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Micromechanics based fatigue modeling using Fast Fourier Transform based homogenization

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“The foolish man seeks happiness in the distance. The wise grows it under his feet.”

James Oppenheim

Resumen

El comportamiento a fatiga de las aleaciones policristalinas depende en gran medida de su microestructura, en particular, del tamaño del grano, la forma y las distribuciones de orientaciones. La caracterización experimental del comportamiento a fatiga requiere una gran campaña experimental, que debe repetirse para cada una de las microestructuras metálicas de interés. Los modelos micromecánicos pueden ser utilizados para predecir la vida útil a fatiga en función de la microestructura, lo que permite reducir el número de experimentos necesarios para la caracterización del material. Esos modelos se basan en la homogeneización computacional, la cual tiene como objetivo vincular la respuesta macroscópica con la microestructura policristalina y el comportamiento del cristal, descrito en este caso por un modelo de plasticidad cristalina (CP), para resolver un problema de valor en el contorno (BVP) dentro de un elemento de volumen representativo periódico (RVE) de la microestructura. Sin embargo, los modelos de vida a fatiga basados en micromecánica presentan algunas limitaciones, (a) el gran coste computacional al resolver la distribución de los microcampos con elementos finitos limita la complejidad de las microestructuras y el muestreo estadístico, (b) los parámetros de los indicadores de fatiga (FIPs), utilizados para cuantificar la fuerza

impulsora para el inicio de la fatiga, dependen en gran medida del tamaño de RVE, y (c) las predicciones de vida no tienen en cuenta la probeta o el tamaño del componente.

En este trabajo se desarrolla una nueva metodología para la predicción de la vida a fatiga basada en la micromecánica que supera las limitaciones de los métodos actuales. Respecto a la limitación (a), aquí se desarrolla la adaptación de un marco de homogeneización basado en la transformada rápida de Fourier (FFT) para el modelado por fatiga de policristales basado en micromecánica. Las principales ventajas de FFT con respecto a los elementos finitos en homogeneización computacional son el alto rendimiento numérico, las condiciones de contorno periódicas naturales y la ausencia de una malla, las cuales permite simular RVEs muy detallados y el uso directo de imágenes o datos tomográficos como input. El marco se basa en el enfoque Galerkin FFT que se adapta en este trabajo para proporcionar microcampos precisos durante las cargas cíclicas para modelos genéricos de plasticidad cristalina y condiciones de carga macroscópicas. En primer lugar, se introducen operadores de proyección discretos para mejorar la suavidad del microcampo. En segundo lugar, se desarrolla un nuevo algoritmo para imponer una carga macroscópica o una historia mixta de carga / gradiente de deformación dentro del enfoque Galerkin FFT de una forma muy eficiente. Tercero, se propone un nuevo método de homogeneización basado en FFT, rápido, robusto y eficiente en memoria, en el que el campo de desplazamientos en el espacio de Fourier es la incógnita a resolver, el DBFFT. Los métodos de FFT se han validado contra simulaciones de elementos finitos y se ha demostrado que las respuestas cíclicas macroscópicas de un policristal usando ambos métodos son idénticas, independientemente del número de ciclos. Las diferencias en los campos microscópicos están por debajo de alrededor del 3 % y la diferencias máximas en las predicciones de vida RVE son del 6 %. Como resumen, el marco de homogeneización FFT desarrollado permite predecir la vida útil a fatiga con una precisión similar a los modelos basados en elementos finitos, pero reduciendo fuertemente el coste computacional. Todos estos desarrollos se han incluido en un nuevo código de homogeneización basado en FFT, FFTMAD, que incluye diferentes esquemas de resolución para problemas lineales y no lineales tanto en pequeñas deformaciones como en grandes. Nuestro código también permite vincular ecuaciones constitutivas de material generalistas provenientes de elementos finitos, p.e. subrutinas de material Abaqus (*umat*s).

Respecto a las limitaciones (b) y (c), se desarrolla un nuevo enfoque estadístico para el modelo de vida de fatiga micromecánico. En este enfoque, se propone una técnica de escalamiento basada en la distribución de Gumbel y el concepto del eslabón más débil para obtener una vida a fatiga macroscópica y dispersión a nivel de probeta/componente, incluyendo millones de granos, a partir de los resultados obtenidos mediante

la simulación de un conjunto estadístico de pequeños RVEs que contienen solo unos pocos cientos de granos. Dado que el enfoque de la vida se basa en los resultados extrapolados a nivel de probeta, los resultados de la vida son independientes del tamaño de RVE y el modelo explica naturalmente el efecto del tamaño de probeta.

Finalmente, el modelo estadístico de vida a fatiga se usa para predecir la respuesta a fatiga de la superaleación base níquel Inconel 718 (IN718) para diferentes casos de carga y dos microestructuras. El comportamiento del cristal se explica por un modelo de CP que incluye todas las características típicas de una superaleación policristalina: efecto Bauschinger, relajación de la tensión promedia y ablandamiento cíclico; y se calibra utilizando un ajuste inverso con diferentes bucles de histéresis de ensayos experimentales de fatiga. Utilizando los resultados de la simulación, se propone una ley potencial para relacionar el parámetro indicador de fatiga a nivel de muestra y el número de ciclos con la iniciación de grieta, en el que los dos parámetros se ajustan a partir de los experimentos. Se ha encontrado una buena correlación con los resultados experimentales de la vida útil a fatiga para todas las microestructuras y casos de carga considerados. Además, el modelo permite estimar el llamado factor de caída de propiedades en fatiga, que relaciona la pérdida de rendimiento en fatiga de una probeta de fatiga respecto a un componente más grande.

Abstract

The fatigue behavior of a polycrystalline alloy is strongly dependent on its microstructure, in particular to the grain size, shape and orientation distributions. The experimental characterization of the fatigue performance requires a large experimental campaign, that should be repeated for each of the metallic microstructures of interest. Micromechanical models can be used to predict fatigue life as function of the microstructure allowing to reduce the number of experiments needed for material characterization. Those models rely on computational homogenization that aims to link macroscopic response with polycrystalline microstructure and crystal behavior, accounted by a crystal plasticity (CP) model, by solving a Boundary Value Problem (BVP) on a periodic Representative Volume Element (RVE) of the microstructure. However, micromechanics based fatigue life models present some limitations, (a) the large computational cost for solving the microfield distribution with Finite Elements limits the complexity of the microstructures and the statistical sampling, (b) fatigue indicator parameters (FIPs), used to quantify the driving force for fatigue initiation, are strongly dependent on the RVE size, and (c) life predictions do not account for the specimen or component size.

In this work a new Micromechanics based fatigue life prediction approach is developed which overcomes the limitations of the current approaches. Respect the limitation (a), a homogenization framework based on Fast Fourier Transform (FFT) is adapted here for micromechanics based fatigue modeling of polycrystals. The main advantages of FFT respect to Finite Elements in computational homogenization are the very high numerical performance, the natural periodic boundary conditions and the absence of a mesh, that allows simulating very detailed RVEs and the direct use of images or tomographic data as input. The framework relies in the Galerkin FFT approach that is adapted in this work to provide accurate microfields during cyclic loading for generic crystal plasticity models and macroscopic loading conditions. First, discrete projection operators are introduced to improve microfield smoothness. Second, a new approach is developed for imposing macroscopic stress or mixed stress/deformation gradient history within the Galerkin FFT approach in a very efficient manner. Third, a fast, robust and memory-efficient new FFT homogenization approach is proposed in which the displacement field on the Fourier space is the unknown to solve, the DBFFT. The FFT framework is validated against Finite Element simulations and it is shown that the macroscopic cyclic responses of a polycrystal using both methods are indistinguishable, irrespective of the number of cycles. The differences in the microscopic fields are below around 3% and the maximum difference in the RVE life predictions are 6%. As a summary, the FFT homogenization framework developed allows to predict fatigue life with a similar accuracy than finite elements based models but strongly reducing the computational cost. All these developments have been included in a new FFT homogenization code, FFTMAD, which includes different resolution schemes for linear and non-linear problems under both small and finite strains. Our code also allows to link generalists material constitutive equations from finite element solvers, i.e. Abaqus material subroutines (*umats*).

Respect the limitations (b) and (c) a new statistical approach for micromechanics fatigue life model is developed. In this approach, an upscaling technique based on Gumbel distribution and the weakest link concept is proposed to obtain macroscopic fatigue life and scatter at specimen/component level, including millions of grains, from the results obtained by the simulation of a statistical ensemble of small RVEs containing only a few hundred of grains. Since the approach for life is based on the extrapolated results at specimen level, the life results are RVE size independent and the model accounts naturally the effect of specimen size.

Finally, the statistical fatigue life approach is applied to predict the fatigue response of the Nickel-base superalloy Inconel 718 (IN718) for different load cases and two microstructures. The crystal behavior is accounted by a CP model that includes all the

typical features of a polycrystalline superalloy: Bauschinger effect, mean stress relaxation and cyclic softening; and is calibrated using inverse fitting with different hysteresis loops of experimental fatigue tests. Using simulation results, a power law is proposed to relate the fatigue indicator parameter at the specimen level and number of cycles to crack initiation, in which the two parameters are adjusted from experiments. A very good agreement with experimental results of fatigue lifetime is found for all the microstructures and load cases considered. Moreover, the model allows to estimate the so-called fatigue knock-down factor, that relates the loss of fatigue performance from a fatigue specimen to a larger component.

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Segio Lucarini San José

*To all those people who, day by day,
help me to become a better person.*

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List of abbreviations

IN718	Inconel 718
LPT	Low Pressure Turbine
FFT	Fast Fourier Transform
FE	Finite Elements
FEM	Finite Elements Method
CP	Crystal Plasticity
RVE	Representative Volume Element
LCF	Low Cycle Fatigue
HCF	High Cycle Fatigue
LEFM	Linear Elastic Fracture Mechanics
BVP	Boundary Value Problem
FIP	Fatigue Indicator Parameter
SVE	Statistical Volume Element

CRSS Critical Resolved Shear Stress

FCC Face Centered Cubic

CDF Cumulative Distribution Function

FFTW Fastest Fourier Transform in the West

DFT Discrete Fourier Transform

IDFT Inverse Discrete Fourier Transform

ODF Orientation Distribution Function

Notation

Ω_0	Domain in reference configuration
$\mathbf{x}, \boldsymbol{\xi}, \mathbf{q}$	Vectors x_i, ξ_i, q_i
$\mathbf{P}, \mathbf{F}, \boldsymbol{\tau}$	Second-order tensors $P_{ij}, F_{ij}, \tau_{ij}$
$\mathbb{C}, \mathbb{G}, \mathbb{K}$	Fourth-order tensors $C_{ijkl}, G_{ijkl}, K_{ijkl}$
$\mathbf{A} = \mathbf{F}^T$	Tensor transpose $A_{ij} = F_{ji}$
$\mathbf{A} = \boldsymbol{\tau} \mathbf{F}$	Dot product $A_{ij} = \tau_{ip} F_{pj}$
$a = \mathbf{F} : \mathbf{P}$	Double dot product $a = F_{ij} P_{ij}$
$\mathbf{P} = \mathbb{C} : \mathbf{F}$	Double dot product $P_{ij} = C_{ijkl} F_{kl}$
$\nabla_0 \cdot \mathbf{P}$	Divergence of tensor field in the reference configuration $\frac{\partial P_{ij}}{\partial X_j}$
$G * P$	Convolution operation
I_{ijkl}	Fourth order identity tensor $I_{ijkl} = \delta_{ik} \delta_{jl}$

1 INTRODUCTION

This PhD thesis is organized as follows. First, in Chapter 1, the motivation and objectives of the work developed here are introduced. Chapter 2 outlines the state of the art and the theoretical background related to micromechanics fatigue models, its application to Ni-base superalloys, and the basis of Fast Fourier Transform (FFT) methods. The FFT homogenization framework developed, including its validation and efficiency study, and new FFT algorithms are presented in Chapter 3. A new statistics based framework for fatigue life prediction is proposed and validated in Chapter 4. Finally, the application of the proposed framework to Inconel 718 (IN718) fatigue life predictions is presented (Chapter 5). In Chapter 6 conclusions and future work are remarked.

1.1 Motivation

Cyclic loading is a typical working condition for many components used in aerospace or automotive industries. Under these conditions, materials —and especially metallic alloys— might suffer progressive internal damage, leading finally to the catastrophic failure of the component. This phenomenon of damage accumulation due to repeating reverse loading is known as fatigue, name introduced about middle 19th century

to describe the type of failures occurring from cyclic stress histories (Stephens et al., 1980). The first famous structural catastrophes/failures attributed to fatigue were the collapse of a molasses tank in 1919 (Boston) for building structures and the accident of two "Comet" aircraft in 1954 for aircraft industry (Suresh, 1998). Since then, fatigue became a fundamental area of research both in solid mechanics and materials science, with the ultimate goal of manufacturing long durability structures subjected to fatigue.

Today, fatigue is still one of the most limiting conditions in the design of many parts in the aerospace industry. This is especially critical in components of jet-engines subjected to high stresses, high temperature and cyclic loading. Precipitation hardened superalloys are the ideal candidates for these applications because of their mechanical performance and corrosion strength (Wagner and Hall, 1965). Among them, the Ni-base IN718 alloy is the most used in Low Pressure Turbine LPT (Figure 1.1) components (disk, shell, blades, etc.) and the core of this thesis. This material is used as cast or machined from wrought raw materials, having a wide variety of microstructures depending on the particular part. The fatigue life of this material is strongly dependent on its microstructure features such as grain size and orientation distribution. In order to optimize the component design, it is fundamental to use the fatigue allowables of for the actual microstructure resulting from the manufacturing process of that particular component. To this aim, it is important to develop mathematical models and simulation techniques that allow the prediction of the fatigue life of the alloy as function of its actual microstructure without the need of large experimental campaigns to characterize each microstructure.

Figure 1.1: Aircraft jet engine scheme with the LPT framed (left) and LPT disk with several blades mounted (right).

The first fatigue models were focused on the macroscopic response of the material when subjected to different levels of fluctuating loads (either strain or stress). These

studies were mainly phenomenological, and do not rely on the microscopic mechanisms leading to the fatigue phenomenon neither consider the influence of the microstructure. Therefore, extensive experimental campaigns were needed to evaluate the performance of the material, translated in an important cost and a time-consuming process (Schütz, 1996; Schijve, 2001). Macroscopic models were developed consisting on the application of plastic strain-based criteria for low cycle fatigue, Low Cycle Fatigue (LCF), or stress-based criteria for high cycle fatigue, High Cycle Fatigue (HCF), transferring results from experimental tests on relatively small scale notched and un-notched specimens to structural components (Bannantine et al., 1990).

Going deeper into fatigue mechanisms, it is known that fatigue life can be divided into two stage: crack initiation (nucleation and early growth) and crack propagation. Following studies including these micromechanisms were mainly focused in crack propagation stage. Paris and Erdogan (1963) introduced the well-known Paris law for Linear Elastic Fracture Mechanics (LEFM) crack propagation, which relates the number of cycles of propagation with the stress intensity factor measure (Griffith and Taylor, 1921). However, these studies do not include the effect the microstructure in the early stages of fatigue. Still nowadays, the combination of stress/strain criteria with LEFM is used for designing structural component, but disregarding microstructural aspects (Castillo and Fernández-Canteli, 2009).

As mentioned before for the case of Inconel 718, it is nowadays well-known that microstructure plays a fundamental role in the fatigue response of engineering alloys (François, 1989). Fatigue crack initiation is due to the development of regions within a single grain where plastic slip is accumulated forming Persistent Slip Bands (PSB) (Suresh, 1998). Due to the heterogeneous distributions of plastic slip at the micro level, persistent slip bands appear in specific grains or in specific bands of a grain which locations are highly influenced by the microstructure. Therefore, a model for predicting the fatigue life of a material, especially if the initiation stage plays an important role, has to take into account the microscopic strain fields developed in the material.

To analyze the mechanical behavior at microscale, polycrystal homogenization is the most interesting technique. It allows to establish the link between micro- and macro- scales solving with some numerical technique the distribution of the microscopic strain and stress fields within a more or less idealized representation of the microstructure. Within this framework, the influence of the microscopic characteristics of the polycrystal (grain size, shape and orientations for instance) on the macroscopic response can be taken into account. Polycrystal homogenization is a very complex non-linear problem that can be solved using two different approximations, namely mean-field methods (Taylor, 1938; Sachs, 1928; Molinari et al., 1987; Lebensohn and

Tomé, 1993) in which microstructure is strongly simplified, and full-field computational homogenization (Miehe et al., 1999; Lebensohn, 2001; Delaire et al., 2000; Raabe et al., 2001; Bhattacharyya et al., 2001; Miehe et al., 2002; Segurado and Llorca, 2013; Segurado et al., 2018).

Polycrystal full-field homogenization implies solving the Boundary Value Problem (BVP) on a complex RVE under some mechanical loads and, to this end, the Finite Elements Method (FEM) is the most common choice. The method uses the concept of RVE (Papanicolau et al., 1978; Hill, 1963; Smit et al., 1999; Suquet, 1985; van der Sluis et al., 1999) to analyze the homogenized properties and behavior of the material at the macroscale. A RVE is defined as the smallest microstructural volume that is statistically representative of the heterogeneous material considering the effect of its microstructural features (Drugan and Willis, 1996; Gitman et al., 2007; Kanit et al., 2003; Melro et al., 2012; Terada et al., 2000). In the case of polycrystalline metals, the RVE consists in an aggregate of grains with size, shape and orientation distributions representative of the microstructure considered. The mechanical behavior of each grain is usually modeled with a Crystal Plasticity (CP) model (Peirce et al., 1983) that includes the relevant features of cyclic plasticity such as kinematic hardening, ratcheting or cyclic softening (Cailletaud, 1992; Cruzado et al., 2017). The results of the full-field homogenization are the field of stress, strains and internal variable within the microstructure that provides fundamental information about fatigue crack initiation and are the basis of micromechanics based fatigue models.

The reasons why the FEM is commonly used are the availability of numerous codes, both commercial or open source, the efficient implicit integration of the non-linear problems and the accurate representation of complex geometries (including smooth interfaces for grain boundaries) achieved by the use of adaptive meshing. Nevertheless, FEM applied to microstructure based fatigue models presents also some limitations, such as the meshing requirement or the high computational cost of the simulations. Due to the stochastic nature of fatigue, tens of RVEs need to be generated, meshed and analyzed, but the generation of quality meshes for a polycrystalline RVEs is not easy to automatize and a common alternative is to use structured voxel models (Castelluccio and McDowell, 2014; Manonukul and Dunne, 2004; Shenoy et al., 2008; McDowell and Dunne, 2010; Sweeney et al., 2014; Cruzado et al., 2017). Finite element voxel models can be automatically generated but the most interesting features of FEM, the adaptation of the mesh to the actual geometry and smooth representation of grain boundaries, are lost when using this type of discretization. The second, and most important, limitation is the computational cost. The models required for an accurate prediction of

fatigue life based on the microfields are particularly large and, in addition, the simulation of several cycles is often required (Cruzado et al., 2017). FEM in its implicit form scales by $O(n^2-n^3)$ depending on the particular boundary conditions and solver used, and this scaling prevents the use of very big meshes or requires the use of largely parallel codes running in computer clusters.

An alternative to FEM that has become very popular in the last years for solving many homogenization problems are the methods based on the FFT or spectral solvers. The original method was introduced by Moulinec and Suquet (1994) and the seminal idea consists in transforming the equilibrium equation for the heterogeneous periodic medium into the equilibrium equation in a homogeneous reference medium subject to body forces and solving the resulting Poisson's equation iteratively using the Green's functions method. The Green's function in the reference medium for a periodic domain can be easily obtained by transforming the equations to the Fourier space using the fast Fourier transform (FFT) algorithm to compute the discrete Fourier transform of the fields. FFT based homogenization has become very popular in the last years due to its excellent numerical performance (the algorithm scales by $n \log n$) that allows the use of very detailed RVEs with a strong reduction in computational cost compared with FEM, being able to speed up the simulations by orders of magnitude (Eisenlohr et al., 2013). For this reason, since its introduction, the framework has been successfully applied for homogenizing the mechanical response of composites (Kabel et al., 2015; Monchiet and Bonnet, 2013), voided materials (Lebensohn et al., 2013; Lebensohn and Cazacu, 2012) and polycrystalline metals (Lebensohn, 2001; Lebensohn et al., 2004; Eisenlohr et al., 2013; Rovinelli et al., 2015) under monotonic loading.

Within this framework, the heterogeneous distribution of stress, strains and other internal variable microfields are resolved, allowing the use of local fatigue criteria to estimate the fatigue life of the alloy Shenoy et al. (2007); McDowell and Dunne (2010); Sangid (2013). Moreover, other microstructural items such as precipitates, non-metallic inclusions and defects, responsible of stochastic response in fatigue, can be explicitly considered Zhang et al. (2015). The fatigue life is estimated from the distribution of some FIP (Sweeney et al., 2012; Wan et al., 2014; Chen et al., 2018), that is a function of the local fields obtained in the simulation of the cyclic behavior and which definition is based on the material crack initiation micro mechanisms. To this aim, an empirical law (Manonukul and Dunne, 2004; Sweeney et al., 2013; Castelluccio and McDowell, 2015) is used to link the FIP value characteristic of the full RVE to the number of cycles to initiation, being this law fitted to one or more fatigue experiments. Since crack nucleation occurs in the hottest point of the microstructure, the FIP value characteristic of the whole RVE corresponds to the region with the largest FIP and because this value

has a large variation for different RVEs of the same size, numerous realizations of different samples of the same microstructure, called Statistical Volume Element (SVE)s, are studied (Przybyla and McDowell, 2010; Przybyla et al., 2013; Sweeney et al., 2015).

The micromechanics based fatigue framework presented is nowadays the most sophisticated approach for microstructure sensitive fatigue life estimation. However, it suffers from some limitations. The first one, already depicted before is that, due to the use of FEM as solver, the size of RVEs used and SVE statistics are very limited, compromising the accuracy of the method or its extension to more complex microstructures. Second, since the FIP characteristic of a given RVE is dependent on its size, the fatigue law is associated to the particular RVE size used in the simulations and cannot be used directly if this condition is changed. Finally, this RVE volume effect is also observed in experiments—the fatigue life of materials decrease with increasing the specimen size (Carpinteri et al., 2009; Furuya, 2008; Sun et al., 2016)—and this specimen size dependency is not accounted in the approach. In summary the objective of this thesis is to overpass these limitations, as it will be proposed in detail in the next section.

1.2 Objectives

The general objective of this thesis is to develop a new micromechanics based fatigue life nucleation framework that overcomes some of the limitations of the current approaches and to apply this framework to predict the fatigue life of Inconel 718 superalloy. In particular, the thesis has three main objectives.

The first objective is then **developing and validating a FFT based homogenization framework for microstructure sensitive fatigue life prediction** that allows to efficiently simulate the cyclic response of statistical ensembles of large RVEs that accurately represent the complex microstructures. This framework should include

- A robust implementation of the FFT based solver including the formulation in finite strains and implicit time integration.
- Direct use of constitutive equations developed for finite element codes, including the material consistent tangents. In particular, in order to allow compatibility with previous work developed in FEM for crystal plasticity, the implementation should allow a direct use of material subroutines written using the Abaqus umat standard.
- An efficient treatment of macroscopic loading conditions including strain, stress and mixed control.

- An assessment of the accuracy of the FFT method when used for fatigue life prediction.
- Development of improvements in the versatility and the efficiency of the FFT based homogenization methods.

Second, a microstructure sensitive robust fatigue approach should be RVE size independent, in contrast to the current state of the art. Moreover, the prediction should allow to account for specimen size effect as an additional parameter to the microstructure. Since the direct simulation of RVEs of sizes in the order of real specimens is not possible, microstructure sensitive fatigue modeling needs to be enhanced by some statistically based extrapolation procedure. Thereby, the second main objective of this thesis consists in **developing an enhanced micromechanics based fatigue life prediction framework** which provides

- The consideration of statistical nature of the SVEs dependent on the size.
- A unique relation between microstructures and RVE independently on size.
- The ability to compute size effects in fatigue for different volumes.

Finally, **this new framework will be applied to a widely used engineering material, the Inconel 718 superalloy**. The result will be the adjustment of the current approach with some experimental tests and the validation of the microstructure fatigue life prediction for independent load cases and microstructures.

2 STATE OF THE ART

A review of different approaches to model the fatigue behavior of metals is presented in this chapter, including the fatigue phenomenon (Section 2.1), the classic macroscopic approaches (Section 2.2) and the recent studies of micromechanics based fatigue methods (Section 2.3). Within micromechanics based models, special emphasis is given to the basis FFT based homogenization methods (in Section 2.4), covering the basic theory and different types of solvers with the non-linear extensions. Finally, a literature review of the application of the micromechanics based fatigue model to IN718 Ni-base superalloy is presented (Section 2.5).

2.1 Fatigue of metallic alloys

Fatigue is the weakening of a material caused by cyclic loading that results in progressive and localized structural damage and the growth of cracks. In metal alloys, this phenomenon may depend on many material factors as: microstructure, temperature, defects, notches, geometry, size, surface roughness, etc. This work is focused in the dependence on the microstructure, hence micromechanisms that are involved in the fatigue process are studied.

Fatigue life is usually divided in two different regimes: crack initiation and crack propagation. Within crack initiation regime, two stages can be identified: crack incubation and microstructurally small crack (MSC) growth (McDowell, 1997; McDowell et al., 2003). In metals, the whole fatigue process is controlled by cyclic plastic deformation. Figure 2.1 represents an illustration of the fatigue life range that takes each fatigue stage.

Figure 2.1: Schematic illustration of the four stages of fatigue in ductile metals until failure taken from Mughrabi (2015).

Before fatigue crack nucleation takes place, irreversible processes occur during the cyclic loading leading to plastic deformation accumulation. Dislocation movement during the loading leads to complex processes of dislocation accumulation, nucleation and structure evolution that finally is traduced into plastic deformation. Irreversible dislocation glide occurs under cyclic loading and usually leads to the development of persistent slip bands (PSBs) (Mughrabi, 1987), extrusions, and intrusions in surface

grains that are optimally oriented for slip. On sub-grain scale, the evolution of persistent slip bands (PSB) is known to be strongly dependent on dislocation interactions and dislocation structure formation and implies a plastic strain localization.

The localized cyclic plastic deformation in the microstructure (cyclic microplasticity) plays a key role in the fatigue crack initiation mode from the micro-scale point of view. Crack initiation accounts for a significant portion of fatigue life (Lankford and Kusenberger, 1973; Mughrabi, 2009) and is controlled by cyclic plastic deformation and PSBs. Fatigue crack initiation and short fatigue crack growth are strongly influenced by the features of underlying microstructure (Tokaji et al., 1988; Suresh, 1998). The heterogeneity of the microstructure such as inclusions and grain boundaries are determinant for crack initiation (Bennett and McDowell, 1999; Simonovski et al., 2007) since they are assumed to be stress concentrators and thus the plastic strain is localized near such regions. The accumulation of plastic deformation within PSBs leads to the fracture of the crystallographic plane and hence the initiation of the crack.

After crack initiation, microstructural small crack propagation takes place, where a microcrack of a length of the grain size starts propagating through several grains. This stage is still very dependent on the microstructure and thus, microstructure again plays a fundamental role. The crack propagation path usually follows crystallographic planes of the adjacent grains (Castelluccio and McDowell, 2015). After the crack overcomes tens of grains, the crack is considered a macrocrack and LEFM is applicable to this stage of fatigue life.

Size effect in fatigue

The effect of specimen size on the fatigue behavior of materials is a topic of great importance in both scientific and engineering aspects. The fatigue characterization of structural components implies testing difficulties and extrapolation of the test results to other sizes is needed. It is known that the fatigue strength of materials decreases with the increase of specimen size. The size dependency can be observed in experiments where the fatigue life of materials decrease with increasing the specimen size (Carpinteri et al., 2009; Furuya, 2008; Sun et al., 2016). In the example figure ()

Figure 2.2: Example of fatigue life data for two different specimen size (Sun et al., 2016).

This well-known phenomenon has been intensively analyzed from the birth of fracture mechanics (Griffith and Taylor, 1921). The first attempt to account for this dependency in brittle fracture was developed by Weibull, the weakest link approach (Weibull, 1939), which states that the probability of failure increases with the specimen size due to a higher probability of finding a critical zone that causes the structural macroscopic failure. Further probabilistic studies show that the higher the microstructural heterogeneity of the material, the more critical is the size effect phenomenon (Freudenthal and Gumbel, 1956).

2.2 Classic fatigue models

Models based on S-N curves

The classic models to characterize fatigue behavior are pure phenomenological approaches in which only the macroscopic stress amplitude $\Delta\sigma$ or strain amplitude $\Delta\varepsilon$ of the cycle is considered and provide a relation with the total fatigue life of a material. A first stress-life approach was developed in (Wohler, 1860; Spangenberg, 1875) by characterizing the fatigue behavior of the materials with the S - N curves, which represent stress amplitude $\Delta\sigma$ versus number of cycles to failure N_f . An example of S - N curve is shown in figure 2.3. The point on the top of the curve corresponds to the tensile ultimate strength, which leads to the failure during the first ramp up of the first cycle. The

horizontal line on the bottom of the figure 2.3 corresponds to the fatigue limit, which is the maximum stress where the test will last infinite time.

Figure 2.3: Example of a the S - N curve taken from Schijve (2001).

In the S - N curves, two different regimes can be observed, namely LCF and HCF. The LCF regime is characterized by the higher macroscopic stress amplitudes, as a consequence the material plastifies and the micro-plastic strain is homogeneously distributed within the microstructure. The macroscopic plastic strain can be observed in the macroscopic hysteresis loop of every cycle. On the contrary, in HCF regime the stress amplitude is lower and cyclic plastic strain only occurs localized in some hotspots of the microstructures being macroscopic plasticity almost negligible.

Basquin (1910) proposed to plot the S - N curve using a log-log scale ($\log \Delta\sigma$ - $\log N$). This representation allows to identify a linear correlation between the number of cycles and the stress amplitude. This relation is known as the Basquin law, where C and n are material constants and follows

$$\Delta\sigma = C \cdot 2N_f^n, \quad (2.1)$$

where C and n are material parameters. This law is still used today in its original form or using an alternative formulation as

$$\frac{\Delta\varepsilon_e}{2} = \frac{\sigma_f}{E} (2N_f)^c. \quad (2.2)$$

where $\Delta\varepsilon_e$ is the elastic strain amplitude, σ_f is a material parameter that scales with tensile strength, E is the Young's modulus of the material and b is the slope of the log-log fitting curve.

Based on the Bauschinger effect (Bauschinger, 1880), which results in a change of the elastic limit during the cyclic loading, Coffin (1954) and Manson (1954) proposed a strain-life approach for load cases in which plasticity is observed in each cycle. As a result, a $\Delta\varepsilon$ - N curves were obtained and, similarly to equation (2.1), a log-linear correlation (equation (2.3)) was observed between the macroscopic plastic strain amplitude $\Delta\varepsilon_p$ and the number of cycles to rupture N_f . This law, known as Coffin-Manson model is given by

$$\frac{\Delta\varepsilon_p}{2} = \varepsilon_f (2N_f)^c \quad (2.3)$$

where ε_f and c are material parameters. the model is still being used today for the design in the LCF regime.

It has been observed experimentally that, in addition to the stress or strain amplitude of the cycles, the mean value of the stress plays a role in the fatigue performance of an alloy. However, previous approaches do not consider this effect. The mean stresses σ_m of a fatigue test is characterized by the load ratio R which is defined as:

$$R = \frac{\sigma_{min}}{\sigma_{max}} \quad \text{or} \quad \sigma_m = \frac{R+1}{2} \sigma_{min} \quad (2.4)$$

Experiments commonly use stress ratios of $R = 0$ and $R = -1$, corresponding to fully tensile loads and fully reversed loads respectively. Soderberg, Goodman and Gerber included in their studies the effect of the mean stress to calculate an equivalent fatigue limit of a pure reversal loads fatigue test (Goodman, 1914).

Alternatives to the Coffin-Manson relation were proposed including the effect of the mean stress. To this aim, a new equation was proposed by Smith et al. (1963) that relates total strain with fatigue life as the sum of the elastic and plastic strains. This new expression implies an extension of the Coffin-Manson law for the cases where the plastic strain amplitude $\Delta\varepsilon_p$ is low and follows

$$\frac{\Delta\varepsilon}{2} = \frac{\Delta\varepsilon_e}{2} + \frac{\Delta\varepsilon_p}{2} = \frac{\sigma_f - \sigma_m}{E} (2N_f)_1^c + \varepsilon_f (2N_f)_2^c \quad (2.5)$$

where c_1 and c_2 are constants of the material. Both contributions can be observed in figure 2.4. The plastic strain contribution is dominant in LCF whereas elastic strain contribution is dominant in HCF.

Figure 2.4: Plastic and elastic strain contributions to $\Delta\varepsilon$ - N curve extracted from Schijve (2001).

Fatigue has a stochastic nature and this nature makes difficult to accurately characterize correctly the average fatigue behavior. A correct experimental characterization implies to perform a large amount of experiments to account for the scatter in the results, as it is shown in Figure 2.5. A large scatter in fatigue life for identical tests conditions is found and the number of cycles in fatigue life can differ in an order of magnitude or more, especially in HCF cases.

Figure 2.5: Experimental fatigue results from Hardrath et al. (1959).

In figure 2.5 it can be also observed that the scatter associated with lower stress amplitudes, close to the fatigue limit, is considerably higher than the scatter associated with high stress amplitudes. This large scatter at low stresses is due to the crack initiation. The location and generation of a crack depends on the hotspots available, that randomly varies from one specimen to other. On the other hand, under high

stresses, more locations undergo plastic strain and the probability to initiate a crack is much higher and it is less dependent on the specific details of the microstructure defects. Experiments can confirm that, under the microscope, the fracture surface shows multi-site initiation for high stress amplitude whereas single crack initiation is found for lower stress amplitudes, close to the fatigue limit (Schijve, 1994).

Classic treatment of the macroscopic scatter found in fatigue experiments consists in fitting the life distribution for a particular stress amplitude to a probabilistic distribution. The most common distributions used to fit fatigue results are the log-normal distribution and the 3-parameter Weibull distribution (Schijve, 2005). The log-normal Cumulative Distribution Function (CDF) is defined by:

$$P(X \leq x) = \frac{1}{\sigma\sqrt{2\pi}} \int_0^x e^{-\frac{1}{2}\left(\frac{\log(y)-\mu}{\sigma}\right)^2} \frac{dy}{y} \quad (2.6)$$

where μ and σ are two parameters defining the statistical function. These are parameters related to the mean and the standard deviation in the logarithmic scale, respectively. The variable x represents the number of cycles until failure N_f . The 3-parameter Weibull distribution CDF is also defined by the expression (2.7).

$$P(X \leq x) = 1 - e^{-\left(\frac{x-\theta}{\lambda}\right)^k} \text{ for } x > \theta \quad (2.7)$$

where k is known as the shape parameter, λ as the scale parameter and finally θ is the location parameter. The location parameter sets a limit below which the probability of occurrence is zero.

Typical normal probability graphs are used to fit test data to a particular statistical distribution. This graph shows the correlation of the statistical distribution to the experimental data and represents the probability of rupture corresponding to a particular value of the logarithm of the number of lifetime cycles 2.6. The CDF of a log-normal distribution is shown as a straight line in this type of plot.

Figure 2.6: Example of test results in a normal probability graph. Log-normal distribution (straight line) and 3-parameter Weibull (curves)). Taken from Schijve (2005).

More advanced and sophisticated fatigue models have been developed taking these seminal studies as their basis (Miner, 1945; Morrow, 1965; Solomon, 1986). Some other studies introduced characteristic homogenized features of the microstructure to include the effect of grain size or defects but from a macroscopic point of view (Tanaka and Mura, 1982a,b; Chan, 2003; McDowell et al., 2003).

Models for crack propagation

In these seminal studies, only the final failure of the complete specimen is considered, and different stages of fatigue life are not described. To determine the influence of existing cracks and the crack growth behavior, linear elastic fracture mechanics were developed by Griffith and Taylor (1921), where stress intensity factor concept was introduced for static cracks stating that the intensity of a crack is a function of the applied stress, the crack length and its geometry. In these works, the basic concept consists in considering the change of elastic energy stored in the material as the driving energy to create new surfaces to propagate the crack. Using these concepts, Paris and Erdogan (1963) proposed a log-log empirical relationship between the range of stress intensity, ΔK , and the crack growth rate $\frac{da}{dN}$ introducing only two further material specific parameters C and n (see Figure 2.7). Note that ΔK depends on the crack length, the particular loading conditions and a geometrical factor.

Figure 2.7: Illustration of a Paris diagram showing crack growth rate per cycle as function of stress intensity factor and the three separated regimes of crack growth during fatigue loading.

The Paris law is valid only for a limited range of stress intensity factor. In order to observe a macroscopic crack growth, the crack length has to overcome a critical length that depends on the geometry and loading conditions and it is characterized by the threshold stress intensity factor ΔK_{Th} . This value depends is highly influenced by the microstructure. On the other hand, if the crack is too large, crack growth becomes unstable and the value defining this characteristic length is given by ΔK_u . Although crack propagation can be accurately predicted using Paris type models, crack nucleation and early growth is not accounted, and this stage can imply a major amount of the total lifetime especially for small loading amplitudes.

Models for size effects

Regarding macroscopic models that capture the size effect, several model have been developed (Paolino et al., 2013; Castillo et al., 1985; Castilio et al., 1987; Castillo and Fernández-Canteli, 2001; Castillo and Fernández-Canteli, 2009). Most of them are statistical approaches based on the extreme value distributions such as the Weibull, Gumbel and Frechet that takes into account the length by using the weakest link principle. This principle establishes that the fatigue lifetime of a longitudinal element is the minimum fatigue life of its constituting pieces and it is calculated by the joint probability of the survival function of each piece.

2.3 Micromechanics based fatigue models

Most of the classic fatigue models used in industry are based on macroscopic data and cannot capture explicitly the influence of the microstructure. As a consequence, large experimental programs are needed to feed the $S-N$ (or $\Delta\varepsilon-N$) curves for every different microstructure. To provide a better understanding of the influence of microstructure in the fatigue behavior, micromechanics based fatigue models are essential tools. They are based on the micromechanical simulations combining computational homogenization and crystal plasticity models. Micromechanics based fatigue models in which the actual microstructure is considered would help in the design of fatigue resistant materials, identifying the key microstructural parameters (such as grain size and crystallographic orientation) and being able to virtually test different microstructures without actually manufacture them (McDowell, 2007; McDowell and Dunne, 2010). Micromechanics based models for predicting fatigue life (McDowell, 2007) aim to reduce the cost and time to obtain reliable fatigue predictions.

Micromechanics based fatigue models rely on the simulation of the mechanical response of a Representative Volume Element (RVE) (consisting in an aggregate of grains, see Section 2.3.1) of the microstructure under cyclic loads by means of computational homogenization. This involves solving the Boundary Value Problem (BVP) on a periodic domain (the RVE of a polycrystal) containing the actual grain size, shape and orientation distributions subjected to cyclic load and extrapolate the results to the macroscale. Single grains within the polycrystal are modeled using a Crystal Plasticity (CP) model as constitutive equation. These models have to take into account all the phenomena exhibited by the material at the crystal level. Different solvers are available for the resolution of the boundary value problem such as the Finite Element Method (FEM) (Manonukul and Dunne, 2004; Korsunsky et al., 2007; Sweeney et al., 2013; Shenoy et al., 2007; Sinha and Ghosh, 2006; Keshavarz and Ghosh, 2013; Cruzado et al., 2017) or fast Fourier transform (FFT) (Lebensohn, 2001; Lebensohn and Cazacu, 2012; Eisenlohr et al., 2013; Rovinelli et al., 2015). Computational homogenization allows to obtain the microfields and microstrain concentration within the polycrystal under a given loads history, being this field distribution within the RVE the basis for fatigue life prediction by calculating some Fatigue Indicator Parameters (FIPs) that are representative of the driving force of fatigue crack initiation.

Micromechanics based fatigue modeling is a well-established framework to predict the crack initiation (or directly fatigue life if crack growth stage is small compared to incubation) from micromechanics simulations (McDowell and Dunne, 2010; Dunne, 2014; Pineau et al., 2016). The approach follows these steps:

1. Synthetic generation of a RVE consisting of a determined number of grains, following real microstructure grain size and orientations distributions
2. Development/adjustment of a crystal plasticity model to account for the grain behavior which reproduces the elasto-visco-plastic behavior of the crystals
3. Simulation of the RVE response under a macroscopic cyclic loading for a relevant number of cycles using computational polycrystalline homogenization
4. Evaluation of a Fatigue Indicator Parameter for every point of the microstructure to obtain the most critical region and the FIP value associated to this particular RVE
5. Prediction of the fatigue life using an empirical fatigue life law that links the FIP of the RVE to the number of cycles to initiation N_i . The law is usually fitted to one or more fatigue experiments

Additionally, is very common to use different random RVEs (defining a set of SVEs) representative of the same microstructure to introduce statistics in the predictions.

Although micromechanics based fatigue models are complex and computationally expensive, they have interesting advantages that include:

- Microplasticity fields can be obtained even for stress/strain ranges in which no macroscopic plastic deformation is exhibited.
- Multiaxial loading conditions can be simulated. Traditional approaches as the S-N curve are limited to a single loading case, which most of the times is uniaxial.
- The effect of the microstructure, including aspects such as grain size, texture, grain shape and size distribution, is naturally introduced through the RVE used.
- The effect of defects such as second phases and voids can be explicitly introduced in the model.
- Statistical studies can be performed, and the expected scatter of a fatigue case can be obtained.

In this section, the different elements of the micromechanics based fatigue framework used are described, including the RVE generation, the crystal plasticity model, the polycrystal homogenization technique and the fatigue life prediction method.

2.3.1 Representation of the microstructure

The first step to perform computational homogenization and to solve the micromechanics problem, consist in the generation of synthetic RVEs of the microstructure. In the case of polycrystalline metals, the RVE corresponds to a periodic domain containing an aggregate of grains (crystals) following the actual microstructure of the material, namely the grain size, shape and orientation distributions. The size of the RVE of a polycrystal for a given macroscopic property is defined as the minimum volume of the microstructure such that the property considered from the RVE (obtained from the computational homogenization macroscopic response) is equal to the effective property of the macroscopic heterogeneous solid.

The generation of synthetic polycrystals consists in dividing the RVE in a set of geometrical domains, each one corresponding to a grain. Crystals are assumed to be homogeneous polyhedra separated by grain boundaries, normally assumed to have no thickness, with a specific orientation. Alternatively, other microstructural features that can be relevant at local level, as second phases or twin boundaries, can be explicitly included into the polycrystal. The most common approach to characterize a polycrystalline microstructure is to determine the grain size and shape distribution, together with the Orientation Distribution Function (ODF) that defines the crystallographic texture of the polycrystal.

This microstructural parametrization allows to virtually generate different RVEs following the same microstructural characteristics. The 3D grain size distributions can be obtained either from optical microscopy micrographs or X-ray diffraction maps, obtaining 2D cross sectional equiaxed grain size distribution and transforming it into 3D grain size distributions (Heilbronner and Bruhn, 1998; Cruzado et al., 2015). Other novel experimental techniques allow to determine the 3D grain size and shape distributions such as microtome or mechanical milling or 3D diffraction-contrast tomography (Alkemper and Voorhees, 2001; Spowart et al., 2003; Ludwig et al., 2008). Further microstructure descriptors can be determined as 2-point statistics (Torquato, 2001).

From the microstructural parameters, the generation of RVE is performed using a geometrical tessellation that can reconstruct the 3D morphology of the grains. The starting point is a cloud of crystal centers, that should be spatially distributed according the grain size corresponding to that crystal. This spatial distribution can be obtained using a Montecarlo method and assuming the grains to be ellipsoids. Then, the geometric definition of the polycrystal consists in assigning any point x in the RVE to a particular grain G_i . This is done by checking a generalized distance of each point with the grain centers that, for or any point x contained in the RVE is defined for the grain

G_i with center $\mathbf{x}_i$ and a radius r_i as

$$\mathbf{x} \in G_i \text{ if } d(\mathbf{x}, \mathbf{x}_i) < d(\mathbf{x}, \mathbf{x}_j) \forall j \neq i \quad (2.8)$$

where $d(\mathbf{x}, \mathbf{x}_j)$ is the metric defining the distance point-grain center. If a Voronoi tessellation is considered, then

$$d(\mathbf{x}, \mathbf{x}_i) = \|\mathbf{x} - \mathbf{x}_i\| \quad (2.9)$$

However, more developed tessellations can be used, as the multiplicative weighted Voronoi tessellation that defines the measure of the distance as

$$d(\mathbf{x}, \mathbf{x}_i) = \frac{\|\mathbf{x} - \mathbf{x}_i\|}{r_i} \quad (2.10)$$

and the Laguerre tessellation (Redenbach et al., 2012) that determines the distance as

$$d(\mathbf{x}, \mathbf{x}_i) = \|\mathbf{x} - \mathbf{x}_i\|^2 - r_i^2 \quad (2.11)$$

Figure 2.8: Left: Voxel type RVE polycrystal. Right: Voronoi type RVE polycrystal.

The digitalization of the tessellation of the RVEs can be performed in two different manners. The first type of digitalization consists in the rasterization of the spatial representation of the tessellation into a regular grid of voxels, yielding into the voxel type models. The second is the representation of the real geometric representation of the tessellation including the polyhedron vertexes, edges, surfaces and volumes resulting in the Voronoi type models. Examples of polycrystals are shown in Figure 2.8. The voxelized model is suitable to model with structured voxel grids and can serve as an input of many types of BVP solvers as finite differences, FFT or FEM. On the contrary, the Voronoi type model should use an adaptive mesh, which usually requires an extra computational effort as a trade of accuracy in the geometry definition.

The RVEs used in this work are cubes with a regular discretization of cubed voxels. This type of RVEs are known as voxel models. Each grain in the RVE is represented by a set of voxels or elements that defines the grain size and shape. The RVEs are synthetically generated to fulfill the statistical distribution of grain sizes of the microstructure of the material. Any equiaxed grain microstructure obtained from experimental measurements usually follows a log-normal distribution defined by the parameters σ and μ . The cubic RVEs including this statistics can be generated nowadays in a quite automated process using any open-source codes, for instance DREAM3D (Dream.3d, 2012), Neper (Quey et al., 2011) and FFTMAD (Appendix B). An example of RVE generated is shown in Figure 2.8.

Finally, another important concept is the Statistical Volume Element (SVE) (Przybyla and McDowell, 2010; Przybyla et al., 2013; Sweeney et al., 2015). The SVEs does not fulfill the properties of a RVE, only a large population of SVEs can statistically indicate the characteristics of a RVE. In this case, the effective properties can be computed as an average of the properties obtained from many SVEs. This type of volume elements is useful when there are computational limitation concerning the size of the volume to study and the characteristic length of the microstructural features.

2.3.2 Crystal plasticity models

The Crystal Plasticity (CP) model is a material constitutive model that aims to reproduce the mechanical behavior of metallic single crystal taking into account the crystallographic nature of the metal. A review on basic concepts on CP models can be found in Roters et al. (2010); Segurado et al. (2018). The seminal work in CP models was developed by Taylor and Elam (1923, 1925) describing the plastic deformation of metallic single crystals as a function of crystallographic slip where the slip only occurs in slip systems. Slip systems are formed by the combination of a slip plane, which are normally the planes containing the highest number of atoms per unit area (close packed planes), and a slip direction, which also are the close packed directions, containing the highest number of atoms per unit length (Hull and Bacon, 2011). In Taylor and Elam (1923, 1925), resolved shear stress on each slip system acts as a driving force of the shear deformation. Taylor (1938) adapted the model to be applied for polycrystal aggregates.

Hill (1966) extended the Taylor model to the continuum mechanics framework for small strains. In the following years the framework was adapted to finite strains and considering a general internal variable thermodynamic formalism in Rice (1971); Hill and Rice (1972). Lee and Liu (1967) introduced the concept of the multiplicative decomposition of the deformation gradient into elastic and plastic parts. CP constitutive

models were adapted for single crystal behavior using rate independent (Peirce et al., 1982, 1983) or viscoplasticity formulations (Asaro and Needleman, 1985). Finally, this framework was enhanced including efficient and well-posed integration methods for the highly nonlinear viscoplastic laws (Cuitiño and Ortiz, 1992) and rigorous integration for the finite deformation framework (Miehe, 1996).

The starting point of the majority of modern CP models for finite strains is the concept that the deformation gradient $\mathbf{F}$ can be split into its elastic, $\mathbf{F}_e$, and plastic, $\mathbf{F}_p$, parts (see Figure 2.9) as a multiplicative decomposition following

$$\mathbf{F} = \mathbf{F}_e \mathbf{F}_p \quad (2.12)$$

where the configuration defined by $\mathbf{F}_p$ represents the relaxed or intermediate configuration. In the context of CP, it is assumed that $\mathbf{F}_p$ leaves the crystal lattice undistorted and unrotated (Rice, 1971; Hill and Rice, 1972) and the rotation of the lattice is determined only by $\mathbf{F}_e$.

Figure 2.9: Multiplicative decomposition of the deformation gradient.

This decomposition defines two configurations of the material, the intermediate (only after plastic strains), and the current (after total strains), as shown in Figure 2.9.

The definition of the velocity gradient, in combination with eq. (2.12), yields into:

$$\mathbf{L} = \dot{\mathbf{F}}\mathbf{F}^{-1} = \dot{\mathbf{F}}_e\mathbf{F}_e^{-1} + \mathbf{F}_e\dot{\mathbf{F}}_p\mathbf{F}_p^{-1}\mathbf{F}_e^{-1} \quad (2.13)$$

So that the plastic velocity gradient defined in the intermediate configuration $\overline{\mathbf{L}}_p$ is extracted from the total velocity gradient as the term

$$\overline{\mathbf{L}}_p = \dot{\mathbf{F}}_p\mathbf{F}_p^{-1} \quad (2.14)$$

In a generic CP framework, the constitutive equations can be derived from the energy density functional formulation expressed in the intermediate configuration $\overline{\Psi}$ (Cuitiño and Ortiz, 1992; Han et al., 2005). Following the internal state variable formalism, the free energy density, $\overline{\Psi}$, can be expressed as

$$\overline{\Psi} = \overline{\Psi}(\mathbf{F}, \boldsymbol{\alpha}) \quad (2.15)$$

where $\boldsymbol{\alpha}$ stands for the vector of internal state variables. The free energy density can be split into the elastic and plastic energy densities (Cuitiño and Ortiz, 1992) following

$$\overline{\Psi} = \overline{\Psi}_e(\mathbf{F}\mathbf{F}_p^{-1}) + \overline{\Psi}_p(\mathbf{F}_p, \boldsymbol{\alpha}) . \quad (2.16)$$

From the derivations of the free energy functional, the stress tensor defined in the intermediate configuration (the second Piola-Kirchhoff $\mathbf{S}$) yields as

$$\mathbf{S} = \frac{\partial \overline{\Psi}_e}{\partial \overline{\mathbf{E}}_e} \quad (2.17)$$

where $\overline{\mathbf{E}}_e$ stands for the Green-Lagrange elastic strain in the intermediate configuration and is given by

$$\overline{\mathbf{E}}_e = \frac{1}{2} (\mathbf{F}_e^T \mathbf{F}_e - \mathbf{I}) \quad (2.18)$$

where $\mathbf{I}$ is the second order identity tensor. The Cauchy stress $\boldsymbol{\sigma}$ can be recovered pushing the second Piola-Kirchhoff stress $\overline{\mathbf{S}}$ from the intermediate configuration to the current configuration according to

$$\boldsymbol{\sigma} = J\mathbf{F}_e\overline{\mathbf{S}}\mathbf{F}_e^T \quad (2.19)$$

where J is the determinant of the deformation gradient $\mathbf{F}$. When the free energy elastic potential, $\overline{\Psi}_e$ in eq. (2.16), is quadratic, a linear expression of the second Piola-Kirchhoff

stress as a function of the Green-Lagrange elastic strain yields, following

$$\bar{\mathbf{S}} = \bar{\mathbb{C}} : \bar{\mathbf{E}}_e, \quad (2.20)$$

where $\bar{\mathbb{C}}$ represents for the fourth order elastic stiffness tensor of the single crystal corresponding to the crystallographic lattice. In Face Centered Cubic (FCC) metals this tensor can be determined by three constants, namely C_{11} , C_{12} and C_{44} , due to cubic symmetries.

The plastic behavior of a crystal plasticity model is dictated by the slip systems corresponding to the crystallographic nature of the crystal lattice. Each slip system k of a single crystal is determined by two orthogonal unit vectors, namely $\mathbf{s}_k$ and $\mathbf{m}_k$, which stand for the slip direction and slip plane normal, respectively and that remain invariant in the intermediate configuration (2.9). In the case of FCC crystals, there are 4 slip planes with 3 possible slip directions each, which means that there are 12 possible slip systems corresponding to the family of $\{111\}$ planes and the $\langle 110 \rangle$ directions.

The plastic slip of a slip system is governed by the conventional flow rule, proposed in Rice (1971). The single crystal plastic behavior follows the geometrical description of the slip systems and it is described by the plastic velocity gradient tensor as the sum of the plastic slip of all the slip systems. The resulting expression of the plastic velocity gradient tensor follows

$$\bar{\mathbf{L}}_p = \sum_k \dot{\gamma}_k \mathbf{s}_k \otimes \mathbf{m}_k \quad (2.21)$$

where $\dot{\gamma}_k$ is the plastic slip in each slip system k and the outer product $\mathbf{s}_k \otimes \mathbf{m}_k$ is the non-symmetric Schmid tensor of the system k .

Crystal plasticity model normally defines the evolution of the plastic slip in a slip system $\dot{\gamma}_k$, as a function of the internal variables $\boldsymbol{\alpha}$ and the resolved shear stress τ_k on the slip plane corresponding to that slip system, following the so-called flow rule ((2.22)).

$$\dot{\gamma}_k = \dot{\gamma}_k(\tau_k, \boldsymbol{\alpha}) \quad (2.22)$$

The resolved shear stress τ_k is obtained as the projection of the applied load in the crystal on the slip plane and direction of the slip system k . Considering that λ is the angle between the direction of the applied force and the slip direction, and that ϕ is the angle between the force and the normal to the slip plane, the resolved shear stress is calculated as shown in equation (2.23) (see Figure 2.10).

Figure 2.10: Projection of the applied load in a slip system (Hull and Bacon, 2011).

$$\tau_k = \frac{F}{A} \cos \phi \cos \lambda \quad (2.23)$$

In eq. (2.23), F is the force applies and A is the cross-section area. In a finite strains context, the resolved shear stress τ_k is defined as (Cuitiño and Ortiz, 1992)

$$\tau_k = \mathbf{F}_e^T \mathbf{F}_e \bar{\mathbf{S}} : \mathbf{s}_k \otimes \mathbf{m}_k \quad (2.24)$$

although this definition is usually simplified as

$$\tau_k = \bar{\mathbf{S}} : \mathbf{s}_k \otimes \mathbf{m}_k \quad (2.25)$$

Finally, the shear rate $\dot{\gamma}_k$ of each slip system k is determined by a flow rule that accounts for the physical phenomena that occurs when slip planes are activated. In parallel, an evolution of the internal variable should be defined within a consistent thermodynamic framework.

Many types of CP models have been developed in the last decades that can be classified as: phenomenological, physically based and strain gradient plasticity models. Among them, phenomenological CP model has been used in this work, due to its simplicity, efficiency and good accuracy.

Phenomenological crystal plasticity models

In the phenomenological CP models, the evolution of internal variables determines the current state of the crystal, similar to classic constitutive equations. This evolution is based on the microscopic physical processes although internal variables are not necessarily physical entities as dislocation densities. Rice (1971); Hill and Rice (1972) introduced the first approach using a rate-independent model and, few years later, viscoplastic formulations became very popular (Peirce et al., 1983; Anand and Kothari, 1996).

In phenomenological CP models, the slip is a consequence of a shear stress acting on a particular slip system. α is the vector of the internal variables that contains the information about the state on the crystal. The accumulated plastic slip γ_k and the Critical Resolved Shear Stress (CRSS) g_k are typical state variables for each slip system. g_k corresponds to the critical value of the resolved shear stress to activate the plastic slip in the k slip system. The slip rate, eq. (2.22), is usually given by a power-law flow rule following

$$\dot{\gamma}_k = \dot{\gamma}_0 \left| \frac{\tau_k}{g_k} \right|^{\frac{1}{m}} \text{sign}(\tau_k) \quad (2.26)$$

where $\dot{\gamma}_0$ and m stand for the reference strain rate and the strain rate sensitivity parameter, respectively. In the original work of Peirce et al. (1983), $\dot{\gamma}_k$ can take only positive values and positive and negative slip directions s_k where considered. In most of the recent viscous formulations, $\dot{\gamma}_k$ (eq. (2.26)) is considered using both signs and only one direction of s_k .

The evolution of the critical resolved shear stress (CRSS) can be determined to account for strain hardening. In the original model by Peirce et al. (1983) only isotropic hardening is considered and follows eq. (2.27), where the CRSS on each system included the explicit contributions of the slip in the same system (self hardening) and of the slip on all the other slip systems (latent hardening) is considered.

$$\dot{g}_k = \sum_l h_{kl} |\dot{\gamma}_l| \quad (2.27)$$

In (2.27), h_{kl} is the matrix containing the latent and self hardening moduli. Peirce et al. (1983) proposed a model defining the hardening moduli as a function of a parameter q determined by the latent hardening and the accumulated shear on all the slip systems $\dot{\gamma}_l$ that reads as

$$h_{kl} = h(\Gamma) (q + (1 - q) \delta_{kl}) \quad (2.28)$$

where q is the coefficient of the latent hardening and where

$$\Gamma = \sum_k \int_0^t \dot{\gamma}_k dt \quad (2.29)$$

The function $h(\Gamma)$ proposed for FCC single crystals takes the form

$$h(\Gamma) = \text{sech}^2 \left(\frac{h_0 \Gamma}{\tau_s - \tau_0} \right) \quad (2.30)$$

where the three parameters stand for the initial CRSS, τ_0 , the saturation CRSS, τ_s , and the initial hardening modulus. Alternatives to this saturation hardening law have been proposed in Tome et al. (1984); Peirce et al. (1983).

To account for cyclic deformation, the phenomenological framework has been improved introducing the effect of a backstress into the constitutive equations. This backstress follows the formulation of kinematic hardening laws at the crystal level (Méric et al., 1991; Cailletaud, 1992; Hu et al., 1992). In the flow rule according to (Cailletaud, 1992), the plastic shear rate stands as a function of the CRSS and the backstress.

$$\dot{\gamma}_k = \begin{cases} \dot{\gamma}_0 \left(\frac{|\tau_k - \chi_k| - g_k}{K} \right)^{\frac{1}{m}} \text{sign}(\tau_k - \chi_k) & \text{if } |\tau_k - \chi_k| \geq g_k \\ 0 & \text{if } |\tau_k - \chi_k| < g_k \end{cases} \quad (2.31)$$

In eq. (2.31), χ_k stands for the backstress corresponding to the slip system k and K is a numerical parameter. Cailletaud (1992) proposed the equation (2.32) for FCC metals, and the evolution of the backstress was defined by the kinematic hardening.

$$\dot{\chi}_k = c \dot{\gamma}_k - d |\dot{\gamma}_k| \chi_k \quad (2.32)$$

where c and d are two material constants that dictates the kinematic hardening. Several approaches have been developed to reproduce the kinematic hardening. The majority are adapted from the macroscopic cyclic behavior to the crystal level. In Méric et al. (1991), the Frederick-Armstrong law for kinematic hardening was adapted to a CP model, following

$$\dot{\chi}_k = c \dot{\gamma}_k - d |\dot{\gamma}_k| \chi_k \quad (2.33)$$

Recently, Cruzado et al. (2017) presented a phenomenological CP model for cyclic loading that includes the effect of cyclic softening and an alternative evolution of the backstress to account for the mean stress relaxation. The plastic slip rate in this model is

expressed as

$$\dot{\gamma}_k = \dot{\gamma}_0 \left| \frac{\tau_k - \chi_k}{g_k} \right|^{\frac{1}{m}} \text{sign}(\tau_k - \chi_k) \quad (2.34)$$

where the evolution of the backstress is obtained as a simplified version of the Ohno-Wang macroscopic model (Ohno and Wang, 1993) limited to the first two terms

$$\dot{\chi}_k = c\dot{\gamma}_k - d|\dot{\gamma}_k|\chi_k \left(\frac{|\chi_k|}{c/d} \right)^r \quad (2.35)$$

where c and d are the parameters of the Frederick-Armstrong model while r is an extra parameter that controls the mean stress relaxation velocity. Finally, the cyclic softening was accounted for through a new internal variable, the cyclic plastic slip, γ_{cyc} , is given by,

$$\gamma_{cyc} = \sum_k \int_0^t |\dot{\gamma}_k| dt - \sum_k \left| \int_0^t \dot{\gamma}_k dt \right| \quad (2.36)$$

which was taken into account in the evolution of the CRSS, decomposing the CRSS g_k into the cyclic $g_{k\text{ cyc}}$ and isotropic hardening $g_{k\text{ iso}}$ parts, and defining $g_{k\text{ cyc}} = g_{k\text{ cyc}}(\gamma_{cyc})$, using a Voce type law with negative slope.

2.3.3 Simulation of the RVE response

This step consists in the resolution of the periodic BVP on a RVE of the microstructure under some macroscopic loading. It allows to link the microstructure descriptors, used for the generation of the RVE, with the constitutive equations (CP) defined for each single phase incorporated into the RVE. The RVE is usually considered periodic, as it is embedded into the microstructure of the material, and the applied loads are assumed to be the far-field equivalent loads. As a result, the homogenized behavior can be calculated and microfields are obtained.

In polycrystal computational homogenization, the BVP becomes non-linear due to non-linear material behavior. If the framework used is formulated in finite strain, non-linear geometry is also considered. The solver used should deal with these non-linearities and to this end, Newton-Raphson method can be used. In this case material tangent is needed and should be provided by the constitutive equations. Often, this tangent is not easy to derive from the constitutive equations and approximated tangents or numerical consistent tangents are used instead (Meier et al., 2014).

Among the different solvers available in computational homogenization approaches,

Finite Element Method (FEM) is the most used for polycrystal homogenization (Castelluccio and McDowell, 2014; Manonukul and Dunne, 2004; Shenoy et al., 2008; McDowell and Dunne, 2010; Sweeney et al., 2014; Cruzado et al., 2017). There are several reasons for this, in particular the availability of many FEM codes, the access to a lot of constitutive equations and the adaptability and smoothness of the geometries that can be achieved with a good meshing. However, FEM approach applied to computational homogenization present also some drawbacks:

- FEM requires a mesh and meshing some microstructures is time consuming and not an easy task even using commercial packages. Moreover, meshing voxel type images requires generating a smooth geometry first.
- Periodic boundary conditions, the standard approach in computational homogenization, require special implementation in finite elements. Elimination of degrees of freedom or Lagrange multipliers are normally used, and the result of these techniques is a loss of diagonal band structure of the stiffness matrix increasing the memory to store it and the efficiency of the linear solvers.
- The method, in its implicit form, scales by $O(n^2 - n^3)$ (n is the number of degrees of freedom) depending on the particular conditions and solving approach. This scaling prevents the use of very big meshes or the need of using largely parallelized codes running in computer clusters.

In FEM, periodic boundary conditions are imposed relating the relative displacement between periodic nodes with the macroscopic (average) deformation gradient $\bar{\mathbf{F}}$ according to equation (2.37) (Segurado and Llorca, 2013; Cruzado et al., 2015).

$$\mathbf{u}_B - \mathbf{u}_A = (\bar{\mathbf{F}} - \mathbf{I})\mathbf{L}_{AB} \quad (2.37)$$

In eq. (2.37), $\bar{\mathbf{F}}$ stands for prescribed macroscopic deformation gradient and $\mathbf{u}_A$ and $\mathbf{u}_B$ the displacement vectors of the nodes A and B in the same location of opposite faces (Segurado and Llorca, 2013; Cruzado et al., 2015). An illustration of periodic boundary conditions is shown in Figure 2.11.

Figure 2.11: Example of periodic boundary conditions in a 2D polycrystal taken from Segurado et al. (2018). (a) Undeformed configuration. (b) Deformed shape under biaxial deformation.

Computational homogenization of polycrystals requires the use of large number of degrees of freedom in the BVP that depends on the discretization of the domain. The minimum discretization needed to accurately represent a RVE is closely related to the characteristic length of the microstructure and the size of the RVE studied. This leads to a computational limitation regarding the maximum size of the RVE or the maximum refinement of the discretization. An efficient alternative to the FEM homogenization is the Fast Fourier Transform (FFT) homogenization, which is based on the seminal work proposed by Moulinec and Suquet (1994). This alternative presents some advantages:

- FFT does not require meshing and voxel type images can be directly plugged in as a grid.
- Periodic boundary conditions are naturally considered since, the geometry and all the fields considered in the algorithm are periodic
- The method scales by $O(N \log N)$, being N the number of degrees of freedom, and allows to solve larger RVEs compared to FEM

This approach is considered more suitable for the study of polycrystals (Lebensohn, 2001; Lebensohn and Cazacu, 2012; Eisenlohr et al., 2013; Rovinelli et al., 2015) due to the necessity of solving large RVEs. Indeed, FFT approaches are the basis of this thesis and for this reason, the method is described exhaustively in Section 2.4.

2.3.4 Fatigue crack initiation: Fatigue indicator parameters and prediction laws

In metals, the mechanisms of fatigue crack initiation are often described in terms of the development of regions of persistent slip bands. In LCF, bulk plastic deformation takes place, but the plasticity is still heterogeneous and therefore localized. On the contrary, in HCF the plastic deformation drastically depends on any defect introduced inside the microstructure where the plasticity can start to localize. In polycrystalline metals with random crystallographic orientations, local stress and plastic strain fields are dictated by the distributions of orientations, grain shapes and sizes. It is expected that localized regions appear where slip localizes and thus crack initiation occurs.

When fatigue crack formation and subcritical growth follows crystallographic paths the evolution of the microfields during the simulation of a loading cycle can be used to predict fatigue life. To this aim, microscopic parameters that reflect the local driving forces for fatigue crack formation, named Fatigue Indicators Parameters (FIPs) (McDowell and Dunne, 2010), are obtained from the microscopic fields obtained in the FFT or FEM solutions of the BVP. These parameters vary across the RVE depending on the local features of the microstructure and can be related to the number of cycles necessary to nucleate a crack.

Different FIPs have been proposed in the literature as driving force to correlate with fatigue life, namely the equivalent plastic slip per cycle (Manonukul and Dunne, 2004; Sweeney et al., 2012), plastic work accumulated per cycle (Sweeney et al., 2014; Wan et al., 2014) and the Fatemi-Socie parameter (Fatemi and Socie, 1988; Shenoy et al., 2007). The local value of the equivalent plastic slip per cycle, P_{cyc} is defined as

$$P_{cyc}(\mathbf{x}) = \int_{cyc} \mathbf{L}_p(\mathbf{x}) : \mathbf{L}_p(\mathbf{x}) dt \quad (2.38)$$

where $\mathbf{L}_p$ is the plastic velocity gradient. The local value of the density of energy dissipated per cycle defines in each slip system defines the plastic work accumulated per cycle FIP, $W_{k\ cyc}$,

$$W_{k\ cyc}(\mathbf{x}) = \int_{cyc} \tau_k \dot{\gamma}_k(\mathbf{x}) dt \quad (2.39)$$

where τ_k is the resolved shear stress and $\dot{\gamma}_k$ is the shear strain rate on the slip system k . Finally, the Fatemi-Socie parameter is calculated as

$$FS_{k\ cyc}(\mathbf{x}) = \frac{\Delta\gamma_{k\ cyc}}{2} \left(1 + K' \frac{\sigma_{n\ k}}{\sigma_y} \right) \quad (2.40)$$

where $\Delta\gamma_{k\ cyc}$ is the maximum range of plastic slip of the plane k over a fatigue cycle,

K' is a constant that controls the effect of normal stress in fatigue crack formation and $\sigma_{n\ k})/\sigma_y$ is the ratio between the maximum tensile stress normal to the slip plane k and the cyclic yield strength.

The physical meaning of these values is the local accumulation of damage per cycle and it must be highlighted that these parameters are computed in each material point. The local value of the FIPs may depend on the actual discretization (Sweeney et al., 2013) and in order to reduce this dependency and also to introduce explicitly a physical volume in which the nucleation process takes place, non-local measures of the FIPs are defined. These non-local FIP values are the average of the corresponding FIP local value in a given integration volume. Then, the maximum value of the non-local FIP map in the RVE is taken as the parameter representative of the fatigue damage accumulation per cycle in the full microstructure and is used to estimate the number of cycles for crack nucleation. Two integration regions are commonly used in the literature, the volume occupied by a grain (Shenoy et al., 2007) and the volume defined, for each integration point, by the bands of a given width contained in the grain and parallel to the slip planes (Castelluccio and McDowell, 2015) (see Figure 2.12). As a result, for a particular RVE two FIP values can be used to predict the fatigue life of a given RVE, the maximum grain averaged FIP per cycle, FIP_{RVE}^g

$$FIP_{RVE}^g = \max_{i=1, n_g} \frac{1}{V_i^g} \int_{V_i^g} FIP_{cyc}(\mathbf{x}) dV_i^g \quad (2.41)$$

where n_g is the total number of grains and V_i is the volume of the i -th grain, and the maximum band averaged FIP per cycle FIP_{RVE}^b ,

$$FIP_{RVE}^b = \max_{i=1, n_b} \left\{ \max_{k_i} \frac{1}{V_i^b} \int_{V_i^b} FIP_{cyc}^{k_i}(\mathbf{x}) dV_i^b \right\} \quad (2.42)$$

where k_i are the different slips systems contained in the slip plane parallel to the band i , V_i is the volume of that band and n_b is the total number of bands in the microstructure. Note that the band averaged versions can only be applied for the crystallographically defined FIPs. The subregions V_i used for FIP averaging correspond either to full grains (V_i is the volume of the i -th grain) or slip bands (V_i is the volume of each band in which the RVE is divided). The geometrical definition of the bands proposed in Castelluccio and McDowell (2014) corresponds to one element/voxel thickness bands contained within each grain, centered in each voxel of the grain, and parallel to the slip planes of the FCC alloy, $\{111\}$ planes.

Figure 2.12: Illustration of FIP volume averaging: grain averaging (left) and band averaging (right)

The number of cycles for nucleating a crack N_i (or directly the fatigue life if nucleation stage is considered much longer than propagation) of a RVE for a given macroscopic cyclic loading history —defined using strain or stress control, multiaxiality, shape of the cycles, asymmetry R and deformation amplitude $\Delta\varepsilon$ — is obtained by a simple empirical relation between the FIP_{RVE} and N_i . This fatigue life law contains one or more parameters of the material, adjusted correlating the FIP obtained in the simulation of one or more real experiments with the actual life measured in those tests.

The simplistic approach proposed by Manonukul and Dunne (2004) hypothesized the existence of a critical value of FIP at the micro-level, FIP_{crit} , which once achieved, leads to crack initiation. Because the stress–strain behavior stabilizes in some point of the cyclic test, the crack initiation criterion may then be rewritten as

$$FIP_{RVE}N_i = FIP_{crit} \quad (2.43)$$

On the other hand, other authors (Shenoy et al., 2007; Musinski and McDowell, 2012) proposed a power type law expression, based on Tanaka and Mura (1981) model, following

$$FIP_{RVE}^2 N_i = \frac{FIP_{crit}}{d_{gr}} \quad (2.44)$$

where FIP_{crit} is a parameter to fit with experimental data using two or more fatigue tests and d_{gr} is the average grain size. In these models, the grain/band with the highest value gives lowest computed value of N_i and it is assumed to incubate a crack.

2.4 FFT based homogenization

FFT or spectral approaches for homogenization are a set of numerical methods to solve the mechanical equilibrium equation in a periodic heterogeneous domain based on the Fast Fourier Transform. There are many different approaches in FFT homogenization and, disregarding other possible classification, the methods can be divided in two groups attending to their formulations.

The first group are methods derived from the original fixed point iteration scheme proposed by Moulinec and Suquet (1994, 1998). These methods are derived from the strong formulation of the equilibrium and are based in the use of Green's functions for a reference medium computed in the Fourier space and the solution of the Lippmann-Schwinger equation. Several improvements of the original method were later developed to improve the convergence of the iterative scheme for high stiffness contrast (Eyre and Milton, 1999; Michel et al., 2000; Monchiet and Bonnet, 2012). Alternatively, some researchers transformed the fixed-point iterative algorithms into a system of equations, solving the resulting system using Krylov solvers (Zeman et al., 2010; Brisard and Dormieux, 2010, 2012; Kabel et al., 2014, 2016).

The second family is derived from the weak formulation of the linear momentum conservation (Vondřejc et al., 2014; Zeman et al., 2017; de Geus et al., 2017). In this case, the Galerkin approach of the equilibrium is written in terms of the trigonometric polynomials, defined through the discrete Fourier Transform. In addition to its smart formulation, this approach can be highlighted because it does not need the definition of a reference medium. In this family, Krylov solvers are also proposed as the kernel of the algorithm.

The most common FFT based homogenization algorithms are detailed in this section, but first, some basic concepts are explained for the sake of completeness.

2.4.1 Fourier transform

The Fourier transform $\mathcal{F}$ is a mathematical linear operation that transforms a function expressed in time or space domain $f(x)$ into the frequency domain $\hat{f}(\xi)$. $f(x)$ stands for an arbitrary function, x for the independent variable, which corresponds to the position or time, ξ is the variable frequency, which is defined in $\xi \in (-\infty, \infty)$, and $\hat{f}$ represents the function f defined in the frequency domain. The Fourier transform is extensively used for image and digital signal processing.

When the Fourier transform is used on a function in time domain, the domain of the new function is frequency, whereas when the original function is expressed in the space

domain, the resulting function is expressed in spatial frequencies. Accordingly, the frequency representation of the original function is determined by the Fourier transform. The expression to calculate the Fourier transform is given by (Föllinger, 1986):

$$\mathcal{F}(f(x)) = \hat{f}(\xi) = \int_{-\infty}^{\infty} f(x) e^{i\xi x} dx \quad (2.45)$$

where $i = \sqrt{-1}$ is the imaginary number.

Conversely, the inverse of this mathematical operation can be computed via the following equation:

$$\mathcal{F}^{-1}(\hat{f}(\xi)) = f(x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \hat{f}(\xi) e^{-i\xi x} d\xi \quad (2.46)$$

yielding into the expression of the inverse Fourier transform.

The Fourier transform is widely used due to the beneficial properties of representing the function in the frequency domain. One of the properties is the expression of the derivative in the frequency domain. It is a straightforward calculation that consists in the original function multiplied by $i\xi$:

$$\mathcal{F}\left(\frac{d}{dx}f(x)\right) = i\xi \hat{f}(\xi) \quad (2.47)$$

Other interesting property of Fourier transform, widely explored in the methods for solving mechanical problems, is the convolution of two functions. Let f and g be two functions (real or complex valued functions) defined in the real space, the function obtained as the convolution of them $h(x)$ is defined as

$$h(x) = (f * g)(x) = \int_{-\infty}^{\infty} (f(x)g(x - y))dy \quad (2.48)$$

The convolution theorem that states that the Fourier transform of the convolution, $\mathcal{F}(h(x)) = \hat{h}(\xi)$, can be obtained as the point wise product of the Fourier transform.

$$\hat{h}(\xi) = \hat{f}(\xi) \cdot \hat{g}(\xi) \quad (2.49)$$

The last interesting property of the Fourier transform is the shift theorem that gives a closed expression for a shifted function and follows (2.50).

$$\mathcal{F}(f(x - x_0)) = e^{-i\xi x_0} \hat{f}(\xi) \quad (2.50)$$

Further properties of the Fourier transform that are not explicitly used in this framework can be found in classical works such as Föllinger (1986); Boyd (1989).

2.4.2 Discrete Fourier transform

The Fourier transform can be applied to a discrete representation of a periodic function. To this end, the Discrete Fourier Transform (DFT) is performed and consists in a Fourier transform on periodic discrete data or function. It should be remarked that the DFT is properly used if the analyzed segment represents one (time or space) period of an infinitely extended periodic function. In a discrete periodic domain of length L , frequencies are discrete and each frequency ξ stands for one wavenumber, where the total number of waves is the total number of points of the input data and therefore the size of the output is the same of the input data. The discretization in the space or time domain is performed by defining discrete equidistant points $x_n \in \mathbb{R}$ inside the periodic spatial domain.

The result of the DFT of the input function f , with N real numbers $f_n = f(x_n)$ defined in a discretized spatial domain (length L) being $n = 0, \dots, N-1$, is the array $\hat{f}(\xi_k)$, with $k = 0, \dots, N-1$ of N wavenumbers for $\xi_0, \dots, \xi_{N-1}$ according to:

$$\hat{f}_k = \hat{f}(\xi_k) = \sum_{n=0}^{N-1} f_n \cdot e^{\frac{i2\pi kn}{N}}, k = 0, \dots, N-1 \quad (2.51)$$

and the resulting values is the representation in the frequency domain of the original function or data. The frequencies are usually chosen as

$$\xi_k \equiv \frac{2\pi k}{L} \text{ for } \begin{cases} k = -\frac{N-1}{2}, \dots, 0, \dots, \frac{N-1}{2} \text{ if } N \text{ odd} \\ k = -\frac{N}{2}, \dots, 0, \dots, \frac{N-1}{2} \text{ if } N \text{ even} \end{cases} \quad (2.52)$$

for the sake of symmetry respect to the frequency 0. In case that the discretization N is even, the highest valued (in absolute terms) frequency ($k = -\frac{N}{2}$) is called the Nyquist frequency and this term does not have symmetric counterpart.

Similarly, the Inverse Discrete Fourier Transform (IDFT) can be performed as:

$$f(x_n) = \frac{1}{N} \sum_{k=0}^{N-1} \hat{f}_k \cdot e^{-\frac{i2\pi kn}{N}}, n = 0, \dots, N-1 \quad (2.53)$$

It gives the values at each discrete spatial point that results from the operations conducted in frequency domain.

When the original function or data is real, the transformed data in frequency domain is symmetric with respect to the origin on the real part and anti-symmetric on the imaginary part. Thus, in the DFT algorithm, it's only required to compute the values of the transform at the half of the frequencies and the rest of the values are computed from the conjugated complex of the first half data. In the same way, for the inverse transform only half of transformed data is needed to transform to a set of real data (Bracewell, 1986).

In eq. (2.51), the array $\hat{f}(\xi_k)$ of the frequency domain representation is obtained from the one dimensional array of the periodic function f_n evaluated in the discretized points x_n . The DFT can be extended to a (two or) three dimensional function depending on a discrete vector $\mathbf{x}$ with components $x_{n_1}, x_{n_2}, x_{n_3}$ being $n_1 = 0, \dots, N_1 - 1; n_2 = 0, \dots, N_2 - 1; n_3 = 0, \dots, N_3 - 1$ yielding into a multidimensional DFT. It consists in the mathematical linear operator that transforms a function or data defined in $x_n \in \mathbb{R}^3$ into the frequency domain, resulting in a discrete function depending on the frequencies $\xi = \{\xi_{k_1}, \xi_{k_2}, \xi_{k_3}\}$ with $k_1 = 0, \dots, N_1 - 1; k_2 = 0, \dots, N_2 - 1; k_3 = 0, \dots, N_3 - 1$, following eq. (2.52) each component. The expression that performs the three dimensional DFT is defined in (2.54) following Neumann et al. (2001).

$$\hat{f}(\xi) = \hat{f}(\xi_{k_1}, \xi_{k_2}, \xi_{k_3}) = \sum_{n_1=0}^{N_1-1} \sum_{n_2=0}^{N_2-1} \sum_{n_3=0}^{N_3-1} f(x_{n_1}, x_{n_2}, x_{n_3}) \cdot e^{i2\pi\left(\frac{k_1 n_1}{N_1} + \frac{k_2 n_2}{N_2} + \frac{k_3 n_3}{N_3}\right)} \quad (2.54)$$

Similarly, the inverse of the multidimensional DFT reads as

$$f(\mathbf{x}) = f(x_{n_1}, x_{n_2}, x_{n_3}) = \frac{1}{N_1 \cdot N_2 \cdot N_3} \sum_{j=0}^{N_1-1} \sum_{k=0}^{N_2-1} \sum_{l=0}^{N_3-1} \hat{f}(\xi_j, \xi_k, \xi_l) \cdot e^{-i2\pi\left(\frac{j n_1}{N_1} + \frac{k n_2}{N_2} + \frac{l n_3}{N_3}\right)} \quad (2.55)$$

The frequencies ξ now are vectors and will be also centered on 0 value for each component. Nyquist frequencies now are considered all the vectors in which any of the components contains a Nyquist value. In the case of a real-valued input function, the same symmetries of the Fourier Transform within the last axis are preserved over. Extra symmetries can be observed so that the number data points in the frequency domain, which are complex, is exactly the half of the number of input data points, which are real.

Fast Fourier transform

The fast Fourier transform (FFT) is an efficient and witty algorithm to perform the DFT operation (2.51) or (2.54). Following the expression (2.51), the computational operations required scale as $O(N^2)$ and therefore, computational time boosts quadratic

with the discretization. The FFT can perform the DFT with $O(N \cdot \log_2 N)$ operations without any approximation. The existence of the FFT is the main reason to use the frequency domain for homogenization problems. The seminal idea of the FFT algorithms was proposed by Cooley and Tukey (1965). This method divides the whole transformation into smaller parts that are simpler to compute. The key point consists on splitting a Fourier transform into two smaller transforms recursively, until reaching lots of transforms of only two elements in the array, x_0, x_1 with $f(x_0)$ and $f(x_1)$, which can be computed easily following:

$$\widehat{f}(x_0) = f(x_0) + f(x_1); \widehat{f}(x_1) = f(x_0) - f(x_1) \quad (2.56)$$

The original algorithm was designed for power of two sized input arrays but extension for all kind of inputs were developed after. All the FFT algorithms shows a poor performance for prime numbers (Bracewell, 1986).

A large portion of the computational time of FFT based homogenization schemes is spent in the calculation of the FFT. Thus, the implementation of FFT should have a good performance including a good CPU parallelization profile and an efficient memory management. Python, the language that has been used as the basis of this work, includes two implementations of FFT, in numpy and scipy modules that are reasonably efficient. Additionally, there is an alternative standard open source FFT which has shown a performance comparable with algorithms available under commercial licenses, the Fastest Fourier Transform in the West (FFTW). This software is licensed under the GNU General Public License. The FFTW package is developed at the Massachusetts Institute of Technology (MIT) by Frigo and Johnson (1993). It is a C subroutine library with interfaces to call it from C or Fortran codes. It can compute the DFT in one or more dimensions. Moreover, it can handle arrays of arbitrary input size and has interface to compute the DFT of real data. It also has multiprocessor support using the Open Multi-Processing (OpenMP). To implement this tool in python, there is a python module that act as a wrapper called pyfftw that links python data with FFTW C library.

2.4.3 Solving non-homogeneous partial differential equations using Green's function

Let $\mathcal{L}$ be a linear differential operator defined in a domain $\Omega \subset \mathbb{R}^n$. A Green's function $G(\mathbf{x}, \mathbf{s})$ at the point $\mathbf{s}$ is any solution of:

$$\mathcal{L}G(\mathbf{x}, \mathbf{s}) = \delta(\mathbf{x} - \mathbf{s}) \quad (2.57)$$

where δ denotes the delta Dirac.

The Green's function can be used to solve a differential equation related to that operator. A large number of differential equation families can be solved using this method, including inhomogeneous partial differential equations (PDE) with boundary conditions (Bayinl, 2006), of particular interest in this work.

Let be a non-homogeneous boundary value problem defined by $\mathcal{L}$ in a domain Ω with boundary Γ . The problem is finding $u(\mathbf{x})$ such that

$$\mathcal{L}u(\mathbf{x}) = f(\mathbf{x}) \quad (2.58)$$

$$\text{with } u(\Gamma) = C \quad (2.59)$$

where $u(\mathbf{x})$ is the solution function, $f(\mathbf{x})$ is the source or non-homogeneous term and C is a constant. If the Green's function corresponding to the linear operator is known, then multiplying the equation 2.57 by $f(s)$, and integrating with respect to s , it is obtained

$$\int_{\Omega} \mathcal{L} (G(\mathbf{x}, s)f(s)) ds = \int_{\Omega} \delta(\mathbf{x} - s)f(s)ds = f(\mathbf{x}) \quad (2.60)$$

The right-hand side reduces merely to $f(\mathbf{x})$ due to properties of the delta function, and because $\mathcal{L}$ is a linear operator acting only on $\mathbf{x}$ and not on s , the left-hand side can be rewritten as $u(x)$.

$$\mathcal{L} (u(\mathbf{x})) = \mathcal{L} \left(\int_{\Omega} G(\mathbf{x}, s)f(s)ds \right) = f(\mathbf{x}) \quad (2.61)$$

whereby it follows that u has the specific integral form

$$u(\mathbf{x}) = \int_{\Omega} G(\mathbf{x}, s)f(s)ds \quad (2.62)$$

In summary, the solution of equation (2.58) can be obtained from the source term and the green function by computing the integral (2.62).

2.4.4 FFT based homogenization: Basic scheme

The seminal idea of homogenization based on the use of the discrete Fourier transform and its FFT algorithm was first introduced by Moulinec and Suquet (1994). This original method proposed, named basic scheme, is based on solving the Lippmann-Schwinger equation yielded from the strong formulation of the mechanical equilibrium on a periodic domain using a fixed-point algorithm. This scheme was first developed for linear elastic materials and it's the example taken below to explain the algorithm.

Let be a heterogeneous microstructure formed by different phases arranged in a periodic domain Ω , usually named Representative Volume Element or RVE (Fig. 2.13).

Figure 2.13: Periodic domain (RVE) with two phases

The heterogeneous microstructure can be described by a function $\mathbb{C}(\mathbf{x})$ that provides the fourth order stiffness tensor of the phase located at the point $\mathbf{x}$. In a small strain framework, the stress can be computed as

$$\boldsymbol{\sigma}(\mathbf{x}) = \mathbb{C}(\mathbf{x}) : \boldsymbol{\varepsilon}(\mathbf{x}) \quad (2.63)$$

where $\boldsymbol{\sigma} = \sigma_{ij}$ is the Cauchy stress, $\boldsymbol{\varepsilon} = \varepsilon_{ij}$ is the small strain tensor and $\mathbb{C} = C_{ijkl}$ is the symmetric fourth order stiffness tensor with major and minor symmetries. The conservation of linear momentum balance, in its strong formulation and in the absence of body forces, reads as

$$\nabla \cdot \boldsymbol{\sigma}(\mathbf{x}) = \mathbf{0} \quad (2.64)$$

The strain field $\boldsymbol{\varepsilon}(\mathbf{x})$ is assumed to be periodic and is chosen as the unknown of the problem. Then the strain field is decomposed into two parts, the spatial average over the volume, denoted as $\langle \boldsymbol{\varepsilon} \rangle = \bar{\boldsymbol{\varepsilon}}$, and a periodic strain fluctuation field $\tilde{\boldsymbol{\varepsilon}}(\mathbf{x})$. This decomposition reads

$$\boldsymbol{\varepsilon}(\mathbf{x}) = \bar{\boldsymbol{\varepsilon}} + \tilde{\boldsymbol{\varepsilon}}(\mathbf{x}) \quad (2.65)$$

It should be noted that the spatial average $\bar{\boldsymbol{\varepsilon}}$ is usually the data of the problem.

If the actual heterogeneous material were replaced by a homogeneous material with $\mathbb{C}^0$ (reference medium), the equilibrium equation would then be given by

$$\nabla \cdot \mathbb{C}^0 : \boldsymbol{\varepsilon}(\mathbf{x}) = \mathbf{0} \quad (2.66)$$

Adding and subtracting the effect of the reference medium in the definition of the local stress of the actual heterogeneous, eq. (2.63) leads to

$$\boldsymbol{\sigma}(\mathbf{x}) = [\mathbb{C}^0 - \mathbb{C}^0 + \mathbb{C}(\mathbf{x})] : (\tilde{\boldsymbol{\varepsilon}}(\mathbf{x}) + \bar{\boldsymbol{\varepsilon}}) = \underbrace{\mathbb{C}^0 : \tilde{\boldsymbol{\varepsilon}}(\mathbf{x}) + \mathbb{C}^0 : \bar{\boldsymbol{\varepsilon}}}_{\text{reference stress}} + [\mathbb{C}(\mathbf{x}) - \mathbb{C}^0] : (\bar{\boldsymbol{\varepsilon}} + \tilde{\boldsymbol{\varepsilon}}(\mathbf{x})) \quad (2.67)$$

where the under-braced term is called polarization tensor, and is given by¹

$$\boldsymbol{\tau}(\mathbf{x}) := \mathbb{C}^0 : \bar{\boldsymbol{\varepsilon}} + [\mathbb{C}(\mathbf{x}) - \mathbb{C}^0] : (\bar{\boldsymbol{\varepsilon}} + \tilde{\boldsymbol{\varepsilon}}(\mathbf{x})) \quad (2.68)$$

Introducing the Cauchy stress (eq. (2.63)) and polarization tensor (eq. (2.68)) into the linear momentum balance (eq. (2.64)) the following non-homogeneous PDE in the reference medium is obtained

$$\operatorname{div} \mathbb{C}^0 : \tilde{\boldsymbol{\varepsilon}}(\mathbf{x}) = -\operatorname{div}(\boldsymbol{\tau}(\mathbf{x})) , \quad (2.69)$$

being the term $-\operatorname{div} \boldsymbol{\tau}(\mathbf{x})$, is the source of the non-homogeneous equation. Moreover, $\operatorname{div} \boldsymbol{\tau}(\mathbf{x})$ plays the role of an external force per unit volume ($\rho \mathbf{b}$ in the equilibrium equation).

If the fluctuating strain field is expressed in terms of fluctuating displacement field ($\tilde{\mathbf{u}}$), $\nabla^s \tilde{\mathbf{u}} = \tilde{\boldsymbol{\varepsilon}}$, and introduced in the previous equation

$$\operatorname{div} (\mathbb{C}^0 : \nabla^s \tilde{\mathbf{u}}(\mathbf{x})) = -\operatorname{div}(\boldsymbol{\tau}(\mathbf{x})) , \quad (2.70)$$

the resulting equation can be solved using the Green's function theorem. In particular, the Green's function of the linear operator of eq. (2.70), $\mathbf{G}(\mathbf{x}, \mathbf{s})$, relates the displacement fluctuation at a point with a unit external force as

$$\tilde{u}_i(\mathbf{x}) = G_{ij}^0(\mathbf{x} - \mathbf{s}) F_j \quad (2.71)$$

Using this function, the fluctuation displacement field can then be obtained as

$$\tilde{\mathbf{u}}(\mathbf{x}) = \int_{\Omega} \mathbf{G}^0(\mathbf{x} - \mathbf{s}) \operatorname{div} \boldsymbol{\tau}(\mathbf{s}) d\mathbf{s} \quad (2.72)$$

In order to obtain directly the strain as function of the polarization, a fourth order tensor field, $\mathbb{I}$, is introduced, that is defined from the directional derivatives of the Green's function

$$\Gamma_{ijkl}^0(\mathbf{x} - \mathbf{s}) := -G_{ki,jl}^0(\mathbf{x} - \mathbf{s}) \quad (2.73)$$

The resulting expression for the strain fluctuations after applying the corresponding symmetries reads as

$$\tilde{\boldsymbol{\varepsilon}}(\mathbf{x}) = \frac{1}{2}(\tilde{u}_{k,j}(\mathbf{x}) + \tilde{u}_{j,k}(\mathbf{x})) = - \int_{\Omega} \Gamma_{ijkl}^0(\mathbf{x} - \mathbf{s}) \tau_{ij}(\mathbf{s}) d\mathbf{s} = -(\mathbb{I}^0 * \boldsymbol{\tau})(\mathbf{x}) \quad (2.74)$$

¹Note that the term $\mathbb{C}^0 : \bar{\boldsymbol{\varepsilon}}$ in the definition of the polarization (eq. (2.68)) is constant and therefore, divergence free, so the actual value of polarization tensor can neglect that term.

If the polarization field is known, as in the case of a region subjected to a stress-free eigenstrain, this integral can be evaluated directly (Kröner, 1972). On the contrary, in our problem the term $\tau(\mathbf{x})$ depends on the actual strain field and the resulting equation is an implicit integral equation, the Lippmann-Schwinger equation.

The Lippmann-Schwinger equation (eq. (2.74)) is implicit and has to be solved numerically. A Fourier transformation of the equation strongly simplifies the problem since the convolution of two functions in the real space (operation of order n^2) can be obtained as a product in of the Fourier transforms of the functions (order n)

$$\widehat{\varepsilon}(\boldsymbol{\xi}) = \bar{\varepsilon} - \widehat{\mathbb{F}}^0(\boldsymbol{\xi}) : \widehat{\tau}(\varepsilon(\mathbf{x})) \quad (2.75)$$

Note that in (2.75), the polarization is defined as function of the strain field ε and local stiffness $\mathbb{C}(\mathbf{x})$ in the real space, so direct $\mathcal{F}(\cdot)$ and inverse $\mathcal{F}^{-1}(\cdot)$ Fourier transforms are required.

Moreover, to solve the equation, Γ_{ijkl} must be found, and this can be easily achieved in the Fourier space. Green's function is the solution of the equilibrium equation for a unit load located at point $\mathbf{s}$

$$C_{ijkl}^0 G_{km,lj}^0(\mathbf{x} - \mathbf{s}) + \delta_{im} \delta(\mathbf{x} - \mathbf{s}) = 0 \quad (2.76)$$

where δ_{im} is delta Kronecker and δ is the Dirac delta function.

Using the substitution rule of the Kronecker delta and with $i^2 = -1$ the expression of the Green's function, which corresponds to the acoustic tensor, is given by

$$\widehat{G}_{km}^0(\boldsymbol{\xi}) = [C_{ijkl}^0 \xi_l \xi_j]^{-1} \quad (2.77)$$

This equation is valid if $\boldsymbol{\xi} \neq 0$. Replacing (2.77) into the definition of $\mathbb{F}$ (eq. (2.73)) the explicit expression of the operator is determined by

$$\widehat{\Gamma}_{ijkl}^0(\boldsymbol{\xi}) = -i^2 \xi_l \xi_j \widehat{G}_{ki}(\boldsymbol{\xi}) = \xi_l \xi_j [C_{ijkl}^0 \xi_l \xi_j]^{-1}, \forall \boldsymbol{\xi} \neq 0 \quad (2.78)$$

For the 0 frequency the wavelength is infinite, so the solution is the macroscopic imposed strain $\bar{\varepsilon}$. The expression of eq. (2.78) can be simplified in the case of an isotropic reference medium to

$$\widehat{\Gamma}_{ijkl}^0(\boldsymbol{\xi}) = \frac{1}{4\mu^0 |\boldsymbol{\xi}|^2} (\delta_{ki} \xi_l \xi_j + \delta_{li} \xi_k \xi_j + \delta_{kj} \xi_l \xi_i + \delta_{lj} \xi_k \xi_i) - \frac{(\lambda^0 + \mu^0)}{\mu^0 (\lambda^0 + 2\mu^0)} \frac{\xi_i \xi_j \xi_k \xi_l}{|\boldsymbol{\xi}|^4} \quad (2.79)$$

being μ^0 and λ^0 the Lamé coefficients of the reference medium.

Finally, to solve the implicit equation ((2.75)), an iterative method is required. The

basic scheme proposed in Moulinec and Suquet (1994) solves that equation using fixed-point iterative procedure. The resulting algorithm is given in the next box. The value of the reference medium $\mathbb{C}^0$ is required. This value is a pure numerical parameter that has an effect in the convergence rate but does not affect the solution. An optimal choice is the average of the elastic property of the phases.

Algorithm 1: Basic scheme

Data: $\mathbb{C}^0, \mathbb{C}(\mathbf{x}), tol, \bar{\varepsilon}$

Result: $\varepsilon(\mathbf{x})$

$\varepsilon^0(\mathbf{x}) = \bar{\varepsilon}$

while $\frac{\|\varepsilon^{i+1}(\mathbf{x}) - \varepsilon^i(\mathbf{x})\|}{\|\varepsilon^{i+1}\|} > tol$ **do**
 $\tau^i(\mathbf{x}) = [\mathbb{C}(\mathbf{x}) - \mathbb{C}^0] : \varepsilon^i(\mathbf{x})$
 $\hat{\tau}^i(\xi) = \mathcal{F}(\tau^i(\mathbf{x}))$
 $\hat{\varepsilon}^{i+1}(\xi) = -\hat{\Gamma}^0(\xi) : \hat{\tau}^i(\xi)$
 $\varepsilon^{i+1}(\mathbf{x}) = \mathcal{F}^{-1}(\hat{\varepsilon}^{i+1}(\xi)) + \bar{\varepsilon}$

end

2.4.5 Approaches derived from the basic scheme

The use of a fixed-point iteration might result in a poor-convergence rate depending on the phase contrast, even for a clever election of the reference medium. To overcome this limitation, several approaches have been developed based on the same concepts than the basic scheme.

The **accelerated scheme** (Michel et al., 2000) is optimized for high contrast composites and is based on the introduction of an auxiliary field $\mathbf{e}$ at each iteration to improve the convergence.

Algorithm 2: Accelerated scheme

Data: $\mathbb{C}^0, \mathbb{C}(\mathbf{x}), tol, \bar{\varepsilon}$

Result: $\varepsilon(\mathbf{x})$

$\varepsilon^0(\mathbf{x}) = \bar{\varepsilon}$

while $\frac{\|\varepsilon^{i+1}(\mathbf{x}) - \varepsilon^i(\mathbf{x})\|}{\|\varepsilon^{i+1}\|} > tol$ **do**
 $\tau^i(\mathbf{x}) = [\mathbb{C}(\mathbf{x}) - \mathbb{C}^0] : \varepsilon^i(\mathbf{x})$
 $\hat{\tau}^i(\xi) = \mathcal{F}(\tau^i(\mathbf{x}))$
 $\hat{\mathbf{e}}^{i+1}(\xi) = -\hat{\Gamma}^0(\xi) : \hat{\tau}^i(\xi)$
 $\mathbf{e}^{i+1}(\mathbf{x}) = \mathcal{F}^{-1}(\hat{\mathbf{e}}^{i+1}(\xi)) + \bar{\varepsilon}$
 $\varepsilon^{i+1}(\mathbf{x}) = \varepsilon^i(\mathbf{x}) + 2 \left(\mathbb{C}(\mathbf{x}) + \bar{\mathbb{C}} \right)^{-1} : \bar{\mathbb{C}} : (\mathbf{e}^{i+1}(\mathbf{x}) - \varepsilon^i(\mathbf{x}))$

end

The **augmented lagrangian scheme** (Michel et al., 2000) is optimal for composites with very soft inclusions stiffness contrast ($E_m \gg E_p \rightarrow 0$). The method introduces two auxiliary fields $\mathbf{e}$, $\mathbf{s}$, and forces their compatibility and equilibrium by minimization with the augmented Lagrangian.

Algorithm 3: Augmented Lagrangian scheme

Data: $\mathbb{C}^0, \mathbb{C}(\mathbf{x}), tol, \bar{\varepsilon}$

Result: $\varepsilon(\mathbf{x})$

$\mathbf{e}^0(x) = \bar{\varepsilon}; \quad \lambda^0(x) = 0$

while $\frac{\varepsilon^{i+1}(x) - \varepsilon^i(x)}{\varepsilon^{i+1}}$ **and** $\frac{\varepsilon^{i+1}(x) - \mathbf{e}^{i+1}(x)}{\bar{\varepsilon}}$ **and** $\frac{\sigma^{i+1}(x) - \mathbf{s}^{i+1}(x)}{\mathbb{C}^0 : \bar{\varepsilon}} > tol$ **do**

$\tau^i(\mathbf{x}) = \lambda^i(x) - \mathbb{C}^0 : \mathbf{e}^i(\mathbf{x})$

$\hat{\tau}^i(\xi) = \mathcal{F}(\tau^i(x))$

$\hat{\varepsilon}^{i+1}(\xi) = -\hat{\Gamma}^0(\xi) : \hat{\tau}^i(\xi)$

$\varepsilon^{i+1}(\mathbf{x}) = \mathcal{F}^{-1}(\hat{\varepsilon}^{i+1}(\xi)) + \bar{\varepsilon}$

$\mathbf{s}^i(\mathbf{x}) = \mathbb{C}^0 : \varepsilon^{i+1}(x) + \lambda^i(x)$

$\mathbf{e}^{i+1}(\mathbf{x}) = (\mathbb{C}(\mathbf{x}) + \mathbb{C}^0)^{-1} : (\mathbb{C}^0 \varepsilon^{i+1}(\mathbf{x}) + \lambda^i(\mathbf{x}))$

$\lambda^{i+1}(\mathbf{x}) = \mathbb{C}^0 : (\varepsilon^{i+1} - \mathbf{e}^{i+1})$

end

The basic scheme can be also used for **non-linear** materials, as shown in Moulinec and Suquet (1998). This scheme is based on the redefinition of the polarization as

$$\tau(\mathbf{x}) = \sigma(\mathbf{x}) - \mathbb{C}^0 : \varepsilon(\mathbf{x}) \quad (2.80)$$

Following the original form of eq. (2.75) and using eq:nlpolsimp the final expression problem yields into the implicit non-linear equation

$$\hat{\varepsilon}(\xi) = \bar{\varepsilon}(\xi) - \hat{\Gamma}^0(\xi) : (\hat{\sigma}(\varepsilon(\mathbf{x})) - \mathbb{C}^0 : \varepsilon(\mathbf{x})) \quad (2.81)$$

Eq. (2.81) can be solved using a fixed point iteration method, where the solution of the strain field in each iteration is obtained from the result of the previous iteration that is introduced in the right hand side of the equation. Michel et al. (1999) extended the formulation to deal with a prescribed stress problem computing iteratively strain controlled problems until reaching the desired macroscopic stress state.

The extension of the basic scheme to **finite strains** can be found in (Lahellec et al., 2003). In this work, and in most of the approaches later, a Lagrangian configuration is chosen, and equilibrium is expressed in the initial configuration using the first Piola-Kichhoff stress and the deformation gradient. In this case, a Newton-Raphson is combined with the fixed point iteration method to solve the non-linear problem and the

resulting expression of the Green's function in the frequency domain is given by

$$\mathbb{T} = \Gamma_{ijkl} = G_{ik}^0 \xi_j \xi_l |_{(ik)(jh)} \quad (2.82)$$

where G^0 stands for the acoustic tensor (eq. (2.77)) and the symbol $(ik)(jh)$ denotes symmetrization with respect to the indices i, k and j, h only.

Further improvements of this approach were focused in the resolution of the linear equilibrium form (2.75). The expression, in linear elastic materials, can be considered as a linear system of equations and solved iteratively using a Krylov method as the Conjugate Gradient method (Zeman et al., 2010; Vondřejc et al., 2010). This solver shows a higher convergence rate compared to the basic or accelerated scheme, but still presents some limitation in term of stiffness contrast of the phases, since the matrix associated to the linear system is becoming ill-posed.

Finally, extensions of the Lippman-Schwinger equations were proposed for **prescribed macroscopic stress** boundary conditions. In Michel et al. (2000), the duality of the stress based basic scheme is explained, being the solution of the inhomogeneity problem computed by using the fixed point iterative scheme and knowing the compliance tensor for every grid point. Eisenlohr et al. (2013) introduced a method which permits to prescribe the components of the macroscopic deformation gradient or the macroscopic Piola-Kirchhoff stress by correcting the prescribed deformation gradient at each Newton iteration. Under this procedure the algorithm still imposes the full macroscopic strain tensor and corrects it in an iterative manner in order to obtain at the end of the iteration process the macroscopic stress tensor components imposed as input. As a result of the corrections to the applied strain during iterations, the number of iterations per step significantly increases respect the strain control. An alternative approach for classic schemes under mixed control was proposed by Kabel et al. (2016). The method consists in modifying the original basic scheme through the introduction of projection tensors to account for the load control and solving the problem using an iterative Krylov solver. This method for stress control is more efficient than the iterative approaches although still requires the definition of a reference medium which properties might influence the convergence rate.

2.4.6 Galerkin approaches

The Galerkin approaches for FFT homogenization (Vondřejc et al., 2014; Zeman et al., 2017; de Geus et al., 2017) are algorithms in which the weak form of the mechanical equilibrium is solve using a spectral approach and the Galerkin approximation of

the weak form. They are based on imposing the compatibility of the fields by a projector operator defined in the frequency domain and on the use of the fundamental trigonometrical functions as shape functions. The resulting expression of the equilibrium is a linear system of equations that are finally solved by a Krylov method. For the sake of generalization, here is presented the Galerkin approach for a finite strain framework.

The objective of the method is finding the equilibrium deformation gradient and stress microfields in a periodic domain Ω_0 representative of the microstructure of a heterogeneous material. The domain Ω_0 in the reference configuration corresponds to a rectangular parallelepiped characterized by three dimensions, namely L_1, L_2 and L_3 . The domain contains different phases, each one having a particular non-linear behavior, and each point of the domain $\mathbf{x} \in \Omega_0$ belongs to one of those phases. The starting point of the method is the linear momentum balance in the domain Ω_0 under periodic boundary conditions.

$$\left\{ \begin{array}{l} \nabla_0 \mathbf{P}(\mathbf{x}) = \mathbf{0} \\ \mathbf{F}(\mathbf{x}) = \bar{\mathbf{F}} + \tilde{\mathbf{F}}(\mathbf{x}) \\ \text{with } \langle \mathbf{F}(\mathbf{x}) \rangle_{\Omega} = \bar{\mathbf{F}} \\ \text{and } \tilde{\mathbf{F}}(\mathbf{x}) \text{ periodic} \end{array} \right. \quad (2.83)$$

being ∇_0 the divergence in the reference configuration, $\mathbf{P}(\mathbf{x})$ the microscopic first Piola-Kirchhoff stress tensor and $\mathbf{F}(\mathbf{x})$ the microscopic deformation gradient. This field is decomposed in its average value in the domain $\bar{\mathbf{F}}$ (macroscopic or far-field deformation gradient) and the fluctuation field $\tilde{\mathbf{F}}(\mathbf{x})$. The stress at each point of the domain is given by a non-linear constitutive law that models the behavior of the material at that point,

$$\mathbf{P}(\mathbf{x}) = \mathbf{P}(\mathbf{F}(\mathbf{x})) \quad (2.84)$$

where $\mathbf{P}(\mathbf{F}(\mathbf{x}))$ represents a non-linear constitutive model defined in finite strains. The deformation gradient solution of the strong formulation of equilibrium (eq. (2.83)) must be a periodic and compatible field. A weak formulation of the equilibrium is derived then using the virtual work principle. The problem statement consists in finding for every time of a given macroscopic deformation gradient history $\bar{\mathbf{F}}(t)$ the deformation gradient field $\mathbf{F}(\mathbf{x})$ that fulfills

$$\int_{\Omega_0} \delta \mathbf{F}(\mathbf{x}) : \mathbf{P}(\bar{\mathbf{F}} + \tilde{\mathbf{F}}(\mathbf{x})) d\Omega_0 = 0 \quad (2.85)$$

being $\delta \mathbf{F}(\mathbf{x})$ any periodic deformation gradient virtual field fulfilling compatibility and

periodicity conditions. In an incremental time scheme, all the fields in (eq. (2.85)) are defined at time t , although this is omitted to relax the formulation. Note that the terms related to the work done by external stress are not included because they vanish due to the periodic boundary conditions. The compatibility of the virtual field $\delta \mathbf{F}(\mathbf{x})$ is imposed using a projection operator $\mathbb{G}$, which is a fourth order rank linear operator that maps any arbitrary second order tensor periodic field, $\zeta(\mathbf{x})$, in its compatible part

$$\delta \mathbf{F}(\mathbf{x}) = (\mathbb{G} * \zeta)(\mathbf{x}) \quad (2.86)$$

where $*$ stands for the convolution. The projection operator $\mathbb{G}$ is equivalent to the Green's function of a reference media $\mathbb{I}$ introduced in classical approaches (Moulinec and Suquet, 1998), but here, no choice of the reference properties is needed. The standard expression of the projection operator and the modified discrete operator version are given below.

Projector operator

The projector operator $\mathbb{G}(\mathbf{x})$ is a fourth order tensor field (with a closed form expression in the Fourier space) that enforces the compatibility of any tensor field via convolution in the real space. In this framework, the projection operator is used to force the compatibility of the deformation gradient tensor field.

The Helmholtz decomposition of an arbitrary tensor field $\mathbf{A}(\mathbf{x})$ allows to express the field as the sum of three contributions

$$\mathbf{A}(\mathbf{x}) = \mathbf{A}_{\parallel}(\mathbf{x}) + \mathbf{A}_{\perp}(\mathbf{x}) + \overline{\mathbf{A}} \quad (2.87)$$

where $\mathbf{A}_{\parallel}(\mathbf{x})$ is a curl-free component (compatible), $\mathbf{A}_{\perp}(\mathbf{x})$ a divergence-free component (incompatible) and $\overline{\mathbf{A}}$ is the average. The Helmholtz decomposition in the Fourier space (Stewart, 2012) is written as

$$\widehat{\mathbf{A}}(\boldsymbol{\xi}) = \widehat{\mathbf{A}}_{\parallel}(\boldsymbol{\xi}) + \widehat{\mathbf{A}}_{\perp}(\boldsymbol{\xi}) + \widehat{\overline{\mathbf{A}}}, \quad (2.88)$$

being the curl-free component

$$\widehat{\mathbf{A}}_{\parallel}(\boldsymbol{\xi}) = \left(\widehat{\mathbf{A}}(\boldsymbol{\xi}) \cdot \frac{\boldsymbol{\xi}}{|\boldsymbol{\xi}|} \right) \otimes \frac{\boldsymbol{\xi}}{|\boldsymbol{\xi}|} \quad (2.89)$$

where $\boldsymbol{\xi}$ represents the (spatial) frequency vector, with dimension of inverse of length (eq. (2.52)). A fourth order tensor, the projection operator $\widehat{\mathbb{G}}$, can be defined from

equation (2.89) which, when contracted with $\widehat{\mathbf{A}}$, returns its compatible part

$$\widehat{\mathbf{A}}_{\parallel} = \widehat{\mathbb{G}} : \widehat{\mathbf{A}} = \widehat{G}_{ijkl} \widehat{A}_{kl} = \widehat{A}_{\parallel ij} = \delta_{ik} \frac{\xi_j \xi_l}{\boldsymbol{\xi} \cdot \boldsymbol{\xi}} \widehat{A}_{kl} \quad (2.90)$$

In this expression it can be observed that the projection operator in the Fourier space accomplish major symmetry $\widehat{G}_{ijkl} = \widehat{G}_{klij}$.

In order to return a zero mean field value, the projection should be a zero fourth order tensor in the null frequency $\boldsymbol{\xi} = (0, 0, 0)$. If the grid is discretized in an even number of frequencies, symmetries of the operator are lost and some properties used to derive the method are no exact. A simple alternative to overcome this issue is to approximate the value of the operator at the highest frequency (Nyquist frequency) to a null fourth order tensor to recover the frequency symmetry. Considering this, the final expression for the projector operator is

$$\widehat{\mathbb{G}}(\boldsymbol{\xi}) = \widehat{G}_{ijkl} = \begin{cases} 0_{ijkl} & \text{for null and Nyquist frequencies} \\ \delta_{ik} \frac{\xi_j \xi_l}{\boldsymbol{\xi} \cdot \boldsymbol{\xi}} & \text{for the rest of frequencies} \end{cases} \quad (2.91)$$

Substituting equation (2.86) into the weak formulation of equilibrium (eq. (2.85)) and exploiting the symmetries of $\mathbb{G}$ lead to the next integral equation

$$\int_{\Omega_0} \boldsymbol{\zeta}(\mathbf{x}) : [(\mathbb{G} * \mathbf{P})(\mathbf{x})] d\Omega_0 = 0 \quad (2.92)$$

that should be fulfilled for every tensor test function $\boldsymbol{\zeta}(\mathbf{x})$ belonging to the space of all square-integrable arbitrary tensor fields. Then, the domain Ω_0 is discretized in a voxelized regular grid containing $n_x \cdot n_y \cdot n_z$ voxels, being each voxel labeled by three integers x, y, z with $1 \leq x \leq n_x$; $1 \leq y \leq n_y$ and $1 \leq z \leq n_z$. The fields $\mathbf{F}(\mathbf{x})$ and $\boldsymbol{\zeta}(\mathbf{x})$ are approximated by $\mathbf{F}^h(\mathbf{x})$ and $\boldsymbol{\zeta}^h(\mathbf{x})$ respectively. These approximate fields are obtained by interpolating the values at the center of each voxel using the fundamental trigonometric polynomials as shape functions (Zeman et al., 2017) with value equal to 1 at the voxel which belongs to and 0 at the rest of voxels and it is defined by the discrete Fourier transform. As an example, the approximation of the deformation gradient $\mathbf{F}^h(\mathbf{x})$ is obtained as

$$\mathbf{F}^h(\mathbf{x}) = \sum_{x,y,z=1}^{n_x, n_y, n_z} N_{xyz}(\mathbf{x}) \mathbf{F}_{xyz} \quad (2.93)$$

where $N_{xyz}(\mathbf{x})$ are the trigonometrical polynomials for the voxel defined by the integers x, y, z and $\mathbf{F}_{xyz}$ is the value of the deformation gradient at that voxel, $\mathbf{F}_{xyz} = \mathbf{F}(\mathbf{x}(x, y, z))$. The use of the approximate fields in the expression of the virtual work leads to

$$\int_{\Omega_0} \boldsymbol{\zeta}^h(\mathbf{x}) : [\mathbb{G} * \mathbf{P}(\mathbf{F}^h(\mathbf{x}))] d\Omega_0 = 0 \quad (2.94)$$

This integral (eq. (2.94)) is computed using the trapezoidal rule, expressing the trigonometrical polynomials in terms of the discrete Fourier coefficients and using the discrete Fourier transform to perform the convolution operation (Zeman et al., 2017). Note that, opposed to standard finite elements, the integration points are the center of the voxels, the same positions defining the approximated fields (eq. (2.93)). The result of the integral is a sum over the voxels given by

$$\sum_{x,y,z=1}^{n_x, n_y, n_z} \boldsymbol{\zeta}_{xyz} : [\mathbb{G} * \mathbf{P}(\mathbf{F}_{xyz})]_{xyz} = 0 \quad (2.95)$$

The equation (2.95) must be fulfilled for any arbitrary discrete voxel field $\boldsymbol{\zeta}_{xyz}$, implying that the right-hand side of the equation has to be zero at every voxel. If the projection operator is defined in the Fourier space and the convolution is performed as a multiplication in the Fourier space also, the conditions of weak equilibrium can be written as

$$\mathbb{G} * \mathbf{P} = \mathcal{F}^{-1} \left\{ \hat{\mathbb{G}} : \mathcal{F}(\mathbf{P}_{xyz}) \right\} = \mathbf{0}_{xyz} \quad (2.96)$$

where $\mathcal{F}$ and $\mathcal{F}^{-1}$ are the discrete Fourier transform and its inverse respectively, $\mathbf{P}_{xyz}$ stands for the first Piola-Kirchhoff stress at the center of each voxel $\mathbf{P}(\mathbf{F}_{xyz})$ and $\hat{\mathbb{G}}$ is the value of the projection operator in the discrete Fourier space. The expression used for the projection operator is given in eq. (2.91). Equation (2.96) is an algebraic system of $9 \cdot n_x \cdot n_y \cdot n_z$ equations and in which the unknown is the value of the deformation gradient at each voxel $\mathbf{F}_{xyz}$. This equation can be written in a simpler way as

$$\mathcal{G}(\mathbf{P}_{xyz}(\mathbf{F}_{xyz})) = \mathbf{0}_{xyz} \quad (2.97)$$

where $\mathcal{G}$ is a linear map on the vector space in which the voxel fields are defined ($\mathbb{R}^{9 \cdot n_x \cdot n_y \cdot n_z}$) acting on a voxel tensor field $\mathbf{A}_{xyz}$ to create a new voxel tensor field $\mathbf{B}_{xyz}$ into the same space and is defined as

$$\mathcal{G}(\mathbf{A}_{xyz}) := \mathcal{F}^{-1} \left\{ \hat{\mathbb{G}} : \mathcal{F}(\mathbf{A}_{xyz}) \right\} = \mathbf{B}_{xyz}. \quad (2.98)$$

In the case of non-linear material behavior, the discrete expression of the weak form

of equilibrium given by equation (2.97) defines a non-linear system of algebraic equations. Moreover, in the case of a material with internal variables, a history of the macroscopic deformation gradient $\bar{\mathbf{F}}(t)$ has to be defined, the time is discretized in increments and a non-linear problem has to be solved for every time increment $t = t_k$. Let $\bar{\mathbf{F}}(t_k)$ be the value of the macroscopic deformation gradient at time t_k , the objective is finding the deformation gradient at the voxels $\mathbf{F}_{xyz}^{t_k}$ solving the equation (2.97) and being the deformation gradient $\mathbf{F}_{xyz}^{t_{k-1}}$ known at the previous time step. This equation can be solved iteratively by the Newton-Raphson method. To this aim, the deformation gradient field is obtained in an iterative manner, and its value for iteration i is given by

$$\mathbf{F}_{xyz}^i = \mathbf{F}_{xyz}^{i-1} + \delta\mathbf{F}_{xyz}. \quad (2.99)$$

The stress field is linearized around the deformation gradient

$$\begin{aligned} \mathbf{P}_{xyz}^i &= \mathbf{P}_{xyz}^{i-1} + \delta\mathbf{P}_{xyz} = \mathbf{P}_{xyz}^{i-1} + \left. \frac{\partial\mathbf{P}}{\partial\mathbf{F}} \right|_{(\mathbf{F}=\mathbf{F}_{xyz}^{i-1})} : \delta\mathbf{F}_{xyz} = \\ &= \mathbf{P}_{xyz}^{i-1} + \mathbb{K}_{xyz}^{i-1} : \delta\mathbf{F}_{xyz} \end{aligned} \quad (2.100)$$

where $\mathbb{K}$ is the (non-symmetric) material tangent. Combining the equilibrium equation (2.97) with the linearization of deformation gradient and stress (eqs. (2.99) and (2.100)) the next equation is derived for the iteration i

$$\mathcal{G}(\mathbb{K}_{xyz}^{i-1} : \delta\mathbf{F}_{xyz}) = -\mathcal{G}(\mathbf{P}(\mathbf{F}_{xyz}^{i-1})) \quad (2.101)$$

If a new linear map is defined, the resulting expression can be written as

$$\mathcal{G}_{\mathbb{K}^{i-1}}(\delta\mathbf{F}_{xyz}) = -\mathcal{G}(\mathbf{P}(\mathbf{F}_{xyz}^{i-1})) \quad (2.102)$$

where the new linear operator $\mathcal{G}_{\mathbb{K}^{i-1}}$ is defined as

$$\mathcal{G}_{\mathbb{K}^{i-1}}(\mathbf{A}_{xyz}) := \mathcal{G}(\mathbb{K}_{xyz}^{i-1} : \mathbf{A}_{xyz}) \quad (2.103)$$

The expression in equation (2.102) is a linear system of equations in which the unknown is the correction at the iteration i of the deformation gradient $\delta\mathbf{F}_{xyz}$, with $\mathbf{F}^i$ obtained in a previous iteration as $\mathbf{F}^i = \bar{\mathbf{F}}(t_k) + \delta\mathbf{F}^1 + \delta\mathbf{F}^2 \dots + \delta\mathbf{F}^{i-1}$. In this system, the coefficient matrix is very large (dimension $(9 \times n_x \times n_y \times n_z)^2$) and dense, but it is not necessary to explicitly compute it because it is fully defined by the linear operator $\mathcal{G}_{\mathbb{K}^{i-1}}$. This type of equation can therefore be solved using a Krylov iterative solver, where instead of computing and storing the coefficient matrix, a linear operator can be used instead. The conjugate gradient method (Hestenes and Stiefel, 1952) has been

chosen to solve the system due to its good performance for this type of systems. Moreover, the system in eq. (2.102) is indefinite so the use of an iterative descent method is mandatory because, contrary to direct solvers, these methods allow to obtain a solution without eliminating any equation (Kaasschieter, 1988). This deficiency in rank of the operator $\mathcal{G}_{\mathbb{K}^{i-1}}$ is due to its symmetries and to the null value of both the zero and Nyquist frequencies.

For a given time increment t_k corresponding to a macroscopic deformation gradient $\bar{\mathbf{F}}(t_k)$, the solution of the linear equation (2.102) provides a new Newton correction of the deformation gradient, and the equilibrium is reached when the right-hand side of the equation $\mathcal{G}(\mathbf{P}_{xyz})$ is sufficiently small. As in any finite element framework, once reached the equilibrium for time t_k and new time increments are solved until reaching the final time. The solving sequence is summarized in Algorithm 4.

Algorithm 4: Non linear time incremental Galerkin scheme for finite strains

Data: $\bar{\mathbf{F}}, \Delta t, t_{final}, tol_{lin}, tol_{nw}$
Result: $\mathbf{F}(\mathbf{x})$
 $t = 0$
 $\mathbf{F}(t = 0) = \mathbf{I}$
while $t \leq t_{final}$ **do**
 $\mathbf{F}^0 = \mathbf{F}(t = t) + \Delta \bar{\mathbf{F}}^{t+\Delta t}$
 while $\|\delta \tilde{\mathbf{F}}^i\| / \|\bar{\mathbf{F}}^{t+\Delta t}\| \geq tol_{nw}$ **do**
 $\mathbf{P}^i = \mathbf{P}(\tilde{\mathbf{F}}^i); \mathbb{K}^i = \frac{\partial \mathbf{P}}{\partial \mathbf{F}}(\mathbf{F}^i)$
 Solve by Conjugate Gradient while *residual* $\geq tol_{lin}$:
 $\mathbb{G} : \mathbb{K}^i : (\delta \tilde{\mathbf{F}}) = -\mathbb{G} : \mathbf{P}(\mathbf{F}^i)$
 $\mathbf{F}^{i+1} = \mathbf{F}^i + \delta \tilde{\mathbf{F}}$
 end
 $\mathbf{F}(t = t + \Delta t) = \mathbf{F}^{i+1}$
 $t = t + \Delta t$
end

The algorithm using a small strains framework is totally equivalent. The resulting equation is similar to (2.101) with the corresponding small strain counterparts, being the Cauchy stress $\boldsymbol{\sigma}$ instead of the first Piola-Kirchhoff stress $\mathbf{P}$, the strain tensor $\boldsymbol{\varepsilon}$ instead the deformation gradient $\mathbf{F}$, and the fourth order stiffness tensor $\mathbb{C} = \frac{\partial \boldsymbol{\sigma}}{\partial \boldsymbol{\varepsilon}}$ instead the material consistent tangent $\mathbb{K} = \frac{\partial \mathbf{P}}{\partial \mathbf{F}}$ yielding into the following expression:

$$\mathcal{G}^s(\mathbb{C}_{xyz}^{i-1} : \delta \boldsymbol{\varepsilon}_{xyz}) = -\mathcal{G}^s(\boldsymbol{\sigma}(\boldsymbol{\varepsilon}_{xyz}^{i-1})) \quad (2.104)$$

where $\mathcal{G}^s$ corresponds to the operator defined in eq. (2.98) but using the symmetrized

version of the fourth order projector operator tensor $\mathbb{G}^s$, which satisfies major and minor symmetries, following

$$\mathbb{G}^s = G_{ijkl}^s = \frac{1}{4} (G_{ijkl} + G_{jikl} + G_{jilk} + G_{ijlk}) \quad (2.105)$$

where G_{ijkl} is defined in eq. (2.91). Now the operator projects an arbitrary tensor field into a symmetric compatible tensor field. This expression corresponds to the Green Function of the *basic scheme* (Moulinec and Suquet, 1994) for an isotropic reference medium with Lamé constants $\lambda = 0$ and $\mu = 0.5$.

If the problem studied is linear elastic ($\boldsymbol{\sigma} = \mathbb{C} : \boldsymbol{\varepsilon}$), the equilibrium equation becomes linear. Then eq. (2.104) results in an expression (eq. (2.106)) where no iteration is needed and the problem can be solved as a linear system of equations as in the basic or derived schemes.

$$\mathcal{G}^s(\mathbb{C}_{xyz} : \tilde{\boldsymbol{\varepsilon}}_{xyz}) = -\mathcal{G}^s(\mathbb{C}_{xyz} : \bar{\boldsymbol{\varepsilon}}_{xyz}) \quad (2.106)$$

The resulting algorithm is summarized in Algorithm 5.

Algorithm 5: Linear elastic Galerkin scheme for small strains

Data: $\bar{\boldsymbol{\varepsilon}}, \mathbb{C}(\mathbf{x}), tol_{lin}$

Result: $\boldsymbol{\varepsilon}(\mathbf{x})$

Solve by Conjugate Gradient while *residual* $\geq tol_{lin}$:

$$\mathbb{G}^s : \mathbb{C}(\mathbf{x}) : (\tilde{\boldsymbol{\varepsilon}}) = -\mathbb{C} : \mathbb{C}(\mathbf{x}) : \bar{\boldsymbol{\varepsilon}}$$

$$\boldsymbol{\varepsilon} = \tilde{\boldsymbol{\varepsilon}} + \bar{\boldsymbol{\varepsilon}}$$

2.4.7 Discrete derivatives

The results obtained by FFT might present the well-known Gibbs oscillation phenomena in microstructures with a large contrast between phases. In the case of a polycrystals this contrast appears due to the differences in the elasto-plastic response of adjacent grains with different orientations and also due to the presence of non-metallic phases. To overcome this numerical problem, discrete differential operators were first introduced in Müller (2002). They replace the partial derivatives of the differential operators in the real space by a finite difference derivation rule. Then, the discrete derivative rule is transformed to the frequency domain and simplified using the sift theorem. The result is a derivation rule in the Fourier space in which the original frequencies $\boldsymbol{\xi}$ are replaced by some functions of them $\boldsymbol{\xi}' = \boldsymbol{\xi}'(\boldsymbol{\xi})$. Berbenni et al. (2014) extended this idea to derive the first and second order differential operators based on central differences for Poisson and Navier equations.

Among the different possible discrete derivative rules in the real space (i.e. centered scheme, forward or backward differences, etc.), Willot (2015) proposed an alternative rule, the rotated scheme, that exhibited a very smooth response. This approach computes the forward difference in a 45° rotated basis, computing then the difference of diagonal adjacent points (2D example in Figure 2.14). The resulting modified frequency vector for the rotated forward differences scheme derivation (Willot, 2015) is given by

$$\xi' = \xi'_k = \frac{2\pi N_k}{L_k} \frac{1}{4} \tan \frac{q_k}{2} (1 + e^{iq_1}) (1 + e^{iq_2}) (1 + e^{iq_3}) , \quad (2.107)$$

being q_k the normalized frequency vector defined by

$$q_k = \frac{\xi_k L_k}{2\pi N_k} \quad (2.108)$$

where L_k and N_k are the length and the number of voxels in k direction respectively, and ξ is the original frequency vector.

Figure 2.14: A regular grid parallel to the Cartesian axis (e_1 , e_2) and the 45° rotated basis (f_1 , f_2) of the derivative rule. The derivative of the field is calculated at the pixel center x (square). The original field lie along the corners (disks). (Willot, 2015)

2.5 Nickel based superalloy IN718

The material studied in this work is the wrought polycrystalline Inconel 718 superalloy, denominated IN718 alloy, which is widely used for structural parts of jet engines working in a range of temperatures below $650-700^\circ\text{C}$. IN718 is an Iron-Nickel based superalloy of γ Ni rich matrix (FCC) and strengthened with γ' -Ni₃(Al,Ti) and γ'' -Ni₃Nb precipitates. The nominal composition of this alloy is 53% Ni, 19% Fe, 19% Cr, 3% Mo, 5% Nb, 1% Ti, 0.6% Al, 0.04% C and 0.004% B (Radavich, 2004) and the volume fractions of γ' and γ'' phases are in the range 3-5% and 10-20%, respectively, depending

on the bulk alloy composition, the heat-treatment and the degree of element segregation (Fayman, 1987). IN718 combines good corrosion and high mechanical properties with an excellent weldability. In its wrought form, it shows a fine microstructure with equiaxed phase grains as the matrix, and a small fraction (about 12%) of δ phase (Ni_3Nb) distributed preferentially at grain boundaries, and a minor amount (about 0.5%) of second phase particles (niobium carbides, and titanium carbonitrides).

Figure 2.15: Microstructure of coarse-grain IN718 Ni-based superalloy from Cruzado et al. (2015). (a) Polycrystal grain structure showing the distribution of metal carbides and δ phase at the grain boundaries, (b) Distribution of γ' and γ'' precipitates within the Ni FCC solid solution.

The main hardening mechanism is the precipitation hardening produced by the γ'' precipitates that act as obstacle for the dislocations. Since the size of those obstacle is $< 50\text{nm}$, the dislocations can shear or overcome the obstacles without changing the slip plane. For this reason, the plastic deformation occur mainly along 12 octahedral $\{111\}$ $\langle 110 \rangle$ slip systems of the FCC matrix γ phase.

In terms of macroscopic mechanical response, IN718 is characterized by a strong Bauschinger effect (Chaboche et al., 1991) or kinematic hardening. This phenomenon is due to two scale effects. At sub-grain level, the dislocation suffer a backstress due to the formation of dislocation structures as a result of the interaction with the precipitates and grain boundaries (Maciejewski and Ghonem, 2014). At microstructure scale, the differences of the effective yield stress of the differently oriented grains can induce a kinematic hardening when reversal plastic deformations. It can also be observed in strain controlled fatigue experiments that mean stress can be relaxed resulting in cyclic creep or ratcheting (Park et al., 2007; Chaboche et al., 1991). Finally, a cyclic softening can be observed an it is attributed to the successive shearing by dislocations of the

coherent and ordered γ'' precipitates, during the cyclic deformation (Xiao et al., 2005; Kalluri et al., 1994).

The main previous works of micromechanics modeling of IN718 can be found in (Chaboche et al., 1991; Gustafsson et al., 2011; Cruzado et al., 2015, 2017; Ghorbanpour et al., 2017). This work were focused on the development of constitutive equations to reproduce the cyclic behavior of IN718 and on the application of these models for micromechanics based fatigue life prediction.

Many experimental studies can be found in the literature (Pineau et al., 2016) characterizing the mechanical behavior of IN718. However, maybe due to its age (it was developed in the 60s) or mid-range properties, only a few physically based models or multiscale studies can be found, in contrast to the extend literature of this kind for other γ' reinforced superalloys. Among them, Chaboche et al. (1991) developed a phenomenological elasto-visco-plastic model including all the relevant plastic phenomena. More recently, Gustafsson et al. (2011) proposed a physically based model at the macroscale, considering the different hardening mechanisms and including the dependency of some microscopic parameters such as volume fraction or size of γ'' precipitates. However, the model still was developed at the macroscale relating macroscopic response with crystal phenomena using Taylor relation. More recently, Cruzado et al. (2017) proposed a phenomenological CP model to simulate the polycrystalline response using FEM homogenization. The model proposed included also all the relevant plastic response features and was applied to study cyclic behavior of IN718. A CP approach was also used in Ghorbanpour et al. (2017) a bit later using a physically based approach which included the evolution of dislocations. Finally the work developed by Cruzado, Segurado and co-workers was later extended to study LCF and grain size effect in this regime.

3 DEVELOPMENT OF A FRAMEWORK FOR FATIGUE SIMULATIONS BASED ON FFT

The efficiency when solving the mechanical boundary value problem is a crucial aspect of micromechanics based fatigue models (Geers et al., 2010; Segurado et al., 2018). More efficient methods allow the use of larger and more realistic Representative Volume Elements (RVEs) of the microstructure or to perform statistical analysis, fundamental for the study of fatigue. FFT based homogenization does not require meshing simplifying the pre-processing and shows a remarkable computational efficiency and low memory allocation compared to Finite Element Method (FEM). The use of iterative methods for solving the resulting discrete linear problem is partially behind this improvement, since FFT has been usually compared with classical implementations of FEM that rely on less efficient direct solvers for the resulting linear systems. Nevertheless, even introducing iterative solvers and using regular grids in FEM, FFT methods still much more efficient. The memory reduction is due first to the fact that in FFT approaches the linear operators do not need to be stored as a sparse matrix, as normally done in FEM. Second, the use of periodic boundary conditions in the FEM by nodal

elimination reduces drastically the sparsity of the stiffness matrix, resulting in additional memory storage and reducing the computational efficiency due to the increase of the number of operations when applying the linear operators. For these reasons, in this thesis special effort has been made for adapting and improving FFT homogenization applied to micromechanics based fatigue life models.

In order to implement the presented framework and to carry out the polycrystal fatigue simulations, a home-made FFT based code has been developed within the work of this PhD. The code, FFTMAD, is programmed in Python, to take advantage of the wide amount of modules available for numerical methods (numpy, scipy) and the use of object oriented programming. The code includes the classical approaches for linear simulations but non-linear approach is implemented following the Galerkin approach to FFT introduced in (Vondřejc et al., 2014; Zeman et al., 2017; de Geus et al., 2017). Additionally, the code is able to use constitutive equations programmed as Python functions and ABAQUS umat subroutines. All the details about the FFTMAD code can be found in Appendix A.

In this chapter, the FFT framework developed for micromechanics based fatigue life prediction is presented. First a small review of the different features used in micromechanics based fatigue framework is presented in Section 3.1. Secondly, Galerkin based FFT homogenization method is adapted for micromechanics based fatigue model, overcoming the treatment of internal variables, the generalization of the use of constitutive equations and the use of discrete derivative definition to improve the accuracy. Further developments of the method are presented in Sections 3.3 and 3.4, where the Galerkin approach is extended for prescribed macroscopic stress or mixed loading histories and a new homogenization solver is disclosed respectively. Finally, the framework is validated in Section 3.5 for fatigue simulation and in Section 3.6 the efficiency of the different approaches is compared.

3.1 Microstructure generation, constitutive equations and fatigue indicator parameters

3.1.1 Polycrystalline RVE generation

The RVE of a polycrystalline material consists in an aggregate of grains following grain shape, size and orientation statistic distributions representative of the actual microstructure (Section 2.3.1). These distributions can be obtained from experimental measurements. To this end, several approaches can be followed, as using 3D tomography, serial sectioning, or 2D measurements based on EBSD or optical microscope.

Focusing on the most simple approach, 2D optical image, the procedure consist first in acquiring microscope images of chemical attacked polished specimen sections. From the microscope images, the area of each grain can be measured by detecting the grain boundary and using an image processing software.

Figure 3.1: Left, microscope microstructure image. Right, grain boundary determination

If an equiaxed microstructure is assumed, then from each area, an equivalent diameter can be defined assuming a circular shape, following

$$d_{eq} = \sqrt{\frac{4A_{grain}}{\pi}} \quad (3.1)$$

The diameter distribution is then fitted to a log-normal distribution, characteristic of this type of measurements.

Secondly, the 2D equivalent diameter distribution can be transformed into a 3D equivalent diameter distribution considering the probability of obtaining a slice of a sphere at different height in the 2D image following (Heilbronner and Bruhn, 1998). The resulting 3D diameter distribution also follows a log-normal distribution and is the experimental input data for the RVE generation.

Figure 3.2: Left, 2D equivalent diameter distribution. Right, 3D equivalent diameter distribution

The synthetic geometrical generation of the microstructures within a RVE following a log-normal grain size distribution, experimentally obtained as explained above, is done using a weighted Voronoi tessellation in which the points defining the grain center and the corresponding weights are defined to fulfill the target grain size distribution and shape (details in Appendix B). Finally, the RVE geometry is discretized by rasterizing the microstructure in voxels for the FFT simulations resolution in a voxel type RVE (Figure 3.3).

Figure 3.3: Example of a synthetically generated microstructure

The last ingredient of the RVE generation is assigning the orientation of each grain. This assignment is done to have an ODF in the RVE that statistically represents the experimentally measured ODF. In this work, uniform textures are assumed, so the orientation of each grain is assigned to be random.

Periodic boundary conditions are attached to a periodic domain. The microstructure should be periodic and, to this end, when placing the grain centers, a copy of the center has to be placed at RVE length distance in the periodicity direction. Finally, the tessellation is performed considering all the grain centers and its copies. In this work the generation of synthetic microstructures, which follows actual microstructure statistical distributions, has been performed using either Neper (Quey et al., 2011) or the home made generation tool (Appendix B).

Further microstructural features could be included in the RVE such as second phases, defects like voids or free surfaces, that may affect to the behavior of the polycrystals. However, in this thesis, only the effects of grain size and orientation distributions are taken into account. The grains are always considered as a single phase, equiaxed, and the microstructures are clean (without defects or inclusions).

3.1.2 Crystal plasticity model

The elasto-visco-plastic cyclic behavior of crystalline grains is considered by a CP phenomenological model proposed by Cruzado et al. (2017). The model reproduces some common features of the response of polycrystalline Ni-based superalloys under cyclic loading such as kinematic hardening, mean stress relaxation and cyclic softening. Moreover, in Cruzado et al. (2017), the model is parametrized to reproduce the cyclic behavior of IN718 superalloy. A summary of the constitutive equations is presented below.

The crystals behave as elasto-viscoplastic solids in which the plastic velocity gradient is defined as the sum of the plastic slip rates for every slip system multiplied by their corresponding Schmidt tensor. In the case of FCC alloys, the slip systems correspond to the octahedral family, where each slip system k is a combination of the four slip planes $\mathbf{m} = \{111\}$ with their corresponding three slip directions $\mathbf{s} = \langle 110 \rangle$. The plastic velocity gradient is then given by a power-law

$$\mathbf{L}^p = \sum_k \dot{\gamma}_k \mathbf{s} \otimes \mathbf{m} ; \text{ with } \dot{\gamma}_k = \dot{\gamma}_0 \left(\frac{|\tau_k - \chi_k|}{g_k} \right)^{\frac{1}{m}} \text{sign}(\tau_k - \chi_k) \quad (3.2)$$

where $\dot{\gamma}_0$ is the reference strain rate, τ_k is the resolved shear stress, m is the rate sensitivity exponent and g_k and χ_k are the critical resolved shear stress (CRSS) and the

backstress for the k slip system respectively. The kinematic hardening contribution is determined by the evolution of χ_k , adapted in Cruzado et al. (2017) from the macroscopic model by Ohno and Wang (1993),

$$\dot{\chi}_k = c\dot{\gamma}_k - d\chi_k|\dot{\gamma}_k| \left(\frac{|\chi_k|}{c/d} \right)^{mk}. \quad (3.3)$$

with c, d and mk the parameters controlling the backstress evolution. The CRSS, g_k , in the model has two contributions, $g_{k(m)}$ and g_c , that arise from the monotonic and cyclic deformation. $g_{k(m)}$ depends on the accumulated plastic slip and follows the Asaro-Needleman model (Asaro and Needleman, 1985).

In this model, self hardening h follows the expression

$$h = \text{sech}^2 \left(\frac{h_0 \int_0^t \sum_k |\gamma_k|}{\tau_s - \tau_0} \right) \quad (3.4)$$

depending on three parameters that stand for the initial CRSS, τ_0 , the saturation CRSS, τ_s , and the initial hardening modulus, h_0 . The monotonic hardening evolution then is given by

$$\dot{g}_{k(m)} = \sum_l q_{kl} h |\gamma_l| \quad (3.5)$$

that includes the effect of self and latent hardening with the coefficients q_{kl} .

The cyclic contribution is negative and evolves with the accumulated cyclic plastic strain following a Voce-type law Tome et al. (1984) defined by three parameters, $\tau_{\Delta s}$, h_1 and h_2 , as described in Cruzado et al. (2017).

$$g_c = -(\tau_{\Delta s} + h_2 \gamma_{cyc}) \left(1 - \exp \left(-\frac{h_1 \gamma_{cyc}}{\tau_{\Delta s}} \right) \right) \quad (3.6)$$

$$\text{with } \gamma_{cyc} = \sum_k \int_0^t |\gamma_k| dt - \sum_k \left| \int_0^t \gamma_k dt \right| \quad (3.7)$$

The parameters of the crystal plasticity model used for this Chapter are given in Table 3.1. The elastic and viscoplastic parameter are take from IN718 (Cruzado et al., 2015). The rest of parameters do not correspond to any specific material and are just set arbitrarily to represent a generic plastic response including kinematic hardening and cyclic softening. These parameters are the basis of the material used in this Chapter.

Elastic	$C_{11}(\text{GPa})$	$C_{12}(\text{GPa})$	$C_{44}(\text{GPa})$	
	233.2	160.8	98.4	
Viscoplastic	m	$\dot{\gamma}_0$		
	0.017	$2.42 \cdot 10^{-3}$		
Isotropic hardening	$\tau_0 \text{ (MPa)}$	$\tau_s \text{ (MPa)}$	$h_0 \text{ (MPa)}$	q_{kl}
	390.5	420.7	2039	1
Kinematic hardening	$c \text{ (MPa)}$	d	mk	
	23625.4	30.3	20.5	
Cyclic softening	$\tau_s^{cyc} \text{ (MPa)}$	$h_1 \text{ (MPa)}$	$h_2 \text{ (MPa)}$	
	29.7	25.5	0.00122	

Table 3.1: Parameters of the crystal plasticity model for a generic polycrystalline alloy

3.1.3 Fatigue indicator parameters and life prediction

The FIPs, introduced in Section 2.3.4, are parameters defined at the microscale, which aim to represent the driving forces of crack nucleation. In microstructure based fatigue life prediction, the distribution FIPs within the RVE is computed from the variation of the microfields and state variables in each point of the model during the last cycle, obtained from the simulation of a few cycles of the RVE response. Different fatigue indicators are proposed in the literature as a function of the plastic slip in each slip system, the resolved shear stress, and some other fields. In this thesis, two FIPs are used, the equivalent plastic strain (eq (2.38)) and the plastic work (eq (2.39)) accumulated per cycle (Manonukul and Dunne, 2004; Wan et al., 2014). Although it is true that, in contrast to other FIPs such as Fatemi-Socie, these parameters do not consider the difference between pure tension and pure compression cycles, they have a more clear physical interpretation.

The number of cycles for nucleating a crack (or directly fatigue life, N_i) of a RVE for a given macroscopic cyclic loading history —defined using strain or stress control, mutiaxiality, shape of the cycles, asymmetry R and deformation amplitude $\Delta\epsilon$ — is obtained by a simple empirical relation between the FIP_{RVE} and N_i . This fatigue life law contains one or more parameters of the material, adjusted correlating the FIP_{RVE} obtained in the simulation of one or more real experiments with the actual life measured

in those tests. In particular, a power type law expression can be used to this purpose,

$$N_i = \frac{FIP_{crit}}{FIP_{RVE}^c} \quad (3.8)$$

that contains two fitting parameters, FIP_{crit} and c , that should be calibrated using two or more fatigue tests. Since FIP_{RVE} corresponds to the maximum value of the average FIP distributions within one RVE, different RVEs of the same microstructure can give very different FIP_{RVE} values and therefore different fatigue lives. This fact can be used to make a statistical treatment by studying several RVEs of the same microstructure, a set of samples known as statistical volume element or SVE. In this case, the result of the model is the complete statistical distribution of the values FIP_{RVE} of the SVEs and therefore the statistical distribution of lives. Although this idea has been applied by many authors providing very accurate predictions of life in fatigue (for example to the Ni-base superalloy IN718), it can be easily observed that the distribution of FIP_{RVE} changes with the size of the RVE used (as quantified in Chapter 4). This dependency implies that the life prediction laws are not objective and are only valid if the size of the models is kept fixed. This problem, and a model proposed to eliminate this dependency, will be covered in next Chapter.

3.2 Adaptation of Galerkin FFT homogenization for cyclic polycrystalline simulations

A FFT homogenization scheme based on the Galerkin approach is adapted here to be used for microstructure based fatigue life prediction of polycrystals. The framework allows the direct use of any CP model developed for finite elements and includes discrete projector operators (Section 3.2.1), a numerical approach that allows a smoother representation of the microfields used to define the FIPs. This approach, based on the variational concepts underlying FEM, introduces several advantages respect to classical schemes. In particular, Galerkin FFT is based on a robust theoretical background, it does not need an analytic reference medium, and its non-linear extension is formally identical to FEM, using Newton method with material tangent matrices. The benefit of not using a reference medium for the linear solver is that it does not require to redefine the reference medium properties every increment to obtain optimal convergence and the convergence is as good as the optimal classical schemes (i.e. accelerated scheme (Michel et al., 1999)). The non-linear extension based on the Newton-Raphson allows to reach quadratic convergence under the same conditions as finite element, being able to use large strain increments. A summary of the main ideas and equations

of the Galerkin approach introduced in Section 2.4 are presented below. Here, these equations are summarized and particularized for constitutive equations with history dependency.

The periodic RVE of the microstructure is embedded in a cuboidal domain Ω with edges lengths L_x, L_y, L_z . The domain is discretized in a regular array of $n_x \cdot n_y \cdot n_z$ voxels, where each voxel belongs to any of the phases represented. The behavior of each of the phases included in the RVE follows a constitutive equation in which the first Piola Kirchhoff stress $\mathbf{P}$ is given as function of the deformation gradient $\mathbf{F}$ and some history variables $\mathbf{q}$

$$\begin{aligned}\mathbf{P} &= \mathbf{P}(\mathbf{F}, \mathbf{q}) \\ \dot{\mathbf{q}} &= f(\mathbf{q}, \mathbf{F})\end{aligned}\tag{3.9}$$

In this study, the law in eq. (3.9), corresponds to the CP model described in the previous section, and the phases are the different grains, modeled with the same CP model, but using a different initial configuration to account for the orientation.

The FFT homogenization problem in finite deformation for a given macroscopic loading history consists in finding, for every time, the compatible microscopic periodic deformation gradient in the RVE which results in an equilibrium stress field. Although the main equations for Galerkin FFT were introduced in Section 2.4.6, a summary of the approach is presented here, explicitly introducing the dependence of the material on the internal variables. The boundary value problem is solved expressing the weak form of the linear momentum balance in the reference configuration

$$\begin{cases} \int_{\Omega} \mathbb{G} * \boldsymbol{\zeta}(\mathbf{x}) : \mathbf{P}(\mathbf{F}(\mathbf{x}), \mathbf{q}) \, d\Omega &= 0 \\ \langle \mathbf{F} \rangle_{ij} &= \overline{\mathbf{F}}(t) \end{cases}\tag{3.10}$$

where $\langle \cdot \rangle$ represents the volume average, $\boldsymbol{\zeta}(\mathbf{x})$ are second order tensor test functions, $\overline{\mathbf{F}}_{ij}(t)$ is the imposed macroscopic deformation gradient history and $\mathbb{G}$ stands for the projector operator that enforces the compatibility of the test functions being $*$ the convolution operation.

The Piola-Kirchhoff stress and the deformation gradient are discretized similarly to the domain using fundamental trigonometrical functions and are integrated with a trapezoidal integration rule (Vondřejc et al., 2014) to derive from the weak form of the equilibrium equation (3.10) a simple algebraic equation using the Fourier space properties. The resulting non-linear system of equations reads as

$$\mathcal{G}(\mathbf{P}) := \mathcal{F}^{-1} \left\{ \widehat{\mathbb{G}} : \mathcal{F} \{ \mathbf{P}(\mathbf{F}, \mathbf{q}) \} \right\} = \mathbf{0}\tag{3.11}$$

where $\mathcal{G}$ is a linear map that acts on a discrete voxel tensor field, the convolution has become a simple dot product in the Fourier space, $\mathbf{P}$. $\mathbf{q}$ and $\mathbf{F}$ represent here the value of the discrete counterparts of the Piola-Kirchhoff stress, internal variables and deformation gradient at the center of the voxels. $\mathcal{F}$ and $\mathcal{F}^{-1}$ stand for the discrete Fourier transform and its inverse. Eq. (3.11) is an algebraic system of $9 \cdot n_x \cdot n_y \cdot n_z$ non-linear equations in which the unknown is the value of the deformation gradient at each voxel $\mathbf{F}$.

For the resolution of the non-linear system of equations (3.11), load history is split in n time increments. The unknown at the end of each increment k is $\mathbf{F}_k = \mathbf{F}(t_k)$, the deformation gradient field corresponding to time t_k . For the shake of clarity, the discrete fields $\mathbf{F}_k$, $\mathbf{q}_k = \mathbf{q}(t_k)$ and $\mathbf{P}_k = \mathbf{P}(t_k)$ will be named $\mathbf{F}$, $\mathbf{q}$ and $\mathbf{P}$ from now on. A Newton-Raphson method is used to solve the non-linear system at time t_k transforming it into a linear system of equations whose solution provides the correction of the displacement, $\delta\mathbf{F}$, at each iteration i . The linear system is given by

$$\mathcal{G}(\mathbb{K}^i : \delta\mathbf{F}) = -\mathcal{G}(\mathbf{P}(\mathbf{F}^i, \mathbf{q}^i)) \quad (3.12)$$

where $\mathbf{F}^i$ is the last iteration of the deformation gradient, $\mathbf{F}^i = \bar{\mathbf{F}}(t_k) + \delta\mathbf{F}^1 + \delta\mathbf{F}^2 + \dots + \delta\mathbf{F}^{i-1}$. $\mathbf{q}^i$ and $\mathbb{K}^i = \left. \frac{\partial \mathbf{P}}{\partial \mathbf{F}} \right|^i$ are the internal variables vector and the material tangent respectively evaluated at the last iteration. The linear system of equations (3.12) is solved using the conjugate gradient method, whose convergence rate, efficiency and memory allocation are optimal for this problem. The time increment k is finished when the correction of the Newton-Raphson $\delta\mathbf{F}$ is below a given tolerance.

3.2.1 Discrete projector operator

In order to reduce the wavy local response which may appear at the grain boundaries where the elastic contrast is high, a discrete definition of the derivatives in the real space is used. The rotated forward difference rule, presented in Section 2.4.7, has been used and in this adaptation is included as a new ingredient of the formulation of the projector operator in the Galerkin FFT. This implies an improvement in the accuracy of the microfields within a RVE, and finally a smoother field of FIPs, which alleviates the localization in such field. Moreover, it has been shown that the use of discrete operators improves the convergence in the case of high phase contrast. This approach consists in the introduction of the modified version of the frequencies (eq. (2.107)) into the original expression of the projector operator (eq. (2.91)) and resulting in a modified

projection operator, $\hat{G}'_{ijkl}$ for every frequency vector ξ that can be expressed as

$$\hat{G}'_{ijkl} = \begin{cases} 0_{ijkl} & \text{for null and Nyquist frequencies} \\ \delta_{ik} \frac{\tan(\frac{q_j}{2}) \tan(\frac{q_l}{2}) L_m^2}{\tan^2(\frac{q_m}{2}) L_j L_l} & \text{for the rest of frequencies} \end{cases} \quad (3.13)$$

where q corresponds to the normalized frequencies (eq. (2.108)). This newly defined projector operator is directly used to solve equilibrium equation (eq. (3.12)). The new operator implies obtaining smoother fields in the resolution of the problem and, in some cases, a better convergence rate of the linear Krylov solver.

3.2.2 Coupling with Abaqus UMATs

The adaptation of a generic framework to define constitutive equations is fundamental to have a FFT code independent of the particular constitutive equations used. For practical reasons, the Abaqus user material subroutine (*umat*) standard has been chosen, since it is widely used to implement new materials models. In addition, Abaqus *umats* is a common election in the materials and solid mechanics community, and this adaptation FFT-umat implies a valuable contribution for the research community, being able to directly plug in into the code already developed material models written as *umats* Fortran codes.

This adaptation to the FFT framework is valid for using a generic non-linear material with internal variables and under finite deformations. It increases the versatility of FFT algorithms, allowing the use of the efficient FFT schemes for already developed micromechanics frameworks. Here, the relations between Abaqus FEM variables and FFT variables needed for each algorithm are disclosed.

The FFT method needs to evaluate at each iteration the constitutive equation (eq. (3.9)) for each point x as function of the deformation gradient at current and previous time increments, $F(t_k)$ and $F(t_{k-1})$ respectively, the last value of the internal variables, $q(t_{k-1})$, and the time step δt . These values are also inputs of a *umat* subroutine and are passed from the FFT code to the *umat* subroutine through the variables `DFGRD1`, `DFGRD0`, `STATEV` and `DTIME` respectively. After the evaluation, the FFT code needs to recover from the constitutive model the first Piola-Kirchhoff stress $P(t_k)$, the value of the state variables at $q(t_k)$ and the material tangent $\mathbb{K}(t_k)$. From here time notation is omitted and the equations considered are posed for a single material point x and at time t_k to relax formulation.

The *umat* subroutine provides the Cauchy stress (σ) in the variable `STRESS`. The first Piola-Kirchhoff stress is recovered within the FFT code from the definition of this

stress and knowing $\mathbf{F}$ following the expression

$$\mathbf{P} = J\boldsymbol{\sigma}\mathbf{F}^{-T} \quad (3.14)$$

with $J = \det(\mathbf{F})$.

In the case of $\mathbb{K}$ an exact transformation of the consistent tangent matrix defined in the *umat* (variable `DDSDDE`) to the material tangent used by the FFT code is fundamental to preserve in FFT the convergence rate obtained with the user material in a finite element simulation. The material Jacobian that should be defined in a user subroutine at finite strain, in an Abaqus *umat* it is the tangent modulus tensor for the Jaumann rate of the Kirchhoff stress, $\mathbb{C}^{ab}$, a fourth order tensor defined as

$$\overset{\nabla}{\boldsymbol{\tau}} = \dot{\boldsymbol{\tau}} - \mathbf{w} \cdot \boldsymbol{\tau} - \boldsymbol{\tau} \cdot \mathbf{w}^T = J \mathbb{C}^{ab} : \mathbf{d} \quad (3.15)$$

where $\boldsymbol{\tau} = J\boldsymbol{\sigma}$ is the Kirchhoff stress is, $\overset{\nabla}{\boldsymbol{\tau}}$ corresponds to the Jaumann rate and $\mathbf{w}$ and $\mathbf{d}$ are the spin tensor and stretch tensor respectively. In the FFT framework, the material tangent needed to define the linear operator of the equilibrium in each iteration, (eq. (3.12)) is defined as

$$\dot{\mathbf{P}} = \mathbb{K} : \dot{\mathbf{F}} \quad (3.16)$$

and the objective then is to derive an explicit expression relating both tensors, $\mathbb{C}^{ab}$ and $\mathbb{K}$.

Combining the definition of the material tangent in FFT, eq. (3.16), and eq. (3.14) it is obtained

$$\mathbb{K} = \frac{\partial \mathbf{P}}{\partial \mathbf{F}} = \frac{\partial (J\boldsymbol{\sigma} \cdot \mathbf{F}^{-T})}{\partial \mathbf{F}} = \frac{\partial (\boldsymbol{\tau} \cdot \mathbf{F}^{-T})}{\partial \mathbf{F}}. \quad (3.17)$$

Expressing the previous expression (eq. (3.17)) in index notation and expanding the derivative of the product in two terms it is obtained

$$K_{ijkl} = \frac{\partial P_{ij}}{\partial F_{kl}} = \frac{\partial (\tau_{ip} F_{jp}^{-1})}{\partial F_{kl}} = \frac{\partial \tau_{ip}}{\partial F_{kl}} F_{jp}^{-1} + \tau_{ip} \frac{\partial F_{jp}^{-1}}{\partial F_{kl}} \quad (3.18)$$

The second term of equation (3.18), the derivative of the inverse of a tensor with respect to itself, is given by (3.19).

$$\frac{\partial F_{jp}^{-1}}{\partial F_{kl}} = -F_{lp}^{-1} F_{jk}^{-1} \quad (3.19)$$

To obtain first term of equation (3.18), the expression in derivatives of equation (3.15) is multiplied by a small time increment yielding into (3.20).

$$\delta \boldsymbol{\tau} - \delta \mathbf{w} \cdot \boldsymbol{\tau} - \boldsymbol{\tau} \cdot \delta \mathbf{w}^T = J \mathbb{C}^{ab} : \delta \mathbf{d} \quad (3.20)$$

and reordering the equation, the Abaqus tangent can be written as

$$\delta \boldsymbol{\tau} = J \mathbb{C}^{ab} : \delta \mathbf{d} + \delta \mathbf{w} \cdot \boldsymbol{\tau} + \boldsymbol{\tau} \cdot \delta \mathbf{w}^T \quad (3.21)$$

where $\delta \mathbf{d}$ and $\delta \mathbf{w}$ are obtained as function of $\mathbf{F}$ and $\delta \mathbf{F}$ as

$$\delta \mathbf{d} = \frac{1}{2} \left[\delta \mathbf{F} \cdot \mathbf{F}^{-1} + (\delta \mathbf{F} \cdot \mathbf{F}^{-1})^T \right] \quad (3.22)$$

and

$$\delta \mathbf{w} = \frac{1}{2} \left[\delta \mathbf{F} \cdot \mathbf{F}^{-1} - (\delta \mathbf{F} \cdot \mathbf{F}^{-1})^T \right]. \quad (3.23)$$

Replacing these expressions eqs. (3.22) and (3.23) into equation (3.21), it is obtained

$$\begin{aligned} \delta \boldsymbol{\tau} = J \mathbb{C}^{ab} : & \frac{1}{2} \left[\delta \mathbf{F} \cdot \mathbf{F}^{-1} + (\delta \mathbf{F} \cdot \mathbf{F}^{-1})^T \right] + \\ & \frac{1}{2} \left[\delta \mathbf{F} \cdot \mathbf{F}^{-1} - (\delta \mathbf{F} \cdot \mathbf{F}^{-1})^T \right] \cdot \boldsymbol{\tau} + \\ & \boldsymbol{\tau} \cdot \frac{1}{2} \left[\delta \mathbf{F} \cdot \mathbf{F}^{-1} - (\delta \mathbf{F} \cdot \mathbf{F}^{-1})^T \right]^T \end{aligned} \quad (3.24)$$

Now, the Kirchhoff stress is also linearized respect the perturbation of the deformation gradient

$$\delta \boldsymbol{\tau} = \frac{\partial \boldsymbol{\tau}}{\partial \mathbf{F}} : \delta \mathbf{F} \text{ in index } \delta \tau_{ip} = \frac{\partial \tau_{ip}}{\partial F_{kl}} \delta F_{kl}. \quad (3.25)$$

If equation (3.24) is written in index notation, the resulting expression reads

$$\begin{aligned} \delta \tau_{ip} = & \frac{J}{2} C_{ipkm}^{ab} \delta F_{kl} F_{lm}^{-1} + \frac{J}{2} C_{ipmk}^{ab} F_{lm}^{-1} \delta F_{kl} + \\ & \frac{1}{2} I_{ipkq} \delta F_{kl} F_{lm}^{-1} \tau_{mq} - \frac{1}{2} I_{ipmq} F_{lm}^{-1} \delta F_{kl} \tau_{kq} + \\ & \frac{1}{2} I_{ipqk} \tau_{qm} F_{lm}^{-1} \delta F_{kl} - \frac{1}{2} I_{ipqm} \tau_{qk} F_{lm}^{-1} \delta F_{kl} \end{aligned} \quad (3.26)$$

and comparing the terms of the last two equations (3.25) and (3.26), considering the minor symmetries of $\mathbb{C}^{ab}$ and the symmetry of $\boldsymbol{\tau}$, the resulting expression is:

$$\begin{aligned} \frac{\partial \tau_{ip}}{\partial F_{kl}} = & J C_{ipkm}^{ab} F_{lm}^{-1} + \\ & \frac{1}{2} \delta_{ik} \delta_{pq} F_{lm}^{-1} \tau_{mq} - \frac{1}{2} \delta_{im} \delta_{pq} F_{lm}^{-1} \tau_{kq} + \\ & \frac{1}{2} \delta_{iq} \delta_{pk} F_{lm}^{-1} \tau_{qm} - \frac{1}{2} \delta_{iq} \delta_{pm} F_{lm}^{-1} \tau_{qk} \end{aligned} \quad (3.27)$$

that can be simplified to

$$\begin{aligned} \frac{\partial \tau_{ip}}{\partial F_{kl}} = & J C_{ipkm}^{ab} F_{lm}^{-1} + \\ & \frac{1}{2} \delta_{ik} F_{lm}^{-1} \tau_{mp} - \frac{1}{2} F_{li}^{-1} \tau_{kp} + \\ & \frac{1}{2} \delta_{pk} F_{lm}^{-1} \tau_{im} - \frac{1}{2} F_{lp}^{-1} \tau_{ik} \end{aligned} \quad (3.28)$$

Finally, introducing eq. (3.28) in the definition of the material tangent (eq. (3.18)) the final expression for the material tangent used in the FFT approach, as function of the Abaqus tangent $\mathbb{C}^{ab}$, deformation gradient $\mathbf{F}$ and Kirchhoff stress $\boldsymbol{\tau}$, is given by

$$\begin{aligned} K_{ijkl} = & (J C_{ipkm}^{ab} F_{lm}^{-1} + \frac{1}{2} \delta_{ik} F_{lm}^{-1} \tau_{mp} - \\ & \frac{1}{2} F_{li}^{-1} \tau_{kp} + \frac{1}{2} \delta_{pk} F_{lm}^{-1} \tau_{im} - \frac{1}{2} F_{lp}^{-1} \tau_{ik}) F_{jp}^{-1} - \tau_{ip} F_{lp}^{-1} F_{jk}^{-1}. \end{aligned} \quad (3.29)$$

and it can be directly introduced in eq. (3.12).

The validity of this expression has been assessed by comparing Abaqus and FFT tangents in materials where both tangents can be analytically solved as a Neo-Hookean model or Saint-Venant-Kirchhoff model.

3.3 Algorithm for stress and mixed control in Galerkin based FFT

The Galerkin approach was initially formulated imposing the history of the macroscopic deformation gradient. In this section, the Galerkin based algorithm for finite strains (de Geus et al., 2017) is extended to use stress and mixed control of the macroscopic load history using a direct method based on a modified project operator and preserving the computational performance of the original method.

3.3.1 Macroscopic stress and mixed control

Generic mixed control is fundamental for many cases of interest as uniaxial tests or creep tests. As explained in Section 2.4, several methods were developed for stress control. Most of them impose the control via modifying iteratively the imposed strain by computing the inverse of a numerical effective tangent (Eisenlohr et al., 2013) or by modifying the formulation of the basic scheme as a stress iterative approach, requiring them computing local compliance matrices (Michel et al., 2000) and being valid for pure stress control. Kabel et al. (2016) introduced a stress control approach for the Newton-Krylov algorithm of the Lippmann-Schwinger equation but it still requires a reference medium. A modification of the projection operator of the Galerkin FFT is here proposed in order to simulate the behavior of the heterogeneous material under any generic stress or mixed stress-strain load history without implying any extra computational effort or iteration.

Macroscopic stress control

This condition corresponds to a stress control uniaxial test or a creep test for instance. The algorithm starts with the assumption that the first Piola-Kirchhoff stress can be split into its average and fluctuating parts

$$\mathbf{P}(\mathbf{F}, \mathbf{q}) = \langle \mathbf{P}(\mathbf{x}, \mathbf{q}) \rangle_{\Omega} + \tilde{\mathbf{P}}(\mathbf{F}, \mathbf{q}) \quad (3.30)$$

and introducing this decomposition into equilibrium equation (3.11), it is obtained

$$\mathcal{G} \left(\langle \mathbf{P} \rangle_{\Omega} + \tilde{\mathbf{P}}(\mathbf{F}, \mathbf{q}) \right) = \mathbf{0} \quad (3.31)$$

The average term of $\mathbf{P}$ vanishes because the projection operator $\hat{\mathcal{G}}$ eliminates the mean part of the field to which is applied and the actual equilibrium equation that is solved corresponds to

$$\mathcal{G} \left(\tilde{\mathbf{P}}(\mathbf{F}, \mathbf{q}) \right) = \mathbf{0} \text{ for } \langle \mathbf{F} \rangle_{\Omega} = \bar{\mathbf{F}} \quad (3.32)$$

where the input data is the averaged value of the deformation gradient and the average stress is unknown and obtained as a result of the simulation.

Let's consider an alternative projection operator $\mathcal{G}^*$ in which the condition of zero mean projection is eliminated. If this operator is applied to the fluctuation of the stress (zero mean value), the redefinition of the operator does not affect the result and the equilibrium equation is identical to the one expressed using the standard operator (eq. (3.32)) coincides

$$\mathcal{G}^* \left(\tilde{\mathbf{P}}(\mathbf{F}, \mathbf{q}) \right) = \mathcal{G} \left(\tilde{\mathbf{P}}(\mathbf{F}, \mathbf{q}) \right) = \mathbf{0}. \quad (3.33)$$

Under stress control the input data is the target macroscopic stress, $\bar{\mathbf{P}}$, and therefore it should be equal to the average stress $\langle \mathbf{P} \rangle_\Omega$. Combining the stress decomposition (equation (3.30)) with equation (3.33), the equilibrium can be expressed as

$$\mathcal{G}^* (\mathbf{P} (\mathbf{F}, \mathbf{q}) - \langle \mathbf{P} \rangle_\Omega) = \mathcal{G}^* (\mathbf{P} (\mathbf{F}, \mathbf{q}) - \bar{\mathbf{P}}) = 0 \quad (3.34)$$

The resulting equilibrium equation consists in finding the value of the full deformation gradient, $\mathbf{F}$, including both fluctuations and the field mean value and corresponds to

$$\text{Find } \mathbf{F} \mid \mathcal{G}^* (\mathbf{P} (\mathbf{F}, \mathbf{q})) = \mathcal{G}^*(\bar{\mathbf{P}}) \text{ for a given } \bar{\mathbf{P}} \quad (3.35)$$

To determine the value of $\mathcal{G}^*$ that preserves equilibrium enforcing that $\langle \mathbf{P} \rangle_\Omega = \bar{\mathbf{P}}$, equation (3.35) is expressed as a convolution in the Fourier space

$$\mathcal{F}^{-1} \left(\widehat{\mathbb{G}}^*(\boldsymbol{\xi}) : \widehat{\mathbf{P}}(\boldsymbol{\xi}) \right) = \mathcal{F}^{-1} \left(\widehat{\mathbb{G}}^*(\boldsymbol{\xi}) : \widehat{\bar{\mathbf{P}}} \right). \quad (3.36)$$

Equation (3.32) implies that both operators should act identically on zero average tensor so $\widehat{\mathbb{G}}^*(\boldsymbol{\xi}) = \widehat{\mathbb{G}}(\boldsymbol{\xi}) \forall \boldsymbol{\xi} \neq 0$, reducing eq. (3.36) to

$$\widehat{\mathbb{G}}^*(\boldsymbol{\xi} = 0) : \widehat{\mathbf{P}}(\boldsymbol{\xi} = 0) = \widehat{\mathbb{G}}^*(\boldsymbol{\xi} = 0) : \bar{\mathbf{P}} \quad (3.37)$$

Finally, the $\mathbb{G}^*$ operator projects an arbitrary tensor field into the sum of its compatible and mean parts. Therefore, the null frequency should project the average part of a field into itself, and this is achieved by defining its value as the fourth order identity tensor. Using the property of the Fourier transform $\widehat{\mathbf{P}}(\boldsymbol{\xi} = 0) = \langle \mathbf{P} \rangle_\Omega$ in equation (3.37), it is enforced $\langle \mathbf{P} \rangle_\Omega$ to be the target macroscopic stress. The new operator is defined as

$$\widehat{G}_{ijkl}^* = \begin{cases} \delta_{ik}\delta_{jl} & \text{for null frequency} \\ 0_{ijkl} & \text{for Nyquist frequencies} \\ \delta_{ik} \frac{\xi_j \xi_l}{\boldsymbol{\xi} \cdot \boldsymbol{\xi}} & \text{for the rest of frequencies} \end{cases} \quad (3.38)$$

In the case of non-linear behavior, the system is also solved iteratively using the same linearization of the original scheme. For each iteration i the correction of the deformation gradient $\delta \mathbf{F}$ is obtained here solving this linear system

$$\mathcal{G}^* (\mathbb{K}^i : \delta \mathbf{F}) = -\mathcal{G}^* (\mathbf{P} (\mathbf{F}^i, \mathbf{q}^i) - \bar{\mathbf{P}}) \quad (3.39)$$

where, contrary to the strain control approach, the correction for the deformation gradient field $\delta \mathbf{F}$ includes a mean value. It can also be observed that when equilibrium is reached ($\delta \mathbf{F} \rightarrow 0$) the average stress reaches the objective. It will be shown in the

numerical examples that the algorithm summarized in equation (3.39) do not require additional iterations, havin the same computational cost than the original scheme for strain control.

Mixed control of macrosopic stress and strain

Load histories combining values of both macroscopic stress and deformation gradient are very common. Such conditions can be found for example in uniaxial or biaxial tests under strain where strain is imposed in some directions, but leaving the others free to deform. The input data now is $\bar{P}_{IJ} = \langle P \rangle_{IJ}$ for components IJ in which stress is imposed and $\bar{F}_{ij} = \langle F \rangle_{ij}$ for the rest of components. The equilibrium equation can be expressed as

$$\text{Find } \mathbf{F}' \mid \begin{cases} \mathcal{G}^* (\mathbf{P} (\bar{\mathbf{F}}_{ij} + \mathbf{F}', \mathbf{q}))_{ij} = 0_{ij} \text{ for a given } \bar{F}_{ij} \text{ in directions } ij \\ \mathcal{G}^* (\mathbf{P} (\bar{\mathbf{F}}_{ij} + \mathbf{F}', \mathbf{q}))_{IJ} = \mathcal{G}^* (\bar{\mathbf{P}})_{IJ} \text{ for a given } \bar{P}_{IJ} \text{ in directions } IJ \end{cases} \quad (3.40)$$

where $\mathbf{F}'$ is the solution of the equilibrium equation under mixed control (eq. (3.40)) and corresponds to a fluctuation term for the ij components ($F'_{ij} = \tilde{F}_{ij}$) and the full deformation gradient term for the IJ components ($F'_{IJ} = F_{IJ}$). These conditions are imposed again by modifying the value of the projection operator for the null frequency. The modified projection operator is obtained following the same reasoning as for stress control and corresponds to

$$\widehat{G}^*_{ijkl} = \begin{cases} \delta_{ik}\delta_{jl} & \text{if } \xi = 0 \text{ for stress controlled } IJ \text{ terms} \\ 0_{ijkl} & \text{if } \xi = 0 \text{ for strain controlled } ij \text{ terms} \\ 0_{ijkl} & \text{for Nyquist frequencies} \\ \delta_{ik} \frac{\xi_j \xi_l}{\xi \cdot \xi} & \text{for } \xi \neq 0 \end{cases} \quad (3.41)$$

This operator should be used as the operator $\mathcal{G}^*$ in equation (3.40) for a mixed control problem. The resulting non-linear system for obtaining the equilibrium is solved by Newton as in the previous cases, and the result is the field $\mathbf{F}'$

3.3.2 Validation of the macroscopic loading control algorithm

Particle reinforced hyperelastic matrix

The first benchmark consists in a non-linear elastic composite. A uniaxial monotonic test of a periodic cubic RVE composed by a hyperelastic matrix reinforced by stiff spherical particles will be simulated under macroscopic strain, stress and mixed control schemes. The RVE contains 4 particles occupying a volume fraction of 0.2 and

the domain is discretized using 64^3 voxels (Fig. 3.4(a)). The matrix and particle mechanical behavior follows a Saint Venant-Kirchhoff hyperelastic model used in Kabel et al. (2014); de Geus et al. (2017). The matrix properties are $\mu = 28\text{Pa}$ and $k = 46.67\text{Pa}$ (shear and bulk modulus) and the particles are one order of magnitude stiffer (both moduli are 10 times larger than the matrix ones). The uniaxial tensile test reaches an elongation of $\lambda_{end} = \frac{L}{L_0} = 0.2$, being L and L_0 the target and initial cell length in the loading direction, and being the other two directions unconstrained. This test is done using three different types of control that imply different loading paths. In all the cases the load is homogeneously divided in 100 load increments and equilibrium is solved in each of them. The load increments are defined introducing a pseudo-time t being the final stage reached at $t = t_{end}$.

Case (1) corresponds to the actual type of control in a uniaxial stress test, a mixed control in which a macroscopic deformation gradient is imposed in x direction as a ramp and the rest of terms are stress free.

$$\bar{\mathbf{F}}^{(1)}(t) = \begin{pmatrix} 1 + \lambda_{end} \frac{t}{t_{end}} & 0 & 0 \\ * & * & 0 \\ * & * & * \end{pmatrix} \quad \text{and} \quad \bar{\mathbf{P}}^{(1)}(t) = \begin{pmatrix} * & * & * \\ 0 & 0 & * \\ 0 & 0 & 0 \end{pmatrix} \quad (3.42)$$

Case (2) is a full stress control, being the stress applied a linear ramp from 0 to the stress $\mathbf{P}_{end}^{(1)}$ obtained as the solution in the first case and here introduced as input.

$$\bar{\mathbf{P}}^{(2)}(t) = \mathbf{P}_{end}^{(1)} \frac{t}{t_{end}} \quad (3.43)$$

Finally, *case (3)* is a full strain control test (the standard boundary conditions in FFT) where all the deformation gradient is imposed using a linear ramp to reach the deformation gradient of previous simulation final solution $\bar{\mathbf{F}}_{end}^{(1)}$.

$$\bar{\mathbf{F}}^{(3)}(t) = \bar{\mathbf{F}}_{end}^{(1)} \frac{t}{t_{end}} \quad (3.44)$$

The longitudinal response of the three tests are represented in Fig. 3.4(b) while the transverse response is represented in Fig. 3.4(c).

Figure 3.4: Particle reinforced RVE (a), first Piola-Kirchhoff stresses for three load cases in hyperelastic model in load direction (b) and transverse directions (c).

All simulations have the same endpoint, but follow different paths. *Cases* (1) and (2) share the path, but differ in the size of the strain increments due to the non-linear behavior. Being the behavior of the hyperelastic material path independent, the macroscopic stress of *cases* (1) and (2) are superposed, as it can be observed in Fig. 3.4(b). *Case* (3) follows a slightly different path because a ramp is applied controlling the full deformation gradient. In this material, the behavior depends non-linearly on the deformation gradient value, implying that the transverse elongation result of a transverse stress free condition depends on the deformation level. The effect of the different loading paths can be observed in the response in both directions being especially clear in the transverse direction (Fig. 3.4 (b)) where under a stress and mixed control transverse stresses are zero while, when using strain control, small compressive stresses are developed. Macroscopic and microscopic results at the endpoint for all the cases are the same within the numerical accuracy.

Polycrystal

The second benchmark is a polycrystal, an example with loading path and strain rate dependencies. The RVE is cube discretized in 64^3 voxels and the model contains around 200 randomly oriented grains (Fig. 3.5(a)). Each grain follows the crystal plasticity model described in Section 3.1.2. A final elongation of $\lambda_{end} = 0.02$ is imposed in 200s, what corresponds in the case of strain control to a uniaxial tensile test with strain rate $5 \cdot 10^{-5}$ and time is discretized in 20 regular increments. Four loading conditions will be studied being the first three cases identical to the previous section. The fourth case consists in a *pseudo-uniaxial* tensile test in which the uniaxial tension condition is approached using full strain control resulting in a isochoric deformation at the final stage. In the absence of an efficient stress-control technique this approach is an approximation to uniaxial test and only exact for incompressible materials, which is a

property of the plastic regime of the material model used here. The resulting deformation gradient follows

$$\bar{\mathbf{F}}^{(4)}(t) = \frac{t}{t_{final}} \begin{pmatrix} \lambda_{end} & 0 & 0 \\ 0 & \left(\sqrt{\frac{1}{1+\lambda_{end}}} - 1\right) & 0 \\ 0 & 0 & \left(\sqrt{\frac{1}{1+\lambda_{end}}} - 1\right) \end{pmatrix} + \mathbf{I} \quad (3.45)$$

Figure 3.5: Polycrystalline RVE (a), first Piola-Kirchhoff stresses for three load cases in crystal plasticity model in load direction (b) and (c) transverse directions.

The results of the simulations are represented in Fig. 3.5. Now *cases* (1) and (2), although very similar, are not exactly superposed do to the effect of the differences in the strain rate during the loading ramp. *Case* (3) reaches the same point as previous two cases but, as it happened for the composite, the path is totally different and compressive transverse stresses are developed during the test. The *case* (4) is a typical approximation made in plastic materials to perform tests emulating uniaxial stress, but controlling the full deformation gradient instead. However, it can be observed that for the properties here selected, the polycrystalline response (Fig. 3.5) is very different from a real uniaxial tensile test. This difference is specially noticeable when comparing the transverse response: in the *pseudo-uniaxial* stress test, the compressive transverse stresses are not zero and grow with the applied strain. This last result indicates that the use of this type of strain control conditions to emulate uniaxial tension can lead to inaccurate results.

3.4 Displacement Based FFT method

The vast majority of FFT based homogenization use the gradient of a potential field (electric field or displacement in the previous cases) as the unknown variable. In this

section, a new full FFT homogenization framework for linear/non-linear mechanical problems is proposed based on the displacement field as the problem unknown and using the preconditioned conjugate gradient method as kernel, the Displacement Based FFT (DBFFT). In this method, a system of linear equations in the frequency domain is derived for the linear behavior, with an associated full-rank Hermitian matrix, which is solved using a Krylov solver with a preconditioner. Moreover, the method allows imposing macroscopic values of strain, stress and mixed conditions maintaining the definiteness of the system and the computational performance. The non-linear extension of the method is totally general and can be used for any local constitutive equation and combination of macroscopic stress and strain history.

3.4.1 The method: Displacement Based FFT

The method aims to find directly the displacement field that satisfies the equilibrium conditions. The properties of the Fourier Transform and the decomposition of the displacement field in its macroscopic part and the fluctuations will be used to solve the periodic boundary value problem. The problem consists in obtaining the displacement field that fulfills the equilibrium in a periodic domain $\Omega \in \mathbb{R}^3$, the RVE. The RVE is a hexahedral box of dimensions $L_1 \cdot L_2 \cdot L_3$ formed by the spatial distribution of two or more phases, being the behavior at a point $x \in \Omega$ defined by the constitutive equation of the phase occupying that point. The boundary conditions are periodic in strain and stress, and the load is introduced through a far-field/macroscopic state.

The domain Ω is discretized in a voxelized regular grid containing $N_1 \cdot N_2 \cdot N_3$ voxels. The fields involved in the problem will then be represented by their value at the center of each voxel. The Fourier space is discretized in the same number of frequencies and the Fourier transform of a function defined in Ω is obtained by the Discrete Fourier Transform of the discrete field and computed using the FFT algorithm. The frequency domain discretization is defined by the frequency vectors in eq. (2.52). The use of even grid implies some assumptions related to the Nyquist frequencies such as neglect them or approximate them. Therefore, for the shake of simplicity, in this section only odd grids will be analyzed.

DBFFT scheme: Small strains

Under macroscopic strain control loading, the prescribed macroscopic strain tensor $\bar{\varepsilon}_{\bar{U}}$ can be written as function of the relative displacement vectors between periodic faces, $\bar{U}$, as

$$[\bar{\varepsilon}_{\bar{U}}]_{ij} = \frac{1}{2} \left(\frac{\bar{U}_{i(j)}}{L_j} + \frac{\bar{U}_{j(i)}}{L_i} \right) \quad (3.46)$$

where $\bar{U}_{i(j)}$ is the relative displacement between the periodic faces normal to direction j , in the direction i being L_j the length of the domain Ω along the direction j . Note that this relation is the same used for periodic boundary conditions in Finite Element homogenization, in which displacements are also the principal unknown Segurado et al. (2018)

The displacement field is split into its fluctuating periodic part $\tilde{\mathbf{u}}(\mathbf{x})$ (with zero average), and a linearly growing part, $\mathbf{u}_{\bar{U}}$, that accounts for the macroscopic strain and is dictated by the relative displacements vectors $\bar{\mathbf{U}}$,

$$\mathbf{u}(\mathbf{x}) = \mathbf{u}_{\bar{U}}(\mathbf{x}) + \tilde{\mathbf{u}}(\mathbf{x}). \quad (3.47)$$

The displacement field contribution due to the macroscopic relative displacement is related to the prescribed macroscopic strain tensor by

$$\mathbf{u}_{\bar{U}}(\mathbf{x}) = \bar{\boldsymbol{\varepsilon}}_{\bar{U}} \cdot \mathbf{x} \quad (3.48)$$

Using this decomposition (eq. (3.47)), the resulting expression for the strain tensor field $\boldsymbol{\varepsilon}(\mathbf{x})$ reads as

$$\boldsymbol{\varepsilon}(\mathbf{x}) = \nabla^s \mathbf{u}(\mathbf{x}) = \bar{\boldsymbol{\varepsilon}}_{\bar{U}} + \nabla^s \tilde{\mathbf{u}}(\mathbf{x}) \quad (3.49)$$

where ∇^s denotes the symmetric gradient.

The starting point of the method is the equilibrium equation in its strong form,

$$\nabla \cdot \boldsymbol{\sigma}(\mathbf{x}) = \mathbf{0}. \quad (3.50)$$

If the phases inside the domain are linear elastic materials, the equation (3.50) can be written as

$$\nabla \cdot [\mathbb{C}(\mathbf{x}) : \nabla^s \mathbf{u}(\mathbf{x})] = \mathbf{0} \quad (3.51)$$

where $\mathbb{C}(\mathbf{x})$ corresponds to the stiffness tensor of the phase located at the point $\mathbf{x}$. Using the displacement field decomposition (eq. (3.47)), the linearity of both the gradient and divergence differential operators and rearranging terms, the equilibrium equation can be rearranged as

$$\nabla \cdot [\mathbb{C}(\mathbf{x}) : \nabla^s \tilde{\mathbf{u}}(\mathbf{x})] = -\nabla \cdot [\mathbb{C}(\mathbf{x}) : \bar{\boldsymbol{\varepsilon}}_{\bar{U}}] \quad (3.52)$$

Equation (3.52) is a partial differential equation in which the displacement fluctuation, $\tilde{\mathbf{u}}$, is the field to solve. This equation is also the starting point of the basic scheme

(Moulinec and Suquet, 1994) but, instead of introducing a reference medium to transform the microstructure dependency $\mathbb{C}(\mathbf{x})$ into an eigenstrain, the equation is transformed in its current form to the Fourier space to compute the derivatives.

Using the definition of the derivative in the Fourier space (eq. (2.47)), the symmetric gradient of the fluctuation field in the real space

$$[\nabla^s \tilde{\mathbf{u}}(\mathbf{x})]_{ij} = \frac{1}{2} \left(\frac{\partial \tilde{u}_i}{\partial x_j} + \frac{\partial \tilde{u}_j}{\partial x_i} \right) \quad (3.53)$$

is transformed to

$$[\mathcal{F}(\nabla^s \tilde{\mathbf{u}}(\mathbf{x}))]_{ij} = \hat{s}_{ijk} \hat{u}_k = \hat{\mathbf{s}}(\boldsymbol{\xi}) \cdot \hat{\mathbf{u}}(\boldsymbol{\xi}) \quad (3.54)$$

being $\hat{\mathbf{s}}$ the symmetric gradient operator and $\hat{\mathbf{u}}$ the displacement field, both fields belonging to the Fourier space and therefore defined in the frequency domain as function of the frequency vector $\boldsymbol{\xi}$. The expression of the symmetric gradient operator $\hat{\mathbf{s}}$ is

$$\hat{\mathbf{s}}(\boldsymbol{\xi}) = \hat{s}_{ijk}(\boldsymbol{\xi}) = \frac{1}{2} (i\xi_j \delta_{ik} + i\xi_i \delta_{jk}) \quad (3.55)$$

and it can be observed that the operator becomes zero for the null frequency $\boldsymbol{\xi} = \mathbf{0}$.

The divergence of a tensor field is defined in the real space as

$$[\nabla \cdot \boldsymbol{\sigma}(\mathbf{x})]_i = \frac{\partial \sigma_{ij}}{\partial x_j} \quad (3.56)$$

and its transformation in the Fourier space corresponds to

$$[\mathcal{F}(\nabla \cdot \boldsymbol{\sigma}(\mathbf{x}))]_i = \hat{d}_{ijk} \hat{\sigma}_{jk} = \hat{\mathbf{d}}(\boldsymbol{\xi}) : \hat{\boldsymbol{\sigma}}(\boldsymbol{\xi}) \quad (3.57)$$

being $\hat{\mathbf{d}}$ the divergence operator and $\hat{\boldsymbol{\sigma}}$ the stress tensor field, both expressed in the frequency domain. The expression of the operator $\hat{\mathbf{d}}$ corresponds to

$$\hat{\mathbf{d}} = \hat{d}_{ijk} = i\xi_k \delta_{ij} \quad (3.58)$$

and it also eliminates the average part of the field.

Finally, transforming the equation linear momentum conservation (eq. (3.52)) to the Fourier space and replacing the differential operators in the real space by their Fourier space counterparts, given by eqs. (3.54) and (3.57), it is obtained

$$\hat{\mathbf{d}} : \mathcal{F} \left(\mathbb{C}(\mathbf{x}) : \mathcal{F}^{-1} \left(\hat{\mathbf{s}} \cdot \hat{\mathbf{u}} \right) \right) = -\hat{\mathbf{d}} : \mathcal{F}(\mathbb{C}(\mathbf{x}) : \bar{\boldsymbol{\varepsilon}}_{\bar{U}}) \quad (3.59)$$

If the fields in the previous equation are replaced by their discrete counterparts in

both real and Fourier spaces and the Fourier transform is computed as the discrete transform, equation (3.59) becomes a linear system of equations of complex numbers in which the unknown is the fluctuation displacement field defined in the Fourier space, $\tilde{\mathbf{u}}$. The size of the system in 3D is $3 \cdot N_1 \cdot N_2 \cdot N_3$ and, if the zero frequency (corresponding to the rigid body motions) terms and real Fourier transform symmetries are removed, the system becomes fully determined with an associated Hermitian matrix. This type of linear systems can be solved with direct or iterative methods. In the case of iterative solvers, the full-rank of the associated matrix allows the use of preconditioners, in contrast to what happens when solving the rank deficient systems resulting from the Galerkin-FFT approach.

DBFFT: Stress control

Many times the macroscopic loading path is prescribed in stress or with a combination of terms in stress and strains. Classically, FFT methods are conceived to have the macroscopic strain as input and resolve the stress and mixed cases by iterative approaches. In the previous section (Section 3.3), a method to include directly the prescribed terms of the macroscopic stress in the formulation for the Galerkin-FFT approach has been proposed. Here, a similar approach for the DBFFT is proposed.

The macroscopic load should be imposed by six different values of either the macroscopic strain or stress tensor. Let $[\bar{\sigma}_{\bar{f}}]_{IJ}$ be the terms of the macroscopic stress tensor that are prescribed and let $[\bar{\epsilon}_{\bar{U}}]_{ij}$ be the terms prescribed of the macroscopic strain, with $IJ \neq ij$. Equivalent to the treatment of the macroscopic strain, the macroscopic stress is imposed through a force vector $\bar{\mathbf{f}}$

$$[\bar{\sigma}_{\bar{f}}]_{ij} = \frac{\bar{f}_{i(j)}}{A_j} \quad (3.60)$$

where $\bar{f}_{i(j)}$ is the force in i direction applied on the face normal to j direction and A_j the area of the Ω domain at the plane normal to j direction. Equilibrium implies that the same forces appear with contrary sign in the opposite directions. The microscopic stress in the terms where the macroscopic stress is prescribed are split in its average part and fluctuations, while the rest of the terms of the tensor are not decomposed. This decomposition is given by

$$\begin{aligned} [\sigma(\mathbf{x})]_{IJ} &= [\bar{\sigma}_{\bar{f}}]_{IJ} + [\sigma^*(\mathbf{x})]_{IJ} \\ [\sigma(\mathbf{x})]_{ij} &= [\sigma^*(\mathbf{x})]_{ij} \end{aligned} \quad (3.61)$$

In equation (3.61) $\sigma^*(\mathbf{x})$ is a non-zero averaged tensor in the components where strain is imposed, ij , and a stress fluctuation (zero average) in the components IJ where stress is imposed. The strain field can be split as

$$\varepsilon(\mathbf{x}) = \nabla^s \mathbf{u}(\mathbf{x}) = \bar{\varepsilon}_{\bar{U}} + \bar{\varepsilon}_{\bar{F}} + \nabla^s \tilde{\mathbf{u}}(\mathbf{x}) \quad (3.62)$$

where $\bar{\varepsilon}_{\bar{F}}$ is the unknown macroscopic strain that appears as a result of the macroscopic prescribed stress $\bar{\sigma}_{\bar{F}}$, and that is zero in the ij components. The tensor $\bar{\varepsilon}_{\bar{U}}$ contains the prescribed components of the macroscopic strain ij and is zero in the components IJ . The displacement field corresponding to the strains defined in eq. (3.62) is given by

$$\mathbf{u}(\mathbf{x}) = \bar{\varepsilon}_{\bar{U}} \cdot \mathbf{x} + \bar{\varepsilon}_{\bar{F}} \cdot \mathbf{x} + \tilde{\mathbf{u}}(\mathbf{x}) \quad (3.63)$$

The displacement field contains now two different unknowns, $\bar{\varepsilon}_{\bar{F}}$ and $\nabla^s \tilde{\mathbf{u}}$. This implies the introduction of additional equations to impose that the IJ components of the average stress equal the corresponding components of the prescribed macroscopic stress. The resulting system of differential equations reads

$$\begin{aligned} \nabla \cdot \sigma(\mathbf{x}) &= 0 \\ [\langle \sigma(\mathbf{x}) \rangle]_{IJ} &= [\bar{\sigma}_{\bar{F}}]_{IJ} \end{aligned} \quad (3.64)$$

where the unknown variable to solve is $\{\tilde{\mathbf{u}} \mid \bar{\varepsilon}_{\bar{F}}\}$. Note that the first equation does not affect the average value, and the second are the additional equations needed to obtain the unknown IJ components of the macroscopic strain $\bar{\varepsilon}_{\bar{F}}$. Again for simplicity, the phases will be considered linear elastic materials, so that, using the displacement field decomposition (eq. (3.63)), equilibrium equation becomes

$$\nabla \cdot [\mathbb{C}(\mathbf{x}) : \nabla^s (\tilde{\mathbf{u}}(\mathbf{x}) + \bar{\varepsilon}_{\bar{F}} \cdot \mathbf{x} + \bar{\varepsilon}_{\bar{U}} \cdot \mathbf{x})] = 0. \quad (3.65)$$

Then, thanks to the linearity of gradient and divergence operators the terms are rearranged, yielding into expression (3.66).

$$\nabla \cdot [\mathbb{C}(\mathbf{x}) : (\nabla^s \tilde{\mathbf{u}}(\mathbf{x}) + \bar{\varepsilon}_{\bar{F}})] = -\nabla \cdot [\mathbb{C}(\mathbf{x}) : \bar{\varepsilon}_{\bar{U}}] \quad (3.66)$$

The system is transformed to the Fourier space using the same differential operators defined in the previous section. The terms inside divergence operations in eq. (3.66), the left-hand side (lhs) and the right-hand side (rhs), are rewritten in the Fourier space

upon the use of eq. (3.54).

$$\begin{aligned}\widehat{\boldsymbol{\sigma}}_{lhs} &= \mathcal{F} \left(\mathbb{C} : \left(\mathcal{F}^{-1} \left(\widehat{\mathbb{s}} \cdot \widehat{\mathbf{u}} \right) + \overline{\boldsymbol{\varepsilon}}_{\overline{F}} \right) \right) \\ \widehat{\boldsymbol{\sigma}}_{rhs} &= \mathcal{F} \left(\mathbb{C} : \overline{\boldsymbol{\varepsilon}}_{\overline{U}} \right)\end{aligned}\tag{3.67}$$

Finally, using eq. (3.57), the system of equations defining the equilibrium (3.64) becomes

$$\begin{aligned}\widehat{\mathbb{d}} : \widehat{\boldsymbol{\sigma}}_{lhs} &= -\widehat{\mathbb{d}} : \overline{\boldsymbol{\sigma}}_{rhs} \\ [\widehat{\boldsymbol{\sigma}}_{lhs}(\mathbf{0})]_{IJ} &= [\overline{\boldsymbol{\sigma}}_{\overline{F}}]_{IJ} - [\widehat{\boldsymbol{\sigma}}_{rhs}(\mathbf{0})]_{IJ}\end{aligned}\tag{3.68}$$

As in the strain controlled version, the system of equations is fully determined and Hermitian if the zero frequency from the first equation is removed and the symmetries of the real Fourier transform are used.

DBFFT: Non-linear finite strains

The extension of the method to finite strains is straightforward expressing the equilibrium in the reference configuration through the first Piola Kirchhoff stress $\mathbf{P}$ and using the deformation gradient $\mathbf{F}$ to characterize the deformed state. For strain control, the prescribed macroscopic state is given by the average deformation gradient $\overline{\mathbf{F}}_{\overline{U}}$ that is related with the relative displacement between opposite RVE faces through

$$[\overline{\mathbf{F}}_{\overline{U}}]_{ij} = \delta_{ij} + \frac{\overline{U}_{i(j)}}{L_j}.\tag{3.69}$$

where δ_{ij} is the Dirac delta and $\overline{U}_{i(j)}$ is the relative displacement between the periodic faces normal to direction j , in the direction i .

The conservation of the linear momentum in the reference configuration is given by

$$\nabla_0 \cdot \mathbf{P}(\mathbf{x}) = \mathbf{0}\tag{3.70}$$

where the first Piola-Kirchhoff stress $\mathbf{P}$ is given for each phase present in the microstructure by a non-linear constitutive equation $\mathbf{P}(\mathbf{F}, \mathbf{L}, \mathbf{q})$ depending in general on the deformation gradient, the velocity gradient, $\mathbf{L}$ and a set of internal variables $\mathbf{q}$. $\nabla_0 \cdot$ represents the divergence in the reference configuration. As in the linear case, the variable in which the problem is defined is the displacement field, in particular the displacement fluctuations $\widehat{\mathbf{u}}$.

The total macroscopic deformation gradient prescribed is split in n increments. The deformation at each increment k , $\overline{\mathbf{F}}_{\overline{U}}^k$, defines the macroscopic relative displacement $\overline{\mathbf{U}}^k$

of the RVE opposite faces and therefore the contribution of this macroscopic displacement into the local field. If all the fields are known at increment k , the displacement at increment $k + 1$ corresponds to

$$\mathbf{u}^{k+1}(\mathbf{x}) = (\bar{\mathbf{F}}_{\bar{U}}^{k+1} - \mathbf{I}) \cdot \mathbf{x} + \tilde{\mathbf{u}}^{k+1}(\mathbf{x}). \quad (3.71)$$

where $\tilde{\mathbf{u}}^{k+1}(\mathbf{x})$ is the unknown field to be solved that corresponds to the fluctuation part of the displacement at increment $k + 1$. The expression for the displacement (eq. (3.71)) is introduced in the equilibrium equation leading to

$$\nabla_0 \cdot \mathbf{P}(\mathbf{I} + \nabla_0(\mathbf{u}^{k+1}(\mathbf{x}))) = \nabla_0 \cdot \mathbf{P}(\bar{\mathbf{F}}_{\bar{U}}^{k+1} + \nabla_0 \tilde{\mathbf{u}}^{k+1}(\mathbf{x})) = 0 \quad (3.72)$$

where, the gradient of the deformation is ∇_0 is also taken in the reference configuration, being $\mathbf{F} = \mathbf{I} + \nabla_0 \mathbf{u}$. Note that a non-linear elastic material has been assumed for simplicity (no dependency on $\mathbf{L}$ and $\mathbf{q}$). The non-linear differential equation defined in eq. (3.72) is solved iteratively by Newton method. For this purpose, the displacement fluctuation field and the Piola stress are linearized around the last iteration i of the displacement field fluctuations, $\tilde{\mathbf{u}}^{k+1,i}(\mathbf{x})$, named $\tilde{\mathbf{u}}^i$ to alleviate the notation.

$$\tilde{\mathbf{u}}^{i+1} = \tilde{\mathbf{u}}^i + \delta \tilde{\mathbf{u}} \quad (3.73)$$

$$\mathbf{P}(\mathbf{I} + \nabla_0(\mathbf{u}^{k+1}(\mathbf{x}))) \approx \mathbf{P}(\bar{\mathbf{F}}_{\bar{U}}^{k+1} + \nabla_0 \tilde{\mathbf{u}}^i) + \mathbb{K}^i : \nabla_0 \delta \tilde{\mathbf{u}} \quad \text{with} \quad \mathbb{K}^i = \frac{\partial \mathbf{P}}{\partial \nabla_0 \delta \tilde{\mathbf{u}}} \quad (3.74)$$

Combining the equilibrium equation (3.72) with the linearization of the stress (eq. (3.74)), the next equation is derived

$$\nabla_0 \cdot \mathbb{K}^i : \nabla_0 \delta \tilde{\mathbf{u}} = -\nabla_0 \cdot \mathbf{P}(\mathbf{I} + \nabla_0 \mathbf{u}^i) \quad (3.75)$$

that is a linear differential equation which unknown is $\delta \tilde{\mathbf{u}}$. In the equation $\nabla_0 \mathbf{u}^i = \bar{\mathbf{F}}_{\bar{U}}^{k+1} - \mathbf{I} + \nabla_0 \tilde{\mathbf{u}}^i$ and $\mathbb{K}^i$ is the material consistent tangent evaluated in the i -th iteration of increment $k + 1$. The iterative Newton starts with $i = 1$ and $\nabla_0 \tilde{\mathbf{u}}^0 = \nabla_0 \tilde{\mathbf{u}}^k$.

Then, following the same approach as in the linear case, the linear differential equation is transformed to the Fourier space and the fields are replaced by their discrete counterparts. The result is a linear system of complex numbers

$$\hat{\mathcal{d}} : \mathcal{F} \left(\mathbb{K}^i : \left(\mathcal{F}^{-1} \left(\hat{\mathcal{g}} \cdot \delta \tilde{\mathbf{u}} \right) \right) \right) = -\hat{\mathcal{d}} : \mathcal{F} \left(\mathbf{P}(\nabla_0 \mathbf{u}^i + \mathbf{I}) \right) \quad (3.76)$$

in which the unknown vector to solve is $\delta \tilde{\mathbf{u}}$. The linear equation to solve the equilibrium in each Newton iteration (3.76) is formally identical to the linear equation obtained for the case of linear elasticity (eq. (3.59)). The difference is that in eq. (3.76) the

gradient operator $\widehat{\mathfrak{G}}$ is no longer symmetric being this operator defined in the Fourier space as

$$[\widehat{\mathfrak{G}}(\boldsymbol{\xi})]_{ijk} = \delta_{ik}\xi_j. \quad (3.77)$$

The resulting system is fully determined removing the zero frequency. As in the other cases, the linear equation can be solved by any iterative solver. The Newton iterations finish when the maximum value of $\nabla_0 \delta \tilde{\mathbf{u}}$ the last linear iteration is below a tolerance set to 10^{-6} .

The stress and mixed control approach followed for the linear elastic problem can be followed almost identically in the non-linear case. The prescribed data in this case is a combination of some components the macroscopic first Piola-Kirchhoff stress $[\bar{\mathbf{P}}_{\bar{f}}]_{IJ}$ and other components of the macroscopic deformation gradient $[\bar{\mathbf{F}}_{\bar{U}}]_{ij}$. The deformation gradient field will be split into the part due to macroscopic imposed Piola stress $\bar{\mathbf{F}}_{\bar{f}}$ and the part due to prescribed deformation gradient $\bar{\mathbf{F}}_{\bar{U}}$.

$$\mathbf{F}(\mathbf{x}) = \mathbf{I} + [\bar{\mathbf{F}}_{\bar{U}} - \mathbf{I}]_{ij} + [\bar{\mathbf{F}}_{\bar{f}} - \mathbf{I}]_{IJ} + \nabla_0 \tilde{\mathbf{u}} \quad (3.78)$$

where $\bar{\mathbf{F}}_{\bar{f}}$ is unknown and is only valued in IJ components where Piola stress is imposed. Dividing the applied load in N increments and solving linearization of the equilibrium in each increment by an iterative Newton approach, the linear system to solve at each Newton iteration i is

$$\begin{aligned} \widehat{\mathfrak{d}} : \mathcal{F} \left(\mathbb{K}i : \left(\mathcal{F}^{-1} \left(\widehat{\mathfrak{G}} \cdot \delta \tilde{\mathbf{u}} \right) + (\bar{\mathbf{F}}_{\bar{f}} - \mathbf{I}) \right) \right) &= \\ &= -\widehat{\mathfrak{d}} : \mathcal{F} \left(\mathbf{P}(\nabla_0 \mathbf{u}^i + \mathbf{I}) \right) \\ \left[\mathcal{F} \left(\mathbb{K}i : \left(\mathcal{F}^{-1} \left(\widehat{\mathfrak{G}} \cdot \delta \tilde{\mathbf{u}} \right) + (\bar{\mathbf{F}}_{\bar{f}} - \mathbf{I}) \right) \right) (\mathbf{0}) \right]_{IJ} &= \\ &= [\bar{\mathbf{P}}]_{IJ} - \mathcal{F} \left(\mathbf{P}(\nabla_0 \mathbf{u}^i + \mathbf{I}) (\mathbf{0}) \right)_{IJ} \end{aligned} \quad (3.79)$$

being $\nabla_0 \mathbf{u}^i = [\bar{\mathbf{F}}_{\bar{U}}^{k+1} - \mathbf{I}]_{ij} + \nabla_0 \tilde{\mathbf{u}}^i$ and starting the algorithm with $\nabla_0 \tilde{\mathbf{u}}^0 = \nabla_0 \tilde{\mathbf{u}}^k$. In (3.79), the unknown to be solved is the variable $\left\{ \widehat{\mathbf{u}} \mid \bar{\mathbf{F}}_{\bar{f}} \right\}$ and, if the zero frequency and doubled terms due to the symmetries of the real Fourier transform are removed in the first equation, the system becomes also fully determined and Hermitian.

Improving the efficiency: Preconditioners

The idea of introducing preconditioners to improve the convergence rate when using Krylov solvers for FFT homogenization was first proposed in Zeman et al. (2010) for the conjugate-gradient version of the basic-scheme applied to an electrostatic problem. However, its practical use has been limited since the application of a pre-conditioner

to a rank-deficient system solved by the conjugate gradient, as the one resulting in the Galerkin-FFT approach, might lead to either non convergence of the algorithm or to solutions not fulfilling compatibility conditions.

On the contrary, in the DBFFT approach, thanks to full rank of the linear systems of equations derived for both linear (eq. (3.59)) and non-linear materials (eq. (3.76)), preconditioners can be applied directly and without any risk in order to improve the convergence when solving iteratively the system.

The linear systems defined in the previous sections are not given as function of a matrix of coefficients but expressed in terms of linear operators as

$$\mathcal{A}(\mathbf{u}) = \mathbf{b} \quad (3.80)$$

where the linear operator $\mathcal{A}$ defines the result of applying the matrix of the system to a vector $\mathbf{u}$ and $\mathbf{b}$ is the right-hand side of the equation.

In terms of linear operators, the preconditioner of the system should be a linear operator $\mathcal{M}$ that provides a good approximation of the inverse of the linear operator $\mathcal{A}$.

$$\mathcal{M}(\mathcal{A}(\mathbf{u})) \approx \mathbf{u} \text{ and } \mathcal{M} \approx \mathcal{A}^{-1} \quad (3.81)$$

If an operator $\mathcal{M}$ were obtained which corresponded exactly to the inverse $\mathcal{A}^{-1}$ then the system could be directly solved applying $\mathbf{u} = \mathcal{M}(\mathbf{b}) = \mathcal{A}^{-1}(\mathbf{b})$. For the systems considered it is not possible to obtain an analytic expression for $\mathcal{A}^{-1}$.

Focusing on the linear case given by eq. (3.59), the inverse of $\mathcal{A}$ would consist in applying from left to right the inverse of the operations defining the action of $\mathcal{A}$ over $\widehat{\mathbf{u}}$. Some of these operations are not invertible but, if the local stiffness matrix $\mathbb{C}(\mathbf{x})$ is replaced at each point by the average stiffness $\overline{\mathbb{C}} = 1/n \sum_{\mathbf{x}_1}^{\mathbf{x}_n} \mathbb{C}(\mathbf{x})$, the modified eq. (3.59) can be inverted. The resulting linear operator is given by

$$[\mathcal{M}(\widehat{\mathbf{u}})]_{\xi} := \mathbf{M}(\xi) \cdot [\widehat{\mathbf{u}}]_{\xi} \quad (3.82)$$

where $\widehat{\mathbf{u}}$ is the discrete vector field of displacement fluctuations in the Fourier space and $[\widehat{\mathbf{u}}]_{\xi}$ is the displacement fluctuation vector in the Fourier point ξ and $\mathbf{M}(\xi)$ is second order tensor defined for each frequency as

$$\mathbf{M}(\xi) = \begin{cases} [\xi \cdot \overline{\mathbb{C}} \cdot \xi]^{-1} & \text{for } \xi \neq \mathbf{0} \\ [\{\mathbf{1}\} \cdot \overline{\mathbb{C}} \cdot \{\mathbf{1}\}]^{-1} & \text{for } \xi = \mathbf{0} \end{cases} \quad (3.83)$$

The second order preconditioner operator is computed once at the beginning of the simulation and does not imply any extra direct or inverse Fourier transform. In the

case of a finite strain non-linear simulation, the definition of the preconditioner $\mathbb{M}$ is very similar, replacing the average stiffness matrix by the average material tangent $\bar{\mathbb{K}}$ and it is computed at the beginning of the increment. This average stiffness matrix can be recomputed once in a while to further improve the convergence.

3.4.2 Numerical results of the DBFFT

The DBFFT method has been added to the code FFTMAD (Appendix A) as a new scheme and programmed combining python and fortran subroutines. All the linear systems are solved using the conjugate gradient method for complex numbers and the preconditioner defined in eqs. (3.82) and (3.83). The conjugate gradient method for complex numbers has been programmed in python to compute the three residuals proposed at each equilibrium iteration. Postprocessing is done using FFTMAD subroutines and deformed plots and field iso plots are generated using *paraview*.

In this section several numerical examples are tested and compared with the Galerkin FFT approach Zeman et al. (2017); de Geus et al. (2017) to benchmark the method proposed. Three types of residual are computed to check the fulfillment of equilibrium condition, strain field compatibility and boundary conditions. The residuals proposed are similar to the ones proposed in Moulinec and Silva (2014) adapted to displacements.

The first residual defines the deviation of the resulting displacement field from the equilibrium, given by the linear momentum balance, and reads

$$\epsilon_{equilibrium} = \frac{\|\nabla \cdot (\boldsymbol{\sigma})\|_{L_2}}{\|\langle \boldsymbol{\sigma} \rangle\|}, \quad (3.84)$$

where $\|\cdot\|$ denotes the Frobenius norm of a second order tensor and $\|\cdot\|_{L_2}$ the L_2 norm of a tensor field. The equilibrium residual tolerance is set to 10^{-8} for all the tests presented here. The second residual quantifies the incompatibility of the strain field and is defined as

$$\epsilon_{compatibility} = \frac{\max(|\nabla \times (\nabla \times (\boldsymbol{\varepsilon}))|)}{\|\langle \boldsymbol{\varepsilon} \rangle\|} \quad (3.85)$$

where $\nabla \times$ denotes the rotational operation, $|\cdot|$ is the absolute value of the field and $\max$ extracts the maximum among all the components of all the tensors forming the discrete field. The last error measure is the loading residual, which checks if the boundary conditions are fulfilled, and is defined by

$$\epsilon_{loading} = \frac{\|\langle \boldsymbol{\varepsilon} \rangle - \bar{\boldsymbol{\varepsilon}}\|}{\|\bar{\boldsymbol{\varepsilon}}\|} \quad (3.86)$$

Under stress control (the macroscopic stress is prescribed), the residual is computed with the stress field σ and the prescribed macroscopic stress $\bar{\sigma}$ instead. The compatibility check and the loading check tolerance are established as 10^{-10} .

Finally, differences in the solution between the two methods are compared by computing the norm of the difference of the solution fields, that follows

$$\text{Diff}(f) = \frac{\|f_{DBFFT} - f_{Galerkin}\|_{L2}}{\|f_{Galerkin}\|_{L2}} \quad (3.87)$$

for a generic field f that can be a vector or a tensor field.

Linear elasticity with strain control: spherical inclusion

In the first numerical benchmark an idealized linear elastic composite with a regular array of spherical inclusions with variable phase contrast is studied. The RVE corresponds to a cubic periodic domain composed by a spherical inclusion embedded in the matrix, occupying the 20% volume fraction and discretized in $63 \cdot 63 \cdot 63$ voxels. The problem is solved prescribing the full macroscopic strain tensor. The elastic properties of each phase are set to $E_m = 70 \text{ MPa}$ and $\nu = 0.3$ for the matrix, while for the inclusion the elastic modulus is $E_m = k \cdot E_m$ and $\nu = 0.3$, where k is the stiffness contrast. The macroscopic strain applied is uniaxial strain, being 0.1% in loading direction and 0 for the rest of the components. The linear system given by eq. (3.59) and using the preconditioner defined in eqs. (3.82) and (3.83) is solved using the Conjugate Gradient method, and at each iterations the three error estimations (eqs. (3.84)-(3.86)) are computed. The iterative process is performed until reaching a tolerance for equilibrium $\epsilon_{equilibrium} < 10^{-8}$ and 10^{-10} for the other two estimations or when the number of iterations reached 10^4 . Ten different cases have been simulated with phase contrasts ranging from very soft inclusions (nearly voids, $k = 10^{-5}$) to stiff inclusions ($k = 10^4$).

To illustrate the results obtained and the ability of the DBFFT method to obtain the deformed shape without any further postprocessing, the deformed shape and the axial stress component in the direction of the applied load are shown in Figure 3.6 for the case of $k = 10^5$. Quantitatively, for all the stiffness contrasts, the strain fields obtained with the DBFFT and the Galerkin approach solution are virtually identical, being the difference between these fields computed using eq. (3.87) below the equilibrium tolerance (10^{-8}). The homogenized response is therefore also identical, within the numerical precision.

When checking the convergence rates, a remarkable difference is found between the two methods, as shown in Fig. 3.7 where the residual decay is represented as function of the number of iterations for the cases with the extreme phase contrast,

Figure 3.6: Deformed shape ($\times 20$) obtained using the displacement field solved directly in DBFFT (left) and stress field in the loading direction of the elastic inclusion model (right) for phase contrast 10^5

$k = 10^{-5}$ and $k = 10^5$. In all the cases considered, the convergence rate of the DBFFT for the same tolerances and linear solver (conjugate gradient) is superior, leading to an improvement in efficiency respect to the Galerkin approach that, for the extreme cases $k = 10^{-5}$ and $k = 10^5$, result in a reduction of the number of iterations up to 40%. It must be noted that the compatibility and loading fulfillment are always accomplished for both methods .

The improvement in the number of iterations is related to the condition number of the matrix representing the linear system of equations. In the case of the DBFFT, the use of a preconditioner reduces the condition number of the matrix and improves the convergence rate allowing to find the solution using less iterations.

Linear elastic with stress control: spherical inclusion

In this section the results of the DBFFT method using macroscopic stress control are assessed solving the same case of the elastic inclusion presented in the previous section. RVE shape, material properties and tolerances are the same but in this case the load applied is a uniaxial macroscopic stress in the loading direction, being the rest of the components 0. As in the previous case, the differences in stress and strain fields between the DBFFT with stress control and the stress control version of the Galerkin scheme proposed in Section 3.3 are below the equilibrium tolerance. Respect the efficiency, a figure summarizing the results obtained for all the stiffness contrasts considered is represented in Figure 3.8 (left) where the number of iterations for both methods

Figure 3.7: Equilibrium residual for the elastic inclusion model when $k = 10^{-5}$ (left) and $k = 10^4$

is represented as function of the phase contrast. In Fig. 3.8 (right) the results obtained in the previous section are represented in the same type of diagram for a better comparison. As it happens under strain control, here in all the cases the compatibility and loading error estimators are fulfilled for both methods. The convergence rates are also higher for the DBFFT algorithm and depend on the stiffness contrast as shown in Figure 3.8. The comparison in number of iterations needed to reach the equilibrium tolerance is almost identical to the strain controlled simulations, a reduction near 40% in the case of compliant inclusions.

Non linear simulation with hyperelastic materials: random array of spherical voids

The third benchmark consists in a non-linear hyperelastic matrix containing a random distribution of 5 spherical pores and a total porosity volume fraction of 0.2. Opposite to FE, in FFT approaches voids cannot be just removed from the grid since Fourier transforms and differential operators act on full fields defined in regular grid in a hex-aedrical domain. For this reason, voids are usually considered as very compliant elastic inclusions, the same approach followed here. The RVE considered is a cube containing 63^3 voxels (Fig. 3.9). The test simulated consists in applying a uniaxial elongation $\lambda = \frac{L}{L_0} = 2$, being L and L_0 the final and initial lengths of the cell in the loading direction, and keeping the other directions undeformed. Both the matrix and the compliant inclusions follow a Saint Venant-Kirchhoff hyperelastic model. The matrix properties are $E = 70 \text{ MPa}$ and $\nu = 0.3$ (Young and Poisson modulus) and the stiffness of the inclusions is 100 times smaller. Load is homogeneously divided in 5 load increments and

Figure 3.8: Number of iterations as a function of the stiffness contrast for elastic linear inclusion: strain control (left) and stress control (right)

the equilibrium is solved in each of them using Newton method, as described in the model description. The tolerance of the Newton iterations is 10^{-6} and the three residuals proposed for the linear simulations are adapted to the non-linear case and used to check the convergence of the linear iterations. In particular, the equilibrium error estimator is computed modifying eq. (3.84) by replacing the stress with the first Piola-Kirchhoff stress and the divergence with the divergence in the reference configuration. The compatibility check is also adapted to finite strain, being computed as

$$\epsilon_{compatibility} = \frac{\max(|\nabla_0 \times (\mathbf{F})|)}{||\langle \mathbf{F} \rangle - \mathbf{I}||} \quad (3.88)$$

where $\nabla_0 \times$ represents the rotational of a tensor field in the reference configuration.

The deformed shape obtained using directly the displacement obtained by the DBFFT method is represented in Fig. 3.9 without any magnification. In the same figure, on the right, the normal component of the first Piola-Kirchhoff stress field in the loading direction is represented for the porous matrix. In the Figure 3.9 it can be observed how the pore shape evolves from spherical ellipsoidal and how the stress in the loading direction is concentrated in the void diameter in planes normal to the loading direction. Respect the accuracy of the solution, the result provided by DBFFT is again almost identical to the one obtained by the Galerkin method, being the differences (eq. (3.87)) in both deformation gradient and stress fields below the equilibrium tolerance (10^{-8}) at the end of each increment. The compatibility and loading requirements are always fulfilled.

Figure 3.9: Deformed shape with the displacement field (left) and first Piola-Kichhoff stress field in the loading direction (right) of the porous matrix

Finally, the efficiency of the method for this non-linear elastic case is analyzed representing the evolution of the equilibrium error estimator (eq. (3.59)) as function of the total iteration number (Fig. 3.10, left), and the total number of iterations per increment at the end of each strain increment (Fig. 3.10, right). The number of iteration in both curves refers to the total number of iterations performed by the conjugate gradient considering all the Newton iterations. From Fig. 3.10(left) it can be observed that DBFFT converges faster and requires less linear iterations per Newton iteration to reach the tolerance resulting in a smaller number of increments for the simulation than the Galerkin method. The total iteration number is reduced by 20%, which is translated in a computational time saving of similar order. It must be noted that the better performance of the DBFFT respect to the Galerkin scheme is reduced in the last increment, at a very large strain. The reason for this reduction in the convergence rate is that the preconditioner used, computed with the initial tangent stiffness, does not improve the condition number of the system for very distorted RVEs.

Non linear with path-dependency: elasto-visco-plastic polycrystal

The last benchmark proposed is a metallic polycrystal. This is an ideal case because it illustrates the behavior of a material with loading path and strain rate dependencies. The RVE is a cube discretized in 63^3 voxels and the model contains around 200 randomly oriented grains (Fig. 3.11). Grain distribution in the RVE is generated using a Voronoi tessellation and grain orientations are random using the generation tool presented in B. Each grain follows a crystal plasticity (CP) explained in Section 3.1.2.

Figure 3.10: Equilibrium residual (left) and number of iterations per increment (right) for the hyperelastic porous matrix model

Strain control is used prescribing the full deformation gradient. A final elongation of $\lambda = 0.02$ is imposed in 400s in the loading direction and a negative strain is applied in transverse direction $\lambda' = 1/\sqrt{\lambda}$ to produce a final isochoric deformation. Shear components of the deformation gradient are set to 0 and time is discretized in 20 regular increments of 20s.

The DBFFT method is able to finish the simulation using the standard error tests, the equilibrium estimator given by (eq. (3.59)) using the Piola stress and 10^{-8} as value of the tolerance. On the contrary, the Galerkin approach after a few increments cease to converge and the error estimator is stacked near the tolerance limit. This lack of convergence for very small tolerances in the case of the polycrystal is due to the ill-condition of the linear operator, that might be caused by the large differences in the local material tangents during the elastic-plastic transition. For this reason, the residual proposed in de Geus et al. (2017) is used instead for the equilibrium check and, in this case, both methods are able to converge. The norm of the difference of deformation gradient field is $5 \cdot 10^{-7}$ and the loading and compatibility check are fulfilled in both methods.

The deformed shape obtained with the displacements obtained with DBFFT method is represented in the left part of Figure 3.11 using a magnification of 10. A smooth deformation of the surface is observed corresponding to the different effective stiffness of the grains due to their orientation. The Von Mises stress invariant of the Cauchy stress is shown in the right image of Figure 3.11. In this case, the concentration of the stress in certain grains can be clearly observed. This stress concentration is due to the

orientation of the grain as well as the orientation of the surrounding grains.

Figure 3.11: Deformed shape ($\times 10$) showing grains (left) and Von Mises stress field (right) of the polycrystal

The convergence is analyzed representing in Figure 3.11 the evolution of the equilibrium error estimator (defined in de Geus et al. (2017)) as function of the total iteration number (left) and the total number of iterations per increment at the end of each strain increment (right). The DBFFT performance is in this case clearly superior to the Galerkin approach. The total number of iterations for the DBFFT is reduced by 60% even considering a tighter equilibrium residual tolerance. Respect to the evolution of the number of iterations per increment, it shows different stages for both methods. In the first increments, corresponding to the elastic response, the number of iterations is very small due to the limited phase contrast. Then, number increases very fast and is kept high (around 200 in the Galerkin and around 70 in the DBFFT) in a strain range corresponding to the elasto-plastic transition. This is due to the very high stiffness contrast at this stage caused by the presence of elastic points with very large stiffness with points fully plastified with tangent stiffness orders of magnitude smaller. After this transition, the number of iterations decreases again and this stage corresponds to the fully plastic regime. Note that during the fully plastic regime the number of iterations per increment in the DBFFT method is kept constant while grows linearly in the Galerkin method.

Figure 3.12: Equilibrium residual (left) and number of iterations per increment (right) for the polycrystal

3.5 Validation for micromechanics based fatigue life prediction

In this section, the validity of the FFT framework proposed for micromechanics based fatigue modeling will be assessed. To this aim, the macroscopic response and microscopic fields obtained for different cyclic loading histories using both the FEM and the FFT framework will be compared. The parameters defining the probability for a given RVE to nucleate a crack computed using both numerical approaches is compared, and the impact of the differences in the fatigue life estimation is analyzed.

3.5.1 Test description

The microstructure of the material is represented using a cubic RVE and the grain geometry is generated using the open source code *Neper* (Quey et al., 2011). The grain sizes follow a log-normal distribution with a mean value of the grain diameter of $10\mu\text{m}$ and standard deviation of 0.5. The grains shape is approximately equiaxial by selecting a target spheroidicity equal to 1. Three different models will be considered in this study. All the models share the same geometry —corresponding to the Voronoi tessellation of a particular arrangement of centers containing 235 grains— but are discretized with different number of voxels, 32^3 , 64^3 and 128^3 , Figs. 3.13 and 3.13. In the case of the finite element simulations, each voxel is used to define a cubic linear element (C3D8 in Abaqus) where the Selective Reduced Integration (SRI) method is

Figure 3.13: Discretization of the RVE using 32^3 voxels, 64^3 voxels and 128^3 voxels

Figure 3.14: Details of a cluster of grains in the models with 32^3 voxels, 64^3 voxels and 128^3 voxels

used to avoid element locking. It must be noted that the complexity of both models is equivalent because the number of independent nodes in the FE model is identical to the number of voxels of the FFT approach.

The models are subjected to a nearly uniaxial-stress cyclic strain history. In order to apply this load history using strain control, the applied deformation gradient is given by

$$\mathbf{F}(t) = \begin{bmatrix} F(t) & 0 & 0 \\ 0 & 1/\sqrt{F(t)} & 0 \\ 0 & 0 & 1/\sqrt{F(t)} \end{bmatrix}, \quad (3.89)$$

that is a purely isochoric deformation which, due to the fully incompressible nature of the plastic deformation, results in a stress state very close to uniaxial stress. The value of the function $F(t)$ is set to represent a triangular cycle with a period $T = 4s$, macroscopic strain amplitude ε_{max} and $R_\varepsilon = 0$. If t' is the time relative to the beginning

of the cycle, the deformation gradient in the loading direction is given by

$$F(t') = \begin{cases} (\frac{1+\varepsilon_{max}}{T})2t' & \text{if } t' < T/2 \\ 1 + 2\varepsilon_{max} - (\frac{\varepsilon_{max}}{T})2t' & \text{if } t' > T/2 \end{cases} \quad (3.90)$$

For the FE simulations, the same deformation history is applied imposing the history of the relative displacement between the corresponding faces in the periodic RVE through the periodic boundary conditions using the master nodes of each face pair, see Segurado and Llorca (2013) for more details. In both simulation frameworks the time increments used are the same in order to allow a direct comparison of the results.

3.5.2 Simulation of the cyclic behavior of polycrystals

In this section the macroscopic and microscopic response of the polycrystal under two different cyclic loading cases and two different number of cycles are obtained using the FFT framework. The model results are compared with the corresponding FEM simulations.

Macroscopic response

First, a cyclic loading following (eq. 3.90) with macroscopic strain amplitude of $\varepsilon_{max} = 1\%$ is applied to the different discretizations of the polycrystal. This strain range is relatively large for fatigue considerations and the resulting fatigue regime for this particular setting is the LCF. The macroscopic stress-strain response in the loading direction obtained in the numerical simulation of three cycles is represented in Figure 3.15 for both FEM and FFT and for two discretizations, 32^3 (Fig. 3.15(a)) and 64^3 voxels (Fig. 3.15(b)). In the case of the FFT simulations the results using standard projection operators and the operators based on the discrete derivatives (Section 3.2.1) are depicted. Note that the 128^3 voxel model is not represented here because the finite element code was not able to simulate a system of that size.

Figure 3.15: Comparative stress-strain curve for a model containing (a) 32^3 voxel/elements and (b) 64^3 voxel/elements

The results in Figure 3.15 show that FEM and FFT macroscopic solutions are practically superposed. From a quantitative view point, a relative error of the stress-strain curve predicted with FFT respect the FE solution at time t is defined as

$$Error(t)[\%] = \frac{|\sigma(t) - \sigma_{FEM}(t)|}{\max(\sigma_{FEM})} \cdot 100, \quad (3.91)$$

and using this definition the maximum error was below 0.9% in the case of 32^3 voxels. When the model is refined to 64^3 the differences became smaller than 0.5%. Finally, it should be noted that the use of projection operators based on discrete derivatives does not influence the macroscopic result of the FFT simulation. These results show the ability of the Galerkin FFT homogenization framework to obtain an accurate effective response for the cyclic behavior of polycrystals.

To analyze the influence of the local history in the global response of the polycrystal two new cyclic simulations are performed. The first case consists in three full cycles with a large macroscopic strain amplitude ($\varepsilon_{max} = 5\%$) and the second one corresponds to 100 cycles with the original value of the macroscopic strain amplitude, $\varepsilon_{max} = 1\%$. In both cases, the differences between FFT, discrete operator FFT and FEM are still very small and the resulting curves are not easy to distinguished.

In the first case, the relative error in the macroscopic response respect the FE result for the model with 64^3 voxels (eq. (3.91)) is represented in Fig. 3.16 (a). It can be observed that the maximum difference is below 0.8% for the full load history and that this difference is almost independent on the applied deformation or stress level.

Moreover, it can also be observed that there is almost no error increase from cycle to cycle. In the second case a numerical experiment under strain amplitude of $\varepsilon_{max} = 1\%$ for 100 cycles is performed using the small models with 32^3 voxel/elements due to the computational cost of FE simulations. In this simulation the stable cycle is reached and its shape is represented in Fig. 3.16 (b) for both FE and FFT. The stable cycle is perfectly captured by the FFT solver showing that there is no substantial error accumulation with the number of cycles. To highlight the stability of the solutions with the number of cycles, Fig. 3.16 (c) represents the difference between FE and FFT solutions as function of the cycle number and it can be observed that this difference does not increase with the accumulation of plastic strain resulting of cyclic loading.

Figure 3.16: (a) Error during 3 cycles of $\varepsilon_{max} \approx 5\%$ test in 64^3 voxel/elements, (b) first and last cycle for a cyclic history of 100 cycles ($\varepsilon_{max}) = 1\%$) in 32^3 voxel/elements (c) evolution of error with the cycles corresponding to the previous load history

Microscopic fields comparison

The use of FFT for microstructure based fatigue modeling implies an accurate prediction of the microscopic fields because the fatigue life is estimated from the extreme values of those fields after a large number of cycles. To assess the ability of the FFT framework to predict accurate values of the microfields, the microscopic Cauchy stress in the loading direction, σ_{xx} , and the local value of the accumulated shear (fatigue indicator parameter P_{cyc}) are compared with the finite element solution. The comparison is presented for the models with 64^3 voxels. The distribution of the stress in the loading direction after the first ramp-up load obtained with FEM, FFT and the discrete projection operator version of FFT is represented in Fig. 3.17. The figure shows the results in one of the RVE faces using the same code for the three simulations. The results are not smoothed out and correspond to the voxel value in the case of FFT and to the average element value in the case of FEM.

Figure 3.17: Microscopic σ_{xx} values in a RVE face, left: FE results, center: FFT results, right: discrete operator version of FFT

The stress field obtained using the FFT approach is qualitatively very similar to the one obtained with FEM, as it can be observed in Fig. 3.17. Respect the two different projection operators used, the local stress maps are (again qualitatively) very similar and only some differences can be found in areas with stress concentrations.

To quantify the differences between any local field $f(\mathbf{x})$ obtained with FFT with the FE simulation result, f_{FEM} , the normalized $L2$ norm of the difference is proposed (using the center of each voxel).

$$Diff(f)[\%] = \frac{\|f - f_{FEM}\|_{L2}}{\|f_{FEM}\|_{L2}} \cdot 100. \quad (3.92)$$

For the stress component parallel to the loading direction this difference in the 32^3 models corresponded to 4.6% and 3.6% for the standard and discrete projection operator respectively. For the finer discretization of 64^3 voxels these differences decreased to 3.4% and 2.6% respectively. Clearly the use of the discrete projection operator in the FFT simulations provided local fields more similar to FEM solution. In addition, as expected, the differences between FFT and FEM are reduced with the mesh refinement.

The local value of a fatigue indicator parameter, P_{cyc} (defined in eq. (2.38)), in one of the RVE faces obtained after three cycles using the three different modeling approaches is represented in Fig. 3.18. Again, the results represented are the local voxel/element values without smoothing. As it happens with the stress field, qualitatively the FIP patterns obtained with the three methods are very close. Quantitatively, the FFT solution seems to present slightly higher FIP concentrations than the FEM prediction and the use of the modified projection operator led to a smoother FIP field that is also closer to the FEM results. Quantitatively, the differences obtained for the P_{cyc} were 30.9% and 23% in 32^3 models for the normal and discrete version respectively, and 25.1% and 18% in 64^3 models. The results obtained for the other FIP considered in this study, W_{cyc} , are

very similar and omitted here for the sake of brevity. Note that differences in the local relative differences found are affected to a very small value of the resulting plastic strain for a strain level of $\varepsilon_{max} = 1\%$. Indeed, this error definition will become singular for small applied macroscopic strains. It is expected that this error will be reduced for larger strain amplitudes. Finally, it should be highlighted that, again the use of discrete projection operators leads to a result more similar to FEM.

Figure 3.18: Microscopic values of P_{cyc} in a RVE face, left: FE results, center: FFT results, right: discrete operator version of FFT

As it was done with the macroscopic response, the microscopic response is evaluated for two different cyclic loading conditions, longer cycles and larger deformations, to assess the response of the FFT framework under different load histories. The evolution of the local field differences between FEM and FFT computed using eq. (3.92) for 100 cycles and $\varepsilon_{max} = 1\%$ is represented in Fig. 3.19 for the model with 32^3 discretization. It can be observed that, as happened with the macroscopic response, both the differences in stress and strain maps are kept almost constant for all the cycles studied. The effect in the local fields of applying a larger value of the strain in each cycle was also studied using a strain range of $\varepsilon_{max} = 5\%$ and the finer models (64^3 voxels). The differences of the stress between FFT and FEM obtained using eq. (3.92) corresponds now 4.7% and 3.3% (standard and discrete projection operators), slightly greater than the ones obtained for $\varepsilon_{max} = 1\%$. On the contrary, the relative differences in P_{cyc} are notably reduced respect the ones obtained for $\varepsilon_{max} = 1\%$ being now 5.3% and 3.7% for the standard and discrete operator respectively. This error reduction is due to the larger value of plastic strain produced for that level of applied strain.

Figure 3.19: (a) Difference of σ_{xx} field during 100 cycles of $\varepsilon_{max} \approx 1\%$ test in 32^3 voxel/elements and (b) Difference of P_{cyc} field during 100 cycles of $\varepsilon_{max} \approx 1\%$ test in 32^3 voxel/elements

3.5.3 Fatigue life estimation

As explained in Section 2.3.4, the local values of the FIPs are not adequate to correlate the fatigue life of a given microstructure due to discretisation errors and fatigue indicators are averaged in some regions to produce non-local measures more adequate to estimate the tendency to nucleate a crack. Therefore, it is expected that the small differences found between the FEM and FFT FIP microfields, after averaging, become much smaller. Moreover, the FIP representative of the full RVE and responsible of the fatigue life predictions is based on the tails of the non-local fatigue indicator parameter distribution so the differences in the microfields in regions with small FIP value will not affect the fatigue life estimation. In this section the differences between the resulting FEM and FFT non-local fatigue indicators parameter distribution will be studied and the implication of this difference in the RVE fatigue life estimation will be analyzed.

Two non-local fatigue indicator parameters will be considered, grain averaged P_{cyc} and the band averaged W_{cyc} and simulations will be done with the 64^3 voxel model. In the case of the grain averaged P_{cyc} , one FIP value is obtained per grain (here 235 values) and a histogram showing the fraction of grains as function of the P_{cyc} is represented in Figure 3.20(a). A similar graph is computed for W_{cyc} and represented in Fig. 3.20(b), but in this case the histogram represents the fraction of averaging bands.

Figure 3.20: FIP histogram for 64³ voxel model in FEM, FFT, and discrete projection operator FFT. (a) grain averaged P_{cyc} and (b) band averaged W_{cyc}

When the FIPs are averaged at grains (Figure 3.20(a)) it can be observed that the distribution of the local FIP through the grains obtained using FE and FFT are very similar, presenting only some small differences for small FIP values (left part of the curve). It can also be observed that when FFT is based on the discrete projection operators the curves become almost identical in the full FIP range. This result highlights the conclusion obtained when comparing the local fields point by point: the modified projection operator produces a response in all the microfields studied (stress, strain and the two FIPs considered) more similar to FE than the standard FFT method. The histogram with the volumetric distribution of W_{cyc} (3.20(b)) shows more differences between FEM and FFT results and, again, the FFT fields obtained with the modified projection operator are closer to the FEM solution. This better agreement with FE obtained using the modified projection operator is very clear in the tail of the distribution for large FIPs, where standard FFT predicts a maximum FIP considerably larger than the other two methods.

Next, the FIP representative of the microstructure—in which fatigue life prediction is based on—is obtained using FE, FFT and FFT based on the discrete operator. To compute this value, ten different RVEs representative of the same microstructure and containing 64³ voxels are simulated (some times called a set of SVEs). Each RVE followed the same grain size distribution previously described and has around 230 grains. The simulations consist in three cycles following the strain history defined in equations (3.89) and (3.90). The maximum FIP of each RVE is extracted from the simulation using equations (2.38) with (2.41) and (2.39) with (2.42), and the FIP representative of the

method is obtained as the average of the FIP of each RVE (ten in total). The relative difference between the two FFT approaches and the reference FE solution is obtained as

$$Err(\%) = 100 \frac{FIP_{FE} - FIP_{FFT}}{FIP_{FE}} \quad (3.93)$$

where FIP_{FE} and FIP_{FFT} stand for the average in FIP value of the different RVE realizations. The average FIP value, the standard deviation and the relative difference respect FE are represented in Table 3.2 for grain averaged P_{cyc} and in Table 3.3 for band averaged W_{cyc} .

	FE	FFT	FFT discrete operator
mean []	2.567e-2	2.603e-2	2.597e-2
std deviation []	6.021e-3	5.845e-3	5.942e-3
difference with FE (eq. (3.93))	0	1.40%	1.17%

Table 3.2: Mean value, standard deviation and difference with FE of the microstructure representative value of grain averaged P_{cyc}

	FE	FFT	FFT discrete operator
mean [N/m]	5.071e6	5.823e6	5.424e6
std deviation [N/m]	5.112e5	8.763e5	6.948e5
difference with FE (eq. (3.93))	0	14.6%	6.8%

Table 3.3: Mean value, standard deviation and difference with FE of the microstructure representative value of band averaged W_{cyc}

The results on Table 3.2 shows that, when grain averaging is used, the value of P_{cyc} representative of the microstructure and obtained using either FEM or FFT are almost identical (differences below 2%), being the value of FFT method slightly larger than FE in all the cases. Respect the standard deviation of the ten FIP values obtained, FE and FFT results are very similar being the scatter found in FFT slightly smaller. In this case the use of a modified projection operator has a small influence in the results. The reason for the strong similarity between FE and FFT is that grain averaging implies integration over many material points and therefore the local differences found are smooth out in the averaging procedure. The second FIP studied, W_{cyc} , is obtained by band averaging and the resulting FIPs and comparison with FE are shown in Table 3.2. It can be observed that the differences are higher compared to the grain averaged P_{cyc} , but they are still quite limited, being always below 15%. Again, FFT results are slightly larger than FE solution. The dispersion between the ten RVEs is larger than for grain averaging, an expected result because the non-local smoothing procedure is

done here in bands containing much less element than a grain. Nevertheless, the most interesting result here is that the introduction of the modified projection operator in the FFT simulation significantly reduces the error with the reference FE solution to less than the half, from 14.6% to 6.8%.

Finally, the influence of the differences found in the FIP representative of the microstructure between FE and FFT will be used to estimate the deviations expected in the fatigue life (number of cycles to nucleate a crack) using both techniques. In light of the previous results it is clear that the modified version of the projection operator has to be used to minimize the difference in the FIP values representative of the microstructure with respect FE. If the fatigue life prediction law is adjusted using FE models, this small differences in FIP will be translated to the fatigue life prediction. In the case of a linear relation to correlate FIP with life (Section 2.3.4), the relative difference found in the FIP will be directly the difference in the number cycles for crack nucleation between FE and FFT and will be limited in the worst situation to 6.8% (band averaging). However, linear relations are not ideal to correlate fatigue because and more complex expressions are proposed as the one described in Section 3.1.3. Considering the maximum error in the FIP_{cyc} prediction with respect FE, 6.8%, the maximum relative deviation expected in fatigue life prediction is $\approx 15\%$. This deviation will be well accepted for fatigue life prediction because the scatter in life of different fatigue experiments is far beyond this difference.

3.5.4 Effect of second phases

The presence of stiff second phases as carbides in the alloy microstructure has a strong effect in the fatigue response due to the stress concentrations produced around them. Considering this situation in microstructure based fatigue life prediction is not a problem using FE but FFT simulations using the standard projection operator might lead to Gibbs oscillations due to the strong phase contrast, and therefore local fields and FIPs might be inaccurate. The introduction of the modified projection operator proposed in this study and based on the discrete derivatives introduced in Willot (2015) will allow to alleviate this problem and extend the use of FFT in fatigue to RVEs containing second phases. In order to assess the validity of this framework in the presence of hard phases, a distribution of particles ten times stiffer than the crystals are included in the polycrystalline model, occupying 1% of the total volume. The particles are introduced as spheres with a diameter following a log-normal distribution of sizes of mean $4\mu m$ and $\sigma = 0.56$ obtained from a experimental measure of carbides inside the microstructure of Inconel 718. In this case, models containing 64^3 voxels are used and

simulations are performed using FE and FFT with the two projection operators considered.

The local result of the simulation with carbides are represented in Fig. 3.21. A straight path crossing a stiff particle is shown as a white line (Fig. 3.21(a)) and the value of the strain component XX along that path obtained using the three simulations is represented in Fig. 3.21(b). In this figure the artificial oscillations in the response obtained using standard FFT are clearly shown and the strong improvement using the discrete projection operator can be observed.

Figure 3.21: (a) Microstructure with stiff particles (in black) and (b) Strain field over the a direction

Regarding the local stress values, the presence of hard particles induces stress concentration around them and the average differences respect FE obtained using the $L2$ norm slightly increased, resulting in 8.6% and 6.9% for the standard and discrete operator respectively. It is worth mentioning that the relative differences in local FIP between FEM and FFT in the case of the discrete operator for the microstructures with stiff particles are very similar to the ones found for pure polycrystals so the effect of considering second phases can be accounted accurately using this FFT approach.

3.6 Analysis of computational performance

The main reason for using FFT is the reduced computational cost respect to finite element simulations. It is well known that FFT is much more efficient solving large models due to the order $n \log n$ growth of the computational cost. Therefore, elastic

simulations or non-linear calculations for small overall strain values can be orders of magnitude faster when using FFT Eisenlohr et al. (2013). Nevertheless, in the case of micromechanics based fatigue simulations the evaluation of the non-linear constitutive equation has a strong impact in the simulation time playing also an important role in the actual performance.

In this section, a comparison of the FFT framework for cyclic simulation of polycrystals with a FEM framework in terms of computational time is presented. The performance of the new developed approaches, Galerkin stress control and DBFFT is analyzed as well.

3.6.1 Performance of the stress and mixed control

The performance of the new approach proposed for stress and mixed control is assessed here. In this case, the objective is comparing the computational cost of using mixed control and strain control, and only Galerkin approach is then considered. The convergence criteria for the iterative linear solver (eq. (3.12)) is the voxel averaged value of the L_2 norm of the residual and for the Newton solver is the maximum deformation gradient correction relative to the averaged deformation gradient. The total computational time of the 4 loading cases studied in Section 3.3 is considered here. The tolerances used are 10^{-8} and 10^{-6} for linear and Newton solvers respectively. First, the total number of conjugate-gradient iterations per load increment is represented as function of the step (Fig. 3.22). This number includes the sum of all the linear iterations performed for each Newton iteration in an increment. In the case of the hyperelastic model (Fig. 3.22(a)) the stress and mixed controlled simulations (*cases* (1) and (2)) took approximately the same number of iterations than using full strain control, illustrating the very good performance of the approach proposed here. The jumps observed in the figure are due to the increase or decrease of one Newton iteration after a given time increment, because each Newton iteration implies several iterations for solving the linear system. In the case of the polycrystal (Fig. 3.22(b)) a similar tendency is achieved. The main difference between the different cases is that, when load control is applied using a ramp (*case* (2)), most of the load increments are elastic and solved in one Newton iteration corresponding the plastic regime only a few steps which require much higher number of iterations.

Figure 3.22: Comparative of convergence for each time increment for (a) particle reinforced hyperelastic and (b) polycrystal. (c) Simulation time comparative for all examples normalized with respect to case (3) time.

The comparative in simulation times for all the cases considered is represented in Fig. (3.22 (c)). The hyperelastic simulations needed almost identical times for every boundary condition. On the contrary, in the polycrystal, differences are found for case (2). As explained before, in this case most of the increments are purely elastic requiring very small simulation time. The plastic regime is then confined only in a few steps and, although each plastic step takes more time than in the other cases, the fast elastic steps compensate the global time and this load case is clearly faster than the others. It must be noted that this is a consequence of using a fixed time step and, for adaptive time stepping, all the cases will require very similar simulation times.

3.6.2 Performance of the DBFFT

Now, the performance of the DBFFT for the particular case of polycrystals is compared to the Galerkin approach. The results obtained shows in all the cases examined an improvement in the convergence rate of the DBFFT method compared to the Galerkin scheme. This leads to a reduction in the computational time proportional to the number of iterations reduced since the heaviest operations for each equilibrium iteration, the direct and inverse Fourier transform of a second order tensor field, are the same in both methods. The rest of operations performed in the conjugate gradient do not represent an important time contribution to the total but DBFFT also presents a small computational saving in this case. This improvement in the conjugate gradient are due to the reduction of the number of components of the solution vector in the system, $1/2$ (small strains) or $1/3$ (finite strains) the size of the methods in which the unknown variable is the strain.

The dependency of the convergence with the stiffness contrast is related to the condition number of the linear system of equations that increases with the phase contrast.

For this reason, preconditioners are fundamental to improve the convergence. This is the main reason why the DBFFT needs less iteration to reach the equilibrium than the Galerkin method that does not admit preconditioners. Moreover, this improvement has been obtained with the preconditioner proposed in this work, but other preconditioners could be found that further improve this behavior.

Regarding memory allocation needs, the Galerkin approach need to store 5 tensor fields while in DBFFT 6 vector fields and 1 tensor field are saved. It can be remarked that in the new method, two third order tensor fields defined in frequencies are used while in the rest of FFT schemes a fourth order tensor needs to be computed, and saved to avoid recomputing them. These considerations imply a reduction of memory around 30%.

3.6.3 Comparison with FE

The superior performance of the FFT approaches respect to FEM might be more limited in the case of micromechanics based fatigue simulations for many reasons, (1) the non-linear constitutive equation (cyclic crystal plasticity) is complex and very expensive to evaluate, (2) the simulations require many cycles including several path changes. The Galerkin FFT framework or the DBFFT used here might be an ideal framework to overcome these limitations thanks to absence of a reference medium, the better performance of the discrete operator and the use of a fully implicit scheme using Newton-Raphson with consistent tangent matrices that allows reducing drastically the number of load increments.

The comparison of the performance between FEM and the two FFT approaches is done using one of the cases presented in the result section, the simulation of the alloy response for three full cycles under quasi-uniaxial loading, strain amplitude of $\varepsilon_{max} = 1\%$ and $R_\varepsilon = 0$. Four different model sizes are considered 32^3 , 64^3 , 128^3 and 256^3 . The simulations were performed in a 120GB RAM 2×8 core Intel Xeon E5-2630 v3 workstation, using 4 cpus for this analysis. The FEM simulations were run using Abaqus/Standard 6.13.3 and the FFT simulation in the home-made code FFTMAD (Appendix A). In the case of FEM both the standard direct LU solver and a Krylov iterative solver are used for the linear problem. Note that this last algorithm is very similar to the linear solver used in the FFT framework so in this case both methods can be fairly compared. In the case of FFT, two different algorithms are used, the Galerkin FFT and the DBFFT. The total time needed for the simulation of each RVE size using both FEM and FFT is graphically represented in Figure 3.23.

Figure 3.23: Simulation time (in hours) for FE and FFT simulations for different RVE sizes

It can be observed that simulation times are similar for 32^3 voxels while the FFT approach is 4 times faster in the 64^3 model compared to the FEM iterative solver and around 10 times faster than FEM using a direct solver. In the case of 128^3 voxel models the comparison with FEM was only possible with the iterative solver because of the memory requirement for the direct solver and in the largest model with 256^3 elements the FEM code was not able to run the simulation with any type of solver. For the models with 128^3 voxels (with more than 2 million voxels) FFT was 6 times faster and required approximately 4 times less memory and than the FEM iterative simulations. These results show that this FFT framework is a reliable option to replace FEM for microstructure based fatigue simulation reducing the computational time and allowing to increase the size and the complexity of the RVEs to improve the accuracy in the fatigue life predictions.

As expected, the DBFFT algorithm presents a superior performance in all the RVE sizes. In the 32^3 voxels the computational time saving is of 10% whereas in the 256^3 voxels the improvement is of $\approx 15\%$ in time. This is due to the higher computational weight of the linear equilibrium resolution in the total time that, for 32^3 voxels, implies around the 20% of the time and, for the 256^3 voxels, involve around the 40% of the

time.

4 A NEW STATISTICAL APPROACH FOR MICROMECHANICS BASED FATIGUE LIFE SIMULATION

As stated in Chapter 2, size effects in fatigue are important to characterize adequately the fatigue behavior of specimens or component. Current models are developed from a macroscopic perspective and using probabilistic models, neglecting the effect of the microstructure in the fatigue performance. In this chapter, a new micromechanics based framework is proposed which aims to obtain fatigue life predictions independent of the RVE size used in the simulations and able to account for the actual size of the specimen/component studied. The chapter is arranged as follows: first a study of the FIP distribution is explained, second the methodology proposed for up-scaling the results from micromechanics to specimen sizes is presented, and finally, the validation including the application of the methodology to real microstructures is shown.

4.1 Statistical distribution of FIPs

The result of a RVE simulation is the distribution of local fields FIPs, and this is the first step towards fatigue life prediction. This local fields are computed in each point and averaged over a region of interest related to the crack initiation zone. The statistical distribution of local averaged FIPs corresponds to an exponential distribution (Fig. 4.1). This type of distributions describes the strong heterogeneity in FIP values, showing a large volume fraction of low FIP values, and a long queue corresponding to the hotspots developing high FIP. Although these points represent a small volume of the RVE, they are the ones controlling the life of that RVE. An example of the distribution of averaged FIPs over three different RVE for a cyclic test can be found in 4.1.

Figure 4.1: Histograms of local FIPs for 3 different 64^3 RVEs with the same size and the same loading condition

The tail (maximum) of this distribution is the value used to characterize the probability of failure of that particular RVE. Due to the large differences found in this FIP_{RVE} , in microstructure sensitive fatigue life models, the definition of RVEs is not enough to characterize the fatigue property and they become SVEs. Thus, an ensemble of SVEs is used and, from the FIP_{RVE} of each element (from here on so-called either RVE or SVE) in the ensemble, a CDF can be found. These FIP_{RVE} distributions (see CDF in Figure 4.2) have been widely used to obtain a life distribution (Przybyla and McDowell, 2010; Przybyla et al., 2013; Sweeney et al., 2015).

In order to have a good description of the fatigue life distribution, it is interesting to study which is the statistical distribution of the maximum FIPs FIP_{RVE} in a set of

SVEs. To this aim, a set of SVEs is generated containing 100 RVEs. This number of RVE samples in the set of SVEs was set as a compromise between having a large statistical population and the computational cost of using a large set of samples. It was found that the use of SVE sets above 50 RVE provide very similar results. For this study the band averaged plastic work FIP W_{RVE} (described in eqs. (2.42) and (2.39)) resulting from cyclic simulations has been selected and the crystal plasticity model used are the one defined in Section 3.1.2. The resulting distribution for RVEs of 64^3 voxels containing about 800 grains is shown in Figure 4.2.

Figure 4.2: Different fitting of a distributions of FIP_{RVE} for a set of 100 64^3 SVEs

In Fig. 4.2, the data defining the CDF are the maximum values within the set of SVEs, representing all the maximums of the exponential distributions of the different SVEs of the ensemble. In fatigue, Weibull and log-normal distributions have been used many times to account for a statistical description of fatigue lives. However, the values in the Figure 4.2 correspond to the tail of an exponential distribution, so it is not clear the these two distributions are able to capture properly the data. Since the final distribution comes from the maximum of sampling an original distribution, is expected that distribution to follow an extreme value distribution.

Among the different extreme value distributions, Gumbel distribution (Gumbel, 1958) is the most adequate one because the original distribution of FIPs within each SVE are themselves tail-shape type distributions (normal or exponential types). The adequacy of Gumbel to the distribution of FIP_{RVE} within a set of SVEs has been already confirmed in Przybyla and McDowell (2010), and will be further assessed here by its ability to accurately described the SVEs data.

The Gumbel CDF is given by

$$CDF(x; \mu, \beta) = \exp\{-\exp\{-(x - \mu)/\beta\}\} \quad (4.1)$$

where μ and β are the two parameters that define the distribution. The mean value of the distribution is $\bar{x} = \mu + \gamma\beta$, where $\gamma = 0.577 \dots$ is the Euler-Mascheroni constant, and its standard deviation $\sigma = \beta\pi/\sqrt{6}$. To verify the ability of the Gumbel function to represent the distributions of FIP_{RVE} , a least squares adjustment of the simulation FIP_{RVE} data set has been made, and the resulting distributions have been represented in Figure 4.2 together with the statistical raw data.

To assess which is the most suitable distribution to reproduce FIPs, in Fig. 4.2, different theoretical distributions have been compared. It can be observed that the adjustment of the Gumbel distribution to the virtual experiments is very accurate. To remark the good correlation, it should be noted that the adjustment of the other aforementioned statistical distributions results in a much greater error as shown in Przybyla and McDowell (2010), resulting in correlation coefficients R of 0.965, 0.991 and 9.999 for the Weibull, log-normal and Gumbel distributions respectively.

Size effects

On the other hand, the statistical distribution of fatigue indicator parameters in an SVE is strongly dependent on the size of the RVE used. To illustrate this dependency, an example is presented using a synthetic polycrystalline microstructure following a log-normal grain size distribution of randomly oriented equiaxed grains. This microstructure is represented using different RVE sizes in which the average discretization of each grain (number of voxels per grain) was kept constant by fixing the voxel size, Fig. 4.8. The resulting distribution obtained for sizes ranging from 15 grains (models with 16^3 voxels) to 20000 grains (256^3 voxels) is represented in Fig. 4.3.

Figure 4.3: Distributions of W_{RVE} for SVEs of different sizes and corresponding fitted Gumbel distribution

In Figure 4.3 it can be clearly observed that the distribution of FIPs shifts to the right when increasing the RVE size. This implies that the larger the size of the RVE, the higher the mean value of the fatigue indicator parameters and therefore the shorter the life predicted. The size dependence of the FIP distributions is maintained throughout all the range of sizes, and distributions do not converge when increasing the RVE size. This leads to the conclusion that defining a minimum size of RVE in fatigue is not possible and implies that the RVEs used in the simulations should have the same number of grains as the actual specimens, something that is computationally unreachable and absolutely inefficient.

4.2 Upscaling statistical approach

In this section an alternative micromechanics based fatigue life approach is presented in which the life prediction law becomes RVE size independent. As in the traditional approach, the method starts with the simulations of the cyclic response of polycrystalline RVEs. These simulations will be carried out with the FFT framework for fatigue (Chapter 3) in order to simulate set of SVEs containing a large number of RVEs to perform FIP statistics. It should be remarked that the term RVE or SVE is used here for referring to each polycrystalline volume element, independently whether the volume element is representative or not to obtain the macroscopic property under study. As a second ingredient, a statistical approach based on the weakest link is proposed to

link the FIP distributions of sets of SVEs with different RVE sizes yielding in unique relation between FIP and microstructure statistics.

The approach proposed here aims to extrapolate the FIP cumulative distribution from a given RVE size to the size of the specimen. The model is based on the weakest link theory Weibull (1939). Let the cumulative distribution function CDF of FIPs (for example W_{RVE}) for a given SVE of size V_0 be

$$CDF_0(x) = P(W > x) \text{ in } V_0, \quad (4.2)$$

which stands for the probability of finding in a RVE of size V_0 a band averaged FIP with $W > x$. If a RVE of volume $V_1 = m V_0$ with $m > 1$ is analyzed, the weakest link theory states that the probability of finding a point in the RVE with $W > x$ in V_1 is greater since it is the probability of finding that critical point for each of the m volumes V_0 contained in V_1 . In particular, the new distribution can be obtained from CDF_0 as

$$CDF_1(x) = P(W > x) \text{ for } V_1 = \prod_{i=1,m} (P(W > x) \text{ for } V_0) = CDF_0^m(x) \quad (4.3)$$

This extrapolation based on the weakest link implies that the CDF of fatigue indicators parameters of any volume can be obtained from the result of the distribution in a size V_0 . The same shifting observed when increasing the RVE size in the virtual experimental data (Fig. 4.3) is also observed when increasing the volume using this theory.

To complete the upscaling model it is necessary to answer two questions, which is the minimum value of V_0 and which is the statistical distribution that best represents the CDF_0 .

The minimum size of V_0 to obtain CDF_0 will be studied numerically in validation stages, but it is expected to be similar to the size needed to adequately represent the macroscopic plastic behavior. Moreover, the minimum V_0 should be large enough that the critical zone of the RVE candidate to cause crack initiation is not affected by its periodic counterparts.

The second question is clear looking at the results of the previous section, Gumbel distribution stands as then perfect candidate for the CDF.

Therefore, combining the weakest link theory (eq. 4.3) with the Gumbel distribution (eq.(4.1)), the upscaling equation from a volume V_0 with $CDF_0(x; \mu_0, \beta_0)$ to V_1 with $V_1 = m V_0$, reads as

$$CDF_1(x) = CDF_0^m(x; \mu_0, \beta_0) = \exp\{-\exp\{-(x - \mu_0 - \beta_0 \ln(m))/\beta_0\}\} \quad (4.4)$$

where the mean $\bar{x}_1$ and standard deviation σ_1 for V_1 are obtained from the distribution of V_0 (μ_0 and β_0 known) as

$$\bar{x}_1 = \bar{x}_0 + \beta_0 \ln(m) = \bar{x}_0 + \sigma_0 \sqrt{6}/\pi \ln(m) \quad \text{and} \quad \sigma_1 = \sigma_0 \quad (4.5)$$

This expression determines the shift of the distribution function, which results in an increase in the mean value of $\ln(m)\sigma_0\sqrt{6}/\pi$ and states that the standard deviation keeps constant from the different scales. It is interesting to note that the shift depends on the standard deviation of the original CDF. If CDF_0 is a step function ($\sigma_0 = 0$) then the extrapolated CDF does not change with the volume. This limit corresponds to the case of a uniformly loaded single crystal—in which every point has the same FIP—which distribution will not be altered by increasing the volume. On the opposite side, for the cases with a very large standard deviations, even small volume increments m , will lead to a large shift of the CDF. According to this unique relation, results obtained with different RVE sizes can be linked, and extrapolated to the specimen size if required.

As a summary, the new approach combines the use of a proper statistical characterization of the FIP distributions from a set of SVEs and the weakest link principle to account for the size effect. These two ingredients are essential to develop an accurate model in microstructure sensitive fatigue.

4.2.1 Length-dependent micromechanics based fatigue model

The incorporation of the upscaling approach to the micromechanics based framework is straightforward, including a new step before adjusting or evaluating the prediction law, the extrapolation of the FIP results to actual specimen size. The new length-dependent micromechanics based fatigue model allows to reduce the computational cost by just computing the distribution in a V_0 with similar size to the one used to predict the average behavior. Moreover, this approach is prone to be a better candidate for predicting fatigue life scatter at specimen size, and opens the opportunity of estimating the size effect that can be found between specimen and component scales (knockdown factor). Given a CP law representing the crystal behavior. The steps to define a fatigue life model using the full length-dependent approach are summarized here:

1. Synthetic generation of a set of N random RVEs of size V_0 representative of the same microstructure (grain size, shape and orientation distribution)
2. Numerical simulation of the response of each RVE of the set under the macroscopic cyclic loading corresponding to the experimental conditions simulated for a relevant number of cycles

3. A FIP_{RVE} value is determined for each RVE of the set (eqs. (2.39) and (2.42))
4. The distribution of FIP_{RVE} is adjusted to a Gumbel distribution (eq.(4.1)) obtaining the parameters μ_0, β_0
5. The Gumbel distribution for V_0 is upscaled using eq. (4.5) to the actual test specimen/component size (defined through m). The new parameters are computed $\mu_1 = \mu_0 + \beta_0 \ln(m)$ and $\beta_1 = \beta_0$
6. An empirical fatigue life law (eq.3.8) is used to predict the fatigue life distribution from the FIP probability distribution at the specimen level obtained using the up-scaled SVE results. As in the standard framework, the empirical law is adjusted using one or more fatigue experimental results. In particular, the fatigue life prediction parameters are obtained linking the mean value of the FIP distribution at the specimen level ($\bar{x}_1$) to the number of cycles to initiation N_i obtained in the corresponding experiment.

Once the empirical fatigue life law is fitted, the new approach (steps 1-6) allows to predict the statistical fatigue life distribution of a polycrystal with the same crystal behavior but any other microstructure (i.e. textured or with a different grain size distribution), loading history or specimen or component dimensions from the simulation of the cyclic response of a SVE of the microstructure.

4.3 Validation of the statistical approach

To demonstrate the validity of the upscaling approach developed, two numerical benchmarks have been proposed. Microstructure generation, FFT simulations, and FIP postprocessing have been made using FFTMAD code (Appendix A and B). Among the different FFT schemes available, the Galerkin-FFT approach combined with the discrete Fourier operator is used here. The simulations are parallelized in *threads*. It should be noted that the use of FFT as an alternative to Finite Elements is fundamental in this validation, since it implies a huge improvement in computational efficiency that allows the use of polycrystalline RVEs of sizes larger than 16 million voxels or the fast simulation of large batteries of calculations to generate the statistical data.

The description of the crystal plasticity model and material parameters can be found in Section 3.1.2. The loading history corresponds to a uniaxial strain controlled fatigue test following a triangular wave with $R_\epsilon = -1$ and a small strain amplitude. The applied strain rate was $\dot{\epsilon} = 5 \cdot 10^{-3} \text{s}^{-1}$. The plastic work FIP (eqs. (2.39) and (2.42)) distributions are extracted from the third fatigue cycle and averaged over the volume of

each grain. The CP model developed in Cruzado et al. (2017) as a *UMAT* material subroutine for Abaqus has been coupled with the spectral solver as shown in Chapter 3.

4.3.1 Validation for 2D models

The first validation benchmark consists in the simulation of simplified polycrystalline 2D microstructures that correspond to a matrix of squared grains composed of 2×2 voxels. The aim of this benchmark is to have a simplified microstructure that allows to reach RVEs of millions of grains, sizes close to the number of grains in a real specimen. The sizes of SVEs used range from 16^2 voxel (64 grains) to 2048^2 voxels, which are over a million grains (Fig 4.4). SVEs sets containing 100 SVEs have been used, except in the case of largest size where the SVE is the result of 20 models. Three SVE sizes have been selected as candidates to define the starting distribution, CDF_0 , 16^2 , 64^2 and 256^2 voxel sizes, and the CDF of these three sizes have been fitted to a Gumbel distribution.

Figure 4.4: 2D polycrystalline models. Left, 16^2 voxels , right 256^2 voxels

The cumulative distribution functions of the grain averaged FIP_{RVE} for the different RVE sizes have been represented in Fig. 4.5 together with the distributions obtained extrapolating the smaller RVEs results to the size of the RVE with 2048 voxels.

In the Figure 4.5 it can be observed that the proposed statistical model is able to predict accurately the distribution of W_{RVE} of a large volume using the upscaling method from the results of RVEs of several orders of magnitude smaller sizes. Regarding the

Figure 4.5: 2D statistics of W_{RVE} for different SVE sizes and upscaling prediction from 16^2 , 64^2 and 256^2 voxel sizes

effect of using 16^2 , 64^2 and 256^2 voxel models as initial distribution V_0 accurately, it can be seen that the extrapolation of models with 16 crystals do not capture the response obtained for the largest models, overestimating the result (Fig. 4.5). On the contrary, both 64^2 and 256^2 models provide very similar and accurate extrapolations. To quantify this, the parameters of the Gumbel μ and β of each set of SVEs has been computed together with the results obtained using the extrapolation procedure. The results are presented in Table 4.1. It can be observed that errors in β were below 8% for SVEs $> 64^3$, while in μ , the errors change from 16% to only 3% in 64^3 . This sudden drop of errors suggests the existence of a minimal V_0 to be used for the procedure proposed.

	μ_{16}	μ_{64}	μ_{128}	μ_{2048}
Original [$\times 10^6$]	2.735	4.203	5.138	7.003
Upscaled to 2048^3 [$\times 10^6$]	8.177	6.790	6.811	7.003
Error [%]	16.76	3.04	2.74	0
	β_{16}	β_{64}	β_{128}	β_{2048}
Original [$\times 10^6$]	5.608	3.733	4.024	4.053
Error [%]	38.37	7.89	0.72	0

Table 4.1: Results of the Gumbel parameter and upscaling of the FIP to 2048^3 RVE size

4.3.2 Validation for 3D models

The second benchmark is designed to ensure that triaxiality effects are correctly upscaled using the proposed methodology. It consists on simplified polycrystalline 3D microstructures which correspond to a polycrystal containing cubic grains composed of $2 \times 2 \times 2$ voxels. The orientations of each grain are assumed to be random. The sizes of RVEs used range from 16^3 voxel (512 crystals) to 256^3 voxels (Fig. 4.6), which are over two million grains. A SVE set of 100 SVEs has been used, except in the case of larger size where the SVE set is the result of 20 models. Starting distributions (CDF_0) are 16^3 , 32^3 and 64^3 sizes, and the CDF of these sizes have been fitted to a Gumbel distribution.

Figure 4.6: Models used for upscaling of 3d cubed grains model. Left, model with 16^3 voxels. Right, model with 256^3 voxels

The statistical results of the simulations for different sizes have been represented in the Figure 4.7 together with the predictions of the proposed model for the results of large volumes. Figure 4.7 shows the very good agreement between the actual distribution of W_{RVE} of large sizes and the proposed statistical model upscale results from the results of RVEs several orders of magnitude smaller. As it happened in 2D, upscaling from sizes smaller than 32^3 (not represented in the Figure) results in inaccurate predictions. These results validate the upscaling model for 3D cases that, even considering the idealized microstructure, contains the correct triaxiality that is included in real microstructures. Quantitatively, the accuracy of the method proposed is summarized in Table 4.2. As in previous 2D validation, a strong jump in error is observed

Figure 4.7: 3D statistics of W_{RVE} for different SVE sizes and upscaling prediction from 32^3 and 64^3 voxel sizes

after reaching a critical size. Here in RVEs of 16^3 voxels, errors are 6 and 24% and when the upscaling is carried out from 32^3 models, the error are reduced to 3 and 8%.

	μ_{16}	μ_{32}	μ_{64}	μ_{256}
Original [$\times 10^6$]	3.143	3.819	4.314	5.293
Upscaled to 256^3 [$\times 10^6$]	5.619	5.483	5.299	5.293
Error [%]	6.16	3.59	0.63	0
	β_{16}	β_{32}	β_{64}	β_{256}
Original [$\times 10^6$]	2.978	2.668	2.369	2.384
Error [%]	24.92	11.91	0.63	0

Table 4.2: Results of the Gumbel parameter and upscaling of the FIP to 2048^3 RVE size

4.3.3 Validation for realistic microstructures

Once the approach has been validated for idealized geometries, here the results of applying the methodology to real microstructures are presented. First, the minimum size of V_0 from which the FIP distributions will be upscaled to the specimen size will be determined for realistic microstructures.

The simulation of the polycrystal behavior is performed using cubic RVEs containing a grain size distribution corresponding to a fine grained homogeneous microstructure and randomly oriented equiaxed grains. Polycrystalline models were also generated using weighted Voronoi (Appendix B) and the grain microstructure was assumed to be periodic, in agreement with the periodic conditions result of the FFT approach. Two examples of voxelized models containing 16^3 and 256^3 voxels can be found in Fig. 4.8.

Figure 4.8: Voxelized RVEs of polycrystals generated using a weighted voronoi tessellation: Left 16^3 voxels (scale $\times 16$), Right 256^3 voxels (scale $\times 1$) (right)

The same type of cyclic simulation has been carried and extracting the FIP from the third fatigue cycle and averaged over the volume of each band within the grains are studied for real microstructures.

Figure 4.9: Left, Hysteresis curve obtained in the simulation of a RVE with 64^3 voxels for the third cycle of a uniaxial strain controlled test. Right, Distribution of the plastic work accumulated during a cycle.

The macroscopic response and microfield distribution within the RVE during several cycles are obtained. The stress strain response of these simulations are hysteresis curves that might evolve from cycle to cycle. An example of a simulation corresponding of a RVE with 64^3 voxels (with approximately 200 grains) is given in Fig. 4.9 where the FIP microfield can be appreciated. It must be noted that the number of crystals in the 64^3 models is representative of the averaged response and larger RVEs provide almost the same result.

To study the dependency of the FIP on the RVE size, RVEs of sizes 16^3 , 32^3 , 64^3 , 128^3 and 256^3 voxel were generated containing approximately 100, 800, 7000, 50000 and 400000 crystals respectively. In all the cases, the average number of voxels per grain is constant. SVEs of 100 RVEs each and 20 models for larger SVEs have been used.

The FIP selected is the plastic work W (eq. (2.39)) and, due to the realistic shape of grains, band averaging ((2.42)) is used to obtain the non-local distribution of FIPs. In order to avoid spurious results for bands that contain only a few voxels, only bands containing more than 10 voxels are considered. W_{RVE} for each RVE is taken as the maximum W_b in the RVE. The cumulative distributions of W_{RVE} and their corresponding Gumbel adjustment are shown in Figure 4.10 for all the RVE sizes studied together with the predictions obtained extrapolating the models with 32^3 , 64^3 and 128^3 voxels to the largest value of 256^3 .

Figure 4.10: Real microstructure statistics of W_{RVE} for different SVE sizes and upscaling prediction from 32^3 and 64^3 voxel sizes

In the Figure 4.10 it can be seen how the statistical approximation works accurately also in 3D models with realistic microstructures at least for the sizes able to be explored (note that 256^3 models already contain 16 millions of voxels but the 400000 grains of these models may still be well below the number of crystals in a real specimen or component). It can be deduced that for this type of microstructure, the minimum V_0 is in the order of 700 grains or RVE sizes between 32^3 and 64^3 , where the error in terms of statistical parameters is below 8.5%. Upscaling predictions from smaller sizes, as 16^3 that corresponds to 100 grains, are inaccurate similar to what happens in the validation cases. Numerical results of the Gumbel distribution parameters together with the calculation of the relative error of the upscaling is shown in Table 4.3.

	μ_{16}	μ_{32}	μ_{64}	μ_{128}	μ_{256}
Original [$\times 10^6$]	1.608	3.259	4.455	5.518	6.585
Upscaled to 256^3 [$\times 10^6$]	7.064	6.438	6.775	6.555	6.585
Error [%]	7.27	2.23	2.89	0.456	0
	β_{16}	β_{32}	β_{64}	β_{128}	β_{256}
Original [$\times 10^6$]	6.561	5.095	5.578	4.987	5.146
Error [%]	27.5	0.99	8.39	3.09	0

Table 4.3: Results of the Gumbel parameter and upscaling of the FIP to 256^3 RVE size

5 SIMULATION OF FATIGUE LIFE OF IN718

The final application of the framework presented in previous chapters is the estimation of fatigue life of polycrystalline alloys. In this chapter the results of the micromechanics based fatigue model are shown for the Ni-base alloy IN718. First, the experimental fatigue tests considered are presented in Section 5.1. In Section 5.2, the classic FFT fatigue framework is used for estimating fatigue life using a cyclic behavior CP model (Section 3.1.2) in the LCF regime. An extension of the CP model is presented considering in this model the influence of the grain size in the mechanical behavior of every single grain by introducing a Hall-Petch type relation into the constitutive equations. Finally (in Section 5.3), the fatigue life distribution of the specimen or component is obtained from the extrapolated FIP distribution using the new proposed statistical method (Chapter 4). This model will also allow to predict the knockdown factor of the fatigue performance from a specimen to an industrial component.

5.1 Microstructures and experimental tests

Two different microstructures of wrought IN718 were investigated in the present study. The average mean grain size was obtained by the measuring the grain areas over a section and according to the methodology described in Section 3.1.1. The first microstructure analyzed corresponds to a fine grain of 8.5 in the ASTM scale, while the second microstructure corresponds to a coarse grain of 3 in the ASTM scale. A SEM image of both fine and coarse grain size microstructures are shown in Fig.5.1. The 3D grain radii distribution measured was approximated by a log-normal function according to the procedure described in Section 3.1.1, obtaining as result grain size distributions of $\sigma = 0.475$ and $\mu = 3.5691$ for the ASTM 3 and $\sigma = 0.544$ and $\mu = 2.031$ for the ASTM 8.5 mean grain sizes.

Figure 5.1: (a) Microstructure of IN718 with ASTM 8.5. (b) Microstructure of IN718 with ASTM 3.

LCF uniaxial tests were conducted at 400°C for the two microstructures according to the standard ASTM E606-04. The axial displacement in the central zone of the specimen was measured using an extensometer directly mounted on the gauge length. A wave form trapezoidal amplitude was applied following $1\text{s}(\text{dwell}) - 5 \cdot 10^{-3}\text{s}^{-1}$ (ramp up) - $1\text{s}(\text{dwell}) - 5 \cdot 10^{-3}\text{s}^{-1}$ (ramp down). The tests were carried with strain amplitudes of $\Delta\varepsilon/\Delta\varepsilon_{\min} = 1, 1.5, 2, 2.5, 3$ and 3.5 in a fully reversed tests $R_{\varepsilon} = -1$ and $\Delta\varepsilon/\Delta\varepsilon_{\min} = 2, 2.5, 3, 3.5, 4.5$ and 5.5 in a mean stress fatigue tests $R_{\varepsilon} = 0$. The experimental fatigue results of this section were provided by ITP Aero and are shown normalized for confidentiality reasons.

Figure 5.2: Experimental LCF hysteresis loops of microstructures ASTM 8.5 and $R_\varepsilon = 0$ (left) and ASTM 3 $R_\varepsilon = -1$ (right).

In Figure 5.2, stress-strain hysteresis loops of fatigue cycles are shown. It can be observed two main effects: the kinematic hardening, and the cyclic softening. The kinematic hardening is observed in the asymmetric yield point of the tensile and compression ramps. The cyclic softening is determined by the reduction of the stress range from the initial loop to the mid-life cycle.

Figure 5.3: Experimental fatigue tests for the microstructures ASTM 8.5 and ASTM 3 in LCF regime and $R_\varepsilon = -1$ (left) and $R_\varepsilon = 0$ (right).

The experimental results of the low cycle fatigue tests for both microstructures are shown in Fig.5.3. Crack initiation is not easy to be detected so, for practical reasons, the number of cycles for crack initiation is take as the cycle in which the maximum load during cyclic loading dropped by 5%. Hysteresis loops of these tests are used for calibrating the CP model parameters related to the cyclic behavior such as kinematic hardening and cyclic softening. Test fatigue lives are used to fit the parameters of the prediction power law (eq. (3.8)) using typically two different strain amplitude tests.

5.2 Fatigue life prediction using classical approach

In this section, fatigue life predictions are carried out using the standard micromechanics based fatigue framework adapted for FFT presented and validated in Chapter 3. The model is used using two different CP models, being the first one grain size independent and the second includes a grain size effect into the constitutive equation yielding into a grain size dependent model.

5.2.1 Grain size independent fatigue model

Cyclic behavior CP model and parameter identification

The cyclic elasto-visco-plastic behavior of the single crystal is dictated by the constitutive equations of the CP model presented in section 3.1.2. The set of CP parameters for monotonic plasticity are taken from Cruzado et al. (2015), where the monotonic stress-strain curve is adapted to the micropillar experiments results for different orientations. In this work, EBSD measures are taken and then single crystal micropillars were machined out by focused ion beam milling and tested in a nanoindenter. However, cyclic tests at nano/microscale are difficult to be carried out and thus only some experimental parameters m , q_{ij} , and $\dot{\gamma}_0$ can be obtained from this type of experiments.

On the other hand, isotropic hardening parameters, τ_0 , τ_s , h_0 , back stress evolution parameters, c , d , k and cyclic softening parameters, τ_s^{cyc} , h^{cyc} are obtained using an inverse fitting strategy presented by Herrera-Solaz et al. (2014). This approach is based on Levenberg-Marquardt iterative algorithm that aims to minimize the differences (in terms of an error measure) between the stress-strain of cyclic or monotonic curves from experiments and the macroscopic behavior obtained by means of computational homogenization of polycrystals.

In the algorithm, the objective function O to minimize is the difference between the experimental hysteresis curves $y_i^{N_x}$ at some different cycles and the value provided by

the simulation using homogenization for the same particular loading conditions.

$$O(\beta) = \sum_{i=1}^{N_1} (y_i^{N_1} - f(x_i, \beta))^2 + \sum_{i=1}^{N_2} (y_i^{N_2} - f^{N_2}(x_i, \beta))^2 + \dots \quad (5.1)$$

where β are the set of parameters to be optimized, N_x are the different loading condition and cycles number hysteresis loops and f^{N_2} are the values of the corresponding simulation. For a given iteration, the variability of the simulation curve respect the variation of the parameters is considered linear as

$$f(x_i, \beta + \delta\beta) = f(x_i, \beta) + \frac{\partial f(x_i, \beta)}{\partial \beta} \cdot \delta\beta = f(x_i, \beta) + \mathbf{J}\delta\beta \quad (5.2)$$

To compute $\mathbf{J} = \frac{\partial f(x_i, \beta)}{\partial \beta}$ some perturbations of the β parameters are tested to evaluate the sensibility of each parameter, requiring to run one simulation for each parameter perturbation and forming this way the Jacobian matrix. The the error function in vector notation yields as

$$O(\beta + \delta\beta) = \|\mathbf{y} - f(\mathbf{x}, \beta) - \mathbf{J} \cdot \delta\beta\|^2 \quad (5.3)$$

Taking the derivative of this objective function with respect to $\delta\beta$ and setting the result to zero gives the final system of equations. Finally, a damped version of the Jacobian is tested using different viscosity coefficient λ and the minimum error solution is chosen. The final linear system of equations reads as

$$(\mathbf{J}^T \mathbf{J} + \lambda \mathbf{I}) \cdot \delta\beta = \mathbf{J}^T \cdot (\mathbf{y} - f(\mathbf{x}, \beta)) \quad (5.4)$$

where $\delta\beta$ an, after solving, the solution is updated as $\beta = \beta + \delta\beta$. This process is repeated until the error reaches the tolerance imposed.

The result is a set of calibrated CP parameters that reproduce accurately the mechanical macroscopic behavior. In this CP model, the parameters are calibrated for the cyclic deformation of IN718 at 400°C as shown in (Cruzado et al., 2017). An illustration of the results of the algorithm for several iterations is shown in Figure 5.4.

Figure 5.4: Fitting data by Levenberg-Marquardt algorithm with two loading conditions.

The resulting set of parameters able to provide very accurate predictions of the experimental fatigue hysteresis loops under a broad range of loading conditions (Cruzado et al., 2017). The set of crystal parameters are shown in Table 5.1 for completeness, normalized by the initial critical resolved shear stress τ_0 , which actual value is omitted here for confidentiality reasons.

Table 5.1: Crystal plasticity parameters for a wrought IN718 at 400°C.

Elastic	C ₁₁ (GPa)	C ₁₂ (GPa)	C ₄₄ (GPa)	
	240	165	101	
Viscoplastic	m	$\dot{\gamma}_0(s^{-1})$		
	0.017	2.42 10 ⁻³		
Isotropic hardening	τ_0 (MPa)	τ_s	h_0	$q_{\alpha\beta}$
	τ_0	0.71 τ_0	-57.13 τ_0	1
Kinematic hardening	c	d	k	
	58.9 τ_0	198.3	17.7	
Cyclic softening	$\tau_{\Delta s}$	h_1	h_2	
	0.076 τ_0	0.07 τ_0	2.33 10 ⁻⁶ τ_0	

These parameters were obtained using FEM homogenization, and its validity using FFT has been checked. The FFT result of two typical hysteresis loops (third cycle) is represented in Figure 5.5. It can be observed how the model is able to accurately capture the cyclic mechanical response.

Figure 5.5: Comparison of simulation and experimental loops of ASTM 8.5 and $R_\varepsilon = -1$ (left) and $R_\varepsilon = 0$ (right).

Results using grain size independent model

The results of the 64^3 voxel models containing around 1000 grains have been used to predict the fatigue life in a Ni-base superalloy IN718, following the steps of the classical micromechanics based fatigue model defined in section 4.2.1. The CP is described in Section 3.1.2 and parameters are given in Table 5.1. The RVEs are synthetically generated using the generator tool of Appendix B and following the fine grain size described in Section 5.1. The loading cases studied correspond to the fatigue test for the ASTM 8.5, $R_\varepsilon = 0$ and $R_\varepsilon = -1$, and strain amplitudes ranging from a small strain ε_{min} (near to HCF) to a large strain of $3.5\varepsilon_{min}$. The FIP used here is the band averaged plastic work, and the maximum value in each RVE is used in the prediction law.

The parameters of the power type prediction law (eq. (3.8)) are obtained from the experimental results corresponding to applied cyclic strain ranges of $\Delta\varepsilon/\Delta\varepsilon_{min} = 1$ and 3.5 and a strain ratio $R_\varepsilon = -1$. It should be noted, that the mean value of the FIPs in the third cycle of several realizations were used to obtain the parameters of the power type prediction law (eq. (3.8)) and the resulting values were $W_{crit} = 1.708 \cdot 10^7 MJ/m^3$ and $m = 1.289$. However, as it was shown on the previous chapter,

since the size of the RVE is always much smaller than the number of grains in the actual tests, the values of the FIP obtained may vary for different RVE sizes and will be much smaller than their value in a RVE of size equivalent to the specimen. Thus, the parameters of the law are only valid for 64^3 voxel size.

The ability of the proposed power type prediction law applied to of IN718 alloy at 400 is shown in Figure 5.6, in which the experimental and the model results for different cyclic strain ranges are plotted for tests carried out with $R_\varepsilon = -1$ and $R_\varepsilon = 0$. Four different numerical results are plotted in Figure 5.6 for each experimental point. The agreement between experiments and simulations was excellent in all cases and the simulation strategy was also able to capture the life reduction induced by $R=0$, as compared with the tests carried out with $R = -1$.

Figure 5.6: Experimental results and model predictions for the fatigue life of IN718 for $R_\varepsilon = -1$ (left) and $R_\varepsilon = 0$ (right). Prediction law parameters calibrated from $\Delta\varepsilon/\Delta\varepsilon_{min} = 1.0, 3.5$ at 400°C .

The model is able to predict accurately the fatigue life under small and large cyclic strain ranges. This is due to the fact that, even though there is almost no plastic deformation in the mechanical response of lower strain amplitudes, the plastic deformation is localized in the most critical regions of the microstructure, being the maximum value the one used for prediction. As a result, the scatter of the predicted fatigue life is larger for this loading conditions. For strain amplitudes lower than the ones studied here and where the fatigue life enters in the HCF regime, other microstructural details such as twin boundaries (Yeratapally et al., 2016), precipitates (Sweeney et al., 2014) and free surfaces (Wan et al., 2016; Przybyla and McDowell, 2012) may play an important role.

These microstructural defects act as stress concentrators, leading to localized plastic microfields in the vicinity of the defects that will be probable sites for the nucleation of persistent slip bands and small cracks. The consideration of these defects will not change very much the present results, but they should definitively be accounted for when predicting the life at lower strain amplitudes.

5.2.2 Grain size dependent fatigue model

Cyclic behavior CP model

The elasto-plastic behavior of IN718 grains is described as an extension of the CP phenomenological model described in Section 3.1.2). The new model is able to reproduce accurately the main cyclic characteristics of IN718, such as kinematic hardening, mean stress relaxation and cyclic softening as well as the grain size effect. The approach used here consists in including the grain size as a parameter in the CP model, and link some of the parameters with this size using a Hall-Petch type relation.

The modification proposed affects to the isotropic hardening initial shear stress value of τ_0 of the evolution of the term $g_{k\ m}$ (eq. (2.30)) that now is described according to the Hall-petch relation as:

$$\tau_0 = \tau'_0 + \frac{k_0}{\sqrt{d}} \quad (5.5)$$

where, τ'_0 corresponds to the initial CRSS of infinitely large grain and k_0 is the Hall-Petch constant and d is the diameter of the corresponding grain size. On the other hand it has been assumed that the effect of the grain size in the flow stress derived from the isotropic and cyclic softening is negligible as these mechanisms depends on the amount of γ'' which is approximately the same in both microstructures.

The dislocation pile-ups at grain boundaries however play an important role in the generation different flow stress behavior for the different grain size. As a result, the Bauschinger effect will be affected by the grain size, as the back stresses produced by dislocation pile-ups will assist motion in the reversal direction. It implies that the grain size effect will affect mainly the kinematic hardening behavior. The kinematic hardening χ^α presented in this material is based on a modified version of the Ohno and Wang model, for which the evolution is given by:

$$\dot{\chi}^\alpha = c\dot{\gamma}^\alpha - d\chi^\alpha|\dot{\gamma}^\alpha| \left(\frac{|\chi^\alpha|}{c/d} \right)^{mk} \quad (5.6)$$

where mk is the parameter that controls the mean stress relaxation velocity and the Hall-Petch type relation has been introduced in the direct hardening modulus c and in

the saturation hardening value, (represented by the ration c/d) according to:

$$c = c' + \frac{k_c}{\sqrt{D}} \quad (5.7)$$

$$\frac{c}{d} = \left(\frac{c}{d}\right)' + \frac{k_{c/d}}{\sqrt{D}} \quad (5.8)$$

where the constants c' and $(c/d)'$ corresponding to the first term of the equation can be described as the direct hardening modulus and saturation value of stress corresponding to a grain with an infinitely large size, respectively. The second parameter of the equation corresponds to the previously explained Hall-Petch hardening effect, where k_c and $k_{c/d}$ are Hall-Petch constants and D is the diameter of the corresponding grain size.

The parameters of the model to simulate the cyclic deformation of IN718 at 400°C are presented in Table. 5.2. The elastic constants are the same as in the grain size independent model. The remaining parameters of the crystal plasticity model and the ones affected by the grain size effect are obtained by trial and error from the experimental results of the cyclic response of IN718 at 400°C under $R_\epsilon = -1$ and the two micro structures. Note that the parameters are normalized by τ'_0 for the shake of confidentiality. The resulting list of parameters for the model are given in Table 5.2.

Elastic	$C_{11}(\text{GPa})$ 240	$C_{12}(\text{GPa})$ 165	$C_{44}(\text{GPa})$ 101		
Viscoplastic	m 0.017	$\dot{\gamma}_0$ $2.42 \cdot 10^{-3}$			
Isotropic softening	$\tau'_0 (\text{MPa})$ τ'_0	τ_s $0.83\tau'_0$	h_0 $57.29\tau'_0$	$q_{\alpha\beta}$ 1	k_0 $8.14 \cdot 10^{-4} \tau'_0$
Kinematic hardening	c' $33.8\tau'_0$	$(c/d)'$ $0.084\tau'_0$	mk 20.49	k_c $1.02 \cdot 10^{-3} \tau'_0$	$k_{c/d}$ $0.145 \tau'_0$
Cyclic softening	τ_s^{cyc} $0.083\tau_0$	h_1 $0.072\tau_0$	h_2 $3.44 \cdot 10^{-6} \tau_0$		

Table 5.2: Mean grain size effect CP model constants for a wrought IN718 at 400°C.

As a result of this calibration, an example of the mechanical response using FFT homogenization of fatigue hysteresis loops of the model is represented together with the experimental loops in the third cycle for the microstructure ASTM 3 and ASTM 8.5 in Figure 5.7. It can be observed that the model shows a good accuracy to reproduce the differences between the behavior of the two microstructures under study but, since a unique model is used for both microstructures, the error between curves is higher than in the grain size independent model.

Figure 5.7: Comparison of simulation and experimental loops of ASTM 8.5 (left) and ASTM 3 (right) $R_\epsilon = -1$.

Results using grain size dependent model

Again, 64^3 voxel RVEs models containing around 1000 grains have been used to predict fatigue life in a Ni-base superalloy IN718, but now generated following two different microstructures. The polycrystal grain sizes follows the fine (ASTM 8.5) and coarse (ASTM 3) grain distributions described in Section 5.1. Cyclic plastic work averaged over bands is used to predict fatigue lives using the power type prediction law (3.8). The cycle from which the FIP is extracted is the third cycle and the parameter of the prediction law were fitted from the mean FIP value of the strain amplitudes of $\Delta\epsilon/\Delta\epsilon_{min} = 1$ and 3.5 and the strain ratio $R_\epsilon = -1$. The parameters of the fatigue life model were $W_{crit} = 1.456 \cdot 10^5 \text{ MJ/m}^3$ and $m = 1.192$.

The predictions of the number of cycles for fatigue crack initiation at 400°C are shown in Fig. 5.8 for both microstructures together with the corresponding experimental results. The agreement between experiments and simulations was excellent in

most cases for both grain sizes. The largest differences in number of cycles are found in the intermediate strain ranges for the coarse grain size where Ni was slightly under-predicted. Moreover, the numerical simulations captured the differences in the fatigue behavior of IN718 alloy when subjected to large and small cyclic strain ranges. At large cyclic strain ranges, plastic deformation is homogeneously distributed throughout the microstructure and the influence of the details of the microstructure (including the average grain size) on the fatigue life is minimum. However, when plasticity is localized in a few grains at low cyclic strain ranges, the effect of the microstructure is noticeable due to the lowest plastic localization in fine grain microstructures.

Figure 5.8: Experimental results and model predictions for the fatigue life of IN718 for $R_\varepsilon = -1$ ASTM 8.5 (left) and ASTM 3 (right). Prediction law parameters calibrated from $R_\varepsilon = -1$, $\Delta\varepsilon/\Delta\varepsilon_{min} = 1.0, 3.5$ at 400°C with ASTM 8.5.

Moreover, it was found that the influence of the microstructure is very large in the case of localized deformation, because the fatigue life is controlled by a continuous accumulation of plastic slip in a few grains. Both factors show the beneficial effect of the small grain size from the fatigue crack initiation viewpoint and explain the longest fatigue life of the alloy with small grain size in this regime.

It should be remarked that, despite the good results shown here, this model is only valid for RVE of 64^3 voxels due to the effect of the RVE size in the FIP value. The number of grains contained in the RVE also affect the life prediction due to the definition of the band averaging of one voxel thickness with a geometrical thickness length that depends on the number of voxel per grain that are introduced into the RVE. The smaller the thickness of the band, the larger the value of the maximum FIP.

5.3 Fatigue life prediction of length-dependent micromechanics fatigue framework

5.3.1 Results using grain size independent model

The results of the 32^3 voxel models have been used to predict fatigue life using the grain size independent CP model (Section 5.2.2), following the steps of the length-dependent micromechanics based fatigue framework defined in Section 4.2.1. The CP parameters are given in Table 5.1. The microstructure corresponds to the fine grained polycrystal and the grain size distribution is represented by a log-normal distribution and generated using a weighted Voronoi tessellation. Tests used here corresponds to the LCF tests defined in the same section for $R_\epsilon = 0$ and $R_\epsilon = -1$ and strain amplitudes ranging from a small strain ϵ_{min} (near to HCF) to a large strain of $3.5\epsilon_{min}$.

Due to the very large number of loading cases studied, in this case the SVEs will contain 50 RVEs and the approximate number of grains of each model will be slightly smaller than the one considered in the previous sections of this chapter. The 50 RVEs were simulated for each loading case considered for the study and, from each RVE, W_{RVE} was obtained as the maximum value of W_i averaged in bands with a minimum threshold of 10 voxels per band. Then, the resulting CDF were extrapolated to the actual specimen size, containing several millions of grains.

The power law of eq. (3.8) is used here and the two fitting parameters, W_{crit} and c should be adjusted with experiments, using as data the average of the upscaled FIP of SVEs and the experimental life (number of cycles N) of at least two different testing conditions. Two different choices of fitting data are explored here, two or three fatigue experiments. The first case considers three strain amplitudes to calibrate the life prediction law, $R_\epsilon = -1$ and $\Delta\epsilon/\Delta\epsilon_{min} = 1.5, 2.5, 3.5$, and the second case uses two strain amplitudes, $R_\epsilon = -1$ and $\Delta\epsilon/\Delta\epsilon_{min} = 1.5, 3.5$. The selection of the strain ranges is made to capture the maximum range of strain amplitudes. The case with $\Delta\epsilon_{min}$ is excluded from the fitting sets since at this strain amplitude it is known that there is a large experimental scatter but we only have one experimental point and this might lead to a large error in the adjustment of the law.

Once the fatigue life prediction law has been fitted, simulations are performed with each RVE of the set for all loading conditions not considered in the fatigue life adjustment. The distribution of W_{RVE} of the SVE is extrapolated to the specimen size and the life prediction equation adjusted (eq. (3.8)) is now applied to transform the probability distribution of FIPs in to the probability distribution of fatigue life of each experiment. Fatigue life CDFs can be obtained from the FIP W_{RVE} distributions (μ and β Gumbel

parameters), assuming that $X = CDF(W_{RVE})$ and corresponds to the Gumbel distribution, reads as

$$X = e^{-e^{-\frac{W_{RVE}-\mu}{\beta}}} \quad (5.9)$$

Therefore, the expression of the a generic W_{RVE} is given by

$$W_{RVE} = \mu - \beta \ln(-\ln X) \quad (5.10)$$

Then, using the power type prediction law (eq. (3.8)), the CDF can be expressed as a function of the calculated fatigue life following

$$N = \frac{(\mu - \beta \ln(-\ln X))^c}{W_{crit}} \quad (5.11)$$

After some mathematical developments, the expression of the CDF as a function of the number of cycles yields as

$$X = CDF(N) = e^{-e^{-\frac{-(N \cdot W_{crit})^{1/c} + \mu}{\beta}}} \quad (5.12)$$

where W_{crit} and c are material constants, and μ and β are the adjusted parameters for a particular microstructure and fatigue test condition.

The results of the CDF of fatigue lives are represented in Figs. 5.9 and 5.10 in which the experimental data is represented with points and the probability distributions of fatigue life are depicted directly such that standard deviation can be observed. Note that, in Fig. 5.9 and 5.10 the results for the seven loading cases with $R_\epsilon = 0$ are pure predictions as well as the four and three cases respectively of $R_\epsilon = -1$ not used for calibrating the fatigue life.

Figure 5.9: Fatigue life prediction distribution for $R_\epsilon = -1$ (left) and $R_\epsilon = 0$ (right), including 99.5% scatter limits (vertical lines). Prediction law parameters calibrated from $\Delta\epsilon/\Delta\epsilon_{min} = 1.5, 3.5$

Figure 5.10: Fatigue life prediction distribution for $R_\epsilon = -1$ (left) and $R_\epsilon = 0$ (right), including 99.5% scatter limits (vertical lines). Prediction law parameters calibrated from $\Delta\epsilon/\Delta\epsilon_{min} = 1.5, 2.5, 3.5$

The results of Fig.5.9 and Fig. 5.10 show that the result of most of the fatigue experiments lie in between the limits of 99.5% of the scatter predicted by the upscaled simulation results. Furthermore, the results show good agreement for both strain ratio

predictions $R_\varepsilon = -1$ and $R_\varepsilon = 0$. This demonstrates the potential capability of length-dependent micromechanics based simulations to predict fatigue life for a wide range of loading conditions. It can also be observed in Figs. 5.9 and 5.10 that the use of two experimental cases is in principle enough to provide an accurate prediction expression. Ideally, the average result of different experiments for the same strain amplitude should be used, being this especially important for very small strain amplitudes where the experimental scatter is very high and a single experiment might lead to unrealistic values of the fatigue life parameters.

Although experimental values of the scatter are not available for every case, in general the model predictions of the scatter slightly underestimate the typical experimental values. This result is a consequence of the lack of defects in the microstructures considered, being the differences in life obtained from one RVE to other only due to the different grain arrangement. On the contrary, in the real specimens, defects are usually present which introduce an additional source of stochasticity.

5.3.2 Knock down factor estimation

Finally, the expression of the CDF of fatigue life as a function of the volume ratio upscaled can be obtained combining eq. (5.12) and the application of the weakest link principle to the parameters of the Gumbel (eq. (4.5)). The final expression yields as

$$CDF(N) = e^{-e^{-\frac{-(N \cdot W_{crit})^{1/c} + \mu + \beta \ln(m)}{\beta}}} \quad (5.13)$$

where W_{crit} and c are material constants, m is the volume ratio, and μ and β are the adjusted parameters for a particular microstructure and fatigue test condition.

In order to show the potential of the technique developed, the life distributions obtained with the fatigue life prediction model for three different volumes are computed and represented in Fig. 5.11. For this example, the loading case of $R_\varepsilon = 0$ and $\varepsilon = 3\varepsilon_{min}$ and the law calibrated with three experiments (Fig. 5.10) are chosen. The strain amplitude corresponds to a case not used for the model calibration and in which the model results are a pure prediction. The volumes selected correspond to a virtual specimen with the volume of the RVE used (orders of magnitude smaller than a real specimen), the typical size of a specimen, and the size of a component several times larger than the specimen.

Figure 5.11: Estimation of the specimen size effect in the of fatigue life distribution for $R_\epsilon = 0$ and $\epsilon = 3\epsilon_{min}$ using as specimen sizes the RVE size, the actual size of a typical fatigue specimen and the size of a component

As it can be observed, the change in the fatigue life predicted for a specimen of the RVE size to the actual sample size is huge. The shift from the specimen to the component was smaller in this case, but implied a reduction of the expected fatigue life of around 40%, from $4 \cdot 10^3$ to $2.5 \cdot 10^3$. These values are in the order of knock down factors used in the industry for the design process. This final example shows the ability of the model to estimate the reduction in the fatigue performance from the value measured in an experiment to the one obtained in a larger component.

6 CONCLUSIONS AND FUTURE WORK

6.1 Conclusions

This work focuses on the development of a fatigue life simulation framework for metallic alloys as function of their microstructure and based on FFT homogenization. One key aspect of this work is the adaptation and further development of FFT approaches for fatigue simulations that allows to simulate efficiently large models to generate the necessary statistics. The other key contribution is the development of a volume dependent micromechanics based fatigue approach to account for the effect of microstructure and specimen size in the fatigue life nucleation, Finally, the framework is applied to predict the fatigue response of the Nickel-base superalloy IN718 for different grain sizes.

Respect the development of a FFT based homogenization framework especially suited for micromechanics based fatigue (chapter 3), first the Galerkin FFT approach is enhanced by the use of discrete projection operators and a novel approach to efficiently apply macroscopic mixed stress/strain loading histories.

- It is shown that the resulting approach is able to reproduce with high fidelity the macroscopic cyclic response and microscopic fields obtained with Finite Elements.
- The modified discrete projection operator provides a smoother microfield distribution, and microscopic results are in better agreement with Finite Elements
- The macroscopic mixed control developed is able to obtain directly the microfield distribution compatible with the combination of macroscopic stress and strain components. Moreover, since no additional iterations are needed, the cost of these simulations is identical to simulations performed under strain control
- The FFT approach results is more than one order of magnitude faster than FE under similar conditions, identical RVE (with linear cubic elements instead of voxels in FE), same CP model and parameters and iterative linear solver.

Additionally, a new FFT homogenization approach based on displacement is developed, the DBFFT, also working for non-linear materials and small and finite strains.

- The method, is validated, and reproduces the same results (within numerical precision) than other FFT schemes.
- The main advantages of the DBFFT is the improvement of the convergence rate (time reduction respect Galerkin approach in linear problems reaching 40% and in polycrystals around 15%)
- The method allows the direct use of standard preconditioners to solve the linear problem, due to the full-rank of the linear operator used in the Fourier space.

The second contribution (chapter 5) is the development of a statistical framework, based on the weakest link approach and extreme value distributions, to estimate fatigue life, accounting for the polycrystalline microstructure and the actual size of the specimen or component under study.

- The framework proposed eliminates the pathological RVE size dependency of life predictions
- The full fatigue life probability distribution is predicted, not only mean values.
- The new framework introduces in the microstructure sensitive fatigue life prediction a fundamental variable, the specimen or component size in which the fatigue behavior is going to be studied.

- The model allows the numerical estimation of the knockdown factor, that is the reduction that has to be applied during design to scale the fatigue performance in a specimen to a full component.

Finally, all this methodology has been used to predict the fatigue life of IN718 alloy for a wide range of cyclic loading conditions and two grain size distributions. The effect of grain size was introduced by modifying the CP parameters of each grain

- The model was able to accurately predict the fatigue life of IN718 alloy showing that the different behavior at small and large cyclic strain ranges was triggered by the localization of the deformation in the former condition against a generalized plastic deformation in the second case
- The model was able to reproduce the experimental trends in the scatter of fatigue life: a large scatter was found at small cyclic strain ranges while a more homogeneous response was found for large applied strains
- In agreement with the experiments, the model did not show any grain size effect on the fatigue life for large applied strain ranges but the predicted fatigue life was considerably longer in the case of alloy with fine grain size for small cyclic strain ranges.

6.2 Future work

Although a great effort has been made to improve the current micromechanics based fatigue approaches, a long way still remains in order to have predictive models for every loading condition and any type of microstructure.

- FFT solvers still present some limitations, one is including voids in the RVEs that kills the convergence rate, reducing the potential benefit of using FFT instead FE. The Augmented Lagrangian scheme was proposed to deal with this problem, but still presents a poor convergence rate. Some other interesting approaches can be found but we believe there is still much space for improvement (Brisard and Dormieux, 2010).
- Finding good preconditioners is fundamental for achieving fast convergence in the case of methods based on linear solvers.

- Micromechanics models rely on the evaluation of some Fatigue Indicator Parameter at the microscale. There are nowadays many different FIPs proposed depending on the alloy, loading case or even research group involved. A more objective and physically motivated classification of FIPs is needed and, very probably, new FIPs should be developed based on complex 3D experiments, as in-situ 3D tomography testing (Rovinelli et al., 2018).
- Considering heterogeneous microstructures at two scales, such as neckless microstructures or the presence of a small amount of very large grains embedded in a fine-grained matrix, is still complicated. The main difficulty is constructing RVEs considering the two grain populations and in this case, we consider that the most clever approach is the use of more complex statistical models.
- Current approach works well if some plasticity localizes at the microstructure. On the contrary, for very small strain or stress ranges well below the macroscopic yield, no plasticity occurs at the microscale and the model tends to overpredict fatigue life. In this case, the regime is HCF to UHCF. A possible approach is including other microstructural features, such as carbides, microcracks or twin boundaries, acting as stress concentrators.

A FFTMAD: A FFT HOMOGENIZATION CODE

In this work, a home-made FFT computational homogenization code, FFTMAD, is developed using python. The code includes the different resolution schemes based on the original approach by Moulinec and Suquet (1994) for linear problems. Non-linear problems for both small and finite strains are also implemented in the code using the Galerkin approach (Vondřejc et al., 2014). This approach allows the use of standard implementation of constitutive equations including tangents and solving non-linear problems using Newton algorithms with quadratic convergence. Material constitutive equations can be directly programmed as functions, but the code also allows the direct use of Abaqus material subroutines (umat), allowing to re-use all the models previously developed for the popular FEM code. The code includes some functions to generate or read RVEs and some postprocessing functions, including the generation of files for Paraview (Ahrens et al., 2005) including displacement, stress, strain and internal variable fields. All the features used in this thesis have been implemented inside the Python script FFTMAD. Here the structure of the code is outlined and input and output files are described together with an example input file in this appendix. Finally, the description of the classes and implemented materials are explained.

Python is an expansive library of open source data analysis tools, web frameworks,

and testing instruments make its ecosystem one of the largest out of any programming community. Moreover, it is an accessible language for new programmers because the community provides many introductory resources. The language is also widely taught in universities and used for working with beginner-friendly devices such as the Raspberry Pi. We selected this programming language because of its ability to perform different simulations using the same project, but defining the input file as a Python script. Therefore, a very simple script allows to perform for standard simulations or for complex operations: for including loops modifying the RVE "on the fly", perform series of simulations...

On the other hand, Python codes have a lower performance than other compiled languages like FORTRAN or C. To overcome this drawback, the Python code use fast compiled libraries for the more time consuming operations like product contractions or Fourier transform.

A.1 Code structure

The homogenization code is designed in four function packages: input generation module, solvers module, operators module and postprocessing module; and two programming classes: simulation class and material class.

Figure A.1: Description of the code

A.1.1 Function packages

Input package

The input generation modules is a package of functions the generates a RVE Ω of the desired dimensions $\Omega = [L_1, L_2, L_3]$ and with the desired discretization $N = [N_x, N_y, N_z]$. In addition, some functions for creating a phase field map inside the RVE have been introduced, like generating one sphere/cubes centered wherever, generating a random distribution of spheres/cubes with a desired volume fraction, generate a RVE with bands, etc. Other option is to read an input file with format: The output of this module is the length of the RVE, the number of the discretized nodes and the phase field map.

Solver package

This package contains all the resolution schemes explained in previous chapter (basic, accelerated, Galerkin, DBFFT...) and the scripts containing the iterative algorithms can solve the linear or non-linear problem.

Operators package

This package contains all the generator for all the operators needed for the different scheme and all the functions used in tensor fields products and differentiation. It also includes some initialization statements for the different solver schemes.

Output package

The main outputs of the analysis are the local strain and stress fields. Also internal state variables for each points is given. This fields will be written in an .vtk file in order to have a view in Paraview (Ahrens et al., 2005) of the stress and strain fields and other interesting values as Von Mises stress, material phase or displacement fields. Moreover the code has the option to plot 2D views of the RVE fields.

A.1.2 Classes

The code uses two classes: simulation class and material class. These classes are described in following paragraphs:

Simulation class

Simulation class contains all the global variables of the resolution procedure. It contains strain and stress field, and the solver schemes for equilibrium equations. These variables are changing during the solution procedure. It also contains auxiliary predefined variables as Green functions.

Inside this class, Fourier points of the discretized mesh grid are contained too. The class reads the material type and properties of every point and relates material models and equations with the corresponding point. Internal variables of the material are saved in this mesh grid.

This class use Python libraries as numpy, scipy or pyfftw. Also wrappers allows to call libraries from another languages as FFTW (C) or own FORTRAN compiled functions.

Material class

The material class is use for defining material properties and material constitutive model equations. This class is initialized with the name of the material and the material type (material model). Later one can set the properties by the function set properties in which arguments must be the properties needed for each type of material.

FFTMAD has three materials models inside: elastic model, elasto-visco-plastic model, hyperelastic model and user defined material model:

- The elastic model defines a elastic stiffness fourth order tensor, that can be isotropic or simple anisotropic.
- Elasto-visco-plastic model is a Von Mises plasticity based model combined with a Perzyna viscoplasticity model.
- The hyperlastic model is based on a Saint Venant–Kirchhoff hyperelastic model.
- The hypoelastic model is based on a NeoHookean model.
- A user defined material model can be introduced in the code. The simplest manner to implement a materials is by a Python code, but also a FORTRAN wrapper has been developed in this work. ABAQUS subroutines materials results haven't been included in this document since this is still an ongoing work.

Material class

An example of an input script is shown below. Note that the input file can be not very intuitive but it is very useful when parametric studies or sequential simulations are wanted to carry out.

```
# General definitions
from INPUT.lucarini_generator import gen_per_poly
from INPUT.orient import rand_ori_umat
from SOLVERS.solverclass import simulation
from MAT_MODELS.materials import material
import numpy as np
import matplotlib.pyplot as plt
from POST.super_extractor_fipru import FIPextraction

# Define simulation and simulation options
my_simulation=simulation('this calculation','non-linear','variational
-nw-cg-finite') #define simulation
```

```

my_simulation.set_options(fftlib='FFTW',einsumlib='f2py',threads=4,
    nlgeom='yes',parallel_mat='umat-omp') # acceleration options of
    the solver
my_simulation.set_tolerances(toler_nw=1e-6,toler_lin=1e-8) #
    tolerances of the solver

# Model geometry
my_simulation.ndim=3 ## dimensions of simulation
my_simulation.n=[16,16,16] ### number of voxels in each direction
my_simulation.L=[20.,20.,20.] ### length of the rve in microns
my_simulation.prop=gen_per_poly(my_simulation.jobname+'micro',
    my_simulation.threads,my_simulation.ndim,\
    my_simulation.n,my_simulation.L,14,0.1,11./2.,17./2.) ### log-normal
    grain size distribution in microns

# Material models and properties
my_materials=[] # initialize the list of materials
elem=np.unique(my_simulation.prop, return_counts=True) # count number
    of elements per grain
ffm = open(my_simulation.jobname+'pmat.txt', 'w');reg=0 # write the
    properties in an output
voxel_vol=my_simulation.L[0]/my_simulation.n[0]*my_simulation.L[1]/
    my_simulation.n[1]*my_simulation.L[2]/my_simulation.n[2] # compute
    the volume of each voxel
for pp in range(np.max(my_simulation.prop)): # for each grain
    if (pp+1)==elem[0][pp-reg]: gr=(6.*elem[1][pp-reg]*voxel_vol/np.
        pi)**(1./3.) # compute the equivalent diameter for each grain
    else: reg+=1 # (exception is grain doesn't exist)
    my_materials.append(material('in718','umat',folder='cp_umat_fath2
        ')) # add a material correspondig to each grain
    my_materials[-1].set_properties(props=np.append(rand_ori_umat()
        [0:6],gr),sdv_num=240) # assign the orientation and grainsize
        to each grain
    ffm.write('%f %f %f %f %f %f %f\n' % (aa[0],aa[1],aa[2],aa[3],aa
        [4],aa[5],gr)) # write the properties in output file
ffm.close() # close output file

#Define loads

```

```

my_simulation.set_load_step(F_ave_goal
    =[[1.005,0,0],[0,1.0,0],[0,0,1.0]],timer=[0.1,1.,0.001,0.5],
    stress_ave_goal=[[0,0,0],[0,0,0],[0,0,0]],info=[216,217,218],frec
    =0,incfix=1,control=[[0,1,1],[1,1,1],[1,1,1]]) # set the first
    ramp up
my_simulation.set_load_step(F_ave_goal
    =[[0.995,0,0],[0,1.0,0],[0,0,1.0]],timer=[0.2,2.,0.002,1.],
    stress_ave_goal=[[0,0,0],[0,0,0],[0,0,0]],info=range(1,240),frec
    =0,incfix=0,control=[[0,1,1],[1,1,1],[1,1,1]]) # set the first
    ramp down
for cycle in range(2): # repeat a cycle X=2 times
    my_simulation.set_load_step(F_ave_goal
        =[[1.005,0,0],[0,1.0,0],[0,0,1.0]],timer=[0.2,2.,0.002,1.],
        stress_ave_goal=[[0,0,0],[0,0,0],[0,0,0]],info=range(1,240),
        frec=0,incfix=0,control=[[0,1,1],[1,1,1],[1,1,1]])
    my_simulation.set_load_step(F_ave_goal
        =[[0.995,0,0],[0,1.0,0],[0,0,1.0]],timer=[0.2,2.,0.001,1.],
        stress_ave_goal=[[0,0,0],[0,0,0],[0,0,0]],info=range(1,240),
        frec=0,incfix=0,control=[[0,1,1],[1,1,1],[1,1,1]])
my_simulation.set_load_step(F_ave_goal
    =[[0.995,0,0],[0,1.0,0],[0,0,1.0]],timer=[0.01,0.01,0.001,0.01],
    stress_ave_goal=[[0,0,0],[0,0,0],[0,0,0]],info
    =[175,179,204,205,206,207,208,209,210,211,212,213,214,215],frec=0,
    incfix=1,control=[[0,1,1],[1,1,1],[1,1,1]]) # extra increment to
    save cyclic state variables

# Solving sequence
my_simulation.generate_green(filterfreq='rotated') # compute
    frequencies and operators
my_simulation.set_FP(my_materials) # assign materials to phases
my_simulation.solve(output=my_simulation.jobname+'result') # run
    simulation

# Postprocessing plot stress strain curve
plt.switch_backend('agg')
fig=plt.figure()
plt.plot((my_simulation.F_ave_inc[:,0,0]-1),my_simulation.
    PK1stress_ave_inc[:,0,0], 'b',label='Pxx')
plt.plot((my_simulation.F_ave_inc[:,0,0]-1),my_simulation.
    PK1stress_ave_inc[:,1,1], 'k',label='Pyy')

```

```
plt.plot((my_simulation.F_ave_inc[:,0,0]-1),my_simulation.
    PK1stress_ave_inc[:,2,2], 'y',label='Pzz')
plt.legend()
plt.savefig(my_simulation.jobname+'resultss.png', format='png', dpi
    =500)
plt.close(fig)
# Postprocessing save in a file the stress strain curve
f=open(my_simulation.jobname+'resultss.txt','w')
for ii in range(len(my_simulation.PK1stress_ave_inc[:,0,0])):
    f.write('%f %f \n' % (my_simulation.F_ave_inc[ii,0,0]-1,
        my_simulation.PK1stress_ave_inc[ii,0,0]))
f.close()
# Postprocessing compute FIPs and make the FIP averaging
FIPextraction(my_simulation.n,1,my_simulation.L,my_simulation.jobname
    +'result')

"""
# Model geometry LOADED
my_simulation.ndim,my_simulation.n,my_simulation.L,my_simulation.prop
    =read_RVE(my_simulation.jobname+'fine.dx') # load the geometry
    from a file

# Material models and Properties LOADED
matt=np.loadtxt(my_simulation.jobname+'mat.txt') # load the
    orintations and grain size from a file
my_materials=[]
for pp in range(np.max(my_simulation.prop)):
    my_materials.append(material('in718','umat',folder='cp_umat_fath2
        '))
    my_materials[-1].set_properties(props=matt[pp],sdv_num=240)
"""
```

B POLYCRYSTAL GENERATION TOOL

A python code has been developed within this work to generate synthetic polycrystals. The code has been incorporated in FFTMAD inputs module and it can be used as a external python function or as a standalone script. The tool performs the weighted Voronoi tessellation and the generates rasterized voxel models from a given grain size distribution. A schematic illustration of the tool is shown in Figure B.1.

Figure B.1: Generation tool scheme

The input of the code is the mean μ and the standard deviation σ of a log-normal distributions of equivalent grain diameters. The limit cut-offs of this distribution is required as input as well, to avoid generating oversized grains or tiny grains even though they are unlikely to be generated. The domain is defined by the length L and the discretization n .

The first step is to calculate the number of grains that will be included in the tessellation. To this end, the log-normal distribution is sampled as many times until the sum of the equivalent volumes of spheres equals (plus minus a tolerance) the volume of the RVE. This step generates a list of sphere diameters that will be included inside the RVE.

Secondly, the sphere centers are placed. The list of diameters is arranged from the largest to the lowest and a Monte Carlo method is used to place the centers of the spheres without or with small overlapping. In this method, the centers are placed randomly, and the position is accepted if no overlapping exists or if the overlapping does not overcome the packing factor, otherwise another random position is tried. The packing factor is variable, and increases with the number of Monte Carlo iterations, allowing the spheres a small penetration that is relative to the sphere diameters.

Finally, the microstructure is rasterized using a weighted Voronoi tessellation for every point belonging to the discretization following eq. (2.10). The output is a map of the different grains considered as different phases in the polycrystal homogenization.

A summarized algorithm is shown in Algorithm 6.

Algorithm 6: RVE generation algorithm

Data: $\mu, \sigma, d_{max}, d_{min}, \mathbf{L}, \mathbf{n}, p_{factor}$
Result: $phase(\mathbf{x})$
 $V_{spheres} = 0$; Initialize d_{list}
 $V_{RVE} = L_x \cdot L_y \cdot L_z$
 $V_{mean} = \frac{1}{6}\pi \exp\{\mu + \sigma^2/2\}^3$
while $V_{spheres} < V_{RVE} - V_{mean}/2$ **do**
 $d_{new} = \text{sample log-normal with } \mu \text{ and } \sigma$
 if $d_{new} > d_{min}$ **and** $d_{new} < d_{max}$ **then**
 Append d_{new} to d_{list}
 $V_{spheres} = V_{spheres} + \frac{1}{6}\pi d_{new}^3$
 end
end
Arrange d_{list}
Initialize x_{list}
for $g1 = 1..N_{grains}$ **do**
 $Placed = False; r_{packing} = 0$
 while $not Placed$ **do**
 $\mathbf{x}_{new} = \text{random position in L}$
 for $g2 = 1..N_{placed\ grains}$ **do**
 $dist_{list} = \text{compute } d(\mathbf{x}_{new}, x_{list})$
 end
 if $any\ dist_{list} < (1 - r_{packing}) \cdot (d_{list}(g1) + d_{list}(g2))/2$ **then**
 $r_{packing} = r_{packing} + p_{factor}$
 continue while
 end
 $Placed = True$
 Append $\mathbf{x}_{new}$ and its periodic replicas to x_{list}
 end
end
for $pos = 1..N_x \cdot N_y \cdot N_z$ **do**
 $dist_{list} = \text{compute for all grain centers } d(\mathbf{x}(pos), x_{list})/d_{list}$
 $phase(pos) = \text{argmin}(dist_{list})$
end

C PERSONAL CONTRIBUTIONS

Publications

Haouala S, Lucarini S, LLorca J, Segurado J (2020) Simulation of the Hall-Petch effect in FCC polycrystals by means of strain gradient crystal plasticity and FFT homogenization. *Journal of the Mechanics and Physics of Solids* 134:103755

Lucarini S, Segurado J (2019) An upscaling approach for micromechanics based fatigue: from RVEs to specimens and component life prediction. *International Journal of Fracture*

Lucarini S, Segurado J (2019) DBFFT: A displacement based FFT approach for non-linear homogenization of the mechanical behavior. *International Journal of Engineering Science* 144:103-131

Lucarini S, Segurado J (2019) An algorithm for stress and mixed control in galerkin-based FFT homogenization. *International Journal for Numerical Methods in Engineering* 119(8):797-805

Lucarini S, Segurado J (2018) On the accuracy of spectral solvers for micromechanics based fatigue modeling. *Computational Mechanics* 63(2):365-382

Ortiz-Roldan J M, Esteban-Manzanares G, Lucarini S, Calero S, Segurado J, Montero-Chacón F, Ruiz-Salvador A R, Hamad S (2018) Fitting electron density as a physically sound basis for the development of interatomic potentials of complex alloys. *Physical Chemistry Chemical Physics* 20(27):18647-18656

Cruzado A, Lucarini S, LLorca J, Segurado J (2018) Crystal plasticity simulation of the effect of grain size on the fatigue behavior of polycrystalline Inconel 718. *International Journal of Fatigue* 113:236-245

Cruzado A, Lucarini S, LLorca J, Segurado J (2018) Microstructure-based fatigue life model of metallic alloys with bilinear Coffin-Manson behavior. *International Journal of Fatigue* 107(Supplement C):40-48

National journals publications

Segurado J, Lucarini S (2019) Simulación del efecto del tamaño de probeta y la dispersión en fatiga de metales mediante micromecánica computacional. *Grupo Español de Fractura*.

Segurado J, Llorca J, Cruzado A, Lucarini S (2016) Un modelo micromecánico del comportamiento en fatiga de una superaleación base Níquel. *Anales de Mecánica de la Fractura* 33

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