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Research plan on novel tools for the prediction of fracture initiation

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1. INTRODUCTION

The Work Package 4 (WP4) "Novel tools for the prediction of fracture in heterogeneous materials" deals with the fundamental scientific problems underlying the NewFrac training network. This report describes the updated objectives of WP4, the specified work plans of the Individual Research Projects (IRPs). The work package is structures in 7 tasks. Each of them is associated to a main Early Stage Researcher (ESR) and a main Supervisor. The goal of this document is to present an updated version of the overall research plan for WP4. In the following, we review the overall objectives, the project partners involved are introduced, and the interactions between them are highlighted. Detailed work plans for the individual Early Stage Researchers (ESRs) and the related tasks in WP are presented in Section 2.

The Lead Beneficiary of this Work Package 4 (WP4) is Sorbone Universite (US). The other participants are Universidad de Sevilla (US), Politecnico di Torino (POLITO), Eidgenoessische Technische Hochschule Zürich (ETH), University of Porto (FEUP), IMT School for Advanced Studies Lucca (IMT), Tel Aviv University (TAU), Robert Bosch GmbH (RB), Foundation for the Research Development and Application of Composite Materials, Airbus Group (FIDAMC).

a. Objectives of Work Package 4

The objective of this Work Package 4 is the development of new virtual testing techniques able to track the initiation and propagation of the fracture phenomena across the scales in the study of complex materials as composites, layered ceramics, photovoltaics, and biomaterials.

We will develop techniques to predict crack nucleation within the Phase-Field (PF) and Finite Fracture Mechanics (FFM) approaches.

Our principal aims are:

1. Identify the key features and limitations of the available PF and FFM techniques in predicting the experimental results for simple (homogenous, isotropic) and complex (e.g. heterogeneous, anisotropic) materials under simple (traction, quasi-static) and complex (multiaxial, fatigue, dynamic) loadings.
2. Improve the available PF and FFM approaches to overcome these limitations.
3. Implement in novel computational tools the proposed improvements and validate them against experimental results.
4. Apply the new techniques to the advanced application contexts of the different ESR (e.g. multi-layer composites, fiber-composites, bones).
5. Perform a critical comparative analysis of the PF and FFM approaches and attempt to propose approaches to combine the benefits of both.

The main idea behind these modelling techniques is the combination of the new Phase Field (PF) approach with the Coupled Criterion of Finite Fracture Mechanics (CCFFM) to simulate fracture phenomena focusing on (sudden) crack initiation and their interactions with interfaces. The CCFFM will be especially suitable for these fracture problems, in the context of analytical and semi-analytical problems. However, the application of CCFFM is currently limited to a specialized community due to a lack of a computational implementation. Thus, the aim of the development of a hybrid approach combining the best of each method, PF and CCFFM, is to cover a relevant gap. Additionally, an extension of the techniques for the application of PF and CCFFM to crack initiation under impacts and to dynamic crack propagation is necessary. The PF approach, very promising for the study of crack branching and fragmentation, will permit overcoming the main flaws typical for other methodologies that have been extensively used to analyze dynamic crack propagation problems. These modeling techniques will be verified against experimental results. The goal is to implement these new strategies for fracture following an application-driven approach based on their use for design and optimization in the industrial environment, because in early design stages and optimization processes, efficient models of fracture initiation and propagation are crucial. Our goal is to make a significant step forward on the key issues in FFM and PF, that will allow developing general computational tools able to solve complex fracture problems tackled in WP5.

Figure 1 bellow gives an overview of all ESRs with a focus on both the key issues addressed by CCFFM/ PF and the advanced applications thereof. In this illustration, the ESRs mainly belonging to work package 5 are shaded in dark grey whereas the ESRs belonging to work packages 4 and 5 are shaded in light grey.

Key issues to be addressed	ESRs 1	2	3	4	5	6	7	8	9	10	11	12	13	Advanced applications
Anisotropy in strength + fracture toughness modeling					●			●		●				Bones
Flat + curved multilayer modeling	●		●		●									Ceramics
Impact + dynamic crack growth	●		●	●			●				●	●		LFRP composites
Inelastic deformation modeling		●	●										●	Microstructure optimization
Fragmentation modeling			●										●	Multigrains
Multifield modeling	●								●					Composites for renewables
Multiscale modeling	●				●	●								SFRP composites
Total energy minimization w/stress condition														

WP 4 | WP 4 and WP 5 | WP 5

Figure 1. Key issues and advanced applications regarding CCFFM/PF addressed by each ESR and allocation to work packages.

In comparison to the grant agreement, slight refinements have been made, which have emerged in the course of more concrete project planning. This figure gives only a very compact representation of the topics covered by the ESRs, a detailed description of the Individual Research Projects (IRPs) follows in Section 2 of this report.

b. Scientific Background: The crack initiation problem.

Correctly modelling the nucleation of new cracks is one of the key issues of fracture mechanics. Within this project it is an essential problem for predicting and enhance the effective toughness of heterogenous material, modelling fracture of biomaterials, or improving the structural strength.

Linear Elastic Fracture Mechanics (LEFM). From a modeling standpoint, the Linear Elastic Fracture Mechanics (LEFM) theory establishes several concepts and principles, which are the basis for the prediction of growth of cracks and analysis of fracture events in brittle and ductile materials. The main limitations of LEFM-based procedures are associated with: (i) the incapacity to predict crack onset around stress concentrations and weak singularities, such as notched or holed specimens, V-notches and multi-material corners, (ii) the notable operative difficulties for their use in complex geometry definitions and/or heterogeneous media, (iii) the limiting modeling framework, since they are restricted to linear elasticity and (iv) the notable effort required for triggering crack branching and coalescence, especially in 3D predictions, among other aspects.

Finite Fracture Mechanics (FFM). This approach establishes the instantaneous appearance of a finite-size crack once the material strength criterion and an energy criterion are satisfied simultaneously. This compromise between the two criteria is proposed since the stress criterion exclusively governs the failure of certain problems (for example in the absence of stress concentrators), whereas in other situations, the energy criterion governs the failure (e.g. solids with sufficiently large cracks). Therefore, the FFM postulates that in "intermediate" cases such as solids with stress concentrators or stress singularities weaker than that corresponding to a crack, fracture will start when both criteria are met. This methodology overcomes one of the main limitations of Griffith's classical criterion for predicting the initiation of a crack in stress concentrators or weak stress singularities. The FFM has shown a great ability to predict crack initiation in a very versatile way in multiple problems and materials. This modeling technique will be applied for predictive analysis in composites (Tasks 4.01, 4.04; ESRs-1, 7,11), hard biological tissues (Tasks 4.05, ESRs-10) and layered ceramics (WP4, Task 4.02; ESR-3).

Phase Field (PF). This computational technique entails a diffuse representation of cracks by a damage variable, which governs the process of material degradation. PF can be considered as special gradient damage model, retrieving a precise energetic equivalence with brittle fracture theory. This formulation also includes a length parameter, to regularize the crack representation in a given band. In recent studies it has been shown that in simple materials this length-scale plays a fundamental role for fracture initiation. For mode-I opening cracks, it can be tuned to recover to experimental traction strength of the materials. However, many issues remains open, e.g. predicting nucleation of cracks under compressive loading or multi-axial loading (task 4.03, ESR 5) , modelling crack of complex materials, as heterogenous materials (tasks 4.04, 4.06, ESR 7-12), anisotropic materials, almost incompressible biological materials (task 4.05, ESR 10), modelling dynamical effect (task 4.07, ESR 13).

Hybrid PF-FFM. Both PF and FFM approaches are based on a common underlying idea of minimization of the total energy functional by using either regularized or discontinuous crack representations, respectively, and considering in same way the stress criterion (very recently in the PF approach). Thus, in the development of new fracture-modeling strategies, two schemes for a consistent hybridization of PF and FFM will be applied, namely staggered and multi-scale hybridizations. In the former, some preliminary ideas of application of stress criteria in PF will be further advanced by applying the coupled stress and energy criterion of FFM (CCFFM) in each time step of PF algorithm to identify/control relevant finite crack advances. In the latter, FFM and PF will be applied at different scales, FFM at micro and PF at meso- or macro-scale. These hybridization schemes of FFM and PF will be conducted in WP4: Tasks 4.01, 4.05 and 4.07 by ESRs-1,8,10,13. These novel fracture-modeling strategies will be also employed for the analysis of several industrial applications under development in WP5: Tasks 5.01-02, 5.05-07 (ESRs- 2,4,8-11).

2. MAIN TASKS, PARTNERS AND EARLY STAGE RESEARCHERS

The project partners US, SU, FEUP, RB, POLITO, ETH, SAFRAN, IMT, and FIDAMC are assigned to Work Package 4. This WP is structured in seven tasks. Each task is associated to a main ESR and a main supervisor. The supervisor in charge of the supervision of the ESR and the coordination of the work of the different partners in the specific task. The following list resumes this organization of the work package:

- Task 4.01 – ESR 1: Development of total energy minimization with stress conditions and a hybrid CCFFM and PF methodology for fracture in anisotropic heterogeneous materials and structures
  Leader: US; Participants: IMT, SU, RB; Supervisor: V. Mantic.

- Task 4.02 – ESR 3: Adaptation of the new techniques to the fracture of ceramics
  Leader: SU; Participants: US, SAFRAN; Supervisor: D. Leguillon.

- Task 4.03 – ESR 5: Methods for compressive crack analysis by PF
  Leader: SU; Participants: ETH, RB; Supervisor: C. Maurini.

- Task 4.04 – ESR 7: Adaptation of the new techniques to the study of debonding
  Leader: POLITO; Participants: ETH, FIDAMC; Supervisor: P. Cornetti.

- Task 4.05 – ESR 10: Adaptation of the CCFFM, PF and hybrid methods to biomaterials
  Leader: ETH; Participants: TAU, SU, RB ; Supervisor : L. De Lorenzis.

- Task 4.06 – ESR 12: Adaptation of the new techniques to the multiscale analysis of composites
  Leader: FEUP; Participants: US, FIDAMC; Supervisor: P.Camanho

- Task 4.07 – ESR 13: Extension of the CCFFM and PF methodologies to dynamic fracture
  Leader: POLITO; Participants: US, IMT, BOTTERO, Supervisor: M.Corrado.

In the next Sections we report the detailed of the research project for each task, by exposing the Individual research plan of the related ESR. We believe that this approach (association of task to ESR) is the best method to assure the supervision and the advancement of the project. The main supervisor of the related ESR is identified as the responsible of the task in the network.

Expected strong collaboration with ESRs

ESRs	1	2	3	4	5	6	7	8	9	10	11	12	13
1			●						●		●		
2	●		●		●					●			
3		●		●							●	●	
4												●	
5						●		●		●			
6					●					●			
7	●										●		●
8		●			●	●				●			
9	●												●
10					●	●		●					
11	●	●	●				●						
12				●									
13	●						●		●				

Figure 2. Overview of all the interaction between the participants ESRs

a. Task 4.01 – ESR 1: Development of total energy minimization with stress conditions and a hybrid CFFM and PF methodology for fracture in anisotropic heterogeneous materials and structures.

Fellow	Host institution	PhD enrolment (Y/N)	Start date	Duration (months)	Deliverables
ESR-01	US	**Y**	**M7**	**36**	**D4.05, D4.12**

Project Title and Work Package(s) to which it is related: *Total energy minimization with stress conditions for mixed mode fracture in anisotropic heterogeneous materials and structures (WP4)*

Objectives: A general and challenging aim of the theoretical developments and computational implementations of this task is an accurate and reliable prediction for mixed mode fracture problems involving simultaneous crack onset, propagation, and interactions with interfaces in piecewise homogeneous anisotropic brittle materials. For this aim a new computational methodology based on the PMTE-SC (Mantic 2014), is expected to be implemented in a FEM code and tested. Although the PMTE-SC is equivalent to the classical formulation of the CCFFM (Leguillon 2002), it appears that PMTE-SC is more suitable for a general-purpose FEM implementation based on a time-stepping procedure (Muñoz-Reja 2020). Application of several methods for a discontinuous representation of cracks will be analysed, e.g. XFEM and its variants as Phantom or Floating Node Methods, VFEM, and/or using a discontinuous damage variable defined elementwise or edgewise in a FEM mesh.

Additionally, optimization strategies suitable for minimization of Total Energy (potential+dissipated) subject to a Stress Condition should be developed. Additionally, in this IRP several possibilities to impose a stress condition in the Phase Field (PF) method for fracture with a regularized/diffused representation of cracks will be explored to get a reliable predictive methodology agreeing with experimental observations. For this objective, e.g., novel forms of the degradation and local fracture energy functions and/or staggered hybrid CCFFM and PF schemes, providing necessary information to the PF algorithm in terms of suitable boundary/interface conditions or prescribed values for PF damage variable in each time step, will be studied. Validation of the computational tools developed by their application to a few industrial fracture problems at different scales in heterogeneous materials and structures.

Principal tasks of ESR-1:

1. *Computational implementation of the PMTE-SC to solve mixed mode fracture problems with interfaces in anisotropic brittle materials.*

1.1 Study of the most successful discontinuous representations of cracks focusing on their prospective application in the PMTE-SC. Especially, either strategies defining the crack path independently of the initial FE mesh, e.g., XFEM/GFEM and its variants as Phantom Node or Floating Node Methods, or defining the crack path as dependent on the initial (sufficiently refined) FE mesh, e.g., with the damage variable defined element-wise or edge-wise leading to "killing element" or splitting mesh nodes+edges approaches. Regarding the crack discretization by the XFEM and its variants, a key issue is to check/ensure the decreasing character of the potential energy for a growing crack, i.e. unzipping nodes along the discretized crack path, which is crucial for the minimization of the total energy.

1.2 Study of previous computational (FEM/BEM) implementations the CCFFM, focusing on implementation strategies, successful features and difficulties found in their applications.

1.3 Proposal of the most promising discretization strategies for PMTE-SC, their preliminary computational implementations (presumably in FEniCS), testing and comparison. Selection of the most suitable strategy for the final implementation.

1.4 Development, testing and comparison of optimization procedures for PMTE-SC, e.g., a modified staggered scheme aimed at global optimization in the feasible parameter-region given by the stress condition taking advantage of the efficiency of its computational implementation.

1.5 General purpose computational implementation in a FEM code of the PMTE-SC for mixed mode fracture problems with interfaces in isotropic and anisotropic brittle materials. Anisotropy of a material implies that both strength and fracture energy are directionally dependent. Testing of the procedure implemented and adjusting its parameters on several benchmark problems.

2. *Computational implementation of strategies to impose stress criteria in the PF*.

2.1 Critical study of different strategies to impose a stress condition in the PF with a regularized/diffused representation of cracks, e.g., by novel forms of the degradation and local fracture energy functions and staggered hybrid CCFFM and PF schemes, providing necessary information to the PF algorithm, e.g., in terms of suitable boundary/interface conditions or prescribed values for PF damage variable in each time step.

2.2 Proposal of the most promising discretization strategies to impose a stress condition in the PF, their preliminary computational implementations (presumably in FEniCS), testing and comparison. Selection of the most suitable strategy for the final implementation.

2.3 General purpose computational implementation in a FEM code of PF with an imposed stress criterion, for mixed mode fracture problems with interfaces in brittle materials. Testing of the procedure implemented and adjusting its parameters on several benchmark problems.

3. *Application of these computational tools to a few challenging industrial problems solved by other ESRs and/or proposed by enterprises by NewFrac TTLab.*
4. *Elaboration of PhD Thesis.*

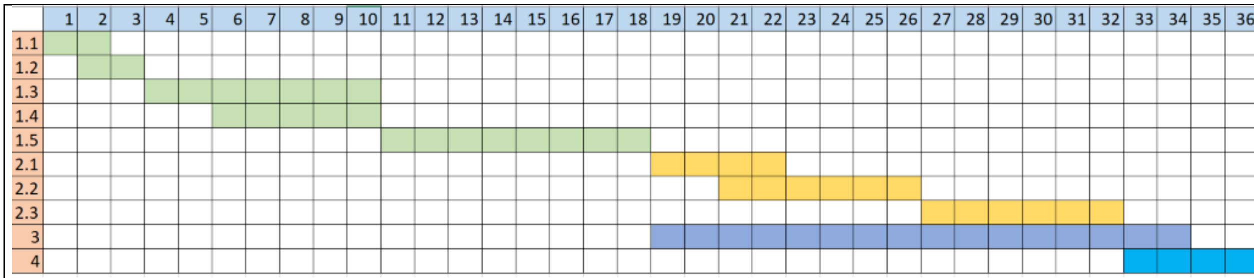

Figure 3. Task/Month - Tentative Gantt Chart of the proposed activities.

Network Interactions: Main interactions of ESR-1 with other ESRs will be initially related to modeling mixed mode fracture in heterogenous (in fact piecewise homogeneous) materials, especially multilayers studied by ESR-3, ESR-9 and ESR-11, and mixed mode studied by ESR-5, among others. Then, ESR-1 will interact with other ESRs in relation to modeling fracture in anisotropic materials, e.g., by ESR-4 and ESR-12. Finally, several ESRs could take advantage of general-purpose procedures and computational tools developed by ESR-1, which could be validated, e.g., by ESR-3, ESR-6 and ESR-9, respectively, on multilayer ceramics, SFRP composites and photovoltaics.

Planned secondment(s): Two secondments in other NewFrac partner's institutions are planned: IMT (Month 10-15) for training in computational implementation of CCFFM and PF and their applications to fracture problems in photovoltaics and RB (Month 35-38) for validation of the developed computational tools solving industrial fracture problems in SFRP composites.

b. Task 4.02 – ESR 3: Adaptation of the new techniques to the fracture of ceramics

Fellow	Host institution	PhD enrolment (Y/N)	Start date	Duration (months)	Deliverables
ESR-03	SU	**Y**	**M7**	**36**	**D4.06, D4.12**

Project Title and Work Package(s) to which it is related: *Fracture analysis of advanced layered ceramics (WP4)*

Objectives: Ceramic materials are widely used in the industry owing to the countless advantages: oxidation and corrosion resistance, high-temperature stability, hardness and wear resistance. However, the main drawback of ceramics is their low fracture toughness, which is related to the spontaneous brittle failure of the component. In this context, advanced layered ceramics, sometimes bio-inspired, are designed to increase strength and energy absorption capacity (toughness). Several applications of these structures can be found in different engineering fields with high economic and societal impacts ranging from biomedicine, automotive engineering, aeronautic and aerospace industries, electronics, and renewable energy systems. A better control of the resistance to failure of these structures is obviously of crucial interest.

The principal aim of this task project will regard the consistent extension of both Phase Field approach (PF) and Coupled Criterion within the Finite Fracture Mechanics framework (CCFFM) modeling, as modelling tools for predicting crack nucleation and growth in layered ceramics and thin films deposited on a substrate. This methodology will allow the robust analysis of the influence of micro- (flaws, grain sizes) and meso-structures (layers, stacking sequences) and will focus in addition on the role of residual stresses of various origins (thermal, chemical…) on the onset and growth of cracks.

Since both methods rely on a characteristic length, which should interact with the already mentioned sizes, it is expected to provide plausible explanations for relationships between the microstructure and fracture properties at the macro-scale. Special attention will be paid to natural structures such as mother-of-pearl, which has exceptional fracture properties. Extensions to other materials with a different microstructure: amorphous (polymers, glass), layered (ceramics, hybrid metal-ceramic composites), among other different typologies, will be considered.

The expected results are all within the same general framework: linking a microscopic description of the structure and its strength properties to the macroscopic fracture properties.

- Influence of the microscopic geometry (layer thickness, grain size, flaw size…) on the macroscopic fracture properties. In this regard, a special attention will be paid to the extreme smallness (thicknesses < 1 μm) of the micro-structure of a natural material like mother-of-pearl.
- Influence of the material parameters (stiffness, strength, toughness) on the macroscopic fracture properties. This is where the effects of residual stresses (due for instance to elaboration but also to aging, oxidation…) will be taken into account.
- Formulation, numerical implementation and even coupling of the two approaches, CCFFM and PF, for layered materials within a multi-field framework.

The PhD thesis of ESR 3 started on November 2, 2020. Principal tasks of ESR-1:

(M X-Y means Month X to Y, X and Y are calculated from the beginning of the PhD thesis)

- Task 1: Getting started with the computer, numerical and theoretical tools. Bibliography. In parallel, start of a study on the comparison between the CC and the line method which can contribute to the learning of the tools. Writing of a paper.
- Task 2: Studying the influence of the microscopic geometry, optimization procedure. Part 1.
- Task 3: First secondment in University of Seville (US). Learning of the PF method and application to layered structures.
- Task 4: Vacations.
- Task 5: First secondment in US. Learning of the PF method and application to layered structures.
- Task 6: Studying the influence of the microscopic geometry, optimization procedure. Part 2. Writing of a paper.
- Task 7: Second secondment in US. Coupling the PF method and the CCFFM.
- Task 8: vacations.M 23: Second secondment in US. Coupling the PF method and the CCFFM.
- Task 9: Studying the influence of the microscopic properties, optimization procedure. Writing of a paper. Writing the manuscript.
- Task 10: Third secondment at Safran Company, proving the industrial applicability of this kind of approaches to fracture of materials for aeronautic applications.
- Task 11: vacations.
- Task 12: Writing of the manuscript. Thesis defense.

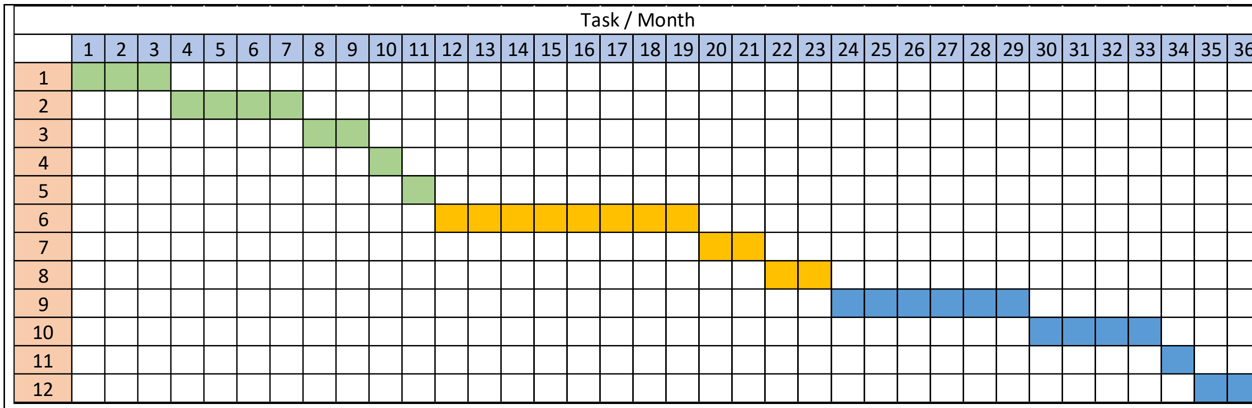

Figure 4. Task/Month - Tentative Gantt Chart of the proposed activities

Network Interactions: ESR-3 will investigate fracture behaviour of advanced layered ceramics and will potentially interact with ESR-2 and 4 in a direct fashion. Further collaborations with ESR-11 and 12 regarding the development of advanced shells with damage capabilities and multi-scale techniques will be of crucial interest for the corresponding projects.

Planned secondment(s): There are two main secondments planned during this PhD thesis. The first one, at University of Seville, to learn the fundamentals of the PF of fracture, specifically devoted to thin walled structures and laminates. The second one will take place at Safran Company. During the latter it is expected to prove the industrial applicability of this kind of approaches to fracture of materials for aeronautic applications.

c. Task 4.03 – ESR 5: Methods for compressive crack analysis by PF

Fellow	Host institution	PhD enrolment (Y/N)	Start date	Duration (months)	Deliverables
ESR-05	**SU**	**Y**	**M9**	**36**	**D4.06, D4.12**

Project Title and Work Package(s) to which it is related: *Nucleation and propagation of compressive cracks (WP4)*

Objectives: Recent results have proved that PF approaches can quantitatively predict crack nucleation for mode-I loading. However, current models [1-3] do not allow for a faithful prediction of the crack nucleation event in more complex loading conditions and materials. A further important limitation of PF models is their difficulty in reproducing fracture propagation under compressive and multiaxial loadings, despite the important amount of research on the subject. The principal aim of the ESR-5 project will be to investigate crack nucleation and propagation under multiaxial loadings and to propose novel extension of the PF approach to overcome the current limitations.

The project will include the following theoretical and numerical developments:

- Task 1: Critical analysis of the existing models and of their limitations in predicting crack nucleation under multiaxial loadings.
- Task 2: Formulation of a new generalized model affecting the crack nucleation under

compressive and multiaxial loadings. The latter, to be adjusted according to shear strength and the compressive strength.

- Task 3: Numerical implementation of the new models and analysis of the localisation modes and dissipation under multi-axial loading. We will study the propagation behaviour after nucleation through theoretical and numerical analysis. The numerical implementation can consider advanced discretisation techniques to avoid potential locking issues.
- Task 4: Analytical and numerical stability and bifurcation analysis of gradient damage models under multiaxial loading. This will apply to the crack nucleation problem an ongoing development in the d'Alembert group on this topic.
- Task 5: Crack nucleation issue for almost incompressible material.
- Task 6: Consider coupled variational damage and plasticity models to correctly account for crack nucleation under multiaxial loading of non-brittle complex material materials. The proposed approach could be extended to model through plasticity the dissipation mechanisms due to friction.
- Task 7: Exploit the development in the application context of biomechanics in collaboration with ESR 8 and ESR 10.
- Task 8: Exploit the development in the application context of SFRP composites in collaboration in collaboration with ESR 6.

	Nov	*Dec*	*Jan*	*Feb*	*Mar*	*Apr*	*May*	*June*	*July*	*Aug*	*Sept*	*Oct*
Year 1	1	1	1	2	2	2	2	3	3	3	3	4
Year 2	4	4	4	5	5	5	5	6	6	6	6	6
Year 3	6	7-8	7-8	7-8	7-8	7-8	7-8	7-8	7-8	7-8	7-8	7-8

Figure 5. ESR-5 Tentative task timeline of the proposed activities

The numerical developments will be based on classic finite element and finite element exterior calculus methods [4], using the FEniCS platform, and will be released into the NEWFRAC collaborative computational framework to benefit other ESRs. The following reports the expected calendar.

Network Interactions: For applications of the numerical codes developed to fracture under compression in SFRP composites ESR 5 will strongly interact with ESR 6, and for fracture under compression in bones with ESR 8 and 10. To model inelastic deformation by PF, ESR 5 can interact with ESR 12, and for multi-field modelling with ESR 3, 9 and 12.

Planned secondment(s): ETH for development of PF applied to fracture in compression and RB for fractures in injection molded SFRP structures under compression

d. Task 4.04 – ESR 7: Adaptation of the new techniques to the study of debonding

Fellow	Host institution	PhD enrolment (Y/N)	Start date	Duration (months)	Deliverables
ESR-07	**POLITO**	**Y**	**M7**	**36**	**D4.05, D5.05, D2.07**

Project Title and Work Package(s) to which it is related: *Debonding of the reinforcement in FRP and FRCM externally strengthened beams (WP5)*

Objectives: Externally reinforced structures are composite structures where the heterogeneity is due to the application of an external reinforcement to an existing structure in order to restore it or to increase its bearing load. The main objective of this ESR project is the analysis of the delamination of the external reinforcement in rectilinear and curved beams strengthened by Fiber Reinforced Composite layers. The problem has a great relevance since external bonding of Fiber Reinforced Composites is nowadays a common practice in strengthening of existing structures in general and in restoring of stone and masonry arches in particular. Furthermore, among the different failure mechanisms of strengthened structures, the reinforcement debonding is probably the most important one to be investigated because of its typical brittle and catastrophic character.

Figure 6: Experimental observations in externally strengthened beams.

The work will start with a general review about fracture mechanics models. It will be also the opportunity for the candidate to share with the supervisors previous research experiences in the field. Then the ESR activity will follow two parallel lines: on one side, he will learn the fundamentals of Finite Fracture Mechanics (FFM); on the other side, he will gather the bibliographical background for the problem of the external reinforcements of structures. Attention will focus on linear elastic fracture mechanics models (LEFM) and Cohesive Crack Models (CCM) for tackling analytically the debonding from rectilinear and curved beams (papers by Paggi, de Lorenzis, Cornetti, among others) and on FFM models for structural assessment of joints (papers by Leguillon, Mantič, Becker, Cornetti, among others).

The analysis developed is expected to be able to model external reinforcements made of Fiber Reinforced Polymers (FRP), Fiber Reinforced Cementitious Matrix (FRCM) composites (with either Carbon or PBO fibers) and Steel Reinforced Grout (SRG). It is important to observe that the debonding behavior of traditional FRP plates differs from the one shown by FRCM or SRG, since debonding occurs within the substrate or at matrix/substrate interface for FRP, while it is mainly governed by the bond between the fiber net and the cement based matrix for FRCM and SRG. In the latter case, the FFM and CCM models have to be improved by taking friction into account. This aspect is relevant, since the mechanical behavior of the FRCM strengthened structure shows a positive pseudo-ductile character. As for the geometries, beams with rectilinear and curved axis will be considered. From a civil engineering point of view, this is an important aspect since external composite reinforcement are often used to strengthen arches and vaults. Debonding will be the kind of failure to be investigated, either from the edges (plate end – PE – debonding) or from the inner part of the reinforcement (Intermediate Crackinduced – IC – debonding). Quasi-static loading condition will be assumed at a first stage; then, the investigation will consider also cyclic and fatigue loadings. Possibly, also thermal loading and the case of pre-stressed reinforcement will be considered.

While the investigation mainly focuses on the debonding of external reinforcements, some outcomes of the research activity of ESR-07 are expected to have a general feature and to be of interest for all ESRs working on FFM. Theoretical insights are expected for what concerns how to tackle friction and residual stresses, competition and interaction among different crack onset points, fatigue and cyclic loadings.

The analytical and numerical results obtained by the ESR will be compared with results taken from the Scientific Literature. Depending on laboratory availability, some ad hoc tests on small-size specimens could be planned. Moreover, cooperation with a research team testing large-size beams from an existing infrastructure undergoing different kinds of retrofitting is also expected.

Network Interactions: ESR-07 will interact with ESR-01, about prediction for mixed mode fracture problems involving simultaneous crack onsets, and with ESR-11, about delamination curved layered structures. Especially, ESR-11 will benefit from the analytical results by ESR-07, while ESR-07 will exploit the knowledge acquired by ESR-13 about FFM and dynamics to assess the strength of FRP-reinforced structures under impact loads.

Planned secondment(s): Two secondements are scheduled: the first at ETH and the second at FIDAMC, where the ESR will share and deepen his knowledge on fatigue loading, phase field modelling and debonding in curved composite structures.

e. Task 4.05 – ESR 10: Adaptation of the CCFFM, PF and hybrid methods to biomaterials

Fellow	Host institution	PhD enrolment (Y/N)	Start date	Duration (months)	Deliverables
ESR-10	**ETH**	**Y**	**M7**	**36**	**D4.05, D5.05, D2.07**

Project Title and Work Package(s) to which it is related: *Phase-field modelling of fracture in the human femur (WP4)*

Objectives: The ESR-10 project aims at developing a phase-field model and related computational framework to predict crack nucleation and propagation in the human femur. From the theoretical point of view, the main difficulties in the predictive simulation of fracture in bones are heterogeneity, to a lesser extent anisotropy, the relevance of complex multiaxial states of loading including significant compressive stresses, and the multiscale nature of the bone structure. The phase-field modeling approach needs some important extensions to handle these aspects effectively. The project will include the following theoretical and numerical developments:

1. *Formulation and testing of a probabilistic approach to describe fracture in heterogeneous materials*. The approach will be first formulated and tested in 1D using both sharp crack and phase-field approaches, and then extended to multiple dimensions.
2. *Investigation of issues related to the length scale parameter in heterogeneous materials*, possibly formulation of a length-scale independent model.

3. *Multiscale formulation* for determination of the macroscopic fracture properties based on microstructural information.

4. If time allows, *incorporation of macroscopically anisotropic fracture properties*, possibly obtained from the multiscale approach at point 3.

The following aspects related to the application to fracture of the human femur will be investigated:

5. *Application of the probabilistic framework to realistic distributions of fracture properties in the human femur* in collaboration with ESR-08. If time allows, also realistic anisotropy scenarios will be considered.
6. *Analysis of crack nucleation and propagation under multiaxial stress states in the human femur*. The type of energy decomposition most suitable to reproduce the strength surface of the bone material under multi-axial stress states will be formulated and studied in collaboration with ESR-08 and ESR-05.
7. *Application of the multiscale formulation to the microstructure of the bone tissues* in collaboration with ESR-08.
8. *Calibration and validation with experimental results* in collaboration with ESR-08.
9. *Extension* of the developments *to the application context of SFRP laminates* in collaboration with ESR-06.

The numerical developments will be based on classical finite element methods, using Matlab or FeniCS, and will be released into the NewFrac collaborative computational framework to benefit other ESRs.

Network Interactions: ESR-10 will strongly interact: with ESR-08 for all aspects related to fracture in bones; with ESR-05 for the modeling aspects related to the energy decomposition; with ESR-06 for the extension of the framework to SFRP laminates.

Planned secondment(s): TAU for application to fracture in bones, RB for extension to fracture in SFRP laminates.

f. Task 4.06 – ESR 12: Adaptation of the new techniques to the multiscale analysis of composites

Fellow	Host institution	PhD enrolment (Y/N)	Start date	Duration (months)	Deliverables
ESR-12	**FEUP**	**Y**	**M7**	**36**	**D4.10, D4.12**

Project Title and Work Package(s) to which it is related: *Fracture in fibre-reinforced thermoplastics (FRTPs) across the scales (WP4)*

Objectives: The advent of new manufacturing capabilities for manufacturing LFRP composites has introduced the possibility of producing highly efficient fibre-reinforced thermoplastics (FRTPs). Due to their inherent characteristics, thermoplastic matrices can overcome the brittle character and difficult recyclability of thermoset matrices. These aspects are of special interest in industrial applications since they encompass higher strain-to-failure, higher fracture toughness and damage tolerance and the ability to reshape and reuse/recycle. However, they also lead to specific challenges for the representation of the inelastic deformation and fracture of coupons or elements manufacture with this class of multi-layered composite materials. The objective of this task concerns the analysis of fracture in FRTPs across the scales, i.e., from the scale of the constituents (micro-scale level) to the scale of the laminate (meso-/macro-scale level). Micro-scale analyses will provide more comprehensive understanding about the potential sources and sequence of damage (fibre-matrix decohesion, matrix cracking, delamination, among others), as well as the prospective damage propagation paths, with particular focus on the role of the thermoplastic matrix. Specific aspects concerning the behaviour of different thermoplastic matrices, such as viscoelastoplasticity and ductile fracture, and the interaction with the reinforcing fibres in terms of damage tolerance will be addressed at this scale. A computational micro-mechanics framework will be developed, integrating robust algorithms that generate reinforcement distributions that are materially and statistically equivalent to real microstructures, constitutive models for the different composite constituents and appropriate definitions of the boundary and loading conditions. Due to the complexity of the geometry and of the boundary and loading conditions of this type of analysis, the PF approach to fracture provides the right context to tackle any general case. A particularly important contribution will be the integration of a PF approach to ductile fracture with three-dimensional viscoelastoplasticity to simulate the nonlinear response and fracture of the thermoplastic matrix, and the integration of the PF approach to fracture with nonlinear elasticity and strength asymmetry to simulate the response of the reinforcing fibres. In addition, PF and cohesive zone models will be coupled to predict the decohesion between fibres and matrix. Analyses at this scale will allow the study of the effect of the nature, properties and distribution of the constituents and ply size effects in the energy dissipation and damage mechanisms in FRTPs. These aspects will be taken into account in the formulation of the appropriate constitutive models for the homogenized orthotropic material at the ply level for meso-/macro-scale analyses. Special attention will be devoted to investigating geometrical effects and loading states in specimens with stress concentrations and holes, which are of relevant practical importance in the aeronautical and aerospace industries. For sufficiently simple coupon and element geometries and loading conditions, analytical or semi-analytical representations of the stress and stress intensity factor fields can be generated, and failure of these coupons and elements predicted using the FFMs approach. Examples of such structures include rectangular notched coupons subjected to uniaxial tensile or compressive loads. However, for more complex geometries and/or boundary conditions, the PF approach to fracture will be employed. These would include notched coupons subjected to multiaxial loads or elements with more complex structural details. Both approaches will be extended to address specific characteristics of the mechanical response and fracture of FRTPs, including pre-failure nonlinearities, strength anisotropy and asymmetry and ductile fracture. This project is conceived for the comprehensive analysis of LFRP at different scales of observations. Due to the high demands in terms of computational capabilities, this project will involve the use of High-Performance Computing Systems (HPCS). Special attention will be paid to the analysis of the role of defects, thermoplastic matrix component, tunnelling cracks in the micromechanical response of LFRP, among many others. he research conducted in this project will employ previous results of Reinoso, Camanho and Arteiro as starting point.

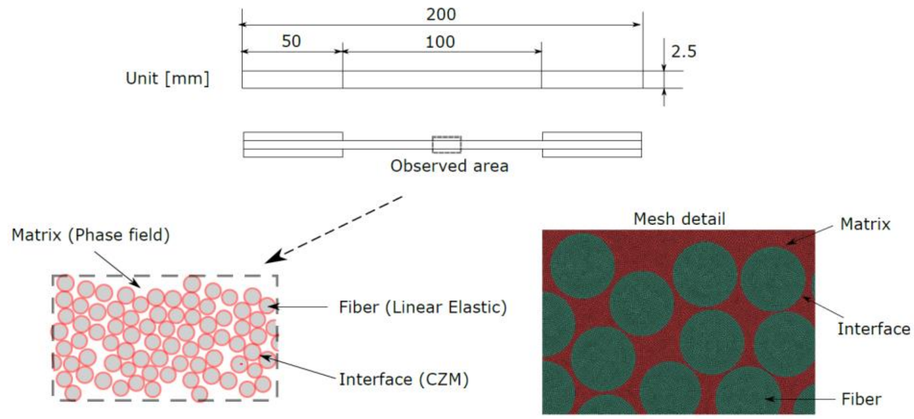

Figure 7. Micro scale example

Principal task of the project:

- Task 1: Literature review: fracture modelling and characterization of FRTPs at different scales.
- Task 2: Development of micro-mechanical models for FRTPs.
- Task 3: Development of constitutive models for FRTP composite constituents based on the PF approach to fracture.
- Task 4: Study the effect of the nature, properties and distribution of the constituents and ply size effects in FRTPs.
- Task 5: Formulation, implementation and validation of constitutive models for FRTPs at the ply (meso-/macro-scale) level.
- Task 6: Development of virtual testing tools for FRTPs based on FFMs and PF in an industrial context.

	UP											US						UP						FIDAMC				UP								
Objectives	M1	M2	M3	M4	M5	M6	M7	M8	M9	M10	M11	M12	M13	M14	M15	M16	M17	M18	M19	M20	M21	M22	M23	M24	M25	M26	M27	M28	M29	M30	M31	M32	M33	M34	M35	M36
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Figure 8. Task/Month - Tentative Gantt Chart of the proposed activities

Network Interactions: ESR-12 will interact with ESR-2, ESR-4, ESR-6 and ESR-9 concerning the development of multiscale approaches of fracture of heterogeneous materials, and with ESR-3, ESR-7 and ESR-11 by interchanging procedures, codes, and common perspectives in the analysis of fracture of different multi-layered composites. Additionally, it is expected that ESR-12 will collaborate with ESR-4 in the definition of robust characterization techniques for advanced composite systems across the scales (from the constituent materials to the multi-layered composites) and to validate the developed models in an industrial context.

Planned secondment(s): US (M12-17) for performing the formulation and numerical implementation of the ductile PF strategies; FIDAMC (M24-27) for training regarding the application of FRTPs in the aeronautical industry and for testing of the developed computational procedures on industrial fracture problems in FRTPs.

g. Task 4.07 – ESR 13: Extension of the CCFFM and PF methodologies to dynamic fracture

Fellow	Host institution	PhD enrolment (Y/N)	Start date	Duration (months)	Deliverables
ESR-13	POLITO	Y	M7	36	D4.11, D4.12

Project Title and Work Package(s) to which it is related: *PF and FFM for fragmentation and dynamic crack propagation in brittle materials and composites (WP4)*

Objectives: In spite of the huge amount of studies carried out and the many advancements achieved in the last decades in the field of dynamic cracking, some aspects still lack of a comprehensive interpretation, such as, for instance, the strengthening and toughening mechanism and the phenomenon of crack branching. In this context, the contribution of the present project consists in the development of numerical and analytical approaches that are robust and devoid of the flaws typical of other methodologies, like the mesh dependency for the cohesive method and the difficulty to manage crack branching and coalescence for the X-FEM, aiming at shedding light on aspects that still lack of a comprehensive interpretation. Besides contributing to answer to open fundamental questions, there are practical issues we want to address. For instance, the fact that the modelling of dynamic processes at an industrial level is almost prohibitive because of complexity of the procedures. Therefore, two complementary strategies are developed:

- Numerical approach based on the Phase Field (PF) model, for a more detailed study of dynamic cracking and fragmentation;
- The extension of Finite Fracture Mechanics (FFM) to dynamics, in order to provide a useful tool for preliminary sizing of materials and structures.

The work will start with a general review about PF and FFM models for quasi-static crack initiation and propagation. Given the very extensive literature in these fields, an accurate selection of papers presenting the bases of the methods and the most interesting applications will be provided to the researcher. Preliminary applications of these methodologies to quasi-static problems will be the opportunity for the researcher to get familiar with a practical use of such approaches and with their prediction capability. Then, the literature review will be extended to the dynamic regime. Concerning the PF, a discrete amount of contributions is available in the literature. They will be critically reviewed, to identify the issues and limitations of this approach to model dynamic cracking. In parallel to the literature review, the researcher will start to acquire hands-on experience with the tools that will be used for numerical simulations during the development of the project (in particular, Python, the finite element library Akantu, and FEniCS).

The objectives of the project are:

- To extend the FFM to dynamics, to provide a reliable tool suitable for preliminary sizing of materials and structures, also for impact loads, thus limiting the use of computationally expensive approaches to the final stage in the structural design. Such an extension will be pursued by introducing an "incubation time" in the stress and energy criteria used to determine the critical load and crack propagation length. The incubation time will allow to include explicitly the loading rate effect in the failure criterion. The inspiration for such a development can come from the reference papers: Petrov Yu.V. "The "quantum" nature of the dynamic fracture in brittle media", 1991 and Kazarinov et al. "Experimental and numerical analysis of PMMA impact fracture" 2020.

- To compare the FFM solutions with the predictions of the well-established Cohesive Crack Model. This step is fundamental to prove the prediction capability of the FFM approach extended to dynamics, given the absolute originality of this development.
- To revise the formulation of PF specifically for dynamic cracking. The formulation of PF derived for quasi-static problems, in fact, does not seem to be suitable also for the dynamic regime. The applications presented in the literature in the dynamic regime highlight severe limitations of the method in getting accurate and realistic predictions of the crack patterns. Some of the evidences are: a reduced number of cracks compared to real fragmentation processes and to predictions given by other modelling methods, difficulties to get micro-branching, enlargement of the dissipation band, loosing sharpness of the crack.
- The implementation of computational methods and Finite Element procedures in research software. In particular, the PF model will be implemented within an explicit time integration scheme. The PF will be also coupled with the Cohesive Zone Model approach, to open the possibility to study in a more efficient way heterogeneous and composite materials.
- To apply the dynamic PF to study fragmentation of materials. A key issue will be the reliability of the method to correctly get the complex crack patterns typical of fragmentation problems. The study case that will be analyzed is the fragmentation of a tempered glass plate, for which a experimental data and also the results obtained with the cohesive crack model are available (Vocialta, Corrado and Molinari, Engineering Fracture Mechanics, 2018). Such a test is particularly suitable because the crack is driven by the internal stress field, thus limiting the spurious effects of boundary conditions.

The development of the project will require the use of highly performant and optimized procedures and numerical libraries to deal with finite element problems having tens of millions of dofs. The codes the supervisors are already familiar with are Akantu (https://akantu.ch/) and FEniCS (https://fenicsproject.org/). Also, the use of a cluster of computers is required. The researcher will have access to the high performance computing center of Politecnico di Torino (HPC@Polito, https://www.hpc.polito.it/).

Network Interactions: Strong collaboration is foreseen with ESR-1, 7 and 9. In particular, ESR-13 will take advantage, for his studies on fragmentation, of the tools for CCFFM and PF developed by ESR-1; and will collaborate with ESR-7 for the development of a FFM approach suitable for dynamic conditions of loading. Interactions with ESR-9 will concern the analysis of the performance of materials for renewable energy applications in dynamics.

3. Summary and Outlook

This report presents an updated version of the working plan of the network on novel tools for modelling fracture initiation. It includes the detailed program of the individual ESR associated to each task. This plan constitutes a sound basis for the development of the Ph.D. projects and to strength the interaction between the different beneficiaries.