crack surface energy $E_s$ for	
	the heterogeneous medium "ref" and the homogeneous medium "homo"	83
3.16	Porous media with $\ell/r = 1.25$ : comparison of F -u relations and crack profiles in	
	the three tests T1, V1 and V2.	84
3.17	Comparison of heterogeneous media (M1) and homogeneous media (M2) in the	
	identification test. In M1, $F_{max} = 0.55$ kN at $\overline{u} = 0.01390$ mm and in M2,	
	$F_{max} = 0.5601$ kN at $\overline{u} = 0.0156$ mm	85
3.18	Validation tests V3, V4 and V5.	86
3.19	Traction test with shorter crack: in heterogeneous media $F_{max} = 1.2353$ kN at	
	$\overline{u} = 0.0166$ mm while in homogeneous media $F_{max} = 1.0393$ kN at $\overline{u} = 0.0178$ mm.	87
3.20	Comparison of heterogeneous media (M1) and homogeneous media (M2) in the	
	complex test: $Fx_{max} = 0.1737$ kN at $\overline{u} = 0.0109$ mm, $Fy_{max} = 0.4916$ kN at	
	$\overline{u} = 0.0110$ mm in M1 and $Fx_{max} = 0.1496$ at $\overline{u} = 0.0111$ mm, $Fy_{max} = 0.4520$	
	kN at $\overline{u} = 0.0113$ mm in M2.	88
3.21	Comparison of heterogeneous media(M1) and homogeneous media (M2) in the	
	double crack test: $F = 0.6959$ kN at $\overline{u} = 0.0124$ mm in M1; and $F = 0.6803$ kN	
	at $u = 0.0164$ mm in M2	88
3.22	Validation test V6: a plate with a centered hole.	89
3.23	Comparison between heterogeneous and homogeneous models: crack patterns for	
	a) $\bar{u} = 0.0195$ mm; (b) $\bar{u} = 0.0255$ mm, (c) $\bar{u} = 0.030$ mm	89
3.24	Test V6 (plate with a centered hole): comparison between the heterogeneous	
	medium response ("ref") and the homogeneous solution ("homo"). $\ldots$ .	89
<u>/</u> 1	A single neuron [76]	09
т. 1 Д Э	A multilaver perceptron MPL [76]	92 02
म.∠ /\ २	a) Original model: b) Surgate model 1 (ANN): c) Surgate model 2 (D ANN)	95 05
т.0	a) original model, b) burdgate model i (ANN), c) burdgate model 2 (D-ANN).	50

4.4	Flowchart of the construction of a surrogate model using an ANN 95
4.5	Examples of data distributions: sampling sequences generated with (a) uniform grid; (b) pseudo-random; (c) Halton; (d) CVT and (e) LCVT. The panel shows the sequences corresponding to 2-D input space with a total of 25 (white circle) and 100 (black points) samples. For high dimensional input, the Halton set is appreciated. [153]
4.6	a) tansig function saturates at $x = 3$ ; b) linear function which is often employed for the output layer
4.7	Comparison of F-u curves of the multiscale model and the surrogate model 99
4.8	Comparison of damage evolution using trained data of the multiscale model(a1,2,3) and the surrogate model(b1,2,3) at three load steps $u = 1.5$ mm, 2.0 mm, 2.5 mm (from top to bottom)
4.9	Application of the surrogate model for the same problem using anisotropic reg- ularization with the mesh H1. Fig a) compares the F-u curves and Fig b) shows the damage profiles at 3 points P1, P2, P3 at the displacement $u = 1.5$ mm, 2.0 mm, 2.5 mm respectively
4.10	Application of the surrogate model for same problem using anisotropic regular- ization with the mesh H2: a) Comparison of the F-u curves; b) Damage profiles at 3 points P1, P2, P3 at the displacement $u = 1.5$ mm, 2.0 mm, 2.5 mm respectively. 102
4.11	Application of the surrogate model for same problem using anisotropic regular- ization with the mesh H3: a) Comparison of the F-u curves; b) Damage profiles at 3 points P1, P2, P3 at the displacement $u = 1.5$ mm, 2.0 mm, 2.5 mm respectively.102
4.12	Comparison some components of $\mathbb{C}_{ijkl}$ computed by the network and by FEM in a monolithic increasing strategy of $\varepsilon_{11}$ with $\Delta \varepsilon = 0.0001$
4.13	Comparison some components of $\mathbb{C}_{ijkl}$ computed by the network and by FEM in a monolithic increasing strategy of $\varepsilon_{11}$ with $\Delta \varepsilon = 0.00005$
4.14	Application of the D-ANN for same problem using anisotropic regularization using mesh H3: a) Comparison of the F-u curves; b) Damage profiles at 3 points P1, P2, P3 at $u = 2$ mm, 2.3 mm, 2.5 mm respectively
4.15	Application of the D-ANN for same problem using anisotropic regularization using mesh H1: a) Comparison of the F-u curves; b) Damage profiles at 3 points A1, B1, C1 at the load steps $u = 1.7$ mm, 2.0 mm, 2.5 mm respectively 107
4.16	Application of the D-ANN for same problem using anisotropic regularization using mesh H3: a) Comparison of the F-u curves; b) Damage profiles at 3 points A2, B2, C2 at the load steps $u = 1.5$ mm, 2.0 mm, 2.5 mm respectively 107

4.17 Application of the D-ANN for same problem using anisotropic regularization using mesh H2: a) Comparison of the F-u curves; b) Damage profiles at 3 points A3, B3, C3 at the load steps u = 1.5 mm, 2.0 mm, 2.5 mm respectively. . . . . 108

# List of Tables

2.1	Material properties of the porous RVE	43
2.2	Material properties of the composite layered RVE.	50
3.1	Identified parameters for the equivalent homogeneous media corresponding to the hard inclusions composite: $\overline{g_c}, \overline{\ell}$ obtained for different regularized lengths $\ell$ in the microscopic phases.	75
4.1	Parameters used to train the ANN.	99
4.2	Parameters used to train the network D-ANN1 and D-ANN2	103

# Contents

1	$\mathbf{Intr}$	oducti	on and literature review	1
	1.1	Backg	ground and motivations	1
	1.2 Numerical methods for fracture modelling			
		1.2.1	Cohesive Zone Models	2
		1.2.2	Extented Finite Element Method (XFEM)	3
		1.2.3	Embedded Finite Element Method EFEM	4
		1.2.4	Continuous damage model without regularization	5
		1.2.5	Non-local damage models	6
		1.2.6	Gradient enhance model	8
		1.2.7	Thick level set method	9
	1.3	Phase	field models for fracture	9
		1.3.1	Representation of cracks in the phase field method	10
		1.3.2	Bourdin, Francfort and Marigo (1998, 2000)	11
		1.3.3	Lancioni and Royer-Carfagni, 2009	12
		1.3.4	Amor et al., 2009	12
		1.3.5	Miehe et al., 2010	13
		1.3.6	Borden et al., 2014	13
		1.3.7	Miehe et al., 2015	14
		1.3.8	Ambati et al., 2015	14
		1.3.9	Degradation function and parameter $\ell$	15
		1.3.10	Discussion on the phase field models	15
1.4 Multiscale modelling of damage		cale modelling of damage	16	
	1.5	Outlin	e of the thesis	20
<b>2</b>	A n	nultisca	ale approach for fracture in heterogeneous media with separated	
	$\mathbf{scal}$	es		<b>21</b>
	2.1	Introd	uction	22
	2.2	Micros	scale fracture model: a phase field approach	23
		2.2.1	Mechanical problem	26
		2.2.2	Phase field problem	26
		2.2.3	Numerical Implementation	29
	2.3	Local	two-scale (FE <sup>2</sup> ) fracture algorithm $\ldots \ldots \ldots$	31
	2.4	A non	local two-scale (FE <sup>2</sup> ) fracture algorithm $\ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots$	33
		2.4.1	Macro regularization	33
		2.4.2	Staggered solving procedure	38
		2.4.3	Computation of the effective elastic tensor	39

	2.5	Numer	rical examples	42
		2.5.1	A plate with a sharp crack (test MS1)	42
		2.5.2	Three-point bending beam (test MS2)	44
		2.5.3	L-shape test	48
		2.5.4	A plate with a hole	48
		2.5.5	Cracked square plate	53
		2.5.6	A plate with two semicircular notches	55
		2.5.7	Snap-back in 4-point bending cracked structure	56
	2.6	Conclu	ision	60
3	Ide	ntificat	ion of fracture models based on phase field for crack propagation	1
	in h	neterog	eneous lattices in a context of non-separated scales	63
	3.1	Introd	uction	64
	3.2	Fractu	are model used for the heterogeneous media $\ldots \ldots \ldots \ldots \ldots \ldots \ldots$	65
	3.3	Fractu	re models for the equivalent homogeneous solid $\ldots \ldots \ldots \ldots \ldots \ldots$	65
		3.3.1	Isotropic effective fracture model	66
		3.3.2	Anisotropic effective fracture model $\ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots$	67
		3.3.3	Numerical implementation	70
		3.3.4	Computation of effective elastic parameters	71
		3.3.5	Effective fracture parameters	72
	3.4	Numer	rical examples	73
		3.4.1	Periodic composite with hard inclusions $\ldots \ldots \ldots \ldots \ldots \ldots \ldots$	73
		3.4.2	Periodic quasi-brittle porous lattice structure: isotropic macroscopic frac-	
			ture model	79
		3.4.3	Periodic porous lattice: anisotropic macroscopic fracture model	85
		3.4.4	Validation tests	86
	3.5	Conclu	ision	90
4	As	urroga	te approach based on neural networks for multi-scale modelling of	f
	frac	ture		91
	4.1	Introd	uction	91
	4.2	Brief r	review of artificial neural network	92
	4.3	Constr	ruction a surrogate model for the multiscale damage model based on ANN	94
	4.4	Applic	ations	98
		4.4.1	A surrogate model using solution 1: ANN model $\ldots \ldots \ldots \ldots \ldots$	98
		4.4.2	A surrogate model using resolution 2 with double ANNs model (D-ANN)	103
	4.5	Discu	ssion and conclusion	106

<b>5</b>	Conclusion					
	5.1	General conclusion	109			
	5.2	Perspectives	110			

# Introduction and literature review

#### **1.1** Background and motivations

Modeling of damage in quasi-brittle heterogeneous materials is of extreme importance in engineering, as it covers several major applicative fields such as civil engineering materials, biomechanics materials (bones), or more recently architectured materials obtained by 3D printing. In such materials, the heterogeneities play a central role in the damage process, by initiating micro cracks which can merge to form macrocracks and then lead to the failure of the structure. To design new materials and optimize their mechanical properties such as strength, understanding and modeling the damage mechanisms from the microscale is required to obtain predictive models. The characteristics of heterogeneous quasi-brittle materials are the complexity of the crack networks (see e.g Fig. 1.1) which form at the macroscale. In random materials such as cementitious materials or cortical bone, a very complex, 3D network of microcracks whose orientation depends on the loading and the local microstructure. In organized materials such as obtained by 3D printing, the cracks may follow preferential directions and induce strongly anisotropic damage.

The main challenges in such problems are listed as follows:

• The modeling and numerical simulation of the initiation and propagation of micro cracks in complex microstructural geometries: the related challenges are associated to the definition of a very robust numerical method and to the large size of simulations involved, especially for 3D microstructures.



Figure 1.1: a) Microstructure of lightweight plaster [27]; b)Microcracks in porous media [151]



Figure 1.2: Schematic representation of a cohesive zone [47].

- The construction of a damage model which can be used at the scale of the structure, as modeling the whole heterogeneities and the related micro crack network is not tractable with available computational resources.
- The right definition of a representative volume element when dealing with quasi-brittle damage, where cracks can propagate through the specimen in very localized regions.
- The inherent numerical difficulties of damage model when solved by numerical methods such as Finite Elements.

The objectives of this Ph.D. thesis will be to propose solutions to the different abovementioned issues with applications to damage in heterogeneous materials with computational multiscale strategies. In the following, we review different methods and methodologies which will be central to this work: (a) numerical methods for fracture modeling, and more specifically the phase field method which we will adopt in our methodologies, and (b) multiscale strategies to model damage.

#### 1.2 Numerical methods for fracture modelling

#### 1.2.1 Cohesive Zone Models

The concept of the Cohesive Zone Models (CZMs) dates back to the work of Dugdale [55] and Barentblatt [9]. According to this approach, a process zone is located ahead of the crack tip as shown in Fig 1.2, associated with a characteristic length. The main idea of CZMs is the introduction of a surface energy term which controls the displacement jump along a known surface where a nonlinear traction-displacement jump relation must be introduced to describe the failure. The method usually associates with finite elements in which the damageable interface is discretized by surfaces where the nodes are doubled to allow jump displacements [79]. The model is consistent with the dissipated energy  $G_c$  in the energy approach of Griffith's theory in some configurations. Additionally, the model was then supported by thermodynamics arguments in [149].



Figure 1.3: a) Bilinear traction-separation law; b)Exponential law.

Many traction-separation laws have been proposed in literature, each being adapted to one specific material. By means of theoretical, experimental and computational techniques, separation laws have been identified in [177] based on by J-integral approach using numerical simulations and inverse analysis [175, 50, 97], and in [95, 206] by multiscale simulation. Fig 1.3 shows two popular types of TSL in brittle materials: the exponential softening law [201] and the bilinear softening law [10, 75, 150]. The intrinsic form of CZMs employs cohesive surface elements in the potential fracture area before computational simulations [200, 84]. Alternatively, cohesive surfaces elements can be inserted during the simulation when a criterion is satisfied. In this way, the model is so-called "extrinsic" [207, 148, 96]. The introduced cohesive element may have a finite thickness or a zero thickness. The drawback of the intrinsic CZM is the requirement of a priori fracture zone while the extrinsic version needs to be employed with an adaptive mesh. CZMs have been efficiently used for stationary cracks on interfaces in [134, 199]. The method has been extended to arbitrary cracks in [33] and to 3D crack in [148], or in combination with other methods like discontinuous Galerkin method [144], among numerous applications in literature. In general, cracks in CZMs propagate by following the boundary of elements, leading to high mesh-dependency issues.

#### 1.2.2 Extended Finite Element Method (XFEM)

In classical Finite Element Method (FEM), the boundaries of the cracks are described explicitly and meshed, requiring complex adaptive meshing strategies which may be highly timeconsuming and not robust for 3D complex configurations. In [12], Belytschko and Black have proposed a partition unity-based method (PUFEM) to minimize this issue which was later developed and renamed as the XFEM method in [127, 44]. By adding discontinuous enrichment functions at nodes, the cracks in XFEM method are described independently of the mesh. In this method, two types of enrichment function can be employed: one for nodes of cracked elements to introduce the strong discontinuity, and one for nodes of elements which contains a



Figure 1.4: Enriched nodes in XFEM method for tracking crack

crack tip to add singular terms. The approximation of the displacement function takes the following form:

$$\mathbf{u}^{h} = \sum_{i \in I} \mathbf{u}_{i} N_{i} + \sum_{j \in J} \mathbf{b}_{j} N_{j} H(\mathbf{x}) + \sum_{k \in K} N_{k} \left( \sum_{l=1}^{n} \mathbf{c}_{k}^{l} F_{l}(\mathbf{x}) \right),$$
(1.1)

where J is the set of crack-enriched nodes; H(x) is the Heaviside function and K is the set of nodes enriched by the crack tip functions  $F_l(x)$  as can be seen in Fig.1.4; **b** and **c** are vectors of additional degrees of freedom. In XFEM, cracks can propagate in an arbitrary direction without dependence to the underlying mesh. Nevertheless, in the classical XFEM, two additional issues remain: (a) the difficulties to deal with many cracks, due to associated level-set functions which must be constructed to describe the position of the crack front; (b) initiation of cracks cannot be dealt with as the method is based on classical fracture mechanics. Despite these drawbacks, XFEM is a good alternative when dealing with fixed cracks and interface problems. Among massive applications and improvements of XFEM, extensions can be mentioned, such as: non-planar 3D crack growth [128, 178, 72], bi-materials [110], dynamic cracks and shear band propagation [176]. Other recent works can be found e.g. in [58, 191, 190].

#### 1.2.3 Embedded Finite Element Method EFEM

The idea within the Embedded Finite Element Method is to introduce discontinuous enrichment inside elements, which vanishes at the boundaries of elements. Then by an appropriate condensation process, the total number of unknowns is not increased as compared to classical FEM. The computation costs of XFEM and EFEM have been compared in [147]. First contributions to E-FEM can be found in [172, 114], in which discontinuities have been assumed to be fixed. Linear jumps have been introduced in [2, 8, 56]. Other drawbacks of EFEM lies on unexpected approximation errors due to the lack of the continuity of the displacement field between two elements leading to strong the mesh-dependency as well as the lack of convergence of the solution with respect to the mesh size. More detail about EFEM, one can find in e.g [147, 194]

On one hand, fracture mechanics with remeshing techniques or XFEM can accurately model

sharp cracks but fail for modeling their initiation and propagation in complex configurations (3D, multiple cracks, merging of independent cracks, etc...). On the other hand, cohesive elements and EFEM suffer from strong mesh dependency and lack of convergence issues. Another strategy for modeling cracks is the use of damage models, as described in the following.

#### 1.2.4 Continuous damage model without regularization

The original concept of damage mechanics should be dated back from the work of Kachanov [87], in which an assumed isotropic degradation function was introduced through a scalar damage parameter d ranging from 0 to 1. The constitutive equation relating the stress field  $\sigma$  and the strain field  $\varepsilon$  of an isotropic damage model is written as:

$$\boldsymbol{\sigma} = (1-d)\mathbb{C}:\boldsymbol{\varepsilon},\tag{1.2}$$

where  $\mathbb{C}$  is the stiffness matrix of the elastic material. In the case of anisotropic damage effects, a damage tensor  $\mathbb{D}$  must be introduced. In addition, an evolution law is necessary for d. This damage law may be chosen such as to reflect the behavior of the considered material. For example, for quasi-brittle materials, the exponential law is usually adopted [155]:

$$d = \begin{cases} 0 & if \quad \kappa < \kappa_0 \\ 1 - \frac{\kappa_0}{\kappa} [(1 - \alpha) + \alpha \exp^{-\beta(\kappa - \kappa_0)}]. \end{cases}$$
(1.3)

In (1.3), the scalar parameter  $\beta$  describes the softening behavior;  $\alpha$  is a scalar which controls the residual state in the post peak stage;  $\kappa_0$  is the threshold for the initiation of damage and  $\kappa$  is a history scalar parameter which takes the largest value of an equivalent strain  $\tilde{\varepsilon}$  which is a function of  $\varepsilon$  (see below). Damage evolution is governed by the Kuhn-Tucker inequalities as follows:

$$\dot{\kappa} \ge 0, \qquad f(\tilde{\varepsilon}, k) \le 0, \qquad df(\tilde{\varepsilon}, k) = 0,$$
(1.4)

where  $f(\tilde{\varepsilon}, k) = \tilde{\varepsilon} - \kappa$  is the loading function driving the evolution of damage. Early developments in the context of numerical methods can be found in [92, 34, 105]. Various definitions for  $\tilde{\varepsilon}$  have been later proposed. For example, according to the Mazars' (1984) criterion [120], cracks can only propagate due to tensile strains, according to:

$$\tilde{\varepsilon}(\boldsymbol{\varepsilon}) = \sqrt{\langle \varepsilon_i \rangle : \langle \varepsilon_i \rangle},\tag{1.5}$$

where  $\varepsilon_i$  are principle strains and  $\langle \varepsilon_i \rangle = \frac{|\varepsilon_i| + \varepsilon_i}{2}$ . For ductile fracture, the modified von Mises equivalent strain is usually defined as:

$$\tilde{\varepsilon}(\varepsilon) = \frac{k-1}{2k(1-2\nu)} I_1(\varepsilon) + \frac{1}{2k} \sqrt{\frac{(k-1)^2}{(1-2\nu)^2}} I_1^2(\varepsilon) + \frac{12k}{(1-\nu)^2} J_2(\varepsilon),$$
(1.6)



Figure 1.5: The double-edge-notched (DEN) specimen tested by Nooru-Mohamed (1992)

where k is the tensile/compressive strength ratio which is adapted depending on the material,  $\nu$  is the Poisson's ratio,  $I_1(\varepsilon) = tr(\varepsilon)$  is the first invariant of the strain tensor,  $J_2(\varepsilon) = \frac{1}{6}(3tr(\varepsilon^2) - tr^2(\varepsilon))$  is the second invariant of the strain tensor.

Another choice is the so-called smooth Rankine calibration [86]

$$\tilde{\varepsilon}(\varepsilon) = \frac{1}{E} \sqrt{\langle \sigma_i \rangle : \langle \sigma_i \rangle}, \qquad (1.7)$$

where  $\langle \sigma_i \rangle$  is the principle stress tensor, E is Young's modulus.

The well-known drawbacks of this model are twofold mesh sensitivities: (i) dependence on the alignment of the mesh (see Fig 1.6) which shows the mesh bias of crack for a double-edgenotched test in Fig 1.5; (ii) the result does not converge with the mesh size as can be seen for the notch beam in Fig. 1.7 and Fig. 1.8. The underlying reason is that the dissipated energy vanishes with the size of the elements. When accumulated damage gets to an extent, the governing equations become ill-posed. Various techniques have been proposed in the literature to remedy for aforementioned mesh sensitivity issues of the local damage model including (i) Cosserat continuum or micropolar model e.g [99, 46]; (ii) adding viscosity [57]; (iii) nonlocal techniques using weight functions to regularize the damage fields [85, 11]; (iv) the addition of higher order gradient of deformation [133, 134]. Pros and cons of these methods have been discussed in [48]. Among those, the two last methods are the most used in computational analysis and are called regularization techniques. A very popular method in this context is the so-called phase field method to fracture [22, 90, 124], which will be detailed in the sequel.

#### 1.2.5 Non-local damage models

We describe here nonlocal damage models based on regularization through a convolution of strain, as firstly developed in  $s = \max_{\tau \in [0,t]} (\hat{\sigma}_1^2 + \hat{\sigma}_2^2)$ . In this context, the localization of damage is kept in a zone defined by a given internal length and thus does not suffer from lack of mesh



Figure 1.6: Influence of mesh type and element size [71] on the crack band trajectory in the test for damage models (a) Rankine type definition of equivalent strain, (b) modified von Mises definition of equivalent strain and (c) micro plane damage model (anisotropic damage model).



Figure 1.7: A test to investigate the convergence w.r.t the mesh [85]: three-point bending test of a concrete beam, corresponding to the results presented in Fig. 1.8.



(a) Load-displacement curves using local damage model

(b) Load-displacement curves using nonlocal damage model

Figure 1.8: Convergence w.r.t the mesh for: local damage model (a) and nonlocal damage models(b), showing the mesh dependency issue [85].

dependence as in local models. Then, the driving force is a function of a nonlocal term  $\bar{\varepsilon}$  defined from the strain, written as:

$$f(\bar{\varepsilon},k) = \bar{\varepsilon} - \kappa, \tag{1.8}$$

where  $\bar{\varepsilon}$  is defined by:

$$\bar{\varepsilon}_{eq}(x) = \frac{\int_{\tilde{\Omega}} g(s)\tilde{\varepsilon}(x-s)dV}{\int_{\tilde{\Omega}} g(s)dV},$$
(1.9)

where the weight function g(s) satisfies  $\int_{\tilde{\Omega}} g(s) dV = 1$ . A popular choice is the Gauss weighting function, written as:

$$g(s) = exp^{-\frac{\|x+s\|^2}{\alpha\ell^2}}.$$
 (1.10)

In (1.10),  $\alpha$  has to be chosen by the users,  $\ell$  is the internal length of the model, and s denotes the relative position vector of a point in  $\tilde{\Omega}$ . Another alternative is the bell-shaped function, where the regularization occurs at a finite distance from one point through a cut-off distance  $r = \|\mathbf{x} - \mathbf{s}\|$ :

$$g(s) = \begin{cases} 1 - \frac{r^2}{R^2} & \text{if } r \le R, \\ 0 & \text{if } r > R. \end{cases}$$
(1.11)

This nonlocal damage model is also referred to in the literature as the integral damage model.

#### 1.2.6 Gradient enhance model

Gradient enhanced damage models [155, 45] are usually mentioned as a differential type nonlocal models, and use another regularization definition of the strain field as follows. Taylor expansion of the term  $\bar{\varepsilon}_{eq}(x+s)$  in Eq. (1.9) gives:

$$\bar{\varepsilon}_{eq}(x+s) = \bar{\varepsilon}_{eq}(x) + \nabla \bar{\varepsilon}_{eq}(x)s + \frac{1}{2!}\nabla^2 \bar{\varepsilon}(x)s^2 + \frac{1}{3!}\nabla \bar{\varepsilon}(x)s^3 + \frac{1}{4!}\nabla^4 \bar{\varepsilon}(x)s^4....$$
(1.12)

Replacing (1.12) into (1.9), we obtain:

$$\bar{\varepsilon}_{eq} = \varepsilon_{eq} + c\nabla^2 \varepsilon_{eq} + d\nabla^4 \varepsilon_{eq} + \dots$$
(1.13)

in which c, d are determined using the weight function g(s) and the volume V. Neglecting higher-order terms, the equivalent strain  $\bar{\varepsilon}$  can be expressed as:

$$\bar{\varepsilon}_{eq} = \varepsilon_{eq} + c\nabla^2 \varepsilon_{eq}. \tag{1.14}$$

Solving such equation involves second-order derivative terms of the local strains and requires  $C^1$  element types to be solved by FEM. By differentiating twice (1.12) and reordering, a practical estimating of  $\bar{\varepsilon}_{eq}$  is written as:

$$\bar{\varepsilon}_{eq} - c\nabla^2 \bar{\varepsilon}_{eq} = \varepsilon_{eq} \tag{1.15}$$

This implicit formula (1.15) is usually solved with an additional boundary condition [101, 130]:

$$\nabla \bar{\varepsilon}_{eq} \cdot \mathbf{n} = 0, \tag{1.16}$$

whose physical meaning is still not well-defined.

Both integral-type and differential-type model can solve the mesh-dependence issues in presence of localization, nevertheless, induce an incorrect crack initiation, as reported in [173]. Improvements to these problems have been proposed in later works (see e.g [69, 137]).

#### 1.2.7 Thick level set method

The thick level set model was introduced in [129, 16] for modelling damage as a propagating level set front. As a constitutive model, it allows capturing complex morphology cracks from the initiation, branching and merging. The potential energy of the model over the domain  $\Omega$  is written as:

$$E(\mathbf{u},\phi) = \int_{\Omega} \Psi(\varepsilon(\mathbf{u}), d(\phi)) d\Omega, \qquad (1.17)$$

where  $\varepsilon$  is the symmetric part of gradient of the displacement field  $\mathbf{u}$ ,  $\phi$  is a level-set function to separate the undamaged zone from the damaged one, d is the increasing damage variable depending on the level set as:  $d(\phi) = 1$  if  $\phi \ge l_c$ ,  $d(\phi) = 0$  if  $\psi \le l_c$ ,  $d'(\phi) > 0$  if  $0 \le \psi \le l_c$ .  $l_c$  is a mesh-size-independent characteristic length leading to the non-local effect of the model. However, TLS induces spurious oscillations in mechanical responses as well as complexity related to self-contact within the crack.

#### 1.3 Phase field models for fracture

A recent powerful nonlocal damage model is the so-called phase field [22, 23, 90, 100, 20], also called as a variational approach to fracture as introduced by Francfort, Marigo and Bourdin [62, 22] and has been popularized later by Miehe by defining an efficient computational framework [124]. The introduced method has combined the advantages of damage models for handling initiation and complex crack patterns, and the theory of fracture through a variational principle which is consistent with Griffith's theory. In the original version, Griffith's theory [73] suffers from several drawbacks such as : (i) it is not able to predict the initiation since it leads to infinite critical stress  $\sigma_c$  when the initial crack goes to zero length; (ii) the construction of criteria for crack initiation is difficult. A short overview of the phase field method and its various extensions will be presented and discussed in the following.

#### 1.3.1 Representation of cracks in the phase field method

Phase field approaches represent a sharp-crack surface topology  $\Gamma$  by means of a surface functional, written as:

$$\Gamma_{\ell}(d) = \int_{\Omega} \gamma(d, \nabla d) dV, \qquad (1.18)$$

where  $\gamma(d, \nabla d)$  is the crack density function per unit volume of the domain  $\Omega$ ; d is a damage variable which ranges between 0 and 1. In the present work, the damage variable is denoted as d, and the intact and fully broken state corresponds to d = 0 and d = 1, respectively. Using the Mumford and Shah type functional to approximate an image segment by Ambrosio and Tortorelli for free discontinuities [5], the regularization functional of Miehe [124] is written as:

$$\gamma(d) = \frac{d^2}{2\ell} + \ell \nabla d. \nabla d, \qquad (1.19)$$

which has been a popular choice in many studies. The field d is the solution of the crack length minimization problem

$$d = \operatorname{Argmin} \int_{\Omega} \gamma(d, \nabla d) dV, \qquad (1.20)$$

which yields the Euler Lagrange equation:

$$d - \ell^2 \Delta d = 0, \tag{1.21}$$

with the boundary condition  $\nabla d.\mathbf{n} = 0$ , where  $\mathbf{n}$  is the output normal vector on the boundary  $\partial \Omega$ .

Various phase field models define the crack density function differently but all depends on (i) a damage variable, (ii) its gradient  $\nabla d$  and (iii) an internal length  $\ell$  which controls the transition zone. For quadratic type functions, those can be recast in the following form:

$$\gamma(d) = \frac{w(d)}{a\ell} + \ell \nabla d^2 / b, \qquad (1.22)$$

where a, b are scalars chosen such that when  $l \to 0$ , the integral of  $\gamma(d)$  is  $\Gamma$  convergent to the surface measure of the crack set.

An alternative form for w(d) is the double-well function, as employed in [90, 39], which can be expressed as:

$$w(d) = d^2 (1-d)^2. (1.23)$$

This choice naturally leads to the irreversibility of crack zones but induces strongly nonlinear equations to be solved to obtain d. For this reason, the quadratic function w(d) is widely used as:

$$w(d) = (1 + \beta s)(1 - s), \qquad s = 1 - d,$$
 (1.24)

leading to a linear problem for d under appropriate evolution schemes (see [126, 143]. One convenient choice is  $\beta = 1$ , e.g  $\gamma(s) = \frac{(1-s^2)}{4c} + c\nabla s \cdot \nabla s$  in (1.28) or  $\gamma(d) = \frac{d^2}{2\ell} + \ell \nabla d \cdot \nabla d$  in



Figure 1.9: Smeared representation of a free discontinuity: (a) diffuse representation of crack in 1D case: The crack density function (1.19) gives  $d = e^{(-|x|/l)}$  in the red lines while (1.33) gives  $d = e^{(-|2x|/l)(1+|2x|/l)}$  in blue lines [195]. Black thick line represents a sharp crack at x = 0; (b) Diffuse representation of crack in 2D case (using (1.19))

(1.30). The reason is that when using  $\beta = 1$ , it yields d = 0 as a minima of the energy function in the absence of mechanical strain. The parameter  $\beta$  is also chosen to be zero e.g. in [22, 119]. A higher order of crack density function has been utilized in [18] to produce smoother crack profiles as can be seen in Fig.1.9a. The parameter  $\ell$  represents the "width" of the smeared crack (see Fig.1.9). The drawback of high order crack density function is that linear elements for solving the phase field problem cannot be used.

#### 1.3.2 Bourdin, Francfort and Marigo (1998, 2000)

To overcome the failure of Griffith's theory to predict the initiation of cracks in the case a crack tip is absent, Francfort and Marigo in [62] proposed a variational approach in which the total potential energy of a cracked body is a function of a buck energy  $E_u$  and a surface energy  $E_s$ , written as:

$$E(\mathbf{u},\Gamma) = E_u(\mathbf{u}) + E_s(\Gamma) = \int_{\Omega} \psi(\mathbf{u},\Gamma) d\Omega + g_c \int_{\Gamma} ds, \qquad (1.25)$$

where **u** is the displacement field, and  $\Gamma$  refers to an admissible crack surface. The variational approach does not involve any crack tip or predefined path and allows the initiation, the branching of cracks, as long as the crack set is the solution of the minimization problem. However, the crack set  $\Gamma$  is unknown, and solving this problem is nontrivial. In a pioneer work of Bourdin et al. [22], Eq. (1.25) was replaced by a regularized version as:

$$E(\mathbf{u}, v) = \int_{\Omega} (g(v) + k)\psi(\mathbf{u})dx + g_c \int_{\Omega} \gamma(v, c)ds, \qquad (1.26)$$

where  $\gamma(v,c) = \frac{(1-v^2)}{4c} + c\nabla v \cdot \nabla v$  is the crack density function. In (1.25) and (1.26), **u** is the displacement field,  $g_c$  is the energy release rate; v is the crack field parameter which varies

smoothly from 1 (undamaged state) to 0 (totally damage state), c is an internal scalar variable representing the width of the cracks, k is small scalar parameter which is added to keep the well-posedness when a node and all its neighbor nodes are totally damaged. When k = 0 and v = 1, the first term in 1.26 turns over to be the classical internal elastic energy. The second term converges to the Hausdorff measure when  $c \to 0$  which implies that in the limit of  $\ell \to 0$  the volume integral tends to the exact surface integrals [22, 23]. This consistency is the consequence of the appropriate degradation function and the crack density function, which will be discussed in the section 1.3.10. In Fig. 1.9 a), the higher order crack density function can give a sharper crack.

The degradation process of material from undamaged state to fractured state was interpreted as a phase change in the work of Kuhn and Muller [93]. This method is now simply called the phase field method in recent literature.

#### 1.3.3 Lancioni and Royer-Carfagni, 2009

In the initial model of Bourdin *et al.* in (1.26), damage can be induced either by a negative or positive strain, leading to a symmetric behavior in traction and compression. For brittle materials, this is unphysical. In addition, for mode II cracks, the obtained crack paths are not realistic. In [100], Lancioni and Royer-Carfagni proposed to split the isotropic elastic energy into spherical and deviatoric parts according to:

$$E(\mathbf{u}, v) = \int_{\Omega} \left( K_n \frac{tr(\varepsilon)^2}{2} + (v^2 + \eta) \mu \varepsilon_D . \varepsilon_D \right) dx + g_c \int_{\Omega} \left( \frac{(1 - v^2)}{4c} + c \nabla v . \nabla v \right) ds, \tag{1.27}$$

where  $K_n = \lambda + \frac{2\mu}{n}$ ,  $\lambda, \mu$  are Lamé's constants,  $\varepsilon_D = \varepsilon - \frac{1}{n}tr(\varepsilon)\mathbf{1}$ ,  $\varepsilon = \frac{1}{2}(\nabla^T \mathbf{u} + \nabla \mathbf{u})$  is the symmetric part of the displacement gradient  $\nabla \mathbf{u}$  and n is the space dimension. Even though this model can capture cracks in mode II, damage still appears in the compression zone.

#### 1.3.4 Amor et al., 2009

To remove damage in compression, Amor *et al.* proposed in [7] a modified regularized formulation in which the elastic energy density is split into two parts and the damage parameter is only associated with the positive part of the energy. This type of decomposition is considered as a modified spherical and deviatoric split:

$$E(\mathbf{u},s) = \int_{\Omega} \left( (s^2 + \eta) \Psi_0^+(\varepsilon) + \Psi_0^-(\varepsilon) \right) dx + g_c \int_{\Omega} \left( (1 - s^2) + \epsilon |\nabla s| \right)^2 ds, \tag{1.28}$$

where  $\Psi_0^+$  and  $\Psi_0^-$  are the hydrostatic and deviatoric part, respectively, and

$$\begin{cases} \Psi_0^+ = \frac{1}{2} K_n \langle tr(\boldsymbol{\varepsilon}) \rangle_+^2 + \mu(\boldsymbol{\varepsilon}^{dev} : \boldsymbol{\varepsilon}^{dev}), \\ \Psi_0^- = \frac{1}{2} K_n \langle tr(\boldsymbol{\varepsilon}) \rangle_-. \end{cases}$$
(1.29)

Note that in (1.28) and (1.26);  $\Psi_0 = \Psi_0^+ + \Psi_0^-$ ,  $K_n = \lambda + \frac{2\mu}{n}$ ,  $\langle a \rangle_{\pm} := \frac{1}{2}(a \pm |a|)$  and  $\varepsilon^{dev} = \varepsilon - \frac{1}{n}\varepsilon \mathbf{1}$ .

#### 1.3.5 Miehe et al., 2010

Miehe et al. proposed in [124] another expression for the potential energy of the cracked solid as:

$$E(\epsilon, c) = \int_{\Omega} g(d)\psi_e^+(\epsilon) + \psi_e^-(\epsilon)d\Omega + g_c \int_{\Omega} \gamma(d)d\Omega, \qquad (1.30)$$

where d denotes the damage variable; g(d) is the degradation function and  $\gamma(d)$  is the crack density function which regularizes the crack. The free energy is split into positive and negative parts using the spectral decomposition of the strain tensor:

$$\begin{cases} \Psi^{+}(\varepsilon) = \frac{\lambda}{2} (\langle Tr(\varepsilon) \rangle_{+})^{2} + \nu Tr\{(\varepsilon^{+})^{2}\}, \\ \Psi^{-}(\varepsilon) = \frac{\lambda}{2} (\langle Tr(\varepsilon) \rangle_{-})^{2} + \nu Tr\{(\varepsilon_{-})^{2}\}, \end{cases}$$
(1.31)

where

$$\varepsilon_{+} = \sum_{i=1}^{D} \langle \varepsilon^{i} \rangle_{+} \mathbf{n}^{i} \otimes \mathbf{n}^{i}, \qquad \varepsilon_{-} = \sum_{i=1}^{n} \langle \varepsilon^{i} \rangle - \mathbf{n}^{i} \otimes \mathbf{n}^{i}, \qquad (1.32)$$

where  $\varepsilon^i$  and  $\mathbf{n}^i$  are the eigenvalues and the eigenvectors of the strain tensor  $\varepsilon_{ij}$ , D = (2,3) is the dimension of the considering problem. This type of decomposition requires more computational effort in comparison with that of (1.29). In this framework, the minimization problem is decoupled and solved in a staggered manner, which is considered as a robust algorithm since it overcomes the convergence difficulty of the monolithic scheme. More details about this model will be presented in Chapter 2.

#### 1.3.6 Borden et al., 2014

Solving the coupled problem in phase field approach requires a nested iterative solver. Since the associated functional is nonconvex, a desired convergence rate is usually difficult to obtain. In [19], Borden *et al.* proposed a fourth-order phase field formulation which improves the convergence of the optimization problem. The crack density function  $\gamma(c)$  is associated with second-order derivatives of the damage variable c as:

$$\gamma(c) = \frac{(1-c^2)}{4\ell} + \frac{\ell |\nabla c|^2}{2} + \frac{\ell^3}{4} (\triangle c)^2.$$
(1.33)

A degradation function  $c^2$  is introduced into the positive part of strain density energy using the decomposition in [124]:

$$\Psi(\varepsilon, c) = c^2 \psi_e^+(\varepsilon) + \psi_e^-(\varepsilon).$$
(1.34)

The potential energy of the proposed model then reads as:

$$E(\varepsilon, c) = \int_{\Omega} c^2 \psi_e^+(\varepsilon) + \psi_e^-(\varepsilon) d\Omega + g_c \int_{\Omega} \gamma(c) d\Omega.$$
(1.35)

The implementation of this model requires at least  $C^1$  elements. Besides, it does not ensure the  $\Gamma$  convergence which is considered to be a condition for the solution of the regularized variational principle to converges to the solution of non-regularized one as  $\ell = 0$ .

#### 1.3.7 Miehe et al., 2015

One drawback of phase field models presented above is that damage occurs within the whole structure, even at small strain and stress local state. To consider the regularized length  $\ell$  as a geometrical parameter only, Miehe et al. in [123] proposed a phase field model with a stress-based criterion, defined as:

$$E(\varepsilon,c) = \int_{\Omega} g(d) \left[ (\psi_e(\varepsilon) - \psi_e^c(\varepsilon)) d\Omega + \int_{\Omega} \psi_e^c(\varepsilon) d\Omega + g_c \int_{\Omega} \gamma_d d\Omega, \right]$$
(1.36)

where  $\psi_e^c(\varepsilon)$  is "a specific fracture energy per unit volume". Among possible choices, one can adopt  $\psi_e^c = \frac{\sigma_c^2}{2E}$ . To ensure the irreversibility, the weak form when solving the damage field in the staggered scheme is modified according to:

$$2\psi_e^c(\varepsilon)\left[d-\ell^2\nabla d\right] = 2(1-d)\mathcal{H},\tag{1.37}$$

where

$$\mathcal{H}(\mathbf{x},t) = \max_{\tau \in [0,t]} \langle \psi_e(\varepsilon) - \psi_e^c(\varepsilon) \rangle, \qquad (1.38)$$

in which,  $\langle . \rangle$  is the Macauley bracket. To distinguish the tension and compression part in (1.38),  $\psi_e(\varepsilon)$  is replaced by  $\psi_e^*(\sigma)$  which is defined as:

$$\psi_e^*(\sigma) = \sup_{\varepsilon} \left[ \frac{\sigma : \varepsilon}{(1-d)^2} - \psi(\varepsilon) \right].$$
(1.39)

#### 1.3.8 Ambati et al., 2015

With the aim to keep the benefit of Miehe's model (1.30), at the computational cost of isotropic model (1.26), a hybrid model has been proposed in [4]:

$$\begin{cases} \sigma(\mathbf{u}, d) = (1 - d)^2 \frac{\partial \Psi(\varepsilon)}{\partial \varepsilon} \\ -\ell^2 \delta d + d = 2 \frac{\ell}{G_c} (1 - d) \mathcal{H} \\ \forall x : \Psi^+ < \Psi^- => d := 0 \end{cases}$$
(1.40)

This model is interpreted as a non-local model using spatial average for d as:

$$d(\mathbf{x}) = \frac{1}{V} \int_{V} g(s) \frac{2l\psi_{0}^{+}(\mathbf{x}+s)/g_{c}}{1+2l\psi_{0}^{+}(\mathbf{x}+s)/g_{c}} ds.$$
(1.41)

The hybrid model saves the computing time since it does not require an iterative solver to solve the displacement problem in the staggered scheme. However, it fails to capture cracks in compressive loading where the negative energy is dominant.

#### **1.3.9** Degradation function and parameter $\ell$

The degradation function plays an important role in the phase field method. Such function governs the non-linear behavior in the post-peak stage and should satisfy the following criteria: (i) a monotonous decreases from d = 0 at the unbroken state to d = 1 to guarantee that there is no enhancement of the effective material stiffness matrix: (ii)  $g_{(d=0)} = 1$  ensure the consistency with the classical elastic problem when no damage appears and g'(d = 1) = 0 when the material is totally damaged; (iii) g'(1) = 0 is to prevent the broadening of damage when complete damage occurs. Several choices for this function include:

$$g(d) = 4(1-d)^3 - 3(1-d)^4,$$
(1.42)

$$g(d) = 3(1-d)^2 - 2(1-d)^3,$$
(1.43)

$$g(d) = (1-d)^2,$$
 (1.44)

in which (1.44) is the most popular. Higher order degradation functions lead to a more linear behavior in the pre-peak stage but lead to solving a nonlinear phase field problem. Recently, a new family of degradation function has been proposed to adapt the behavior of material at the initiation stage [168]:

$$g(d,k,n,w) = (1-w)\frac{1-e^{-k(1-d)^n}}{1-e^{-k}} + wf_c(d)$$
(1.45)

where k, n and w are scalars such that  $k > 0, n \ge 2$  and  $w \in [0, 1]$ . These parameters are used to adjust the pre-peak behavior according to the considering material. In the mentioned work, an approximation of the second order derivative term was proposed as:  $g''(d) = \frac{g'(d)}{1-d}$ .

As in other damage models, regularization involves an internal length  $\ell$  which not only constrains the mesh size but also plays a role as a threshold of damage except using another threshold for energy. The choice of the numerical parameter  $\ell$  has been discussed e.g. in [7, 20, 157, 142]. For this reason, it is considered as a material parameter which is related to the Young modulus and the critical energy release rate. The relation according to phase field formulations has been summarized in [94].

#### 1.3.10 Discussion on the phase field models

In spite of achievements obtained in several works, meshfree technique [13, 54], XFEM [44, 192] or thick level-set method [129, 16, 182] still can hardly handle 3D complex crack problems, especially involving multiple cracks, with initiation, propagation and merging of complex cracks.

Even though the phase field model can be seen as a continuous gradient damage model, it differs from the above models by the following aspects: (i) the evolution of the damage variable involves a global problem, and not an integration law at each Gauss point, which makes the


Figure 1.10: Direct simulation of crack in in a realistic sample concrete for different unit cells comprising: (a) 0.5 million elements; (b) 5 million elements; (c) 9 million elements; (d) 17 million elements and (e) 30 million elements [141].

algorithm more robust; (ii) in its simplest form, the phase field only involves classical FEM without intrusive modifications in the discretization schemes and (iii) it has been shown to provide remarkably predictive results as compared to experiments [138, 196] in heterogeneous quasi-britle materials. The success of phase field models for crack modeling ranges in a variety of problems from static cracks in concrete [143], polycrystals [37, 138], to dynamic cracks [26, 81, 169, 32], coupling with hydraulic forces [193, 197, 77], thermal shock damage [171], shrinkage cracks [119], cohesive cracks [186, 187], or in anisotropy damage [107, 139, 36, 77, 107] among many other works.

#### 1.4 Multiscale modelling of damage

Prediction of damage in quasi-brittle heterogeneous materials from the knowledge of microstructural constituents is an enormous challenge in engineering. Nowadays, experimental imaging techniques such as X-ray microtomography and 3D image correlation allow obtaining very rich information about microstructures in complex materials such as concrete and to follow microcracks during loading. In [141], the phase field method has been used to reproduce complex crack paths in lightweight concrete from realistic 3D micro-CT images (see Fig. 1.10). However, solving such a problem for small volumes of materials constitutes in itself a challenge. Then, solving the damage problem of heterogeneous structures with an explicit description of all the microstructural constituents is not tractable with nowadays computational resources.

A possible solution to overcome this obstacle is to use multiscale approaches and more specifically computational homogenization methods, where the local behavior at the fine scale is upscaled at the macroscale, at which the material is assumed to be homogeneous. Computational homogenization methods in the linear case have been described e.g. in [179, 208]. However, in the nonlinear case, even when no damage is involved, much tougher issues arise associated with: (a) the intrinsic complexity associated with nonlinear problems at both scales; (b) the definition of the macroscale behavior, which has either to be postulated and identified



Figure 1.11: (a) Linear homogenization scheme; (b) Nonlinear homogenization (FE<sup>2</sup> scheme).



Figure 1.12: Multiscale modelling of the cohesive crack [144]: the homogenization is related to the traction separation laws whereas the position of crack is known a priori at macroscale

[180] or obtained numerically by concurrent approaches (FE<sup>2</sup> methods [60]), or in some cases by the construction of a numerical mapping through e.g. interpolation or using techniques like machine learning [102]. The schematic of FE<sup>2</sup> is depicted in Fig. 1.11. Another ingredient which is usually included is the scale separation, implies that the size of the RVE should be small enough in comparison which the size of the macroscale structure  $l_m \ll L_M$ . In the context of damage at the microscale, applications can be found e.g. in [43, 68, 106, 160]

One specific issue when applying  $FE^2$  methods to damage problems is that local damage within the RVE, inducing softening at the macroscale and bringing all mentioned issues related to local damage models, like the loss of uniqueness of the solution [112] or the mesh dependency. Another specific difficulty relies on the right definition of the RVE when localization or cracks cross the RVE.

An alternative to the use of homogenization methods is to describe the cracking in some

small regions, where the response of the subdomain is coupled with the homogeneous structural model away from the crack. This type of multiscale, called in the literature "Arlequin method" [51] or "Bridging domain method" [198] cannot be easily applied to study complex heterogeneous materials like concrete, but can be useful to study the evolution of one region within the structure.

Attempts to adapt  $FE^2$  method for damage problems are reviewed as follows. In [117], the problem of internal localization has been studied in a periodic mortar phase. The localization was detected through the acoustic tensor as  $det(\mathbf{n}.\mathbf{C}_M.\mathbf{n}) \leq 0$ , where  $\mathbf{C}_M$  denotes the tangent stiffness obtained from RVE calculations. A similar approach was proposed in Belytschko *et al.* [14] where the cracks evolve at macroscale from the unit cell at the microscale. This work presents a multiscale aggregating discontinuity method which split the deformation corresponding to material failure from the bulk deformation and defines an equivalent discontinuity or several discontinuities that would be injected into the coarser-scale model and the normal vector  $\mathbf{n}$  is found by solving a minimization problem [74].

Cohesive zone models have been integrated with a multiscale framework in [185] for piezoelectric microsystems, where the computational homogenization is employed in the cohesive layer. After detecting the damage, the continuous damage at microscale is bridged to explicit discontinuities at macroscale through the traction-opening relation. Sharing the same ideas, a multiscale framework has been proposed in [145], where the traction-separation law at the macro scale is proved to be size independent when the average is taken over the damage zone only. Then, one can define an RVE to generate a cohesive law. In [118], a multiscale cohesive model has been proposed to couple the failure at the microscale and the macroscopic constitutive relationship in which the bridging between scale relies on Hill's energy equivalence lemma for traction - displacement jump relation. Broadening the study of [118] to the general case of finite deformations has been shown in [80], in which the RVE underlying the macro scale damage layer is modeled as a nonlinear finite-element BVP to be solved; a technique to model simultaneously the failure process at two scales through a nested scheme in [96]. In [38], Coenen *et al.* have developed an extension of  $FE^2$  to damage by introducing a discontinuous enrichment at the macroscale, where the traction-opening response of the discontinuity and the stress-strain response of the surrounding 'bulk' material are both extracted from a single microstructure volume element (MVE) analysis. A multiscale continuum approach has been proposed in [146] which used a regularized representation of the fracture at both scales based on the cohesive layer. This approach ensures the surface energy between two scales and keeps the homogenization process basically the same as it traditional form however predefined cohesive zones are required at both scales (see Fig. 1.13). A dispersive multi-scale crack model for quasi-brittle heterogeneous materials under impact loading [89] has been studied using TSL.

FEM approaches have been coupled with other methods in a multiscale framework to study



Figure 1.13: Continuum multiscale model [146]: (a) failure cell with inclusions and cohesive bands; (b) geometrical characterization of the failure mode at the microscale.



Figure 1.14: An L-shaped panel test using adaptive multiscale phase field [152].

fracture, e.g micro-BEM with macro-FEM in [170] or micro-DEM and macro-FEM in [88, 109], among many other works.

Apart from FE<sup>2</sup>-like methods, domain decomposition methods constitute another family of approaches to handle damage in heterogeneous structures. The domain decomposition method in [74], which includes discontinuities modeled by XFEM, was proposed with a global/local solving procedure based on the LATIN method [98]. Other domain decomposition methods embedding discontinuities were proposed based on Usawa's algorithm [167], and adaptive multigrid solvers for XFEM approximations [188]. Most of the above methods involve either costly computations related to concurrent multilevel calculations, and domain decomposition methods still have difficulties regarding convergence when propagating cracks occur. Recently a non-intrusive global/local approach to brittle fracture using the phase field method has been presented in [66]. Even though this approach can produce the same result as the corresponding DNS, it may lead to a higher computational cost. Some attempts to apply phase field methods within computational homogenization are mentioned here: Chakraborty [35] used a hierarchical multi-scale approach to study the sensitive of pore distribution in the microstructure in capturing the growth of crack using a phase field based fracture model. Housain *et al.* [83] identified the effective toughness



Figure 1.15: Crack propagation in multiscale modelling with phase field method using adaptive mesh [152].

of the heterogeneous media and the macroscopic evolution law. An adaptive multiscale phase field method for brittle fracture has been proposed in [152] in which the displacement field is transferred from the coarse mesh to the finer mesh based on basis functions (AMPFM). This requires updating the fine mesh region as can be seen in Fig1.15 in an L-shaped panel test (Fig 1.14). Although phase field models are powerful when capturing successfully a wide range of fracture phenomena, it doesn't help to solve inherent difficulties in the multiscale framework for the softening process of materials.

#### 1.5 Outline of the thesis

The content of this thesis is organized as follow:

In this first chapter, we provided a review of numerical methods for modeling damage models, the related current issues and the recent proposed methodologies for multiscale simulations. In Chapter 2, we propose a numerical two-scales approach involving the phase field method to handle damage in heterogeneous quasi-brittle in the case of separated scales. In Chapter 3, we treat the case of non-separated scales, by proposing a simplified method to the construction of homogeneous damageable models based on the identification of an anisotropic phase field model at the macro scale. To alleviate the calculations costs of  $FE^2$  approaches, a tentative of construction of a surrogate model based on neural networks is proposed in the context of damageable microstructures in Chapter 4. Finally, conclusions and perspectives are drawn in Chapter 5.

# Chapter 2

# A multiscale approach for fracture in heterogeneous media with separated scales

# Contents

2.1	Introduction									
2.2	Micros	Microscale fracture model: a phase field approach $\ldots \ldots \ldots$								
	2.2.1	Mechanical problem	26							
	2.2.2	Phase field problem	26							
	2.2.3	Numerical Implementation	29							
2.3	Local two-scale (FE <sup>2</sup> ) fracture algorithm $\ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots$									
2.4	A non	non local two-scale (FE <sup>2</sup> ) fracture algorithm $\ldots \ldots \ldots \ldots \ldots \ldots \ldots$								
	2.4.1	Macro regularization	33							
	2.4.2	Staggered solving procedure	38							
	2.4.3	Computation of the effective elastic tensor	39							
2.5	5 Numerical examples									
	2.5.1	A plate with a sharp crack (test MS1) $\ldots$	42							
	2.5.2	Three-point bending beam (test MS2) $\ldots \ldots \ldots \ldots \ldots \ldots \ldots$	44							
	2.5.3	L-shape test	48							
	2.5.4	A plate with a hole	48							
	2.5.5	Cracked square plate	53							
	2.5.6	A plate with two semicircular notches $\ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots$	55							
	2.5.7	Snap-back in 4-point bending cracked structure	56							
2.6	Conclusion									



(a) compression test

(b) shear test

Figure 2.1: Examples of distributed cracks giving rise to a macroscopic diffuse damage: (a) experimental results in a compression test [164]; (b) simulation results obtained by the phase field method.

# 2.1 Introduction

The objective of this first chapter is to model numerically the fracture in heterogeneous media with separated scales, i.e. in which the characteristic dimensions of the heterogeneities are much smaller than the dimensions of the structure. We assume here that the damage due to microcracking is diffuse, i.e. that locally the microcracks are blocked by the heterogeneities and do not propagate over the whole structure (see Fig. 2.1), giving rise to a diffuse damage at the macroscale. In this framework, it is thus possible to define the macroscale behavior through the local analysis of a Representative Volume Element (RVE) which provides the effective damageable response at the macro scale.

The adopted strategy here relies on a numerical multilevel analysis (FE<sup>2</sup> approach [59, 60]) where the macroscale behavior is not known a priori and fully provided by the local resolution of an RVE associated with each point (Gauss points in a Finite Element discretization) of the structure (see Fig. 2.2).

At the micro scale, crack propagation is explicitly described by the phase field method (see section 2.2) and its evolution is induced by the macroscopic strain prescribed on the RVE. The effective macro stress and the associated softening behavior is then fully induced by the microstructure. At the macro scale, we introduce a regularization procedure to avoid meshdependency issues. The main contribution of the proposed scheme as compared to a direct application of  $FE^2$  with regularization at the macro scale relies in the use of a nested staggered scheme where the macro scale problem appears as an elastic problem at a given iteration, and where the regularization is performed in another iteration, avoiding the use of  $C^1$  FEM approximation at the macro scale.

The organization of this chapter is as the follows: section 2.2 reviews the phase field model which is employed to describe the micro cracking evolution at the microscale; section 2.3 presents the straightforward  $FE^2$ -like local damage model where no particular regularization treatment is performed at the macro scale; section 2.4 introduces several strategies for regularization of the



Figure 2.2: Schematic of the  $FE^2$  method: the macroscopic behavior is provided by the local mechanical state of an RVE associated which each Gauss point of the macroscopic mesh associated with the structure.

macro damage problem within the 2-scale approach, and more specifically a staggered scheme at both scales which removes the need for evaluating the tangent effective tensor. Finally, numerical examples are presented in section 2.5 to show the potential of the proposed scheme to model the damage induced at the micro scale by the microstructure.

# 2.2 Microscale fracture model: a phase field approach

The phase field method is adopted here at the microscale to model the damage through microcracking within the microstructure. The formulations and numerical implementation details are reviewed in this section.

Starting from the pioneering works of Francfort and Marigo [62], difficulties arising in the classical fracture framework can be overcome by a variational-based energy minimization framework (see section 1.3) for brittle fracture [25, 156, 24, 30, 7]. An important ingredient of the method relies on a regularized description of the discontinuities related to the crack front: the surface of the crack is replaced by a smooth function, using a Mumford-Shah functional [131]. The original functional is substituted by an Ambrosio-Tortorelli approximation [5, 6]. It has been shown that the solution of the associated variational problem converges to the solution of the sharp crack description implying discontinuities in the  $\Gamma$ - convergence sense [116, 28, 29]. The approximation then regularizes a sharp crack surface topology in the solid by a scalar auxiliary variable, interpreted as a phase field describing broken and unbroken parts of the solid. Such a method has the quality that it does not require any prior knowledge about the sharp



Figure 2.3: (a) solid containing a sharp crack; (b) solid containing a regularized description of the crack.

geometry and allows crack nucleation and branching, providing a very robust framework for crack propagation simulation. It has been adapted to quasi-static fracture problems in [24, 21], dynamic crack propagation [26, 82], and in a multiphysics context in [126, 1]. Remarkably, the regularized model may be regarded as a damage model of the gradient type [108, 113, 15, 154, 63] with critical differences in the choice of the free energy and dissipation function. Recently, the problem of cohesive fracture has been reformulated in the context of phase field [184].

For an elastic cracked body defined in a domain  $\Omega \subset \mathbb{R}^3$  containing sharp cracks denoted collectively as  $\Gamma$  (see Fig. 2.3 (a)), the total energy of the system is defined as:

$$E = \int_{\Omega} \Psi(\boldsymbol{\varepsilon}, \Gamma) d\Omega + g_c \int_{\Gamma} d\Gamma, \qquad (2.1)$$

where  $\Psi(\boldsymbol{\varepsilon}, \Gamma)$  is the elastic strain density function and  $g_c$  is the critical energy release rate in the sense of Griffith. The above energy form can be replaced by a regularized one, given by:

$$E = \int_{\Omega} \Psi(\varepsilon, d) d\Omega + g_c \int_{\Omega} \gamma(d, \nabla d) d\Omega, \qquad (2.2)$$

where  $\gamma$  is a crack density function, whose model can be chosen among several possible forms, leading to a class of shapes for the regularized damage field near the crack (see e.g. [125]). In this regularized framework, the cracks are no more described by surfaces but by a smooth field  $d(\mathbf{x})$  (see Figs. 2.4 and 2.3). In (2.1),  $\Psi$  can be decomposed according to:

$$\Psi(\boldsymbol{\varepsilon}) = g(d)\Psi^+ + \Psi^- \tag{2.3}$$

to only affect the damage to traction modes, and where g(d) is a degradation function such that g(0) = 1, g(1) = 0 and g'(1) = 0 and  $\Psi^+(\varepsilon^+)$  and  $\Psi^-(\varepsilon^-)$  denote parts of the strain density related to tensile and compressive parts of the strain tensor, respectively. For isotropic media, the following form has been proposed by Miehe et al. [124] as:

$$\Psi^{\pm}(\boldsymbol{\varepsilon}) = \lambda (\langle Tr(\boldsymbol{\varepsilon}) \rangle_{\pm})^2 / 2 + \mu Tr\{(\boldsymbol{\varepsilon}^{\pm})^2\}.$$
(2.4)



Figure 2.4: Regularized representation of a crack: one dimensional case: (a) sharp crack model, taking unitary value of d(x) at  $x = x_{\Gamma} = L/2$  (crack); (b) regularized representation through phase field [143].

This form allows avoiding interpenetration when the cracks are closed without any special algorithm for auto-contact, which renders the implementation very simple. In (2.4),  $\lambda$  and  $\mu$  denote the elastic Lamé's constants in each phase. The operator  $\langle . \rangle_{\pm}$  is defined as  $\langle x \rangle_{\pm} = (x \pm |x|)/2$ ,  $\varepsilon^+$  is the tensile part while  $\varepsilon^-$  is the compression part of the strain tensor obtained by the spectral decomposition:

$$\boldsymbol{\varepsilon}_{\pm} = \sum_{i=1}^{n} \langle Tr(\boldsymbol{\varepsilon}) \rangle_{\pm} \mathbf{v}_i \otimes \mathbf{v}_i, \qquad (2.5)$$

in which  $\mathbf{v}_i$  are the eigenvectors of the strain tensor  $\boldsymbol{\varepsilon}$ . Other decompositions have been proposed as in [7, 100].

Variational approach to damage in tandem with regularization, called in the literature "phase field method", implies the minimization of the total energy with respect to the displacement field **u** and the minimization of the energy with respect to the scalar field *d* describing the crack surface in a smooth manner. The second minimization is subjected to an inequality constraint  $\dot{d} \ge 0$ . To formulate this minimization problem in a simpler setting, a time-stepping  $\mathcal{T} = \{t^0, t^1, ..., t^n, t^{n+1}, ..., t^N\}$  can be introduced. At each time step  $t^{n+1}$ , the problem is to find the displacement fields  $\mathbf{u}^{n+1}$  and  $d^{n+1}$  such that

$$\mathbf{u}^{n+1}, d^{n+1} = \underset{\substack{\mathbf{u} \in \mathcal{K}_A\\ 0 < d^n < d^{n+1} < 1}}{\operatorname{Argmin}} E$$
(2.6)

where  $\mathcal{K}_A$  is a set of kinematically admissible fields. One possible algorithm to solve this problem is to use sequential solving of both minimization problems as

$$D_{\delta \mathbf{u}}E = 0, \tag{2.7}$$

$$D_{\delta d}E = 0, \quad 0 \le d^n \le d^{n+1},$$
(2.8)

where  $D_{\delta} \mathbf{v} f(\mathbf{u})$  is the Gateaux derivative, defined as:

$$D_{\delta \mathbf{v}} f(\mathbf{u}) = \left\{ \frac{f}{d\alpha} \left( f \left( \mathbf{u} + \alpha \ \delta \mathbf{v} \right) \right) \right\}_{\alpha = 0}.$$
 (2.9)

The first equation (2.7) defines the mechanical problem while the second one (2.8) defines the phase field problem. These two problems are coupled as both involve the fields  $\mathbf{u}$  and d.

# 2.2.1 Mechanical problem

Eq. (2.7) can be developed according to:

$$\int_{\Omega} \frac{\partial \Psi}{\partial \boldsymbol{\varepsilon}}(\boldsymbol{\varepsilon}, d) : \boldsymbol{\varepsilon}(\delta \mathbf{u}) d\Omega - \int_{\partial \Omega_F} \mathbf{F}^* \cdot \delta \mathbf{u} d\Gamma = 0, \qquad (2.10)$$

where

$$\frac{\partial \Psi}{\partial \boldsymbol{\varepsilon}}(\boldsymbol{\varepsilon}, d) = \boldsymbol{\sigma}.$$
(2.11)

For the choice

$$g(d) = \left( (1-d)^2 + k \right), \tag{2.12}$$

where k is a small scalar parameter introduced to avoid ill-conditioning when elements are fully damaged, and with  $\Psi$  defined as in (2.3) we obtain:

$$\boldsymbol{\sigma} = \left( (1-d)^2 + k \right) \left\{ \lambda \left\langle Tr\boldsymbol{\varepsilon} \right\rangle_+ \mathbf{1} + 2\mu\boldsymbol{\varepsilon}^+ \right\} + \lambda \left\langle Tr\boldsymbol{\varepsilon} \right\rangle_- \mathbf{1} + 2\mu\boldsymbol{\varepsilon}^-.$$
(2.13)

It yields the classical weak form of the mechanical problem as:

$$\int_{\Omega} \boldsymbol{\sigma} : \boldsymbol{\varepsilon}(\delta \mathbf{u}) \ d\Omega = \int_{\partial \Omega_F} \mathbf{F}^* \cdot \delta \mathbf{u} \ d\Gamma \ \forall \delta \mathbf{u} \in H_0^1(\Omega).$$
(2.14)

The Euler-Lagrange equation (strong form) associated with Eq. (2.14) is given by:

$$\nabla \cdot \boldsymbol{\sigma} = 0, \quad \boldsymbol{\sigma} \mathbf{n} = \mathbf{F}^* \text{ over } \partial \Omega_F, \quad \mathbf{u} = \mathbf{u}^* \text{ over } \partial \Omega_u.$$
 (2.15)

## 2.2.2 Phase field problem

The first equation in (2.8) can be developed as:

$$\int_{\Omega} \frac{\partial \Psi}{\partial d} \delta d \ d\Omega + g_c \int_{\Omega} D_{\delta d} \gamma(d) \Omega = 0.$$
(2.16)

Choosing  $\gamma$  as (1.19) we obtain:

$$\int_{\Omega} \left\{ \frac{\partial \Psi}{\partial d} \delta d + \frac{g_c}{\ell} \left( d\delta d + \ell^2 \nabla d \cdot \nabla(\delta d) \right) \right\} d\Omega = 0, \qquad (2.17)$$

or

$$\int_{\Omega} \left\{ \left( \frac{\partial \Psi}{\partial d} + \frac{g_c}{\ell} d \right) \delta d + \ell g_c \nabla d \cdot \nabla(\delta d) \right\} d\Omega = 0$$
(2.18)

$$= \int_{\Omega} \left\{ \left( g'(d) \left[ \Psi^+ \right] + \frac{g_c}{\ell} d \right) \delta d + \ell g_c \nabla d \cdot \nabla(\delta d) \right\} d\Omega.$$
(2.19)

Choosing  $g(d) = (1 - d)^2$ , we obtain:

$$\int_{\Omega} \left\{ \left( -2(1-d) \left[ \Psi^+ \right] + \frac{g_c}{\ell} d \right) \delta d + g_c \ell \nabla d \cdot \nabla(\delta d) \right\} d\Omega = 0, \qquad (2.20)$$

or

$$\int_{\Omega} \left( 2 \left[ \Psi^+ \right] + \frac{g_c}{\ell} \right) d\delta d + g_c \ell \nabla d \cdot \nabla (\delta d) d\Omega = \int_{\Omega} 2 \left[ \Psi^+ \right] \delta dd\Omega.$$
(2.21)

Using the equality

$$\nabla d \cdot (\delta d) = \nabla \cdot (\delta d \nabla d) - \Delta d \,\,\delta d, \qquad (2.22)$$

we obtain

$$\int_{\Omega} g_c \ell \nabla d \cdot \nabla (\delta d) d\Omega = \int_{\Omega} g_c \ell \nabla \cdot (\delta d \nabla d) - g_c \ell \Delta d \,\,\delta dd\Omega \tag{2.23}$$

and using the divergence theorem:

$$\int_{\Omega} g_c \ell \nabla d \cdot \nabla(\delta d) d\Omega = \int_{\partial \Omega} g_c \ell \delta d\nabla d \cdot \mathbf{n} d\Gamma - \int_{\Omega} g_c \ell \Delta d \, \delta dd\Omega.$$
(2.24)

Then, the associated Euler-Lagrange equations to (2.29) are given by:

$$\left(2\left[\Psi^{+}\right] + \frac{g_{c}}{\ell}\right)d - \ell g_{c}\Delta d = 2\left[\Psi^{+}\right],\tag{2.25}$$

$$\nabla d \cdot \mathbf{n} = 0 \text{ over } \partial \Omega, \quad d = 1 \text{ over } \Gamma,$$
 (2.26)

where  $\Delta d$  denotes the Laplacian operator. Enforcing the irreversibility condition can be prescribed in several ways (see e.g. [31, 125], by enforcing the Dirichlet condition d = 1 at the nodes where the phase field has reached a value of d = 1 or by enforcing numerically  $d^n \leq d^{n+1}$ numerically at each node in the iterative algorithm. Alternatively, the formulation of Miehe [125] introduces a history function  $\mathcal{H}$  which substitutes  $\Psi^+$  to handle loading and unloading and defined as:

$$\mathcal{H}(\mathbf{x},t) = \max_{\tau \in [0,t]} \left\{ \Psi^+(\mathbf{x},\tau) \right\}.$$
(2.27)

It leads to:

$$\left(2\mathcal{H} + \frac{g_c}{\ell}\right)d - \ell g_c \Delta d = 2\mathcal{H}, \quad \nabla d \cdot \mathbf{n} = 0 \text{ on } \partial \Omega_G, \quad d = 1 \text{ on } \Gamma,$$
(2.28)

and to the corresponding weak form:

$$\int_{\Omega} \left( 2 \left[ \Psi^+ \right] + \frac{g_c}{\ell} \right) d\delta d + g_c \ell \nabla d \cdot \nabla (\delta d) d\Omega = \int_{\Omega} 2 \left[ \Psi^+ \right] \delta dd\Omega.$$
(2.29)

Nguyen et al. have shown in [143] that the problem (2.25) can be obtained from thermodynamics considerations, by applying the maximum dissipation principle to the free energy form identified from Eq. (2.2).

Assuming isothermal process, the Clausius-Duhem inequality states that:

$$\phi = \boldsymbol{\sigma} : \dot{\boldsymbol{\varepsilon}} - \dot{W} \ge 0 \tag{2.30}$$

where W is the free energy,  $\sigma$  is the Cauchy stress and  $\phi$  is the dissipation. We can re-write (2.30) as:

$$\boldsymbol{\sigma}: \dot{\boldsymbol{\varepsilon}} - \frac{\partial W}{\partial \boldsymbol{\varepsilon}}: \dot{\boldsymbol{\varepsilon}} - \frac{\partial W}{\partial d} \dot{\boldsymbol{d}} = \left(\boldsymbol{\sigma} - \frac{\partial W}{\partial \boldsymbol{\varepsilon}}\right): \dot{\boldsymbol{\varepsilon}} - \frac{\partial W}{\partial d} \dot{\boldsymbol{d}} \ge 0.$$
(2.31)

It follows that if no damage occurs, i.e. for  $\dot{d} = 0$ , then  $\phi = 0$  and

$$\sigma = \frac{\partial W}{\partial \varepsilon}.\tag{2.32}$$

A reduced form of the Clausius-Duhem inequality can be re-written as:

$$\mathcal{A}d \ge 0 \tag{2.33}$$

where  $\mathcal{A} = -\frac{\partial W}{\partial d}$  is the thermodynamic force associated with d.

At this stage, a threshold function  $F(\mathcal{A})$  such that no damage occurs is assumed in the form:

$$F\left(\mathcal{A}\right) = \mathcal{A} \le 0. \tag{2.34}$$

Assuming the principle of maximum dissipation then requires the dissipation  $\mathcal{A}d$  to be maximum under the constraint (2.34). Using the method of Lagrange multipliers and the following Lagrangian:

$$\mathcal{L} = -\mathcal{A}\dot{d} + \lambda F(\mathcal{A}) \tag{2.35}$$

yields the Kuhn-Tucker equations:

$$\frac{\partial \mathcal{L}}{\partial \mathcal{A}} = 0, \quad \lambda \ge 0, F \le 0, \lambda F = 0.$$
(2.36)

The first equality in (2.36) gives:

$$\dot{d} = \lambda \frac{\partial F(\mathcal{A})}{\mathcal{A}} = \lambda.$$
 (2.37)

Using the second inequality in (2.36), we obtain  $\dot{d} \ge 0$ . Identifying the free energy in (2.2) as  $W = \Psi + g_c \gamma(d, \nabla d)$ , we obtain, for  $\dot{d} > 0$ , F = 0:

$$F = -\frac{\partial W}{\partial d} = -\frac{\partial \Psi(\mathbf{u}, d)}{\partial d} - g_c \delta \gamma(d) = 0, \qquad (2.38)$$

where

$$\delta\gamma(d) = \frac{d}{l} - l\Delta d, \qquad (2.39)$$

which matches Eq. (2.25) for  $\Psi$  and g(d) choosen as (2.3) and (2.12), respectively.

#### 2.2.3 Numerical Implementation

In this thesis work, the different problems are solved numerically with finite elements. First, a mesh of elements in constructed over the domain  $\Omega$ . Let [d] denoting the vector which contains the nodal values of the field d and [ $\delta$ d] the vector containing the nodal values of the test function  $\delta d$ . Then we have in each element:

$$d(\mathbf{x}) = [\mathbf{N}_d(\mathbf{x})] [\mathbf{d}], \quad \delta d(\mathbf{x}) = [\mathbf{N}_d(\mathbf{x})] [\delta \mathbf{d}], \qquad (2.40)$$

$$\nabla d(\mathbf{x}) = [\mathbf{B}_d(\mathbf{x})] [\mathbf{d}], \quad \nabla \delta d(\mathbf{x}) = [\mathbf{B}_d(\mathbf{x})] [\delta \mathbf{d}], \quad (2.41)$$

where  $\mathbf{N}_d(\mathbf{x})$  and  $\mathbf{B}_d(\mathbf{x})$  denote the matrices of shape functions and shape functions derivatives, respectively. Introducing the above discretization in (2.29) gives rise to the following discrete linear system to be solved for the unknown field  $d(\mathbf{x})$  at load increment k + 1:

$$\left[\mathbf{K}_{d}\right]\left[\mathbf{d}\right] = \left[\mathbf{F}\right]_{d},\tag{2.42}$$

where :

$$[\mathbf{K}_{d}] = \int_{\Omega} \{ (2\mathcal{H} + \frac{g_{c}}{\ell}) [\mathbf{N}_{d}]^{T} [\mathbf{N}_{d}] + g_{c}\ell [\mathbf{B}_{d}^{T}] [\mathbf{B}_{d}] \} d\Omega,$$

$$[\mathbf{F}_{d}] = 2 \int_{\Omega} [\mathbf{N}_{d}^{T}] \mathcal{H} d\Omega.$$
(2.43)

In (2.43), the crack driving force  $\mathcal{H}$  is computed according to (2.27).

Similarly, for the mechanical problem, we denote by  $[\mathbf{u}]$  the vector containing the nodal values of the displacement components  $\mathbf{u}$  and  $[\delta \mathbf{u}]$  the vector containing the corresponding nodal values of the test functions  $\delta \mathbf{u}$ . Then, the approximation within elements is defined by:

$$\mathbf{u}(\mathbf{x}) = [\mathbf{N}(\mathbf{x})] [\mathbf{u}]; \delta \mathbf{u}(\mathbf{x}) = [\mathbf{N}(\mathbf{x})] [\delta \mathbf{u}].$$
(2.44)

For a 2D problem, we introduce the vector forms of strain and stress tensors as  $[\boldsymbol{\sigma}] = [\sigma_{11}; \sigma_{22}; \sqrt{2}\sigma_{12};]$  and  $[\boldsymbol{\varepsilon}] = [\varepsilon_{11}; \varepsilon_{22}; \sqrt{2}\varepsilon_{12};]$ . In this context, we have:

$$[\boldsymbol{\varepsilon}] = [\mathbf{B}(\mathbf{x})] [\mathbf{u}]; \quad [\delta \boldsymbol{\varepsilon}] \equiv [\boldsymbol{\varepsilon}(\delta \mathbf{u})] = [\mathbf{B}(\mathbf{x})] [\delta \mathbf{u}], \qquad (2.45)$$

where  $\mathbf{B}(\mathbf{x})$  is the classical matrix of shape functions derivatives. For later use, we introduce the matrix  $[\mathbf{C}_{\lambda}]$  as:

$$\left[\mathbf{C}_{\lambda}\right] = \begin{bmatrix} \lambda & \lambda & 0 \\ \lambda & \lambda & 0 \\ 0 & 0 & 0 \end{bmatrix}.$$
 (2.46)

Furthermore, we adopt the approximation proposed in [143]:

$$\boldsymbol{\varepsilon}_{n+1}^+ \simeq \mathbb{P}_n^+ : \boldsymbol{\varepsilon}_{n+1}, \quad \boldsymbol{\varepsilon}_{n+1}^- \simeq \mathbb{P}_n^- : \boldsymbol{\varepsilon}_{n+1},$$

$$(2.47)$$

and

$$\langle Tr\varepsilon_{n+1}\rangle_{\pm} \simeq \mathcal{R}^{\pm}(\varepsilon_n) \ tr\varepsilon_{n+1},$$
 (2.48)

$$\mathcal{R}^{\pm}(\boldsymbol{\varepsilon}_n) = (sign(\pm tr\boldsymbol{\varepsilon}_n) + 1)/2, \qquad (2.49)$$

which is used to report the nonlinearity associated with the spectral decomposition (2.5) to the previous iteration of the algorithm. In this context,  $[\mathbf{P}^+]$  is the matrix form of the projection tensor  $\mathbb{P}^+$  in (2.47). Introducing the above discretization in (2.29), we obtain the linear system:

$$\mathbf{K}_{u}\left[\mathbf{u}\right]_{n+1} = \left[\mathbf{F}\right]_{n+1},\tag{2.50}$$

$$\mathbf{K}_{u} = \left\{ \left[ \mathbf{K}_{1} \right] \left( \mathbf{d}_{n+1}, \mathbf{u}_{n} \right) + \left[ \mathbf{K}_{2} \right] \left( \mathbf{u}_{n} \right) \right\},$$
(2.51)

where

$$[\mathbf{K}_{1}] (\mathbf{d}, \mathbf{u}_{n}) = (g(d) + k) \int_{\Omega} [\mathbf{B}]^{T} ([\mathbf{C}_{\lambda}] \mathcal{R}^{+} + 2\mu [\mathbf{P}^{+}]) [\mathbf{B}] d\Omega;$$

$$[\mathbf{K}_{2}] (\mathbf{u}_{n}) = \int_{\Omega} [\mathbf{B}]^{T} ([\mathbf{C}_{\lambda}] [\mathcal{R}^{-}] + 2\mu [\mathbf{P}^{-}]) [\mathbf{B}] d\Omega,$$

$$[\mathbf{F}] = \int_{\partial \Omega_{F}} [\mathbf{N}]^{T} [\mathbf{F}^{*}] d\Gamma.$$

$$(2.52)$$

# 2.3 Local two-scale (FE<sup>2</sup>) fracture algorithm

In this section, we describe the straightforward implementation of the  $FE^2$  scheme [60] when the RVE is subjected to damage. The problem to be solved at both scales is given, in the absence of body forces, by:

$$\nabla \cdot \overline{\boldsymbol{\sigma}} \left( d(\mathbf{x}), \overline{\boldsymbol{\varepsilon}} \right) = 0 \quad \text{in} \overline{\Omega}, \tag{2.53}$$

which must be completed by boundary conditions, such as e.g. Dirichlet boundary conditions  $\overline{\mathbf{u}} = \overline{\mathbf{u}}^*$  or Neumann tractions  $\overline{\boldsymbol{\sigma}} \cdot \overline{\mathbf{n}} = \overline{\mathbf{F}}^*$  on the corresponding boundaries  $\partial \overline{\Omega}_u$  and  $\partial \overline{\Omega}_F$ , and

$$\nabla \cdot (\mathbf{C} (d(\mathbf{x})) : \overline{\boldsymbol{\varepsilon}}(\mathbf{x})) = 0 \text{ in } \Omega, \qquad (2.54)$$
$$\left(2\mathcal{H} + \frac{g_c}{\ell}\right) d - \ell G_c \Delta d = 2\mathcal{H} \text{ in } \Omega,$$
$$\nabla d \cdot \mathbf{n} = 0 \text{ on } \partial \Omega_G, \quad d = 1 \text{ on } \Gamma, \qquad (2.55)$$

where  $\overline{\sigma}$  and  $\overline{\varepsilon}$  denote macroscopic stress and strain tensors,  $d(\mathbf{x})$  is the damage at the microscale (defined in the RVE),  $\overline{\Omega}$  is the domain associated with the structure (macro scale),  $\varepsilon(\mathbf{x})$  is the local strain (defined in the RVE), and  $\Omega$  is the domain associated with the RVE. The problems at both scales are coupled by the following relationships (assuming perfect interfaces at the micro scale):

$$\langle \boldsymbol{\varepsilon}(\mathbf{x}) \rangle = \overline{\boldsymbol{\varepsilon}}$$
 (2.56)

$$\langle \boldsymbol{\sigma}(\mathbf{x}) \rangle = \overline{\boldsymbol{\sigma}}$$
 (2.57)

where  $\langle . \rangle$  denotes spatial averaging over the RVE. Condition (2.56) corresponds to boundary conditions to be applied on the boundary of the RVE  $\partial \Omega$ , as (see details e.g. in [203]):

$$\mathbf{u}(\mathbf{x}) = \overline{\boldsymbol{\varepsilon}}\mathbf{x} + \tilde{\mathbf{u}}(\mathbf{x}),\tag{2.58}$$

where  $\tilde{\mathbf{u}}(\mathbf{x})$  is a periodic function over  $\Omega$ . Solving problems (2.53), (2.54) and (2.55) induce two difficulties: (a) they form coupled nonlinear equations and (b) problem (2.54) must be solved at each Gauss point of the macroscopic mesh associated with the structure. The weak form associated with (2.53) is given by:

$$\int_{\overline{\Omega}} \overline{\boldsymbol{\sigma}} \left( \overline{\boldsymbol{\varepsilon}}, d(\mathbf{x}) \right) : \delta \overline{\boldsymbol{\varepsilon}} d\Omega - \int_{\partial \overline{\Omega}_F} \overline{\mathbf{F}}^* \cdot \delta \mathbf{u} d\Gamma = \overline{R} = 0.$$
(2.59)

This problem is nonlinear and can be solved iteratively, e.g. by a Newton method. Firstorder Taylor expansion of (2.59) gives:

$$\overline{R}\left(\overline{\mathbf{u}}^{k+1}\right) = \overline{R}\left(\overline{\mathbf{u}}^{k}\right) + D_{\Delta\overline{\mathbf{u}}}\overline{R}\left(\overline{\mathbf{u}}^{k}\right) = 0, \qquad (2.60)$$

where  $D_{\delta \mathbf{u}}F(\mathbf{u})$  denotes the Gâteaux derivative of F with respect to  $\mathbf{u}$  in the direction  $\delta \mathbf{u}$  and is defined as:

$$D_{\delta \mathbf{u}}F(\mathbf{u}) = \left[\frac{d}{d\alpha}F(\mathbf{u} + \alpha\delta\mathbf{u})\right]_{\alpha=0},$$
(2.61)

where  $\alpha$  is a scalar parameter. We obtain the linearized macro problem as:

$$D_{\Delta \overline{\mathbf{u}}} \overline{R} \left( \overline{\mathbf{u}}^k \right) = -\overline{R} \left( \overline{\mathbf{u}}^k \right)$$
(2.62)

where

$$D_{\Delta \overline{\mathbf{u}}} \overline{R} \left( \overline{\mathbf{u}}^k \right) = \int_{\overline{\Omega}} \frac{\partial \overline{\boldsymbol{\sigma}}}{\partial \overline{\boldsymbol{\varepsilon}}} : \overline{\boldsymbol{\varepsilon}} \left( \Delta \mathbf{u} \right) : \overline{\boldsymbol{\varepsilon}} \left( \delta \mathbf{u} \right) d\Omega,$$
(2.63)

where

$$\frac{\partial \overline{\sigma}}{\partial \overline{\varepsilon}} = \overline{\mathbb{C}}_{tan} \tag{2.64}$$

is identified as the tangent elastic tensor. Introducing a classical FEM discretization  $\overline{\mathbf{u}}(\mathbf{x}) = [\mathbf{N}(\mathbf{x})] [\Delta \overline{\mathbf{u}}]; \ \Delta \overline{\mathbf{u}}(\mathbf{x}) = [\mathbf{N}(\mathbf{x})] [\Delta \overline{\mathbf{u}}]; \ \boldsymbol{\varepsilon}(\Delta \overline{u})(\mathbf{x}) = [\mathbf{B}(\mathbf{x})] [\Delta \overline{\mathbf{u}}]; \ \boldsymbol{\varepsilon}(\delta \overline{\mathbf{u}})(\mathbf{x}) = [\mathbf{B}(\mathbf{x})] [\delta \overline{\mathbf{u}}] \text{ in } (2.62)-(2.63) \text{ leads to the linearized problem:}$ 

$$\left[\overline{\mathbf{K}}_{tan}\right]\left[\Delta\overline{\mathbf{u}}\right] = -\left[\overline{\mathbf{R}}\right],\tag{2.65}$$

where

$$\left[\overline{\mathbf{K}}_{tan}\right] = \int_{\Omega} \left[\mathbf{B}^{T}\right] \left[\overline{\mathbf{C}}_{tan}\right] \left[\mathbf{B}\right] d\Omega, \qquad (2.66)$$

$$\left[\overline{\mathbf{R}}\right] = \int_{\Omega} \left[\mathbf{B}^{T}\right] \left[\overline{\boldsymbol{\sigma}}^{k}\right] d\Omega, \qquad (2.67)$$

where  $[\overline{\sigma}^k]$  is the vector containing the components of the macroscopic stress in each Gauss point, known at iteration k, and  $[\overline{\mathbf{C}}_{tan}]$  is the matrix form associated with  $\overline{\mathbb{C}}_{tan}$ . The operator  $[\overline{\mathbf{C}}_{tan}]$  must be evaluated by perturbation.



Figure 2.5: a) Gauss distribution with l = 0.2 see (1.10) and b) Shape bell distribution with R = 0.2 (1.11)

# 2.4 A non local two-scale (FE<sup>2</sup>) fracture algorithm

In this section, we describe a non-local two-scale model based on the damage of an RVE which may fully induce the anisotropic behavior at the macroscopic scale, while maintaining the convergence and mesh-independence at the macro scale. The main aim of this proposed algorithm is to avoid convolution approaches (see section 2.4.1.1) and  $C^1$  FEM approximations induced by the strain gradient approaches.

#### 2.4.1 Macro regularization

In this section, we first review classical numerical treatments for regularization of the strain field, which can substitute the local strain to remove mesh-dependency issues in damage problems. The different types of regularization techniques are illustrated in a cracked plate problem in Fig. 2.7.

#### 2.4.1.1 Convolution regularization

The convolution regularization was introduced in Pijaudier-Cabot and Bažant in [158]. In this approach, the local strain field is replaced by a regularized one defined by a Gauss-filter approximation in the form:

$$\tilde{\varepsilon}_{ij}(x) = \int_{\tilde{\Omega}} g(s)\overline{\varepsilon}_{ij}(x+s)d\Omega, \qquad (2.68)$$

where  $\tilde{\Omega}$  is usually a circular domain around x and g(s) is a kernel weighting function satisfying  $\int_{\tilde{\Omega}} g(s) d\Omega = 1$ . Two popular choices for g(s) include Gauss distribution and bell-shaped function (see an illustration in Fig. 2.5).

#### 2.4.1.2 Strain gradient approach: Isotropic Regularization (IR)

Convolution regularization is well-known to induce spurious effects such as wrong prediction of crack initiation [173]. Alternatively, the strain gradient regularization [155] replaces the local strain field by a regularized one satisfying:

$$\tilde{\varepsilon}_{ij} - c\ell^2 \nabla^2 \tilde{\varepsilon}_{ij} = \overline{\varepsilon}_{ij}.$$
(2.69)

The parameter c is usually chosen as c = 1/2, where  $\ell$  is an internal length of the material.

#### 2.4.1.3 Strain gradient approach: Anisotropic Regularization (AR)

The classical integral and differential non-local models use a constant gradient parameter c which leads to spurious damage growth since the energy is allowed to be transferred from the fracture zone to its vicinity [65]. Beside this, other drawbacks, such as wrong prediction of damage initiation [173] and spurious distribution of damage in shear-bands [137], have motivated the development of anisotropic nonlocal models. The general idea is using a weighted regularization, which can include "over-nonlocal" formulation [159], stress-based nonlocal models [69], or evolving length scale [135] among others. In [181], the anisotropic regularization (AR) was proposed using a stress-based evolving matrix  $\mathbf{c}(\sigma_{1,2})$  to replace c in (1.15), rewritten as:

$$\tilde{\varepsilon}_{eq} - \ell^2 \nabla .(\mathbf{c} \nabla) \tilde{\varepsilon}_{eq} = \overline{\varepsilon}_{eq}.$$
(2.70)

$$\mathbf{c} = \begin{bmatrix} c_1 & 0\\ 0 & c_2 \end{bmatrix}, \tag{2.71}$$

where

$$c_{1,2} = \frac{\hat{\sigma}_{1,2}}{2f_t} \tag{2.72}$$

are anisotropic gradient coefficients depending on principal stresses  $\hat{\sigma}_{1,2}$  and the tensile strength  $f_t$ . To remove spurious oscillations of the damage field, especially when using low order finite elements, the equation (2.72) was modified in [137] according to:

$$c_{1,2} = \left(\frac{\kappa_0}{max(\kappa, \varepsilon_{eq})}\right)^2 \frac{\overline{\sigma}_{1,2}}{2f_t^2},\tag{2.73}$$

where  $\kappa_0$  is the damage threshold which can be calibrated from the tensile strength and the Young's modulus  $\kappa_0 = f_t/E$ ,  $\varepsilon_{eq}$  is the equivalent strain,  $\overline{\sigma}_{1,2}$  are non-local stress using the convolution regularisation which was called smooth stress by the author.

The anisotropic regularization parameters in (2.72)-(2.73) requires the knowledge of the tensile strength  $f_t$  which is assumed to be unknown at macroscale in this work. We propose

here a simple stress-based anisotropic regularization model which requires only the stress field and the history stress at the material point, as:

$$c_{1,2} = \frac{\hat{\sigma}_{1,2}^2}{2s},\tag{2.74}$$

where

$$s = \max_{\tau \in [0,t]} (\hat{\sigma}_1^2 + \hat{\sigma}_2^2).$$
(2.75)

In 2D problem,  $\hat{\sigma}_{1,2} = \frac{\tilde{\sigma}_{11} + \tilde{\sigma}_{22}}{2} \pm \sqrt{\left(\frac{\tilde{\sigma}_{11} - \tilde{\sigma}_{22}}{2}\right)^2 + \tilde{\sigma}_{12}^2}$ , the computation of *s* avoids singularity when full damage occurs in one element. The regularisation formula is now reformulated as:

$$\tilde{\varepsilon}_{ij} - \ell^2 \nabla . (\mathbf{c} \nabla) \tilde{\varepsilon}_{ij} = \overline{\varepsilon}_{ij}.$$
(2.76)

Note that the gradient term is estimated in the coordinate of principle stress.

#### 2.4.1.4 A two-scale nonlocal staggered scheme based on strain gradient

In what follows, we adopt the strain gradient approach and show the link with phase field regularization process at the macroscopic scale. The macro energy of the structure is expressed by:

$$\overline{E} = \int_{\overline{\Omega}} \overline{\boldsymbol{\sigma}} \left( \overline{\boldsymbol{\varepsilon}}, d(\mathbf{x}) \right) : \overline{\boldsymbol{\varepsilon}} d\Omega - \int_{\partial \overline{\Omega}_F} \overline{\mathbf{F}}^* \cdot \overline{\mathbf{u}} d\Gamma.$$
(2.77)

We recall the definition of the regularized strain  $\tilde{\varepsilon}$  satisfying:

$$\overline{\boldsymbol{\varepsilon}} = \tilde{\boldsymbol{\varepsilon}} - c \overline{\ell}^2 \Delta \tilde{\boldsymbol{\varepsilon}} \tag{2.78}$$

where  $\overline{\ell}$  is here the regularization length at the macro scale (see a discussion on the choice of  $\overline{\ell}$  in section 2.5), and  $\Delta \tilde{\varepsilon}$  denotes Laplacian of each component of  $\overline{\varepsilon}$ , i.e. in indicial notation:

$$\overline{\varepsilon}_{ij} = \tilde{\varepsilon}_{ij} - c\overline{\ell}^2 \frac{\partial^2 \tilde{\varepsilon}_{ij}}{\partial x_k^2}.$$
(2.79)

The macroscopic equilibrium equation:

$$\nabla \cdot \left(\overline{\mathbb{C}} : \overline{\varepsilon}\right) = 0 \quad \text{in } \overline{\Omega} \tag{2.80}$$

then becomes:

$$\nabla \cdot \left(\overline{\mathbb{C}} : \left[\tilde{\varepsilon} - c\overline{\ell}^2 \Delta \tilde{\varepsilon}\right]\right) = 0 \quad \text{in } \overline{\Omega}.$$
(2.81)

We can show in what follows that such form is equivalent to adding a regularization term in the macro energy in the form

$$\overline{E} = \int_{\overline{\Omega}} \overline{\boldsymbol{\sigma}} \left( \overline{\boldsymbol{\varepsilon}}, d(\mathbf{x}) \right) : \overline{\boldsymbol{\varepsilon}} d\Omega + c_2 \overline{\ell}^2 \nabla \overline{\boldsymbol{\varepsilon}} \stackrel{\cdot}{:} \nabla \overline{\boldsymbol{\varepsilon}} - \int_{\partial \overline{\Omega}_F} \overline{\mathbf{F}}^* \cdot \overline{\mathbf{u}} d\Gamma$$
(2.82)

where

$$\nabla \overline{\varepsilon}_{ijk} = \frac{\partial \overline{\varepsilon}_{ij}}{\partial x_k} \tag{2.83}$$

denotes the strain gradient and  $\nabla \overline{\varepsilon}$ :  $\nabla \overline{\varepsilon} = \nabla \overline{\varepsilon}_{ijk} \nabla \overline{\varepsilon}_{ijk}$  denotes triple contraction of indices. Adding the regularization term  $c_2 \overline{\ell}^2 \nabla \overline{\varepsilon}$ :  $\nabla \overline{\varepsilon}$  in (2.82) penalizes large strain gradients and then avoids localization in an infinitely narrow band of elements with the refinement of the mesh. Starting from (2.81), we obtain:

$$\nabla \cdot \left(\overline{\mathbb{C}} : \tilde{\varepsilon}\right) - \nabla \cdot \left(\overline{\mathbb{C}} : c\overline{\ell}^2 \Delta \tilde{\varepsilon}\right) = \nabla \cdot \left(\overline{\mathbb{C}} : \tilde{\varepsilon}\right) - \nabla \cdot \left(\overline{\mathbb{C}} : c\overline{\ell}^2 \nabla \cdot \nabla \tilde{\varepsilon}\right) = 0.$$
(2.84)

Since the right-hand term is introduced only for regularization purpose, it can be substituted by the following simplified formula:

$$\nabla \cdot \left(\overline{\mathbb{C}} : \tilde{\epsilon}\right) - \nabla \cdot \left(c_2 \bar{\ell}^2 \nabla \cdot \nabla \tilde{\epsilon}\right) = 0, \qquad (2.85)$$

where  $c_2$  is a scalar constant. Setting  $\overline{\sigma} = \overline{\mathbb{C}} : \tilde{\varepsilon}$ , multiplying (2.85) by a test function  $\delta \mathbf{u}$  and integrating over  $\overline{\Omega}$  we obtain:

$$\int_{\overline{\Omega}} \nabla \cdot \overline{\boldsymbol{\sigma}} \cdot \delta \overline{\mathbf{u}} d\Omega - \int_{\overline{\Omega}} \left( \nabla \cdot \left( c_2 \overline{\ell}^2 \nabla \cdot \nabla \tilde{\boldsymbol{\varepsilon}} \right) \right) \cdot \delta \overline{\mathbf{u}} d\Omega = 0.$$
(2.86)

For later use, we introduce the following properties. For  $\mathbf{b}$  a real-valued vector field and  $\mathbf{A}$  a second-order tensor field, it can be shown that:

$$\nabla \cdot (\mathbf{A}\mathbf{b}) = (\nabla \cdot \mathbf{A}) \cdot \mathbf{b} + \mathbf{A} : \nabla \mathbf{b},$$

or in indicial notations:

$$\frac{\partial}{\partial x_i} \left( A_{ij} b_j \right) = \frac{\partial A_{ij}}{\partial x_i} b_j + A_{ij} \frac{\partial b_j}{\partial x_i}.$$
(2.87)

Let  $\mathcal{A}$  a third-order tensor and  $\mathbf{B}$  a second-order tensor, then:

$$\nabla \cdot (\mathcal{A} : \mathbf{B}) = (\nabla \cdot \mathcal{A}) : \mathbf{B} + \mathcal{A} : \nabla \mathbf{B},$$

or

$$\frac{\partial}{\partial x_i} \left( A_{ijk} B_{jk} \right) = \frac{\partial A_{ijk}}{\partial x_i} B_{jk} + A_{ijk} \frac{\partial B_{jk}}{\partial x_i}.$$
(2.88)

We then introduce the following relations obtained from the divergence theorem:

$$\int_{\Omega} \nabla \cdot (\mathbf{A}\mathbf{b}) \, d\Omega = \int_{\partial \Omega} \mathbf{n} \cdot \mathbf{A}\mathbf{b} d\Gamma, \qquad (2.89)$$

and

$$\int_{\Omega} \nabla \cdot (\mathcal{A} : \mathbf{B}) \, d\Omega = \int_{\partial \Omega} \mathbf{n} \cdot \mathcal{A} : \mathbf{B} d\Gamma.$$
(2.90)

Using property (2.87), we obtain:

$$\int_{\overline{\Omega}} \nabla \cdot (\overline{\boldsymbol{\sigma}} \delta \overline{\mathbf{u}}) \, d\Omega - \int_{\overline{\Omega}} \overline{\boldsymbol{\sigma}} : \overline{\boldsymbol{\varepsilon}} (\delta \overline{\mathbf{u}}) d\Omega$$
$$- \int_{\overline{\Omega}} \nabla \cdot \left( \left( c_2 \overline{\ell}^2 \nabla \cdot \nabla \widetilde{\boldsymbol{\varepsilon}} \right) \delta \overline{\mathbf{u}} \right) d\Omega + \int_{\overline{\Omega}} \left( c_2 \overline{\ell}^2 \nabla \cdot \nabla \widetilde{\boldsymbol{\varepsilon}} \right) : \overline{\boldsymbol{\varepsilon}} (\delta \overline{\mathbf{u}}) d\Omega = 0$$

Using (2.89):

$$\int_{\overline{\Omega}} \overline{\boldsymbol{\sigma}} : \overline{\boldsymbol{\varepsilon}}(\delta \overline{\mathbf{u}}) d\Omega - \int_{\overline{\Omega}} \left( c_2 \overline{\ell}^2 \nabla \nabla \widetilde{\boldsymbol{\varepsilon}} \right) : \overline{\boldsymbol{\varepsilon}}(\delta \overline{\mathbf{u}}) d\Omega = \int_{\partial \overline{\Omega}} \overline{\boldsymbol{\sigma}} \overline{\mathbf{n}} - \left( c_2 \overline{\ell}^2 \nabla \cdot \nabla \widetilde{\boldsymbol{\varepsilon}} \right) \overline{\mathbf{n}} \cdot \delta \overline{\mathbf{u}} d\Gamma.$$
(2.91)

Using Neumann boundary condition  $\overline{\sigma \mathbf{n}}$  and assuming  $\nabla \tilde{\boldsymbol{\varepsilon}} \cdot \overline{\mathbf{n}} = 0$ , we obtain:

$$\int_{\overline{\Omega}} \overline{\boldsymbol{\sigma}} : \overline{\boldsymbol{\varepsilon}}(\delta \overline{\mathbf{u}}) d\Omega - \int_{\overline{\Omega}} \left( c_2 \overline{\ell}^2 \nabla \cdot \nabla \widetilde{\boldsymbol{\varepsilon}} \right) : \overline{\boldsymbol{\varepsilon}}(\delta \overline{\mathbf{u}}) d\Omega = \int_{\partial \overline{\Omega}_F} \overline{\mathbf{F}}^* \cdot \delta \overline{\mathbf{u}} d\Gamma.$$
(2.92)

Using (2.88), we have:

$$(\nabla \cdot \nabla \tilde{\varepsilon}) : \varepsilon(\delta \overline{\mathbf{u}}) = \nabla \cdot (\nabla \tilde{\varepsilon} : \varepsilon(\delta \overline{\mathbf{u}})) - \nabla \tilde{\varepsilon} : \nabla \varepsilon(\delta \overline{\mathbf{u}}).$$
(2.93)

Then using (2.90):

$$-\int_{\overline{\Omega}} (\nabla \nabla \tilde{\boldsymbol{\varepsilon}}) : \boldsymbol{\varepsilon}(\delta \overline{\mathbf{u}}) d\Omega = \int_{\overline{\Omega}} \nabla \tilde{\boldsymbol{\varepsilon}} : \nabla \boldsymbol{\varepsilon}(\delta \overline{\mathbf{u}}) d\Omega - \int_{\overline{\Omega}} \nabla \cdot (\nabla \tilde{\boldsymbol{\varepsilon}} : \overline{\boldsymbol{\varepsilon}}(\delta \overline{\mathbf{u}})) d\Omega$$
$$= \int_{\overline{\Omega}} \nabla \tilde{\boldsymbol{\varepsilon}} : \nabla \boldsymbol{\varepsilon}(\delta \overline{\mathbf{u}}) d\Omega - \int_{\partial \overline{\Omega}} \nabla \tilde{\boldsymbol{\varepsilon}} \cdot \overline{\mathbf{n}} : \overline{\boldsymbol{\varepsilon}}(\delta \overline{\mathbf{u}}) d\Gamma.$$
(2.94)

By assuming the boundary condition  $\nabla \tilde{\boldsymbol{\varepsilon}} \cdot \mathbf{\overline{n}} = 0$  on  $\partial \Omega$ , we finally obtain

$$\int_{\overline{\Omega}} \overline{\boldsymbol{\sigma}} \left( \overline{\boldsymbol{\varepsilon}}, d(\mathbf{x}) \right) : \delta \overline{\boldsymbol{\varepsilon}} d\Omega + c_2 \overline{\ell}^2 \nabla \overline{\boldsymbol{\varepsilon}} \stackrel{\cdot}{:} \nabla \left( \overline{\delta \boldsymbol{\varepsilon}} \right) = \int_{\partial \overline{\Omega}_F} \overline{\mathbf{F}}^* \cdot \overline{\mathbf{u}} d\Gamma.$$
(2.95)

which corresponds to the weak form obtained by minimizing the energy with respect to the displacement field, or more specifically by evaluating

$$D_{\delta \mathbf{u}}\overline{E} = 0 \tag{2.96}$$

with  $\overline{E}$  given in the form (2.82).

#### 2.4.2 Staggered solving procedure

We summarize the equations to be solved at the macros scale:

$$\nabla \cdot \left(\overline{\mathbb{C}} : \overline{\varepsilon}\right) = 0 \quad \text{in } \overline{\Omega},\tag{2.97}$$

$$\tilde{\varepsilon} - c \bar{\ell}^2 \Delta \tilde{\varepsilon} = \bar{\varepsilon} \quad \text{in } \overline{\Omega}.$$
 (2.98)

We propose here a staggered solving procedure involving the following steps:

- 1. Assuming known  $\overline{\mathbb{C}}$ , solve (2.97) to obtain the strain field  $\overline{\varepsilon}$  (macro problem);
- 2. Given  $\overline{\varepsilon}$ , solve (2.98) to obtain the strain field  $\tilde{\varepsilon}$  (macro problem);
- 3. Given  $\tilde{\boldsymbol{\varepsilon}}$ , solve the RVE problem at each Gauss point, involving solving the local coupled displacement/phase field problems, given the local damage field from previous load steps to update the damage field  $d(\mathbf{x})$  and to evaluate the effective elastic tensor  $\overline{\mathbb{C}}(d(\mathbf{x}))$ .

These different steps are described in the following.

#### 2.4.2.1 Computation of the regularized strain field

Given  $\overline{\epsilon}$ , we propose to solve (2.98) by solving an independent global problem on each component of  $\tilde{\epsilon}$ . The detailed FEM procedure is described below.

Multiplying (2.69) by a test function  $\delta \tilde{\varepsilon}_{ij}$  and integrating over  $\Omega$ , we have:

$$\int_{\Omega} \delta \tilde{\varepsilon}_{ij} \tilde{\varepsilon}_{ij} d\Omega - \int_{\Omega} \delta \tilde{\varepsilon}_{ij} c \ell^2 \nabla^2 \tilde{\varepsilon}_{ij} d\Omega = \int_{\Omega} \delta \tilde{\varepsilon}_{ij} \overline{\varepsilon}_{ij} d\Omega.$$
(2.99)

Using (2.87), we have:

$$\nabla(\delta\tilde{\varepsilon}_{ij}(c\ell^2\nabla)\tilde{\varepsilon}_{ij}) = \nabla.\delta\tilde{\varepsilon}_{ij}(c\ell^2\nabla)\tilde{\varepsilon}_{ij} + \delta\tilde{\varepsilon}_{ij}\nabla(c\ell^2\nabla)\tilde{\varepsilon}_{ij}, \qquad (2.100)$$

or

$$\int_{\Omega} \delta \tilde{\varepsilon}_{ij} \nabla . (c\ell^2 \nabla) \tilde{\varepsilon}_{ij} d\Omega = \int_{\Omega} \nabla (\delta \tilde{\varepsilon}_{ij} (c\ell^2 \nabla) \tilde{\varepsilon}_{ij}) d\Omega - \delta \tilde{\varepsilon}_{ij} \nabla (c\ell^2 \nabla) \tilde{\varepsilon}_{ij} d\Omega.$$
(2.101)

Then using (2.89) we have:

$$\int_{\Omega} \nabla (\delta \tilde{\varepsilon}_{ij} (c\ell^2 \nabla) \bar{\varepsilon}_{ij}) d\Omega = \int_{\partial \Omega} \delta \tilde{\varepsilon}_{ij} (c\ell^2 \nabla) \tilde{\varepsilon}_{ij} \mathbf{n} d\Gamma.$$
(2.102)

From the assumption  $\nabla \tilde{\varepsilon}_{ij} \mathbf{n} = 0$ , the weak form in (2.99) can now be rewritten as:

$$\int_{\Omega} \tilde{\varepsilon}_{ij} \delta \tilde{\varepsilon}_{ij} d\Omega + \int_{\Omega} c \ell^2 \nabla \left( \tilde{\varepsilon}_{ij} \right) \nabla \left( \delta \tilde{\varepsilon}_{ij} \right) d\Omega = \int_{\Omega} \overline{\varepsilon}_{ij} \delta \tilde{\varepsilon}_{ij} d\Omega.$$
(2.103)

This problem must be solved for each component of  $\overline{\varepsilon}_{ij}$ . Then in 2D, 3 problems must be solved to obtain  $\tilde{\varepsilon}$ . Let  $[\hat{\varepsilon}_{ij}]$  denotes as a vector of numerical values of  $\tilde{\varepsilon}$ , using linear finite element shape functions, the nonlocal equivalent strain is expressed in each element as:

$$[\tilde{\varepsilon}_{ij}] = [\mathbf{N}] (\mathbf{x}) [\hat{\varepsilon}_{ij}]; [\nabla \tilde{\varepsilon}_{ij}] = [\mathbf{B}] (\mathbf{x}) [\hat{\varepsilon}_{ij}].$$
(2.104)

Introducing (2.104) in (2.103) leads to

$$[\delta\hat{\varepsilon}_{ij}]^T \int_{\Omega} [\mathbf{N}]^T [\mathbf{N}] d\Omega [\hat{\varepsilon}_{ij}] + [\delta\hat{\varepsilon}_{ij}]^T c\ell^2 \int_{\Omega} [\mathbf{B}]^T [\mathbf{B}] d\Omega [\hat{\varepsilon}_{ij}] = [\delta\hat{\varepsilon}_{ij}]^T \int_{\Omega} [\mathbf{N}]^T [\boldsymbol{\varepsilon}_{ij}] d\Omega \quad (2.105)$$

and due to the arbitrariness of  $[\delta \hat{\varepsilon}_{ij}]$ , we obtain the linear system:

$$[\mathbf{K}] \left[ \hat{\varepsilon}_{ij} \right] = [\mathbf{F}] \tag{2.106}$$

where

$$[\mathbf{K}] = \int_{\Omega} [\mathbf{N}_e]^T [\mathbf{N}_e] d\Omega + c\ell^2 \int_{\Omega} [\mathbf{B}_e]^T [\mathbf{B}_e] d\Omega$$
(2.107)

and

$$[\mathbf{F}] = \int_{\Omega} \left[ \mathbf{N}_e \right]^T \left[ \overline{\varepsilon_{ij}} \right] d\Omega.$$
(2.108)

Note that solving such problem only requires linear  $(C^0)$  FEM discretization.

Let  $\theta$  denotes as the angle between the macroscopic coordinate (x, y) and the principal stress direction  $(x_1, y_1)$ . In the case of anisotropic regularization, we introduce the rotation matrix  $[\mathbf{R}]$  as:

$$[\mathbf{R}] = \begin{bmatrix} \cos(\theta) & \sin(\theta) \\ -\sin(\theta) & \cos(\theta) \end{bmatrix}.$$
 (2.109)

and the scalar c in (2.107) is then replaced by  $[\tilde{\mathbf{c}}]$ , defined by:

$$[\tilde{\mathbf{c}}] = [\mathbf{R}^T] c[\mathbf{R}]. \tag{2.110}$$

#### 2.4.3 Computation of the effective elastic tensor

Given  $\tilde{\varepsilon}$  at each Gauss point of the macroscopic structure, the boundary conditions (2.58) are prescribed on the boundary of the RVE  $\partial \Omega$ . The local problems (2.54) and (2.55) are then solved to obtain the local strain field  $\varepsilon(\mathbf{x})$  and local damage field  $d(\mathbf{x})$ . Given the new damage field, the effective elastic tensor is computed according to

$$\overline{\mathbb{C}}(d(\mathbf{x})) = \left\langle \mathbb{C}(d(\mathbf{x})) : \mathbb{A}(d(\mathbf{x})) \right\rangle, \qquad (2.111)$$

Figure 2.6: The traction test to clarify the convergence of the regularised strain before a sharp crack tip: at the bottom, displacements are locked in both the direction X, and Y; at the upper, the displacement along X axis equals zero while a prescribed in  $\delta u = 0.01$  is applied in Y axis. The regularised length  $\ell$ = 0.05 mm.



where  $\mathbb{A}(\mathbf{x})$  is the fourth-order localization tensor relating micro and macroscopic strains such that:

$$A_{ijkl}(\mathbf{x}) = \varepsilon_{ij}^{(kl)}(\mathbf{x}). \tag{2.112}$$

where  $\varepsilon_{ij}^{(kl)}(\mathbf{x})$  is the strain solution obtained by solving the elastic problem (2.54) (for a fixed value of  $d(\mathbf{x})$ ) when prescribing a macroscopic strain  $\overline{\boldsymbol{\varepsilon}}$  using the boundary conditions (2.58) with:

$$\overline{\boldsymbol{\varepsilon}} = \frac{1}{2} \left( \mathbf{e}_i \otimes \mathbf{e}_j + \mathbf{e}_j \otimes \mathbf{e}_i \right)$$
(2.113)

where  $\mathbf{e}_i$  (i = 1, 2, 3) are unitary basis vectors.

#### 2.4.3.1 Overall algorithm

The overall algorithm is summarized as follows.



Figure 2.7: Evolution of the component  $\varepsilon_{22}$  strain field with the mesh refinement in four cases:(a)- no regularization treatment ;(b)- convolution regularization with Gauss distribution ; (c) - gradient isotropic regularization (IR);(d) - gradient anisotropic regularization (AR)

```
LOOP at each load increment t^{n+1}

1 Update external tractions \overline{\mathbf{F}}^{n+1}

2 Given \overline{\mathbb{C}}^{k+1} = \overline{\mathbb{C}} (\tilde{\varepsilon}^k, d^k(x));

Solve \nabla (\overline{\mathbb{C}}^k : \bar{\varepsilon}^{k+1}) = 0 with boundary conditions \overline{\mathbf{F}}^{n+1} for \bar{\varepsilon}^{k+1}

3 Given \bar{\varepsilon}^{k+1}

Solve \tilde{\varepsilon}^{k+1} - c\ell^2 \nabla^2 \tilde{\varepsilon}^{k+1} = \bar{\varepsilon}^{k+1} for \tilde{\varepsilon}^{k+1};

4 Given \tilde{\varepsilon}^{k+1}

Loop over all Gauss points (RVEs)

Prescribe boundary conditions u(x) = \tilde{\varepsilon}^{k+1} + \tilde{u}

Solve displacement problem

Solve phase field problem for d^{k+1}(x)

Given d^{k+1}(x) compute \overline{\mathbb{C}}^{k+1} = \langle \mathbb{A}(x) : \overline{\mathbb{C}}(d^{k+1}(x)) \rangle

end loop

5 \overline{\mathbb{C}}^k = \overline{\mathbb{C}}^{k+1}, d^k = d^{k+1}(u)

END
```

Figure 2.8: Algorithm: proposed 2-scale nonlocal staggered damage model.

# 2.5 Numerical examples

In this section, we investigate the proposed algorithm in Fig. 2.8 proposed in section 2.4.

#### 2.5.1 A plate with a sharp crack (test MS1)

In this example, a plate of size  $L \times H = 20 \times 80 \text{ mm}^2$  as shown in Fig. 2.9 a) is studied to investigate the convergence of the proposed scheme w.r.t the mesh size at the macro scale. The geometry and the mesh of the microstructure RVE are shown in Fig. 2.9. The material parameters are shown in Table 2.1 where  $\mu_m$ ,  $\lambda_m$  are Lamé's constants of the matrix,  $g_{cm}$ denotes and the Griffith-type critical energy release rate and  $\ell_m = 0.1$  mm is the regularized length of the microstructure.

At the macro scale, the regularization parameter  $\ell_M$  must be chosen and has a strong influence on the results. In this work, we have chosen this parameter such as it is small as compared to the dimensions of the structure, to induce a mesh size not too fine in the vicinity of the crack path. However, we are aware that a more pertinent procedure should be developed to identify this parameter. One possibility could be to use a simulation on a fully discretized heterogeneous structure (see Chapter 3), which could be used to obtain a reference curve to fit this parameter. For reason of lack of time we report this discussion to future works. In this example, the internal length was chosen as  $\ell_M = 5$  mm which is equals to L/20.



Figure 2.9: a) Geometry of a plate with a sharp crack in the traction test, b) Mesh 1: h = 2 mm (302 elements), c) Mesh 2: h = 1 mm (738 elements), d) Mesh 3: h = 0.5 mm (1430 elements).



Figure 2.10: Three sizes of RVE: a) one unit cell, b) two unit cells, c) four unit cells.

Parameter	Value	Unit
$\lambda_m$	121.15	MPa
$\mu_m$	80.77	MPa
$g_{cm}$	0.0027	$\mathrm{kN}/\mathrm{mm}$
$\ell_m$	0.1	$\mathrm{mm}$

Table 2.1: Material properties of the porous RVE.



Figure 2.11: F-u curves for the plate with sharp crack gradient regularisation (isotropic).



Figure 2.12: Test MS2: geometry of the three-point bending beam.

Traction tests on the plate are conducted by applying incremental prescribed displacements at the upper and bottom ends along the y-direction with a displacement increment  $\Delta u = 0.005$ mm. To investigate the convergence at macroscale, three mesh sizes are taken into consideration: 302 elements, 738 elements, and 1430 elements corresponding to three mesh element sizes h =2 mm, 1 mm, 0.5 mm as shown in Fig. 2.9.

As an illustration, the obtained force-displacement curve is examined for strain gradient regularization approach in Fig. 2.11. To show the convergence with respect to the mesh size, three mesh sizes, described in Fig. 2.9 b)-d) have been investigated. We obtain for the corresponding respective curves critical forces values of 8.2769 kN, 8.1504 kN and 8.0728 kN at u = 0.185 mm which show the convergence.

#### 2.5.2 Three-point bending beam (test MS2)

In this example, a beam with dimensions  $H \times L = 102 \times 408 \text{ mm}^2$  is investigated. The regularization parameter at the macroscale is chosen as  $\ell_M = 5 \text{ mm}$ . Four refined mesh as shown in Fig. 2.13 are employed to show the convergence of the results with respect to the mesh size. The bending test is implemented by prescribing the displacement in the middle of the upper



Figure 2.13: Three refined meshes in the vicinity of the crack path: a) H1 = 5 mm (630 elements), b) H2 = 2.5 mm (1290 elements), c) H3 = 1 mm (2762 elements), d) H4 = 0.5 mm (5080 elements)

edge of the beam with increments  $\Delta u = 0.1$  mm. In this test, both isotropic gradient (IR) regularization and anisotropic gradient regularization (AR) are utilised and compared.

First, we analyze the convergence of the response with respect to the RVE size. Three RVEs are considered, as shown in Figs. 2.10 (a-c). At the macro scale, the coarse mesh in Fig. 2.13 a) is employed. The results are presented in Fig. 2.14, evidencing the convergence with respect to the RVE size and the existence of an RVE here. As there is no noticeable difference between the results, we use the RVE with one unit cell (Fig. 2.10 a) in the next examples when we refer to the porous structure).

Secondly, the convergence of the response with respect to the mesh at the macro scale for both IR and AR regularization processes is analyzed in Fig. 2.15. It can be shown that both IR and AR induce the convergence with respect to the mesh size but the deviation is higher in the AR case.

Next, damage profiles are compared. Fig. 2.16 and Fig. 2.17 show damage profiles plotted at the end of the simulation for IR case and AR case, respectively. Denoting by  $c_{ijkl}^0$  the material matrix components of the RVE in the sound state, we define a macroscopic damage indicator  $\bar{d}$ as:  $\bar{d} = max(1 - \bar{c}_{ijkl}/c_{ijkl}^0)$ . Figs. 2.16 and 2.17 show the convergence of the damage zone with respect to the mesh size for both IR and AR. However, for the same value of internal length by  $\bar{\ell}$ , the bandwidth of damage in the AR case is smaller than in the IR case.

Finally, Fig. 2.18 compares the evolution of damage in both IR and AR cases. It can be seen that at the first stage, the difference between the two damage profiles is small, but the improvement of the spuriousness in the AR case is larger in later stage. The reason is the inherent broadening of damage in the IR case, while in the AR case, the broadening of damage stops when a component of a principal stress reaches zero.



Figure 2.14: F-u curves for 3 different RVE sizes.



Figure 2.15: Comparison of F-u curves with respect to the four mesh sizes H1, H2, H3 and H4 using isotropic gradient regularization: (a) isotropic regularization (IR) and (b) anisotropic regularization (AR).



Figure 2.16: Comparison of damage profiles w.r.t the four mesh sizes H1 (a), H2 (b), H3 (c), H4 (d) (Fig. 2.13) using isotropic gradient regularization IR (plotted at the end of the simulation).



Figure 2.17: Comparison of damage profile w.r.t the four mesh sizes H1 (a), H2 (b), H3 (c), H4 (d) in Fig. 2.13 using anisotropic gradient regularization AR (plotted at the end of the simulation).



Figure 2.18: Left: evolution of damage using isotropic regularization (IR); Right: anisotropic regularization (AR) (the mesh H3 in Fig. 2.13 is employed).



Figure 2.19: L-shaped structure: (a) macrostructure geometry of the L-shape test with dimensions L = H = 500 mm, d = 30 mm; (b) mesh involving 2650 elements,  $h_{min} \approx 3.5 \text{ mm}.$ 

#### 2.5.3 L-shape test

Next, an L-shaped structure is studied. The geometry and discretization are depicted in Fig. 2.19. At y = 0, the displacement is fixed in both direction. The regularized length at macroscale is chosen as  $\ell_M = 5$  mm. A displacement is prescribed in point A in Fig. 2.19 a). The considered microstructure is the porous one (case 1) as in the previous section. Both IR and AR are tested. The damage profiles are plotted in Fig. 2.20 a) and b) at steps  $\Delta u = 3.5$ ; 4.5; 5.5; 6.5 mm which correspond to the points (A1, B1, C1, D1) and (A2, B2, C2, D2) in Fig. 2.21 showing the F-u responses of the isotropic regularization (IR) and stress-based regularization (AR) respectively.

In both cases, the crack starts from the inner corner of the structure and gradually propagates to the left similarly with the trend in the literature. However, the crack is more directed than in the case of a homogeneous isotropic material. The reason is that the considered RVE actually induces a directed damage along the x- direction because of the periodicity of the underlying microstructure.

## 2.5.4 A plate with a hole

The objective of this new series of examples is to show that the present multiscale framework is able to induce an anisotropic damage at the macroscale from the only knowledge of the RVE. For this purpose, two RVEs are investigated:

- Case 1: A porous RVE associated with Fig. 2.10 (a).
- Case 2: A composite laminate RVE with a layers orientation of 45°, as depicted in Fig. 2.22, where the phase 2 (yellow color) is 10 times stiffer than the phase 1 (in blue). The different properties are provided in Table 2.2.



Figure 2.20: Evolution of damage of the L-shaped test using isotropic regularization (first row) and anisotropic regularization (second row).



Figure 2.21: Force-displacement curves for the L-shape test.



Figure 2.22: Composite RVE layers orientation of  $45^{\circ}$ .

Name	$\lambda_{m1}$	$\mu_{m1}$	$g_{cm1}$	$\lambda_{m2}$	$\mu_{m2}$	$g_{cm2}$	$\ell_{m1} = \ell_{m2}$
Values	121.15	80.77	0.0027	242.30	161.54	0.027	0.05
Unit	MPa	MPa	kN/mm	MPa	MPa	kN/mm	mm

 Table 2.2: Material properties of the composite layered RVE.



Figure 2.23: a) Geometry of the macro structure of the test in sec. 2.5.4; b) Macro mesh for the porous microstructure using 1296 elements with refinement is in the damage zone h = 2 mm, c) Macro for the composite layered microstructure with refinement is in the damage zone h = 2 mm.

A plate with dimensions  $H \times L = 200 \times 100 \text{ mm}^2$  with a hole in the center is investigated, as shown in Fig. 2.23 (a). The radius of the hole is 25 mm. The regularized length used at the macroscale is chosen as  $\ell_M = 3$  mm. Fig. 2.23 shows the macroscale geometry (a) and the meshes used for case 1 (b) and case 2 (c). For both cases, the plate is subjected to prescribed displacements on both left and right ends simultaneously with the increment of  $\Delta u = 0.002$ mm while their corresponding displacements along y are fixed. The damage profiles at four load steps are plotted in Fig. 2.24 (a), (b), (c) and (d) at four load increments A, B, C and D in Fig. 2.24 (e). The corresponding damage inside the RVE is depicted in Fig. 2.23.

For case 2, we can observe from Fig. 2.26 a clear induced orientation of the macro crack due to the directed microstructure in the RVE, and showing the potential of the present approach to describe an anisotropic damage behavior from the only knowledge of the microstructure. Damage within the RVE at different stages of the load is shown in Fig 2.26.



Figure 2.24: Damage profiles in case 1 of the plate with a hole (sec. 2.5.4) at the point A ( $\Delta u = 0.202$  mm), B ( $\Delta u = 0.206$  mm), C ( $\Delta u = 0.208$  mm), D ( $\Delta u = 0.214$  mm)in Fig.2.25 are depicted in (a) (b) (c) (d), respectively.



Figure 2.25: The force-displacement curve and damage images of the underlying microstructure at the gauss point (center) of the element M in Fig. 2.23


Figure 2.26: Damage profiles in case 2 of the plate with a hole (sec. 2.5.4) at load steps A (u = 0.1120 mm), B (u = 0.1200 mm), C (u = 0.1400 mm), D (u = 0.1600 mm) in Fig.2.27 are depicted in (a) (b) (c) (d), respectively.



Figure 2.27: Force-displacement curve in case 2 and damage profiles for an RVE at point M in Fig. 2.23.



Figure 2.28: Cracked square plate: a) Geometry at macroscale; b) Mesh 1:  $h \approx 1mm$  (3098 elements); c) Mesh 2:  $h \approx 1mm$  (3393 elements).

#### 2.5.5 Cracked square plate

Again, the aim of this example is to show the capability of the model to capture an anisotropic behavior only induced by the geometry of the RVE. The geometry of the macrostructure is depicted in Fig. 2.28 a) with dimensions  $L \times H = 100 \times 100 \text{ mm}^2$ . The regularised length at the macroscale  $\ell_M = 2 \text{ mm}$ . The loading is performed by prescribing the displacement at the top border an increasing displacement along the y- direction while the displacement along xequals zero. At the bottom, the prescribed displacement along x and y is blocked.

Similarly, as in the previous example, the two RVE with porous and laminated microstructures are considered. Damage profiles are depicted in both corresponding cases in Fig. 2.29 at different load steps, showing the oriented crack induced by the oriented laminate RVE.

The corresponding response curves are provided in Figs. 2.30.

Next, the same structure is considered but a shear load is prescribed. The loading is performed by prescribing an increasing displacement at the top border along the x-direction while the displacement along y equal zeros. At the bottom, the prescribed displacement along x and y is fixed. Again, both RVEs are used. A comparison of the obtained damage profiles for both cases is provided in Figs. 2.31 and 2.32. In both cases, AR and IR are tested.



Figure 2.29: Damage profiles for the cracked square plate in traction for case 1 (porous RVE) at u = 0.63 mm (a1), u = 0.70 mm (b1), u = 0.80 mm (c1), u = 1 mm (d1); and for case 2 (laminated RVE): u = 0.2300 mm u = 0.2390 mm, u = 0.2490 mm, u = 0.2590 mm. The IR has been used.



Figure 2.30: Force-prescribed displacement curves in two case of microstructure



Figure 2.31: Evolution of damage using isotropic regularization (first row) and anisotropic regularization (second row) in the shear test with the porous RVE.



Figure 2.32: Evolution of damage using isotropic regularization (first row) and anisotropic regularization (second row) in the shear test with composite RVE.

The comparison of obtain response curves is provided in Figs. 2.33.

#### 2.5.6 A plate with two semicircular notches

Here, a comparison of the effects of both RVEs is conducted in a more complex configuration. A plate with two asymmetric semicircular notches is considered. The regularized length is chosen as  $\ell_M = 2$  mm. At the bottom, the displacement in both directions is fixed. At the upper,



Figure 2.33: Force-prescribed displacement curves of the square plate in the shear test using isotropic regularization (IR case) and anisotropic regularization (AR case): a) with the porous RVE ; b) with the composite RVE.

the displacements along y are prescribed an increasing  $\Delta u$  whereas those along x equal zeros. Two cases of the microstructure (as the previous example) will be considered: case 1 using the porous microstructure, case 2 using the laminate composite microstructure.

In case 1: the load is applied by increasing the prescribed displacement  $\Delta u = 0.002$  mm. The damage profile at four steps are depicted in Fig. 2.35 (a-d) corresponding two 4 points A (u = 0.2240 mm), B (u = 0.2300 mm), C (u = 0.2400 mm), D (u = 0.2500 mm) of the F-u curve in Fig. 2.37a. The damage band first goes straight and then tends to change direction at later steps.

In case 2: prescribing  $\Delta u = 0.005$  mm, the damage profile at four steps are depicted in Fig. 2.35(a-d) corresponding to 4 points A (u = 0.3150 mm), B (u = 0.3250 mm), C (u = 0.3500 mm), D (u = 0.4000 mm) in Fig. 2.36b). We observe that the crack changes its direction at the early stage of the damage. We can appreciate again in this example the influence of the RVE on the crack path at the macro scale.

The force-displacement curves for both cases are depicted in Fig. 2.37.

#### 2.5.7 Snap-back in 4-point bending cracked structure

In this last example, we combine the present two scale approach with an arc-length control procedure to handle possible instabilities at the macro scale. Indeed, in the previous studied cases, the load and geometries did not induce such instabilities. We then introduce at the macro scale an arc-length control procedure (see e.g. [41, 163]) where the problem is solved with Risk's method at the macroscale, and where the arc-length is updated based on the Crisfield's formula. The algorithm is summarized in Fig. 2.38. In this algorithm: both the displacement field, denoted by  $[\mathbf{u}_M]$ , and the external force  $[\mathbf{F}_{ext}]$  are unknowns. The latter  $[\mathbf{F}_{ext}]$  is the



Figure 2.34: Geometry and the mesh:  $H \times L = 80 \times 40$  mm, H1 =30 mm, R = 5 mm; the mesh size  $h_{size} \approx 1$  mm, 2914 elements;



Figure 2.35: Damage profile of the plate with two asymmetric semicircular notches (a) u = 0.224 mm, (b) u = 0.230 mm, (c) u = 0.240 mm, (d) u = 0.250 mm which correspond the point A,B,C,D in Fig.2.37 (a).



Figure 2.36: Damage profile of the plate two asymmetric semicircular notches; (a) u = 0.3150 mm, (b) u = 0.3250 mm, (c) u = 0.3500 mm, (d) u = 0.4000 mm which correspond the points A,B,C,D in Fig.2.37 (b).



Figure 2.37: Force-prescribed displacement curves in two case of microstructure

external force vector which is defined through  $[\mathbf{F}_{hat}]$  and  $\lambda$ . Note that  $[\mathbf{F}_{hat}]$  is also named as the normalized force vector while  $\lambda$  is the Lagrange multiplier which controls the arc-length and which is updated by the increment  $dd\lambda$ .

**Initial values:**  $[\mathbf{F}_{hat}]$  where  $[\mathbf{F}_{hat}](n1) = 1$ ,  $[\mathbf{F}_{hat}](n2) = 10$ ,  $\lambda = \lambda_0$ , where n1 and n2 are the degree of freedom associated with nodes suffering the external load. **WHILE**  $i < n_{step}$ - Compute  $[\mathbf{C}_{eff}]$  and the global stiffness matrix  $[\mathbf{K}_{globalM}]$ - Compute  $[\mathbf{F}_{ext}] = \lambda [\mathbf{F}_{hat}]$  $[\mathbf{Du_1}] = [\mathbf{K}_{globalM}] \setminus [\mathbf{F}_{ext}];$ - if i = 1:  $D\lambda_1 = \lambda_{pre}$  $[\mathbf{Du_1}] = [\mathbf{du_{prev}}];$ else  $D\lambda_1 = \lambda_{pre};$  $\lambda = \lambda + D\lambda;$ - Update:  $[\mathbf{u}_M] = [\mathbf{u}_M] + [\mathbf{D}\mathbf{u}_1];$  $[\mathbf{D}\mathbf{u}_{\mathbf{M}}] = [\mathbf{D}\mathbf{u}_{1}]; \qquad D\lambda = D\lambda_{1}.$ - Compute:  $[\mathbf{F}_{int}]$ - Compute :  $[\mathbf{R}] = [\lambda \mathbf{F}_{hat}] - [\mathbf{F}_{int}]$ - while  $norm(\mathbf{R}) < tol$ Update  $[\mathbf{u}_M] = [\mathbf{u}_M] + [\mathbf{ddu}]$ Compute  $[\mathbf{F}_{int}]$ Compute  $[\mathbf{R}] = [\lambda \mathbf{F}_{hat}] - [\mathbf{F}_{int}]$ Compute  $[\mathbf{du_1}] = [\mathbf{K}_{globalM}] \setminus [\mathbf{F}_{hat}]$ Compute  $[\mathbf{du_2}] = [\mathbf{K}_{globalM}] \setminus [\mathbf{R}]$ Compute the variation of arc-length:  $dd\lambda = -[\mathbf{Du_1}].[\mathbf{du_2}]/[\mathbf{Du_1}].[\mathbf{du_1}]$ Compute:  $[\mathbf{ddu}] = \lambda [\mathbf{du_1}] + [\mathbf{du_2}]$  $D\lambda = D\lambda + dd\lambda$  $\lambda = \lambda + dd\lambda$  $Compute[\mathbf{u}_M] = [\mathbf{u}_M] + [\mathbf{ddu}]$ end while -  $[\mathbf{d}\mathbf{u}_{\mathbf{prev}}] = [\mathbf{D}\mathbf{u}_{\mathbf{M}}];$  $\lambda_{pre} = D\lambda$ Compute the macroscale nonlocal strain field  $[\tilde{\varepsilon}]$ - Compute phase field problem at microscale using  $[\tilde{\varepsilon}]$  as the boundary condition. - Update the damage state [d] the microstructure. END

Figure 2.38: Algorithm for the SEN beam test.

The considered structure is depicted in Fig. 2.39. The beam has 1 notch at the center of the upper border, one roller and one pin at the upper border. The blue parts of the beam in Fig 2.39 are elastic and cannot be damaged, with material elastic properties 10 times larger than the effective ones of the RVE. The beam is loaded at two points, one near the left corner one point near the center of the bottom at a distance of 20 mm, with the magnitude 1F and 10F.



Figure 2.39: Single edge notch beam: the dimension is in mm; a) Load and displacement boundary conditions and b) Mesh and geometry.



Figure 2.40: Damage profile at the end of simulation.

The regularized length at microstructure is  $\ell_M = 4$  mm while the underlying microstructure is the porous one as in 2.5.1, whose geometry and material properties are in Fig. 2.10 a) and Table 2.1.

The result of the simulation is depicted in Fig. 2.40 and 2.41 which show the potential of the framework. We can clearly observe from Fig. 2.41 a snap-back response of the structure, characterizing an instability. It is worth noting that in Fig. 2.40 the main crack is not curved as in experiments for the same geometry. This is due to the anisotropic macroscopic behavior induced by the microstructure.

#### 2.6 Conclusion

In this chapter, a multiscale approach to quasi-brittle anisotropic damage has been proposed with a new macroscopic regularization procedure. The main idea follows the  $FE^2$  method, where we consider quasi-brittle damage within the RVE simulated by the phase field. At the



Figure 2.41: Force-displacement response where displacements are reported at point B.

macroscopic scale, the effective anisotropic damage behavior is fully induced by the geometry and local damage state of the RVE. We do not assume an a priori empirical damage model. As the macroscopic behavior is a softening one due to the damage within the RVE, a regularization process at the macro scale is required to avoid mesh-dependency issues. We have introduced an original procedure for this purpose by introducing a regularization term in the macroscopic energy. We have shown that by adopting an appropriate staggered scheme, we can solve this problem by solving separately the RVE problem, the macroscopic problem given the effective elastic behavior of the RVE within the iteration, and a regularization procedure of the strain field by solving a diffusion equation. We have shown that this framework can be used to solve several heterogeneous structural problems with heterogeneous microstructures when scales are separated, and that we can capture anisotropic macroscopic damage fully induced by the RVE geometry and local properties. Then, another original contribution of this chapter is the application of such a framework to induced-anisotropy due to the RVE damage. Finally, we have shown preliminary results regarding an extension of this framework to the case of instabilities, by combining this procedure with an arc-length method at the macro scale.

Regarding the regularization procedure, we have investigated two regularization processes (Isotropic and anisotropic). We have observed that the anisotropic process limits the broadening of the damage zone during the simulation. Finally, some issues remain. First, a regularization length has to be defined at the macro scale. This constitutes an issue, as such method is aimed at avoiding any tuning parameter at the macro scale. One possible way to obtain this parameter would be to conduct a full simulation (one scale) in a heterogeneous structure corresponding to the RVE and to use the response as a reference to fit the macro regularization length parameter. The second issue is related to the RVE definition. Even if in some cases the convergence with respect to the number of unit cells within the RVE is achieved, this convergence is not guaranteed

for more complex loading (not oriented with main directions). This second points would deserve more investigations in future studies.

### Chapter 3

# Identification of fracture models based on phase field for crack propagation in heterogeneous lattices in a context of non-separated scales

#### Contents

3.1	Introduction			
3.2	Fracture model used for the heterogeneous media			
3.3	Fracture models for the equivalent homogeneous solid			
	3.3.1	Isotropic effective fracture model	66	
	3.3.2	Anisotropic effective fracture model	67	
	3.3.3	Numerical implementation	70	
	3.3.4	Computation of effective elastic parameters	71	
	3.3.5	Effective fracture parameters	72	
3.4	Nume	Numerical examples		
	3.4.1	Periodic composite with hard inclusions	73	
		3.4.1.1 Test for identification of macroscopic parameters	73	
		3.4.1.2 Validation tests	78	
	3.4.2	Periodic quasi-brittle porous lattice structure: isotropic macroscopic frac-		
		ture model	79	
	3.4.3	Periodic porous lattice: anisotropic macroscopic fracture model	85	
	3.4.4	Validation tests	86	
3.5	Concl	Conclusion		

#### 3.1 Introduction

In this chapter, the construction of a homogeneous medium equivalent to a heterogeneous one under quasi-brittle fracture is investigated in the case of non-separated scales. At the microscale, the phase field method to fracture is employed. At the scale of the homogeneous medium, another phase field model either isotropic or anisotropic, depending on the microscale characteristic length and on the underlying microstructure, is assumed. The coefficients of the unknown phase field model for the homogeneous model are identified through the mechanical response of a sample subjected to fracture whose microstructure is fully described and estimated numerically. We show that the identified models can reproduce both the mechanical force response as well as overall crack paths with good accuracy in other geometrical configurations than the one used to identify the homogeneous model. Several numerical examples, involving cracking in regular lattices of both hard particles and pores, are presented to show the potential of the technique.

As reviewed in Chapters 1 and 2, homogenization of damage behavior in heterogeneous media induces tough issues, such as: (a) the intrinsic nonlinearity of the problem; (b) the difficulty to define an RVE due to sharp localization [70, 145]; (c) the numerical lack of convergence and stability at the macroscale and (d) the definition of the characteristic length scale at both scales. Numerically, we have seen in Chapter 2 that heavy computational costs are induced by the FE<sup>2</sup> procedure. The aim of this chapter is two-fold: (a) propose a homogenized model which does not require 2-scale nested computations to alleviate the computational costs; (b) propose a model which can handle the case of non-separated scales, i.e. when the ratio between the characteristic dimensions of heterogeneities is not small with respect to the dimensions of the structure.

This chapter is rewritten from [136]. In this work, we follow [83] by identifying the different parameters of a damage model at the macroscale, which can then be used without concurrent computations for the macroscale calculations. The phase field method was used at the microscale to calibrate the effective toughness, defined as the macroscopic energy release rate required at the boundary of a heterogeneous representative domain to propagate the crack over a macroscopic distance. However, in contrast to the mentioned work, we directly identify all the different parameters of the model, by fitting a typical mechanical test response under crack initiation and propagation in a structure where all heterogeneities are explicitly described. More specifically, the macroscopic damage model is based on the phase field method and its extensions to anisotropic crack propagation [12,13,37,46], to handle the effects of preferential crack propagation in regular lattices.

In the following, section 3.2 reminds the phase field method to fracture employed for the heterogeneous medium which is considered as the reference solution. In section 3.3, the proposed fracture models for the homogeneous medium, including both isotropic and anisotropic phase

field models, are described. The identification procedure is provided. Numerical examples involving heterogeneous media including regular lattices with both hard inclusions and pores are provided in section 3.4 to evaluate the accuracy of the constructed models.

#### 3.2 Fracture model used for the heterogeneous media

The modeling of fracture in the fully detailed model is the classical isotropic phase field method described in section 2.2. The phase field is employed here again because we deal with complex heterogeneous media, and more specifically regular lattices. In such structures, the microcracks initiate, coalesce, and can form very complex set of tens or hundreds of microcracks. The reader can report to section 2.2 for a description of the phase field and numerical implementation.

#### 3.3 Fracture models for the equivalent homogeneous solid

In the sequel, we seek to define models describing the fracture process for an equivalent homogeneous medium, where all details of heterogeneities are avoided (see figure 3.4).

The domain associated with the homogeneous solid is defined in an open domain  $\Omega \subset \mathbb{R}^D$ , where D denotes the space dimension. The corresponding boundary of  $\Omega$  is denoted by  $\partial\Omega$ , where  $\partial\Omega = \partial\Omega_u \cup \Omega_F$ ,  $\partial\Omega_u \cap \Omega_F = \emptyset$ , where traction forces  $\mathbf{F}^*$  are prescribed over the boundary  $\partial\Omega_F$  and displacements  $\mathbf{u}^*$  are prescribed over the boundary  $\partial\Omega_u$ . The quantities associated with the homogeneous medium are denoted by  $\overline{(.)}$ , to distinguish them from their counterparts in the fully heterogenous medium. Note that we assume that the scales are not separated, i.e. that the effective nonlinear properties at one point of the homogeneous structure cannot be obtained from the response of an RVE. Then, the approach we propose is to define models for the homogeneous medium based on the phase field method and to identify their characteristic parameters from specific fracture tests involving crack initiation and propagation in a fully heterogeneous medium. We will consider two cases: the first one when an isotropic phase field model for crack can be adopted, and the second one when an anisotropic model must be used to describe the crack propagation.

Under conditions on spatial distributions of heterogeneities, the effective elastic material can be found as isotropic, either under sufficient symmetry conditions within the microstructure [52], or for random microstructures. However, these conditions do not necessarily lead to an isotropic damage description of the material, as the microcracks can be strongly oriented by the microstructure, the load history, or a nonlinear behavior of the phase, among others. In a context of regularized brittle fracture, the cracks have finite width and the ratio between this width and the characteristic size of the heterogeneities is another criterion leading or not to an effective anisotropic damage, as shown in the following examples

#### 3.3.1 Isotropic effective fracture model

In this first case we consider an isotropic effective damage model for the homogeneous medium. Such model is usually not realistic in heterogeneous quasi brittle materials, as the load induces an orientation of the microcracks [61]. However, we show in the following examples that in a context of regularized brittle fracture, this assumption can be acceptable for regular lattices when the characteristic length in the phases of the heterogeneous medium is of the order of the dimensions of the heterogeneities or larger.

We remind that for quasi-brittle materials, it has been shown that the internal length  $\ell$  can be defined as a finite material parameter characterizing the medium, and that can be evaluated qualitatively from simple 1D considerations [7, 94, 142], or identified quantitatively by inverse approach by combining simulations and experiments [142, 140]. For the above conditions of isotropic damage assumption of the homogeneous medium, we use the same model for the homogeneous model than the one in the heterogeneous medium, the only difference stemming from the values of the material parameters, which will be defined in the sequel. First, the equations of the mechanical problem for the homogeneous medium are given by:

$$\nabla \cdot \overline{\boldsymbol{\sigma}} = 0, \quad \overline{\boldsymbol{\sigma}} \mathbf{n} = \mathbf{F}^* \text{ over } \partial \Omega_F, \quad \overline{\mathbf{u}} = \mathbf{u}^* \text{ over } \partial \Omega_u,$$

$$(3.1)$$

with

$$\overline{\boldsymbol{\sigma}} = \left( (1 - \overline{d})^2 + k \right) \left\{ \overline{\lambda} \left\langle tr \overline{\boldsymbol{\varepsilon}} \right\rangle_+ \mathbf{1} + 2\overline{\mu} \overline{\boldsymbol{\varepsilon}}^+ \right\} + \overline{\lambda} \left\langle Tr \overline{\boldsymbol{\varepsilon}} \right\rangle_- \mathbf{1} + 2\overline{\mu} \overline{\boldsymbol{\varepsilon}}^-.$$
(3.2)

The corresponding weak form is obtained as:

$$\int_{\Omega} \overline{\boldsymbol{\sigma}} : \overline{\boldsymbol{\varepsilon}}(\delta \overline{\mathbf{u}}) \ d\Omega = \int_{\partial \Omega_F} \mathbf{F}^* \cdot \delta \overline{\mathbf{u}} \ d\Gamma \quad \forall \delta \overline{\mathbf{u}} \in H_0^1(\Omega).$$
(3.3)

The equations of the phase field problem are given by:

$$\left(2\overline{\mathcal{H}} + \frac{\overline{g_c}}{\overline{\ell}}\right)\overline{d} - \overline{\ell}\overline{g_c}\Delta\overline{d} = 2\overline{\mathcal{H}}$$
(3.4)

with the boundary conditions

$$\nabla \overline{d} \cdot \mathbf{n} = 0 \text{ over } \partial \Omega, \quad \overline{d} = 1 \text{ over } \overline{\Gamma}.$$
 (3.5)

The corresponding weak form is given by:

$$\int_{\Omega} \{ (2\overline{\mathcal{H}} + \frac{\overline{g_c}}{\overline{\ell}}) d\delta \overline{d} + \overline{g_c} \overline{\ell} \nabla \overline{d} \cdot \nabla (\delta \overline{d}) \} \ d\Omega = \int_{\Omega} 2\overline{\mathcal{H}} \delta \overline{d} \ d\Omega \quad \forall \delta \overline{d}(\mathbf{x}) \in H_1^0(\Omega).$$
(3.6)

In the above,  $\overline{d}$  is the unknown fracture field for the homogeneous medium,  $\overline{\lambda}$  and  $\overline{\mu}$  are homogeneized elastic parameters defined in section 3.3.4, and  $\overline{g_c}$  and  $\overline{\ell}$  are parameters to be identified (see section 3.3.5). In the above,  $\overline{\mathcal{H}}$  is a function similar to  $\mathcal{H}$  but using homogeneous quantities.

#### 3.3.2 Anisotropic effective fracture model

When the microscopic characteristic length  $\ell$  is much lower than the size of the heterogeneities, the micro cracks strongly interact with the heterogeneities and this can induce preferential orientations of the cracks. In that case, an isotropic model for fracture is no longer valid to describe the crack propagation in the homogeneous medium. In such situation, even though the microstructure induces isotropic homogeneous elastic properties, the damage behavior can be fully anisotropic, as it is the case in regular lattices like honeycombs [162]. Then, we propose to employ the anisotropic phase field model proposed in [138, 139], which is an extension to the model proposed in [36] to n preferential directions, to describe the fracture process in the homogeneous medium. Considering n preferential directions induced by the microstructure, which are assumed to be identified *a priori* from the microstructure knowledge, we define the total energy as:

$$E(\overline{\mathbf{u}}, \overline{d}_1, \overline{d}_2, ..., \overline{d}_n) = \int_{\Omega} \overline{\Psi}(\boldsymbol{\varepsilon}(\overline{\mathbf{u}}), \overline{d}_1, \overline{d}_2, ..., \overline{d}_n) \ d\Omega + \overline{g_c} \sum_{i=1}^n \int_{\Omega} \tilde{\gamma}_i(\overline{d}_i) \ d\Omega - \int_{\partial\Omega_F} \mathbf{F}^* \cdot \overline{\mathbf{u}} d\Gamma, \quad (3.7)$$

where  $\overline{d}_1, \overline{d}_2, ..., \overline{d}_n$  are independent phase fields associated with each preferential direction i, and

$$\overline{\Psi}(\overline{\mathbf{u}}, \overline{d}_1, \overline{d}_2, ..., \overline{d}_n) = (\prod_{i=1}^n g_i(\overline{d}_i) + k)\overline{\Psi^+} + \overline{\Psi^-},$$
(3.8)

where  $\overline{\Psi}^+$  and  $\overline{\Psi}^-$  are given by:

$$\overline{\Psi}^{\pm}(\overline{\varepsilon}) = \overline{\lambda}(\langle tr(\overline{\varepsilon}) \rangle_{\pm})^2 / 2 + \overline{\mu} tr\{(\overline{\varepsilon}^{\pm})^2\},\tag{3.9}$$

where  $\overline{\lambda}$  and  $\overline{\mu}$  are given by 3.22. In Eq. (3.8),  $g_i(\overline{d}_i) = (1 - \overline{d}_i)^2$  is the degradation function associated with the damage variable  $\overline{d}_i$ . The crack density function  $\tilde{\gamma}_i(\overline{d}_i, \nabla \overline{d}_i, \boldsymbol{\omega}_i)$  associated to the *i*-th direction is defined as:

$$\tilde{\gamma}_i(\overline{d}_i, \nabla \overline{d}_i, \boldsymbol{\omega}_i) = \frac{1}{2\overline{\ell}} \overline{d}_i^2 + \frac{\overline{\ell}}{2} \boldsymbol{\omega}_i : \nabla \overline{d}_i \otimes \nabla \overline{d}_i, \qquad (3.10)$$

where  $\omega_{i}$  is a second-order orientation tensor defined by:

$$\boldsymbol{\omega}_i = \mathbf{I} + \overline{\beta}_i (\mathbf{I} - \mathbf{n}_i \otimes \mathbf{n}_i), \tag{3.11}$$

where  $\mathbf{n}_i$  is the unit normal vector to the preferential direction or plane of the damage and  $\mathbf{I}$  is the second-order identity tensor. The anisotropic effect is parameterized by the coefficients  $\overline{\beta}_i$ . When  $\overline{\beta}_i = 0$  and n = 1, the isotropic phase field model is recovered. The new variational principle is written as a minimization with respect to  $\overline{\mathbf{u}}$  and the fields  $\overline{d}_i$ , i = 1, 2, ..., n:

$$\overline{\mathbf{u}}^{n+1}, \overline{d}_i^{n+1} = \operatorname{Argmin}_{\substack{\overline{\mathbf{u}} \in \mathcal{K}_A \\ 0 \le \overline{d}_i^n \le \overline{d}_i^{n+1}}} E, \quad i = 1, 2, ..., n.$$
(3.12)

In the sequel, we assume that the homogeneous material is elastically isotropic, but the fracture process is anisotropic. This simplifies the definition of the model for separation into tensile and compressive parts in (3.9). Other type of splitting the energy can be choosen (see [7] for isotropic elastic case and [49] and for anisotropic elastic case). The mechanical problem is then described by (3.1) with

$$\overline{\boldsymbol{\sigma}} = \left(\prod_{i=1}^{n} g_i(\overline{d}_i) + k\right) \left\{ \overline{\lambda} \left\langle tr\overline{\boldsymbol{\varepsilon}} \right\rangle_+ \mathbf{1} + 2\overline{\mu}\overline{\boldsymbol{\varepsilon}}^+ \right\} + \overline{\lambda} \left\langle Tr\overline{\boldsymbol{\varepsilon}} \right\rangle_- \mathbf{1} + 2\overline{\mu}\overline{\boldsymbol{\varepsilon}}^-.$$

The weak form remains unchanged as in (3.3). The minimization process with respect to each  $\overline{d}_i$  field gives:

$$\int_{\Omega} \left\{ -2(1-\overline{d}_i)\delta \overline{d}_i \prod_{i\neq j} g_j(\overline{d}_j)\Psi^+ + \frac{\overline{g_c}}{\overline{\ell}} \overline{d}_i \delta \overline{d}_i + \overline{g_c} \overline{\ell} \nabla \overline{d}_i \boldsymbol{\omega}_{\mathbf{i}} \nabla (\delta \overline{d}_i) \right\} d\Omega = 0,$$

$$i = 1, 2, ..., n. \quad (3.13)$$

To ensure irreversibility of the fields  $\overline{d}_i$ , we use the history function defined in [138] as:

$$\hat{\mathcal{H}}_i = \max_{\tau \in [0,t]} \{ \prod_{i \neq j} g_j(d_j) \overline{\Psi}^+(\mathbf{x},\tau) \}.$$
(3.14)

Replacing (3.14) into (3.13), the weak form for the i-th phase field problem is finally obtained as:

For post-processing visualization purpose, an equivalent phase field  $d_{eq}$  is calculated from  $\overline{d}_i$ (i = 1,2,...,n) such that:

$$(1 - d_{eq})^2 = \prod_{i=1}^n g_i(\overline{d}_i)^2.$$
(3.16)

In this model, in addition to the effective elastic parameters  $\overline{\lambda}$  and  $\overline{\mu}$ , the following fracture parameters have to be identified:  $\overline{g_c}$ ,  $\overline{\ell}$ ,  $\overline{\beta_i}$ , i = 1, 2, ..., n. For the sake of simplification, we assume that  $\overline{\beta_1} = \overline{\beta_2} = , ... = \overline{\beta_n} = \overline{\beta}$ . Then, three material parameters need to be identified instead of the two in the case of using the same model for the homogeneous model. It is worth noting that in (3.11), the different preferential orientations  $\mathbf{n_i}$  have to be identified. In the present work, we consider simple microstructures where these orientations can be assumed a priori based on simple geometric considerations (see e.g. Fig. 3.1).



Figure 3.1: Three favourable orientations of crack in the periodical porous media (a); the porous media is replaced by homogeneous one with there preferential directions where  $\mathbf{n}_1, \mathbf{n}_2, \mathbf{n}_3$  are normal vectors (c)

In the following, we investigate the anisotropic effects in (3.7) employed for the periodic media in Fig. 3.1, in which the distribution of the microvoids is assumed to lead to 3 preferential directions. We'll show that the anisotropic damage effect depends on both to parameters  $\bar{\beta}$  and  $\bar{\ell}$ . For this purpose we consider a circle sample (R = 0.32 mm) with a hole at the center (r = 0.03 mm) with the critical energy release rate  $g_c = 1$ N/mm<sup>2</sup>. The dimension is depicted in Fig.3.1b. The heterogeneous medium will be replaced by a homogeneous media with 3 preferential directions. The corresponding normal vectors of those directions are defined by  $\mathbf{n_1} = [-1/2; \sqrt{3}/2]; \mathbf{n_2} = [-1; 0]; \mathbf{n_3} = [-1/2; -\sqrt{3}/2].$ 

According to the Griffith's theory, the crack will start to propagate when the surface energy reaches its critical value. In other words, in the domain, a surface will be created at the position where the created surface energy is maximum. To illustrate this, we apply  $d_{i(i=1,2,3)} = 1$  in the inner hole and solve the phase field problem in the absence of the elastic problem. We consider the average surface energy  $Gs(\theta)$  (N/mm<sup>2</sup>) in different directions around the center. The average  $Gs(\theta)$  is computed as:

$$Gs(\theta) = \frac{1}{r_2 - r_1} \int_{r_1}^{r_2} g_c dr.$$
 (3.17)

In this investigation,  $r_1 = r$  and  $r_2 = r_1 + 0.1$  mm as in Fig. 3.1c. We set  $\beta = 50$  while



Figure 3.2: The polar plot of  $G_s(\theta)$  w.r.t  $\ell$  when  $\beta = 50$ : anisotropic effect is clear in three cases of  $\ell$  when the number of preferential direction n = 1.

varying the length scale parameters  $\ell = 0.005$  mm; 0.01 mm; 0.02 mm and plot the average surface energy along different directions. As can be seen in Fig. 3.2, the anisotropic is clear in all these cases. Next, we combine the results of three preferential directions. We can observe in Fig. 3.3 that the anisotropic effect depends on both  $\beta$  and  $\ell$  or the product  $\beta \ell$ . This can be interpreted by reformulating (3.10) as:

$$\tilde{\gamma}_i(\overline{d}_i, \nabla \overline{d}_i, \boldsymbol{\omega}_i) = \frac{1}{2\overline{\ell}} \overline{d}_i^2 + \frac{\overline{\ell}}{2} \nabla \overline{d}_i^2 + \frac{\overline{\beta}\ell}{2} (\mathbf{I} - \mathbf{n}_i \otimes \mathbf{n}_i) : \nabla \overline{d}_i \otimes \nabla \overline{d}_i.$$
(3.18)

It can be seen in (3.18) that the anisotropic part of the surface energy density comes from the third term on the right-hand side of the formula which varies w.r.t the product  $\overline{\beta \ell}$ .

#### 3.3.3 Numerical implementation

The numerical implementation for the isotropic phase field model has been presented in sec 2.2.3. Herein, only the numerical implementation of phase field problem in the anisotropic case will be presented. The matrix form of (3.13) to solve damage fields  $d_{i(i=1,2..n)}$  at step k+1:

$$\left[\mathbf{K}_{d_i}\right] \left[ \overline{\mathbf{d}_i} \right] = \left[ \mathbf{F}_{d_i} \right], \tag{3.19}$$



Figure 3.3: The polar plot of  $G_s(\theta)$  with respect to  $\beta$  and  $\ell$ : when  $\beta = 50$ , the convexity is clear in case  $\ell = 0.01$  (b) while it is not obvious in case  $\ell = 0.005$ (a).

where :

$$\begin{cases} [\mathbf{K}_{di}] = \int_{\Omega} \{ (2\overline{\mathcal{H}_{i}} + \frac{\overline{g_{c}}}{\overline{\ell}}) [\mathbf{N}_{d}]^{T} [\mathbf{N}_{d}] + \overline{g_{c}} \overline{\ell} [\mathbf{B}_{d}^{T}] \omega_{\mathbf{i}}(\overline{\beta}) [\mathbf{B}_{d}] \} d\Omega, \\ \\ [\mathbf{F}_{d}] = 2 \int_{\Omega} [\mathbf{N}_{d}^{T}] \overline{\mathcal{H}_{i}} d\Omega. \end{cases}$$
(3.20)

The formulation for elastic problem is the same as in (2.50) except a new degradation function will be employed, then:

$$[\mathbf{K}_1](\mathbf{d}_{i(n+1)}), \mathbf{u}_n) = \left(\prod_{i=1}^n g_i(\bar{d}_i) + k\right) \int_{\Omega} [\mathbf{B}]^T \left( [\mathbf{C}_{\lambda}] \mathcal{R}^- + 2\mu \left[ \mathbf{P}^+ \right] \right) [\mathbf{B}] \ d\Omega.$$
(3.21)

#### 3.3.4 Computation of effective elastic parameters

The effective elastic parameters are computed by means of classical computational homogenization. For 2D plane strain isotropic material, the effective coefficients are deduced from (2.111) by:

$$\overline{\lambda} = \overline{C}_{1122}, \quad \overline{\mu} = \frac{\overline{C}_{1111} - \overline{C}_{1122}}{2}. \tag{3.22}$$



Figure 3.4: Identification procedure for constructing the equivalent homogeneous medium

#### 3.3.5 Effective fracture parameters

To determine the unknown fracture parameters related to the homogeneous medium, an inverse approach employing numerical simulations over the heterogeneous medium as a reference for the identification of the parameters is proposed. In the case of the isotropic fracture model, the unknown parameters are  $\overline{g_c}$  and  $\overline{\ell}$ , while in the anisotropic model the unknown parameters are  $\overline{g_c}$ ,  $\overline{\ell}$  and  $\overline{\beta}$ . A schematic of the overall identification procedure is provided in Fig. 3.4. First, a fracture simulation is performed on a structure whose heterogeneities are explicitly described and fully meshed. We recall that we assume a non-separation of scales, i.e. that the characteristic size of the heterogeneities is not too small as compared to the characteristic dimensions of the structure. A force-displacement-curve is obtained, which is used as data for the identification. Then, the same problem is solved for the homogeneous model, and the unknown fracture parameters are adapted until a tolerance criterion is reached. In the present work, we have used the following functional:

$$J = \int_0^{u_{max}^*} \left( F^{homo}(u^*) - F^{ref}(u^*) \right)^2 du, \qquad (3.23)$$

where  $u_{max}^*$  is the maximum applied displacement in the simulation involving the full heterogeneous structure,  $F^{homo}$  is the force response of the homogeneous structure, and  $F^{ref}$  is the reference response of the heterogeneous structure. The problem to identify the unknown



Figure 3.5: Periodic hexagonal lattice of circular inclusions or pores

parameters is then given by

$$\left\{\overline{g_c}, \overline{\ell}, \overline{\beta}\right\} = \operatorname{Arg\ min}\ J. \tag{3.24}$$

It is worth noting that in the present work, we did not introduced in the optimization problem an objective related to the error in the direction of the crack. This point should be investigated in future studies. To ensure a right reproduction of main crack directions, we have then constrained the values of  $\overline{\beta}$  to sufficiently large ranges.

As the problem (3.24) is non-convex and may involve many local minima, efficient optimization algorithms must be employed. In the present work, we have used the simplex search algorithm described in [3], while many other strategies are possible from the vast literature on optimization algorithms.

#### 3.4 Numerical examples

In this section, the procedure described in sections 3.3.4, 3.3.5 to construct the homogeneous damage model is applied to several practical examples, including hard particles-matrix composites and porous media with regular lattices. For all the examples, linear 3-node elements have been used for the different meshes.

#### 3.4.1 Periodic composite with hard inclusions

#### 3.4.1.1 Test for identification of macroscopic parameters

We consider the heterogeneous structure depicted in Fig. 3.6, composed of a matrix and circular inclusions which are distributed over a periodic hexagonal lattice (see Fig. 3.5). The radius of inclusions is r = 0.025 mm and the distance h between the inclusions centers is equal to 0.08 mm. The material parameters of the matrix are:  $\mu_1 = 121.15$  MPa,  $\lambda_1 = 80.77$  MPa,  $g_c^1 = 0.0027$  kN/mm, where  $\mu_1$ ,  $\lambda_1$  and  $g_c^1$  denote the matrix Lamé's parameters and Griffith-type critical energy release rate associated with the matrix, respectively. The material parameters for the inclusions are chosen as twice those of the matrix:  $\mu_2 = 2\mu_1 \lambda_2 = 2\lambda_1$  MPa,  $g_c^2 = 2g_c^1$ . To analyze the influence of the microstructural damage parameters on the identified homogeneous



Figure 3.6: Test (T1) used to identify the parameters of the homogeneous crack propagation model: heterogeneous media (left) and homogeneous media (right).

model, different crack width values are considered:  $\ell = \{r/5, 2r/5, r, 2r\}$ . The corresponding meshes for the heterogeneous structure (see Fig. 3, left) contain:  $3.4 \times 10^5$ ,  $8.8 \times 10^4$ ,  $8.8 \times 10^4$ and  $2.2 \times 10^4$  elements respectively. The corresponding meshes for the homogeneous structure (see Fig. 3, left) contain  $3.2 \times 10^5$ ,  $8.0 \times 10^4$ ,  $8.0 \times 10^4$  and  $2.0 \times 10^4$  elements respectively. We note that both discretizations for heterogeneous and homogeneous structures contain similar number of elements. This has been chosen for validation purpose. However, once identified, the homogeneous model can be used within a context of adaptive mesh refinement, to drastically reduce computational times as compared to directly solve the heterogeneous structure problem.

In each case, we first identify the macroscopic damage parameters  $\overline{g_c}$  and  $\overline{\ell}$  and validate the model through several tests implying crack initiation and propagation for other configurations. The test used to identify the parameters is described in Fig. 3.6. The size of the samples is  $L \times H = 1 \times 1 \text{ mm}^2$ . In the following tests, dimensions L and H will remain unchanged.

In this first case, we assume that  $\ell$  is of the order of the radius r of the inclusions. We recall that  $\ell$  is here regarded as a material parameter for the matrix. It has been shown experimentally and numerically in [140] that when this parameter is larger than the heterogeneities in the medium, then the crack path is not much affected by these heterogeneities, and an isotropic damage model can accurately reproduce the crack propagation. However as expected, the equivalent medium involves both elastic and damage parameters which take different values than in the matrix. Then, under these assumption (the case when  $\ell \ll R$  will be treated in section 3.4.3), we use the same phase field model for the macroscopic scale, but identify the unknown parameters  $\overline{\ell}$  and  $\overline{g_c}$  by the procedure described in section 3.3.5.

In that case, the isotropic damage model described in section 3.3.1 is used for the homogeneous model. The first step is to compute the effective elastic parameters of the homogeneous

case	$\overline{\ell},$	$\overline{g_c}$
$\ell = 0.005$	$4.950\times 10^{-3}$	$3.797\times 10^{-3}$
$\ell = 0.010$	$1.012\times 10^{-2}$	$3.700\times10^{-3}$
$\ell = 0.025$	$2.525\times 10^{-2}$	$3.595\times10^{-3}$
$\ell = 0.050$	$5.000\times 10^{-2}$	$3.491\times 10^{-3}$

**Table 3.1:** Identified parameters for the equivalent homogeneous media corresponding to the hard inclusions composite:  $\overline{g_c}, \overline{\ell}$  obtained for different regularized lengths  $\ell$  in the microscopic phases.

domain from the RVE described in Fig. 3.5. The results give  $\overline{\mu} = 101.66$  MPa and  $\overline{\lambda} = 149.70$  MPa. In a second step, we identify the parameters of the macroscopic phase field model using the tension test described in Fig. 3.6, called (T1). The sample includes an initial horizontal crack of length 0.5*L* at y = 0.5H. Displacements are fixed along x- and y- direction on the lower end (y = 0). On the upper end (y = H), the displacements are fixed along x-direction and prescribed along the y-direction through  $u_y = \overline{u}$ . Incremental displacements steps  $\Delta u = 10^{-4}$  mm are prescribed until complete failure of the specimen.

A force-displacement curve is obtained for the heterogeneous medium (see Fig. 3.6) and used as a reference solution for the identification. The same test is conducted on the homogeneous medium to fit the unknown effective coefficients  $\overline{g_c}$  and  $\overline{\ell}$ .

In the following examples, we use as an initial guess for the optimization procedure the following values:  $\ell^0 = \ell$  and  $g_c^0 = f_1 g_c^1 + f_2 g_c^2$ , where  $f_1$  and  $f_2$  are the respective volume fractions of each phase.

Table 3.1 shows the resulting effective parameters  $(\overline{g_c}, \overline{\ell})$  in four cases, corresponding to different crack widths at the microscale:  $\ell = \{r/5, 2r/5, r, 2r\}$ . We can note that the optimized values of  $\overline{\ell}$  do not vary significantly as compared to  $\ell$  which is expected as the crack path is not much affected by the presence of the inclusions in that case. However, we can note that  $\overline{g_c}$  take different values as compared to the matrix and that the lower the microscopic crack width is, the larger the macroscopic toughness.

Fig. 3.7 compares the force-displacement responses and their corresponding energy-dispacement curves using the identified parameters for different values of micro crack widths  $\ell$ . We can note that the larger  $\ell$ , the better agreement between micro and effective response or crack patterns is found. Even though the homogeneous model is not able to capture all branching and secondary microcracks as in the microscopic model, the main direction and length of the crack is well captured with the homogeneous model. With smaller  $\ell$ , the microscopic heterogeneous model



Figure 3.7: Comparison between reference solution, "ref" (heterogeneous medium) and equivalent homogeneous medium, "homo": (a) Force - displacement curve and (b) Energy- displacement curve for the traction test (T1).



d)ℓ= 0.05mm

Figure 3.8: Crack networks for the traction test (T1): comparison between the reference solution (heterogeneous medium) and the equivalent homogeneous medium.

induces more fluctuations, and then the macroscopic model only captures the averaged trends, which is expected.

#### 3.4.1.2 Validation tests



(b) The double cracks test(V2)

Figure 3.9: Validation tests of periodic composite structure with hard inclusions: a shear test (V1) and a double crack test (V2).

In this section, the identified homogeneous model is validated on other configurations than the one used to identify the effective parameters. The first validation test (called V1) uses the same cracked sample as described above, but the loading induces shear. The second validation test (V2) involves a doubly cracked specimen. Both tests are described in Fig. 3.9. For the shear test, the geometry of the sample is the same as in the traction test. The displacements are blocked along both direction on the lower end. On the upper end, the displacements are fixed along the y-direction and are prescribed along the x- direction with displacement increments  $\Delta u_X = 5 \times 10^{-5}$  mm. In the double cracks test depicted in Fig. 3.9 (b), the rectangular domain contains two initial cracks whose lengths are a = 0.25 mm and their position is defined by h = 0.25 mm. The displacements are blocked along both direction on the lower end. On the lower end. On the lower end.

upper end, the displacements are fixed along the x-direction and are prescribed along the ydirection with displacement increments  $\Delta u_Y = 1 \times 10^{-4}$  mm.

Results are presented in Figs (3.10-3.13). Here again, a good agreement is found between the reference model and the homogeneous one. When the microscopic crack width  $\ell$  is small as compared to the heterogeneities, the homogeneous model no more captures the local fluctuations of both response and microcrack networks, but the overall trends are well captured.

## 3.4.2 Periodic quasi-brittle porous lattice structure: isotropic macroscopic fracture model

In this section, we consider a porous lattice structure with periodic distribution of pores on a hexagonal lattice (see Fig. 3.5). The material properties of the skeleton are  $\mu = 121.15$  MPa,  $\lambda = 80.77$  MPa,  $g_c = 0.0027$  kN/mm and the crack width is  $\ell = 0.025$  mm. To evaluate the influence of the ratio  $\ell/r$ , we consider two sizes of pores while maintaining the same value for  $\ell$  and using r = 0.02 mm , h = 0.064 mm and r = 0.01 mm, h = 0.032 mm. The test used to identify the macroscopic parameters of the phase field model is the same as in the previous example (Fig. 3.6, Test (T1)), except that the heterogeneities are here voids. We will show that in the case where  $\ell$  is of the same order than r, an isotropic phase field can provide a good approximation for the response of the heterogeneous model, but with some restrictions. The case when  $\ell$  is much lower than the radius of the pores will be treated in section 3.4.3. It is worth noting that here again, the elastic effective medium is isotropic.

We first consider the case  $\ell/r = 2.5$ , corresponding to a porosity of 0.345. In this case, the effective elastic parameters for the RVE depicted in Fig. 3.5 are obtained as  $\overline{\mu} = 35.96$  MPa;  $\overline{\lambda} = 42.86$  MPa and the identified parameters for the effective phase field model are obtained as:  $\ell = 0.025$  mm and  $\overline{g_c} = 0.0017624$  kN/mm.

In a second case,  $\ell/r = 1.25$ , r = 0.02 mm and h = 0.064 mm (see Fig. 3.5), which induces a porosity of 0.33. The effective elastic parameters are in this case obtained as:  $\overline{\mu} = 32.06$  MPa,  $\overline{\lambda} = 40.10$  MPa. The identified damage parameters for the homogeneous model are obtained as:  $\overline{g_c} = 0.001827$  KN/mm;  $\overline{\ell} = 0.0250$  mm.

Two validation tests, called V1 and V2, have been performed in both case. The validation test V1 involves a shear load as described in Fig. 3.9 (a) while the test V2 implies a sample with two initial cracks as described in Fig. 3.9 (b). The conditions and geometries are identical as in the previous examples. The results are presented in Fig. 3.14 and 3.16.

In the case  $\ell/r = 2.5$ , we can observe from both tests V1 and V2 (see Figs. 3.14 and 3.16), that the force-displacement curve as well as the crack path are accurately reproduced by the homogeneous model. In Fig. 3.15(a), (b), the energy - displacement  $E - \overline{u}$  and surface energy - displacement  $E_s - \overline{u}$  are plotted for both models, showing a good agreement. Results for the porous medium with  $\ell/r = 1.25$  are provided in Fig. 3.16. We can note that in this case,



Figure 3.10: Comparison between the response of homogeneous media ("homo") and heterogeneous media ("ref") using equivalent parameters in the Table 1: Force - displacement (first column) and Energy- displacement (second column) in the validation shear test (V1).



Figure 3.11: Comparison of F-u curves and E-u curves of the heterogeneous media and homogeneous media in the double cracks test (V2) with various regularized length.



d) $\ell$  = 0.05mm

d) $\ell$  = 0.05mm

Figure 3.12: Comparison of phase field distribution of the heterogeneous media and the homogeneous media in shear test (V1) with various regularized length.

Figure 3.13: Comparison of phase field distribution of the heterogeneous media and homogeneous media in the double cracks test (V2)with various regularized length.

even though the force-displacement curve is in good agreement with the reference model, the crack path tends to deviate. This show the limits of the isotropic model for the homogeneous medium in the case  $\ell < r$ . To circumvent this issue, the anisotropic phase field model described in section 3.3.2 is adopted in the next section, to treat the case  $\ell \ll r$ .



a) Force - displacement curves b) heterogeneous medium c) homogeneous medium

Figure 3.14: Porous media with  $\ell/r = 2.5$ : comparison of F -u relations and crack profiles in three tests: T1,V1,V2



Figure 3.15: Comparison between (a) the total energy and (b) the crack surface energy  $E_s$  for the heterogeneous medium "ref" and the homogeneous medium "homo".



a) Force - displacement curves b) heterogeneous media c) homogeneous medium

Figure 3.16: Porous media with  $\ell/r = 1.25$ : comparison of F -u relations and crack profiles in the three tests T1, V1 and V2.



Figure 3.17: Comparison of heterogeneous media (M1) and homogeneous media (M2) in the identification test. In M1,  $F_{max} = 0.55$  kN at  $\overline{u} = 0.01390$  mm and in M2,  $F_{max} = 0.5601$  kN at  $\overline{u} = 0.0156$  mm.

#### 3.4.3 Periodic porous lattice: anisotropic macroscopic fracture model

In this example, we assume that the internal length  $\ell$  is much smaller that the size of the pores. In this case, the isotropic model for fracture propagation described in section 3.3.1 can no longer describe some preferential crack paths induced by the microstructure. Then, the anisotropic phase field framework described in section 3.3.2 is adopted. The porous media with parameters r = 0.02 mm and h = 0.064 mm (see Fig. 3.5) is employed. Here,  $\ell = 0.0025$  mm, which corresponds to  $\ell = r/8$ . In that context, there are three damage parameters to be identified, in addition to the effective elastic parameters:  $\bar{\ell}, \bar{g_c}$ , and the parameter related to anisotropy  $\bar{\beta}$  in Eq. (3.20).

Note that regarding elastic properties, the media remains isotropic, and can be characterized by the two effective Lamé's parameters  $\overline{\lambda}$  and  $\overline{\mu}$ . These two effective parameters have the same values as in the previous example. In the studied lattice of Fig. 3.5 there are three obvious main preferential directions for crack propagation, corresponding to n = 3 in Eq 3.7. The above phase field parameters are identified using the traction test described in Fig. 3.6, where 175 load increments  $\Delta u_Y = 1.5 \times 10^{-4}$  mm are prescribed in the first 50 steps and  $\Delta u_Y =$  $1 \times 10^{-4}$  mm during the following steps. A comparison between the homogeneous model and the reference heterogeneous one are depicted in Fig. 3.17, showing that the homogeneous model is able to capture the preferential direction for the crack path induced by the microstructure. The following macroscopic parameters are obtained through the optimization procedure:  $\overline{g_c} =$  $2.388 \times 10^{-3}$  kN/mm,  $\overline{\ell} = 0.0082$  mm and  $\overline{\beta} = 50.002$ .

#### 3.4.4 Validation tests



Figure 3.18: Validation tests V3, V4 and V5.

In this section, we validate the anisotropic model on several different configurations. The first set of tests consist in cracked samples as described in Figs. 3.18.

The first one, described in Fig. 3.18 (a), involves the same geometry than used for identification of the model, but a more complex loading involving both traction and shear on the upper end of the structure. On the lower end, displacements are fixed in both directions while prescribed in both directions with increments  $\Delta u_Y = \Delta u_X = 1 \times 10^{-4}$  on the upper end. Comparison between the reference solution (heterogeneous medium) and the homogeneous one is provided in Fig. 3.20. Remarkably, both force response and crack paths are well described by the homogeneous model. We can even note that the set of microcracks which develop on the upper-right-end are captured by the homogeneous model.

Next, a traction test is considered, where the crack is shorter that in the test used for identification, as described in Fig.3.18 (b). The boundary conditions are the same than in the identification test. The crack length is equal to 0.1 L. Results are presented in Figs. 3.19. We can note from Fig. 3.19 (a) that the main direction of the crack is well captured. Here, even though the global shape of the response is similar, we note in Fig. 3.19 (b) some discrepancies between both solution for Force-displacement curves: in the heterogeneous medium  $F_{max} = 1.23$ 



Figure 3.19: Traction test with shorter crack: in heterogeneous media  $F_{max} = 1.2353$  kN at  $\overline{u} = 0.0166$  mm while in homogeneous media  $F_{max} = 1.0393$  kN at  $\overline{u} = 0.0178$  mm.

kN at u = 0.0166 mm while in homogeneous media  $F_{max} = 1.04$  kN at u = 0.0178 mm. The error in the maximum force is about 15 %.

The third test implies a porous lattice structure containing two cracks as depicted in Fig. 3.18(c). Displacements are fixed in both directions on the lower end (y = 0) and prescribed along the y- direction with 300 displacement increments  $\Delta u_Y = 1 \times 10^{-4}$  mm. Results are presented in Fig.3.21. We can observe from 3.21(a) that the crack path are accurately captured by the homogeneous model and the second preferential direction is activated, this cannot be achieved by using one preferential direction. However, we note from Fig. 3.21 (b) that even though the maximum force is well captured, the failure of the sample occurs later in the homogeneous model. This issue might be corrected in future studies by modifications of the degradation function g(d) and by formulations implying a threshold (see e.g. [123]). Note that these formulations imply more parameters, which should then be also identified in the present framework. Another source of discrepancy comes from the fact that the crack propagation is strongly influenced by the environment of the onset of the crack, which can be complex in the heterogeneous medium. Then, room for improvement of the method is possible.

Finally, a lattice structure with periodic pores is considered, which contains a large hole in its center, as depicted in Fig. 3.22. The dimensions of the sample are  $L \times H = 2 \times 1.2 \text{ mm}^2$ . Displacements are fixed in both directions on the lower face (y = 0) and only y-displacements are prescribed on the upper face y = H during 200 displacement increments  $\Delta u_Y = 1.5 \times 10^{-4}$ . Comparisons between the full-field (micro) model and the homogeneous model are presented in Figs. 3.23 and 3.24). We can note a good agreement between both models, both regarding the evaluation of the traction response and on the crack paths whose overall directions are accurately captured.


(b) Force- displacement curves

Figure 3.20: Comparison of heterogeneous media (M1) and homogeneous media (M2) in the complex test:  $Fx_{max} = 0.1737$  kN at  $\overline{u} = 0.0109$  mm,  $Fy_{max} = 0.4916$  kN at  $\overline{u} = 0.0110$  mm in M1 and  $Fx_{max} = 0.1496$  at  $\overline{u} = 0.0111$  mm,  $Fy_{max} = 0.4520$  kN at  $\overline{u} = 0.0113$  mm in M2.



Figure 3.21: Comparison of heterogeneous media(M1) and homogeneous media (M2) in the double crack test: F = 0.6959 kN at  $\overline{u} = 0.0124$  mm in M1; and F = 0.6803 kN at u = 0.0164 mm in M2



Figure 3.22: Validation test V6: a plate with a centered hole.



Figure 3.23: Comparison between heterogeneous and homogeneous models: crack patterns for a)  $\bar{u} = 0.0195$  mm; (b) $\bar{u} = 0.0255$  mm, (c)  $\bar{u} = 0.030$  mm.



Figure 3.24: Test V6 (plate with a centered hole): comparison between the heterogeneous medium response ("ref") and the homogeneous solution ("homo").

#### 3.5 Conclusion

A procedure was proposed to construct an equivalent homogeneous model for heterogeneous lattices submitted to crack propagation in the case of non-separated scales. Unlike the case of separated scales where an RVE can be considered for the micro scale, for non-separated scales, i.e. when the characteristic dimensions of inclusions are much smaller than the dimensions of the structure, the notion of RVE does not exist anymore. In the present work, we have proposed to use at the scale of the homogeneous medium phase field models, whose parameters are identified through numerical crack propagation tests in fully heterogeneous samples. Two main cases have been considered: when the microscale crack width is comparable with the dimensions of the heterogeneities, and when the crack width is much smaller. For the first case, we have shown that an isotropic phase field model accurately captures both mechanical response of the sample as well as overall crack paths. In the second case, the microstructure interacts much more with the cracks, inducing preferential directions in regular lattices, and requiring an anisotropic phase field. The results show that the homogeneous model is able to reproduce both force response and crack paths also in this situation. The identified models for crack propagation in heterogeneous media have then been validated through numerical tests involving different configurations, showing the applicability of the method. The identified model can then be used for crack propagation simulations without the need for meshing implicitly all heterogeneities.

## Chapter 4

# A surrogate approach based on neural networks for multi-scale modelling of fracture

#### Contents

4.1	Introduction							
4.2	Brief review of artificial neural network							
4.3	Construction a surrogate model for the multiscale damage model based on ANN 94							
4.4	Applications							
	4.4.1	4.4.1 A surrogate model using solution 1: ANN model						
		4.4.1.1 Test of the ANN model with isotropic regularisation 99						
		4.4.1.2 The bending beam using anisotropic regularisation 100						
		4.4.1.3 An RVE simulation						
	4.4.2 A surrogate model using resolution 2 with double ANNs model (D-ANN)							
4.5	Discu	sion and conclusion $\ldots \ldots \ldots$						

### 4.1 Introduction

In this chapter, we investigate the development of a data-driven approach based on neural networks to construct a surrogate model able to replace the costly local RVE calculations in a two-scale method such as the one presented in Chapter 2. Indeed, the computational costs in such methods are so high that it prevents their use for practical engineering applications. Even though various methods such as reduced order models [204, 78], hyper-reduction [205] or parallel computing [40] have been proposed to reduce the computational costs in FE<sup>2</sup> methods, industrial and 3D applications are still limited. A more recent technique, named self-consistent clustering analysis, has been presented in [111] can be cited as a new method based on NTFA method [166] with an efficient way of defining local clusters of constant anelastic strain field and is combined with an efficient Fourier technique to compute local solutions.

In recent years, data sciences have grown exponentially in the context of artificial intelligence, machine learning and image recognition, among many others. Application to mechanical



Figure 4.1: A single neuron [76]

modeling is more recent (see e.g. [103] for an application in case of hyperelastic heterogeneous materials). Initial applications of the machine-learning technique for modeling material behaviors can be traced back to the 1990s in the work [67], which has pointed out that the feed-forward artificial neural network can be used to replace a mechanical constitutive model. Later, various works have utilized fitting techniques including the artificial neural network (ANN) to build material laws from the experimental data, such as in [64, 104, 202, 91].

Basically, the surrogate model for a multiscale approach is a mathematical model which is constructed in order to replace the microscopic scale (RVE) calculations by an approximate surrogate model, fast to evaluate. Besides ANN, other techniques can be used in engineering applications, such as response surface methodology (RSM)[132] or Kriging [174].

Recently Le et al. proposed in [103] to construct the response of nonlinear hyperelastic RVE in a  $FE^2$  context by replacing the effective behavior response by a neural network. Recent extensions to stochastic models [17] or in combination with reduced order model [111], have substituted the computation of the RVE by a network. A notable work employing a hybrid data-driven approach to bridge through 2 length scales was presented in [189] which used the recursive neural network to replace DEM-FEM-FEM multiscale simulations.

In this chapter, we propose a numerical strategy to construct a surrogate model for the RVE response using neural networks in the case of a damageable RVE. The main difficulty here as compared to hyperelastic materials [103] is the influence of loading history, which will be handled here through the history of the damageable effective elastic tensor used as inputs for the network. Applications to 2-scale damageable heterogeneous structures are investigated.

#### 4.2 Brief review of artificial neural network.

Artificial Neural Networks (ANN) have been inspired by human brains. In such a model, each neuron is defined as a simple mathematical function. Though some concepts have appeared earlier, the origin of the modern neural network traces back to the work of Warren McCulloch



Figure 4.2: A multilayer perceptron MPL. [76]

and Walter Pitts [121] who have shown that theoretically, ANN can reproduce any arithmetic and logical function.

The simplest architecture of a neuron is depicted in Fig 4.1 where p is the net input, w is the input weight parameter, b is the bias, n denotes the net input which enters into the activation function or transfer function f, and a is the net output which is defined as:

$$a = f(wp + b). \tag{4.1}$$

When the net input and the net output are vectors, (4.1) can be rewritten as

$$a_i^k = f\left(\sum_{i=1}^m w_{ki}p_i + b_k\right),\tag{4.2}$$

where k denotes for neuron number k in the network, m is the number of input signals. Though bias scalars  $b_k$  are usually interpreted as the linear shift of the transfer output, they can be simply considered as a type of weighting scalars parameters.

Depending on the aim of the network, the ANN can be classified into unsupervised networks or supervised networks. The former corresponds to the clustering problem while the latter aims to the regression and classification problem. Various structures and applications can be found in literature such as for data series problems or extrapolation problems, one may need a recurrent neural network (RNN), or long-short term memory RNN, or a nonlinear autoregressive exogenous model (NARX). Principally, an RNN can be transferred to feed-forward ANN somehow. However, this issue is out of the scope of this section which is restricted to a feed-forward ANN devoted to an approximation problem. The name "feed-forward" refers to the data flow in the network. As can be seen in a multilayer network, also called as a multilayer perceptron (MPL) in Fig 4.2, the information moves from the input to output in contrast with the RNN where the output of one layer may enter its previous layer(s).

The key idea of the ANN surrogate is to map the given input to the given output through a network. It means that one has to specify the employed lost function (or performed function), the structure of a network associated with the number of layers and number of neurons in each layer, the activation function of each neuron. After choosing a network structure, the process estimating the weights and bias is called "the training process" or "the learning process" of the network. Various learning algorithms have been proposed in the literature which may be based on gradient such as gradient descent back-propagation (with/without momentum and adaptive learning rate), Levenberg-Marquardt, Bayesian Regularization or base on Genetic Algorithm (GA). These algorithms aim to find the information of the network to optimize the lost function which is used to evaluate the quality of the network.

### 4.3 Construction a surrogate model for the multiscale damage model based on ANN

In this section, the construction of an ANN-based surrogate model will be presented. Considering the staggered scheme proposed in section 2.4, the damage at macro scale is induced through the degradation of the material stiffness matrix  $\overline{\mathbb{C}}(d(\mathbf{x}))$ . Evaluating the macroscale material matrix requires a significant effort as it requires a phase field simulation followed by a homogenization problem on the RVE. In the following, we investigate the possibility to construct an ANN to replace the response of the RVE.

The strategy to construct a surrogate model using ANN is illustrated in Fig. 4.4. It includes:

- 1. Define the input and the output for the network.
- 2. Collect data: conduct calculations on the RVE which will be provided as input for the ANN.
- 3. Design the surrogate model: for ANN, it includes determining the number of layers and neurons, the activation function, the lost function.
- 4. Select a training algorithm: Lavenberg-Marquardt, Bayesian Regularization, Genetic Algorithm... or a combination of training algorithms.
- 5. Train the network: use the constructed data to fit the different parameters and weighting functions in the ANN. Various factors can affect the training time which can be defined by the trainer. In case the expected performance is obtained, the training process is stopped and the result will be employed. In contrast, when the performance does not reach the



4.3. Construction a surrogate model for the multiscale damage model based on ANN 95

Figure 4.3: a) Original model; b) Surogate model 1 (ANN); c) Surogate model 2 (D-ANN).



Figure 4.4: Flowchart of the construction of a surrogate model using an ANN.

expectation, another training process may be conducted with a change in the parameters (e.g the number of echoes, the minimum gradient, the learning rate in gradient-based training algorithm ...).

- 6. Analyse the performance: check the quality of the trained model, if the model does not satisfy the accuracy criteria, go back to step 2 to add data or steps 3,4,5 to obtain a new model.
- 7. Use the network: the application of network is limited by the input range which has been chosen before training.

The aim of this section is to define an ANN-based surrogate for the multiscale framework in the chapter 2 to remove the RVE calculations.

According to the multiscale framework defined in 2.4, at one macroscale the loading step,  $\overline{\mathbb{C}}_{ijkl}^{t+1}$  will depend the history of damage and on actual load. We propose to define the dependence of  $\overline{\mathbb{C}}_{ijkl}^{t+1}$  to  $\overline{\mathbb{C}}_{ijkl}^{t}$  and to the macro strain field applying on the microstructure  $\overline{\varepsilon}^{t}$ . In the 2D case, the symmetric stiffness matrix  $[\overline{\mathbb{C}}]$  is associated with 6 components which act as input parameters, in addition to the 3 independent components of the strain field yielding 9 dimensions for the input layer. In the following, we will present two surrogate solutions for the multiscale problem.

• The first solution is illustrated in Fig. 4.3b) which uses 1 network, called simply "ANN model" in the next section, to transfer between scales. The input and output are written explicitly as:

$$Input = \left[\overline{C}_{1111}^t, \overline{C}_{1122}^t, \overline{C}_{1112}^t, \overline{C}_{2222}^t, \overline{C}_{2212}^t, \overline{C}_{1212}^t, \overline{\varepsilon}_{11}^t, \overline{\varepsilon}_{22}^t, \overline{\varepsilon}_{12}^t\right]',$$

which requires 9 neurons for the input layer where as the output includes 6 neurons, written as:

$$Output = \left[\overline{C}_{1111}^{t+1}, \overline{C}_{1122}^{t+1}, \overline{C}_{1112}^{t+1}, \overline{C}_{2222}^{t+1}, \overline{C}_{2212}^{t+1}, \overline{C}_{1212}^{t+1}\right].$$

• The second solution is illustrated in Fig. 4.3c) which employs 2 networks and named as "D-ANN model" in the sequence. The first network D-ANN1 has the Input1 = Input as in the first solution while will produce the surface energy  $E_s$  or  $Output1 = [E_s]$ . The output of this network will take part in the input of the second network. Explicitly, the input and output of the second network D-ANN2 are written as:

$$Input2 = \left[\overline{C}_{1111}^t, \overline{C}_{1122}^t, \overline{C}_{1112}^t, \overline{C}_{2222}^t, \overline{C}_{2212}^t, \overline{C}_{1212}^t, \overline{\varepsilon}_{11}^t, \overline{\varepsilon}_{22}^t, \overline{\varepsilon}_{12}^t, E_s\right]',$$

which requires 10 neurons for the input layer where as the output includes 6 neurons, written as:

$$Output2 = \left[\overline{C}_{1111}^{t+1}, \overline{C}_{1122}^{t+1}, \overline{C}_{1112}^{t+1}, \overline{C}_{2222}^{t+1}, \overline{C}_{2212}^{t+1}, \overline{C}_{1212}^{t+1}\right].$$

4.3. Construction a surrogate model for the multiscale damage model based on ANN 97



Figure 4.5: Examples of data distributions: sampling sequences generated with (a) uniform grid; (b) pseudo-random; (c) Halton; (d) CVT and (e) LCVT. The panel shows the sequences corresponding to 2-D input space with a total of 25 (white circle) and 100 (black points) samples. For high dimensional input, the Halton set is appreciated. [153].

The essential material to extract a data-driven model obviously is the data. The distribution of data can affect the training time and the obtained result. The method to sample the data may be stochastic or deterministic or geometrical methods. Among those, the uniform grid method may be the simplest but having a pure coverage. Other geometrical method is Latin hypercube sampling (LHS) [122] which is supposed to induce a faster convergence but is being claimed for produces clustering of sampling points at high dimensions [153]. Besides, various methods in literature such as Centroidal Voronoi Tessellation (CTV)[53], Latinized CVT [165], Opposition Based Learning [161], Pseudo Random [115], Haltonset [153] have their own benefits and drawbacks in which the Haltonset method is supposed to give a good coverage with a minimum amount of data in case of the high dimension of input (n > 5).

The high dimensionality of the input layer induces some difficulties to obtain a good surrogate model in approximation problem using neural networks such as requirements of a large amount of data, the gradient vanishing problem when training with gradient-based learning methods, and probability of overfitting. Unfortunately, while three strain fields of the input data can be considered independent, six other fields of the effective stiffness matrix are not. In other words, the difficulty relating to the 'big data' or 'the curse of dimensionality' [183] is avoided. However, in this way, it raises difficulties for a sampling strategy.

To our best knowledge, there is no general rule to specify the optimal structure and training algorithm for large classes of problems. The training is a trying and testing process and no automated construction of network is available at the time this thesis is written, even though we can guess that this will be treated in a near future. For an approximation problem, the ANN with one hidden layer can give the expected result for any continuous function [42] while the MLP is usually applied to the classification problem. Nevertheless, when the data is extremely nonlinear, an MLP is usually employed for a good performance with a reasonable time of training.

The activation function is chosen based on the purpose of the network. Herein, for regression,



Figure 4.6: a) tansig function saturates at x = 3; b) linear function which is often employed for the output layer.

the activation function at the output layer is usually chosen to be linear, while in hidden neurons, the activation must be nonlinear. One can mainly define any nonlinear function as the transfer function. However, sigmoid or sigmoid-like functions are popular because of the correlation with their derivatives. Note that, depending on the choice of the activation, transforming the data to a suitable range is necessary to avoid the saturation.

In this section, the network is trained using Matlab®toolbox. The classical transfer function *tag-sigmoid* is employed, written as:

$$f(x) = \frac{e^x - e^{-x}}{e^x + e^{-x}},$$
(4.3)

which varies in the range [-1; 1] and starts to be saturated when x > 3 as can be seen in Fig. 4.6. This causes the vanishing gradient problem and the training will get stuck at some points. To avoid this issue, a classical normalisation is applied to the input data:

$$\mathbf{x} = 2\frac{\mathbf{x} - \mathbf{x}^{min}}{\mathbf{x}^{max} + \mathbf{x}^{min}} - 1, \tag{4.4}$$

which transfers the input to the range [-1;1]. Note that the normalisation depends on both the activation function and the input, e.g if the input is in a recommendation range for the activation function, it is not necessary to normalise. Another linear technique is available in literature, written as:  $\mathbf{x} = (\mathbf{x} - \mathbf{x}^{mean}) . / \mathbf{x}^{std}$ , where  $\mathbf{x}^{mean}$  is the average value of the input vectors in the data set, and  $\mathbf{x}^{std}$  is the vector containing the standard deviations of each element of the input vectors. Apart from these linear transformations, one may need an appropriate nonlinear transformation to improve the quality of the networks.

#### 4.4 Applications

#### 4.4.1 A surrogate model using solution 1: ANN model

In this section, the data from a simulated numerical example is used to define a model which is then used for cases where the input can be considered to be in the same range. Specifically,



Figure 4.7: Comparison of F-u curves of the multiscale model and the surrogate model.

a data-driven model from the saved results of the multiscale scheme from the bending beam in section 2.5.2 are employed. The data is doubled based on the symmetric of the microstructure including 56700 data sets of which 70% is randomly selected for training.

Name	Number of inputs	Hidden layers	Number of outputs	Performance	Number of echos
26.114	0	0	2	10.04	2000
Model 1	9	9	6	16 %	3000
Model 2	9	10-10	6	12.1~%	3000
Model 3	9	10-10-6	6	2.65%	3000

 Table 4.1: Parameters used to train the ANN.

To generate the surrogate model, several simple to complex network structures were chosen for the training whose results are shown in Tab. 4.1. The ANN has learned through Levenberg Marquart algorithm, which is the most popular choice for the approximation problem, using the mean square error (mse) for the performance function. For the best performance, the Model 3 is selected for applications in the next section.

#### 4.4.1.1 Test of the ANN model with isotropic regularisation

The selected model is employed to reproduce the beam test defined in section 2.5.2, which was used to generate the trained data. Fig. 4.7 compares the F-u curves of the damage multiscale model (DMs) and ANN model. We can see that despite having employed a complex structure



Figure 4.8: Comparison of damage evolution using trained data of the multiscale model(a1,2,3) and the surrogate model(b1,2,3) at three load steps u = 1.5 mm, 2.0 mm, 2.5 mm (from top to bottom).

with three hidden layers to reach a mean square error of 2.65%, a discrepancy is observed when using the surrogate model to re-compute the test. The critical forces are obtained respectively as 5.5602 kN (at u = 1.8 mm) and 5.0641 kN (at u = 1.6 mm), which yields a discrepancy of 8.9%. Though the ANN model fails to guess the exact value of the force but still captures the degradation trend. Comparison of the evolution of damage when using the surrogate model and the reference model is depicted in Fig 4.8 which shows that the surrogate gives a satisfying distribution of damage.

#### 4.4.1.2 The bending beam using anisotropic regularisation

The ANN is here employed to simulate the degradation of the beam bending test in section 4.4.1.1 where the applied strain on the RVE is regularized by the anisotropic process (AR) using three mesh sizes H1, H2, H3 as in Fig. 2.13. Here again, we remind that the input for the network should are in the same range than the trained input. At the present time, using very different ranges for the input parameters as compared to actual values yields large errors which are difficult to control. When using different regularization processes, different values of strain are obtained but ranges are not far from the given input.

Three mesh sizes of the damage zone are investigated. With each mesh, F-u curves of the ANN model and the anisotropic damage model are compared. Damage profiles are plotted at 3 steps: u = 1.5 mm, u = 2.0 mm, u = 2.5 mm.

Fig. 4.9 reports the results of mesh H1: the discrepancy between of critical force 5.0748 kN (u = 1.6 mm) and 4.7090 kN (u = 1.5 mm) is 7.2082 % between the DMs model and the ANN model respectively. Those of mesh H2 are 4.5050 kN (u = 1.5 mm), 4.3121 kN (u = 1.4 mm) with a difference of 4.2815% (see Fig 4.10) and of mesh H3 are 4.4857 kN (u = 1.5 mm), 4.1725



Figure 4.9: Application of the surrogate model for the same problem using anisotropic regularization with the mesh H1. Fig a) compares the F-u curves and Fig b) shows the damage profiles at 3 points P1, P2, P3 at the displacement u = 1.5 mm, 2.0 mm, 2.5 mm respectively.

kN (u = 1.4 mm) which differs at 6.9824% (see Fig 4.11). However, it is notable that after some accumulative damage, the result in the surrogate model fluctuates which prevents the damage evolving to a total fracture.

#### 4.4.1.3 An RVE simulation

To investigate the cause of the low accuracy of the ANN model, the degradation of the material stiffness matrix in a single RVE is investigated. Specifically, we prescribe 2 series of load steps with 150 strains increment of  $\Delta \varepsilon_{11} = \begin{bmatrix} 1 \times 10^{-4} & 5 \times 10^{-5} \end{bmatrix}$  on the RVE. At each step, the effective stiffness matrix is stored, and denoted by  $\overline{\mathbf{C}}^{fem}$ .

The ANN model is then employed in the two following situations:

• Case 1: the ANN is tested with every single set of input which is computed from the multiscale simulation. It means that  $\overline{\mathbf{C}}$  at time t is evaluated using the applied strain and the previous value  $\overline{\mathbf{C}}^{fem(t-1)}$ 

$$\overline{\mathbf{C}} = f_{ann} \left( \overline{\mathbf{C}}^{fem(t-1)}, \overline{\varepsilon}^t \right)$$
(4.5)

• Case 2: the effective stiffness matrix is evaluated by the ANN model completely. Specifically, the  $\overline{\mathbf{C}}$  at the time t + 1 is evaluated using the applied strain and the previous value  $\overline{\mathbf{C}}^{ann(t)}$ 

$$\overline{\mathbf{C}} = f_{ann} \left( \overline{\mathbf{C}}^{ann(t)}, \overline{\boldsymbol{\varepsilon}}^t \right)$$
(4.6)



Figure 4.10: Application of the surrogate model for same problem using anisotropic regularization with the mesh H2: a) Comparison of the F-u curves; b) Damage profiles at 3 points P1, P2, P3 at the displacement u = 1.5 mm, 2.0 mm, 2.5 mm respectively.



Figure 4.11: Application of the surrogate model for same problem using anisotropic regularization with the mesh H3: a) Comparison of the F-u curves; b) Damage profiles at 3 points P1, P2, P3 at the displacement u = 1.5 mm, 2.0 mm, 2.5 mm respectively.

The results of some selected components of the material matrix are depicted in Fig. 4.12 and Fig. 4.13 in which column (a) and (b) present the result of (4.5) and (4.6) respectively. The good match in column (a) implies that as long as the input is well evaluated, the output of the surrogate model is reliable. Meanwhile, in column (b), discrepancy appears after some degradation. It is supposed to be due to the cumulative error from previous steps, which induces the drop of the material stiffness sooner than in the FEM model. This explains the sooner degradation in previous examples (sec 4.4.1.1, 4.4.1.2) in comparison with their references.

Some additional reasons can be the cause of the above under-expected results: (i) the effective material stiffness depends on the degradation of each element in the micro-structure, so that using the material stiffness matrix is a simplification which may not give enough information for damage distribution in the microstructure; (ii) the noise of data, which is a consequence of the previous cause, not only requires an effort to train but also the good performance of the trained data does not ensure the reliability when applying for the new input.

# 4.4.2 A surrogate model using resolution 2 with double ANNs model (D-ANN)

The second test uses 2 networks to substitute the multiscale framework as shown in 4.3 c). Multiple structures were employed trying to find the substitution as showed in Table 4.2.

Name	Number of inputs	Hidden layers	Number of outputs	Performance	Number of echos
D-ANN1 (1)	9	10	1	0.00008~%	500
D-ANN1 $(2)$	9	10-10	1	0.00007~%	1000
D-ANN1 $(3)$	9	20-20	1	0.00005~%	1000
D-ANN2 $(1)$	10	10	6	13.4~%	2000
D-ANN2 (2)	10	10-10	6	3.53~%	3000
D-ANN2 $(3)$	10	20-20	6	1.32%	3000

Table 4.2: Parameters used to train the network D-ANN1 and D-ANN2.

The selected results to replace the multiscale for the double surrogate model are D-ANN1 (3) and D-ANN2 (3). Note that the output of D-ANN1 is the surface energy of the microstructure which will be one component of the input vector for D-ANN2 to generate the effective stiffness matrix. In the following we present results of D-ANN for the test in sec 4.4.1.1, 4.4.1.2.

• For the beam test using isotropic regularization and H1 mesh (sec 4.4.1.1), the critical



Figure 4.12: Comparison some components of  $\mathbb{C}_{ijkl}$  computed by the network and by FEM in a monolithic increasing strategy of  $\varepsilon_{11}$  with  $\Delta \varepsilon = 0.0001$ .



Figure 4.13: Comparison some components of  $\mathbb{C}_{ijkl}$  computed by the network and by FEM in a monolithic increasing strategy of  $\varepsilon_{11}$  with  $\Delta \varepsilon = 0.00005$ .



Figure 4.14: Application of the D-ANN for same problem using anisotropic regularization using mesh H3: a) Comparison of the F-u curves; b) Damage profiles at 3 points P1, P2, P3 at u = 2 mm, 2.3 mm, 2.5 mm respectively.

force in D-ANN is 5.5963 kN at u = 2.0 mm in comparison with their references are (5.5602 kN, 1.9 mm) which yields a 0.55 % differences at the peak. The discrepancy in the post peak can be explained by the cumulative error in 4.12.

The second test is made with the same beam but using isotropic regularization (sec 4.4.1.2): three mesh sizes (H1, H2, H3) will be taken into consideration. The results are shown in Fig. 4.15, 4.16 and 4.17 respectively. For the three mesh sizes, after reaching the peak, good agreement between the surrogate model and the original model is obtained until u = 2 mm. For the H1 mesh, the critical force of D-ANN model is 4.9680 kN at u = 1.7 mm in comparison with their references are (5.0748 kN, 1.6 mm). Those for the mesh H2 and H3 are (4.4866 kN, 1.5 mm, 4.5050 kN, 1.6 mm, 0.41%) and (4.3347 kN, 1.6 mm, 4.4857 kN, 1.6 mm, 3.37%). We can see that at the early stage of damage evolution, the D-ANN model can produce reasonable results as very small differences are observed in this stage.

#### 4.5 Discussion and conclusion

This chapter presented an attempt to replace the costly RVE calculations in the two-scale strategy developed in Chapter 2 through the development of a surrogate model based on Artificial Neural Networks (ANN). Such ANN can be viewed as a "black box" model, where the relationship between input and output are defined by a set of interconnected functions which define the network. The different coefficients of the functions are identified during an optimization phase



Figure 4.15: Application of the D-ANN for same problem using anisotropic regularization using mesh H1: a) Comparison of the F-u curves; b) Damage profiles at 3 points A1, B1, C1 at the load steps u = 1.7 mm, 2.0 mm, 2.5 mm respectively.



Figure 4.16: Application of the D-ANN for same problem using anisotropic regularization using mesh H3: a) Comparison of the F-u curves; b) Damage profiles at 3 points A2, B2, C2 at the load steps u = 1.5 mm, 2.0 mm, 2.5 mm respectively.



Figure 4.17: Application of the D-ANN for same problem using anisotropic regularization using mesh H2: a) Comparison of the F-u curves; b) Damage profiles at 3 points A3, B3, C3 at the load steps u = 1.5 mm, 2.0 mm, 2.5 mm respectively.

called "learning" step, based on advanced optimization techniques. In this work, we have used such a technique to define the relationship between the components of the damageable elastic tensor as a function of its history through its components at previous time steps and as a function of the actual effective strain state. Using data obtained from direct simulations on the RVE (sampled through the full FE<sup>2</sup> procedure), the constructed model is observed to provide reasonable results, even though discrepancies are noted, especially in the post-peak response. We have applied this technique (for the first time to our best knowledge) in the 2-scale framework and have obtained encouraging results regarding macroscopic damage profile. The computational gains are enormous, as a typical 2-scale calculation iteration can take around 252 seconds on a parallel 8-core workstation, whereas the proposed approach with the ANN surrogate model takes typically around 1 second on 1 core. However, we have to include in the ANN strategy the data construction, which implies many RVE calculations. Due to a lack of time, we could not investigate more deeply this approach, and many issues remain, e.g.: (a) the dependence to history is only done through an influence of effective elastic tensor at previous steps, which could be improved via other choices; (b) a control of the accuracy of the ANN surrogate model, especially for data set different from the range of values used for the learning step; (c) a more automatic strategy for the construction of the networks, which implies many technical choices and (d) the large computational times required to construct the data base used to train the ANN, as such technique requires a large set of data to give reasonable accuracy. In conclusion, this first attempt in constructing a reduced modem for  $FE^2$  approaches provided interesting hints and first results but showed that a large room for improvement of such techniques remains in future studies.

# Chapter 5 Conclusion

### 5.1 General conclusion

In this work, contributions to numerical multiscale methods for modeling fracture in heterogeneous quasi-brittle materials have been presented. First, we have proposed in Chapter 2 a two-scale approach in the case of separated scales, where the fracture occurs at the microscale. The local damage is modeled by the phase field method, which is fully adapted to model initiation, propagation, and merging of complex, multiple cracks such as occurring in heterogeneous media. We have proposed an original algorithm based on a staggered scheme combined with strain gradient regularization, which offers the following advantages: (a) it removes meshdependence and convergence issues which occur by direct application of classical FE<sup>2</sup> schemes in presence of damage at the microscale; (b) it does not require  $C^1$  approximation at the macroscopic scale, even though it is a strain gradient based scheme. The method has been applied to porous and composite materials, and it has been shown that such an approach is able to capture an anisotropic behavior fully induced by the microstructure. An original application of oriented cracks at the macro scale and induced by an orientation of layers at the RVE scale has been presented. However, such approach requires heavy computational times and memory, as sequences of elastic and phase field problems need to be solved at each Gauss point of the structure, and all the local damage fields must be stored for next iterations.

Secondly, in Chapter 3, we have proposed to the first time to our best knowledge, a simple method to construct a homogenized fracture model in heterogeneous media by directly identifying an anisotropic phase field model at the macro scale whose coefficients are identified by performing preliminary simulations on fully meshed and detailed heterogeneous structures such as lattice porous structures or periodic composites. The main advantage of such a technique is that once identified, the model can be used at the macro scale without new RVE calculations. In addition, non-separated scales can be handled, i.e. the homogeneous fracture model is able to operate in the case when the dimensions of the heterogeneities are not much small as compared to the characteristic dimensions of the structure. Several numerical examples have shown that once identified, very satisfying load response and mean crack paths could be captured by the model, even in configurations very different from the structure used for the identification procedure.

Finally, to alleviate these computational costs, a surrogate approach based on neural net-

works has been proposed in Chapter 4. The proposed technique builds a numerical input-output response model by learning from a collection of RVE data, for several states of macroscopic strains and damage history. Even though high dimensionality and non-independence of variables can cause difficulties for sampling and training, the surrogate model can capture the damage zone reasonably and can be evaluated at low computational costs at the macro scale. The preliminary investigations conducted in this chapter have shown that the accuracy of such a model strongly depends on the evolution of damage in the RVE and requires a large number of preliminary simulations to provide satisfactory results.

#### 5.2 Perspectives

The perspectives of this work are numerous, first from the new contributions developed, but also due to some remaining issues and limitations. Some of the possible perspectives are described as follows.

- In the case of separated scales, the right definition of the RVE in the case of fracture at the microscale remains to be clarified. Even though we have assumed localized microcracks within the RVE, a more in-depth analysis would be required to show the convergence of the macroscopic response at the macro scale in different configurations.
- The proposed two-scale strain gradient approaches inherits some drawbacks of strain gradient approaches to damage, i.e. the "broad" damage region within the crack path which required very fine meshes in the associated regions. Other formulations leading to sharper damage profiles are required to alleviate this issue.
- Direct identification of empirical anisotropic phase field models is a practical solution and can be useful in many cases, especially in the case of lattice structures where the preferential damage directions are known in advance due to the microstructure symmetries. However, a more automatic methodology to construct such homogeneous fracture models for general, 3D or random heterogeneous media still required exciting works in the future.
- The data-driven approach to multiscale damage models seems promising, but many issues remain to make such model efficient in term of learning phase (limitation of costs related to preliminary calculations) and accurate for general macroscopic loading. The main issue is the history-dependence at the RVE scale, which requires a simplified definition to be defined as an input for the neural network, and the correct definition of the sampling strategy. More specifically, feed-forward artificial networks have shown limitations in such problems. For future works, different types of network could be investigated, such as recurrent neuron network (RNN), or adaptive neuro-fuzzy inference system (ANFIS).

# Bibliography

- A. Abdollahi and I. Arias. Phase-field modeling of crack propagation in piezoelectric and ferroelectric materials with different electromechanical crack conditions. *Journal of the Mechanics and Physics of Solids*, 60:2100–2126, 2012.
- [2] J. Alfaiate, A. Simone, and LJ. Sluys. Non-homogeneous displacement jumps in strong embedded discontinuities. *International Journal of Solids and Structures*, 40(21):5799– 5817, 2003.
- [3] M. Ambati, T. Gerasimov, and L. De Lorenzis. Convergence properties of the Nelder-Mead simplex method in low dimensions. SIAM Journal od optimization, 1(9):112–143, 1998.
- [4] M. Ambati, T. Gerasimov, and L. De Lorenzis. A review on phase-field models of brittle fracture and a new fast hybrid formulation. *Computational Mechanics*, 55(2):383–405, 2015.
- [5] L. Ambrosio and V.M. Tortorelli. Approximation of functionals depending on jumps by elliptic functionals via Γ-convergence. Comm. Pure Appl. Math., 43:999–1036, 1990.
- [6] L. Ambrosio and V.M. Tortorelli. On the approximation of free discontinuity problems. Boll. U.M.I., 6-B:105–123, 1992.
- [7] H. Amor, J.-J. Marigo, and C. Maurini. Regularized formulation of the variational brittle fracture with unilateral contact: Numerical experiments. *Journal of the Mechanics and Physics of Solids*, 57(8):1209–1229, 2009.
- [8] P.M.A. Areias, J.M.A. Cesar de Sa, C.A. Conceicao Antonio, J. Carneiro, and V.M.P Teixeira. Strong displacement discontinuities and lagrange multipliers in the analysis of finite displacement fracture problems. *Computational Mechanics*, 35(1):54–71, 2004.
- [9] G.I. Barenblatt. Concerning equilibrium cracks forming during brittle fracture. the stability of isolat cracks. relationships with energetic theories. *Journal of Applied Mathematics* and Mechanics, 23(5):1273–1282, 1959.
- [10] Z.P. Bažant and E. Becq-Giraudon. Statistical prediction of fracture parameters of concrete and implications for choice of testing standard. *Cement and concrete research*, 32(4):529–556, 2002.
- [11] Z.P. Bažant and B.H. Oh. Crack band theory for fracture of concrete. Matériaux et construction, 16(3):155–177, 1983.

- [12] T. Belytschko and T. Black. Elastic crack growth in finite elements with minimal remeshing. International journal for numerical methods in engineering, 45(5):601–620, 1999.
- [13] T. Belytschko, L. Gu, and Y-Y. Lu. Fracture and crack growth by element free galerkin methods. Modelling and Simulation in Materials Science and Engineering, 2(3A):519, 1994.
- [14] T. Belytschko, S. Loehnert, and J.H. Song. Multiscale aggregating discontinuities: a method for circumventing loss of material stability. *International Journal for Numerical Methods in Engineering*, 73(6):869–894, 2008.
- [15] A. Benallal and J.-J. Marigo. Bifurcation and stability issues in gradient theories with softening. *Model. Simul. Mater. Sc.*, 15:S283–S295, 2007.
- [16] P-E. Bernard, N. Moës, and N. Chevaugeon. Damage growth modeling using the thick level set (tls) approach: Efficient discretization for quasi-static loadings. *Computer Meth*ods in Applied Mechanics and Engineering, 233:11–27, 2012.
- [17] M. A. Bessa, R. Bostanabad, Z. Liu, A. Hu, D. W. Apley, C. Brinson, W. Chen, and W. K. Liu. A framework for data-driven analysis of materials under uncertainty: Countering the curse of dimensionality. *Computer Methods in Applied Mechanics and Engineering*, 320:633–667, 2017.
- [18] M.J. Borden. Isogeometric Analysis of Phase-field Models for Dynamic Brittle and Ductile Fracture. PhD thesis, The University of Texas at Austin, 2012.
- [19] M.J. Borden, T.J.R. Hughes, CM. Landis, and C.V.. Verhoosel. A higher-order phasefield model for brittle fracture: Formulation and analysis within the isogeometric analysis framework. *Computer Methods in Applied Mechanics and Engineering*, 273:100–118, 2014.
- [20] M.J. Borden, C.V. Verhoosel, M.A. Scott, T.J.R. Hughes, and CM. Landis. A phase-field description of dynamic brittle fracture. *Computer Methods in Applied Mechanics and Engineering*, 217:77–95, 2012.
- [21] B. Bourdin. Numerical implementation of the variational formulation of quasi-static brittle fracture. *Interface Free Bound.*, 9:411–430, 2007.
- [22] B. Bourdin, GA. Francfort, and J-J. Marigo. Numerical experiments in revisit brittle fracture. Journal of the Mechanics and Physics of Solids, 48(4):797–826, 2000.
- [23] B. Bourdin, GA. Francfort, and J-J Marigo. The variational approach to fracture. Journal of elasticity, 91(1-3):5–148, 2008.

- [24] B. Bourdin, G.A. Francfort, and J.J. Marigo. Numerical experiments in revisited brittle fracture. Journal of the Mechanics ad Physics of Solids, 48:797–826, 2000.
- [25] B. Bourdin, G.A. Francfort, and J.J. Marigo. The Variational Approach to Fracture. Springer-Verlag, Berlin, 2008.
- [26] B. Bourdin, C. Larsen, and C. Richardson. A time-discrete model for dynamic fracture based on crack regularization. *Int. J. Fract.*, 168:133–143, 2011.
- [27] A. Bouterf. Comportement mécanique de la plaque de plâtre étudié par tomographie et essais mécaniques in-situ. PhD thesis, Ecole normale supérieure Cachan, 2014.
- [28] D.P. Braides. Approximation of Free Discontinuity Problems. Springer Verlag: Berlin, 1998.
- [29] D.P. Braides.  $\Gamma$ -Convergence for Beginners. Oxford University Press: New York, 2002.
- [30] M. Buliga. Energy minimizing brittle crack propagation. J. Elast., 52:201–238, 1999.
- [31] R. Müller C. Kuhn, A. Schlüter. On degradation functions in phase field fracture models. *Computational Material Science*, 108:374–384, 2015.
- [32] T. Cajuhi, L. Sanavia, and L. De Lorenzis. Phase-field modeling of fracture in variably saturat porous media. *Computational Mechanics*, 61(3):299–318, 2018.
- [33] G. T. Camacho and M. Ortiz. Computational modelling of impact damage in brittle materials. International Journal of solids and structures, 33(20-22):2899–2938, 1996.
- [34] J-L. Chaboche. Continuum damage mechanics: Part ii—damage growth, crack initiation, and crack growth. Journal of applied mechanics, 55(1):65–72, 1988.
- [35] P. Chakraborty, Y. Zhang, and Michael R. Tonks. Multi-scale modeling of microstructure dependent intergranular brittle fracture using a quantitative phase-field based method. *Computational Materials Science*, 113:38–52, 2016.
- [36] J.D. Clayton. Defects in nonlinear elastic crystals: differential geometry, finite kinematics, and second-order analytical solutions. ZAMM-Journal of Applied Mathematics and Mechanics/Zeitschrift für Angewandte Mathematik und Mechanik, 95(5):476–510, 2015.
- [37] J.D. Clayton and J. Knap. Phase field modeling and simulation of coupled fracture and twinning in single crystals and polycrystals. *Computer Methods in Applied Mechanics and Engineering*, 312:447–467, 2016.

- [38] E.W.C. Coenen, V.G. Kouznetsova, E. Bosco, and M.G.D. Geers. A multi-scale approach to bridge microscale damage and macroscale failure: a nest computational homogenization-localization framework. *International journal of fracture*, 178(1-2):157–178, 2012.
- [39] F. Corson, M. Adda-Bedia, H. Henry, and E. Katzav. Thermal fracture as a framework for quasi-static crack propagation. *International journal of fracture*, 158(1):1–14, 2009.
- [40] F. Covezzi, S. de Miranda, F. Fritzen, S. Marfia, and E. Sacco. Comparison of reduced order homogenization techniques: prbmor, nutfa and mxtfa. *Meccanica*, 53(6):1291–1312, 2018.
- [41] M.A. Crisfield. A fast incremental/iterative solution procedure that handles "snapthrough". In Computational Methods in Nonlinear Structural and Solid Mechanics, pages 55–62. Elsevier, 1981.
- [42] G. Cybenko. Approximation by superpositions of a sigmoidal function. Mathematics of control, signals and systems, 2(4):303–314, 1989.
- [43] C. Dascalu, G. Bilbie, and E.K. Agiasofitou. Damage and size effects in elastic solids: a homogenization approach. *International Journal of Solids and Structures*, 45(2):409–430, 2008.
- [44] C. Daux, N. Moës, J. Dolbow, N. Sukumar, and T. Belytschko. Arbitrary branched and intersecting cracks with the extended finite element method. *International Journal for Numerical Methods in Engineering*, 48(12):1741–1760, 2000.
- [45] R.H.J Peerlings R De and J De Vree. Gradient enhanced damage for quasi-brittle materials. International Journal for numerical methods in engineering, 39(3391-3403):68, 1996.
- [46] R. De Borst. Simulation of strain localization: a reappraisal of the cosserat continuum. Engineering computations, 8(4):317–332, 1991.
- [47] R. De Borst, M. A Crisfield, J.J.C Remmers, and C.V. Verhoosel. Damage Mechanics, chapter 6, pages 67–218. Wiley-Blackwell, 2012.
- [48] R. De Borst, L.J. Sluys, H.B. Muhlhaus, and J. Pamin. Fundamental issues in finite element analyses of localization of deformation. *Engineering computations*, 10(2):99–121, 1993.
- [49] L. De Lorenzis, A. McBride, and B.D. Reddy. Phase-field modelling of fracture in single crystal plasticity. *GAMM-Mitteilungen*, 39(1):7–34, 2016.

- [50] J.L.A. De Oliveira e Sousa and R. Gettu. Determining the tensile stress-crack opening curve of concrete by inverse analysis. *Journal of engineering mechanics*, 132(2):141–148, 2006.
- [51] H.B. Dhia. Problèmes mécaniques multi-échelles: la méthode arlequin. Comptes Rendus de l'Académie des Sciences-Series IIB-Mechanics-Physics-Astronomy, 326(12):899–904, 1998.
- [52] M.S. Dresselhaus and G. Dresselhaus. Note on sufficient symmetry conditions for isotropy of the elastic moduli tensor. *Journal of Materials Research*, 6(5):1114–1118, 1991.
- [53] Q. Du, M. Gunzburger, and L. Ju. Advances in studies and applications of centroidal voronoi tessellations. Numerical Mathematics: Theory, Methods and Applications, 3(2):119–142, 2010.
- [54] M. Duflot and H. Nguyen-Dang. Fatigue crack growth analysis by an enriched meshless method. Journal of Computational and Applied Mathematics, 168(1):155–164, 2004.
- [55] D.S. Dugdale. Yielding of steel sheets containing slits. Journal of the Mechanics and Physics of Solids, 8(2):100–104, 1960.
- [56] J. Dujc, B. Brank, and A. Ibrahimbegovic. Stress-hybrid quadrilateral finite element with embedded strong discontinuity for failure analysis of plane stress solids. *International* journal for numerical methods in engineering, 94(12):1075–1098, 2013.
- [57] G. Etse and K. Willam. Failure analysis of elastoviscoplastic material models. Journal of Engineering Mechanics, 125(1):60–69, 1999.
- [58] G. Ferté, P. Massin, and N. Moës. 3d crack propagation with cohesive elements in the extended finite element method. *Computer Methods in Applied Mechanics and Engineering*, 300:347–374, 2016.
- [59] F. Feyel. Multiscale FE<sup>2</sup> elastoviscoplastic analysis of composite structure. Computational Material Science, 16(1-4):433-454, 1999.
- [60] F. Feyel and J-L. Chaboche. Fe 2 multiscale approach for modelling the elastoviscoplastic behaviour of long fibre sic/ti composite materials. *Computer methods in applied mechanics* and engineering, 183(3):309–330, 2000.
- [61] S. Fichant, C. La Borderie, and G. Pijaudier-Cabot. Isotropic and anisotropic descriptions of damage in concrete structures. *Mechanics of Cohesive-frictional Materials: An International Journal on Experiments, Modelling and Computation of Materials and Structures*, 4(4):339–359, 1999.

- [62] G.A. Francfort and J.J. Marigo. Revisiting brittle fracture as an energy minimization problem. Journal of the Mechanics and Physics of Solids, 46(8):1319–1342, 1998.
- [63] M. Frémond and B. Nedjar. Damage, gradient of damage and principle of virtual power. International Journal of Solids and Structures, 33:1083–1103, 1996.
- [64] T. Furukawa and G. Yagawa. Implicit constitutive modelling for viscoplasticity using neural networks. International Journal for Numerical Methods in Engineering, 43(2):195– 219, 1998.
- [65] M.G.D. Geers, R. De Borst, W.A.M. Brekelmans, and R.H.J. Peerlings. Strain-based transient-gradient damage model for failure analyses. *Computer methods in applied mechanics and engineering*, 160(1-2):133–153, 1998.
- [66] T. Gerasimov, N. Noii, O. Allix, and L. De Lorenzis. A non-intrusive global/local approach applied to phase-field modeling of brittle fracture. Advanced Modeling and Simulation in Engineering Sciences, 5(1):14, 2018.
- [67] J. Ghaboussi, JH Garrett Jr., and X. Wu. Knowledge-based modeling of material behavior with neural networks. *Journal of engineering mechanics*, 117(1):132–153, 1991.
- [68] S. Ghosh, J. Bai, and D. Paquet. Homogenization-based continuum plasticity-damage model for ductile failure of materials containing heterogeneities. *Journal of the Mechanics* and Physics of Solids, 57(7):1017–1044, 2009.
- [69] C. Giry, F. Dufour, and J. Mazars. Stress-based nonlocal damage model. International Journal of Solids and Structures, 48(25-26):3431–3443, 2011.
- [70] I.M. Gitman, H. Askes, and LJ. Sluys. Representative volume: existence and size determination. *Engineering fracture mechanics*, 74(16):2518–2534, 2007.
- [71] P. Grassl and M. JiráSek. On mesh bias of local damage models for concrete. Proceedings of FraMCoS-5, Vail, USA, pages 252–262, 2004.
- [72] A. Gravouil, N. Moës, and T. Belytschko. Non-planar 3d crack growth by the extended finite element and level sets—part ii: Level set update. *International Journal for Numerical Methods in Engineering*, 53(11):2569–2586, 2002.
- [73] A.A. Griffith. The phenomena of flow and rupture in solids: Phil. Trans. Roy. Soc. Lond. Ser. A, 221:163–198, 1920.
- [74] P-A. Guidault, O. Allix, L. Champaney, and C. Cornuault. A multiscale extended finite element method for crack propagation. *Computer Methods in Applied Mechanics and Engineering*, 197(5):381–399, 2008.

- [75] G.V. Guinea, J. Planas, and M. Elices. A general bilinear fit for the softening curve of concrete. *Materials and structures*, 27(2):99–105, 1994.
- [76] M. T. Hagan, H. B. Demuth, M. H. Beale, and O. De Jesús. Neural network design. ebook, 2nd Edition.
- [77] Y. Heider and B. Markert. A phase-field modeling approach of hydraulic fracture in saturat porous media. *Mechanics Research Communications*, 80:38–46, 2017.
- [78] J.A. Hernández, J. Oliver, A. E. Huespe, M. A. Caicedo, and J. C. Cante. Highperformance model reduction techniques in computational multiscale homogenization. *Computer Methods in Applied Mechanics and Engineering*, 276:149–189, 2014.
- [79] A. Hillerborg, M. Modéer, and P. E. Petersson. Analysis of crack formation and crack growth in concrete by means of fracture mechanics and finite elements. *Cement and concrete research*, 6(6):773–781, 1976.
- [80] C.B. Hirschberger, S. Ricker, P Steinmann, and N. Sukumar. Computational multiscale modelling of heterogeneous material layers. *Engineering Fracture Mechanics*, 76(6):793– 812, 2009.
- [81] M. Hofacker and C. Miehe. Continuum phase field modeling of dynamic fracture: variational principles and staggered fe implementation. *International Journal of Fracture*, pages 1–17, 2012.
- [82] M. Hofacker and C. Miehe. A phase field model of dynamic fracture: Robust field updates for the analysis of complex crack patterns. *International Journal for Numerical Methods* in Engineering, 93:276–301, 2013.
- [83] M.Z. Hossain, C.J. Hsueh, B. Bourdin, and K Bhattacharya. Effective toughness of heterogeneous media. *Journal of the Mechanics and Physics of Solids*, 71:15–32, 2014.
- [84] Z.H. Jin, G. H. Paulino, and R. H. Dodds Jr. Cohesive fracture modeling of elastic– plastic crack growth in functionally graded materials. *Engineering Fracture Mechanics*, 70(14):1885–1912, 2003.
- [85] M. JiráSek. Nonlocal damage mechanics. Revue européenne de génie civil, 11(7-8):993– 1021, 2007.
- [86] M. JiráSek and M. Bauer. Numerical aspects of the crack band approach. Computers & Structures, 110:60–78, 2012.
- [87] L. M. Kachanov. Time of the rupture process under creep conditions, izy akad. Nank SSR Otd Tech Nauk, 8:26–31, 1958.

- [88] A. Karami and D. Stead. Asperity degradation and damage in the direct shear test: a hybrid fem/dem approach. Rock mechanics and rock engineering, 41(2):229–266, 2008.
- [89] A. Karamnejad and L.J. Sluys. A dispersive multi-scale crack model for quasi-brittle heterogeneous materials under impact loading. *Computer Methods in Applied Mechanics* and Engineering, 278:423–444, 2014.
- [90] A. Karma, D.A. Kessler, and H. Levine. Phase-field model of mode iii dynamic fracture. *Physical Review Letters*, 87(4):045501, 2001.
- [91] T. Kirchdoerfer and M. Ortiz. Data-driven computational mechanics. Computer Methods in Applied Mechanics and Engineering, 304:81–101, 2016.
- [92] D. Krajcinovic. Constitutive equations for damaging materials. Journal of applied Mechanics, 50(2):355–360, 1983.
- [93] C. Kuhn and R. Müller. A phase field model for fracture. PAMM, 8(1):10223–10224, 2008.
- [94] C. Kuhn, A. Schlüter, and R. Müller. On degradation functions in phase field fracture models. *Computational Materials Science*, 108:374–384, 2015.
- [95] M.G. Kulkarni, P.H. Geubelle, and K. Matouš. Multi-scale modeling of heterogeneous adhesives: Effect of particle decohesion. *Mechanics of Materials*, 41(5):573–583, 2009.
- [96] M.G Kulkarni, K Matouš, and P.H Geubelle. Coupled multi-scale cohesive modeling of failure in heterogeneous adhesives. International Journal for Numerical Methods in Engineering, 84(8):916–946, 2010.
- [97] S.H. Kwon, Z. Zhao, and S.P. Shah. Effect of specimen size on fracture energy and softening curve of concrete: Part ii. inverse analysis and softening curve. *Cement and Concrete Research*, 38(8-9):1061–1069, 2008.
- [98] P Ladevèze, J-C Passieux, and D Néron. The latin multiscale computational method and the proper generalized decomposition. *Computer Methods in Applied Mechanics and Engineering*, 199(21-22):1287–1296, 2010.
- [99] R. S. Lakes, S. Nakamura, J. C. Behiri, and W. Bonfield. Fracture mechanics of bone with short cracks. *Journal of biomechanics*, 23(10):967–975, 1990.
- [100] G. Lancioni and G. Royer-Carfagni. The variational approach to fracture mechanics. a practical application to the french panthéon in paris. *Journal of elasticity*, 95(1-2):1–30, 2009.

- [101] D. Lasry and T. Belytschko. Localization limiters in transient problems. International Journal of Solids and Structures, 24(6):581–597, 1988.
- [102] B.A. Le, J. Yvonnet Q.-C., and He. Computational homogenization of nonlinear elastic materials using neural networks. *Int. J. Numer. Meth. Eng.*, 104(12):1061–1084, 2015.
- [103] B.A. Le, J. Yvonnet, and Q-C. He. Computational homogenization of nonlinear elastic materials using neural networks. *International Journal for Numerical Methods in Engineering*, 104(12):1061–1084, 2015.
- [104] M. Lefik and B. A. Schrefler. Artificial neural network as an incremental non-linear constitutive model for a finite element code. *Computer methods in applied mechanics and engineering*, 192(28-30):3265–3283, 2003.
- [105] J. Lemaitre and J-L. Chaboche. Mechanics of solid materials. Cambridge university press, 1994.
- [106] F. Lene and D. Leguillon. Homogenized constitutive law for a partially cohesive composite material. *International Journal of Solids and Structures*, 18(5):443–458, 1982.
- [107] B. Li, C. Peco, D. Millán, I. Arias, and M. Arroyo. Phase-field modeling and simulation of fracture in brittle materials with strongly anisotropic surface energy. *International Journal for Numerical Methods in Engineering*, 102(3-4):711–727, 2015.
- [108] T. Liebe, P. Steinmann, and A. Benallal. Theoretical and computational numerical aspects of a thermodynamically consistent framework for geometrically linear gradient damage. *Computer Methods in Applied Mechanics and Engineering*, 190:6555–6576, 2001.
- [109] A. Lisjak, BSA. Tatone, G. Grasselli, and T. Vietor. Numerical modelling of the anisotropic mechanical behaviour of opalinus clay at the laboratory-scale using fem/dem. *Rock mechanics and rock engineering*, 47(1):187–206, 2014.
- [110] X.Y. Liu, Q.Z. Xiao, and B. L. Karihaloo. Xfem for direct evaluation of mixed mode sifs in homogeneous and bi-materials. *International Journal for Numerical Methods in Engineering*, 59(8):1103–1118, 2004.
- [111] Z. Liu, M. A. Bessa, and W. K. Liu. Self-consistent clustering analysis: an efficient multi-scale scheme for inelastic heterogeneous materials. *Computer Methods in Applied Mechanics and Engineering*, 306:319–341, 2016.
- [112] S. Loehnert and T. Belytschko. A multiscale projection method for macro/microcrack simulations. International Journal for Numerical Methods in Engineering, 71(12):1466– 1482, 2007.

- [113] E. Lorentz and A. Benallal. Gradient constitutive relations: numerical aspects and applications to gradient damage. Computer Methods in Applied Mechanics and Engineering, 194:5191–5220, 2005.
- [114] H.R. Lotfi and P.B. Shing. Embedded representation of fracture in concrete with mixed finite elements. International journal for numerical methods in engineering, 38(8):1307– 1325, 1995.
- [115] G. Marsaglia, W. W. Tsang, et al. The ziggurat method for generating random variables. Journal of statistical software, 5(8):1–7, 2000.
- [116] G. Dal Maso. An Introduction to  $\Gamma$ -Convergence. Birkhäuser Verlag: Boston, 1993.
- [117] T.J. Massart, R.H.J. Peerlings, and M.G.D. Geers. An enhanced multi-scale approach for masonry wall computations with localization of damage. *International journal for numerical methods in engineering*, 69(5):1022–1059, 2007.
- [118] K. Matouš, MG. Kulkarni, and P.H Geubelle. Multiscale cohesive failure modeling of heterogeneous adhesives. Journal of the Mechanics and Physics of Solids, 56(4):1511– 1533, 2008.
- [119] C. Maurini, B. Bourdin, G. Gauthier, and V. Lazarus. Crack patterns obtained by unidirectional drying of a colloidal suspension in a capillary tube: experiments and numerical simulations using a two-dimensional variational approach. In *Fracture Phenomena in Nature and Technology*, pages 75–91. Springer, 2014.
- [120] J. Mazars. Application of Continuous Damage Mechanic to Non-Linear Behavior of Concrete Structures. PhD thesis, PhD Thesis, Paris 6 University, Paris.(in French), 1984.
- [121] W. S. McCulloch and W. Pitts. A logical calculus of the ideas immanent in nervous activity. The bulletin of mathematical biophysics, 5(4):115–133, 1943.
- [122] M. D. McKay, R. J. Beckman, and W. J. Conover. Comparison of three methods for selecting values of input variables in the analysis of output from a computer code. *Technometrics*, 21(2):239–245, 1979.
- [123] C. Miehe, M. Hofacker, L-M Schaenzel, and F. Aldakheel. Phase field modeling of fracture in multi-physics problems. part ii. coupled brittle-to-ductile failure criteria and crack propagation in thermo-elastic-plastic solids. *Computer Methods in Applied Mechanics* and Engineering, 294:486–522, 2015.
- [124] C. Miehe, M. Hofacker, and F. Welschinger. A phase field model for rate-independent crack propagation: Robust algorithmic implementation based on operator splits. *Computer Methods in Applied Mechanics and Engineering*, 199(45):2765–2778, 2010.

- [125] C. Miehe, M. Hofacker, and F. Welschinger. A phase field model for rate-independent crack propagation: Robust algorithmic implementation based on operator splits. *Computer Methods in Applied Mechanics and Engineering*, 199:2776–2778, 2010.
- [126] C. Miehe, F. Welschinger, and M. Hofacker. A phase field model of electromechanical fracture. Journal of the Mechanics and Physics of Solids, 58:1716–1740, 2010.
- [127] N. Moës, J. Dolbow, and T. Belytschko. A finite element method for crack growth without remeshing. International journal for numerical methods in engineering, 46(1):131–150, 1999.
- [128] N. Moës, A. Gravouil, and T. Belytschko. Non-planar 3d crack growth by the extended finite element and level sets—part i: Mechanical model. International Journal for Numerical Methods in Engineering, 53(11):2549–2568, 2002.
- [129] N. Moës, C. Stolz, P-E. Bernard, and N. Chevaugeon. A level set based model for damage growth: the thick level set approach. *International Journal for Numerical Methods in Engineering*, 86(3):358–380, 2011.
- [130] H.-B. Mühlhaus and E.C. Alfantis. A variational principle for gradient plasticity. International Journal of Solids and Structures, 28(7):845–857, 1991.
- [131] D. Mumford and J. Shah. Optimal approximations by piecewise smooth functions and associated variational problems. *Commun. Pure Appl. Math.*, 42:577–685, 1989.
- [132] R. H Myers. Response surface methodology—current status and future directions. Journal of Quality Technology, 31(1):30–44, 1999.
- [133] A. Needleman. Material rate dependence and mesh sensitivity in localization problems. Computer methods in applied mechanics and engineering, 67(1):69–85, 1988.
- [134] A. Needleman. An analysis of tensile decohesion along an interface. Journal of the Mechanics and Physics of Solids, 38(3):289–324, 1990.
- [135] G. D. Nguyen. A damage model with evolving nonlocal interactions. International Journal of Solids and Structures, 48(10):1544–1559, 2011.
- [136] N. Nguyen, J. Yvonnet, J. Réthoré, and A.B. Tran. Identification of fracture models based on phase field for crack propagation in heterogeneous lattices in a context of non-separat scales. *Computational Mechanics*, pages 1–22, 2018.
- [137] T.H.A. Nguyen, T.Q. Bui, and S. Hirose. Smoothing gradient damage model with evolving anisotropic nonlocal interactions tailored to low-order finite elements. *Computer Methods* in Applied Mechanics and Engineering, 328:498–541, 2018.

- [138] T.T Nguyen, J Réthoré, and Marie-C Baietto. Phase field modelling of anisotropic crack propagation. European Journal of Mechanics-A/Solids, 65:279–288, 2017.
- [139] T.T. Nguyen, J. Rethoré, J. Yvonnet, and M.C. Baietto. Multi-phase-field modeling of anisotropic crack propagation for polycrystalline materials. *Comput. Mech.*, 60(2):289– 314, 2017.
- [140] T.T. Nguyen, J. Yvonnet, M. Bornert, and C. Chateau. Direct comparisons of 3D crack networks propagation in cementitious materials between phase field numerical modeling and in-situ microtomography experimental images. J. Mech. Phys. Solids, 95:320–350, 2016.
- [141] T.T Nguyen, J. Yvonnet, M. Bornert, C. Chateau, F. Bilteryst, and E. Steib. Large-scale simulations of quasi-brittle microcracking in realistic highly heterogeneous microstructures obtained from micro ct imaging. *Extreme mechanics letters*, 17:50–55, 2017.
- [142] T.T. Nguyen, J. Yvonnet, M. Bornert, C. Chateau, K. Sab, R. Romani, and R. Le Roy. On the choice of parameters in the phase field method for simulating crack initiation with experimental validation. *International Journal of Fracture*, 197(2):213–226, 2016.
- [143] T.T. Nguyen, J. Yvonnet, Q.-Z. Zhu, M. Bornert, and C. Chateau. A phase field method to simulate crack nucleation and propagation in strongly heterogeneous materials from direct imaging of their microstructure. *Engineering Fracture Mechanics*, 139:18–39, 2015.
- [144] V. P. Nguyen. Discontinuous galerkin/extrinsic cohesive zone modeling: Implementation caveats and applications in computational fracture mechanics. *Engineering fracture mechanics*, 128:37–68, 2014.
- [145] VP. Nguyen, O. Lloberas-Valls, M. Stroeven, and LJ Sluys. Homogenization-based multiscale crack modelling: from micro-diffusive damage to macro-cracks. *Computer Methods* in Applied Mechanics and Engineering, 200(9):1220–1236, 2011.
- [146] J. Oliver, M. Caicedo, E. Roubin, A. E. Huespe, and J.A. Hernández. Continuum approach to computational multiscale modeling of propagating fracture. *Computer Methods in Applied Mechanics and Engineering*, 294:384–427, 2015.
- [147] J. Oliver, A.E. Huespe, and P.J. Sánchez. A comparative study on finite elements for capturing strong discontinuities: E-fem vs x-fem. Computer methods in applied mechanics and engineering, 195(37-40):4732–4752, 2006.
- [148] M. Ortiz and A. Pandolfi. Finite-deformation irreversible cohesive elements for threedimensional crack-propagation analysis. *International journal for numerical methods in engineering*, 44(9):1267–1282, 1999.

- [149] N. S. Ottosen. Thermodynamic consequences of strain softening in tension. Journal of engineering mechanics, 112(11):1152–1164, 1986.
- [150] K. Park, G.H. Paulino, and J.R. Roesler. Determination of the kink point in the bilinear softening model for concrete. *Engineering Fracture Mechanics*, 75(13):3806–3818, 2008.
- [151] E. M. Passmore. Strength-grain size-porosity relations in alumina. Jour. of the Amer. Ceramic Society, 48(1), 1965.
- [152] R.U. Patil, B.K. Mishra, and I.V. Singh. An adaptive multiscale phase field method for brittle fracture. *Computer Methods in Applied Mechanics and Engineering*, 329:254–288, 2018.
- [153] M. Pedergnana, S. G. García, et al. Smart sampling and incremental function learning for very large high dimensional data. *Neural Networks*, 78:75–87, 2016.
- [154] R.H.J. Peerlings, R. de, W.A.M. Brekelmans, and H.P.J. de Vree. Gradient-enhanced damage for quasi-brittle materials. *International Journal for Numerical Methods in En*gineering, 39(39):3391–3403, 1996.
- [155] R.H.J. Peerlings, R. De Borst, WAM. Brekelmans, and M.G.D. Geers. Gradient-enhanced damage modelling of concrete fracture. *Mechanics of Cohesive-frictional Materials: An International Journal on Experiments, Modelling and Computation of Materials and Structures*, 3(4):323–342, 1998.
- [156] K. Pham and J.-J. Marigo. The variational approach to damage: I. the foundations. C. R. Mecanique, 338:191–198, 2010.
- [157] K. Pham, J.-J. Marigo, and C. Maurini. The issues of the uniqueness and the stability of the homogeneous response in uniaxial tests with gradient damage models. J. Mech. Phys. Solids, 59(6):1163–1190, 2011.
- [158] G. Pijaudier-Cabot and Z.P. Bažant. Nonlocal damage theory. Journal of engineering mechanics, 113(10):1512–1533, 1987.
- [159] L. H. Poh and S. Swaddiwudhipong. Over-nonlocal gradient enhanced plastic-damage model for concrete. *International Journal of Solids and Structures*, 46(25-26):4369–4378, 2009.
- [160] P. Raghavan and S Ghosh. A continuum damage mechanics model for unidirectional composites undergoing interfacial debonding. *Mechanics of Materials*, 37(9):955–979, 2005.
- [161] S. Rahnamayan, H. R. Tizhoosh, and M. M. A. Salama. Opposition-based differential evolution. *IEEE Transactions on Evolutionary computation*, 12(1):64–79, 2008.
- [162] J. Réthoré, TBT. Dang, and C. Kaltenbrunner. Anisotropic failure and size effects in periodic honeycomb materials: A gradient-elasticity approach. *Journal of the Mechanics* and Physics of Solids, 99:35–49, 2017.
- [163] E Riks. An incremental approach to the solution of snapping and buckling problems. International journal of solids and structures, 15(7):529–551, 1979.
- [164] R. Romani, M. Bornert, D. Leguillon, R. Le Roy, and K. Sab. Detection of crack onset in double cleavage drilled specimens of plaster under compression by digital image correlation-theoretical predictions based on a coupled criterion. *European Journal of Mechanics-A/Solids*, 51:172–182, 2015.
- [165] V. J. Romero, J. V. Burkardt, M. D. Gunzburger, and J. S. Peterson. Comparison of pure and "latinized" centroidal voronoi tessellation against various other statistical sampling methods. *Reliability Engineering & System Safety*, 91(10-11):1266–1280, 2006.
- [166] S. Roussette, J.C. Michel, and P. Suquet. Non uniform transformation field analysis of elastic-viscoplastic composites. *Composite Science and Technology*, 69:22–27, 2009.
- [167] E. Rudoy. Domain decomposition method for crack problems with nonpenetration condition. ESAIM: Mathematical Modelling and Numerical Analysis, 50(4):995–1009, 2016.
- [168] J.M. Sargado, E. Keilegavlen, I. Berre, and J.M. Nordbotten. High-accuracy phase-field models for brittle fracture based on a new family of degradation functions. *Journal of the Mechanics and Physics of Solids*, 2017.
- [169] A.; Schlüter, A.; Willenbücher, C. Kuhn, and R Müller. Phase field approximation of dynamic brittle fracture. *Computational Mechanics*, 54(5):1141–1161, 2014.
- [170] G.K. Sfantos and M.H. Aliabadi. Multi-scale boundary element modelling of material degradation and fracture. *Computer Methods in Applied Mechanics and Engineering*, 196(7):1310–1329, 2007.
- [171] P. Sicsic, J-J. Marigo, and C. Maurini. Initiation of a periodic array of cracks in the thermal shock problem: a gradient damage modeling. *Journal of the Mechanics and Physics of Solids*, 63:256–284, 2014.
- [172] J. C. Simo, J. Oliver, and F. Armero. An analysis of strong discontinuities induced by strain-softening in rate-independent inelastic solids. *Computational mechanics*, 12(5):277– 296, 1993.
- [173] A. Simone, H. Askes, and LJ. Sluys. Incorrect initiation and propagation of failure in non-local and gradient-enhanced media. *International Journal of Solids and Structures*, 41(2):351–363, 2004.

- [174] T. W. Simpson, T. M. Mauery, J. J. Korte, and F. Mistree. Kriging models for global approximation in simulation-based multidisciplinary design optimization. AIAA journal, 39(12):2233–2241, 2001.
- [175] V. Slowik, B. Villmann, N. Bretschneider, and T Villmann. Computational aspects of inverse analyses for determining softening curves of concrete. *Computer Methods in Applied Mechanics and Engineering*, 195(52):7223–7236, 2006.
- [176] J.H. Song, P.M.A. Areias, and T. Belytschko. A method for dynamic crack and shear band propagation with phantom nodes. *International Journal for Numerical Methods in Engineering*, 67(6):868–893, 2006.
- [177] B. F. Sørensen and T. K. Jacobsen. Determination of cohesive laws by the j integral approach. *Engineering fracture mechanics*, 70(14):1841–1858, 2003.
- [178] N. Sukumar, D.L. Chopp, and B. Moran. Extended finite element method and fast marching method for three-dimensional fatigue crack propagation. *Engineering Fracture Mechanics*, 70(1):29–48, 2003.
- [179] P.M. Suquet. Elements of homogenization for inelastic solid mechanics, homogenization tech—niques for composite media,(sanchez-palencia, e. and zaoui, a., ed.),(1987).
- [180] K. Terada, M. Hori, T. Kyoya, and N. Kikuchi. Simulation of the multi-scale convergence in computational homogenization approaches. *International Journal of Solids and Structures*, 37(16):2285–2311, 2000.
- [181] Q-T. Tran, T. Rabczuk, Y. Bazilevs, and G. Meschke. A higher-order stress-based gradient-enhanced damage model based on isogeometric analysis. *Computer Methods* in Applied Mechanics and Engineering, 304:584–604, 2016.
- [182] F.P. Van Der Meer and L.J. Sluys. The thick level set method: sliding deformations and damage initiation. Computer Methods in Applied Mechanics and Engineering, 285:64–82, 2015.
- [183] V. Vapnik. Estimation of dependences based on empirical data. Springer Science & Business Media, 2006.
- [184] C. Verhoosel and R. de Borst. A phase-field model for cohesive fracture. International Journal for Numerical Methods in Engineering, 96:43–62, 2013.
- [185] C.V.. Verhoosel, J-JC. Remmers, and MA. Gutiérrez. A partition of unity-based multiscale approach for modelling fracture in piezoelectric ceramics. *International journal for numerical methods in engineering*, 82(8):966–994, 2010.

- [186] C.V. Verhoosel, J.J.C Remmers, M.A. Gutiérrez, and R De Borst. Computational homogenization for adhesive and cohesive failure in quasi-brittle solids. *International Journal* for Numerical Methods in Engineering, 83(8-9):1155–1179, 2010.
- [187] J. Vignollet, S. May, René DB, and C.V.. Verhoosel. Phase-field models for brittle and cohesive fracture. *Meccanica*, 49(11):2587–2601, 2014.
- [188] H. Waisman and L. Berger-Vergiat. An adaptive domain decomposition preconditioner for crack propagation problems modeled by xfem. *International Journal for Multiscale Computational Engineering*, 11(6), 2013.
- [189] K. Wang and W. Sun. A multiscale multi-permeability poroplasticity model linked by recursive homogenizations and deep learning. *Computer Methods in Applied Mechanics* and Engineering, 334:337–380, 2018.
- [190] Y. Wang, C. Cerigato, H. Waisman, and E. Benvenuti. Engineering Fracture Mechanics, 178:148–168, 2017.
- [191] Z. Wang, Ti. Yu, T.Q. Bui, S. Tanaka, C. Zhang, Sohichi Hirose, and J-L Curiel-Sosa. 3-d local mesh refinement xfem with variable-node hexahedron elements for extraction of stress intensity factors of straight and curved planar cracks. *Computer Methods in Applied Mechanics and Engineering*, 313:375–405, 2017.
- [192] G.N. Wells and L.J. Sluys. A new method for modelling cohesive cracks using finite elements. International Journal for Numerical Methods in Engineering, 50(12):2667–2682, 2001.
- [193] Z.A. Wilson and C.M. Landis. Phase-field modeling of hydraulic fracture. Journal of the Mechanics and Physics of Solids, 96:264–290, 2016.
- [194] J.Y. Wu, F.B. Li, and S.L. Xu. Extended embedded finite elements with continuous displacement jumps for the modeling of localized failure in solids. *Computer Methods in Applied Mechanics and Engineering*, 285:346–378, 2015.
- [195] J.Y. Wu and V.P. Nguyen. A length scale insensitive phase-field damage model for brittle fracture. Journal of the Mechanics and Physics of Solids, 2018.
- [196] T. Wu, A. Carpiuc-Prisacari, M. Poncelet, and L De Lorenzis. Phase-field simulation of interactive mixed-mode fracture tests on cement mortar with full-field displacement boundary conditions. *Engineering Fracture Mechanics*, 182:658–688, 2017.
- [197] L. Xia, J. Yvonnet, and S. Ghabezloo. Phase field modeling of hydraulic fracturing with interfacial damage in highly heterogeneous fluid-saturat porous media. *Engineering Fracture Mechanics*, 186:158–180, 2017.

- [198] S.P. Xiao and T. Belytschko. A bridging domain method for coupling continua with molecular dynamics. *Computer methods in applied mechanics and engineering*, 193(17-20):1645–1669, 2004.
- [199] X-P. Xu and A. Needleman. Void nucleation by inclusion debonding in a crystal matrix. Modelling and Simulation in Materials Science and Engineering, 1(2):111, 1993.
- [200] X.-P. Xu and A. Needleman. Numerical simulations of fast crack growth in brittle solids. Journal of the Mechanics and Physics of Solids, 42(9):1397–1434, 1994.
- [201] X. P. Xu and A. Needleman. Numerical simulations of dynamic crack growth along an interface. *International Journal of Fracture*, 74(4):289–324, 1996.
- [202] G. J. Yun, J. Ghaboussi, and A. S. Elnashai. A new neural network-based model for hysteretic behavior of materials. *International Journal for Numerical Methods in Engineering*, 73(4):447–469, 2008.
- [203] J. Yvonnet. Computational Homogenization With Finite Elements. Springer, to appear, 2019.
- [204] J. Yvonnet and Q.C. He. The reduced model multiscale method (r3m) for the non-linear homogenization of hyperelastic media at finite strains. *Journal of Computational Physics*, 223(1):341–368, 2007.
- [205] M. J. Zahr, P. Avery, and C. Farhat. A multilevel projection-based model order reduction framework for nonlinear dynamic multiscale problems in structural and solid mechanics. *International Journal for Numerical Methods in Engineering*, 112(8):855–881, 2017.
- [206] X. Zeng and S. Li. A multiscale cohesive zone model and simulations of fractures. Computer methods in applied mechanics and engineering, 199(9-12):547–556, 2010.
- [207] Z. Zhang, G. H. Paulino, and W. Celes. Extrinsic cohesive modelling of dynamic fracture and microbranching instability in brittle materials. *International Journal for Numerical Methods in Engineering*, 72(8):893–923, 2007.
- [208] T.I. Zohdi, J.T. Oden, and G.J. Rodin. Hierarchical modeling of heterogeneous bodies. Computer methods in applied mechanics and engineering, 138(1-4):273–298, 1996.