COMPUTATIONAL CHARACTERIZATION AND OPTIMIZATION OF HYBRID COMPOSITES REINFORCED WITH TWO TYPES OF FIBER OF DIFFERENT MATERIALS

Filipe José Sequeira Leal

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Supervisors: Prof. Helder Carriço Rodrigues
Prof. José Arnaldo Pereira Leite Miranda Guedes

Examination Committee
Chairperson: Prof. João Orlando Marques Gameiro Folgado
Supervisor: Prof. José Arnaldo Pereira Leite Miranda Guedes
Member of the Committee: Prof. Paulo Rui Alves Fernandes

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Abstract

The objective of this work was to develop a finite element based model to computationally characterize and optimize hybrid composites reinforced with two types of long-fibers of different materials. To that extent, two Matlab computer programs were developed and one other modified to meet the requirements of the problem. All three are thoroughly described. The investigation was based on the concepts described by homogenization theory. As such, the parametrization of the structure was reduced to that of a representative element volume. Two cross-sectional microstructures were analyzed: one with random and other with geometric fiber distributions. The results show optimum microstructural configurations for a number of loading cases, considering three possible filling fiber pairs: carbon fiber/E glass fiber, carbon fiber/epoxy fiber and carbon fiber/void; where the matrix material is epoxy. Additionally, stress distributions within the microstructure of a selected group of case studies are displayed. Further observation on the results has led to the conclusion that the microstructural arrangement type of the fibers does not have a major impact on the homogenized stiffness of the composite. However, it was found that a geometric fiber distribution shows a value up to 48.77% less on the maximum Von Mises element stress compared with a random fiber distribution under the exact same optimization conditions. Alongside, it was observed that it is possible to lower the tensile stress peaks in the random fiber distribution configurations, with minimal loss of structural stiffness, if a stress constraint is applied to the optimization problem.

Keywords: Hybrid Composites; Homogenization Method; Finite Elements; Microstructural Optimization; Stress Distribution
Resumo

O objectivo deste trabalho foi desenvolver um modelo computacional para caracterizar e optimizar materiais compósitos híbridos reforçados por dois tipos de fibras contínuas de materiais distintos. Com esse objectivo, desenvolveram-se dois programas de raiz em Matlab, e modificou-se um terceiro para que satisfizesse as necessidades do problema. Os três são descritos em detalhe. A investigação baseou-se nos conceitos descritos pela teoria da homogeneização. Como tal, a parametrização da estrutura foi reduzida à de um elemento de volume representativo. Foram analisados dois tipos de secções transversas da microestrutura: uma apresentando uma distribuição aleatória das fibras, e a outra uma distribuição geométrica. Os resultados mostram configurações óptimas das microestruturas para diferentes carregamentos, considerando três tipos de pares de fibras de enchimento: carbono/vidro tipo E, carbono/epoxy e carbono/vazio; em que o material da matriz é epoxy. Adicionalmente, apresenta-se a distribuição de tensão na microestrutura de alguns dos casos. A observação dos resultados levou a concluir que o arranjo microestrutural das fibras não possui uma influencia significativa na rigidez homogeneizada do compósito. No entanto, descobriu-se que uma distribuição geométrica das fibras apresenta um valor até 48,77% inferior na tensão de Von Mises máxima observada nos elementos, quando comparada com uma distribuição aleatória sob as mesmas condições de optimização. Ao mesmo tempo, observou-se que é possível reduzir os picos na tensão de tracção nas configurações com distribuição de fibras aleatória, com uma perda mínima na rigidez da estrutura, se for aplicado um constrangimento de tensão ao problema de optimização.

Palavras-chave: Materiais Compósitos Híbridos; Método da Homogeneização; Elementos Finitos; Optimização Microestrutural; Distribuição de Tensões
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Acronyms

CAD – Computer Aided Design
CFRP – Carbon Fiber Reinforced Polymer
DMO – Discrete Material Optimization
FEA – Finite Element Analysis
FEM – Finite Element Method
RVE – Representative Volume Element
SIMP – Solid Isotropic Material with Penalization
SQP – Sequential Quadratic Programming
CHAPTER 1 – Introduction

The first chapter sets out the background to the research study that was conducted and further described in this document. First, an introduction regarding topics such as composite materials, micromechanics and structural optimization will be addressed. An overview over the current state of art concerning the assembly of these three topics within the context of the thesis will follow. There will be a brief text on the reasons why this research was carried out, succeeded by a succinct statement on the aims and objectives of the dissertation. The chapter will be closed with an outline on the organization of this document.

1.1 Composite materials

A composite material can be defined as the resulting material from the combination of two, or more, different materials [1]. The materials used to build it often have very different physical properties and can be divided into two different groups: matrix and reinforcement. The outcome of their mixture is a material that combines their individual characteristics, giving the composite very unique and interesting properties. One of the major driving forces towards the manufacture of composite materials nowadays relates to their high relative stiffness, and strength, to weight [2].

In a composite, the reinforcement are the fibers. These are used to add strength and stiffness to the matrix. The reinforcement fibers can be cut, aligned, placed in different ways to affect the properties of the resulting composite [2]. The matrix, normally a form of resin, surrounds and binds the reinforcement, keeping the fibers in place and allowing that applied loads can be effectively transferred along the composite. Plus, it protects the reinforcement from chemical and/or environmental attacks [2].

Natural composites exist in both animals and plants [1]. For instance, wood and bones are two natural composite materials. Mankind has been making composites for thousands of years: one early example is mud bricks made by mixing mud and straw together [1, 3]. These combine the compressive strength of the dried mud with the tensile strength of the straw, creating a brick that is resistant to both squeezing and tearing [1]. Many ancient civilizations used mud bricks to build their houses and main infrastructures, some of which can still be seen today. Even nowadays these building blocks are used in regions where other resources are scarce.

The first modern composite material was fiberglass: a material made by combining a polymeric matrix with a glass reinforcement [1]. This glass reinforcement is usually sold as a roll of fabric. It is then cut according the needs of the piece to be manufactured, each layer laid randomly across each other and held together by the polymeric matrix. A composite made using this process is called a laminate composite. Although this is not the only method fiberglass can be made, it encompasses one of the different techniques to create composite materials in general. Other types of reinforcements used to create composite materials are
summarized in Figure 1. The research study reported in this document will focus on continuous fiber reinforced composites.

The top reason why, in many applications, composites are chosen over more traditional materials lies in their weight to stiffness/strength ratios. For example, carbon fiber reinforced composites can be five times stronger than 1200 grade steel while having only one fifth of the weight [2]. Another example is the 6061 grade aluminum; this one is much closer in weight to carbon fiber composites. Still, the composite can have twice the modulus and up to seven times the strength [2]. Choosing appropriate combinations between matrix and reinforcement can lead to a countless number of possibilities. Composite materials can be made to exactly meet the requirements of a particular application [1]. An additional advantage relates to the design flexibility composites provide as many of them can be molded into complex shapes [1]. On the other hand, cost arises as the major drawback since raw materials to build composites are often expensive.

The new Airbus 380, the world’s largest passenger airliner, makes use of modern composites in its design [1]. This has been the airline’s gradually increasing policy since the 1980s when it started by using 5% composite materials in its A310-300 [4]. In this new aircraft, more than 20% of composites – about 25% according to [5] – were used as part of the total airframe. Mainly of which a polymeric matrix reinforced with carbon fibers (see Figure 2). Yet another more radical example is their next generation: A350XMB. The latter consists of 53% composite materials spread all over from the nose section, through the fuselage, up to the rear fuselage [4, 5]. Both A380 and A350XMB are in commercial service since October 2007 and January 2015, respectively.
With the continuous evolution of technology, composites are, each day, reaching higher standards. New materials are coming into play, making composites increasingly become a noticeable option for many applications. Some advanced composite materials are now being made using carbon reinforcements, instead of glass. Such materials are lighter and stronger but also more expensive to produce than fiberglass. They are, for example, being used in aircraft structures and expensive sports equipment as golf clubs. Carbon and boron nitride nanotubes have also been successfully used to make new composites. These, besides being even lighter than regular carbon fibers, are also stronger. The possibilities for their application huddle in the automotive and aircraft industries. Lower fuel consumption might be at a small step away, as soon as their manufacturing process comes at a lower cost.

1.1.1 Hybrid composite materials

Hybrid composite materials represent a particular case within composite materials as they result from the incorporation of various different types of fibers/particles into a single matrix, or by using different material plies in a composite laminate. This kind of materials have extensive engineering application where strength to weight ratio, ease of fabrication and low cost are required. Hybrid composites deliver a combination of properties such as tensile modulus, compressive strength and impact strength that are beyond the reach of regular composite materials. As is common amongst composite materials, hybrid composite’s behavior can be translated as a sum of the individual performance of its components. In this specific case, resulting in an even more favorable balance between the material’s inherent advantages and disadvantages. Furthermore, having two or more types of fibers/particles/plies makes it possible to better complement the
lacking properties on one specific fiber/particle/ply type with the favorable properties of the others [9]. Hybrid composites are usually used when, for instance, a precise combination of properties of different fibers needs to be achieved, or when longitudinal as well as lateral, good, mechanical performances are required [8]. Recently, hybrid composites have been established as highly efficient, high performance structural materials and, as a result, their use is seen rapidly increasing in industries such as: aeronautical, maritime, wind power generation, civil construction and telecommunications [8].

The research documented throughout this paper focuses, precisely, on the computational characterization and optimization analysis of hybrid composites having two different long-fiber reinforcement types.

1.2 Basic concepts in micromechanics

Nowadays, many industrial and engineering materials, as well as most biological materials, are inhomogeneous [10]. This means that they aggregate two or more different, distinguishable, constituents (or “phases”) at some small length scale – a microstructural scale. Each constituent has its own properties and material orientations and may itself be an inhomogeneous material at a smaller length scale [10]. Figure 3 shows an example of a typical microstructure of an inhomogeneous material as well as a symbolic representation of its manufacture.

![Figure 3 – Macroscopic versus microscopic structures of an inhomogeneous material [11].](image)

The macroscopic characteristics of such materials result from a combination of the cumulative response from the distinct “pure” materials [11]. For example, adding several particles or fibers in a binding material is a relatively inexpensive to enhance that material’s properties so that a specific macroscopic response is obtained. Composites, along with concrete, polycrystalline materials, porous and cellular materials, among
others, are well-known examples of inhomogeneous materials. Much of what was previously described about composite materials constitutes a specification of the nature, behavior and philosophy of application of inhomogeneous materials.

The importance of micromechanical analysis lies in the inherent microscale inhomogeneities present in this sort of materials. If one were to attempt to perform a numerical simulation over a macroscopic structure made with a microheterogeneous material, a very fine mesh – e.g. that from a finite element mesh – would have to be applied over the structure in order to capture all the microscale details [11]. The resulting system of equations would contain an extraordinary number of unknowns. Naturally, such mesh would require a huge computational power to be solved. That from a computing machine that does not exist so far. Even if it did, the information resulting from the analysis of such a system would be so complex as to be practically incomprehensible. Moreover, it would be practically impossible to find and ascertain the position of all the heterogeneities under the surface of the material [11]. The solution that the engineers came across was: homogenization.

The idea is simple: “to compute a constitutive ‘relation between averages’, relating volume averaged field variables” [11]. This is, to compute effective, or apparent, properties (the designations may vary upon the authors) that describe the microscopic behavior of the structure in macroscopic terms. This technique is oftentimes referred in literature as homogenization method, or theory. The volume averaging occurs over a statistically representative sample of material, often denoted to as representative volume element (RVE) [11]. Figure 4 illustrates this idea.

![Diagram of actual structure and structure with effective properties](image)

Figure 4 – Determining effective properties of inhomogeneous materials in structural engineering [11].
In Figure 4, $IE^{(1)}$ and $IE^{(2)}$ represent the elasticity tensor of the two different materials, 1 and 2, $IE^*$ refers to the effective elasticity tensor of the macroscopic structure, while $\langle \sigma \rangle$ and $\langle \varepsilon \rangle$ are the volume averaged stress and strain fields within the statistically representative volume element (RVE).

The analysis of microheterogeneous materials is not a recent issue as there are publications related with estimates of effective responses of different materials under assumptions on the internal fields of the microstructure dating back to more than 150 years ago [11]. Nonetheless, the first analysis of the effective mechanical properties of a microheterogeneous material is credited to Voigt, with a paper published in 1889 [11]. Despite being an issue that has been subject of study for a long time now, micromechanics is more and more a topic of interest nowadays, and which deserves especial attention, particularly due to the sharp growth in the use of composites.

1.3 Structural design optimization

One of mankind’s most important and distinctive quality is the capability of decision making. It does not matter the field of activity one belongs to; whether it is economic, political, military or technological, decisions are constantly demanded and have a far reaching influence in our lives [12]. For this same reason, optimization tools play an important role in structural design: their very purpose is often to find the best way of building a specific structure so that maximum benefit can be taken out of it with minimal use of resources [12]. Hence, these are many times a key factor helping the designer making an informed choice and, ultimately, taking a decision.

The first “high speed” digital computers only started to appear in the 1950s, however optimization can be said to have occurred throughout the human history. Prior to that time, the lack of resources made the process much more difficult and time-consuming; often characterized by small and painstaking steps towards the optimum [13]. Structural optimization methods and the finite element analysis (FEA) began to develop roughly at the same time, but despite their close relationship they followed a much different path [14]. On one hand, the finite element method (FEM) was well up to date and widespread in commercially available software since the early 1990s; on the other hand, only more recently optimization technology got to a point where it has gained some mainstream popularity and could be considered close to a fully matured subject [14, 15].

“The optimal structural design will always constitute the best compromise between a number of contradictory demands and wishes for the structure” [13]. In other words, structural design optimization denotes the challenge of finding the best design available given the performance criteria and restrictions defined by the engineer. A solution is then obtained via iteratively improving an initial design, judging and selecting each time better and better design parameters. Whenever no further improvement can be made the design is said to be optimal.
Stegmann [13] gives a simple, practical, example that helps understand the concept behind the “[…] contradictory demands and wishes for the structure”. He explains that despite being of great interest for an airliner manufacturer to increase the overall profitability of their aircrafts (by increasing the number of passengers they can carry and their maximum speed while reducing operation costs and weight) it may not be possible due to interdependency between variables and other internal and/or external constraints. For instance, increasing the number of passengers would increase the weight and reduce the speed of the airplane, whereas an increased speed would increase its operation costs. Moreover, limitations introduced by the airports’ architecture (length of the runway, height of the gates, etc.) would directly interfere with the conceivable size of the plane. Even the size or capacity of the manufacturer’s production units could introduce constraints in the design of the aircrafts.

As the reader may now realize, structural design optimization is a subject that is far from being straightforward. Over the recent decades, authors like Bazaraa et al. (2006) [16] or Luenberger and Ye (2008) [17] have put their efforts on formulating and compiling algorithms to successfully achieve it. But despite all its complexity, optimization problems can be stated in a mathematical form that is rather simple. Equation (1) presents the canonical form of such problems:

\[
\begin{align*}
\text{Objective:} & \quad \min_x f(x) \\
\text{Subject to:} & \quad x_{\text{min}} \leq x \leq x_{\text{max}} \\
& \quad h(x) = 0 \\
& \quad g(x) \leq 0
\end{align*}
\]

In (1), \( x \) represents the design variable, \( f \) is the objective function to be minimized, \( x_{\text{min}} \) and \( x_{\text{max}} \) the minimum and maximum attributable values of \( x \), and \( h(x) \) and \( g(x) \) denote the equality and inequality constraints applied to the problem, respectively. In order to get to such formulation there are a series of steps that shall be followed. These are schematically illustrated in Figure 5.

The problem formulation process starts by developing a descriptive statement of the problem/project, which is usually done by the project’s sponsor/owner. This first step serves the purpose of describing the overall objectives of the project and requirements to be met [18].

The development of a mathematical formulation for any design optimization problem requires the presence of relevant information such as material properties, performance requirements, resource limits, cost of raw materials, etc. Together with the description of the analysis’ procedures and tools used to tackle the problem, this is the goal of step number two. Many times the problem statement is vague and assumptions must be made in order to formulate it and solve it. In such cases a clear specification of such information needs to be stated later in the formulation process [18].
Step number three is used to identify the set of variables that describe the system. These are called design variables. The design variables shall be, as far as possible, independent from each other and regarded as free because one should be able to assign them any value. The number of independent design variables sets the number of degrees of freedom of the problem. If proper design variables are not selected for a problem, its formulation may be either incorrect or impossible at all. The following considerations summarize the concerns that shall be taken care when identifying design variables for a problem [18]:

- Design variables should be independent from each other as far as possible;
- A minimum number of design variables required to properly formulate a design optimization problem exists;
- As many independent variables as possible should be elected as design variables at the problem formulation phase; and
- Valid design variables should specify a trial design of the system when assigned with concrete numerical values.

To compare all the different possible designs and assess which are better or worse, a criterion must be defined. In step number four, one is expected to choose a criterion that serves this purpose. This criterion must be a scalar function whose numerical value can be obtained once a design is specified. In other words, it must be a function of the design variables vector $x$. Such criterion is often called an objective function for the design optimization problem and the goal is to maximize it or minimize it depending on the problem requirements. Emphasis is placed on the importance that a valid objective function must be, directly or
indirectly, influenced by the variables of the design problem; otherwise, it is not a meaningful objective function. One should note that an optimized design results in the best value for the objective function, maximum or minimum [18].

Finally, step number five aims at identifying all the restraints placed on the design and develop mathematical expressions for them. In terms of the problem formulation process, these are collectively called constraints. Most realistic systems must be designed and manufactured within given resources and performance requirements. For example, structural members should not fail under normal operating loads and they must fit into available amounts of space. Constraints regulating these and other aspects of the behavior of such elements must depend on the design variables since, only then, do their values change with different trial designs. I.e., a meaningful constraint must be a function of at least one design variable. The constraints can be divided in: linear or nonlinear, equality or inequality and implicit constraints. Linear constraints have only first-order terms in the design variables whereas nonlinear comprise more general optimization problems. Equality constraints fix an explicit value for those particular constraints while the solution for inequality constraints ranges in an interval of admissible values. Lastly, implicit constraint is the designation given to more complex constraints that are indirectly influenced by the design variables [18].

Only after these being successfully stated and assessed one must go forward and try to solve the design optimization problem. In terms of the theoretical problem presented in (1), the goal would be to gradually update the values of the design variable, \( x \), according to a series of algorithms as the ones compiled in [18], [16] or [17], with or without derivative information, until the lowest value (since it was formulated as a minimization problem) of the objective function, \( f \), is found. This point sets the optimal design parameters to the design problem. With respect to the problem explored in this document, the aim will be to find the stiffest possible layout for the fiber reinforced composite; where the design variables will represent the material to be applied to each of the existing fibers – from two possible options with distinct stiffnesses – and the constraints will comply material volume and average stress limitations.

1.4 State of the art and Motivation

In 1984, Schmit [19] posed the following sentence: “Historically, the desire to reduce structural weight while preserving structural integrity, particularly in aerospace applications, has been a strong driving force behind the development of structural optimization methods. Today, the need for energy conservation in transportation systems via weight reduction provides further motivation for the application of structural optimization methods. The growing use of fiber composite materials in structures is likely to increase the demand for modern analytical tools that will make it possible to fully exploit the design potential offered by these new materials” (as cited in [14]). Albeit having been made over 30 years ago, this sentence unveils issues that are still being dealt today. It gives not only a starting point for the initial development of structural optimization tools but also pinpoints the direction Schmit expected it to follow. And turns out he was correct.
since structural optimization methods, together with composite materials, became major objects of research in modern society.

Topology optimization emerged as a first mathematical approach towards the search for extensive efficiency and performance gains in continuous and discrete structures. This method is usually followed by two others: shape optimization and size optimization (see Figure 6).

![Figure 6 – Two-dimensional structure subjected to topology, shape and size optimizations [13].](image)

These are three generic classes of methods commonly used for doing structural design optimization. Topology optimization (left) deals with the distribution of a limited amount of material over a specific domain and, as such, can introduce holes within the structure. The result is usually a rough outline of the structure so shape optimization (middle) can be used to make the boundaries smoother. Finally, size optimization (right) can be used to find the optimal thickness distribution over the structure. See, for example, [20] for an academic literature on the subject. Detailed studies on the three structural optimization methods applied in the design of an aircraft’s wing box and leading edge droop nose ribs can be found in [21] and [22]. Emphasis is placed on the topology optimization stage since optimization assisted design processes strongly rely on its ability to generate a highly efficient initial concept.

Structural design optimization of composite structures lies within the same principles as for isotropic material structures but having an increased design freedom. While the different forms of composites were already presented in Figure 1, their predominant usage in industry is via composite laminates where thin fiber reinforced orthotropic plies are stacked on top of each other in several orientations to form a shell structure. Composite layer stacking optimization problems along with material selection problems are subjects that have been extensively studied in past years and are now fairly well documented. A major breakthrough happened when Stegmann and Lund (2005) [23] developed a novel method for doing material optimization of general composite shell structures labelled Discrete Material Optimization (DMO). This came as a follow up from previous works on Solid Isotropic Material with Penalization (refer to Zhou and Rozvany (1991) [24], Bendsøe et al. (2000) [25], Bendsøe and Sigmund (2003) [20] and references therein), the so-called SIMP approach, and to its generalization to multiphase topology optimization (Sigmund and Torquato (1998) [26]). From there, more recent studies such as [27], [28] and [29] could be established. [27] targets a design problem on the maximization of the buckling load factor of laminated multi-material composite shell structures using the DMO methodology; the authors illustrate with a practical case study of a simplified shell model of a spar cap from a wind turbine. [28] proposes an optimization strategy for maximizing the ductility of fiber reinforced concrete with long textile fibers – a material that opens up a new field for concrete
applications in the future – considering the nonlinearity of the materials involved. Finally, [29] focuses on the vibro-acoustic optimization of laminated composites plates in order to minimize the sound power radiated from their surface to the surrounding acoustic medium when subjected to an external time-harmonic mechanical load. Such investigations as the one conducted in [29] could potentially lead to a new way to create sound insulation in transportation systems, especially if coupled with a mechanical performance optimization.

Despite being a well-established, powerful, tool that can generate highly efficient and often innovative structural design concepts, researchers have been trying to find ways to fill in the shortcomings of topology optimization regarding structural design optimization of shell structures. While solid/void density distributions are the only choice in structures made with isotropic materials, for shell structures intermediate densities can be interpreted as different thicknesses and their penalization can potentially lead to inefficient structures. It has been shown in [30] that an optimization method solely based on the optimization of the thicknesses throughout the shell structure also provides meaningful results, and may be used as an alternative to topology optimization. Such optimization method is referred in [30, 31] as free size optimization and it works by defining the thickness of every single shell element as a design variable. This method is presented and described in [30] and [31]. [30] exhibits the method applied to an academic problem while [31] addresses the specific case of the optimization of an aircraft underbelly fairing under hypothetical operation conditions. Another, more complete and exhaustive, document on the subject can be found in [32]. In the latter it is interesting to observe the composite laminate acquire truss-like contours when subjected to benchmark structural optimization examples such as the cantilever beam with a vertical load at the opposite end.

More recently hybrid composite materials began having a little closer attention due to their undeniable flexibility to reach on demand properties. A large portion of the research existing today pays attention to the use of hybrid composites filled with natural fibers, trying to understand their mechanics and searching for natural alternatives to synthetic fiber composites. Examples are presented in [33], [34] and [35]. In [33] the authors evaluate the static and dynamic mechanical properties of a palmyra palm leaf stalk fiber and jute fiber reinforced polyester matrix and compare its performance with hybrid composites reinforced with natural/glass fibers; the outcome shows positive results and opens up its application to the manufacture of lightweight automotive parts. [34] aims to the assessment of the mechanical properties of hybrid glass/sisal and glass/jute fiber reinforced epoxy composites, exhibiting a comparison between the resulting properties of both materials. Lastly, [35] presents a study where the mechanical and thermal properties of raw jute fiber reinforced hybrid composites versus jute/banana fiber reinforcements, in an epoxy matrix, are investigated and compared; the tests carried out by the authors lead to the conclusion that the addition of banana fibers result in an increase in the mechanical and thermal properties of the hybrid composite. A particularly interesting review article, in a slightly different scope, is documented in [36]. It explains about natural fiber/nanoclay hybrid systems and their prospective use in food packing. At the same time, gives an
overview about the most recent advances and emerging new aspects of nanotechnology for the
development of hybrid composites environmentally compatible as food packing materials.

Even though the market for natural fiber reinforced hybrid composites has the potential to sharply grow in
the near future, more demanding engineering applications will still require synthetic reinforcements to take
place. Automotive and aerospace come along as some of the industries where hybrid composites constitute
an important class of materials due to their lower density, higher specific strength and better physical and
mechanical properties compared to pure materials. The following papers reveal some of their potential use
in aerospace applications: [37], [38] and [39]. In [37] the authors investigate the mechanical response and
the industrial manufacturability of Carbon Fiber Reinforced Polymer (CFRP)/titanium hybrid composite
laminates using a spacecraft payload adaptor as an example. [38] presents a study on the mechanical and
wear properties of hybrid metal matrix composites enhanced with mica and SiC ceramic particles. Finally,
[39] presents an analysis on the fatigue behavior of CFRP/steel hybrid composites, a material that appears
to be a very promising solution to increase bolt bearing strength in future composite aerospace structures.

Hybrid composite materials make up a subject that, despite the research work conducted in recent years,
still has great room for development. This is especially true with regard to the computational characterization
and microstructural optimization of the hybrid composites. That, together with the market opportunities for
composite materials, constitute the main reasons why this investigation was carried out.

1.5 Objectives

Nowadays, it is commonly accepted that numerical simulation tools are an important input in predicting more
accurately structural responses of every sort of mechanical components. More particularly, with regard to
the use of composite materials, to predict their micro-macro structural responses. Ideally, in an attempt to
reduce laboratory expense associated with experimental testing, one would like to be able to anticipate a
new material’s behavior only by numerical simulations. The primary goal being to accelerate the trial and
error laboratory development of new high performance materials. To this end, the tool described in this
monograph proposes, through the analysis of a number of case studies, to give some insight on the optimal
distribution of two different types of fibers within a hybrid composite material, as well as to provide a mean
to achieve such optimization.

1.6 Outline of the thesis

The thesis is organized in five main chapters.

Chapter 1 – Introduction, introduces the background concepts addressed in the document. This includes
brief descriptions about topics like composite materials, micromechanics, structural design optimization and
the state of the art.
CHAPTER 2 – Methodology is dedicated to the detailing of the research procedure. Here, the scope of the problem and its formulation are presented, alongside with the description of the computer programs used to solve it and the characterization of the case studies that were investigated.

CHAPTER 3 – Results deals with the presentation of the optimization results obtained for the different case studies that were analyzed. Results concerning a random fiber distribution RVE as well as a geometric fiber distribution RVE for different pairs of filling fibers and loading conditions are shown.

CHAPTER 4 – Discussion is devoted to a critical assessment of the results. The optimal microstructural configurations are analyzed in terms of compliance with the loading condition, their performance in terms of stiffness and stress distribution is comparatively measured and potential ways to apply such results in real context are identified.

CHAPTER 5 – Conclusions summarizes the conclusions drawn from the present work.
CHAPTER 2 – Methodology

The second chapter details the way the research was conducted. It presents and justifies the research methods, sources of information and computational tools that were used to tackle the topic. First, a clear description of the scope of the problem will be addressed. An overview over the approach that was used in conducting the research will follow. Finally, there will be provided a thorough description of the computational procedure, as well as all the intermediate steps (gathering of information, hypotheses, and so forth), that was undertaken in order to reach the solution of the problem.

2.1 Scope of the problem

As mentioned in the introductory chapter, hybrid composites come as a result of the incorporation of more than one type of reinforcements in a binding matrix; or through the use of plies of different materials in the case of composite laminates. Due to their very heterogeneous nature, questions related to the optimal distribution of the different kinds of reinforcements within the matrix may naturally arise. What is the best volume fraction for each of the reinforcements? Which are the ideal regions to place them? These are just examples of what this document intends to portray. And since in this research only continuous fiber reinforced composites were studied (review Figure 1), from now on these will be the ones subject to observation.

The first problem lies within the computational characterization of the fiber reinforced hybrid composite itself. How to turn a structural domain where heterogeneities are distributed in a completely random way into something measurable? How to keep the computations within acceptable limits given the current state of computer technology? In order to get some truthfulness in the results one needed to consider the stochastic distribution of the fibers throughout the composite domain. The goal was to simulate, as far as possible within the framework of a master’s thesis, a material that could be built from a real manufacturing process.

The second problem relates to the structural design optimization applied to hybrid composites. Which material shall be assigned to each of the fibers considering their position within the composite? Is there any difference in the final layout if the materials attributable to the fibers are changed? What is the difference between the imposition of a volume or an average stress constraint? Figure 7 shows the Computer Aided Design (CAD) model of the RVE used in this work. This helps to better understand the concepts mentioned earlier. On the left, a bundle of fibers randomly distributed across the domain by a computer program specifically designed for that matter (see “Overview of the approach” or “RAND_uSTRU_GEN” sections for a reference) and, on the right, their matching matrix.
As seen in Figure 7, there are three types of fiber conditions: full fibers (4, 5, 7, 8, 10, 11, 12, 14, 15 and 16), fibers split into two (2, 3, 6, 9 and 13) and corner fibers (1). From this point ahead, the problem is then how to assign the two different fiber materials to fibers 1, 2, 3, …, 16, according to an external load and to a volume constraint, or an average stress constraint, so that a requirement such as the maximization of the stiffness is met. Where the volume constraint serves the purpose of limiting the number of possible existing fibers assigned with a specific material, and the stress constraint aims at limiting the maximum possible values of stress throughout the domain of the RVE.

The fiber distribution layout presented in Figure 7 will be used as the standard model throughout the whole document. This particular arrangement was chosen because it contains all three types of fiber conditions and due to its compatibility with the chosen mesh size. One was able to notice that, depending on the mesh sizes chosen to discretize the RVE, some of the layouts produced by the random fiber distribution generator resulted in meshes with overlapping elements when using Abaqus (FEA commercial software) meshing module. A more detailed description of the standard RVE (Figure 7), the role of Abaqus in solving the problem, as well as the meshing error it produced in some of the generated layouts, will be detailed in subsequent sections.

2.2 Overview of the approach

The solution to the problem was achieved through the use of four main computer programs: one to generate a random distribution of a given number of fibers in a two-dimensional RVE (RAND_uSTRU_GEN), another to transform the RVE in a three-dimensional domain and build a suitable mesh (3DMeshGENAbaqus2D – where Abaqus was used as part of the process), a program to compute the homogenized properties of the
composite characterized by that particular RVE/microstructure (Premat), and, finally, one to carry out the optimization of the fiber’s material (CompositeOpt). Both RAND_uSTRU_GEN and Premat were preexisting programs which were modified in order to fulfill the needs associated with the problem. RAND_uSTRU_GEN is the name given to the algorithm developed by Melro, Camanho and Pinho (2008) [40], whose designation derives from an acronym of Random Microstructure Generator. The algorithm is built as a Matlab computer program, which easily enables its use. In [40] the reader can see a detailed description of how the algorithm works; later in this document a broader analysis of its functioning will also be covered. Premat is a computer program authored by Guedes and Kikuchi (1990) [41], developed in Fortran, whose purpose is to compute the homogenized properties of linear elastic composite materials. Combined with Postmat, these two programs can be used to model the composite’s mechanical behavior; where Postmat is used to compute localized (microstructural) information such as displacements, stresses and strains after a finite element procedure has been already used to solve the general structure. [41] presents all the theory and mathematical formulations behind the homogenization method and underlying issues related to its implementation into Premat and Postmat.

In accordance with what was discussed in the introductory subchapter “Basic concepts in micromechanics”, the use of the homogenization theory assumes that the RVE constitutes a representation of the microscopic level that is sufficiently general so that its behavior can be extended, with minimal loss of information, to the macroscopic level. With this being said, the method then considers that the composite material is locally formed by the spatial repetition of very small structures – microscopic cells – when compared with the overall macroscopic dimensions of the structure of interest [41]. In other words, this means that the macroscopic structure is constructed as a collage of successive RVEs next, above and below each other, as represented in Figure 8.

![Figure 8](image)

Figure 8 – Microscopic periodicity of the macroscopic domain defined by the RVE.

Thereby, the material properties are assumed to be periodic functions of the microscopic variable, where the period is very small when compared to the macroscopic variable. The computation of the equivalent, or
effective, material properties is consequently enabled by performing a limiting process when the microscopic cell size is reduced to zero. The homogenization method is a rigorous mathematical theory which can as well provide reasonable solutions for problems where experimental data is unavailable or inexistent, or when only bounds for the equivalent material constants can be found by other theories [41].

### 2.2.1 Overall scheme of the solution

An overall scheme representing the way the solution to the problem was built is depicted in Figure 9, as a flowchart. Figure 9 shows the most important inputs required by the different computer programs, the main outputs they produce, as well as the linkage and how the data flows across them. The figure is divided into three columns, each of them displaying the summarized flowcharts of the three Matlab programs used to tackle the problem: RAND_uSTRU_GEN, 3DMeshGENAbaqus2D and CompositeOpt. Premat is not individually shown since it works more as a subroutine of CompositeOpt. As indicated in Figure 9, Premat is divided into two different modules – the meshing and homogenization modules – which can be used as individual computer programs to avoid generating additional data that may be unnecessary for the ongoing processes.

**Figure 9 – Flowchart of the program’s network.**
Besides generating a random fiber distribution across the RVE, a subroutine was created in RAND_uSTRU_GEN in order to make it generate a geometric fiber distribution. This geometric distribution has shown to be an important tool in an attempt to understand if the results from the optimization really made any sense according to one’s mechanical perception of the problem. Examples of the optimization of a sixteen fibers reinforced RVE, for a set of five different loading conditions, are presented in “Volume constraint case studies”, “Geometric fiber distribution” section.

3DMeshGENAbaqus2D works solely based on the python script file produced by the modified RAND_uSTRU_GEN program and the number of existing fibers in the RVE. It calls Abaqus as a subroutine to read and execute the python script file which, in turn, orders Abaqus to generate a CAD model of the RVE, mesh it and save all the important mesh information into a text file. From there, 3DMeshGENAbaqus2D continues by reading the text file and store its data: element nodal coordinates, connectivities and number of the elements belonging to the matrix and to the fibers. The next step deals with transforming the two-dimensional RVE mesh into a tri-dimensional mesh. After all this being done, the new 3D mesh information is saved into a new text file.

The 3D mesh text file produced by 3DMeshGENAbaqus2D is read by the meshing module of Premat and the periodicity conditions are settled. The periodicity conditions target the surface nodes of the RVE and their purpose is to let Premat know that those are the points that connect with the surrounding “RVEs”. CompositeOpt program uses the output file from Premat meshing module and some more input variables entered by the user, including the imposed strain (which acts as the loading condition) and the initial value for the design variables, to start running the design optimization analysis. The design variables are directly related to the material assigned to each of the fibers. Therefore, their initial default value is given so that every fiber has the same starting opportunity to follow any material’s direction. Only the extremes of the interval constitute a meaningful engineering result since intermediate values represent a mixture of the two possible materials. It is therefore very important that the algorithm is able to reach what in topology optimization is often referred as a black and white design, grey areas avoided. CompositeOpt runs a cycle that updates the design variables in every iteration according to the gradient of the objective function, for every fiber, and checks if the algorithm converged to a solution. The program halts if the stopping criteria are met or by user intervention.

2.3 Problem formulation and parametrization of design

The first step in formulating a structural design optimization problem is the problem statement (recap Figure 5). This step has been already addressed in “Scope of the problem” subchapter. The following paragraphs deal with the description of the tasks that had to be performed in each of the four remaining steps to develop a mathematical formulation and parametrization for the design optimization problem. These four steps are: data and information collection, identification/definition of the design variables, identification of a criterion to be optimized and identification of the constraints.
2.3.1 Data and information collection

The problem is clear with regard to its purpose. There are three different materials within the RVE: the material from the matrix, the material of the fibers type 1 and the material of the fibers type 2. The matrix keeps the same material throughout the optimization, whereas the fibers may be assigned with a different material – material of fibers type 1 or type 2 – during the process. The ultimate goal of the optimization process is to achieve a better mechanical performance of the composite structure with regard to a criterion that is yet to be selected.

One of the important steps in gathering information on the problem was, therefore, the choice of the constituent materials. To have significant, interesting, results in an engineering point of view, the author chose to have two fiber material types with real context application and quite dissimilar mechanical properties. With that being, their combination delivers a wider range of possible applications. The material from the matrix was based on its compatibility with those from the fibers; aimed towards the potential manufacture of a real composite containing all three materials. The material properties, namely the Young’s modulus and Poisson’s ratio, of the matrix and fiber types 1 and 2 are presented in Table 1.

Table 1 – Material properties of the matrix and fiber types 1 and 2 [42, 43, 44, 45].

<table>
<thead>
<tr>
<th>Material</th>
<th>Young’s Modulus, $E$ [GPa]</th>
<th>Poisson’s Ratio, $\nu$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Matrix (Epoxy resin)</td>
<td>3.53</td>
<td>0.347</td>
</tr>
<tr>
<td>Fiber type 1 (Carbon fiber)</td>
<td>436</td>
<td>0.270</td>
</tr>
<tr>
<td>Fiber type 2 (E Glass fiber)</td>
<td>72.0</td>
<td>0.200</td>
</tr>
</tbody>
</table>

As indicated in Table 1, the materials assigned to the matrix and fiber types 1 and 2 were, respectively, epoxy resin, carbon and E glass. This table only shows the Young’s modulus and Poisson’s ratio because it was assumed that these three materials are isotropic. Isotropic materials have only two independent elastic constants, from which the remaining can be calculated. Young’s modulus and Poisson’s ratio were chosen because this is one of the sets of properties that Premat is programmed to accept as an input. The particular choice of epoxy resin, carbon and E glass has no other special reason than these being engineering materials with plenty of current application in engineering related industries, such as automotive, aerospace, among others. Their costs as raw materials were not taken into consideration because this work focuses on achieving a qualitative study on the optimization of fiber material distribution, more than assessing aspects related with the actual manufacture of the composite.

The main assumptions made in carrying out this work, some of which already mentioned, are summarized in the following items:

- Matrix and fiber materials are isotropic materials;
- There is a seamless connection between the matrix and the fibers, i.e., they are perfectly bound to each other;
• The deformations undergone by the composite material are in the range of linear elastic deformation;
• The composite material can be described, without major loss of information, as having a periodic microstructure.

Despite these hypotheses, the problem continues to have a general scope both as an academic case study as a potential source of information for the manufacturing of real hybrid fiber reinforced composites. The matrix and fiber materials were considered to be isotropic because Premat is coded to handle isotropic materials. A perfect binding between fibers and matrix was assumed to avoid having to dive into deeper micromechanical problems such as stress concentration on the border between the fibers and the matrix, or de-bonding, for instance. This work focuses only in the range of linear elastic deformation because the purpose of the study is not to deal with stress states that produce yielding of the material. Also because this assumption is reasonable for many engineering materials and engineering design scenarios, since most of the engineering parts are projected to work within the linear elastic range of the deformation curve. Finally, the forth hypothesis comes as a premise of the homogenization theory itself.

2.3.2 Identification/Definition of the design variables

The design problem of a hybrid composite structure with two fiber types can be compared with that of a topology optimization problem. Or on a similar perspective, to a DMO problem with only two materials to choose from. In topology optimization, one considers a mechanical element as a body occupying a domain \( \Omega^{mat} \) which is part of a larger reference domain \( \Omega \) in \( \mathbb{R}^2 \) or \( \mathbb{R}^3 \). The reference domain \( \Omega \) is chosen such as to allow the definition of the applied loads and boundary conditions. The concern is in the determination of the optimal placement of a given isotropic material in \( \Omega \) as to finding the best possible value for a certain condition; which often is the maximization of the stiffness of the structure. This is, one seeks for the points in space that shall be material points and which shall be voids (no material). \( \Omega^{mat} \) is the name given to the group of material points [20].

When the goal is to maximize the stiffness of the structure, one can state the optimal design problem as the particular problem of finding the optimal choice of the stiffness tensor \( E_{ijkl}(x) \), which is a variable over the reference domain \( \Omega \). The set of admissible stiffness tensors are the ones that attain the material properties of a given isotropic material in \( \Omega^{mat} \) and zero properties elsewhere [20]. Mathematically, this translates into the equation in (2):

\[
E_{ijkl}(x) = 1_{\Omega^{mat}}E^0_{ijkl}, \quad 1_{\Omega^{mat}} = \begin{cases} 1 & \text{if } x \in \Omega^{mat} \\ 0 & \text{if } x \in \Omega \setminus \Omega^{mat} \end{cases} \\
\int_\Omega 1_{\Omega^{mat}} d\Omega = Vol(\Omega^{mat}) \leq V
\]

(2)

Where the inequality in (2) expresses a limit, \( V \), on the amount of material available to the construction of \( \Omega^{mat} \), so that the maximum stiffness design is for a limited volume. The absence of such condition would
result in $\Omega^{\text{mat}}$ being the same as $\Omega$. The tensor $E_{ijkl}^0$ is the stiffness tensor for the given isotropic material. The way $E_{ijkl}(x)$ is expressed in (2) denotes that a distributed, discrete valued design problem, was formulated (a 0-1 problem) [20].

The most frequently used approach to solve this problem is to replace the integer variables with continuous variables and introduce a way to penalize any intermediate values in order to steer the solution back to discrete 0-1 values. The design problem for the fixed domain is formulated as a sizing problem by modifying the stiffness matrix so that it has a continuous dependence on a function which is interpreted as a density of material. This function is then the design variable. The requirement is that, in the end, the design consists almost entirely of material or no material regions. One way to force the values of this artificial density function to reach the 0-1 objective is through the use of SIMP model; a method that has proven very popular and extremely efficient [20]. Equation (3) shows how these concepts apply to the computation of $E_{ijkl}(x)$, which is now a continuous function:

$$E_{ijkl}(x) = \rho(x)^p E_{ijkl}^0, \quad p > 1$$

$$\int_{\Omega} \rho(x) d\Omega \leq V, \quad 0 \leq \rho(x) \leq 1, \quad x \in \Omega$$

(3)

Here, $\rho(x)$ is the design function, frequently designated as “density”, $E_{ijkl}^0$ still represents the material properties of a given isotropic material and $p$ denominates the material exponent, or penalization factor, used in the power law. The difference in (3) is that the relationship between $E_{ijkl}(x)$ and $E_{ijkl}^0$ is no longer discrete, it defines now a continuous problem.

In the specific problem being examined, there is no such thing as the distinction between $\Omega$ and $\Omega^{\text{mat}}$ domains. Although, there is a distinction between what can be defined as the matrix domain, $\Omega^{\text{matrix}}$, and the fibers domain, $\Omega^{\text{fibers}}$. If $\Omega^{\text{matrix}}$ is discarded of the equation, since nothing is changed there during the optimization process, and the whole attention turns to $\Omega^{\text{fibers}}$, it gets clear that there is an analogy between the concepts used in topology optimization and the ones trying to be addressed in this work. What in topology optimization is a matter of searching for material points and voids, in the hybrid composite optimization problem the issue is choosing between fiber type 1 and fiber type 2 materials. Thus, also here the notion of “density” as design function applies. Figure 10 shows the idea of “densities” adapted to the optimization of fiber reinforced hybrid composites.
Solving this problem through computational means demands the adoption of appropriate computational methods. A typical approach, and the one used throughout this monograph, as seen Figure 10, is to discretize the problem using finite elements. Finite element method is a classic, well-established, technique in topology optimization problems, which also perfectly served the purposes of the problem under consideration.

The notion of “densities” is, in topology optimization, applied to each single element that discretizes the domain. This causes mesh refinement to be a major issue regarding the result that outcomes from the optimization, in visual and structural terms. In the optimization of fiber reinforced hybrid composites, the “density” refers not to a single element but to the bundle of elements that constitute the fiber. Here, the size of the elements is particularly important to achieve a smoother evaluation of the field variables, not causing a direct interference on the graphical look (the frame) of the final, optimized, RVE (which is fixed), although it can potentially lead to different final solutions.

### 2.3.3 Identification of a criterion to be optimized

The problem was investigated in terms of the pursuit for the maximum stiffness of the structure. More specifically, the optimization problem intended to maximize the elastic deformation energy of the composite, i.e., the energy stored by the material through elastic distortion caused by mechanical work. Its mathematical equation is presented in (4):

\[
U_{\text{elastic deformation}} = \epsilon^0_i E^H_{ijkl} \epsilon^0_k \quad i, j, k, l = 1, \ldots, 3
\]  

(4)
Where $\varepsilon_{ij}^0$ and $E_{ijkl}^H$ represent, respectively, the strain and the homogenized stiffness tensors. The problem was formulated so that the loading condition is applied in the RVE by means of an imposed displacement, which, in turn, is introduced by the user via the definition of an average, macroscopic, strain tensor $\varepsilon_{ij}^0$. It becomes then easy to observe that with $\varepsilon_{ij}^0$ being a constant, the maximization of the elastic deformation energy ($U_{\text{elastic deformation}}$) can only occur by increasing the homogenized stiffness of the composite material.

In simple, graphical, terms, this translates into the image displayed in Figure 11.

![Figure 11 – Hypothetical initial and final stress-strain curves of the composite.](image)

Figure 11 shows what the stress-strain curves of the composite material could look like before and after the optimization process. In this image, $\sigma$ denotes the stress, $\varepsilon$ represents the strain, $\varepsilon_0$ is the limit value of strain in the elastic range of the deformation, and $E_i$ and $E_f$ are the initial and final Young’s modulus of the composite – given by the slope of the respective lines. Figure 11 illustrates a different, simplified, way to comprehend the dependence between the elastic deformation energy (area below the elastic portion of the curves) and the stiffness (measured by the Young’s modulus, in this representation). In the particular case of being imposed a strain value equal to $\varepsilon_0$, it is clear to understand that the elastic deformation energy (the green area) will be larger the greater the slope of the curve is, which, in Figure 11, represents the measure of stiffness.

Unlike what is intended in topology optimization, in the fiber reinforced hybrid composite optimization problem one is interested in the determination of the optimal placement of a number of isotropic materials (two in this specific case) in a confined area in space. The way $E_{ijkl}(x)$ varies along the domain, as well as its dependence in terms of the design variables is, therefore, different. To tackle this individual sub problem, DMO methodology was used. DMO is a method that allows transforming a discrete optimization problem into a continuous optimization problem when there is more than one material to choose from, or when there is one material that can be used in different orientations (orthotropic material). This method computes the
constitutive tensor of each fiber, $E_{ijkl}$, as a weighted sum of a finite number of constitutive tensors, $E_{ijkl}^n$, predefined and fixed. Each of these different tensors correspond to a different candidate; in this case fiber type 1 and fiber type 2 materials. The general expression for the computation of the stiffness tensor of a fiber $f$ from a $n$ number of possible candidates is given in (5):

$$E_{ijkl}^f = \sum_{n=1}^{N_c} w_{nf} E_{ijkl}^n = w_{1f} E_{ijkl}^1 + w_{2f} E_{ijkl}^2 + \cdots + w_{Ncf} E_{ijkl}^{Nc}, \quad 0 \leq w_{nf} \leq 1 \quad (5)$$

Where $N_c$ is the total number of candidates and the $w_{nf}$ are the weight functions associated with each of the candidates. The goal in DMO is to assign the value 1 to a single weigh function, all others being zero at the end of the optimization process. (6) expresses the formulation for a problem having only two materials to choose from:

$$E_{ijkl}^f = w_{1f} E_{ijkl}^1 + w_{2f} E_{ijkl}^2 = w_{1f} E_{ijkl}^1 + (1 - w_{1f}) E_{ijkl}^2, \quad 0 \leq w_{nf} \leq 1, \quad n = 1, 2 \quad (6)$$

Where a simplification allowing the existence of only one weight function was derived due to the increased straightforwardness of such problems. The parametrization employed in solving the fiber reinforced hybrid composite optimization problem is then found in (7):

$$E_{ijkl}^f = \rho_{fp} E_{ijkl}^1 + (1 - \rho_{fp}) E_{ijkl}^2, \quad p > 1, \quad f = 1, \ldots, 16 \quad (7)$$

Where variables showing a $f$ subscript are individually computed for each of the sixteen existing fibers. $E_{ijkl}^1$ and $E_{ijkl}^2$ correspond to the isotropic fiber type 1 and fiber type 2 materials, respectively. And the weighted function can be replaced by the penalized design variable, $\rho_{fp}$. This is possible because in this particular situation, since the aim is that $\rho_{fp}$ are assigned the values 1 or 0, when they are attributed one of these two values, due to the formulation of (7), one of the $E_{ijkl}^n|_{n=1,2}$ is automatically cancelled. It is then clear to see that the density interpolates between the material properties $E_{ijkl}^1$ and $E_{ijkl}^2$:

$$E_{ijkl}^f(\rho_f = 0) = E_{ijkl}^2, \quad E_{ijkl}^f(\rho_f = 1) = E_{ijkl}^1 \quad (8)$$

Meaning that if the final design has density zero or one in all fibers, that design is comparable with a black-and-white design from topology optimization. And such result gives a positive clue about the correct evaluation of the physical model and the performance of the optimization process.

### 2.3.4 Identification of the constraints

Once set the optimality criterion and the design variables, the next, and final, step corresponded to the identification of the constraints. These are usually applied in order to guarantee that specific performance requirements of the structure are met. This problem was formulated under two main constraints: a fiber type
volume constraint and an average stress constraint; independently applied to different case studies. The fiber type volume constraint in presented in (9):

$$\sum_{f=1}^{N_f} A_f \rho_f \leq V, \quad 0 \leq \rho_f \leq 1$$

(9)

Where $N_f$ is the total number of existing fiber in the RVE (sixteen in the standard RVE) and $A_f$ denotes the transversal area of the fiber, which is a constant since every fiber has the same dimensions. This constraint intends to limit the number of fibers having a specific fiber type material. As observed in (8), when the densities are assigned with value 1 the fibers are given fiber type 1 material, which happens to be the stiffest material (see Table 1). Since one is trying to reach the stiffest possible configuration, without such constraint every fiber would be given fiber type 1 material. It is therefore concluded that the lower the value of $V$, the lower the number of fibers being assigned with fiber type 1 material. An actual example is, for instance, when quantity $V/A_f$ equals 8. Such number means that there are eight densities, $\rho_f$, assigned with value 1.

When a RVE has, as the standard RVE, sixteen fibers, this leads to a final layout having 50%/50% distribution of fiber types 1 and 2 materials. If, on the other hand, the RVE had only, for instance, 10 fibers, this ratio would increase to 80%/20%.

The mathematical expression used to introduce the average stress constraint is featured in (10):

$$\sigma_{ij}^0 \sigma_{ij}^0 \leq S, \quad i, j = 1,...,3$$

(10)

Where $S$ expresses a limit on the maximum possible value of the square of the Euclidean norm of the stress tensor $\sigma_{ij}^0$, which was considered to be a valid indicator about the magnitude of the stresses within the RVE. The stress tensor, $\sigma_{ij}^0$, was computed as shown in (11):

$$\sigma_{ij}^0 = E_{ijkl}^\text{h} \varepsilon_{kl}$$

(11)

Regardless of being a constraint mainly focused on controlling the stress distribution within the RVE, the limitation introduced by (11) also acts indirectly as a fiber type volume restriction, and could thus be applied independently of its existence. This happens as a result from the very presence of two different types of fibers within the RVE. With one being stiffer than the other, they contribute differently to the overall stress state. Since the material with greater stiffness introduces, for a same strain condition, a higher stress contribution than the lower stiffness material, the constraint acts to control the number of fibers assigned with it. Figure 11 also helps understand this concept: if one imagines that $E_i$ is the Young’s modulus of the weaker fiber type material (fiber type 2 material) and $E_f$ is the Young’s modulus of the stronger fiber type material (fiber type 1 material), when imposed the same strain value, $\varepsilon_0$, the stronger material shows a stress value that is higher. Once the average stress constraint seeks to impose a limit on the maximum
stress value observed inside the RVE, then it automatically also limits the number of fibers being assigned with fiber type 1 material.

Having been gathered all the required information for the formulation of the problem, this could finally be established as presented in (12):

\[
\text{Objective: } \max_{\rho \in \Omega_{\text{fibers}}} U_{\text{elastic deformation}} = \varepsilon_{ij}^0 E_{ijkl}^H \varepsilon_{kl}^0 \\
\text{Subject to: } \begin{cases} 
0 \leq \rho_f \leq 1, & f = 1, ..., 16 \\
\sum_{f=1}^{N_f=16} A_f \rho_f \leq V \quad (\text{Volume}) \\
or \\
\sigma_{ij}^0 a_{ij}^0 \leq S \quad (\text{Stress})
\end{cases}
\]

(12)

The problem formulation in (12) translates the descriptive statement of the design optimization problem, presented in "Scope of the problem" subchapter, into a well-defined mathematical statement. The remaining computational work was based on the pursuit for its solution.

2.4 Description of the computer programs

The following sections are fully dedicated to the description of the computer programs that were developed with the purpose of solving the fiber reinforced hybrid composite design optimization problem, as well as all the important details that characterize them. The computer problems will be lectured in the following order: RAND_uSTRU_GEN, 3DMeshGENAbaqus2D and CompositeOpt. Exhaustive flowcharts graphically depicting their working processes can be found in Appendix A.

2.4.1 RAND_uSTRU_GEN

RAND_uSTRU_GEN is the name of a fairly recent algorithm whose purpose is to generate transversal cross-sections of long-fiber reinforced composite materials. This algorithm was created by Melro, Camanho and Pinho (2008) [40] to fulfill a common setback within the existing methods at that time: their incapacity to generate high fiber volume fraction composite models. In an industry demanding, every day, more and more the use of composite materials, companies are searching for cost-effective techniques capable to accurately predict the elastic properties of composites from the properties of their constituents. Traditional methods like conducting a full experimental campaign in order to characterize a given mixture of constituents for a given reinforcement's volume fraction are becoming increasingly rare, as they require a considerable amount of human, financial and time resources. The current trend is to decrease the dependence on experimental data by complementing it with numerical and/or analytical processes based on knowledge from micromechanics coupled with the application of FEA. It is precisely in the computational characterization stage of the process that RAND_uSTRU_GEN proves quite useful. A flowchart describing
the functioning of the algorithm is found in Figure 57 (Appendix A). For more detailed information about the program and the principles behind its operation, the reader is recommended to read [40].

2.4.1.1 Geometric reinforcement distribution

The aim of building a complementary algorithm to generate a geometric distribution of the reinforcements was, in first place, to create a tool that could help better understanding if the results obtained at the end of the optimization phase made sense according to the user’s own intuition. Secondly, to create a point of comparison between the random and geometric designs in order to conclude on the advantages and disadvantages of one against the other. The flowchart of this algorithm is presented in Figure 61 (Appendix A).

The geometric fiber distribution algorithm is only run in the end of RAND_uSTRU_GEN routine so it has access to all the important information used in building the random fiber distribution RVE. Namely: the real number of fibers, \( N_{\text{fibre}\_\text{real}} \), in the RVE (half fibers and corner fibers are only count once), the fiber radius, \( R \), and the width, \( a \), of the RVE (this algorithm is only prepared to generate square RVEs). The results, as shown in Figure 61, come in one of two possible ways: as an array containing the coordinates of the center of the fibers in the RVE, or as an error message – whenever the algorithm cannot find a geometric distribution that fits inside the RVE boundaries. There are four different types of fiber distribution layouts that the algorithm can generate. Examples are displayed in Figure 12.

![Figure 12 – Four types of geometric fiber distribution layouts.](image)

(a) (b) (c) (d)

Figure 12 – Four types of geometric fiber distribution layouts. a) \( x \times x \) type of layout, b) \( x + x + \cdots \) type of layout, c) \( x + (x - 1) + x + \cdots \) type of layout and d) \( (x - 1) + x + (x - 1) + \cdots \) type of layout; where \( x \) designates the number of fibers in the row with higher number of fibers.

Their specific designations are related to the number of fibers per row and the number of existing rows. To that extent, layouts having a number of fibers, \( N_{\text{fibre}\_\text{real}} \), that is a perfect square are designated “\( x \times x \)”; the remaining, depending on the number of fibers they have in each row, are designated “\( x + x + \cdots \)”, “\( x + (x - 1) + x + \cdots \)” and “\( (x - 1) + x + (x - 1) + \cdots \)”, where the number of sums corresponds to the number of rows.

2.4.1.2 Modifications

The modifications were mainly at the level of the outputs generated by the program. Since Abaqus was intended to make a first, bi-dimensional, mesh on the RVE – for the sake of ease and time saving –
RAND_uSTRU_GEN output module had to be accordingly changed to meet its needs. RAND_uSTRU_GEN is, by default, programmed to code a python script file that can be run by Abaqus to generate a sketch of the RVE, as exemplified in Figure 13 (left). However, this code was taken a step further to automatically undertake the whole process that goes from the sketching to the mesh generation phase (Figure 13, on the right), and the creation of an output text file containing all the necessary mesh information to serve as an input to 3DMeshGENAbaqus2D.

In summary, the steps that were incorporated/adjusted in the output module are, in sequential order, pinpointed in the following; these are transversal steps for building and meshing a CAD model in regular FEA commercial software:

- Draw the matrix and each fiber in disjointed sketches;
- Assign different parts to every sketch;
- Create materials for the matrix and the fibers;
- Assemble the parts;
- Generate a mesh for every part;
- Merge the meshes of every part to create a unique, assembled, mesh; and finally
- Write an Abaqus input file.

The reason why fibers were programmed to be drawn in different sketches is related to the need of making traceable the mesh elements that constitute them. Another detail lies within the creation of matrix and fiber materials inside Abaqus. Even though this option was made available, there is no need to assign any
particular material properties in such an early phase since they need to be manually introduced in a later stage of the process.

2.4.1.3 The standard RVE

The standard RVE (see Figure 7 or Figure 10) is a sixteen fiber reinforced RVE having a 50.27% fiber volume fraction. It is a square RVE, like all other RVE examples presented in this document. But it could be as well a rectangular RVE since all programs developed in this study are set up to support an RVE with a rectangular shape (exception made to the geometric fiber distribution algorithm). Square RVEs were chosen as a matter of simplicity and symmetry. A high fiber volume fraction was used to demonstrate the potential of RAND_uSTRU_GEN, although not very high not to overload the RVE with fibers. Finally, the RVE was chosen to contain sixteen reinforcements in an attempt to exhibit results on a representative volume with medium dimensions. The major limitation to this number was undoubtedly the time it required to perform the optimization process, which was found to increase exponentially with the size of the RVE.

In RAND_uSTRU_GEN, the relationship between the fiber radius, $R$, the width, $a$, and height, $b$, of the RVE is set by a parameter called delta, $\delta$. This parameter is defined as the ratio expressed in (13):

$$\delta = \frac{\text{RVE width, } a}{\text{Fiber radius, } R} \quad (13)$$

Where both $\delta$ and $R$ are entered by the user and the width and height of the RVE are computed accordingly. In case the user wants a rectangular RVE, a constant has to be manually introduced in the respective line of the Matlab file where these dimensions are calculated. In this particular study, a $\delta$ and $R$ values equal to 10 and 0.01 were, respectively, used. Trias et al. (2006) [46] demonstrated that, for long-fiber reinforced composites made of carbon fiber and epoxy matrix, a $\delta$ equal to 50 should be used to consider the RVE representative of the composite material. Unfortunately, that input could not be employed into this work as it would result in an unaffordable need for computational power. This also applies to the mesh size: the element size used was $\frac{a}{19}$; while not resulting in an excessively coarse mesh (see Figure 10), it could certainly be more refined so that there was a more fluid variation of the field variables. Anyway, the real object of study of this work is to show that there is an optimum distribution of the available fiber materials, which can be calculated to take greater profitability of the composite. The author tried to take the RVE to its potentially conceivable limits within the available timeframe.

Regarding the fiber distribution layout in the RVE, it was randomly selected from an endless number of options with a single criterion: the arrangement should have both half fibers and corner fibers. There is no explanation behind this option other than, once more, show the potential of RAND_uSTRU_GEN algorithm. While the layout design of the fiber distribution is naturally an important variable, a research by Matsuda et al. (2003) [47], which compared the elastic-viscoelastic behavior of long-fiber reinforced laminates subjected to in-plane tensile loading using homogenization theory, concluded that the spatial distribution of the reinforcements in the RVE does not affect the macroscopic response of laminates, but it significantly affects
the microscopic stress distribution. From where one can conclude that the fiber distribution layout can be especially interesting in studies dealing with the onset and propagation of damage in the matrix.

2.4.2 3DMeshGENAbaqus2D

3DMeshGENAbaqus2D is a program that was particularly designed to act as part of the solution of the research problem discussed in this document. It functions as a bridge connecting RAND_uSTRU_GEN and CompositeOpt. Its construction only took place because one realized that a 3D mesh entirely generated in Abaqus on top of a, built from scratch, tridimensional RVE CAD model would not possess the necessary requirements to be directly used in Premat meshing module. The reason being the lack of symmetry between the opposite surfaces of the mesh, i.e., the nodal positions of the elements situated in the surface of the representative volume did not match across the RVE’s thickness, width and/or height. This problem was producing an inability of Premat correctly generating the periodicity conditions. Consequently, a more disaggregated solution where Abaqus was only used to generate a bi-dimensional mesh over a bi-dimensional RVE model was preferred, being every other additional steps made outside Abaqus.

3DMeshGENAbaqus2D is divided in five different submodules: a routine that calls and opens an Abaqus window to show the user the different parts (matrix and fibers) and the mesh, another to read the text file generated by Abaqus and store its information, two other modules to add thickness to the bi-dimensional RVE mesh, add intermediate points and discretize the new tridimensional domain using tetrahedral elements, and a final routine to output all this new information into a text file. A flowchart describing in more detail the operation processes of the 3DMeshGENAbaqus2D is found in Figure 58 (Appendix A).

2.4.2.1 Generation of the tridimensional mesh

As mentioned above, the tridimensional mesh was built on top of a bi-dimensional mesh generated by Abaqus. To accomplish this, the process was divided into three distinct phases. First, thickness, \( t \), was added to the mesh. This was achieved by creating a second layer of mesh elements and moving them apart, in parallel, from the first of a certain distance equal to the desired thickness. In computational terms this translates into running a loop where command (14) is executed in each iteration:

\[
\text{position}(i + N^{\text{nodes}}, j) = \begin{cases} 
    i + N^{\text{nodes}} & \text{for } j = 1 \\
    \text{position}(i, j) & \text{for } j = 2 \text{ or } 3, \quad i = 1, ..., N^{\text{nodes}}, \quad j = 1, ..., 4 \\
    t & \text{for } j = 4 
\end{cases} 
\]  

(14)

Where \( \text{position} \) refers to the array storing element’s nodal information (nodal number in the first column, \( x \), \( y \) and \( z \) coordinates in the second, third and fourth columns, respectively) and \( N^{\text{nodes}} \) is the total number of nodes of the bi-dimensional mesh. A schematic representation of the procedure is presented in Figure 14. The number of nodes are, consequently, duplicated by the end of this cycle. The second layer of mesh elements shares the exact same \( x \) and \( y \) coordinates with the original one, but having a \( z \) coordinate equal to the thickness, \( t \), assuming that the original bi-dimensional mesh is situated in the origin of the \( z \) axis. The value assigned to the thickness is not particularly important because it does not influence the
homogenization process. In this work, this specific value was set equal to $a/5$, where $a = 0.1$. A value big enough to add visual depth to the 3D RVE and small enough to avoid excessively high aspect ratio tetrahedral elements.

The second step was the creation of additional, intermediate, nodes in order to prepare the mesh for the third, and final, step: dividing the mesh into tetrahedral elements. The discretization of the 2D RVE model was done using triangular mesh elements (as seen in the meshed RVE from Figure 13, or in Figure 14). This means that when the second layer is generated, the three-dimensional mesh is composed of triangular prismatic elements. These, in addition to making a poor, unsatisfactory, discretization of the RVE since, for instance, do not allow the variation of the field variables in the thickness direction, are not supported by Premat. The solution to overcome this problem was dividing each triangular prism into three tetrahedrons. Figure 15 illustrates this process.

The intermediate nodes were introduced in the middle of the edges that join each of the vertices $a$, $b$, $c$, $d$, $e$ and $f$ of the respective tetrahedrons (see Figure 15). The elements used to discretize the 3D RVE were, therefore, 10-node tetrahedrons. These were preferred to 4-node tetrahedral elements because they enable a more accurate assessment of the phenomena that take place inside the domain.

An additional, and final, remark is left regarding Abaqus meshing module. The author decided to force the user to manually close Abaqus window, instead of just running Abaqus in the background, so that the user has the opportunity to verify the non-occurrence of meshing errors as the one exposed in Figure 16.
Figure 16 – Abaqus meshing error.

Figure 16 shows a mesh containing overlapping elements. This error is likely to occur for element sizes that are too large to describe the smallest details of the RVE. The author’s experience has demonstrated that such error creates a discontinuity in the mesh, preventing the affected elements to be properly processed in further steps of the optimization process.

2.4.2.2 Influence of the element size

The influence of the mesh size in the time required to perform the optimization process was already mentioned in “The standard RVE” section. This next segment presents a brief study that clearly shows the relationship between the element size and the time 3DMeshGENAbaqus2D and Premat homogenization module take to build the tridimensional mesh and complete the homogenization process, respectively. Three distinct meshes were analyzed: the coarser having an element size equal to \( \frac{a}{10} \), the intermediate having an element size equal to \( \frac{a}{19} \) and the more refined having an element size equal to \( \frac{a}{30} \); all three used to discretized the same RVE, the standard RVE. The three meshes are displayed in Figure 17.

Figure 17 – Standard RVE meshed with \( \frac{a}{10} \), \( \frac{a}{19} \) and \( \frac{a}{30} \) element sized meshes.

Table 2 summarizes the results, showing also complementary information such as the number of elements and nodes that each of the meshes contains. Additionally, it provides an estimate of the minimum total time required to perform the optimization process.
Table 2 – Analysis of the relationship between mesh element size and running time of the computer programs.

<table>
<thead>
<tr>
<th>Element size</th>
<th>No. of elements</th>
<th>No. of nodes</th>
<th>Time to build 3D mesh [s]</th>
<th>Time to perform homogenization [s]</th>
<th>Time to perform optimization [h]</th>
</tr>
</thead>
<tbody>
<tr>
<td>a/10</td>
<td>1224</td>
<td>2595</td>
<td>≈43</td>
<td>≈16</td>
<td>≈0.31–0.89</td>
</tr>
<tr>
<td>a/19</td>
<td>2460</td>
<td>5157</td>
<td>≈172</td>
<td>≈135</td>
<td>≈2.63–7.50</td>
</tr>
<tr>
<td>a/30</td>
<td>6432</td>
<td>13245</td>
<td>≈1299</td>
<td>Unable to run^2</td>
<td>-</td>
</tr>
</tbody>
</table>

The author draws the reader’s attention to the fact that the standard RVE – the one that will be featured in “CHAPTER 3 – Results” – was discretized using a mesh element size equal to $\frac{a}{19}$. Table 2 shows that the time per run increases very quickly to completely unsustainable values for relatively small decreases in the element size. Last column indicates, with good, although conservative, approximation, the time intervals required to perform each optimization analysis, concerning the volume constrained case studies. This time frame was computed based on the average number of runs required to achieve convergence of the solutions. In most cases, these range between 70 and 200, where each run is particularly characterized by the time it takes to perform the homogenization process. Such estimate was therefore obtained as a result of the multiplication between the times in “Time to perform homogenization” column and the average number of runs for solution convergence.

The estimate does not include the application of the stress constraint because, as further mentioned in “Design variables update algorithms” section, the methods used to perform the optimization process for these two constraints were different. With the time-to-convergence in stress constrained case studies being much more variable (see number of cumulative internal loops/runs in Table 5). An estimate of the computation time for these examples can also be obtained by multiplying the number of internal loops by 135s. Additionally, Table 5 shows that, for the lower third of the results, the number of cumulative internal loops was kept around, or under, 200. This was ultimately achieved through an experimental process of trial and error, by introducing simple measures to increase the convergence tolerance and limit the number of internal loop iterations of the optimization algorithm.

2.4.3 CompositeOpt

CompositeOpt is the third, and last, Matlab program involved in the solution of the problem. The outputs it generates are the final optimization results, which can be analyzed by the user. This program’s structure is slightly more complex than the previous two. Figure 59 and Figure 60 (Appendix A) show an in-depth, descriptive, flowchart of CompositeOpt’s computational routine. From all the processes that make up CompositeOpt, the author highlights the most important as being: the routines that call mesh3d and hmg3d

---

1 These times refer to an estimate based on the average number of runs required to achieve solution convergence in the optimization process of the volume constrained case studies. The stress constrained case studies were excluded of this assessment due to the unpredictability in their optimization process (refer to “Design variables update algorithms” for more detailed information on the optimization algorithms).

2 The memory required to store the stiffness matrix exceeds the limit allowed by the Fortran compiler used to compile Premat.
(Premat meshing and homogenization modules, respectively) and store their data, the module that computes the objective function and the module that updates the design variables. These constitute the core of the program.

The general idea of the program is to apply a fixed deformation, through a strain imposition, to the RVE and, based on the gradient of the objective function and the restrictions on the design, compute the layout that best responds to that loading condition. While the explicit expressions of the objective function and the volume and stress constraints were already stated in “Problem formulation and parametrization of design” section, the mathematical formulation of their gradients was not presented yet. The gradient of the objective function derives from the mathematical equation of the objective function as follows:

\[
\frac{\partial}{\partial \rho_f} (U_{\text{elastic deformation}}) = \frac{\partial}{\partial \rho_f} (\varepsilon_{ij}^0 E_{ijkl}^H \varepsilon_{kl}^0) = \varepsilon_{ij}^0 \frac{\partial E_{ijkl}^H}{\partial \rho_f} \varepsilon_{kl}^0 \quad i, j, k, l = 1, ..., 3 \tag{15}
\]

Where the derivatives of the homogenized coefficients, \(E_{ijkl}^H\), in order to the design variables, \(\rho_f\), was computed as mathematically formulated in [20] (refer to pp. 124 of the previous reference).

And the gradient of the volume and stress constraints can be expressed as stated in (16) and (17), respectively:

\[
\frac{\partial}{\partial \rho_f} \left( \sum_{f=1}^{N_f} A_f \rho_f \leq V \right) \iff \sum_{f=1}^{N_f} \frac{\partial}{\partial \rho_f} (A_f \rho_f) \leq \frac{\partial}{\partial \rho_f} (V) \iff \sum_{f=1}^{N_f=16} A_f \leq 0 \tag{16}
\]

\[
\frac{\partial}{\partial \rho_f} (\sigma_{ij}^0 \sigma_{ij}^0 \leq S) \iff \frac{\partial}{\partial \rho_f} (\sigma_{ij}^0 \sigma_{ij}^0) \leq \frac{\partial}{\partial \rho_f} (S) \iff 2 \frac{\partial \sigma_{ij}^0}{\partial \rho_f} \sigma_{ij}^0 \leq 0 \iff 2 \frac{\partial E_{ijkl}^H}{\partial \rho_f} \varepsilon_{kl}^0 E_{ijkl}^H \varepsilon_{kl}^0 \leq 0 \tag{17}
\]

Collected all this information, the update of the design variables comes down to the use of an algorithm specifically built for that matter. Many algorithms can be found in the literature addressing this issue. Examples of works covering this subject – such as [16] and [17] – have already been presented in the introductory chapter. The next paragraphs are occupied with describing the options chosen in this work.

### 2.4.3.1 Design variables update algorithms

Due to the natural resemblance, already highlighted in the previous sections, of the fiber reinforced hybrid composite optimization and topology optimization problems, the algorithm chosen to perform the update of the design variables derived, very naturally, from a proposal described in Topology Optimization – Theory, Methods and Application [20], written by Bendsøe and Sigmund (2003). This updating scheme, referred by its authors as condition of optimality, is presented in (18):

\[3\]

3 The variables \(\rho_K\), \(\rho_{K+1}\) and \(B_K\) in expressions (18) and (19) are fiber dependent. This dependency is not clearly stated in order to ease the comprehension of the expressions.
\[ \rho_{K+1} = \begin{cases} \max\{(1-\zeta)\rho_K, \rho_{\text{min}}\} & \text{if } \rho_K B_K^\eta \leq \max\{(1-\zeta)\rho_K, \rho_{\text{min}}\} \\ \min\{(1+\zeta)\rho_K, 1\} & \text{if } \min\{(1+\zeta)\rho_K, 1\} \leq \rho_K B_K^\eta \\ \rho_K B_K^\eta & \text{otherwise} \end{cases} \] (18)

Where \( \rho_K \) denotes the value of the design variable (density) at iteration step \( K \), \( \rho_{\text{min}} \) symbolizes the minimum attributable density value, \( \zeta \) is a move limit and \( \eta \) is a tuning parameter. Both \( \zeta \) and \( \eta \) were used to control the changes that can happen at each iteration step. They can be adjusted, by experiment, for efficiency of the method. [20] sets typical values of \( \zeta \) and \( \eta \) as being 0.2 and 0.5, respectively. A lower bound, \( \rho_{\text{min}} \), was introduced on the density in order to prevent the appearance of any possible singularities in the mathematical calculations related to the stiffness matrix of the homogenized composite. Although, as it is, such occurrence being impossible by the DMO formulation employed. \( B_K \) is, in this particular problem, given by the expression:

\[ B_K = \frac{\varepsilon_{ij}^0 \left( \frac{\partial E_{ijkl}^\eta}{\partial \rho} \right)_K \varepsilon_{kl}^0}{\lambda_k} \] (19)

Here \( \lambda_k \) refers to the Lagrange multiplier of the constraints in (9) and (10). Notice, however, that they are never present simultaneously. \( B_K \) is directly related to the fulfillment of the volume constraint. Bottom line, (19) is a necessary condition for optimum. When \( B_K \) equals a unitary value, it means that a local optimum was reached. Other possibilities are \( B_K > 1 \) and \( B_K < 1 \), to which the algorithm responds by, respectively, “adding” and “removing” material in those regions (in topology optimization terminology). In other words, increasing or decreasing the value of that specific \( \rho_f \) being updated. This action is, as seen in (19), dependent on the elastic deformation energy. More precisely, on its sensitivity to a variation in the values of the design variables; where the “addition” or “removal” of material from a specific region of the domain is determined according its influence on the overall stiffness of the structure, in comparison to other, different, regions. In this context, the Lagrange multiplier acts as the mediator value which determines the regions to be stiffened, while ensuring, at the same time, the compliance with the volume/stress constraint.

It is emphasized that, in this previous discussion, whenever the author referred to the “addition” or “removal” of material, in hybrid composite terminology this translates into assigning a stiffer or less stiff material – a fiber type 1 or fiber type 2 material. A second remark to the fact that it was assumed that the bounds limiting the values of the densities are not violated in any of the aspects discussed in the preceding paragraph; the very formulation of (18) does not allow this to happen. In addition, a final observation to clarify that expressions (18) and (19) are fiber dependent. This dependence was not introduced in their formulation to avoid an overload of indexes, which would difficult their comprehension. In topology optimization they would be, for instance, elementwise dependent. For a descriptive and more technical analysis on the derivation of equation (19), the significance of Lagrange multiplier \( \lambda \), its influence in the design variables and, overall, their meaning within the context of the problem, the reader is recommended to take a look in the first chapter of [20].
This updating scheme works predominantly well with constraints that have a direct dependence on the design variables, such as the volume constraint, as observed in (9). In contrast, the implementation of this scheme to a problem with a stress constraint as the one formulated in (10) is extremely inefficient. This happens because the update $\rho_{K+1}$ depends on the present value of the Lagrange multiplier, $\lambda_K$, and thus $\lambda_K$ needs to be constantly adjusted in an inner iteration loop in order to satisfy the active constraint (it being volume, stress, or other). If this adjustment cannot be done quickly, as with the stress constraint, due to the need to, at every new design variable’s set, compute a new stress tensor – meaning that a new homogenization process needs to be undertake – the method becomes very slow.

To solve problems constrained by a stress restriction, the author then decided to use Matlab’s optimization tool fmincon with a SQP algorithm. Other optimization methods have been tested, such as: steepest descent and the conjugate gradient method (Fletcher and Reeves). Fmincon was eventually chosen by the superior quality of the results. All fmincon, steepest descent and conjugate gradient proved very slow tools/algorithms, so that, in an attempt to potentially find an improvement for this problem, a penalization of the objective function was introduced. In mathematical terms this is described as:

$$f_{\text{penalty}} = \varepsilon_{ij} E_{ijkl} e_{kl}^0 + \frac{1}{2} c \max(0, \sigma_{ij}^0 \sigma_{ij}^0 - S)^2$$  \hspace{1cm} (20)

$$\frac{\partial f_{\text{penalty}}}{\partial \rho_f} = \varepsilon_{ij} \frac{\partial E_{ijkl}}{\partial \rho_f} e_{ij}^0 + 2c \max(0, \sigma_{ij}^0 \sigma_{ij}^0 - S) \frac{\partial E_{ijkl}}{\partial \rho_f} e_{kl}^0 e_{kj}^0 e_{kl}$$  \hspace{1cm} (21)

Where (20) and (21) correspond, respectively, to the penalized objective function and its gradient. A penalized formulation of the objective function aims, precisely, to penalize structural designs that violate the constraints and, hopefully, steer the optimization process more proficiently to the solution. This is accomplished by the very formulation of the penalized function which acts as stated in (22):

$$f_{\text{penalty}} = \begin{cases} U_{\text{elastic deformation}} & \text{if } \sigma_{ij}^0 \sigma_{ij}^0 - S \leq 0 \\ \infty & \text{if } \sigma_{ij}^0 \sigma_{ij}^0 - S > 0 \end{cases}$$  \hspace{1cm} (22)

Naturally, assigning infinity to the value of the penalized function is exaggerated. But the level of penalization is subject to be controlled by the parameter $c$, oftentimes called penalty factor. Its value depends on each specific case being investigated but, typically, there is a $c$ that makes the solution tend to a constant. After that threshold, higher penalty factors do not add any worthwhile value to the solution.

Fmincon is prepared to deal with minimization problems. Because the problem addressed in this document was formulated as a maximization problem, changes had to be made to make it solvable by fmincon. The relationship between maximization and minimization problems in presented in (23):

$$\max f(x) = - \min(-f(x))$$  \hspace{1cm} (23)
A maximization problem corresponds to minus the result of the minimization of the negative of the objective function. (23) allows the transformation of maximization problems into minimization problems, or vice versa, and it was successfully used to convert the problem under investigation.

2.4.3.2 Convergence criteria
The application of the volume and stress constraints to the problem formulation adds different levels of complexity to the optimization algorithm. Accordingly, the criteria used to assess for solution convergence in each of them were left different. Due to the increased complexity introduced by the stress constraint, coupled with the apparent lack of convergence of the solutions obtained by fmincon, the author decided to leave the convergence assessment task in charge of the user. It should be noted as well that the “apparent lack of convergence” referred in the last sentence comes as a result, not of an inability of fmincon to generate satisfactory solutions, but with the difficulty to merge the solution to a 0-1 type of design.

Regarding the case of the volume constraint, a criterion resulting from a combination of three sub-criteria was applied:

- Convergence in terms of the values of the design variables;
- Convergence in terms of the value of the objective function; and
- Convergence in terms of the limit values of the design variables.

The first and second criteria set that the values of the design variables and the objective function, between iterations $K$ and $K + 1$, must be within a given tolerance specified by the user. The third checks for the so-called black and white (0-1) type of solution by inspecting whether the values of the design values are close to their possible limits, within a certain quantified margin. The first two are assessed together on an “or” basis, meaning that both of them are accepted as a measure of convergence. However, these are judged on an “and” basis with the third criterion to guarantee that the solution really is what the user is expecting. This combination came as a natural result from experience dealing with the optimization algorithm and, although highly demanding, it assures that, when the algorithm stops, the solution is adequate. On the other hand, this characteristic makes it hard, sometimes, for the algorithm to stop by itself. To overcome this problem, and avoid the generation of unnecessary iterations, the program asks the user if he wants stop or if he wants to change the material exponent to help the solution converge faster.

2.5 Case studies characterization
Several case studies were analyzed as part of this work. As previously mentioned, examples with a random fiber distribution RVE, as well as a geometric fiber distribution RVE, were considered. On top of that, three different cases of filling fiber pairs were studied. The first pair being the already revealed fiber type 1/fiber type 2 or, in terms of the nomenclature of the materials themselves, carbon fiber/E glass fiber. The second pair was fiber type 1/matrix, or carbon fiber/epoxy “fiber”; where the weaker fiber material was assigned the same material of the matrix. The objective in this one was to find out, among a number of possibilities...
defined a priori, which positions are the best if a certain number of fibers is to be placed within the RVE. The third, and final, pair was fiber type 1/void. And here the aim was similar to the previous but with an additional detail: the positions that are not filled with fibers remain as voids in the RVE. In either case, the default initial value assigned to the design variables, \( \rho_f \), was 0.5 to avoid giving the optimization routine any sort of early suggestion on the direction where to follow.

All the case studies were analyzed for a set of five different loading conditions. These are schematically presented in Figure 18.

This specific spectrum was chosen as a mean to explore and to get an insight on the quality of the results generated by the optimization tool described in this monograph. Figure 18 shows a variety of microstructural loading conditions that the author thought being representative enough of the various possible types of external loads applied on the composite structure. The conditions signaled by (d) and (e) cannot be considered completely hydrostatic loadings due to the way they are introduced in CompositeOpt. CompositeOpt is only prepared to generate a strain condition based on individual inputs of singular strains in the different directions. I.e., one can only say that wants a certain imposed strain in a specific direction, to which can be added other, individual, imposed strains with different values and directions. But this is not the same as having a strain loading that acts both, at the same time, in directions \( x \) and \( y \), for instance.

In all the examples the author attempted achieving a same volume fraction of 50% between the two types of filling fibers – it being fiber type 1 material, fiber type 2 material, matrix “fiber” or void. This means, concerning the particular RVEs used to perform this investigation (the standard RVE and the sixteen geometrically distributed fibers RVE), that the end result of the optimization was intended to be always a \( 8/8 \) fiber distribution between the two materials of the fiber pairs. With respect to the volume constraint, this was quite straightforward; regarding the stress constraint, an investigation had to be made in order to find the limit value, \( S \), that could lead to such result. There is no specific reason on why this particular division of the number of fibers was made. It should not influence the overall performance of the optimization.
program. However, this same fraction was kept equal among all the examples so they can be compared to each other.

For some case studies, a stress distribution analysis within the microstructure was conducted. The election of the examples was based on their potential interest for mutual comparison with other, different, layouts, given the same loading condition. For instance, comparing the stress distribution within a RVE constrained by a volume restriction and a RVE constrained by a stress restriction, loaded with case (a) from Figure 18. All these findings are displayed in CHAPTER 3 – Results.
CHAPTER 3 – Results

The third chapter addresses the results from the optimization analyses that have been undertaken on the demand for solving the problem described in the previous segment. First, a brief introduction to the color code used in the displayed figures is presented. Next, the results concerning the introduction of the volume constraint will be shown. The exhibition of the results obtained by the application of the stress constraint will follow. The final section of this chapter is devoted to presenting the outcome of the stress distribution analysis within the microstructure of the RVE, achieved through the use of Postmat.

3.1 Color code

All images follow the same color code: dark blue represents lower density materials and dark red represents higher density materials. Ideally the lower and higher density materials should always have densities equal to zero and one, respectively; meaning that a complete convergence of the solution was achieved. The real density value of the lower and higher density materials, as well the density value for the intermediate density material, is always displayed in a colored label below the image to which is assigned. Figure 19 shows an example of such label.

![Density Color Code](image)

Figure 19 – Standard label of the RVE’s optimization result images.

It should be noted that not always – namely in the volume constrained case studies – the lower density material will possess a density equal to zero due to the introduction of the lower bound, \( \rho_{\text{min}} \), on the attributable values for the densities. Second, the matrix has by default, in all cases, a density equal to 0.5 and, therefore, the color associated with it. Lastly, a recall regarding expression (8), which states that \( \rho_f = 0 \) corresponds to the weaker fiber material (E glass fiber, matrix “fiber” or void, depending the examples) and \( \rho_f = 1 \) corresponds to the stronger fiber material (always carbon fiber).

3.1.1 Stress distribution analysis results

A similar color code applies to the stress distribution analysis results. In this case, however, the label below each image shows the range of stress values, in MPa, present within the microstructure. The dark blue color still representing the lower value of the range and dark red the higher. Each image refers to a specific stress condition and is categorized accordingly. Figure 20 shows a practical example.
Where Figure 20 relates to an example of a uniaxial tensile stress in direction $x$, computed elementwise (EL Stress 11). The other possible categories are summarized in Table 3.

**Table 3 – Summary of the category designations of the RVE’s stress analysis images.**

<table>
<thead>
<tr>
<th>Category</th>
<th>Designation</th>
</tr>
</thead>
<tbody>
<tr>
<td>EL Von Mises Stress</td>
<td>Elementwise Von Mises stress distribution ($\sigma_{VM}$)</td>
</tr>
<tr>
<td>EL Stress 11</td>
<td>Elementwise uniaxial stress in direction $x$ ($\sigma_{xx}$)</td>
</tr>
<tr>
<td>EL Stress 12</td>
<td>Elementwise shear stress in the $xy$ plane ($\tau_{xy}$)</td>
</tr>
<tr>
<td>EL Stress 13</td>
<td>Elementwise shear stress in the $xz$ plane ($\tau_{xz}$)</td>
</tr>
<tr>
<td>EL Stress 22</td>
<td>Elementwise uniaxial stress in direction $y$ ($\sigma_{yy}$)</td>
</tr>
<tr>
<td>EL Stress 23</td>
<td>Elementwise shear stress in the $yz$ plane ($\tau_{yz}$)</td>
</tr>
<tr>
<td>EL Stress 33</td>
<td>Elementwise uniaxial stress in direction $z$ ($\sigma_{zz}$)</td>
</tr>
</tbody>
</table>

Although it may be obvious, the author notices that in this particular study, in contrast with the former, the matrix is not assigned any specific color because it is also part of the analysis.

### 3.2 Volume constraint case studies

The following sections present the results of the analysis carried out on the RVE subjected with a volume constraint. The examples begin with the random fiber distribution RVE, for all three cases of filling fiber pairs. This exposition will then continue with the exact same examples but for the geometric fiber distribution RVE.

#### 3.2.1 Random fiber distribution (standard RVE)

The subsequent case studies, Figure 21 and Figure 22, relate to the optimization of the standard RVE for filling fibers pair carbon fiber/E glass fiber, with the introduction of a volume constraint that limits the use of the stronger fiber material in 50% of the total number of fibers; in the particular case of the volume constraint examples, that will always translate into a maximum of 8 fibers.
Figure 21 – Optimization results of the random fiber distribution RVE filled with carbon/E glass fibers, with a volume constraint (part 1 of 2). a) Imposed uniaxial strain in the $x$ direction, b) imposed shear strain in the $xy$ plane, c) imposed uniaxial strain in the $z$ direction and d) imposed “hydrostatic” $\varepsilon_{xx} + \varepsilon_{yy}$ strain loading.
Figure 22 – Optimization results of the random fiber distribution RVE filled with carbon/E glass fibers, with a volume constraint (part 2 of 2). e) Imposed rotated shear $\varepsilon_{xx} + \varepsilon_{xy}$ strain loading; compressive component in x direction.

Charts depicting the evolution of the value of the objective function along the iterative process to the results presented in Figure 21 and Figure 22 can be found in Figure 62 (Appendix B).

The following case studies, Figure 23 and Figure 24, refer to the optimization of the standard RVE for filling fibers pair carbonfiber/epoxy “fiber”, with the introduction of the 50% limitation on the volume of fibers assigned with the stronger fiber material.

$U_{elast\,def} = 294.45 \text{ MPa}$

$U_{elast\,def} = 182.43 \text{ MPa}$

$U_{elast\,def} = 684.41 \text{ MPa}$

Figure 23 – Optimization results of the random fiber distribution RVE filled with carbon/epoxy fibers, with a volume constraint (part 1 of 2). a) Imposed uniaxial strain in the x direction and b) imposed shear strain in the xy plane.
Figure 24 – Optimization results of the random fiber distribution RVE filled with carbon/epoxy fibers, with a volume constraint (part 2 of 2). c) Imposed uniaxial strain in the $z$ direction, d) imposed “hydrostatic” $\varepsilon_{xx} + \varepsilon_{yy}$ strain loading and e) imposed rotated shear $-\varepsilon_{xx} + \varepsilon_{xy}$ strain loading; compressive component in $x$ direction.

Charts depicting the evolution of the value of the objective function along the iterative process to the results presented in Figure 23 and Figure 24 can be found in Figure 63 (Appendix B).

The final case studies within this segment, Figure 25 and Figure 26, relate to the optimization of the standard RVE for filling fibers pair carbon fiber/void, with the introduction of the 50% limitation on the volume of fibers assigned with the stronger fiber material. These are shown below.
Figure 25 – Optimization results of the random fiber distribution RVE filled with carbon fibers/voids, with a volume constraint (part 1 of 2). a) Imposed uniaxial strain in the $x$ direction, b) imposed shear strain in the $xy$ plane, c) imposed uniaxial strain in the $z$ direction and d) imposed "hydrostatic" $\varepsilon_{xx} + \varepsilon_{yy}$ strain loading.
Figure 26 – Optimization results of the random fiber distribution RVE filled with carbon fibers/voids, with a volume constraint (part 2 of 2). e) Imposed rotated shear $-\varepsilon_{xx} + \varepsilon_{xy}$ strain loading; compressive component in $x$ direction.

Charts depicting the evolution of the value of the objective function along the iterative process to the results presented in Figure 25 and Figure 26 can be found in Figure 64 (Appendix B).

### 3.2.2 Geometric fiber distribution

The subsequent case studies, Figure 27 and Figure 28, relate to the optimization of the geometric fiber distribution RVE for filling fibers pair carbon fiber/E glass fiber, with the introduction of a volume constraint that limits the use of the stronger fiber material in 50% of the total number of fibers.

Figure 27 – Optimization results of the geometric fiber distribution RVE filled with carbon/E glass fibers, with a volume constraint (part 1 of 2). a) Imposed uniaxial strain in the $x$ direction and b) imposed shear strain in the $xy$ plane.
Figure 28 – Optimization results of the geometric fiber distribution RVE filled with carbon/E glass fibers, with a volume constraint (part 2 of 2). c) Imposed uniaxial strain in the \( z \) direction, d) imposed “hydrostatic” \( \varepsilon_{xx} + \varepsilon_{yy} \) strain loading and e) imposed rotated shear \( -\varepsilon_{xx} + \varepsilon_{yy} \) strain loading; compressive component in \( x \) direction.

Charts depicting the evolution of the value of the objective function along the iterative process to the results presented in Figure 27 and Figure 28 can be found in Figure 65 (Appendix B).

The following case studies, Figure 29 and Figure 30, refer to the optimization of the geometric fiber distribution RVE for filling fibers pair carbon fiber/epoxy “fiber”, with the introduction of the 50% limitation on the volume of fibers assigned with the stronger fiber material.
Figure 29 – Optimization results of the geometric fiber distribution RVE filled with carbon/epoxy fibers, with a volume constraint (part 1 of 2). a) Imposed uniaxial strain in the $x$ direction, b) imposed shear strain in the $xy$ plane, c) imposed uniaxial strain in the $z$ direction and d) imposed “hydrostatic” $\varepsilon_{xx} + \varepsilon_{yy}$ strain loading.
Figure 30 – Optimization results of the geometric fiber distribution RVE filled with carbon/epoxy fibers, with a volume constraint (part 2 of 2). e) Imposed rotated shear $-\varepsilon_{xx} + \varepsilon_{yy}$ strain loading; compressive component in $x$ direction.

Charts depicting the evolution of the value of the objective function along the iterative process to the results presented in Figure 29 and Figure 30 can be found in Figure 66 (Appendix B).

The final case studies within this segment, Figure 31 and Figure 32, relate to the optimization of the geometric fiber distribution RVE for filling fibers pair carbon fiber/void, with the introduction of the 50% limitation on the volume of fibers assigned with the stronger fiber material. These are shown below.

Figure 31 – Optimization results of the geometric fiber distribution RVE filled with carbon fibers/voids, with a volume constraint (part 1 of 2). a) Imposed uniaxial strain in the $x$ direction and b) imposed shear strain in the $xy$ plane.
Figure 32 – Optimization results of the geometric fiber distribution RVE filled with carbon fibers/voids, with a volume constraint (part 2 of 2). c) Imposed uniaxial strain in the $z$ direction, d) imposed “hydrostatic” $\varepsilon_{xx} + \varepsilon_{yy}$ strain loading and e) imposed rotated shear $-\varepsilon_{xx} + \varepsilon_{xy}$ strain loading; compressive component in $x$ direction.

Charts depicting the evolution of the value of the objective function along the iterative process to the results presented in Figure 31 and Figure 32 can be found in Figure 67 (Appendix B).

A summary table, Table 4, containing the final optimization values of the objective function and the volume constraint violation, as well as the number of runs required to achieve full solution convergence and the reference maximum and minimum possible values of the objective function, can be found in Appendix B. This table includes both the random and geometric fiber distribution case studies.
3.3 Stress constraint case studies

The following sections present the results of the analysis carried out on the RVE subjected with a stress constraint. Examples will be presented regarding the random fiber distribution RVE, for all three cases of filling fiber pairs. A consistent, converged, solution could not be achieved for any of the geometric fiber distribution cases. Consequently, these results will not be displayed. The very same problem happened with the cases with an imposed uniaxial strain in the $z$ direction. However, these were kept in order to maintain a coherent structure with the results presented in the “Volume constraint case studies” section. These also serve to demonstrate the appearance of non-converged results. The reasons why convergence could not be achieved in any of these cases will be regarded to “CHAPTER 4 – Discussion”.

The optimization process for the volume constraint was much more difficult and time consuming due to the need to be able to compute the limit stress value, $S$, that would lead to a final 8/8 fiber type materials distribution (recall equation (10)). In certain cases, this value had to be adjusted in between iterations in order to attempt to steer the results to the desired final solution. Still, not always such distribution was attained; with the number of strong material fibers ranging from 6 to 9 in some cases. Additionally, at this stage, the author chose to present a wider range of case studies than to show results with better convergences because. Even without being achieved full convergence, these solutions show strong trends that point towards the optimal result.

3.3.1 Random fiber distribution (standard RVE)

The subsequent case studies, Figure 33 and Figure 34, relate to the optimization of the standard RVE for filling fibers pair carbon fiber/E glass fiber, with the introduction of a stress constraint that attempts to limit the use of the stronger fiber material to roughly 50% of the total number of fibers.
Figure 33 – Optimization results of the random fiber distribution RVE filled with carbon/E glass fibers, with a stress constraint (part 1 of 2). a) Imposed uniaxial strain in the $x$ direction, b) imposed shear strain in the $xy$ plane, c) imposed uniaxial strain in the $z$ direction and d) imposed “hydrostatic” $\varepsilon_{xx} + \varepsilon_{yy}$ strain loading.
Figure 34 – Optimization results of the random fiber distribution RVE filled with carbon/E glass fibers, with a stress constraint (part 2 of 2). e) Imposed rotated shear $-\varepsilon_{xx} + \varepsilon_{xy}$ strain loading; compressive component in $x$ direction.

Charts depicting the evolution of the value of the objective function along the iterative process to the results presented in Figure 33 and Figure 34 can be found in Figure 68 (Appendix B).

The following case studies, Figure 35 and Figure 36, refer to the optimization of the standard RVE for filling fibers pair carbon fiber/epoxy "fiber", with the introduction of a stress limitation that attempts to restrict the total number of fibers assigned with the stronger fiber material by roughly 50%.

Figure 35 – Optimization results of the random fiber distribution RVE filled with carbon/epoxy fibers, with a stress constraint (part 1 of 2). a) Imposed uniaxial strain in the $x$ direction and b) imposed shear strain in the $xy$ plane.
Figure 36 – Optimization results of the random fiber distribution RVE filled with carbon/epoxy fibers, with a stress constraint (part 2 of 2). c) Imposed uniaxial strain in the \( z \) direction, d) imposed “hydrostatic” \( \varepsilon_{xx} + \varepsilon_{yy} \) strain loading and e) imposed rotated shear \(-\varepsilon_{xx} + \varepsilon_{yy}\) strain loading; compressive component in \( x \) direction.

Charts depicting the evolution of the value of the objective function along the iterative process to the results presented in Figure 35 and Figure 36 can be found in Figure 69 (Appendix B).

The final case studies within this segment, Figure 37 and Figure 38, relate to the optimization of the standard RVE for filling fibers pair carbon fiber/void, with the introduction of a stress limitation that attempts to restrict the total number of fibers assigned with the stronger fiber material by roughly 50%. These are shown below.
Figure 37 – Optimization results of the random fiber distribution RVE filled with carbon fibers/voids, with a stress constraint (part 1 of 2). a) Imposed uniaxial strain in the $x$ direction, b) imposed shear strain in the $xy$ plane, c) imposed uniaxial strain in the $z$ direction and d) imposed “hydrostatic” $\varepsilon_{xx} + \varepsilon_{yy}$ strain loading.
Figure 38 – Optimization results of the random fiber distribution RVE filled with carbon fibers/voids, with a stress constraint (part 2 of 2). e) Imposed rotated shear $-\varepsilon_{xx} + \varepsilon_{yy}$ strain loading; compressive component in $x$ direction.

Charts depicting the evolution of the value of the objective function along the iterative process to the results presented in Figure 37 and Figure 38 can be found in Figure 70 (Appendix B).

A summary table, Table 5, containing the final optimization values of the objective function, average stress (computed as the square of the Euclidean norm of the stress tensor $\sigma_{ij}^0$) and constraint violation, as well as the total number of iterations and cumulative inner loop iterations required to achieve a satisfactory solution convergence, the reference maximum and minimum possible values of the objective function, and the average stress constraint limitation value, can be found in Appendix B.

### 3.4 Microstructural stress distribution analysis

The following sections present the results of the microstructural stress distribution analyses carried out on top of some of the optimal layouts shown in the preceding subchapters. The examples begin with the analysis of the optimal layouts of the random and geometric distribution RVEs for both volume and stress constraints, which were under an imposed uniaxial $\varepsilon_{xx}$ strain loading, with filling fibers pair carbon/E glass. This exposition will then continue with the analysis of the correspondent layouts for an imposed shear $\varepsilon_{xy}$ strain loading, with filling fibers pair carbon/epoxy. The subchapter will close with the presentation of the results for the optimal layouts under an imposed “hydrostatic” $\varepsilon_{xx} + \varepsilon_{yy}$ strain loading, when the filling fibers pair was carbon/voids.

The order of display of the results was slightly changed in this subchapter in order to facilitate the comparison between the various analyses. Due to the lack of space, not all the categories/stress conditions referred in Table 3 could be presented. The criterion of selection was the value of the tensile stress in the
most loaded element(s); the four stress conditions showing the highest values were chosen. Given the low quality of the images – result of their shrinkage – the reader has available Table 6, Table 7 and Table 8 (Appendix C) which list the maximum, intermediate and minimum values displayed in the label correspondent to each of the figures.

3.4.1 Filling fibers pair carbon/E glass, $\varepsilon_{xx}$ strain loading

The subsequent analyses, Figure 39, relate to the microstructural stress distribution of the layout previously shown in Figure 21 (a), where the loading condition was an imposed uniaxial strain in the $x$ direction, the filling fiber pair was carbon/E glass and the optimization process was subjected to a volume constraint.

![Microstructural stress distribution analysis](image)

Figure 39 – Microstructural stress distribution analysis for the optimal, random fiber distribution, layout subjected to an imposed $\varepsilon_{xx}$ strain, filling fiber pair carbon/E glass and a volume constraint. a) Von Mises stress distribution, b) uniaxial stress in direction $x$, c) uniaxial stress in direction $y$ and d) uniaxial stress in direction $z$. 
The following analyses, Figure 40, refer to the microstructural stress distribution of the layout previously shown in Figure 27 (a), where the loading condition was an imposed uniaxial strain in the $x$ direction, the filling fiber pair was carbon/E glass and the optimization process was subjected to a volume constraint.

Figure 40 – Microstructural stress distribution analysis for the optimal, geometric fiber distribution, layout subjected to an imposed $\varepsilon_{xx}$ strain, filling fiber pair carbon/E glass and a volume constraint. a) Von Mises stress distribution, b) uniaxial stress in direction $x$, c) uniaxial stress in direction $y$ and d) uniaxial stress in direction $z$.

The final analyses within this segment, Figure 41, relate to the microstructural stress distribution of the layout previously shown in Figure 33 (a), where the loading condition was an imposed uniaxial strain in the $x$ direction, the filling fiber pair was carbon/E glass and the optimization process was subjected to a stress constraint.
Figure 41 – Microstructural stress distribution analysis for the optimal, random fiber distribution, layout subjected to an imposed $\varepsilon_{xx}$ strain, filling fiber pair carbon/E glass and a stress constraint. a) Von Mises stress distribution, b) uniaxial stress in direction $x$, c) uniaxial stress in direction $y$ and d) uniaxial stress in direction $z$.

A complementary table, Table 6, listing the maximum, intermediate and minimum values displayed in the labels correspondent to the three previous figures is available in Appendix C. In addition to these, Table 6 also shows the values of the stress conditions that were not presented in the figures.

### 3.4.2 Filling fibers pair carbon/epoxy, $\varepsilon_{xy}$ strain loading

The subsequent analyses, Figure 42, relate to the microstructural stress distribution of the layout previously shown in Figure 23 (b), where the loading condition was an imposed shear strain in the $xy$ plane, the filling fiber pair was carbon/epoxy and the optimization process was subjected to a volume constraint.
Figure 42 – Microstructural stress distribution analysis for the optimal, random fiber distribution, layout subjected to an imposed $\varepsilon_{xy}$ strain, filling fiber pair carbon/epoxy and a volume constraint. a) Von Mises stress distribution, b) uniaxial stress in direction $x$, c) shear stress in the $xy$ plane and d) uniaxial stress in direction $y$.

The following analyses, Figure 43, refer to the microstructural stress distribution of the layout previously shown in Figure 29 (b), where the loading condition was an imposed shear strain in the $xy$ plane, the filling fiber pair was carbon/epoxy and the optimization process was subjected to a volume constraint.
Figure 43 – Microstructural stress distribution analysis for the optimal, geometric fiber distribution, layout subjected to an imposed $\varepsilon_{xy}$ strain, filling fiber pair carbon/epoxy and a volume constraint. a) Von Mises stress distribution, b) uniaxial stress in direction $x$, c) shear stress in the $xy$ plane and d) uniaxial stress in direction $y$.

The final analyses within this segment, Figure 44, relate to the microstructural stress distribution of the layout previously shown in Figure 35 (b), where the loading condition was an imposed shear strain in the $xy$ plane, the filling fiber pair was carbon/epoxy and the optimization process was subjected to a stress constraint. As could be observed, the final solution depicted in Figure 35 (b) did not fully converge. As such, in order to make it possible to compare with the rest, convergence was manually induced by setting the eight fibers with higher densities with $\rho = 1$ and the remaining with $\rho = 0$, prior to the stress distribution analysis.
Figure 44 – Microstructural stress distribution analysis for the optimal, random fiber distribution, layout subjected to an imposed $\varepsilon_{xy}$ strain, filling fiber pair carbon/epoxy and a stress constraint. a) Von Mises stress distribution, b) uniaxial stress in direction $x$, c) shear stress in the $xy$ plane and d) uniaxial stress in direction $y$.

A complementary table, Table 7, listing the maximum, intermediate and minimum values displayed in the labels correspondent to the three previous figures is available in Appendix C. In addition to these, Table 7 also shows the values of the stress conditions that were not presented in the figures.

### 3.4.3 Filling fibers pair carbon/void, $\varepsilon_{xx} + \varepsilon_{yy}$ strain loading

The subsequent analyses, Figure 45, relate to the microstructural stress distribution of the layout previously shown in Figure 25 (d), where the loading condition was an imposed “hydrostatic” $\varepsilon_{xx} + \varepsilon_{yy}$ strain, the filling fiber pair was carbon/void and the optimization process was subjected to a volume constraint.
Figure 45 – Microstructural stress distribution analysis for the optimal, random fiber distribution, layout subjected to an imposed “hydrostatic” $\varepsilon_{xx} + \varepsilon_{yy}$ strain, filling fiber pair carbon/void and a volume constraint. a) Von Mises stress distribution, b) uniaxial stress in direction $x$, c) uniaxial stress in direction $y$ and d) uniaxial stress in direction $z$.

The following analyses, Figure 46, refer to the microstructural stress distribution of the layout previously shown in Figure 32 (d), where the loading condition was an imposed “hydrostatic” $\varepsilon_{xx} + \varepsilon_{yy}$ strain, the filling fiber pair was carbon/void and the optimization process was subjected to a volume constraint.
Figure 46 – Microstructural stress distribution analysis for the optimal, geometric fiber distribution, layout subjected to an imposed “hydrostatic” $\varepsilon_{xx} + \varepsilon_{yy}$ strain, filling fiber pair carbon/void and a volume constraint. a) Von Mises stress distribution, b) uniaxial stress in direction $x$, c) uniaxial stress in direction $y$ and d) uniaxial stress in direction $z$.

The final analyses within this segment, Figure 47, relate to the microstructural stress distribution of the layout previously shown in Figure 37 (d), where the loading condition was an imposed “hydrostatic” $\varepsilon_{xx} + \varepsilon_{yy}$ strain, the filling fiber pair was carbon/void and the optimization process was subjected to a stress constraint. As could be observed, the final solution depicted in Figure 37 (d) did not fully converge. As such, in order to make it possible to compare with the rest, convergence was manually induced by setting the eight fibers with higher densities with $\rho = 1$ and the remaining with $\rho = 0$, prior to the stress distribution analysis.
Figure 47 – Microstructural stress distribution analysis for the optimal, random fiber distribution, layout subjected to an imposed “hydrostatic” $\varepsilon_{xx} + \varepsilon_{yy}$ strain, filling fiber pair carbon/void and a stress constraint. a) Von Mises stress distribution, b) uniaxial stress in direction $x$, c) uniaxial stress in direction $y$ and d) uniaxial stress in direction $z$.

A complementary table, Table 8, listing the maximum, intermediate and minimum values displayed in the labels correspondent to the three previous figures is available in Appendix C. In addition to these, Table 8 also shows the values of the stress conditions that were not presented in the figures.
CHAPTER 4 – Discussion

The fourth chapter is devoted to the discussion of the results that were presented in “CHAPTER 3 – Results”. Firstly, an observation predominately focused in analyzing and comparing the different optimized layouts in terms of the objective function will be made. Next, a similar comparison, now concerning the microstructural stress distribution. The third section of this chapter will be dedicated to the discussion of various issues particularly related with the optimization process. The chapter will close with a reference about the applicability of this work in real context and future work ideas will be left.

With the lack, to nonexistence, of previous works addressing the subject depicted in this dissertation (at least as far as the knowledge of the author), it became hard to carry an informed assessment of the results that were achieved. The remaining option was, therefore, to make a judgement based on one’s own intuition.

4.1 Overall analysis of the optimal layouts

Looking at each individual layout trying to assess its legitimacy can be a rather ambiguous task. This is particularly true for the random fiber distribution case studies. A good way to start is, therefore, to analyze the geometric fiber distribution cases. In such cases, due to the symmetry of the distribution, it is a good first indicator if the final, optimized, configuration demonstrates some sort of symmetry itself.

With respect to the geometric case studies having filling fibers pair carbon/E glass (Figure 27 and Figure 28), it is clear to see that all of them resulted in a very similar final solution. Much like a nucleus of hard, horizontally aligned (in the \(x\) direction), fibers surrounded by the weaker fibers. Such solution seems to be correct in a mechanical point-of-view for the imposed uniaxial \(\varepsilon_{xx}\) strain loading. The reason being that the agglomeration of the stronger fibers in the direction of the loading may certainly be a factor that positively influences the overall stiffness of the structure. On the other hand, this sort of configuration does not appear to have a straightforward explanation for the remaining loading conditions.

Additionally, it is possible to observe a behavior that distinguishes the layouts from Figure 27 (b) and Figure 28 (e) from the rest. Those show an abdication of a strong fiber from the horizontal band and its placement on an upper layer. What might seem an isolated and occasional behavior may also derive from a meaningful mechanical phenomenon given that these two case studies are subjected to loading conditions that can be represented by the same Mohr’s circle (see Figure 48). Figure 48 shows a bi-dimensional representative element loaded with a pure shear stress condition and the way it translates in terms of the principal stresses space (on the left), and the correspondent Mohr’s circle (on the right). It becomes clear that these two types of loading are closely interconnected.
In the examples concerning the case studies having filling fibers pair carbon/epoxy (Figure 29 and Figure 30) it is particularly interesting to observe how a simple change in the weaker fiber properties generates such different optimal configurations from the first. It is emphasized that in this case the weaker fiber assumes the same properties of the matrix. For all purposes, the structural performance of the composite will then be purely a result of the introduction of carbon fibers. Here the variety of the configurations is much higher than the previous cases. This is curious because one could, at the outset, expect all final configurations to match regardless of the materials assigned to the fibers. The optimization program searches for the fiber positions where it is advantageous to place the stronger fibers for a given loading condition. Once these were found, it would be plausible that these would keep constant independently of any possible changes in the weaker fiber material. The results show that the problem may be much deeper than that, and other phenomena may come into play when substantial changes are made into elementary variables such as the fiber material.

Here, the imposed uniaxial $\varepsilon_{xx}$ strain loading case study (Figure 29 (a)) still shows a recognizable pattern. The difference is in the placement of the horizontal stronger fiber band, which is now located on the top layers. It is interesting to notice because such solution, in macroscopic terms, is no different from the one presented in Figure 27 (a). Either way, the agglomeration of the strong fibers in the loading direction remains, which reinforces the earlier conjecture. To confirm that such configuration is transverse to the uniaxial strain loading in the $x$ and $y$ directions, the author carried out, as a demonstration, an optimization process for the geometric fiber distribution RVE subjected to an imposed uniaxial $\varepsilon_{yy}$ strain loading for all three filling fibers types. The results are shown in Figure 49.
Figure 49 – Optimization results of the geometric fiber distribution RVE subjected to an imposed uniaxial strain in the $y$ direction, with a volume constraint. a) Filling fibers pair carbon fiber/E glass fiber, b) filling fibers pair carbon fiber/epoxy fiber and c) filling fibers pair carbon fiber/void.

The configurations shown in Figure 49 clearly resemble those from the imposed uniaxial $\epsilon_{xx}$ strain loading case studies – Figure 27 (a) and Figure 29 (a). It is, however, emphasized the gap between Figure 49 (c) and Figure 31 (a), which the author was expecting to be comparable, by a $90^\circ$ angle. In an attempt to understand such difference, one discovered an interesting but undesirable result: the final solutions seem to show a dependence on the optimization process. More specifically, the optimization process seems to be leading some solutions to local optima depending on the updating scheme of the material exponent, $mat_{\text{exp}}$. This short analysis led to the conclusion that is not an advantage to maintain $mat_{\text{exp}}$ constant for a number of runs such as twenty (as done in this work), but rather update it every ten runs (as done in the optimization process for Figure 49), for instance.

The difference in the objective function can be overwhelming for some of the configurations. If Figure 31 (a) kept the same layout that was found in Figure 27 (a), the elastic deformation energy would rise from a mere $63.56 Nm/m^3$ (see Table 4) to $139.09 Nm/m^3$, which is more than double. This outcome brings to surface, once again, the idea that, after all, there may be an optimum layout that is unique for a particular loading condition, regardless of the fiber materials. To better understand this phenomenon and its implications on the results to a full extent, further study would be necessary. Such investigation will be left as future work.

It is also observed that, for filling fiber pairs carbon/epoxy (Figure 29 and Figure 30) and carbon/void (Figure 31 and Figure 32), the resemblance between the configurations for the imposed shear $\epsilon_{xy}$ and the rotated shear $-\epsilon_{xx} + \epsilon_{yy}$ strain loadings is no longer present. However, they show a placement of the strong fibers which is clearly oriented in the direction of action of the principal stresses; $45^\circ/-45^\circ$ for the pure shear $xy$ strain loading (Figure 29 (b) and Figure 31(b)) and $0^\circ/90^\circ$ for the rotated shear $-\epsilon_{xx} + \epsilon_{yy}$ strain loading (Figure 30 (e) and Figure 32 (e)).

With regard to the random fiber distribution solutions, both volume and stress constrained, albeit more difficult, it is still possible to identify some common ground with the characteristics pinpointed in the geometric fiber distribution case studies’ analysis. An example of that are Figure 21 (a), Figure 23 (a) and Figure 25 (a), for the volume constrained case studies, and Figure 33 (a) and Figure 35 (a), for the stress
constrained case studies, demonstrating a preferential orientation of the strong fibers in the \( x \) direction. One can also observe an arrangement of the strong fiber in a 45° angle which is particularly noticeable in Figure 21 (b) and Figure 23 (b), for the volume constrained case studies, and Figure 33 (b) for the stress constrained case studies. All other configurations, and particularly those deriving from an RVE subjected to an imposition of a uniaxial strain in the \( z \) direction, are plausible but much harder to assess based on concrete engineering knowledge.

4.2 Performance of the optimal layouts in terms of stiffness

A more interesting analysis consists in comparing the influence of the fiber distribution type – random or geometric – and the type of constraint – volume or stress – in terms of the elastic deformation energy of the optimized RVE and, consequently, on the homogenized stiffness of the composite structure. Figure 50 graphically displays the data recorded in Table 4 and Table 5.

![Graphical display of data recorded in Table 4 and Table 5](image)

Figure 50 – Performance of the optimized layouts in terms of the elastic deformation energy of the RVE.

Figure 50 provides some interesting information. Despite being quite tiptoed with each other, it is possible to see a slight trend that shows that, for most cases, a geometric fiber distribution results in a stiffer structure. These are followed up by the random fiber distribution layouts subjected to the volume constraint. Additionally, the author stresses that the values of the elastic deformation energy shown in Figure 50 are for the exact same configurations presented in “CHAPTER 3 – Results”. Meaning that, since most of the stress constrained case studies did not fully converge, this comparison is a little biased towards the
“Random (Stress)” configurations because the majority of them ended up having $\sum_{f=1}^{N_f=16} \rho_f > 8$. It would, however, be natural to expect that the volume constrained, random fiber distribution, configurations led to a stiffer design. The purpose of the stress constraint is undoubtedly more demanding for the optimization process. While the volume constraint allows any material distribution within the RVE, provided it is not exceeded a give number of fibers assigned with carbon, the stress constraint goes beyond that point and demands the microstructural stress distribution to be limited.

In a study by Guedes et al. (2003) [51], the authors describe a computational model for approximating energy bounds for two-phase composite materials under multiple load cases. While such results could possibly set a comparison background for the elastic deformation energy attained in the case studies with filling fibers pair carbon/epoxy, the author could not use them to establish a direct judgement on the findings in this document because Guedes et al. formulated the problem as a minimization of the homogenized compliance. Such formulation involves the introduction of the loading condition as a stress state, in opposition with the construction based on the definition of the strain used in this work.

Pryz [52, 53] observed that the transverse constitutive behavior of polymeric matrix composites is a function of the spatial arrangement of the reinforcements. Such result is, in a way, reaffirmed in this document. Moreover, this work raises the dependency of the transverse constitutive behavior of polymeric matrix composites in the internal fiber type distribution, for a same microstructural design of the RVE, in hybrid composite materials with two fiber types.

In a field of study that goes beyond the scope of this dissertation, Brockenbrough et al. (1991) [54] have shown that in the plastic regime, the transverse deformation cannot be correctly predicted if a periodic fiber distribution is used to model the composite material. Such result dictates that, despite possibly showing the best performance regarding the overall stiffness of the composite structure in the elastic regime, geometric fiber distributions cannot be fully characterized using numerical simulation tools in predicting micro-macro structural responses of the composite. Thus, experimental testing may always be required, with the laboratory costs it entails.

### 4.3 Performance of the optimal layouts in terms of stress distribution

One other scrutiny that is quite interesting involves analyzing the way the stress field distributes within the different microstructures. In this sense, the data recorded in Table 6, Table 7 and Table 8 were put into the graphical form that can be seen in Figure 51. Figure 51 shows and compares the maximum tensile stress values present inside the microstructures generated by the optimization program for the particular set of case studies provided in “Microstructural stress distribution analysis” results section.
Figure 51 – Performance of the optimized layouts in terms of the microstructural stress within the RVE.

First, the author would like to point out that the very high stress values shown in Figure 51 are due to the mistreatment of the imposed strain values introduced as input as part of the optimization process. Some of these even show tensile stress values that go beyond the ultimate tensile strength of the individual E glass and carbon fibers. After a brief search the author found reference values for the ultimate tensile strength of E glass and carbon fibers to be, respectively, 3.1 – 3.8MPa [55] and \( \approx 3.5 \text{GPa} \) [56]. The values shown in Figure 51 are, naturally, in most cases too high so that they could represent authentic conditions of application of such composite structures. The Von Mises stress peak in the carbon/E glass fibers pair case, for instance, would, in an engineering project analysis, for sure, be a serious cause for concern. This fact, however, was not considered here as the presence of a linear elastic behavior was always assumed. As a future work, one could look into the characterization and optimization of a composite material having in mind a more authentic behavior, particularly in view of the potential plastic deformation of the composite.

Figure 51 confirms the results that would, a priori, be expected from an introduction of a stress limitation in the design optimization. It is quite clear that the random configurations generated under a stress constraint led to a microstructural stress distribution with lower tensile peaks in the elements, when compared with the volume constrained version. More specifically, it can be observed a decrease of 1.73%, 37.9% and 6.95% in the Von Mises maximum stress peak in the stress constrained (random fiber distribution) carbon/E glass, carbon/epoxy and carbon/void fiber pair configurations, respectively, when compared with the homologous volume constrained configurations. Moreover, Figure 51 reveals some other trends. For instance, it shows that the geometric fiber distributions spread even more effectively the stress across the domain. Namely, it
can be observed a decrease of 42.0%, 48.77% and 11.23% in the Von Mises maximum stress peak in the volume constrained (geometric fiber distribution) carbon/E glass, carbon/epoxy and carbon/void fiber pair configurations, respectively, when compared with the homologous random fiber distribution configurations.

One of the major surprises is to realize that for filling fibers pair carbon/epoxy – or in words, for a normal, one fiber type, composite material – the random, stress constrained, configurations outperform the geometric, volume constrained, distributions. It must, however, be emphasized that such comparison is not completely equivalent given the different nature of their constraints. In a follow-up of this study, it would be interesting to see which would be the behavior of a geometric distribution if also subject to a stress constraint. Such research is also left as future work.

Again, reference is made to the results reported by Matsuda et al. (2003) [47] which, remind, compared the elastic-viscoelastic behavior of long-fiber reinforced laminates subjected to in-plane tensile loading using homogenization theory. They concluded that the spatial distribution of the reinforcements in the RVE does not affect the macroscopic response of laminates, but it significantly affects the microscopic stress distribution. Here, the author was able to conclude a very similar result: while the different designs show homogenized stiffnesses that are fairly constant across fiber distribution types and internal fiber type configurations, the influence of such variables in the microscopic stress distribution appears to be much more volatile. Once more time, such outcome confirms similar conclusions a bit across literature emphasizing the importance to consider the transverse randomness of the fiber distribution. For instance, as referred in [40], and previously mentioned in this work, for studying the evolution of damage in the matrix.

A particularly interesting observation refers to Figure 45, Figure 46 and Figure 47. These describe the microstructural stress distribution within the microstructure of the carbon/void filled case studies presented in “Filling fibers pair carbon/void, $\epsilon_{xx} + \epsilon_{yy}$ strain loading”. One can recognize stress concentration spots mainly occurring in the periphery of the voids. Hence, such result also shows that the presence of singularities like voids may represent a crucial role in crack onset and propagation, and may therefore jeopardize the integrity of the composite structure.

The author would like to close this segment with a short investigation on the legitimacy to manually induce 0-1 convergence in Figure 35 (b) and Figure 37 (d) to reach the results presented in Figure 44 and Figure 47, as clearly stated in their preceding texts. Figure 52 and Figure 53 depict, respectively, the evolution of the densities along the optimization process for each of the sixteen fibers up to the optimal configurations portrayed in Figure 35 (b) and Figure 37 (d).
Figure 52 – Evolution process that led to the configuration presented in Figure 35 (b).

Figure 53 – Evolution process that led to the configuration presented in Figure 37 (d).

Figure 52 and Figure 53 demonstrate that the great majority of the fibers show a monotonous behavior as the optimization process evolves. When the last iteration is reached, apart for a limited number of exceptions (particularly in Figure 52), the value of the density has shown a steady progression. Despite the inconsistency verified in some of the fibers, the author thought it would be reasonable to assume that the trend shown at the end of the last iteration would be the one that would lead to the final, fully converged, configuration, if such configuration could have been attained.

4.4 Optimization process related issues

In this section some issues related with the optimization process are addressed in a disaggregated way. First, a reflection on the motive why the optimization algorithm failed to converge any of the stress
constrained case studies subjected to an imposed uniaxial strain in the z direction (Figure 33 (c), Figure 36 (c) and Figure 37 (c)). The only reason the author can think of to explain such occurrence comes from a mixture of insufficiency in the domain discretization and fmicon's inability to deal with very close objective function gradient values. The mesh discretization employed in the direction of the thickness was, despite the use of the tetrahedral elements, still very rough. A mesh with at least two layers of elements, by contrast with the current mesh which has only one, is advised for future work. Still, it was noticeable, albeit very small, some difference in the values of the gradients of the objective function for the different fibers. Nevertheless, the author failed in getting fmicon to effectively guide the optimization to a discrete solution.

With regard to the stress constrained geometric fiber distribution cases, the author believes the problem was very similar. While here the discretization may not have been one of the causes, the differences in the objective function gradients, for each fiber, were also notably small. And thus, once again, one was faced with fmicon's inability to guide the solution to a discrete result (fibers with different densities).

It remains then to understand why this problem did not first occur in the homologous, volume constrained, case studies. The author believes the explanation for this fact lies in the density update algorithm that was employed: the updating scheme described in equation (18) is a simpler solution, characterized by a more mechanical modus operandi. Fmincon, in turn, is a much more complex tool, whose functioning is not quite clear. Simplicity may have been more successful in this situation. Overall, the author was disappointed with fmicon's performance in this study and, as a suggestion for future work, recommends other optimization algorithm to be used.

The next issue concerns the charts depicting the evolution of the value of the objective function along the iterative process to the results shown in “Stress constraint case studies” (Figure 68, Figure 69 and Figure 70). In first place, it is noted the fact that each line represents an entire run in fmincon. A run that led from an initial design to an intermediate/final design – symbolized by the first and last points on those lines. The reason why, in most of the cases, fmincon does not show the same initial point in the current iteration as the end point of the previous iteration is due to the change in the material exponent. Figure 54 helps understand the concept by representing the influence of the power law in the value of the densities.
If the reader remembers the parametrization employed in solving the fiber reinforced hybrid composite optimization problem (recall equation (7)), it becomes clear that every time the material exponent, \( mat_{\exp} \), or \( p \) as named in Figure 54 and equation (7), is increased, the value of the intermediate densities gets lower. Consequently, the value of the objective function decreases since lower values of the densities are assigned to the weaker, fiber type 2, material. This is the exact same reason why Figure 62 to Figure 67 show that staggered behavior.

One other fact that deserves to be noted is the reason why the last points from each line in Figure 68, Figure 69 and Figure 70 do not always show a growing progress, which should be expected given the fact that the optimization process is attempting to maximize the objective function. The reason for this phenomenon may fall upon two main factors: the first related to the fmincon’s inability to always reach a design that stands right on top of the limit set by the constraint (oftentimes the design showed a significant gap, by default, to the limit), and the second associated with the adjustments made to the constraint in-between iterations. The author recalls that such adjustments were meant to assure that the stress constrained case studies would reach a final configuration with a 50%/50% fiber type material distribution.

Finally, a brief observation on the data recorded in Table 4, particularly focused on the total number of runs required to converge each of the examples. It is clear to see that this number gradually increases as fiber type material 2 becomes weaker. While the author cannot think of a reasoned explanation for this occurrence, it is still interesting to notice.

### 4.5 Real context impact and future work

The fundamental purpose of this research is to show – and provide a numerical tool for that matter – that there is an optimal fiber configuration which leads to maximum usage of the potential offered by the composite material, hybrid or not. How these results can be applied in real composite structures is a completely different issue. Current composite manufacturing technologies, in general, do not seem to be particularly prepared to work with the level of accuracy required by the results presented in this document.
Additionally, only a small fraction of them work with single, continuous, fibers as raw materials; these are filament winding and pultrusion [58]. Yet, it is possible that in a near future one will be able to successfully incorporate hybrid composite optimization knowledge into composite manufacturing.

Simple adjustments could, almost immediately, potentially open room for improvement. For instance, in pultrusion, whose scheme is shown in Figure 55. This process is limited to components with constant, or near constant, cross-sections. However, if one could figure a way to control the arrangement of the fibers before they were dipped into the resin bath, it would be, for example, possible to produce pre-impregnated composite sheets, whose distribution of the fibers would be optimized to suit a particular application. These, in turn, could be subsequently processed by autoclave or roll forming to produce all sorts of different parts and/or composites laminates.

![Composite Pultrusion Manufacturing Process](image1)

*Figure 55 – Composite pultrusion manufacturing process [59].*

Another possibility, perhaps a more ambitious idea, could be its application on filament winding process, which is, to some extent, similar to composite pultrusion (see Figure 56). Here, a deeper investigation combining the microstructure and the deposition of the fiber layers, as well as their relation with the structural response of the composite, would certainly be required.

![Composite Filament Winding Manufacturing Process](image2)

*Figure 56 – Composite filament winding manufacturing process [60].*
Out of curiosity, in 2015 NASA acquired an industrial automated fiber placement tool, which is nothing more than a gigantic robot, which, using filament winding technology, is expected to build the biggest, lightweight, composite parts ever made for space vehicles [61]. Such parts will, says Preston Jones, deputy director of Marshall’s Engineering Directorate, be possibly used to build part of the space vehicles that will carry humans on exploration missions to Mars and other places [61].

Even though the author attempted to cover the randomness of the arrangement of the fibers within the microstructure, the results presented in this paper are limited to a chosen random microstructure. Each microstructure has its own dynamics. Therefore, these specific results may, at most, be taken as a reference for other research works; namely because they show preferred patterns for the arrangement of the fiber types in the microstructure. The author considers this particularity as one of the major limitations of this dissertation.

Composite materials, due to their complex, heterogeneous, nature, are still an issue with some room for progress. In that context, the author suggests some investigations to be held, in addition to those proposed along the chapter:

- Examine case studies with filling fibers having volume fractions other than 50%/50%;
- Experimentally corroborate the results described in this paper;
- Develop or adapt computational methods which can, by one hand, make faster the optimization process and, on the other hand:
  - Help mitigate convergence to local optimum solutions;
  - Be designed to support multi-objective and multi-load conditions;
  - Consider different stress constraints (e.g. hydrostatic pressure, Von Mises stress, maximum principle stresses, etc.)
  - Consider local stress constraints;
- Study practical ways to incorporate this technology in conventional composite manufacturing methods;
- Link microstructural plie optimization with composite layer stacking optimization problems.
CHAPTER 5 – Conclusions

The objective of this work was to develop a finite element based model to computationally characterize and optimize hybrid composites reinforced with two types of long-fibers of different materials. The platforms of implementation have been computer aided finite element analysis tool Abaqus and software programming environment Matlab. A number of other, non-commercial, computer programs were used and modified according the needs of the investigation. As a result, two new computer programs were created to meet the proposed target.

The dissertation was started with a brief description of the three main background topics: composite materials, micromechanics and structural design optimization. A few sections describing the problem in detail followed. The problem was presented as an optimal allocation issue of the two possible fiber type materials among a fixed number of fibers, subjected to a volume or an average stress constraint. The author proceeded with the formulation of the problem. Firstly, the matrix and fiber type materials used to perform the optimization problem were established. Alongside, the main, relevant, assumptions and limitations of the optimization process were clearly stated. Then, the mathematical formulation of the problem was introduced. The inherent similarity between the topology optimization and the hybrid composite optimization problems was highlighted. The mathematical equations that allowed the computation and assessment of the objective function and the constraints were settled. This concluded the problem formulation stage. Next, the Matlab computer programs – RAND_uSTRU_GEN, 3DMeshGENAbaqus2D and CompositeOpt – used in reaching a solution to the hybrid composite optimization problem were described. This included a portrayal of the most important features in each one of them. The third chapter was dedicated to the presentation of the results. Case studies with both geometric and random fiber distributions were displayed. Additionally, a series of figures showing the microstructural stress distribution inside some of the previous case studies was introduced. The thesis was concluded with a thorough analysis on the results.

This research serves, above all, the purpose of showing that there is an optimal fiber and fiber material microstructural distribution within the composite which can be calculated and that enables greater profitability of the material. Due to the lack of previous work addressing this same problem, the author had to rely on its own knowledge to assess the results. It was observed a good correlation between the results and the theory, with a decent amount of the results visibly showing a trend on the distribution of the stronger fibers in the direction of the principal stresses. The author also noticed, however, that some of the solutions may not represent the configuration that generates the stiffest structure; seeming like the algorithm may have converged to a local optima.

Some of the most interesting results came from the comparison between the impact of the random fiber distribution and the geometric fiber distribution configurations in the overall composite structure response. The analyzed data showed that in terms of overall stiffness of the structure there is little impact between
having one or the other. Yet, with a slight trend pointing towards the geometric fiber configurations being the stiffer. On the other hand, when the object of analysis was the stress field distribution within the microstructure, a strong trend indicating that the geometric fiber distribution configurations are able to disperse more uniformly the stress across the matrix and fibers was observed; resulting in considerably lower tensile stress peaks in the elements. Here, another interesting result could also be observed: it is possible to lower the tensile stress peaks in the random fiber distribution configurations, with minimal loss of structural stiffness, if a stress constraint is applied to the optimization problem.

Composite manufacturing technologies existing today seem, in general, unprepared to work with the level of accuracy required by the results presented in this document. In addition, only a small portion of those are specially dedicated to work with continuous fibers as raw materials. Nevertheless, the author thinks it may be possible to implement the results described herein, or similar, in a near future if further validation on their actual influence on the structural response of the composite material is achieved. And, naturally, if that impact justifies any potential investments.

Composite materials market is growing at an extraordinary rate. Key economic indicators and market dynamics suggests that such trend will continue in the upcoming years. The rising demand for lighter structural materials is a fact. It is anticipated by 2020 approximately 65 percent of U.S. composites growth will be driven by the aerospace, transportation and construction industries. It becomes then clear the need to study every possible aspect of these, whose estimates say, will be the materials of the future.
References


[57] A. Orlando and M. Luege, "Topology Optimization".


Appendix A

A.1 Computer programs detailed flowcharts

Figure 57 – RAND_uSTRU_GEN descriptive flowchart.
Figure 58 – 3DMeshGENAbaqus2D descriptive flowchart.

**FEA commercial software:**
Runs RAND_FDISP.py or GEO_FDISP.py python script files which are programmed to automatically generate a 2D mesh on the RVE and output it as a text file. Shows ABAQUS workspace so that the user can observe and access any mesh details.

**Important outcomes:**
ABAQUS-auto.inp - text file with nodal position, conectivities and information about which elements belong to the matrix or fibers

**Main Variables:**
- position - array containing mesh elements nodal coordinates
- conectivities - array containing mesh elements nodal numbering
- elset - array with information of the elements belonging to matrix and each of the different fibers

Makes an offset of the 2D mesh points according to the magnitude of the thickness that is intended to give the RVE, in the z coordinate. Creates intermediate nodes to divide the triangular prismatic elements into three tetrahedral elements.

**Main Variables:**
- position (updated)

Divides each triangular prismatic element into three tetrahedral elements.

**Main Variables:**
- ijk - an updated version of conectivities but giving additional information on the sets of elements belonging to a same fiber
- elset (updated)

Generates Mesh.inp.txt, to be read by Premat meshing module

**Mesh.inp.txt** - Text file with 3D mesh nodal position and conectivities information.
Figure 59 – CompositeOpt descriptive flowchart (part 1 of 2).
Figure 60 – CompositeOpt descriptive flowchart (part 2 of 2).
A.2 Geometric fiber distribution algorithm flowchart

![Flowchart Diagram]

- **Begin**
- **Acquire the number of fibers**
- **N_fibre_real is a perfect square**
  - **Y**: Distribute fibers in a $x\times x$ layout
  - **N**: Check how many fibers fit in a row
    - **Y**: Attempt a $x+(x-1)+x+(x-1)+\ldots$ layout
    - **N**: Attempt a $(x-1)+x+(x-1)+x+\ldots$ layout
      - **Y**: Compute fiber center position
      - **N**: Error message

- **Compute fiber center position**
  - Computes the coordinates of the center of the fibers based on the fiber distribution (number of fibers per row and number of rows) and the RVE’s geometry (width)

- **Attempt succeeded?**
  - **Y**: A
  - **N**: End

**N_fibre_real - number of fibers in the RVE; half fibers and corner fibers are not counted individually in this variable**

**x representing the number of fibers per row. A $x\times x$ layout being a physical arrangement with $x$ fibers in a row, and $x$ rows. A $x+(x-1)+x+(x-1)+\ldots$ layout having $x$ fibers in the first row, $(x-1)$ fibers in the second row, and so on until the last row which can have both $x$ or $(x-1)$ fibers**

Figure 61 – Geometric fiber distribution algorithm flowchart.
Appendix B

B.1 Optimization process detailing figures

Figure 62 – Evolution of the objective function along the optimization process of the random fiber distribution RVE filled with carbon/E glass fibers, with a volume constraint. a) Imposed uniaxial strain in the $x$ direction, b) imposed shear strain in the $xy$ plane, c) imposed uniaxial strain in the $z$ direction, d) imposed “hydrostatic” $\varepsilon_{xx} + \varepsilon_{yy}$ strain loading and e) imposed rotated shear $-\varepsilon_{xx} + \varepsilon_{yy}$ strain loading; compressive component in $x$ direction. $mat_{exp}$ increased by 3 every twenty runs.
Figure 63 – Evolution of the objective function along the optimization process of the random fiber distribution RVE filled with carbon/epoxy fibers, with a volume constraint. a) Imposed uniaxial strain in the $x$ direction, b) imposed shear strain in the $xy$ plane, c) imposed uniaxial strain in the $z$ direction, d) imposed “hydrostatic” $\varepsilon_{xx} + \varepsilon_{yy}$ strain loading and e) imposed rotated shear $-\varepsilon_{xx} + \varepsilon_{yy}$ strain loading; compressive component in $x$ direction. $mat_{exp}$ increased by 3 every twenty runs from run 1 to 140, and every 10 runs thereafter.
Figure 64 – Evolution of the objective function along the optimization process of the random fiber distribution RVE filled with carbon fibers/voids, with a volume constraint. a) Imposed uniaxial strain in the $x$ direction, b) imposed shear strain in the $xy$ plane, c) imposed uniaxial strain in the $z$ direction, d) imposed “hydrostatic” $\varepsilon_{xx} + \varepsilon_{yy}$ strain loading and e) imposed rotated shear $-\varepsilon_{xx} + \varepsilon_{yy}$ strain loading; compressive component in $x$ direction. $mat_{exp}$ increased by 3 every twenty runs from run 1 to 140, and every 10 runs thereafter.
Figure 65 – Evolution of the objective function along the optimization process of the geometric fiber distribution RVE filled with carbon/E glass fibers, with a volume constraint. a) Imposed uniaxial strain in the $x$ direction, b) imposed shear strain in the $xy$ plane, c) imposed uniaxial strain in the $z$ direction, d) imposed “hydrostatic” $\varepsilon_{xx} + \varepsilon_{yy}$ strain loading and e) imposed rotated shear $-\varepsilon_{xx} + \varepsilon_{yy}$ strain loading; compressive component in $x$ direction. $mat_{exp}$ increased by 3 every twenty runs.
Figure 66 – Evolution of the objective function along the optimization process of the geometric fiber distribution RVE filled with carbon/epoxy fibers, with a volume constraint. a) Imposed uniaxial strain in the $x$ direction, b) imposed shear strain in the $xy$ plane, c) imposed uniaxial strain in the $z$ direction, d) imposed “hydrostatic” $\varepsilon_{xx} + \varepsilon_{yy}$ strain loading and e) imposed rotated shear $-\varepsilon_{xx} + \varepsilon_{yy}$ strain loading; compressive component in $x$ direction. $mat_{exp}$ increased by 3 every twenty runs from run 1 to 140, and every 10 runs thereafter.
Figure 67 – Evolution of the objective function along the optimization process of the geometric fiber distribution RVE filled with carbon fibers/voids, with a volume constraint. a) Imposed uniaxial strain in the $x$ direction, b) imposed shear strain in the $xy$ plane, c) imposed uniaxial strain in the $z$ direction, d) imposed “hydrostatic” $\varepsilon_{xx} + \varepsilon_{yy}$ strain loading and e) imposed rotated shear $-\varepsilon_{xx} + \varepsilon_{yy}$ strain loading; compressive component in $x$ direction. $mat_{exp}$ increased by 3 every twenty runs from run 1 to 140, and every 10 runs thereafter.
Figure 68 – Evolution of the objective function along the optimization process of the random fiber distribution RVE filled with carbon/E glass fibers, with a stress constraint. a) Imposed uniaxial strain in the $x$ direction, b) imposed shear strain in the $xy$ plane, c) imposed uniaxial strain in the $z$ direction, d) imposed "hydrostatic" $\varepsilon_{xx} + \varepsilon_{yy}$ strain loading and e) imposed rotated shear $-\varepsilon_{xx} + \varepsilon_{yy}$ strain loading; compressive component in $x$ direction.
Figure 69 – Evolution of the objective function along the optimization process of the random fiber distribution RVE filled with carbon/epoxy fibers, with a stress constraint. a) Imposed uniaxial strain in the $x$ direction, b) imposed shear strain in the $xy$ plane, c) imposed uniaxial strain in the $z$ direction, d) imposed "hydrostatic" $\varepsilon_{xx} + \varepsilon_{yy}$ strain loading and e) imposed rotated shear $-\varepsilon_{xx} + \varepsilon_{yy}$ strain loading; compressive component in $x$ direction.
Figure 70 – Evolution of the objective function along the optimization process of the random fiber distribution RVE filled with carbon fibers/voids, with a stress constraint. a) Imposed uniaxial strain in the $x$ direction, b) imposed shear strain in the $xy$ plane, c) imposed uniaxial strain in the $z$ direction, d) imposed "hydrostatic" $\varepsilon_{xx} + \varepsilon_{yy}$ strain loading and e) imposed rotated shear $-\varepsilon_{xx} + \varepsilon_{xy}$ strain loading; compressive component in $x$ direction.
## B.2 Optimal solution summary tables

Table 4 – Summary of the final/optimal solution data regarding the volume constraint optimization process, for the random and geometric fiber distribution RVEs. The table presents the final values of the solutions' objective function and volume constraint violation, the total number of runs and reference values for the objective function when all fibers are assigned with $\rho = 1$ (maximum possible value) and $\rho = 0$ (minimum possible value).

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Table 5 – Summary of the final/optimal solution data regarding the stress constraint optimization process, for the random fiber distribution RVE. The table presents the final values of the solutions' objective function, average stress (computed as the square of the Euclidean norm of the stress tensor $\sigma_{ij}^0$) and constraint violation, the total number of iterations and cumulative inner loop iterations, the reference values for the objective function when all fibers are assigned with $\rho = 1$ (maximum possible value) and $\rho = 0$ (minimum possible value), and the average stress constraint limitation value.\(^4\)

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\(^4\) The values related to the $\varepsilon_{33}$ loading condition are shaded because they do not represent a meaningful optimization final, converged, result.
## Appendix C

### C.1 Microstructural stress analysis complementary tables

Table 6 – Microstructural stress distribution analysis label values for the optimal, random and geometric distribution, layouts subjected to an imposed $\varepsilon_{11}$ strain loading and filling fiber pair carbon/E glass.

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<th>Middle value [MPa]</th>
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Table 7 – Microstructural stress distribution analysis label values for the optimal, random and geometric distribution, layouts subjected to an imposed $\varepsilon_{12}$ strain loading and filling fiber pair carbon/epoxy.

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Table 8 – Microstructural stress distribution analysis label values for the optimal, random and geometric distribution, layouts subjected to an imposed “hydrostatic” $\varepsilon_{11} + \varepsilon_{22}$ strain loading and filling fiber pair carbon/E glass.

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