A NUMERICAL REPRESENTATIVE VOLUME ELEMENT ON THE MESOSCALE FOR PARTS MANUFACTURED THROUGH FUSED DEPOSITION MODELING AND REINFORCED WITH SHORT FIBERS

A Thesis by

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The following faculty members have examined the final copy of this thesis for form and content, and recommend that it be accepted in partial fulfillment of the requirement for the degree of Master of Science with a major in Aerospace Engineering.

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Nicholas D. Smith, Committee Chair

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Davood Askari, Committee Member
DEDICATION

To Art and Science
To Master Hirasawa
ACKNOWLEDGEMENTS

I thank the Fulbright Program, embodied in the Department of State’s Fulbright division and the Moroccan American Commission for Educational and Cultural Exchange MACECE, for the incredible opportunity I have been given: through their funding and support, I was able to come to the United States, conduct the research I am devoted to and passionate about and go through the rich experience that is living in the land of the free.

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I hope and intend for this work and the rest of my endeavors to honor the combined time and effort invested in me.
ABSTRACT

The analysis and certification of parts manufactured through Fused Deposition Modeling and reinforced with short fibers are the main drawback of the emerging technology. The present work builds a framework for the discrete modeling of these parts through the construction of a Representative Volume Element on the mesoscale, which will account for the properties of the material and the features of the manufacturing process and can be used as a building bloc on the mesoscale. To this end, a study conducted in two main steps has been performed: a first analysis of the Representative Volume Element on the microscopic scale of a short fiber embedded in a matrix has been conducted. Studies in convergence ensured the use of optimal mesh and an analysis of orientation determined the reliability of coupling numerical stiffness with orientation averaging, as well as the closure approximation used. The second step consisted of building a Representative Volume Element on the mesoscopic scale, containing the homogenized microscopic oriented stiffness and taking into consideration fibers' distribution and void. The accuracy of the study and carry through of the periodicity and stiffness application were assessed through the comparison of the numerical stiffness tensors with the analytical solution and the stiffness obtained from a unit cell with the resulting one from a periodic structure. An initial framework has therefore been established that takes a minimal input in properties from the microscale and delivers an averaged oriented stiffness tensor on the mesoscale.
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<td>Additive Manufacturing</td>
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LIST OF SYMBOLS

\( \nu \) Poisson’s Ratio

\( \sigma \) Stress

\( \varepsilon \) Strain

\( a_{ij} \) Second Order Orientation Tensor

\( a_{ijkl} \) Fourth Order Orientation Tensor

\( a_{ijkl}^L \) Fourth Order Orientation Tensor according to linear closure approximation

\( a_{ijkl}^Q \) Fourth Order Orientation Tensor according to quadratic closure approximation

\( a_{ijkl}^H \) Fourth Order Orientation Tensor according to hybrid closure approximation

\( C_{ijkl} \) Stiffness Tensor

\( v_f \) Fiber Volume Fraction

\( v_{RVE_i} \) Volume of the Representative Volume Element

\( S \) Eshelby’s Stiffness Tensor

\( A_E \) Eshelby’s Strain Concentration Tensor

\( A_{MT} \) Mori-Tanaka’s Stiffness Tensor

\( A_{Tot} \) Mori-Tanaka’s Strain Concentration Tensor

\( C_f \) Fiber Stiffness Tensor

\( C_m \) Matrix Stiffness Tensor

\( U \) Strain Energy
A  Aspect Ratio
C  Spacing
p  Orientation Vector
Ψ(p)  Distribution Function
E_i  Young’s Modulus of principal direction i
G_i  Shear Modulus of principal direction i
δ_{ij}  Kronecker Delta function
a_i  Boundary force
\bar{P}  First Piola-Kirchoff Stress Tensor
x_i  Current Position
X_i  Original Position
w_i  Displacement Fluctuation
A_i  Discrete Vector
CHAPTER 1
INTRODUCTION

Load-bearing components go through extensive testing and analysis. The certification process can be particularly onerous in these cases and will require different resources, time and computation methods being the most expensive.

In the field of aeronautics and aerospace, the constraints are more demanding and the timelines tighter. Therefore, to a on the techniques and codes behind the analysis, continuous advancement is conducted on the methodologies of simulation and modeling, both requiring a solid knowledge of the material in use, the manufacturing process and the conditions under which the parts operate.

This last point represents one of the main challenges facing additive manufacturing in its transition to a trusted manufacturing process used for load-bearing parts. While several institutes and companies are already improving their parts by using different 3D printing techniques, their simulation and analysis methods are somewhat lacking: The investigative models presently used rely either on a classic analysis approach or an experimental one; the parts are assigned properties extracted from mechanical tests of dogbone 3D printed specimens. Extensive meshing is used to capture the smaller phases of a heterogeneous material and statistical mechanics allow the evaluation of the average properties from random batches of testing data. In cases of additive manufacturing techniques using powder, the Finite Element models used are either alloy models or converging towards it.

In the case of additive manufacturing techniques such as Fused Deposition Modeling, the manufacturing process has a great impact on the load bearing capabilities
of the part, and its input material is neither powder nor alloy. Producing load-bearing parts through FDM can be achieved through short fiber-reinforced polymer material. This adds to the anisotropy of the part, thus making traditional analysis very inaccurate if used to assess the mechanical properties of the component. Figure 1 gives an overview of the Fused Deposition Modeling: The process is achieved through the deposition of heated polymer in layers. The layers are gradually built from single long filament called beads. These filaments are presented in Figure 2, and are usually stacked close enough to overlap, which allows their walls to fuse together and create cohesive regions between the different layers.

![Figure 1: Fused Deposition Modeling process](image-url)
In this current research, we approach the dilemma of analyzing the structure of a part manufactured through FDM and reinforced with short fibers by building a multi-scale model that will take into consideration the different variables impacting the properties of the components at different scales. Figure 3 gives an overview of the framework of our approach. On the microscopic scale, we study the homogenized RVE that takes into consideration the properties of short fibers, their spacing and distribution as well as their orientation. On the mesoscopic scale as a first step, we develop a homogenized model that uses the effective stiffness tensors built from the previous study, and takes into consideration the beads’ geometry and layout. As a second, we construct the array of beads visible to the naked eye. We take into consideration the presence of the voids and the stiffness tensor obtained from the mesoscale study.
We consequently establish a modeling procedure in three main steps for FDM parts reinforced with short fibers, that rely on an initial input of mechanical properties and orientation state and delivers a final homogeneous stiffness tensor that accounts for manufacturing, material properties and orientation state.
CHAPTER 2
LITERATURE REVIEW

The following chapter summarizes several findings used throughout the research: Fused Deposition Modeling as an Additive Manufacturing technique is presented, along with its process and parameters. The use of short fibers in FDM is explained, their analytical characterization and their orientation are presented along with the impact of process conditions during modeling/injection on their properties. An overview of the field of micromechanics and the homogenization technique is also introduced.

2.1 Additive Manufacturing

Additive Manufacturing – Or Rapid Prototyping and 3D printing – has quickly transitioned from a hobbyist trend to a production asset. The aerospace and aeronautics industries practically believe in the process as a compulsory milestone in the future of space conquest, and account for around 17% of the AM field revenue. Airbus[1],[2], Boeing[3],[4] and GE[5] have already investigated and or incorporated 3D printed parts within their products, from airplanes’ bodies to turbo-engines and satellites.

Additive manufacturing existed since the 80s, but particularly soared in the last decade. Generally, the process relies on the layer-by-layer creation of a part from a CAD model previously post-processed into an STL (Stereolithography) file format.

Previously, additive manufacturing was used to create rapid prototypes (hence the naming). Now, it is being used in broader applications thanks to a wide range of advantages. It is particularly efficient in rendering complex CAD features, otherwise difficult through traditional manufacturing, without the need of patterns, molds or tooling.
In the case of small complex parts, manufacturing time and cost are decreased. In addition to that, the technique is easy to learn, implement and doesn’t allow room for human error during the manufacturing process. The waste is reduced to a minimum, and the recyclability of the debris makes it an environment-friendly process.

There are still several challenges to take in Additive Manufacturing: the prices of the certain machines can reach 1.5 million US dollars. To a certain extent, post-processing of the parts may be required in some cases, and the limitations of the heated bed can be problematic for big parts. Yet, several investigations are conducted in respect to these drawbacks: Companies are investigating large-scale parts through Additive Manufacturing [6], [7], [8]. Also, some AM processes can already ensure great mechanical properties for challenging parts such as blades and nozzles [9], [10], [11] and few have already been certified and incorporated in aircrafts.

Due to the features of the additive manufacturing techniques, most materials used are either plastics or metal powder. The type of material or technique of AM used plays a significant role in the price, the time it will take to make the part and the mechanical properties the final product will have. Depending on the material, Additive Manufacturing can be divided into the following categories:

- Liquid Based Additive Layer Manufacturing such as SLA (Stereolithography Apparatus ) uses a raw material is in its liquid phase. The machine uses a high energy electron or laser beam to process and cure the material into the final, solid part. Figure 4 is an overview of the SLA process: a vat of liquid resin that is UV-curable and a UV laser are used to build parts one layer at a time. On each layer,
the laser beam traces a part cross-section pattern on the surface of the liquid resin. The component is ready after a final curation in a UV over.

Figure 4: Stereolithography Apparatus

- Powder Based Additive Layer Manufacturing such as SLS (Selective laser Sintering) or SLM (Selective Laser Melting) relies on powder (nylon, steel, alloys, titanium...). Laser or electron beam heat is used to melt fine powdered material into the required shape. Figure 5 shows the main parts of the SLS process: a laser beam is used on metal powder to sinter it and compact it into the desired shape.
Solid Based Additive Layer Manufacturing: These systems use a solid raw material, which often comes in thin wires, as an input. Then, an electron beam, heating path or laser beam are used to melt the material into the required shape. The following systems are examples of solid based additive manufacturing systems: LOM (Laminated Object Modeling), MJM (Multi-Jet Modeling) and FDM (Fused Deposition Modeling). Figure 6 illustrates the LOM process: a pre-rolled material sheet is cut using a guided laser. The next sheet is rolled over and glued before undergoing the same process. The outcome is a block of the laminated metal product and the supports to dispose of.
2.1.1 Fused deposition modeling

Fused Deposition Modeling is one of the earliest developed AM processes. It is also one of the cheapest, safest and requires the least amount of training. The main input is plastic wires. The parts are constructed layer by layer through deposition. The material, typically thin wires of plastic, is heated through the machine and extruded through nozzles.

2.1.1.1 Procedure

The FDM machine typically comes with a station and software. The CAD model of the part is then exported to a general format: The export converts the 3D part into the stereolithography -STL- format. This format allows the tessellation of the part into a set of simple triangles, thus allowing the simplification of the part without too much loss on the details. The accuracy on the other hand is reduced but usually kept within the manufacturing's error range. Once the STL is ready, the slicer of the FDM (Quickslice,
Simplify 3D, Ideamaker…etc) will convert the file into thin sections, thus creating the layers that the nozzle will deposit and stack.

Figure 7: FDM Apparatus

Figure 7 shows the main parts of the FDM process. When the process plan is generated, the thin wires - or filaments – are fed to the machine and go through a heating path or element in order to be melted. Once the material reaches the nozzle, it is in semi-molten state. The extrusion nozzle moves around the X-Y plane while the platform moves according to Z. It follows the process plan fed to the machine and deposits on the base of the machine, previously heated, or on another layer. In the latter case, the new layer fuses with the deposited one. If the part will use supports to be disposed of later, it is possible to use a second nozzle that will deposit the support material during the main deposition.
2.1.1.2 Parameters

Parts manufactured through FDM have anisotropic properties [12]. Regardless of the nature of the material used to create them, the parameters of the manufacturing process play a significant role into shaping the properties of the part [13].

Previous studies determined significant manufacturing variables [14],[15],[16] impacting the Ultimate Tensile Strength, UTS, the build time, the surface quality and the bonding of the layers of the part. The rest of the parameters are either of qualitative nature (color), redundant (nozzle’s diameter, bead’s height…etc), considered constant (humidity, deposition speed…) or uncontrollable and noise factors (chamber temperature, humidity…). The ones retained are as follows:

- **Bead Width**: The bead is the term coined for the line (road) that the nozzle deposits on the platform. The width of the bead is its thickness. It will depend on the nozzle’s head and varies between 0.2mm-1mm (0.0078" - 0.0393701”). The bead’s width can improve the surface quality and increase the build time.

- **Air Gap**: Since the beads are extruded in cylindrical shape, their fusing doesn’t involve the whole surface. The space left between the beads is defined as the air gap. The gap can be positive (the beads are not touching), or negative (the beads are overlapping the same space to a certain extent). It impacts the density of the part, thus resulting in longer build time and a decrease in void fraction.

- **Temperature of the build**: Heating is a compulsory part of material transformation and deposition. It controls the viscosity and the fusing of the layers. The crystallization behavior and the cohesiveness between the beads is significantly influenced by the temperature of the build.
• **Raster Orientation:** the beads of the material will be oriented according to the nozzle’s path. This is defined as the raster orientation and it is taken relatively to the loading direction of the FDM part. This variable impacts the direction of the highest load bearing capacity of the bead, and the strength properties of the final component.

• **Air temperature:** This variable describes the temperature of the air within the FDM machine throughout the process. It is therefore a tricky parameter to track due to its fluctuation depending on the time and the location. It primarily affects the fusing of the layers and thus the cohesive nature of the beads and their load bearing capacity.

Of the five variables, air gap and raster orientation have the most impact on the stiffness of the part: the tensile and compressive strengths of the part increase with a decreasing air gap, whereas the raster orientation ensures higher load-bearing when the alignment of the load is the same than the bead’s deposition.

### 2.1.1.3 Materials used in FDM

Since FDM relies on the heating and deposition of material to stack the layers and fuse them together, the feeding and support materials are regularly polymers, in particular thermoplastics such as PLA (PolyLActide), PPSF (PolyPhenylSulFone), ABS (Acrylonitrile Butadiene Styrene) or combinations of them.

While these materials are homogeneous, available and cheap, their mechanical properties do not generally allow use as load-bearing components [17]. Moreover, due to the FDM parameters, the parts will have a high degree of anisotropy despite the initially
homogeneous nature of the material. This has prompted an investigation in the possible other materials that can be used in FDM.

2.1.2 FDM with short fibers:

One of the solutions to reinforce FDM parts is to add short fibers to the thermoplastic. Short fibers are cheaper and more available than long fibers. Besides, they are hard to recycle and include in other practices. 30 to 40% of pristine carbon fibers are wasted during the process of manufacturing and difficult to salvage afterwards. Yet, it has been demonstrated that recycling carbon fiber will be cost effective and energy efficient compared to the alternative, producing virgin fibers. Therefore, adding short fibers to thermoplastics used in FDM has been investigated by several sources.

Zhong et al. [18] studied the addition of glass fiber in ABS and observed an improvement of the mechanical properties of the filament. Marcus Ivey et al. [19] compared specimens made out of PLA with PLA reinforced with short carbon fibers (PLA/CF). The tensile tests conducted showed a significant increase in the Young's modulus in the PLA/CF parts in comparison to PLA ones. Tekinalp et al. [20] studied the addition of short fibers to ABS and manufactured specimens of different fiber volume fraction for tensile testing. They observed an increase in strength and modulus of the ABS reinforced composites.

The studies mentioned have taken an experimental approach in assessing the properties of the coupons. Others used analogies of the laminate theory to predict the properties of the FDM manufactured parts [21], [22], [23]: the layer by layer structure and oriented state allows the use of the orthotropic material model and the laminate stacking
approach and calculate the average mechanical properties. The effective modulus calculated correlated reasonably with the FEA simulations and the experimental testing.

These methods require an extremely fine mesh and a homogeneous input material. One of the main reasons is the lack of an exclusive discretized methodology to model and simulate 3D printed coupons on software. Attempts have not been found for FDM parts reinforced with short fibers. It is however a crucial step to investigate in order to use FEA for simulation and certification purposes: load-bearing parts have to answer rigorous requirements in analysis and certification. Studies or lifecycle at least, have to be conducted. In the case of advanced industries such as aerospace, the requirements of study cases are diverse and extensive. Conducting physical testing gives data that can be used as a first reference and an early draft for material cards. But the understanding of the heterogeneous and anisotropic nature of the FDM manufactured part, as well, as the overall properties it will have, is the key to deliver accurate material models and generalized properties for the part, in order to include it in the FEA process.

2.2 Micromechanics and multiscale modeling of heterogeneous media

Composites are anisotropic materials whose properties aren’t computed directly like alloys. A study of the components of the composite has to be conducted beforehand to take into consideration the properties of the phases of the composite. Table 1 illustrates the degree of anisotropy in common composites, compared to steel and aluminum.
Table 1: Comparison between composites and alloys in degree of anisotropy

<table>
<thead>
<tr>
<th>Material</th>
<th>$E_1/E_2$</th>
<th>$E_1/G_{12}$</th>
<th>$F_{1}/F_{2t}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Aluminum</td>
<td>1.00</td>
<td>3.08</td>
<td>1.00</td>
</tr>
<tr>
<td>Steel</td>
<td>1.00</td>
<td>2.58</td>
<td>1.00</td>
</tr>
<tr>
<td>S-Glass/Epoxy</td>
<td>2.44</td>
<td>5.06</td>
<td>28.00</td>
</tr>
<tr>
<td>E-Glass/Epoxy</td>
<td>4.42</td>
<td>8.76</td>
<td>17.70</td>
</tr>
<tr>
<td>Carbon/Epoxy</td>
<td>13.64</td>
<td>19.10</td>
<td>41.40</td>
</tr>
<tr>
<td>UHM/Epoxy</td>
<td>40.00</td>
<td>70.00</td>
<td>90.00</td>
</tr>
<tr>
<td>Kevlar/Epoxy</td>
<td>15.30</td>
<td>27.80</td>
<td>260</td>
</tr>
<tr>
<td>Aramide/Epoxy</td>
<td>15.82</td>
<td>39.55</td>
<td>3.82</td>
</tr>
</tbody>
</table>

For laminated composites, taking a Representative Volume Element -RVE- allows the computation of the ply's averaged properties. Following this logic, several elementary models have already being constructed. For instance, in the case of laminate theory, the effective properties are obtained through Voigt[24] and Reuss[25], thus allowing the calculations of the properties of every lamina, and thus the laminate. Coupon testing on laminates also delivers exploitable data that accurately describes the properties obtained through analytical averaging.

2.2.1 The need for micromechanics

As the heterogeneity of the composite increases, and the variables governing its properties increase, there is a need to take these variables into consideration, to find new ways to average properties and to be able to come up with results and physical testing data that can be comparable. To answer such need amongst others, micromechanics is dedicated to materials and their related phenomenon (such as cracks, voids…) on the microscale.
One of the main arcs of micromechanics is the homogenization of heterogeneous media: in order to capture the properties of the different phases constituting a material, a process of averaging their properties over a representative volume on the microscale allows building a homogeneous model, easier to handle in the constitutive equations, and transitionable to the macroscale in use. Mean-field methods, such as the self-consistent method, the two-step bounding method...etc are used in the following step to average a large number of inclusions over the volume.

Most of the mean-field methods used in the homogenization process rely on the existence of the strain tensor (or strain localization tensor) to develop their homogeneous model. Rao et al.[26] used the asymptotic homogenization to develop his equivalent homogeneous model:

\[ <\sigma_{ij}> = C_{ijkl}^H \varepsilon_{kl} \]  

(2.2.1)

With \( C_{ijkl}^H \) the equivalent homogenized stiffness tensor
\( \varepsilon_{kl} \) the volume averaged strain
\(<\sigma_{ij}> \) The volume averaged stress given over the RVE given by: 

\[ <\sigma_{ij}> = \frac{1}{V_e} \int_{V_e} \sigma_{ij} \, dV_e \]

The strain tensor developed by Eshelby is considered an elegant and analytical solution to the homogenization problem.

**2.2.2 Eshelby’s tensor for inclusions in an infinite media**

The Eshelby’s model[27] is the analytical solution for the homogeneous stiffness of an inclusion within an infinite media: Using the superposition principle of linear elasticity and the Green’s function, Eshelby related the constrained strain to the inclusion’s eigenstrain.
Variationally, heterogeneous inclusions were described by Sokolnikoff[28] as the study of an energy functional:

We recall that the energy within a volume of a homogeneous material (linear, elastic, without body forces) is proportional to the dot product of the strain and stress tensors.

For the case of a heterogeneous material though, our definition of energy will be calculated in a piece-wise fashion, according to the different phases, but will use the same relation within each subdomain (or phase) of the material.

The microscopic energy within a phase is defined as:

\[ U_{Microscopic} = \frac{1}{2} \varepsilon(x) : C(x) : \varepsilon(x) \]  

(2.2.2)

With C being the stiffness tensor.

Once the expression is average throughout the material's domain, we get the equivalent energy functional:

\[ U_{Equivalent} = < U_{Microscopic} >= < \frac{1}{2} \varepsilon(x) : C(x) : \varepsilon(x) > \]  

(2.2.3)

On the other hand, if the heterogeneous material is assumed to be homogeneous, it will yield a “macroscopic” energy, such as:

\[ U_{Macroscopic} = \frac{1}{2} \varepsilon(x) : C_h(x) : \varepsilon(x) \]  

(2.2.4)

For an array of anisotropic elastic heterogeneous materials, both energies are related, as \( U_{macroscopic} \) is the average of the \( U_{Microscopic} \). Therefore, we can relate their stiffnesses such as:

\[ \frac{1}{2} < \varepsilon(x) : C(x) : \varepsilon(x) > = \frac{1}{2} < \varepsilon(x) > : C_h(x) : < \varepsilon(x) > \]  

(2.2.5)

The minimum potential energy principle stipulates that there is a strain field \( \varepsilon \) minimizing the trial energy functional. It applies to periodic materials as well. Bensoussan
et al.[29] proved that the boundary conditions will be over the RVE and vanish because of the periodicity.

The stiffness tensor $C_h$ computed from the expression will inherit C’s features: it will be symmetric and positive definite.

### 2.2.3 The Self-consistent method

One of the mean-field methods used in dilute models and based on the Eshelby’s solution is the self-consistent method: The self-consistent method tends to overestimate the interactions between inclusions. While a closed-form solution can be found for continuous fibers, using SC for short fibers requires iteration and the accuracy is decreased.

The essential assumption of the method is that every inclusion is embedded within an equivalent medium of as-yet-unknown stiffness, according to the following equation:

$$A^{SC} = [I + S_c C_c^{-1}(C_f - C_c)]^{-1}$$  \hspace{1cm} (2.2.6)

With

$$C_c = C_M + V_f (C_f - C_c)$$  \hspace{1cm} (2.2.7)

Where $C_i$ are the respective stiffness tensors of the composite, the matrix and the fiber, and $S_c$ the Eshelby’s tensor of the composite.

### 2.2.4 The Mori-Tanaka model

While the Eshelby tensor is an important foundation in the homogenization process, it doesn’t give an accurate evaluation of stiffness in concentrated suspensions.

The Mori-Tanaka[30] model offers an analytical approximation for heterogeneous media with higher concentrations of suspensions. Mori-Tanaka’s model is an “explicit” solution to the inclusions’ problem when their concentration is higher and their
geometrical structures are significantly small. Mori-Tanaka rely on the linear elasticity of the matter to include the stiffness while taking into consideration their aspect ratio and length. The methodology is valid for ellipsoidal inclusions with finite dimensions: The strain concentration tensor according to Mori-Tanaka $A^{MT}$ is defined using the Eshelby strain concentration tensor $A^E$ relating the inclusion’s strain to that of the matrix:

$$A^{MT} = A^E (V_f A^E + V_m I)^{-1}$$

(2.2.8)

With $V_f$ the fiber volume fraction and $V_m$ the matrix volume fraction, and

$$A^E = [IS(C_m)^{-1}(C_f - C_m)]^{-1}$$

(2.2.9)

Summing over the different inclusions and their volume fraction of every orientation of the heterogeneous material, we find the general strain concentration tensor $A$ such as:

$$A = \sum V_i A_i^{MT}$$

(2.2.10)

The stiffness is computed using the following expression:

$$C = C_m + V_f (C_f - C_m) A$$

(2.2.11)

The Eshelby model is the foundation of homogenization techniques. It is also the only analytical solution available for the inclusion problem. Its accuracy however decreases with higher volume fraction. On the other hand, Mori-Tanaka may not necessarily offer a local accurate answer but the averaged properties correlate with the available results. FEA and laminate theory display similar values.

Jiang et al.[31] compared the computed effective moduli of a composite for an aspect ratio $\gamma$ using different mean field methods and laminate theory. Figure 8 summarizes the comparison: Mori-Tanaka offers the most reasonable agreement with the improved self-consistent method and the Hashin-Shtrikman’s lower bound.
Figure 8: Comparison between different micromechanics model vs fiber volume ratio: (a) in-plane bulk modulus; (b) in-plane shear modulus; (c) longitudinal shear modulus
Grimal et al.[32] compared the computed stiffness values calculated from the Mori-Tanaka analytical solution with the results obtained different FEA runs.

Figure 9 is a comparison between stiffness terms computed through FEA and Mori-Tanaka: The solid line represents the results from the analytical solution. The crosses, circles and dots represent the results obtained from FE models of RVE.

*Figure 9: Comparison of stiffness coefficients obtained through different methods*
Freour et al.[33] compared the macroscopic and local stresses of the T300/5208 composites in the central ply of the [+55/-55]_s laminate calculated using the Mori-Tanaka approach and the SC method. Figure 10 summarizes the findings: SC - Self-Consistent values are calculated using self-consistent method. MT values are computed using Mori-Tanaka approach.

![Figure 10: Comparison between stresses calculated using SC (Self-Consistent) and Mori-Tanaka](image)

2.2.5 Boundary conditions for micromechanical models

While following the numerical guidelines of finite element methods, the discretization process of micromechanical models has to answer specific goals: computing average properties, allowing an accurate transition between scales and the recovery of local states in the different inclusions involved. In our case, our aim is to compute the stiffness properties of the equivalent homogeneous model. Therefore, a specific set of boundary conditions is required for a heterogeneous RVE that will give
results for the effective stiffness tensor. Hill and Mandel[34] constructed the macro-heterogeneity condition based enforcing the consistency of the energy within the two models: if we consider a media as a discrete and cohesive particle system, the volume average of the virtual work applied at the boundaries of the micro-structure and the virtual work of a macroscopic material point must be equal. Therefore, they have to satisfy the following condition:

\[ \bar{P}: \delta \bar{F} = \frac{1}{v} \sum_{i=1}^{n} a_i \delta x_i \]  \hspace{1cm} (2.2.12)

Where \( \bar{P} \) is the homogeneous first Piola-Kirchoff stress tensor,

\( \bar{F} \) is the homogeneous deformation gradient

\( a_i \) is the boundary force

\( x_i \) is the current position vector

The resulting statement to solve for is:

\[ \frac{1}{v} \sum_{i=1}^{n} (a_i - \bar{P}A_i)(\delta w_i) = 0 \]  \hspace{1cm} (2.2.13)

Where \( A_i \) is the finite area vector

\( w_i \) the local fluctuation

Three common types of boundary conditions can be used to satisfy the equation:

**2.2.5.1 Periodic boundary conditions**

They are best suited for periodic structures, hence their optimal results for RVE and multi scale studies. If we consider a RVE to have positive and negative faces, periodic boundary conditions impose the same displacement on the boundaries facing one another:

\[ x_i^+ - x_i^- = \bar{F}(X_i^+ - X_i^-) \]  \hspace{1cm} (2.2.14)

where \( x_i^+ \) is the current position of the point,
and $X_i^+$ is the initial position of the point, related to $x_i^+$ by the deformation gradient $\bar{F}$ and a local fluctuation $w_i$ by the following relation:

$$x_i = \bar{F}X_i + w_i$$  \hfill (2.2.15)

Applying periodic traction will follow the same logic, except the nature of periodicity: to respect the law of equilibrium, traction should be antiperiodic.

In the case of periodic boundary conditions, we formulate them as follows:

$$w_i'^+ = w_i'^-$$ for displacement at the boundaries, and $$a_i'^+ = -a_i'^-$$ for traction at the boundaries.

### 2.2.5.2 Homogeneous displacement

Homogeneous displacement boundary conditions assume zero micro-scale fluctuations, making them less accurate than periodic boundary conditions for RVE models and resulting in stiffer results. In the case of larger RVE, they converge towards the periodic boundary conditions results.

Homogeneous displacement is formulated as follows: $$w_i'^+ = w_i'^- = 0$$ at the boundaries.

### 2.2.5.3 Homogeneous traction

Since the boundary forces $a_i$ are determined from the first Piola-Kirchoff stress tensor $\bar{P}$ and the vector $A_i$, it follows that on the boundary, we have:

$$a_i = \bar{P}A_i$$  \hfill (2.2.16)

The equation establishes homogeneous traction boundary conditions and provides softer results compared to periodic boundary conditions. In the case of larger RVE, they converge towards the periodic boundary conditions results.
2.3 Characterization of short fibers and suspensions

Short fibers are defined by their material’s properties (transverse isotropic properties) and their geometrical features: aspect ratio and spacing.

- The aspect ratio $A$ is defined through the fiber’s diameter and its length.
- The spacing $C$ gives an average distance between the short fibers within the matrix. It can be evaluated through the fiber concentration by volume.
- The orientation state of the short fibers play a significant role in the mechanical properties of the part due to the degree of anisotropy of the fibers.

Spacing and aspect ratio are important in determining the mechanical properties of the parts and assessing the suspension’s concentration in the matrix as well as the interaction of the short fibers with one another.

The common classification scale for suspensions depending on inclusions dimensions is:

- Dilute suspension: $C<<A^2$.
- Semi-concentrated $A^2<C<A$
- Concentrated $C>A$

In the case of concentrated composites, they are the ones commonly found in the market: commercial composites usually contain 10% to 50% fibers by weight. To assess other properties of the inclusions such as fiber orientation, the interaction between short fibers has to be taken into consideration. This is achieved through an interaction coefficient proposed and developed by Folgar and Tucker[35].
Semi-concentrated composites are modeled using Dinh and Armstrong’s[36] model: the bulk deformation of the fluid to track the orientation of the short fibers in rigid state within homogeneous flow.

For dilute suspensions, the orientation state doesn’t take into consideration the interactions of the fibers in its equation of change. This current research uses dilute suspensions. The orientation state is described details in the following section.

2.4 Orientation-Averaging

To be able to assess parts manufactured with a heterogeneous material made out of short fiber and polymers and manufactured through the molding/injection processes, it is essential to be able to evaluate such impact and quantify the properties accordingly, thus paving the way to a framework to discretizing the parts and coming up with analysis and certification protocols.

When it comes to FDM with short fibers, the main feature that manufacturing impacts is the orientation pattern of the short fibers in the viscous flow. Fibers’ alignment is a dominant feature in the composite’s structural properties. In the case of short fibers composites, the orientation pattern of the fibers as they navigate the flow during the manufacturing process becomes a key feature. In order to evaluate the mechanical properties of the heterogeneous material, the properties of both phases are averaged over the continuum. The anisotropy and orientation are weighted by an orientation distribution function. This procedure is known as orientation averaging and requires an understanding and correct evaluation of the orientation state. To quantify this property, several choices of variables have been proposed and studied: Nomura and Kawai[37] used sets of orientation factors depending on symmetry and Eulerian angles to describe
orientation state. Hermans described fiber orientation with axisymmetric parameters through assumptions over symmetry assumptions or primary orientation of the axis [38]. White and Spruiell investigated the use of angles between the material axes and the Cartesian coordinate reference axes defining the machine and exploiting the symmetry of the transverse direction of the films [39].

In the present work, we choose to adopt Advani and Tucker’s [40] approach to describing orientation: They rely on tensorial parameters to describe the orientation of short fibers in injection molding processes: starting from the coordinates of the vector \( \mathbf{p} = \langle p_1, p_2, p_3 \rangle \) - illustrated in figure 11 - describing the orientation state of a short fiber, and an orientation distribution function \( \Psi(\mathbf{p}) \), the following second-order tensor is constructed:

\[
a_{ij} = \int p_i p_j \Psi(\mathbf{p}) \, d\mathbf{p} \quad (2.4.1)
\]

![Figure 11: Fiber orientation in spherical coordinates](image)

\( a_{ij} \) is a symmetric and normalized tensor that describes the orientation state of the fibers within a volume. Figure 12 shows examples of orientation distribution and the \( a_{ij} \) terms describing it. In the case of short fibers completely aligned with the \( x_2 \)-direction,
the diagonal terms of $a_{ij}$ are 0 except for $a_{22} = 1$. In the case of random orientation, the $a_{ii}$ terms are all equal to 0.33 and $a_{ii} = 1$.

![Figure 12: Fibers orientation description using $a_{ij}$](image)

The fourth order orientation tensor, $a_{ijkl}$, is used to describe the orientation state and provide a closed system to the stiffness calculations. Like the second order tensor, it relies on the unit vector describing the fiber orientation and the orientation distribution function:

$$a_{ijkl} = \oint p_ip_jp_kp_l \Psi(p)dp$$  \hspace{1cm} (2.4.2)

In particular, Advani & Tucker prove mathematically and physically that the second and fourth order of the tensorial parameters are sufficient to determine the stiffness tensor taking into consideration the fiber orientation state. Since the stiffness tensor is a fourth degree order tensor, higher orders of orientation tensors will not improve its values. This particular approach represents a more general take on the orientation study, mainly because of the independence of the referential of study as well as the compact and unified shape of the formulas used. The use of tensorial parameters implies the following assumptions:

- The fibers are assumed to be rigid cylinders, uniform in length and diameter.
- The fiber concentration within the matrix is spatially uniform.

- Orientation distribution function is a sufficient description for the orientation state to compute stiffness properties.

Moreover, the 4th order tensor provides complete information of the 2nd one. Finally, the orientation tensors allow the recovery of the distribution function.

The need of a 4th order orientation tensor arises from the need of the tensorial parameters to account for processing conditions when computing orientation. The equation of motion of suspensions in a uniform flow introduces material derivatives that result in the presence of the next even order tensor, the fourth order orientation tensor. Computing the equation of change with the fourth order tensor will cause the sixth order one to appear in the expression, leading to an open set of equations. This is known as a closure problem. Consequently, we use closure approximations to obtain a closed system.

Building closure approximations is part of the orientation averaging process. While there are several closure approximations, we restrict ourselves to the following main types, as they were extensively used and tested for inclusions in polymer flow.

2.4.1 The linear closure approximation

The linear closure was suggested by Hand[41]. It is an exact closure for completely random distributions of fibers and allows the computation of the 4th order orientation tensor through the following equation:

\[
a_{ijkl} = A(\delta_{ij}\delta_{kl} + \delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}) + B(a_{ij}\delta_{kl} + a_{ik}\delta_{jl} + a_{il}\delta_{jk} + a_{jl}\delta_{ik} + a_{jk}\delta_{il})
\]

(2.4.3)
with A and B constants depending on the dimension of the orientation space, such that:

A=-1/35 and B=1/7 for 3D orientation states, and A=-1/24 and B=1/6 for 2D orientation states.

2.4.2 The quadratic closure approximation

The quadratic closure was introduced by Doi[42]. It is an exact solution for perfect uniaxial alignment in flow[43], [44]. and allows the computation of the 4th order orientation tensor through the following equation:

$$a_{ijkl} = a_{ij} a_{kl}$$  \hfill (2.4.4)

It is the exact solution for completely aligned distributions of fibers and doesn’t involve additional parameters.

2.4.3 The hybrid closure approximation

The hybrid closure, introduced by Advani and Tucker[45], is a mix of the linear and quadratic closures. It gives an accurate approximation for all orientation states, and allows the computation of the 4th order orientation tensor through the following equation:

$$a_{ijkl} = (1 - f) a_{ijkl}^L + f a_{ijkl}^Q$$  \hfill (2.4.5)

With $a_{ijkl}^L$ the 4th order orientation tensor computed using the linear closure approximation.

And $a_{ijkl}^Q$ the 4th order orientation tensor computed using the quadratic closure approximation.

And f a parameter such as :

$$0 < f < 1$$

$$f = A a_{ij} a_{ji} - B$$
For 3D orientation states, $A=3/2$ and $B=1/2$. For 2D orientation states, $A=2$ and $B=1$.

From the shape of $f$, the hybrid closure approximation will be the same than the linear closure in case of random orientation, and will be exactly equal to the quadratic closure approximation in case of perfectly aligned orientation.

Randy and Tucker [46], [47], [48] conducted experiments to assess the accuracy of the tensorial parameters in predicting the elastic properties of short fibers composites and proved the accuracy of the methodology for regular flow fields and low fiber volume fraction. In the case of three-dimensional flow fields, care should be given as the configuration allows more freedom of motion. More recently, Müller and Böhlke [49] used micro-computed tomography to compare orientation tensor predictions to experimental microstructure data. The deviations observed using only the second order orientation tensor were relatively high and pressed the importance of using a fourth order orientation tensor to describe more accurately the microstructure data. They also observed that on the experimental scale, the detectors don’t pick up on the shortest fibers, which can amount to more than 50% of the fiber volume fraction, thus explaining the deviation between the comparisons and the need to account for the fibers with small aspect ratio.

For our current work, we choose to use the orientation tensors along with the linear, hybrid and quadratic closure approximations for our orientation averaging before relying on the one giving the least deviation.

### 2.5 Manufacturing impact on short fibers

The Fused Deposition Modeling process involves the injection and melting of the raw material before deposition. This impacts the short fibers on different aspects:
-Crystal composition: due to heat, the crystal structure of the composite transitions through different phases and changes from the raw material to the end result used in layer deposition.

-Inclusions’ dimensions: The short fibers’ original length is impacted by the injection process and the original aspect ratio decreases significantly by the end of the process. Severe fiber attrition[50] can happen due to higher fiber concentration and longer fiber length, resulting in a higher degree of fiber-fiber interaction and increased fiber-wall contacts.

-Inclusions’ distribution: the short fibers are usually thrown within the polymer with little adjustment. The resulting orientation is random. It has been observed however, that due to injection and/or molding process, the fibers closer to the walls of the injecting pipe are aligned with the longitudinal direction of the wall. As the short fibers progress to the inner flow, the orientation assumes as random state until a transversal one.

Mazahir et al. [51] conducted experiments using a center-gated disk to evaluate fiber orientation. They observed two distinguishable layers of orientation through the thickness, known as the shell and the core layer. Fibers within the shell layer tend to align in the direction of the flow. Fibers in the core layer tend to align in the transversal layer. In-between, a transition layer exhibits a random orientation.

Yazdi et al[52] worked on a similar study on how short fibers are affected by viscous effects. They observed that in places far enough from vortices, fiber orientation was not affected by the matrix’s features, but near contraction walls, fibers are more orientated for polymer matrices. Vortex intensity was reciprocally related to fiber
orientation in the vortex region. An increase in fiber aspect ratio or concentration also results in a slightly more orientated state and a more intense vortex.
CHAPTER 3

OBJECTIVE

Amongst the challenges FDM faces as a novel manufacturing process, certification and analysis come as prominent milestones. Load-bearing parts require extensive and rigorous calculations in order to pass the requirements in both testing and analysis. FDM using short fiber composites represent the additional challenge of taking into consideration the complex features of the material and the manufacturing process. These two main points aren't taken into consideration during the analysis or testing of a dogbone sample manufactured using FDM: the mesh can't be so fine as to pick up individual fibers' properties. The geometry can't represent every orientation state of every fiber within the part on a microscopic scale. Overall, traditional FEA methods won't take into consideration the voids, cohesive zones between beads and orientation features and distributions of a part made out of short fiber composite and manufactured through Fused Deposition Modeling.

To answer these challenges, our research aims at setting up an RVE for FDM components made out of short fiber composites, taking the unique features of FDM with short fibers composites into calculations, and using it as the building block for the meshing type during discretization step, as illustrated in Figure 13.
Our current study focuses on the construction of a framework for the analysis of an RVE of the FDM part made out of short fiber composites. This implies the study of the RVE on a microscopic scale, which will take into consideration the features of the short fiber, and the study of the RVE on the mesoscopic scale, which will incorporate the manufacturing process impact.
CHAPTER 4
MICROSCOPIC SCALE

The following chapter covers the work performed on the representative volume element -RVE- on the microscopic scale, of the short fiber composite part manufactured through the FDM process. Our main objective is to prove the accurate use of a combined stiffness tensor with the orientation tensor to represent the average stiffness over a RVE. An overview of the input data is detailed, a study in convergence is conducted prior to the RVE analysis. Finally, an analytical and FE studies are performed and compared.

4.1 Analysis Set Up

The following section describes the common configuration used for the convergence and orientation studies.

4.1.1 Representative volume element at the microscopic scale

A Representative Volume Element is defined as a basic building block of the material, and should neither be too big as to have iterated features, nor so small that it misses some features of the heterogeneity of the material. In the case of short-fiber composites, in order to render their structural features accurately, we take into consideration their spacing and their aspect ratio. Consequently, as shown in figure 14, our RVE is a cube containing two short fibers, a central complete one and the other divided into quarters and distributed symmetrically, therefore taking into consideration the distribution’s features. We choose an idealized cubic volume for the overall RVE, and an idealized cylinder for the short fibers.
The dimensions are picked such as there is possibility to orient the central fiber within the matrix volume. This restrains the value of the fiber volume fraction and the aspect ratio for the first iteration.

4.1.2 Hypothesis of the study

The following assumptions are adopted for the microscopic RVE:

- Fibers are assumed to be isotropic.
- Matrix is assumed to be isotropic.
- Fiber and matrix are perfectly bonded.
- Fibers’ length is not impacted by the manufacturing process and maintained to its initial dimensions.
- There are neither voids nor cracks within the RVE.
4.1.3 Material’s information

The short fibers are made out of T300. The matrix is PPS. The aspect ratio is assumed to be 5 in the first iteration due to limitations in computational resources and need of a less dilute fiber volume fraction that can accommodate different orientation states for the central fiber. We also assume a fiber volume fraction of $V_f = 3.63\%$.

Table 2 summarizes the material properties used throughout this study, extracted from the respective datasheets of T300 [53] and PPS [54] :

<table>
<thead>
<tr>
<th>Fiber Properties</th>
<th>Matrix Properties</th>
</tr>
</thead>
<tbody>
<tr>
<td>Tensile Strength</td>
<td>3530 Mpa</td>
</tr>
<tr>
<td>Tensile Modulus</td>
<td>230 Gpa</td>
</tr>
<tr>
<td>Poisson Ratio</td>
<td>0.2</td>
</tr>
<tr>
<td>Strain</td>
<td>1.50%</td>
</tr>
<tr>
<td>Density</td>
<td>1.76 g/cm³</td>
</tr>
<tr>
<td>Fiber Diameter</td>
<td>5 μm</td>
</tr>
</tbody>
</table>

<p>| | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Tensile Modulus</td>
<td>3.8 GPa</td>
</tr>
<tr>
<td>Poisson Ratio</td>
<td>0.4</td>
</tr>
<tr>
<td>Density</td>
<td>1.34 g/cm³</td>
</tr>
<tr>
<td>Cube length</td>
<td>30 μm</td>
</tr>
</tbody>
</table>

4.1.4 Model Orientation

Figure 15 illustrates the three main orientations of the core fiber, used in our study:

a. Both fibers are aligned according to the z-axis.

b. The divided fiber is aligned to the z-axis, while the central fiber is aligned at 45° relatively to it.

c. The divided fiber is aligned to the z-axis, while the central fiber is aligned at 90° relatively to it.
4.1.5 Periodic boundary conditions

Throughout this study, we use the periodic boundary conditions to simulate the periodicity of microscopic RVE. The periodic boundary conditions are particularly powerful when it comes to minimizing the functional describing the RVE and ensuring energy conservation between the heterogeneous model and the equivalent homogeneous one. The comparison between the two models allows the construction of the effective stiffness of the homogenized model through the properties of the different phases of the material.

Therefore, to construct the stiffness tensor, we apply one strain corresponding to the tensor’s column we wish to compute and leave the others as zero. Assuming a local coordinate axis \((x_1, x_2, x_3)\) for the cubic RVE, we fix the geometric center of the structure in all directions to avoid rigid body motion and we apply the following sets of boundary conditions as shown from Figure 16 through 21:

\[
\begin{array}{cccccc}
C_{11} & C_{12} & C_{13} & 0 & 0 & 0 \\
C_{12} & C_{22} & C_{23} & 0 & 0 & 0 \\
C_{13} & C_{23} & C_{33} & 0 & 0 & 0 \\
0 & 0 & 0 & C_{22} & 0 & 0 \\
0 & 0 & 0 & 0 & C_{33} & 0 \\
0 & 0 & 0 & 0 & 0 & C_{11} \\
\end{array}
\]

Apply Strain in the 1-direction

\[
\epsilon_{ij} = \{\epsilon_{x1}, 0, 0, 0, 0, 0\}^T \text{ applied to the negative 11-face}
\]

Antiperiodicity in 11-dir on the positive and negative 11-faces

Periodicity for all directions applied to the rest of the faces

Figure 16 : Periodic Boundary Conditions corresponding to the Tension_11 case
Figure 17: Periodic Boundary Conditions corresponding to the Tension_22 case

Figure 18: Periodic Boundary Conditions corresponding to the Tension_33 case

Figure 19: Periodic Boundary Conditions corresponding to the Shear_23 case

Figure 20: Periodic Boundary Conditions corresponding to the Shear_13 case

Figure 21: Periodic Boundary Conditions corresponding to the Shear_12 case
4.1.6 Analytical homogenization

Unlike Eshelby’s model that provides an accurate and analytical solution for dilute suspensions (<1%), Mori-Tanaka model gives an accurate explicit solution to composites with higher concentration. In our case, \( V_f = 3.63\% \) and will therefore require the Mori-Tanaka model: its construction relies on the Eshelby strain concentration tensor but takes into consideration partitioned fiber volume fractions instead of a unique value.

To construct the stiffness taking into consideration the orientation state of the RVE according to Mori-Tanaka method, we assume that the cube is partitioned into a laminate of three plies with the following stacking according to y-axis:

a. \([0]_2\).

b. \([0/45]\).

c. \([0/90]\).

We calculate Eshelby strain concentration tensor for every ply using the following equation:

\[
A^\alpha = [I + S^\alpha (C_m)^{-1}(C_f - C_m)]^{-1}
\] (4.1.1)

With: \( A \) the strain concentration tensor of the fiber oriented at angle \( \alpha \).

\( I \) the neutral tensor.

\( S^\alpha \) the Eshelby tensor of the fiber oriented at angle \( \alpha \).

\( C_f \) The fiber stiffness tensor.

\( C_m \) The matrix stiffness tensor.

We then calculate the total strain concentration tensor:

\[
A^{Tot} = \sum_{\alpha_i} v_{\alpha_i} A^E_{\alpha_i}
\] (4.1.2)
With : \(v_i\) the fiber volume fraction corresponding to every Eshelby strain concentration tensor

\(A^E_i\) the strain concentration tensor of the fiber oriented at angle \(\alpha_i\).

This allows us to compute the concentration strain tensor according to Mori-Tanaka, using the following equation:

\[
A^\alpha_{MT} = A^E_\alpha [(1 - v_f)I + A^{Tot}]^{-1}
\]  

(4.1.3)

Finally, we can compute the effective stiffness of the whole RVE with the equation:

\[
C_{eff} = C_m + v_\alpha (C_f - C_m)A^\alpha_{MT} + v_\beta (C_f - C_m)A^\beta_{MT}
\]  

(4.1.4)

With: \(v_\alpha\) the fiber volume fraction of the ply where the short fiber is oriented at angle \(\alpha\).

\(v_\beta\) the fiber volume fraction of the ply where the short fiber is oriented at angle \(\beta\).

\(A^\alpha_{MT}\) and \(A^\beta_{MT}\) respectively the strain concentration tensors corresponding to the plies with orientations \(\alpha\) and \(\beta\).

In the cases of the sequences [0]_2, [0/45] and [0/90], the resulting stiffness tensors according to Mori-Tanaka are shown on Table 3 to 5:
Table 3: Stiffness (in GPa) according to MT method for [0]_2

<table>
<thead>
<tr>
<th></th>
<th>8.53</th>
<th>5.64</th>
<th>5.62</th>
<th>0.00</th>
<th>0.00</th>
<th>0.00</th>
</tr>
</thead>
<tbody>
<tr>
<td>8.53</td>
<td>5.64</td>
<td>5.62</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
</tr>
<tr>
<td>5.64</td>
<td>8.53</td>
<td>5.62</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
</tr>
<tr>
<td>5.65</td>
<td>5.65</td>
<td>9.35</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
</tr>
<tr>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>1.56</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
</tr>
<tr>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>1.56</td>
<td>0.00</td>
<td>0.00</td>
</tr>
<tr>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>1.53</td>
<td></td>
</tr>
</tbody>
</table>

Table 4: Stiffness (in GPa) according to MT method for [0/45]

<table>
<thead>
<tr>
<th></th>
<th>9.05</th>
<th>5.73</th>
<th>5.64</th>
<th>0.00</th>
<th>0.00</th>
<th>0.18</th>
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<tbody>
<tr>
<td>5.71</td>
<td>8.63</td>
<td>5.64</td>
<td>0.00</td>
<td>0.00</td>
<td>0.18</td>
<td>0.00</td>
</tr>
<tr>
<td>5.62</td>
<td>5.64</td>
<td>8.53</td>
<td>0.00</td>
<td>0.00</td>
<td>-0.01</td>
<td></td>
</tr>
<tr>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>1.54</td>
<td>0.01</td>
<td>0.00</td>
<td></td>
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<tr>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.01</td>
<td>1.56</td>
<td>0.00</td>
<td></td>
</tr>
<tr>
<td>0.10</td>
<td>0.10</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>1.74</td>
<td></td>
</tr>
</tbody>
</table>

Table 5: Stiffness (in GPa) according to MT method for [0/90]

<table>
<thead>
<tr>
<th></th>
<th>8.94</th>
<th>5.63</th>
<th>5.64</th>
<th>0.00</th>
<th>0.00</th>
<th>0.00</th>
</tr>
</thead>
<tbody>
<tr>
<td>5.63</td>
<td>8.94</td>
<td>5.64</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
</tr>
<tr>
<td>5.63</td>
<td>5.63</td>
<td>8.53</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
</tr>
<tr>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>1.55</td>
<td>0.00</td>
<td>0.00</td>
<td></td>
</tr>
<tr>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>1.55</td>
<td>0.00</td>
<td></td>
</tr>
<tr>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>1.56</td>
<td></td>
</tr>
</tbody>
</table>

The results obtained correspond to a dilute short fiber volume fraction within a matrix. The abnormal values for the [0/45] are due to the explicit calculations and error range used (0.01) accumulating through the inverse operations.
4.2 Convergence study

We conducted a convergence study in order to establish the impact of the mesh refinement on our results: due to the limited computational resources at the time of this research, we seek to establish the most optimal mesh given the resources, the ability to converge and the accuracy of the results. The reported values are compared to the analytical ones predicted by the Mori-Tanaka method and to the extra-fine mesh.

4.2.1 Mesh quality

Comsol offers an automated mesh option: Physics controlled mesh. The mesh refinement is available in nine types. For our study, we pick five refined configurations: Coarse, Normal, Fine, Finer and Extra Fine.

Table 6 summarizes the mesh details of every model:

*Table 6: Mesh Details for the different models and refinement options*
4.2.2 Convergence Analysis

Using the periodic boundary conditions detailed in the previous section, we extract the local stresses and strains of every configuration and every mesh type. We compute the stiffness tensors and compare them with the Mori-Tanaka analytic stiffness. Table 7 through Table 9 summarize the findings:

Table 7: Comparison between Comsol and MT stiffness for $[0]_2$

<table>
<thead>
<tr>
<th></th>
<th>Stiffness From Comsol - Coarse</th>
<th>Comparison with Mori-Tanaka</th>
</tr>
</thead>
<tbody>
<tr>
<td>Coarse</td>
<td>8.54  5.64  5.59  0.00  0.00  0.00</td>
<td>-0.10%  0.08%  0.48%  0.00%  0.00%  0.00%</td>
</tr>
<tr>
<td></td>
<td>6.54  8.54  5.59  0.00  0.00  0.00</td>
<td>0.08%  -0.10%  0.48%  0.00%  0.00%  0.00%</td>
</tr>
<tr>
<td></td>
<td>5.59  10.11 0.00  0.00  0.00  0.00</td>
<td>1.03%  1.03%  -8.03%  0.00%  0.00%  0.00%</td>
</tr>
<tr>
<td></td>
<td>0.00  0.00  0.00  1.46  0.00  0.00</td>
<td>0.00%  0.00%  0.00%  0.00%  0.00%  0.00%</td>
</tr>
<tr>
<td></td>
<td>0.00  0.00  0.00  0.00  1.46  0.00</td>
<td>0.00%  0.00%  0.00%  0.00%  0.00%  4.61%</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th></th>
<th>Stiffness From Comsol - Normal</th>
<th>Comparison with Mori-Tanaka</th>
</tr>
</thead>
<tbody>
<tr>
<td>Normal</td>
<td>8.54  5.64  5.59  0.00  0.00  0.00</td>
<td>-0.09%  0.05%  0.45%  0.00%  0.00%  0.00%</td>
</tr>
<tr>
<td></td>
<td>6.54  8.54  5.59  0.00  0.00  0.00</td>
<td>0.05%  -0.09%  0.46%  0.00%  0.00%  0.00%</td>
</tr>
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<td></td>
<td>5.59  10.09 0.00  0.00  0.00  0.00</td>
<td>0.96%  0.97%  -7.85%  0.00%  0.00%  0.00%</td>
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<td>0.00  0.00  0.00  1.46  0.00  0.00</td>
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<td>0.00  0.00  0.00  0.00  1.46  0.00</td>
<td>0.00%  0.00%  0.00%  0.00%  6.57%  0.00%</td>
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<td></td>
<td>0.00  0.00  0.00  0.00  0.00  1.46</td>
<td>0.00%  0.00%  0.00%  0.00%  0.00%  4.75%</td>
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</table>

<table>
<thead>
<tr>
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<th>Stiffness From Comsol - Fine</th>
<th>Comparison with Mori-Tanaka</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fine</td>
<td>8.54  5.64  5.59  0.00  0.00  0.00</td>
<td>-0.09%  0.03%  0.45%  0.00%  0.00%  0.00%</td>
</tr>
<tr>
<td></td>
<td>6.54  8.54  5.59  0.00  0.00  0.00</td>
<td>0.03%  -0.09%  0.45%  0.00%  0.00%  0.00%</td>
</tr>
<tr>
<td></td>
<td>5.59  10.09 0.00  0.00  0.00  0.00</td>
<td>0.95%  0.95%  -7.83%  0.00%  0.00%  0.00%</td>
</tr>
<tr>
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<td>0.00  0.00  0.00  1.46  0.00  0.00</td>
<td>0.00%  0.00%  0.00%  6.58%  0.00%  0.00%</td>
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<td>0.00  0.00  0.00  0.00  1.46  0.00</td>
<td>0.00%  0.00%  0.00%  0.00%  6.58%  0.00%</td>
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<tr>
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<td>0.00%  0.00%  0.00%  0.00%  0.00%  4.79%</td>
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<th></th>
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<th>Comparison with Mori-Tanaka</th>
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<tbody>
<tr>
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<td>8.53  5.63  5.59  0.00  0.00  0.00</td>
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</tr>
<tr>
<td></td>
<td>6.53  8.53  5.59  0.00  0.00  0.00</td>
<td>0.16%  0.03%  0.41%  0.00%  0.00%  0.00%</td>
</tr>
<tr>
<td></td>
<td>5.58  10.07 0.00  0.00  0.00  0.00</td>
<td>1.14%  1.14%  -7.61%  0.00%  0.00%  0.00%</td>
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<td>0.00%  0.00%  0.00%  6.61%  0.00%  0.00%</td>
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<td>0.00%  0.00%  0.00%  0.00%  6.61%  0.00%</td>
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<td>0.00  0.00  0.00  0.00  0.00  1.46</td>
<td>0.00%  0.00%  0.00%  0.00%  0.00%  4.88%</td>
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<td>0.15%  0.01%  0.51%  0.00%  0.00%  0.00%</td>
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<td></td>
<td>5.58  10.04 0.00  0.00  0.00  0.00</td>
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</tr>
<tr>
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<td>0.00%  0.00%  0.00%  0.00%  0.00%  4.92%</td>
</tr>
<tr>
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<td>Comparison with Mori-Tanaka</td>
<td></td>
</tr>
<tr>
<td>-------------------------------</td>
<td>-----------------------------</td>
<td></td>
</tr>
<tr>
<td>8.68 5.63 5.72 0.00 0.05 0.00</td>
<td>4.11% 1.64% -1.40% 0.00% 0.00% 0.00%</td>
<td></td>
</tr>
<tr>
<td>5.63 8.54 5.61 0.00 -0.06 0.00</td>
<td>1.41% 1.10% 0.57% 0.00% 0.00% 0.00%</td>
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</tr>
<tr>
<td>5.72 5.61 9.47 0.00 0.04 0.00</td>
<td>-1.71% 0.48% -11.07% 0.00% 0.00% 0.00%</td>
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</tr>
<tr>
<td>0.00 0.00 1.46 0.00 0.00 0.00</td>
<td>0.00% 0.00% 0.00% 4.95% 0.00% 0.00%</td>
<td></td>
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<tr>
<td>0.00 0.00 0.00 0.00 1.58 0.00</td>
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<th>Comparison with Mori-Tanaka</th>
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<tr>
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<td>4.13% 1.60% -1.43% 0.00% 0.00% 0.00%</td>
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<tr>
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<td>1.39% 1.10% 0.53% 0.00% 0.00% 0.00%</td>
</tr>
<tr>
<td>5.72 5.61 9.46 0.00 0.04 0.00</td>
<td>-1.76% 0.41% -10.92% 0.00% 0.00% 0.00%</td>
</tr>
<tr>
<td>0.00 0.00 1.46 0.00 0.00 0.00</td>
<td>0.00% 0.00% 0.00% 4.99% 0.00% 0.00%</td>
</tr>
<tr>
<td>0.00 0.00 0.00 0.00 1.58 0.00</td>
<td>0.00% 0.00% 0.00% 0.00% 15.96% 0.00%</td>
</tr>
<tr>
<td>0.00 0.00 0.00 0.00 0.00 1.46</td>
<td>0.00% 0.00% 0.00% 0.00% 15.96% 0.00%</td>
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<td>4.23% 1.72% -1.32% 0.00% 0.00% 0.00%</td>
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<tr>
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<td>1.42% 1.20% 0.58% 0.00% 0.00% 0.00%</td>
</tr>
<tr>
<td>5.72 5.60 9.43 0.00 0.00 0.00</td>
<td>-1.63% 0.56% -10.56% 0.00% 0.00% 0.00%</td>
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<tr>
<td>0.00 0.00 1.46 0.00 0.00 0.00</td>
<td>0.00% 0.00% 0.00% 5.07% 0.00% 0.00%</td>
</tr>
<tr>
<td>0.04 -0.06 0.04 0.00 1.58 0.00</td>
<td>0.00% 0.00% 0.00% 0.00% 15.98% 0.00%</td>
</tr>
<tr>
<td>0.00 0.00 0.00 0.00 0.00 1.46</td>
<td>0.00% 0.00% 0.00% 0.00% 15.98% 0.00%</td>
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<table>
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<th>Stiffness From Comsol - Extra-Fine</th>
<th>Comparison with Mori-Tanaka</th>
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<tr>
<td>8.66 5.63 5.71 0.00 0.00 0.00</td>
<td>4.25% 1.74% -1.20% 0.00% 0.00% 0.00%</td>
</tr>
<tr>
<td>5.63 8.53 5.61 0.00 0.00 0.00</td>
<td>1.42% 1.20% 0.58% 0.00% 0.00% 0.00%</td>
</tr>
<tr>
<td>5.73 5.61 9.45 0.00 0.00 0.00</td>
<td>-1.82% 0.39% -10.77% 0.00% 0.00% 0.00%</td>
</tr>
<tr>
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<td>0.00% 0.00% 0.00% 5.07% 0.00% 0.00%</td>
</tr>
<tr>
<td>0.04 -0.06 0.04 0.00 1.58 0.00</td>
<td>0.00% 0.00% 0.00% 0.00% 16.09% 0.00%</td>
</tr>
<tr>
<td>0.00 0.00 0.00 0.00 0.00 1.46</td>
<td>0.00% 0.00% 0.00% 0.00% 16.09% 0.00%</td>
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</tbody>
</table>

Table 8: Comparison between Comsol and MT stiffness for [0/45]
Table 9: Comparison between Comsol and MT stiffness for [0/90]

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<th>Stiffness From Comsol - Coarse</th>
<th>Comparison with Mori-Tanaka</th>
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<tr>
<td>Coarse</td>
<td>9.32 5.62 5.60 0.00 0.01 0.00</td>
<td>-4.24% 0.19% 0.76% 0.00% 0.00% 0.00%</td>
</tr>
<tr>
<td></td>
<td>5.62 8.54 5.62 0.00 0.00 0.00</td>
<td>0.18% 4.47% 0.36% 0.00% 0.00% 0.00%</td>
</tr>
<tr>
<td></td>
<td>0.00 0.00 0.00 1.46 0.00 0.00</td>
<td>0.00% 0.00% 0.00% 0.00% 5.60% 0.00%</td>
</tr>
<tr>
<td></td>
<td>0.00 0.00 0.00 0.00 1.46 0.00</td>
<td>0.00% 0.00% 0.00% 0.00% 5.52% 0.00%</td>
</tr>
<tr>
<td></td>
<td>0.00 0.00 0.00 0.00 0.00 1.46</td>
<td>0.00% 0.00% 0.00% 0.00% 6.59% 0.00%</td>
</tr>
</tbody>
</table>

<table>
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<tr>
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<th>Stiffness From Comsol - Normal</th>
<th>Comparison with Mori-Tanaka</th>
</tr>
</thead>
<tbody>
<tr>
<td>Normal</td>
<td>9.31 5.62 5.60 0.00 0.00 0.00</td>
<td>-4.17% 0.14% 0.73% 0.00% 0.00% 0.00%</td>
</tr>
<tr>
<td></td>
<td>5.62 8.54 5.62 0.00 0.00 0.00</td>
<td>0.13% 4.48% 0.36% 0.00% 0.00% 0.00%</td>
</tr>
<tr>
<td></td>
<td>5.60 5.62 9.32 0.00 0.00 0.00</td>
<td>0.48% 0.13% -9.30% 0.00% 0.00% 0.00%</td>
</tr>
<tr>
<td></td>
<td>0.00 0.00 0.00 1.46 0.00 0.00</td>
<td>0.00% 0.00% 0.00% 5.67% 0.00% 0.00%</td>
</tr>
<tr>
<td></td>
<td>0.00 0.00 0.00 0.00 1.46 0.00</td>
<td>0.00% 0.00% 0.00% 5.56% 0.00% 0.00%</td>
</tr>
<tr>
<td></td>
<td>0.00 0.00 0.00 0.00 0.00 1.46</td>
<td>0.00% 0.00% 0.00% 6.71% 0.00% 0.00%</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th></th>
<th>Stiffness From Comsol - Fine</th>
<th>Comparison with Mori-Tanaka</th>
</tr>
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<tbody>
<tr>
<td>Fine</td>
<td>9.31 5.62 5.60 0.00 0.00 0.00</td>
<td>-4.12% 0.13% 0.71% 0.00% 0.00% 0.00%</td>
</tr>
<tr>
<td></td>
<td>5.62 8.54 5.62 0.00 0.00 0.00</td>
<td>0.12% 4.48% 0.35% 0.00% 0.00% 0.00%</td>
</tr>
<tr>
<td></td>
<td>5.60 5.62 9.32 0.00 0.00 0.00</td>
<td>0.46% 0.11% -9.28% 0.00% 0.00% 0.00%</td>
</tr>
<tr>
<td></td>
<td>0.00 0.00 0.00 1.46 0.00 0.00</td>
<td>0.00% 0.00% 0.00% 5.69% 0.00% 0.00%</td>
</tr>
<tr>
<td></td>
<td>0.00 0.00 0.00 0.00 1.46 0.00</td>
<td>0.00% 0.00% 0.00% 5.56% 0.00% 0.00%</td>
</tr>
<tr>
<td></td>
<td>0.00 0.00 0.00 0.00 0.00 1.46</td>
<td>0.00% 0.00% 0.00% 6.74% 0.00% 0.00%</td>
</tr>
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<table>
<thead>
<tr>
<th></th>
<th>Stiffness From Comsol - Finer</th>
<th>Comparison with Mori-Tanaka</th>
</tr>
</thead>
<tbody>
<tr>
<td>Finer</td>
<td>9.38 5.61 5.59 0.00 0.00 0.00</td>
<td>-4.92% 0.29% 0.96% 0.00% 0.00% 0.00%</td>
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<tr>
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<td>0.20% 4.55% 0.52% 0.00% 0.00% 0.00%</td>
</tr>
<tr>
<td></td>
<td>5.59 5.61 9.30 0.00 0.00 0.00</td>
<td>0.74% 0.40% -9.04% 0.00% 0.00% 0.00%</td>
</tr>
<tr>
<td></td>
<td>0.00 0.00 0.00 1.46 0.00 0.00</td>
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<tr>
<td></td>
<td>0.00 0.00 0.00 0.00 0.00 1.46</td>
<td>0.00% 0.00% 0.00% 6.86% 0.00% 0.00%</td>
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<table>
<thead>
<tr>
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<th>Stiffness From Comsol - Extra-Fine</th>
<th>Comparison with Mori-Tanaka</th>
</tr>
</thead>
<tbody>
<tr>
<td>Extra fine</td>
<td>9.30 5.62 5.60 0.00 0.00 0.00</td>
<td>-3.95% 0.17% 0.69% 0.00% 0.00% 0.00%</td>
</tr>
<tr>
<td></td>
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<td>0.21% 4.55% 0.38% 0.00% 0.00% 0.00%</td>
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<tr>
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<td>0.54% 0.18% -8.98% 0.00% 0.00% 0.00%</td>
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<td>0.00% 0.00% 0.00% 5.76% 0.00% 0.00%</td>
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<td>0.00% 0.00% 0.00% 5.59% 0.00% 0.00%</td>
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<td>0.00% 0.00% 0.00% 6.84% 0.00% 0.00%</td>
</tr>
</tbody>
</table>

Observations:

- There is a difference between the stiffness tensor calculated through Comsol and the one obtained through Mori-Tanaka method.

- The deviation doesn’t vary much depending on the mesh refinement: we observe a deviation of less than 1% in the principal terms, and less than 0.5% in the other terms.

- The extra-fine mesh doesn’t guarantee the least deviation in every term.

Table 10 through 12 illustrates the comparison of the extra-fine stiffness tensor with the other configurations for the three cases.
Table 10: Comparison between Comsol's extra-fine mesh and the other refinements for $[0]_2$

<table>
<thead>
<tr>
<th>Stiffness From Comsol</th>
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<th>Normal</th>
<th>Fine</th>
<th>Finer</th>
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<tr>
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<tr>
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</tbody>
</table>

Table 11: Comparison between Comsol's extra-fine mesh and the other refinements for $[0/45]$

<table>
<thead>
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<th>Coarse</th>
<th>Normal</th>
<th>Fine</th>
<th>Finer</th>
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<td></td>
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<tr>
<td>8.68 5.63 5.72 0.00 0.05 0.00</td>
<td>-0.14% -0.10% -0.20% 0.00% 0.00% 0.00%</td>
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</tr>
<tr>
<td>5.63 8.54 5.61 0.00 -0.06 0.00</td>
<td>-0.01% -0.07% 0.03% 0.00% 0.00% 0.00%</td>
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<tr>
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<th>Stiffness From Comsol</th>
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<th>Normal</th>
<th>Fine</th>
<th>Finer</th>
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</tr>
<tr>
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<tr>
<td>0.00 0.00 0.00 0.00 0.00 1.46</td>
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<th>Normal</th>
<th>Fine</th>
<th>Finer</th>
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<tr>
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<td>-0.09% -0.16% -0.21% 0.00% 0.00% 0.00%</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>5.64 8.54 5.61 0.00 -0.06 0.00</td>
<td>-0.08% -0.07% -0.01% 0.00% 0.00% 0.00%</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>5.72 5.61 9.45 0.00 0.04 0.00</td>
<td>0.05% 0.02% -0.06% 0.00% 0.00% 0.00%</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.00 0.00 0.00 0.00 1.46 0.00</td>
<td>0.00% 0.00% 0.00% 0.00% 0.00% 0.00%</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.00 0.00 0.00 0.00 0.00 1.46</td>
<td>0.00% 0.00% 0.00% 0.00% 0.00% 0.00%</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>8.66 5.63 5.72 0.00 0.00 0.00</td>
<td>-0.02% -0.02% -0.12% 0.00% 0.00% 0.00%</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>5.63 8.53 5.61 0.00 -0.08 0.00</td>
<td>0.00% 0.00% 0.00% 0.00% 0.00% 0.00%</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>5.72 5.60 9.43 0.00 0.00 0.00</td>
<td>0.00% 0.00% 0.00% 0.00% 0.00% 0.00%</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.00 0.00 0.00 0.00 1.46 0.00</td>
<td>0.00% 0.00% 0.00% 0.00% 0.00% 0.00%</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.00 0.00 0.00 0.00 0.00 1.46</td>
<td>0.00% 0.00% 0.00% 0.00% 0.00% 0.00%</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

48
Table 12: Comparison between Comsol’s extra-fine mesh and the other refinements for [0/90]

<table>
<thead>
<tr>
<th></th>
<th>Stiffness From Comsol - Coarse</th>
<th>Comparison with Extra-fine</th>
</tr>
</thead>
<tbody>
<tr>
<td>Coarse</td>
<td>9.32  5.62  5.60  0.00  0.01  0.00  -0.28%  0.02%  0.06%  0.00%  0.00%  0.00%</td>
<td></td>
</tr>
<tr>
<td></td>
<td>5.62  8.54  5.62  0.00  0.00  0.00  -0.03%  -0.09%  -0.01%  0.00%  0.00%  0.00%</td>
<td></td>
</tr>
<tr>
<td></td>
<td>5.60  5.62  9.33  0.00  0.01  0.00  0.00%  0.00%  -0.40%  0.00%  0.00%  0.00%</td>
<td></td>
</tr>
<tr>
<td></td>
<td>0.00  0.00  0.00  1.46  0.00  0.00  0.00%  0.00%  -0.17%  0.00%  0.00%  0.00%</td>
<td></td>
</tr>
<tr>
<td></td>
<td>0.00  0.00  0.00  0.00  1.46  0.00  0.00%  0.00%  0.00%  0.00%  0.00%  -0.27%</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th></th>
<th>Stiffness From Comsol - Normal</th>
<th>Comparison with Extra-fine</th>
</tr>
</thead>
<tbody>
<tr>
<td>Normal</td>
<td>9.31  5.62  5.60  0.00  0.00  0.00  -0.20%  -0.02%  0.03%  0.00%  0.00%  0.00%</td>
<td></td>
</tr>
<tr>
<td></td>
<td>5.62  8.54  5.62  0.00  0.00  0.00  -0.08%  -0.08%  -0.02%  0.00%  0.00%  0.00%</td>
<td></td>
</tr>
<tr>
<td></td>
<td>5.60  5.62  9.32  0.00  0.00  0.00  -0.06%  -0.05%  -0.29%  0.00%  0.00%  0.00%</td>
<td></td>
</tr>
<tr>
<td></td>
<td>0.00  0.00  0.00  1.46  0.00  0.00  0.00%  0.00%  0.00%  0.00%  0.00%  0.00%</td>
<td></td>
</tr>
<tr>
<td></td>
<td>0.00  0.00  0.00  0.00  1.46  0.00  0.00%  0.00%  0.00%  0.00%  -0.03%  0.00%</td>
<td></td>
</tr>
<tr>
<td></td>
<td>0.00  0.00  0.00  0.00  1.46  0.00  0.00%  0.00%  0.00%  0.00%  0.00%  -0.15%</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th></th>
<th>Stiffness From Comsol - Fine</th>
<th>Comparison with Extra-fine</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fine</td>
<td>9.31  5.62  5.60  0.00  0.00  0.00  -0.17%  -0.04%  0.01%  0.00%  0.00%  0.00%</td>
<td></td>
</tr>
<tr>
<td></td>
<td>5.62  8.54  5.62  0.00  0.00  0.00  -0.09%  -0.07%  -0.04%  0.00%  0.00%  0.00%</td>
<td></td>
</tr>
<tr>
<td></td>
<td>5.60  5.62  9.32  0.00  0.00  0.00  -0.08%  -0.07%  -0.28%  0.00%  0.00%  0.00%</td>
<td></td>
</tr>
<tr>
<td></td>
<td>0.00  0.00  0.00  1.46  0.00  0.00  0.00%  0.00%  0.00%  0.00%  -0.08%  0.00%</td>
<td></td>
</tr>
<tr>
<td></td>
<td>0.00  0.00  0.00  0.00  1.46  0.00  0.00%  0.00%  0.00%  0.00%  -0.03%  0.00%</td>
<td></td>
</tr>
<tr>
<td></td>
<td>0.00  0.00  0.00  0.00  1.46  0.00  0.00%  0.00%  0.00%  0.00%  -0.11%  0.00%</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th></th>
<th>Stiffness From Comsol - Finer</th>
<th>Comparison with Extra-fine</th>
</tr>
</thead>
<tbody>
<tr>
<td>Finer</td>
<td>9.38  5.61  5.59  0.00  0.00  0.00  -0.93%  0.13%  0.27%  0.00%  0.00%  0.00%</td>
<td></td>
</tr>
<tr>
<td></td>
<td>5.62  8.54  5.61  0.00  0.00  0.00  -0.01%  -0.01%  0.14%  0.00%  0.00%  0.00%</td>
<td></td>
</tr>
<tr>
<td></td>
<td>5.59  5.61  9.30  0.00  0.00  0.00  0.21%  0.22%  -0.05%  0.00%  0.00%  0.00%</td>
<td></td>
</tr>
<tr>
<td></td>
<td>0.00  0.00  0.00  1.46  0.00  0.00  0.00%  0.00%  0.00%  0.00%  0.00%  0.00%</td>
<td></td>
</tr>
<tr>
<td></td>
<td>0.00  0.00  0.00  0.00  1.46  0.00  0.00%  0.00%  0.00%  0.00%  0.02%  0.00%</td>
<td></td>
</tr>
<tr>
<td></td>
<td>0.00  0.00  0.00  0.00  1.46  0.00  0.00%  0.00%  0.00%  0.00%  0.00%  0.02%</td>
<td></td>
</tr>
</tbody>
</table>

Observations:

- The deviation between the values of the extra-fine stiffness and the other configuration is generally less than 1%.
- In the case of the normal refinement, the deviation of all terms of stiffness for all cases is less than 0.5%.

4.2.3 Convergence study conclusion

By comparing stiffness values between the Mori-Tanaka method and Comsol's given values for different configurations and different refinements, we observed:

- The deviation between the stiffness tensor obtained through Comsol and the one calculated using Mori-Tanaka’s method is less than 1%.
Using an extra-fine mesh doesn’t guarantee the smallest value of deviation, even less in all terms.

The difference in stiffness values between the extra-fine configuration and the coarser refinements is less than 1%.

In particular, the normal mesh delivers results within 0.5% of the extra-fine ones.

For the rest of the study, we will use a normal mesh to compute our results. Thus ensuring an optimal number of degrees of freedom to solve for within the computational means and the requirements of accuracy.

4.3 Orientation study

The objective of the orientation study is to establish the accuracy of using the numerical stiffness of an RVE coupled with an orientation tensor compared to using an RVE with an oriented fiber. Our goal is to establish the first step of our framework: using an aligned RVE taking into consideration spacing and short fiber’s properties and an orientation tensor, we can compute an effective stiffness taking the orientation into consideration.

Table 13 summarizes the three cases of study conducted following different orientation states:

<table>
<thead>
<tr>
<th></th>
<th>Case 1</th>
<th>Case 2</th>
<th>Case 3</th>
</tr>
</thead>
<tbody>
<tr>
<td>$a_{ij}$</td>
<td>$\begin{bmatrix} 0.25 &amp; 0 &amp; 0 \ 0 &amp; 0.25 &amp; 0 \ 0 &amp; 0 &amp; 0.5 \end{bmatrix}$</td>
<td>$\begin{bmatrix} 0.33 &amp; 0 &amp; 0 \ 0 &amp; 0.33 &amp; 0 \ 0 &amp; 0 &amp; 0.33 \end{bmatrix}$</td>
<td>$\begin{bmatrix} 0 &amp; 0 &amp; 0 \ 0 &amp; 0 &amp; 0 \ 0 &amp; 0 &amp; 1 \end{bmatrix}$</td>
</tr>
</tbody>
</table>
4.3.1 Stiffness tensors of RVE’s used

4.3.1.1 RVE\textsubscript{1}

The RVE\textsubscript{1} takes into consideration the spacing and aspect ratio of the short fibers. It is modeled with two fibers, one central and one partitioned on quarters, both aligned according to z-axis. Its main purpose is capturing the spacing and the effect of differently oriented fibers within the same RVE, as displayed in Figure 22:

![Figure 22: RVE\textsubscript{1} used for the case 1 in orientation study](image)

Table 14 is the stiffness tensor of RVE\textsubscript{1} calculated through Comsol:

<table>
<thead>
<tr>
<th></th>
<th>8.54</th>
<th>5.64</th>
<th>5.59</th>
<th>0.00</th>
<th>0.00</th>
<th>0.00</th>
</tr>
</thead>
<tbody>
<tr>
<td>5.64</td>
<td>8.54</td>
<td>5.59</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
</tr>
<tr>
<td>5.59</td>
<td>5.59</td>
<td>10.09</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
</tr>
<tr>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>1.46</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
</tr>
<tr>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>1.46</td>
<td>0.00</td>
<td>0.00</td>
</tr>
<tr>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>1.46</td>
<td></td>
</tr>
</tbody>
</table>
4.3.1.2 RVE$_2$

The RVE$_2$ allows more flexibility in modeling orientation states. It is modeled with one central short fiber aligned according to y-axis. Its main advantage is the relative ease of modeling orientation states, as displayed in Figure 23:

![Figure 23: RVE$_2$ used for the case 2 in orientation study](image)

Table 15 is the stiffness tensor of RVE$_2$ calculated through Comsol:

<table>
<thead>
<tr>
<th></th>
<th>8.34</th>
<th>5.51</th>
<th>5.53</th>
<th>0.00</th>
<th>0.00</th>
<th>0.00</th>
</tr>
</thead>
<tbody>
<tr>
<td>5.51</td>
<td></td>
<td></td>
<td></td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
</tr>
<tr>
<td>5.53</td>
<td></td>
<td></td>
<td></td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
</tr>
<tr>
<td>0.00</td>
<td></td>
<td></td>
<td></td>
<td>1.41</td>
<td>0.00</td>
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<tr>
<td>0.00</td>
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<td></td>
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<td>1.40</td>
<td>0.00</td>
</tr>
<tr>
<td>0.00</td>
<td></td>
<td></td>
<td></td>
<td>0.00</td>
<td>0.00</td>
<td>1.41</td>
</tr>
</tbody>
</table>
4.3.1.3 RVE$_3$

The RVE$_3$ allows more flexibility in modeling orientation states. It is modeled with one central short fiber aligned according to z-axis. Its main advantage is the relative ease of modeling orientation states, as displayed in Figure 24:

![Image](image-url)

*Figure 24: RVE$_3$ used for the case 3 in orientation study*

Table 16 is the stiffness tensor of RVE$_3$ calculated through Comsol:

<table>
<thead>
<tr>
<th></th>
<th>8.34</th>
<th>5.53</th>
<th>5.51</th>
<th>0.00</th>
<th>0.00</th>
<th>0.00</th>
</tr>
</thead>
<tbody>
<tr>
<td>5.53</td>
<td>8.34</td>
<td>5.51</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
</tr>
<tr>
<td>5.51</td>
<td>5.51</td>
<td>9.13</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
</tr>
<tr>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>1.41</td>
<td>0.00</td>
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<td>0.00</td>
<td>0.00</td>
<td>1.41</td>
<td>0.00</td>
<td>0.00</td>
</tr>
<tr>
<td>0.00</td>
<td>0.00</td>
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<td>0.00</td>
<td>0.00</td>
<td>1.40</td>
<td></td>
</tr>
</tbody>
</table>

4.3.2 Constructed volumes used

4.3.2.1 Volume$_1$

To compare the accuracy of the RVE coupled with an orientation tensor, we compare it to a volume made out of the RVE and displaying the orientation state described by the tensor.
The Array Volume\textsubscript{1} is made out of 3x3x2 RVE. It accounts for 36 fibers, with 9 fibers oriented according to x-axis, 9 according to y-axis and 18 oriented according to z-axis. Figure 25 illustrates the volume\textsubscript{1} used on Comsol.

4.3.2.2 Volume\textsubscript{2}

The Array Volume\textsubscript{2} is made out of 3x3x3 RVE. It accounts for 27 fibers, each 9 fibers oriented according to a principal direction. Figure 26 illustrates the volume\textsubscript{2} used on Comsol.
### 4.3.2.3 $\text{Volume}_3$

The Array $\text{Volume}_3$ is made out of $3 \times 3 \times 3$ RVE. It accounts for 27 fibers, all of which are oriented according to the $z$-direction. Figure 27 illustrates the $\text{volume}_3$ used on Comsol.

![Volume 3](image)

*Figure 27: $\text{Volume}_3$ for case 3*

### 4.3.3 Orientation averaging

To model the orientation state of the RVE, we use a second order orientation tensor and a fourth orientation tensor. Since our orientation states were picked along the principal directions, the second orientation tensor will be diagonal. We populate the trace terms. The trace should be equal to 1.

Table 17 summarizes the orientation tensors for every case:

<table>
<thead>
<tr>
<th>$a_{ij}$</th>
<th>Case 1</th>
<th>Case 2</th>
<th>Case 3</th>
</tr>
</thead>
<tbody>
<tr>
<td>$0.25$</td>
<td>$0$</td>
<td>$0.33$</td>
<td>$0$</td>
</tr>
<tr>
<td>$0.25$</td>
<td>$0$</td>
<td>$0.33$</td>
<td>$0$</td>
</tr>
<tr>
<td>$0$</td>
<td>$0$</td>
<td>$0$</td>
<td>$0$</td>
</tr>
<tr>
<td>$0$</td>
<td>$0.5$</td>
<td>$0$</td>
<td>$0$</td>
</tr>
<tr>
<td>$0$</td>
<td>$0.33$</td>
<td>$0$</td>
<td>$0$</td>
</tr>
</tbody>
</table>

*Table 17: Orientation tensor $a_{ij}$ for cases 1, 2 and 3*
The orientation averaging calculation requires the construction of the fourth order orientation tensor from the second order one, $a_{ij}$. To this end, several closure approximations were developed. We use the following three: the linear closure approximation, the quadratic and the hybrid ones.

We compute the stiffness tensor of the RVE with every orientation tensor and for the three closure approximations. Table 18 through 20 summarize the oriented stiffness tensors obtained:

Table 18: Oriented Stiffness (in GPa) for the RVE

<table>
<thead>
<tr>
<th>Stiffness of RVE - Linear Closure</th>
</tr>
</thead>
<tbody>
<tr>
<td>8.85</td>
</tr>
<tr>
<td>5.64</td>
</tr>
<tr>
<td>5.68</td>
</tr>
<tr>
<td>0.00</td>
</tr>
<tr>
<td>0.00</td>
</tr>
<tr>
<td>0.00</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Stiffness of RVE - Quadratic Closure</th>
</tr>
</thead>
<tbody>
<tr>
<td>8.78</td>
</tr>
<tr>
<td>5.67</td>
</tr>
<tr>
<td>5.73</td>
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<td>0.00</td>
</tr>
<tr>
<td>0.00</td>
</tr>
<tr>
<td>0.00</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Stiffness of RVE - Hybrid Closure</th>
</tr>
</thead>
<tbody>
<tr>
<td>8.85</td>
</tr>
<tr>
<td>5.64</td>
</tr>
<tr>
<td>5.69</td>
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<tr>
<td>0.00</td>
</tr>
<tr>
<td>0.00</td>
</tr>
<tr>
<td>0.00</td>
</tr>
</tbody>
</table>
Table 19: Oriented Stiffness (in GPa) for RVE2

<table>
<thead>
<tr>
<th></th>
<th>Stiffness of RVE2 - Linear Closure</th>
<th></th>
<th>Stiffness of RVE2 - Quadratic Closure</th>
<th></th>
<th>Stiffness of RVE2 - Hybrid Closure</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>8.54  5.56  5.56  0.00  0.00  0.00</td>
<td></td>
<td>8.49  5.58  5.58  0.00  0.00  0.00</td>
<td></td>
<td>8.54  5.56  5.56  0.00  0.00  0.00</td>
</tr>
<tr>
<td></td>
<td>5.56  8.54  5.56  0.00  0.00  0.00</td>
<td></td>
<td>5.58  8.49  5.58  0.00  0.00  0.00</td>
<td></td>
<td>5.56  8.54  5.56  0.00  0.00  0.00</td>
</tr>
<tr>
<td></td>
<td>5.56  5.56  8.54  0.00  0.00  0.00</td>
<td></td>
<td>5.58  5.58  8.49  0.00  0.00  0.00</td>
<td></td>
<td>5.56  5.56  8.54  0.00  0.00  0.00</td>
</tr>
<tr>
<td></td>
<td>0.00  0.00  0.00  1.49  0.00  0.00</td>
<td></td>
<td>0.00  0.00  0.00  1.46  0.00  0.00</td>
<td></td>
<td>0.00  0.00  0.00  1.49  0.00  0.00</td>
</tr>
<tr>
<td></td>
<td>0.00  0.00  0.00  0.00  1.49  0.00</td>
<td></td>
<td>0.00  0.00  0.00  0.00  1.49  0.00</td>
<td></td>
<td>0.00  0.00  0.00  0.00  1.49  0.00</td>
</tr>
<tr>
<td></td>
<td>0.00  0.00  0.00  0.00  0.00  1.49</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
Table 20: Oriented Stiffness (in GPa) for RVE\textsubscript{3}

<table>
<thead>
<tr>
<th>Stiffness of RVE\textsubscript{3} - Linear Closure</th>
</tr>
</thead>
<tbody>
<tr>
<td>8.27</td>
</tr>
<tr>
<td>5.51</td>
</tr>
<tr>
<td>5.60</td>
</tr>
<tr>
<td>0.00</td>
</tr>
<tr>
<td>0.00</td>
</tr>
<tr>
<td>0.00</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Stiffness of RVE\textsubscript{3} - Quadratic Closure</th>
</tr>
</thead>
<tbody>
<tr>
<td>8.34</td>
</tr>
<tr>
<td>5.53</td>
</tr>
<tr>
<td>5.51</td>
</tr>
<tr>
<td>0.00</td>
</tr>
<tr>
<td>0.00</td>
</tr>
<tr>
<td>0.00</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Stiffness of RVE\textsubscript{3} - Hybrid Closure</th>
</tr>
</thead>
<tbody>
<tr>
<td>7.99</td>
</tr>
<tr>
<td>5.41</td>
</tr>
<tr>
<td>5.97</td>
</tr>
<tr>
<td>0.00</td>
</tr>
<tr>
<td>0.00</td>
</tr>
<tr>
<td>0.00</td>
</tr>
</tbody>
</table>

Observations

As predicted by the behavior of the hybrid closure approximation, in the case of pure random orientation (case 2), the linear closure approximation is given exactly by the hybrid closure. In the case of pure alignment (case 3), the quadratic closure approximation is given exactly by the hybrid closure. In the case of a hybrid orientation, the values resulting from the hybrid closure approximation lie between the values of the linear and quadratic closure approximation.
4.3.4 Orientation analysis

We run the volumes in Comsol, extract the local stresses and strains and compute the respective stiffness tensors. Table 21 through 23 summarize their comparison with the Mori-Tanaka oriented stiffness tensors calculated for the RVEs.

*Table 21: Comparison between the stiffness (in GPa) of Volume 1 and the oriented stiffness of RVE 1*

<table>
<thead>
<tr>
<th>Stiffness of Volume 1 Comsol</th>
<th>Comparison with RVE 1 - Linear Closure</th>
</tr>
</thead>
<tbody>
<tr>
<td>8.91</td>
<td>0.63% -0.56% -1.71% 0.00% 0.00% 0.00%</td>
</tr>
<tr>
<td>5.57</td>
<td>-1.21% 0.04% -1.95% 0.00% 0.00% 0.00%</td>
</tr>
<tr>
<td>5.58</td>
<td>-1.85% -1.43% 3.75% 0.00% 0.00% 0.00%</td>
</tr>
<tr>
<td>0.00</td>
<td>0.00% 0.00% 0.00% -10.12% 0.00% 0.00%</td>
</tr>
<tr>
<td>0.00</td>
<td>0.00% 0.00% 0.00% 0.00% -10.13% 0.00%</td>
</tr>
<tr>
<td>0.00</td>
<td>0.00% 0.00% 0.00% 0.00% 0.00% -10.20%</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Comparison with RVE 1 - Quadratic Closure</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.41% -1.09% -2.60% 0.00% 0.00% 0.00%</td>
</tr>
<tr>
<td>-1.75% 0.83% -2.84% 0.00% 0.00% 0.00%</td>
</tr>
<tr>
<td>-2.75% -2.32% 5.36% 0.00% 0.00% 0.00%</td>
</tr>
<tr>
<td>0.00% 0.00% 0.00% -3.28% 0.00% 0.00%</td>
</tr>
<tr>
<td>0.00% 0.00% 0.00% -3.29% 0.00% 0.00%</td>
</tr>
<tr>
<td>0.00% 0.00% 0.00% 0.00% -6.77% 0.00%</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Comparison with RVE 1 - Hybrid Closure</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.63% -0.56% -1.88% 0.00% 0.00% 0.00%</td>
</tr>
<tr>
<td>-1.21% 0.04% -2.12% 0.00% 0.00% 0.00%</td>
</tr>
<tr>
<td>-2.03% -1.61% 3.86% 0.00% 0.00% 0.00%</td>
</tr>
<tr>
<td>0.00% 0.00% 0.00% -9.43% 0.00% 0.00%</td>
</tr>
<tr>
<td>0.00% 0.00% 0.00% -9.44% 0.00% 0.00%</td>
</tr>
<tr>
<td>0.00% 0.00% 0.00% 0.00% 0.00% -9.51%</td>
</tr>
</tbody>
</table>
Table 22: Comparison between the stiffness (in GPa) of Volume_2 and the oriented stiffness of RVE_2

<table>
<thead>
<tr>
<th>Stiffness of Volume_2 - Comsol</th>
<th>Comparison with RVE_2 - Linear Closure</th>
</tr>
</thead>
<tbody>
<tr>
<td>8.61 5.52 5.51 0.00 0.00 0.00</td>
<td>-0.82% 0.77% 0.83% 0.00% 0.00% 0.00%</td>
</tr>
<tr>
<td>5.52 8.53 5.52 0.00 0.00 0.00</td>
<td>0.78% 0.17% 0.78% 0.00% 0.00% 0.00%</td>
</tr>
<tr>
<td>5.51 5.52 8.61 0.00 0.00 0.00</td>
<td>0.83% 0.78% -0.83% 0.00% 0.00% 0.00%</td>
</tr>
<tr>
<td>0.00 0.00 0.00 1.41 0.00 0.00</td>
<td>0.00% 0.00% 0.00% 5.81% 0.00% 0.00%</td>
</tr>
<tr>
<td>0.00 0.00 0.00 0.00 1.41 0.00</td>
<td>0.00% 0.00% 0.00% 0.00% 5.85% 0.00%</td>
</tr>
<tr>
<td>0.00 0.00 0.00 0.00 0.00 1.41</td>
<td>0.00% 0.00% 0.00% 0.00% 0.00% 5.81%</td>
</tr>
</tbody>
</table>

Table 23: Comparison between the stiffness (in GPa) of Volume_3 and the oriented stiffness of RVE_3

<table>
<thead>
<tr>
<th>Stiffness of Volume_3 - Comsol</th>
<th>Comparison with RVE_3 - Quadratic Closure</th>
</tr>
</thead>
<tbody>
<tr>
<td>8.34 5.53 5.51 0.00 0.00 0.00</td>
<td>-1.20% -0.54% 1.88% 0.00% 0.00% 0.00%</td>
</tr>
<tr>
<td>5.53 8.34 5.51 0.00 0.00 0.00</td>
<td>-0.54% -1.20% 1.88% 0.00% 0.00% 0.00%</td>
</tr>
<tr>
<td>5.51 5.51 9.16 0.00 0.00 0.00</td>
<td>1.88% 1.88% -1.38% 0.00% 0.00% 0.00%</td>
</tr>
<tr>
<td>0.00 0.00 0.00 1.41 0.00 0.00</td>
<td>0.00% 0.00% 0.00% 7.09% 0.00% 0.00%</td>
</tr>
<tr>
<td>0.00 0.00 0.00 0.00 1.41 0.00</td>
<td>0.00% 0.00% 0.00% 0.00% 7.09% 0.00%</td>
</tr>
<tr>
<td>0.00 0.00 0.00 0.00 0.00 1.40</td>
<td>0.00% 0.00% 0.00% 0.00% 0.00% -2.34%</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Stiffness of Volume_3 - Comsol</th>
<th>Comparison with RVE_3 - Hybrid Closure</th>
</tr>
</thead>
<tbody>
<tr>
<td>8.34 5.53 5.51 0.00 0.00 0.00</td>
<td>0.00% 0.00% 0.00% 0.00% 0.00% 0.00%</td>
</tr>
<tr>
<td>5.53 8.34 5.51 0.00 0.00 0.00</td>
<td>0.00% 0.00% 0.00% 0.00% 0.00% 0.00%</td>
</tr>
<tr>
<td>5.51 5.51 9.16 0.00 0.00 0.00</td>
<td>0.00% 0.00% 0.00% 0.00% 0.00% 0.00%</td>
</tr>
<tr>
<td>0.00 0.00 0.00 1.41 0.00 0.00</td>
<td>0.00% 0.00% 0.00% 0.00% 0.00% 0.00%</td>
</tr>
<tr>
<td>0.00 0.00 0.00 0.00 1.41 0.00</td>
<td>0.00% 0.00% 0.00% 0.00% 0.00% 0.00%</td>
</tr>
<tr>
<td>0.00 0.00 0.00 0.00 0.00 1.40</td>
<td>0.00% 0.00% 0.00% 0.00% 0.00% -0.20%</td>
</tr>
</tbody>
</table>
Observations:

- The comparison of the stiffness of the Volume\textsubscript{1} vs the oriented stiffness of RVE\textsubscript{1} has deviations that are less than 8% for the linear closure, less than 5% for the quadratic closure and less than 11% for the hybrid closure.

- The comparison of the stiffness of the Volume\textsubscript{2} vs the oriented stiffness of RVE\textsubscript{2} has deviations that are less than 6% for the linear closure, less than 4% for the quadratic closure and less than 8% for the hybrid closure.

- The comparison of the stiffness of the Volume\textsubscript{3} vs the oriented stiffness of RVE\textsubscript{3} has deviations that are less than 8% for the linear closure, less than 0.3% for the quadratic closure and less than 0.3% for the hybrid closure.

- The shear terms present the most deviation through the three models.

4.3.5 Orientation study conclusion

We performed the orientation study to assess the impact of using a combination of a RVE numerical stiffness with an orientation tensor to come up with an effective oriented tensor, compared with the Mori-Tanaka’s oriented stiffness. We compared the results with volumes of oriented short fibers. The observed deviations were overall less than 11%. The use of hybrid closure approximation resulted in the highest deviations overall (11% for Volume\textsubscript{1}, 8% for Volume\textsubscript{2} and 0.3% for Volume\textsubscript{3}). The use of the quadratic closure approximation resulted in the smallest deviations (5% for Volume\textsubscript{1}, 04% for Volume\textsubscript{2} and 0.3% for Volume\textsubscript{3}).

Therefore, we will use the quadratic closure approximation for the construction of the fourth order orientation tensor and the computation of the effective oriented stiffness.
tensor of the RVE combined with the numerical stiffness obtained from local stresses and strains of Comsol.

4.4 Conclusion

The following chapter summarized the work performed in the microscopic study: our goal was to establish a framework of orientated stiffness construction for RVE of FDM parts made out of short fiber composites. We modeled an idealized RVE that takes into consideration the structural and mechanical properties of short fibers composites. We conducted a convergence study to assess the impact of the meshing refinement available on the accuracy of the results and established the optimal accuracy of a normal mesh. Finally, we performed an orientation study on three cases to choose the optimal closure approximation that incorporates the orientation averaging to the stiffness tensor with the least deviation from the oriented stiffness of the original RVEs. We established the use of quadratic closure approximation.
CHAPTER 5
MESOSCOPIC SCALE

The following chapter covers the work performed on the representative volume element -RVE- on the mesoscopic scale, of the short fiber composite part manufactured through the FDM process. Our main objective is to assess the homogeneous stiffness constructed from the bead, using the oriented stiffness tensors built on the microscopic scale. An overview of the input data is detailed, a study of stiffness is performed.

5.1 Analysis set up

The following section summarizes the additional setup used for the bead modeling on the mesoscopic scale.

5.1.1 Representative volume element at the mesoscopic scale

The mesoscopic RVE should capture the periodic features of the deposited layers of the FDM process. It should be big enough to capture the bead and the manufacturing effect on it, yet small enough to avoid redundancy and be computed as a basic building block.

Beads generally come as long cylindrical deposits of melted material. Due to the process and the additional deposited beads on the z-direction, their top and bottom surfaces are flattened and their sides, whether with negative or positive overlap, keep their round features, leaving space for air.

From micro-tomography images and based on average dimensions observed, we constructed the following idealized RVE displayed in figure 28:
5.1.2 RVE partitioning

Due to the injection process and the viscous flow transporting the short fibers through the FDM machine, the alignment of the inclusions changes from the original configuration.

In the case of injection modeling, as the bead exists the nozzle head, two main layers of orientation state are observed, an outer layer called the shell layer where short fibers are aligned along the wall of the pipes, this making them completely aligned along
the z principal direction, and a core layer where the short fibers have a random orientation state.

In our current study, the beads are deposited through Fused Deposition Modeling, and to our knowledge, there was no found literature on the inner distribution of short fibers inside. The micro-tomographic data available displays a rather uniform alignment of fibers as shown on figure 29, but further experimental data should be acquired before formulating a reasonable hypothesis.

![Micro-tomographic image of a cross-section of a part manufactured using FDM. Details of the fibers’ alignment in case of the 0° and 90° beads](image)

In our study, we chose to study three cases of orientation distribution as summarized by table 24:

![Table 24: Cases analyzed in the mesoscopic scale](image)
In the case of the partitioned bead, two layers are created. Due to the lack of literature regarding the volume of the shell for FDM parts with reinforced short fibers, the shell layer is taken 20% of the total volume fraction, based on injection molding. Figure 30 illustrates the geometry used for case 3.

*Figure 30: Partitioned mesoscopic RVE with the shell layer in blue*
5.1.3 Parameters of the analysis

We use the oriented stiffness tensors numerically calculated from the microscopic RVEs combined with the quadratic closure approximation to describe the stiffness properties of the beads.

We use the periodic boundary conditions detailed during the microscopic study over the flat faces. We omit the round faces to take the shape into consideration.

5.2 Mesoscopic RVE analysis

We conduct the set of six study cases to compute the averaged stiffness over the mesoscopic RVE. We extract the local stresses and strains to perform the calculation.

5.2.1 Case 1

Table 25 displays the result in stiffness of case 1:

Table 25: Stiffness (in GPa) from Comsol of the mesoscopic RVE - case 1

<table>
<thead>
<tr>
<th>Stiffness from Comsol of the RVE Case1</th>
</tr>
</thead>
<tbody>
<tr>
<td>7.15</td>
</tr>
<tr>
<td>3.72</td>
</tr>
<tr>
<td>4.32</td>
</tr>
<tr>
<td>0.00</td>
</tr>
<tr>
<td>0.00</td>
</tr>
<tr>
<td>0.00</td>
</tr>
</tbody>
</table>

Table 26 is the comparison between the oriented stiffness tensor used as input data from the microscale study and the resulting one calculated from Comsol.
Table 26: Comparison between the stiffness input and outcome from Comsol

<table>
<thead>
<tr>
<th>Stiffness from Comsol of the RVE Case 1</th>
<th>Comparison</th>
</tr>
</thead>
<tbody>
<tr>
<td>7.15  3.49  2.92  0.00  0.00  0.00</td>
<td>14.21%  36.84%  46.94%  0.00%  0.00%  0.00%</td>
</tr>
<tr>
<td>3.72  7.01  2.96  0.00  0.00  0.00</td>
<td>32.61%  15.98%  45.97%  0.00%  0.00%  0.00%</td>
</tr>
<tr>
<td>4.32  4.18  7.09  0.00  0.00  0.00</td>
<td>21.51%  24.19%  22.31%  0.00%  0.00%  0.00%</td>
</tr>
<tr>
<td>0.00  0.00  0.00  1.41  0.00  0.00</td>
<td>0.00%   0.00%   0.00%   0.00%   0.00%   0.00%</td>
</tr>
<tr>
<td>0.00  0.00  0.00  0.00  1.41  0.00</td>
<td>0.00%   0.00%   0.00%   0.00%   0.00%   0.00%</td>
</tr>
<tr>
<td>0.00  0.00  0.00  0.00  0.00  1.40</td>
<td>0.00%   0.00%   0.00%   0.00%   0.00%   0.00%</td>
</tr>
</tbody>
</table>

There is a drop a values of stiffness overall. The shear terms are not affected.

Table 27 is the resulting Young’s moduli from the input and output stiffness tensors and their comparison.

Table 27: Comparison of the Young’s moduli from the input and output stiffness tensors

<table>
<thead>
<tr>
<th></th>
<th>Input</th>
<th>Output</th>
<th>Comparison</th>
</tr>
</thead>
<tbody>
<tr>
<td>E1 (GPa)</td>
<td>4.05</td>
<td>4.73</td>
<td>-16.96%</td>
</tr>
<tr>
<td>E2 (GPa)</td>
<td>4.05</td>
<td>4.63</td>
<td>-14.39%</td>
</tr>
<tr>
<td>E3 (GPa)</td>
<td>4.75</td>
<td>4.75</td>
<td>0.13%</td>
</tr>
</tbody>
</table>

The values of E_i are overestimated compared to the stiffness tensor used as an input. This is a predictable outcome given the use of homogeneous displacement. The deviation is the least in the main direction.

5.2.2 Case 2

Table 28 displays the result in stiffness of case 2
Table 28: Stiffness (in GPa) from Comsol of the mesoscopic RVE - case 2

<table>
<thead>
<tr>
<th>Stiffness from Comsol of the RVE Case 2</th>
</tr>
</thead>
<tbody>
<tr>
<td>7.40</td>
</tr>
<tr>
<td>3.81</td>
</tr>
<tr>
<td>4.40</td>
</tr>
<tr>
<td>0.00</td>
</tr>
<tr>
<td>0.00</td>
</tr>
<tr>
<td>0.00</td>
</tr>
</tbody>
</table>

Table 29 is the comparison between the oriented stiffness tensor used as input data from the microscale study and the resulting one calculated from Comsol.

Table 29: Comparison between the stiffness input and outcome from Comsol

<table>
<thead>
<tr>
<th>Stiffness from Comsol of the RVE Case 2</th>
<th>Comparison</th>
</tr>
</thead>
<tbody>
<tr>
<td>7.40</td>
<td>3.68</td>
</tr>
<tr>
<td>3.81</td>
<td>7.31</td>
</tr>
<tr>
<td>4.40</td>
<td>4.42</td>
</tr>
<tr>
<td>0.00</td>
<td>0.00</td>
</tr>
<tr>
<td>0.00</td>
<td>0.00</td>
</tr>
<tr>
<td>0.00</td>
<td>0.00</td>
</tr>
</tbody>
</table>

There is a drop in values of stiffness overall. The shear terms are not affected.

Table 30 is the resulting Young’s moduli from the input and output stiffness tensors and their comparison.

Table 30: Comparison of the Young’s moduli from the input and output stiffness tensors

<table>
<thead>
<tr>
<th>E1 (GPa)</th>
<th>E2 (GPa)</th>
<th>E3 (GPa)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Input</td>
<td>4.16</td>
<td>4.16</td>
</tr>
<tr>
<td>Output</td>
<td>4.84</td>
<td>4.67</td>
</tr>
<tr>
<td>Comparison</td>
<td>-16.38%</td>
<td>-12.42%</td>
</tr>
</tbody>
</table>
The values of $E_i$ are overestimated compared to the stiffness tensor used as an input. This is a predictable outcome given the use of homogeneous displacement. The deviation is the least in the main direction.

### 5.2.3 Case 3

Table 31 displays the result:

*Table 31: Stiffness (in GPa) from Comsol of the Mesoscopic RVE*

<table>
<thead>
<tr>
<th>Stiffness from Comsol of the Mesoscopic RVE</th>
</tr>
</thead>
<tbody>
<tr>
<td>7.16</td>
</tr>
<tr>
<td>3.72</td>
</tr>
<tr>
<td>4.33</td>
</tr>
<tr>
<td>0.00</td>
</tr>
<tr>
<td>0.00</td>
</tr>
<tr>
<td>0.00</td>
</tr>
</tbody>
</table>

This resulting effective stiffness is computed from the random oriented stiffness tensor of the core layer and the aligned according to $z$-axis stiffness tensor of the shell layer. To perform an assessment over the accuracy of the value, we compare the resulting Comsol stiffness with the one computed through the rule of mixtures of the input used, the oriented stiffness tensors.
Table 32: Compliance Tensors (in 1/GPa) of the oriented stiffness tensors used and the mesoscopic RVE computed through Comsol

<table>
<thead>
<tr>
<th>Compliance of RVE₂ - Quadratic Closure</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Volume Fraction 0.8</td>
<td></td>
</tr>
<tr>
<td>0.25</td>
<td>-0.10</td>
</tr>
<tr>
<td>-0.10</td>
<td>0.25</td>
</tr>
<tr>
<td>-0.10</td>
<td>-0.10</td>
</tr>
<tr>
<td>0.00</td>
<td>0.00</td>
</tr>
<tr>
<td>0.00</td>
<td>0.00</td>
</tr>
<tr>
<td>0.00</td>
<td>0.00</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Compliance of RVE₃ - Quadratic Closure</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Volume Fraction 0.2</td>
<td></td>
</tr>
<tr>
<td>0.25</td>
<td>-0.11</td>
</tr>
<tr>
<td>-0.11</td>
<td>0.25</td>
</tr>
<tr>
<td>-0.08</td>
<td>-0.08</td>
</tr>
<tr>
<td>0.00</td>
<td>0.00</td>
</tr>
<tr>
<td>0.00</td>
<td>0.00</td>
</tr>
<tr>
<td>0.00</td>
<td>0.00</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Compliance of Mesoscopic RVE</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>0.21</td>
<td>-0.07</td>
</tr>
<tr>
<td>-0.07</td>
<td>0.22</td>
</tr>
<tr>
<td>-0.10</td>
<td>-0.10</td>
</tr>
<tr>
<td>0.00</td>
<td>0.00</td>
</tr>
<tr>
<td>0.00</td>
<td>0.00</td>
</tr>
<tr>
<td>0.00</td>
<td>0.00</td>
</tr>
</tbody>
</table>

Table 32 displays the values of compliance for the stiffness tensors used. The Young’s modulus in the principal z-direction are calculated from the compliance tensors of the microscopic RVEs and combined using the rule of mixture.

The result is displayed in Table 33, along with a comparison the Young’s modulus obtained from the compliance of the mesoscopic RVE.

Table 33: Young’s Modulus (in GPa) comparison between the rule of mixture and the mesoscopic RVE

<table>
<thead>
<tr>
<th></th>
<th>RVE₂</th>
<th>RVE₃</th>
<th>Rule of Mix</th>
<th>RVE - FE</th>
<th>Comparison</th>
</tr>
</thead>
<tbody>
<tr>
<td>E3 (Gpa)</td>
<td>3.96</td>
<td>4.75</td>
<td>4.11</td>
<td>4.11</td>
<td>0.00%</td>
</tr>
</tbody>
</table>
5.2.4 Mesoscopic RVE conclusion:

From the calculations, we conclude the drop of the stiffness overall. There is a drop in the main z-direction as a direct effect of the void taken into consideration by excluding the curved surfaces from the periodic boundary conditions. The extent of deviations noted on every term are close in cases 1 and 2. The z-direction is not only the main deposition and fiber alignment one, it is also the direction with the main void fraction.

By inputting the oriented stiffness tensors obtained from the microscopic RVEs, we were able to calculate the averaged stiffness of case 3. To assess its accuracy, we used the rule of mixtures and computed the Young’s moduli then compared them, finding the effective property to be the same.

We will analyze array of beads given the same stiffness tensors of cases 1, 2 and 3 to assess FE’s accuracy in carrying the effective oriented stiffness tensors through the scaling process.

5.3 Mesoscopic RVE volume study

To ensure that Comsol takes into consideration the periodicity of the mesoscopic RVE and accounts for the voids built during the FDM process properly, we conducted a study over an array of mesoscopic RVE. Our goal is to assess the average stiffness resulting from the analysis and compare it to the mesoscopic RVE constructed.

5.3.1 Model’s details

The volume used in this study is 2x2x2 mesoscopic RVEs. The material’s properties, oriented stiffness tensors from the microscopic RVEs, are maintained. The mesh type is normal. Figure 31 illustrates the geometry used.
5.3.2 Homogeneous displacement

Due to convergence issues while using periodic boundary conditions on the array of beads, we decided to use homogeneous displacement boundary conditions. Figure 32 through 37 summarizes the boundary conditions used for the six cases:

![Figure 32: Homogeneous Displacement corresponding to the Tension_11 case](image)
Figure 33: Homogeneous Displacement corresponding to the Tension_22 case

Figure 34: Homogeneous Displacement corresponding to the Tension_33 case

Figure 35: Homogeneous Displacement corresponding to the Shear_23 case

Figure 36: Homogeneous Displacement corresponding to the Shear_13 case

Figure 37: Homogeneous Displacement corresponding to the Shear_12 case
5.3.3 Mesoscopic volume analysis

Using Comsol, for every case, we launch the set of six study cases and extract local stresses and strains, which we use to build the average stiffness tensors.

5.3.3.1 Case 1

Table 34 summarizes the stiffness calculated from the array of beads

*Table 34 : Stiffness (in GPa) from Comsol of the array under homogeneous displacement*

<table>
<thead>
<tr>
<th>Stiffness from Comsol of the Array 2x2x2 Case 1</th>
</tr>
</thead>
<tbody>
<tr>
<td>7.47  3.61  3.06  0.00  0.00  0.00</td>
</tr>
<tr>
<td>4.19  7.08  3.26  0.00  0.00  0.00</td>
</tr>
<tr>
<td>4.64  4.25  7.26  0.00  0.00  1.41</td>
</tr>
<tr>
<td>0.00  0.00  0.00  1.41  0.00  1.40</td>
</tr>
<tr>
<td>0.00  0.00  0.00  0.00  0.00  1.40</td>
</tr>
</tbody>
</table>

We compute the values of the Young’s modulus from the following values. The results are displayed in table 33 along with a comparison to the values of Young’s moduli from the input stiffness and the Comsol stiffness of the mesoscopic RVE:

*Table 35 : Young’s Modulus (in GPa) of the array of bead under homogeneous displacement conditions*

<table>
<thead>
<tr>
<th>Array</th>
<th>Input</th>
<th>Comparison</th>
<th>RVE Case1</th>
<th>Comparison</th>
</tr>
</thead>
<tbody>
<tr>
<td>E1 (Gpa)</td>
<td>4.77</td>
<td>4.05</td>
<td>-17.97%</td>
<td>4.73</td>
</tr>
<tr>
<td>E2 (Gpa)</td>
<td>4.48</td>
<td>4.05</td>
<td>-10.73%</td>
<td>4.63</td>
</tr>
<tr>
<td>E3 (Gpa)</td>
<td>4.75</td>
<td>4.75</td>
<td>0.13%</td>
<td>4.75</td>
</tr>
</tbody>
</table>

As expected, the homogeneous displacement overestimates the Young’s moduli compared to the input. The results recovered from the array are within 3.5% of deviation from the FE computed stiffness tensor of the mesoscopic RVE.

We established additional comparisons to evaluate our resulting stiffness : Table 36 summarizes the comparison between the stiffness of the array and the RVE. Table 37
compares the stiffness tensor of the array to the RVE stiffness resulting from Comsol of case 1. Table 30 is the comparison between the Young’s moduli of the array and the RVE.

Table 30: Comparison between the input stiffness in Comsol and the resulting stiffness of the array 2x2x2 from Comsol (in GPa)

| Stiffness of RVE1 - Quadratic Closure | 8.34 | 5.53 | 5.51 | 0.00 | 0.00 | 0.00
|--------------------------------------|------|------|------|------|------|------
|                                      | 5.53 | 8.34 | 5.51 | 0.00 | 0.00 | 0.00
|                                      | 5.51 | 5.51 | 9.13 | 0.00 | 0.00 | 0.00
|                                      | 0.00 | 0.00 | 0.00 | 1.41 | 0.00 | 0.00
|                                      | 0.00 | 0.00 | 0.00 | 0.00 | 1.41 | 0.00
|                                      | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 1.40

<table>
<thead>
<tr>
<th>Comparison between the Array 2x2x2 and the Stiffness Input</th>
</tr>
</thead>
<tbody>
<tr>
<td>10.45%</td>
</tr>
<tr>
<td>24.22%</td>
</tr>
<tr>
<td>15.82%</td>
</tr>
<tr>
<td>0.00%</td>
</tr>
<tr>
<td>0.00%</td>
</tr>
<tr>
<td>0.00%</td>
</tr>
</tbody>
</table>

Table 31: Comparison between the resulting stiffness of the case 1 of mesoscopic RVE and the resulting stiffness of the array 2x2x2 from Comsol (in GPa)

| Stiffness from Comsol of the Array 2x2x2 Case 1 | 7.47 | 3.61 | 3.08 | 0.00 | 0.00 | 0.00
|-----------------------------------------------|------|------|------|------|------|------
|                                              | 4.19 | 7.08 | 3.28 | 0.00 | 0.00 | 0.00
|                                              | 4.64 | 4.25 | 7.26 | 0.00 | 0.00 | 0.00
|                                              | 0.00 | 0.00 | 0.00 | 1.41 | 0.00 | 0.00
|                                              | 0.00 | 0.00 | 0.00 | 0.00 | 1.41 | 0.00
|                                              | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 1.40

<table>
<thead>
<tr>
<th>Comparison between the Array 2x2x2 and the Stiffness of case 1</th>
</tr>
</thead>
<tbody>
<tr>
<td>-4.39%</td>
</tr>
<tr>
<td>-12.78%</td>
</tr>
<tr>
<td>-7.25%</td>
</tr>
<tr>
<td>0.00%</td>
</tr>
<tr>
<td>0.00%</td>
</tr>
<tr>
<td>0.00%</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Stiffness of Mesoscopic RVE Case1 - Comsol Output</th>
</tr>
</thead>
</table>
| 7.15 | 3.49 | 2.92 | 0.00 | 0.00 | 0.00
| 3.72 | 7.01 | 2.98 | 0.00 | 0.00 | 0.00
| 4.32 | 4.18 | 7.09 | 0.00 | 0.00 | 0.00
| 0.00 | 0.00 | 0.00 | 1.41 | 0.00 | 0.00
| 0.00 | 0.00 | 0.00 | 0.00 | 1.41 | 0.00
| 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 1.40

The deviations are minimal between the values of stiffness of the array and the mesoscopic RVE calculated from Comsol. The deviation’s values between the array’s stiffness and the input stiffness are similar to the ones observed in case 1 for the mesoscopic RVE.
5.3.3.2 Case 2

Table 38 summarizes the stiffness calculated from the array of beads

Table 38: Stiffness (in GPa) from Comsol of the array under homogeneous displacement

<table>
<thead>
<tr>
<th>Stiffness from Comsol of the Array 2x2x2 Case 2</th>
</tr>
</thead>
<tbody>
<tr>
<td>7.70  3.68  3.13  0.00  0.00  0.00</td>
</tr>
<tr>
<td>4.26  7.32  3.34  0.00  0.00  0.00</td>
</tr>
<tr>
<td>4.72  4.34  6.71  0.00  0.00  0.00</td>
</tr>
<tr>
<td>0.00  0.00  0.00  1.49  0.00  0.00</td>
</tr>
<tr>
<td>0.00  0.00  0.00  0.00  1.49  0.00</td>
</tr>
<tr>
<td>0.00  0.00  0.00  0.00  0.00  1.49</td>
</tr>
</tbody>
</table>

We compute the values of the Young’s modulus from the following values. The results are displayed in table 39 along with a comparison to the values of Young’s moduli from the input stiffness and the Comsol stiffness of the mesoscopic RVE:

Table 39: Young’s Modulus (in GPa) of the array of bead under homogeneous displacement conditions

<table>
<thead>
<tr>
<th>E1 (Gpa)</th>
<th>Input</th>
<th>Comparison</th>
<th>RVE Case2</th>
<th>Comparison</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>4.88</td>
<td>-17.40%</td>
<td>4.84</td>
<td>-0.87%</td>
</tr>
<tr>
<td>E2 (Gpa)</td>
<td>4.58</td>
<td>-10.24%</td>
<td>4.67</td>
<td>1.94%</td>
</tr>
<tr>
<td>E3 (Gpa)</td>
<td>4.16</td>
<td>0.00%</td>
<td>4.08</td>
<td>-1.78%</td>
</tr>
</tbody>
</table>

As expected, the homogeneous displacement overestimates the Young’s moduli compared to the input. The results recovered from the array are within 2% of deviation from the FE computed stiffness tensor of the mesoscopic RVE.

We established additional comparisons to evaluate our resulting stiffness: Table 40 summarizes the comparison between the stiffness of the array and the RVE. Table 41 compares the stiffness tensor of the array to the RVE stiffness resulting from Comsol of case 2.

Table 40: Comparison between the input stiffness in Comsol and the resulting stiffness of the array 2x2x2 from Comsol (in GPa)
Table 41: Comparison between the input stiffness in Comsol and the resulting stiffness of the array

\[ 2 \times 2 \times 2 \text{ from Comsol (in GPa)} \]

<table>
<thead>
<tr>
<th>Stiffness of RVE2 - Linear Closure</th>
</tr>
</thead>
<tbody>
<tr>
<td>8.54</td>
</tr>
<tr>
<td>5.56</td>
</tr>
<tr>
<td>5.56</td>
</tr>
<tr>
<td>0.00</td>
</tr>
<tr>
<td>0.00</td>
</tr>
<tr>
<td>0.00</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Comparison between the Array 2x2x2 and the Stiffness Input</th>
</tr>
</thead>
<tbody>
<tr>
<td>9.89% 33.82% 43.63% 0.00% 0.00% 0.00%</td>
</tr>
<tr>
<td>23.32% 14.34% 39.95% 0.00% 0.00% 0.00%</td>
</tr>
<tr>
<td>15.18% 22.02% 21.46% 0.00% 0.00% 0.00%</td>
</tr>
<tr>
<td>0.00% 0.00% 0.00% 0.00% 0.00% 0.00%</td>
</tr>
<tr>
<td>0.00% 0.00% 0.00% 0.00% 0.00% 0.00%</td>
</tr>
<tr>
<td>0.00% 0.00% 0.00% 0.00% 0.00% 0.00%</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Stiffness from Comsol of the Array 2x2x2 Case 2</th>
</tr>
</thead>
<tbody>
<tr>
<td>7.70 3.68 3.13 0.00 0.00 0.00</td>
</tr>
<tr>
<td>4.26 7.32 3.34 0.00 0.00 0.00</td>
</tr>
<tr>
<td>4.72 4.34 6.71 0.00 0.00 0.00</td>
</tr>
<tr>
<td>0.00 0.00 0.00 1.49 0.00 0.00</td>
</tr>
<tr>
<td>0.00 0.00 0.00 0.00 1.49 0.00</td>
</tr>
<tr>
<td>0.00 0.00 0.00 0.00 0.00 1.49</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Comparison between the Array 2x2x2 and the stiffness of Case 2</th>
</tr>
</thead>
<tbody>
<tr>
<td>-4.00% -0.05% -4.08% 0.00% 0.00% 0.00%</td>
</tr>
<tr>
<td>-11.93% -0.02% -6.36% 0.00% 0.00% 0.00%</td>
</tr>
<tr>
<td>-7.14% 2.01% -2.73% 0.00% 0.00% 0.00%</td>
</tr>
<tr>
<td>0.00% 0.00% 0.00% 0.00% 0.00% 0.00%</td>
</tr>
<tr>
<td>0.00% 0.00% 0.00% 0.00% 0.00% 0.00%</td>
</tr>
<tr>
<td>0.00% 0.00% 0.00% 0.00% 0.00% 0.00%</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Stiffness of Mesoscopic RVE Case2 - Comsol Output</th>
</tr>
</thead>
<tbody>
<tr>
<td>7.40 3.68 3.01 0.00 0.00 0.00</td>
</tr>
<tr>
<td>3.81 7.31 3.14 0.00 0.00 0.00</td>
</tr>
<tr>
<td>4.40 4.42 6.53 0.00 0.00 0.00</td>
</tr>
<tr>
<td>0.00 0.00 1.49 0.00 0.00 0.00</td>
</tr>
<tr>
<td>0.00 0.00 0.00 1.49 0.00 0.00</td>
</tr>
<tr>
<td>0.00 0.00 0.00 0.00 1.49 0.00</td>
</tr>
</tbody>
</table>

The deviations are minimal between the values of stiffness of the array and the mesoscopic RVE calculated from Comsol. The deviation’s values between the array’s stiffness and the input stiffness are similar to the ones observed in case 2 for the mesoscopic RVE.

5.3.3.3 Case 3

Table 42 summarizes the stiffness calculated from the array of beads.
We compute the values of the Young’s modulus from the following values. The results are displayed in table 43 along with a comparison to the values of Young’s moduli from the input stiffness and the Comsol stiffness of the mesoscopic RVE:

**Table 43 : Stiffness (in GPa) from Comsol of the array under homogeneous displacement**

<table>
<thead>
<tr>
<th>Stiffness from Comsol of the Array 2x2x2 case 3</th>
</tr>
</thead>
<tbody>
<tr>
<td>7.63</td>
</tr>
<tr>
<td>4.21</td>
</tr>
<tr>
<td>4.68</td>
</tr>
<tr>
<td>0.00</td>
</tr>
<tr>
<td>0.00</td>
</tr>
<tr>
<td>0.00</td>
</tr>
</tbody>
</table>

As expected, the homogeneous displacement overestimates the Young’s moduli compared to the input. The results recovered from the array are within 5.5% of deviation from the FE computed stiffness tensor of the mesoscopic RVE, the highest deviation of the three cases.

We established additional comparisons to evaluate our resulting stiffness: Table 44 summarizes the comparison between the stiffness of the array and the RVE. Table 45 compares the stiffness tensor of the array to the RVE stiffness resulting from Comsol of case 3.

**Table 44 : Young’s Modulus (in GPa) of the array of bead under homogeneous displacement conditions**

<table>
<thead>
<tr>
<th></th>
<th>Array</th>
<th>Input - RoM</th>
<th>Comparison</th>
<th>RVE Case3</th>
<th>Comparison</th>
</tr>
</thead>
<tbody>
<tr>
<td>E1 (Gpa)</td>
<td>4.90</td>
<td>3.98</td>
<td>-23.12%</td>
<td>4.65</td>
<td>-5.29%</td>
</tr>
<tr>
<td>E2 (Gpa)</td>
<td>4.58</td>
<td>3.98</td>
<td>-14.97%</td>
<td>4.55</td>
<td>-0.57%</td>
</tr>
<tr>
<td>E3 (Gpa)</td>
<td>4.27</td>
<td>4.11</td>
<td>-3.87%</td>
<td>4.11</td>
<td>-3.87%</td>
</tr>
</tbody>
</table>
Table 45: Comparison between the input stiffness in Comsol and the resulting stiffness of the array 2x2x2 from Comsol (in GPa)

<table>
<thead>
<tr>
<th>Stiffness of Mesoscopic RVE (2 Regions - RoM)</th>
<th>Comparison between the Array 2x2x2 and the Stiffness from RoM</th>
</tr>
</thead>
<tbody>
<tr>
<td>8.34 5.51 5.51 0.00 0.00 0.00</td>
<td>8.54% 35.21% 44.83% 0.00% 0.00% 0.00%</td>
</tr>
<tr>
<td>5.51 8.34 5.51 0.00 0.00 0.00</td>
<td>23.55% 13.43% 40.67% 0.00% 0.00% 0.00%</td>
</tr>
<tr>
<td>5.51 5.51 8.50 0.00 0.00 0.00</td>
<td>15.12% 22.65% 20.39% 0.00% 0.00% 0.00%</td>
</tr>
<tr>
<td>0.00 0.00 0.00 1.41 0.00 0.00</td>
<td>0.00% 0.00% 0.00% -4.56% 0.00% 0.00%</td>
</tr>
<tr>
<td>0.00 0.00 0.00 0.00 1.41 0.00</td>
<td>0.00% 0.00% 0.00% 0.00% 0.00% 0.00%</td>
</tr>
<tr>
<td>0.00 0.00 0.00 0.00 0.00 1.41</td>
<td>0.00% 0.00% 0.00% 0.00% 0.00% 0.00%</td>
</tr>
</tbody>
</table>

Table 46: Comparison between the resulting stiffness of the case 3 of mesoscopic RVE and the resulting stiffness of the array 2x2x2 from Comsol (in GPa)

<table>
<thead>
<tr>
<th>Stiffness from Comsol of the Array 2x2x2 case 3</th>
<th>Comparison between the Array 2x2x2 and the stiffness of case 3</th>
</tr>
</thead>
<tbody>
<tr>
<td>7.63 3.57 3.04 0.00 0.00 0.00</td>
<td>-6.57% -2.14% -3.83% 0.00% 0.00% 0.00%</td>
</tr>
<tr>
<td>4.21 7.22 3.27 0.00 0.00 0.00</td>
<td>-13.24% -3.02% -9.65% 0.00% 0.00% 0.00%</td>
</tr>
<tr>
<td>4.68 4.26 6.77 0.00 0.00 0.00</td>
<td>-8.07% -1.99% -4.65% 0.00% 0.00% 0.00%</td>
</tr>
<tr>
<td>0.00 0.00 0.00 1.47 0.00 0.00</td>
<td>0.00% 0.00% 0.00% 0.00% 0.00% 0.00%</td>
</tr>
<tr>
<td>0.00 0.00 0.00 0.00 1.47 0.00</td>
<td>0.00% 0.00% 0.00% 0.00% 0.00% 0.00%</td>
</tr>
<tr>
<td>0.00 0.00 0.00 0.00 0.00 1.47</td>
<td>0.00% 0.00% 0.00% 0.00% 0.00% 0.00%</td>
</tr>
</tbody>
</table>

The deviations are minimal between the values of stiffness of the array and the mesoscopic RVE calculated from Comsol. The deviation’s values between the array’s stiffness and the input stiffness are similar to the ones observed in case 3 for the mesoscopic RVE.

5.3.4 Mesoscopic volume conclusion

Throughout this study, we conducted analysis on the mesoscopic array of RVE while using the effective stiffness of the mesoscopic RVE. Using the same partitioning on
a 2x2x2 array of beads, we computed stiffness terms under homogeneous displacement boundary conditions and compared them with the stiffness calculated of the mesoscopic RVE. The resulting terms displayed small deviations compared to the unit cell. This can be explained through the use of homogeneous displacement conditions, less accurate and presenting a lower bound to the periodic boundary conditions results.

5.4 Conclusion

This chapter summarizes the findings on the mesoscopic scale: using the effective oriented stiffness tensors constructed from the microscopic study, we modeled the mesoscopic RVE, assessed its intake of the input stiffness tensor and the drop of stiffness after calculation. The voids taken into consideration and aligned in the main direction of deposition z cause a drop of stiffness overall, and in the main direction in particular. We then studied an 2x2x2 array to evaluate the difference in stiffness between the unit cell and the volume. The results were close and lower than the original ones, as predicted because of the use of homogeneous displacement.

The FEA software is carrying on the periodicity state of the stacked cells and the voids’ effect is taken into consideration in the same fashion than in the mesoscopic RVE calculation.
CHAPTER 6

CONCLUSIONS AND FUTURE STUDY

6.1 Conclusions

To provide a framework for FE modeling and analysis of FDM parts reinforced with short fibers, we conducted a study on two main steps and built an RVE on the mesoscale that can be used as a basic building block for the discrete model.

During the first step of the analysis, we worked on the microscopic RVE and took into consideration the short fibers' spacing, aspect ratio and orientation state. Using Mori-Tanaka model and Comsol's FE results, we were able to build a microscopic RVE which, based on the orientation tensor, the hybrid closure and the numerical stiffness, provides an effective stiffness tensor taking into consideration the significant properties of the short fibers in the matrix.

During the second step of the analysis, we worked on the mesoscopic RVE and took into consideration the geometry of the bead and the orientation distribution of the short fibers. Using the effective stiffness tensors of the microscopic RVE, we were able to compute the homogeneous stiffness tensor of the bead.

The final step was the evaluation of the homogeneous stiffness tensor on an array of 2x2x2 to assess the FEA software ability to carry on the effective stiffness and geometry structure (presence of voids). To this end, we applied homogeneous displacement boundary conditions to the volume made out of mesoscopic RVE and compared the resulting stiffness tensor with that of the original unit cell. The observed discrepancy was expected due to the use of the homogeneous displacements, less accurate compared to the periodic boundary conditions. A comparison between the
Young’s moduli display an insignificant deviation between the recovered homogenized properties.

6.2 Future Study

The present work builds a framework that describes a discretization process starting with the basic properties of short fibers and resulting in a homogeneous stiffness tensor that can be used as a material model for the bead’s discrete models.

Further investigation considering the fiber length variation and distribution will refine the results of the microscopic scale studies and give more insight on the extent of the deviations and homogenized properties that can be recovered.

In addition, including interlaminar fracture properties as cohesive zones between beads will allow failure analysis. A comparison with experimental data will help in the final evaluation of the numerical framework and its accuracy for a macroscale model.

The final outcome would be setting up a program that can automate the framework and rely on minimal input to produce a homogeneous stiffness model that can be used for FDM manufactured components reinforced with short fibers and will spare potential users meshing issues, fiber properties input and extensive computation time.
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