Uncertainty Quantification in Composite Materials

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ABSTRACT

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The random nature of the micro-structural attributes in materials in general and composite material systems in particular requires expansion of material modeling in a way that will incorporate their inherent uncertainty and predict its impact on material properties and mechanical response in multiple scales. Despite the importance of capturing and modeling material randomness, there are numerous challenges in structural characterization that are yet to be addressed.

The work presented in this essay takes a few steps towards an improved material modeling approach which encompasses structural randomness in order to produce a more realistic representation of material systems. For this end a computational framework was developed to generate a realistic representative volume element which reflects the inherent structural randomness. First stochastic structural elements were identified and registered from imaging data and parameters were assigned to represent those elements. Statistical characterization of the random attributes was followed by the construction of a representative volume element which shared the same structural statistical characteristics with the original material system. The resultant statistical equivalent representative volume element (SERVE) was then used in finite element simulations which provided homogenized properties and mechanical response predictions. The suggested framework was developed and then implemented on 3 different material systems.

Image processing and analysis in one of the material systems extended the original scope of this work to solving a machine vision and learning problem. Object segmentation for the purpose object and pattern recognition has been a long standing subject of interest in the field of machine vision. Despite the significant attention given to the development of segmentation and recognition methods, the critical challenge of separating merged objects did not share the spotlight. A simple
yet original approach to overcome this hurdle was developed using unsupervised classification and separation of objects in 3D. Lower dimensionality classifiers were joined to provide a powerful higher dimensionality classification tool. The robustness of this approach is illustrated through its implementation on two case studies of merged objects. Applications of this methodology can further extend from structural classification to general problems of clustering and classification in various fields.
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"As far as the laws of mathematics refer to reality, they are not certain, and as far as they are certain, they do not refer to reality."

— Albert Einstein
1. Introduction

1.1 Composite materials

The limitless design possibilities, superior mechanical properties and relatively low production costs are only a few of the reasons that made composite materials popular and attractive to use. Technological advances provide the means for improving the design of existing material systems and for developing new ones. Moreover, the design and analysis of materials are extending to multiple scales ranging from the macroscopic scale to the atomic scale.

Material systems with a complex microstructure are becoming increasingly common and so is the need to characterize their properties and predict their behavior. Physical tests remain essential to the study of materials and are vital for the design of new material systems. In the past two decades models and simulations have been incorporated in the study of materials. Improved computational resources and capabilities contributed to the accuracy and reliability of the complementary computational tools.

When coupled with physical tests, virtual tests are a powerful tool in the development of material systems and structural components. Accurate models and reliable simulations are necessary for relying on virtual tests and for performing fewer experimental procedures. A dependable characterization of materials which accounts for the complexity of the material
system is vital for extending the use of virtual tests [1, 2]. A truly reliable characterization must also account for the inherent uncertainty in materials. Generating virtual specimens of composite materials, which capture the geometrical variability and stochastic nature of the material systems, has been at the focus of several studies.

Figure 1.1: Multi-scale integration of physical and virtual tests.
1.2 Uncertainty in materials

The structural uncertainty in material systems, caused mainly by the stochastic nature of the manufacturing process, points to the limitations of deterministic material models. As a result, structural attributes (such as inclusions, defects and other imperfections) are one of the factors contributing to structural randomness. Quantification or characterization of the random nature of the material’s architecture becomes even more challenging in finer scales, as the structural uncertainty increases.

The effect of structural uncertainties and imperfections on the mechanical and thermal properties of a composite material has long been confirmed [3–6]. For example, random defects can potentially become stress concentration regions which may evolve to become sites for damage initiation. The deviation from the ideal architecture, which is mainly introduced to the material system during manufacturing, can be found at various scales of the material and must be accounted for while modeling the material structure. In a realistic micro-mechanical capturing, characterizing and modeling the micro-scale random structural attributes are imperative as well.

1.3 Material characterization

1.3.1 Homogenization

The classical phenomenological approach for the mechanical characterization of material, which is based on effective material properties, yields a lower and upper bounds of material properties. For the past two decades characterization of material systems was done by using detailed finite element models which resulted in an accurate mechanical analysis. Despite the numerous advantages of finite element analysis (FEA), as the structure of materials become more complex, modeling and analysis become more difficult and costly.

Various homogenization methods enable derivation of the constitutive laws of material
systems. Effective properties are determined based on a representative volume element (RVE) or a periodic unit cell (PUC) constructed at a finer scale. The formulation of reliable RVEs and PUCs for heterogenous materials, has been an on going effort in the past decades [7–13].

1.3.2 Random heterogeneous materials

Two of the key aspects that have been addressed within the framework of homogenization of random heterogeneous materials, are the structural randomness, and the stochastic nature of mechanical processes in material systems. The more common approach for incorporating structural randomness in particle reinforced materials for example, focuses on the particles structural randomness pertaining mostly to their size and location [14, 15], while some aspects of the structural randomness, namely defects, pores, voids, micro-cracks etc., are usually ignored. Another approach for capturing the uncertain nature of materials, focuses on modeling micro-structural failure processes as a stochastic processes [16–18]. Nevertheless, the inherent randomness of the initial micro-structure of material systems has not been fully realized and still poses a challenge in realistic micro-mechanical models.

One philosophy for accounting for the material randomness, advocates the use of statistical tools to model structurally driven material randomness indirectly. One such approach is stochastic homogenization based on the first order perturbation [19]. Bayesian framework has been employed to address material uncertainty by assuming prior statistical model, based on known information, and by characterizing the unknown parameters using their posterior distributions [20]. Poisson and uniform distributions were used to approximate the distribution of structural elements and flaws in order to infer the cumulative probability of damage descriptors in concrete, such as failure and volume of fracture process zone [21].

The work of Torquato in the field of heterogeneous random materials [22], motivated a more direct statistical approach for structurally driven material randomness. A statistically similar representative volume element (SSRVE) was generated in [23] in order to formulate a simplified artificial microstructure, and its statistical similarity was evaluated using Minkowski functionals
1. Introduction

and lineal-path function.

Another direct approach to represent material randomness has been employed in [24], where material discontinuity was introduced via Gauss quadrature. The structural randomness was expressed by the random assignment of material properties to the Gauss quadrature points. Although the physical size of the discontinuities was not considered, the method was further improved in [25, 26] by using random functions, which were based on the size of the discontinuities, for the allocation of material properties at each Gauss point in the RVE.

A different concept of volume element representation, called statistically equivalent periodic unit cell (SEPUC), was first introduced in [27] and was implemented in [28, 29]. The variability of a real microstructure was characterized using statistical descriptive functions such as n-point probability functions and lineal path function [22]. First a parametric model of a unit cell was chosen. In the next stage the differences between the real microstructure and the parametric model were defined using objective functions that quantified the differences between two models. The parameters of the parametric model were then determined by an optimization process that minimized the objective functions.

1.3.2.1 Woven composites

Generating virtual specimens of composite materials, which capture the geometrical variability and stochastic nature of material systems, has been at the focus of several studies on composite woven materials. The characterization of a three dimensional textile composite geometry and of its variability by [30] lead to the formulation of an algorithms for textile composite virtual specimens generation. A one-dimensional tow representation combined the spatial tow loci variability in [31] to provide a more realistic model. In [32] the variabilities in tow cross-sectional area, aspect ratio and orientation were considered to produce a three-dimensional tow representation. The stochastic framework for characterizing the structural variability and uncertainty was extended and used in multi-scale modeling by [33, 34].

While several studies have considered the material randomness in woven materials the major
micro-structural variability discussed was that of the fibers or tows (such as tow orientation and misalignment, cross-sectional area etc.). In [35] a single inclusion was represented as an ellipsoid, though smaller inclusions were not considered in the SEPUC model. Large pores (average pore volume equal to $100 \mu m^3$) were introduced to the matrix phase of the model presented in [36] as an approximation of the porosity observed in the material. The shape and distribution of pores were characterized, approximated as equivalent spheroids and combined in a micro-mechanical model to calculate the effective properties [37]. In order to predict random meso-level crack initiation, micro-level discontinuities were represented as ellipsoids [38] based on their distribution in [18].

### 1.3.2.2 Particle reinforced composites

Additional difficulty arises when discussing virtual specimens for particle reinforced materials in general and when the material system of interest is concrete in particular. The random nature of inclusions (aggregates) and defects (pores, voids and micro-cracks), adds to the uncertainty in the material characterization [25, 39]. Considering concrete not as a material but as a material system, has led to the study of various structural scale levels and their interactions. At the macro-level the internal architecture is smeared. A clear distinction between aggregates and cement occurs at the meso-level and the cement microstructure is considered at the micro-level. Atomistic level simulations are often needed to resolve nano-mechanical properties of the major constituent phases (either hydrated or not) present in cementitious material systems [40].

Structural randomness in the modeling of particle reinforced materials has been considered in the past using a morphological approaches, whether through the formulation of a unit cell or as a part of the formulation of a constitutive model, based on continuum damage mechanics. In particle reinforced materials, such as concrete, the particles morphology (shape and size) and location would be the main causes for any structural randomness.

A methodology for generating statistically optimal unit cell based on 3D reconstruction of polydisperse particulate composites from $\mu CT$ images was presented in [41], where n-point statistical descriptors were used to characterize and generate discrete inclusions in a unit cell.
One-point, two-point and three-point probability functions were used to discretize the inclusions probability space and to characterize the statistical morphology of a pack of spherical glass beads, which was assumed to be isotropic. An optimal representative unit cell was generated by minimizing objective functions that were based on the one-point and two-point probability functions of the pack and the unit cell. The generated cell had a good agreement with the original pack in the first and second order probabilities, but not with the third order probabilities.

In a recent study [42] an efficient algorithm was developed for generating a unit cell with randomly distributed inclusions. The parametric method allowed to generate unit cells with various shapes of inclusions with up to 45% packing fraction. Expanding the variety of inclusions enabling to generate unit cells with complex random distribution of inclusions such as chopped fibers (in 2D and 3D) and 3D granular inclusions. Moreover, a three steps hierarchical approach for preventing inclusions overlapping contributed to the computational efficiency of the method.

The random characterization the shape and size of aggregates is frequently described using sieve analysis and grading curves in general and Fuller curve in particular. In one of the earliest studies, the structural randomness was directly introduced by modeling aggregates randomness using concrete sieving curve [43]. A similar approach was used in [44] where spherical aggregates formed the basis for constructing a concrete unit cell model. The development of a concrete unit cell was also addressed in [45], where randomly distributed spherical aggregates were at the base of the suggested unit cell. The use of Fuller curve was accompanied by sieve analysis as an underlying assumption of aggregates distribution in generating the unit cell. This was followed by another noteworthy contribution in [46], where the sieve analysis, Fuller curve and direct access were used as a part of the homogenization approach for predicting effective material properties. Sieve analysis was used to generate spherical aggregates in [47] as well, where the effect of the cement matrix and aggregates on the failure behavior of plain concrete was examined. This approach for aggregate modeling was also adopted by [48] in the context of diffusivity predictions in concrete.

As noted previously, particles size accounts for one aspect of the random nature of particle reinforced material systems. Most of the aforementioned studies have used spherical
simplification of particles, thus describing the randomness by a single parameter - radius. In order to improve inelastic modeling of particle reinforced material systems in general and aggregate reinforced concrete in particular, a non-spherical description has been explored. Such modeling philosophy was employed in [49], where ellipsoids and ellipsoid based modified shapes were chosen to model aggregates, having a size distribution which was based on the Fuller curve. Spherical, ellipsoidal and polyhedral aggregates were used to model damage behavior of concrete in [50], also in conjunction with the Fuller curve. Another study that generated non-spherical aggregates (using a grading curve), attempted to mimic the manufacturing process of concrete [51]. An alternative approach for introducing randomness in characterizing aggregates shape and size in concrete modeling in 2D, was suggested in [52], where the aggregates were described by random radii and angles.

Departing from the conventional methodologies, a different approach for developing a random morphological model for concrete microstructure was presented in [53]. The model considered two families of morphological criteria: aggregates size distribution aggregates distribution in space. The size distribution (and formulation) was based on the sieve analysis and curves for concrete, using a limited number of sieves. As in most other studies on the subject, the aggregate size has been characterized using a single size parameter - radius or equivalent radius. The sample specific morphological characterization was based on pixel intensity levels observed in slices of CT imaging. These morphological properties have been used to evaluate the equivalency between an original sample and a generated model. The covariance of aggregates was defined and measured based on image intensity values and not on any structural metric, which was not relevant given the size differences in that model.

Another element of randomness in modeling particles in particle reinforced material systems is the position of particles in space. Various packing algorithms and placement methods were used in modeling concrete systems. In most studies particles were randomly placed from largest to smallest, while avoiding particles overlap [45, 49, 52], a method also known as take and place method. A free fall simulation of particles was used to mimic the random physical placement of
aggregates in a cement matrix in [54].

Generating a concrete model is the stepping stone for evaluating equivalent mechanical properties and predicting fracture and failure in concrete. Experimentally supported isotropic distribution was used to characterize the distribution of micro-cracks, which were caused by the activation and growth of micro-defects, in a micro-mechanical constitutive modeling of the nonlinear response of concrete [55]. A multi-scale model for the quasi-brittle strength of cement paste and mortar was developed in [56]. The effects of concrete morphology, more specifically aggregates, on failure behavior and fracture propagation were addressed in [47].
1. Introduction

1.4 Scope

Although significant attention has been given to the modeling of random heterogeneous materials, we believe that there are still several issues to be addressed. In composite woven materials, despite their importance in determining the material behavior, structural imperfections such as pores, voids, micro-voids, cracks and micro-cracks were considered only in a few studies. Accounting for defects would better explain the fracture and damage behavior. In particle reinforced composite materials, particularly in concrete, the existing methods rely on sieves analysis, grading curves and Fuller curve for the characterization of aggregates randomness. Furthermore, when generating aggregates in the context of a unit cell or RVE formulation, the aggregates morphology is limited to single parameter - radius or equivalent radius. Three dimensional characterization with multiple size parameters would provide a more realistic characterization of aggregates geometry.

The primary goal of the work presented here is to provide a methodology for accurate characterization of structural randomness in material systems. This was done by developing a framework for generating a statistically equivalent representative volume element (SERVE) which incorporated material specific structural randomness. The challenges faced in the process gave rise to a secondary goal in the field of machine vision and learning. Geometric structural characterization required development of tools for separation and classification of objects in 3D.

Structural geometric information was extracted from imaging data, such as micrographs and micro computed tomography (µCT). Structural elements, for instance inclusions, were assigned a simplified geometric representation, such as ellipsoids. Parameters of the geometric representation were studied and the correlations between parameters and their distributions were characterized, thus enabling to capture the nature of random phenomena. The suggested framework (illustrated in Fig. 1.2) was created, tested and successfully implemented on several material systems representing three different families of composite materials: ceramic matrix composite, particle reinforced composites and fiber reinforced composites.
1. Introduction

Figure 1.2: Generating statistically equivalent representative volume element.

1.4.1 Material systems

1.4.1.1 Sic/SiNC

For the ceramic matrix composite family, a ceramic matrix composite (CMC), Sic/SiNC (S-200H), was considered in this work. The material system consists of a SiC (Hi-Nicalon™) fibers and a matrix comprised of Si, N and C (Silicon, Nitrogen and Carbon respectively) with a weak interface coating for the required imparting toughness [57] The fibers in the material were arranged in an eight-harness weave (8HW) architecture at 24 EPI with 45% volume fraction (Fig. 1.3). The material was molded in compression, pushing adjacent tows together, making the identification of individual tows far from trivial. This class of CMC\(^1\) has been previously studied in [57, 59–61].

Figure 1.3: Eight-harness weave illustration.

\(^1\)The work presented on this material was funded by the U.S. Air Force Research Laboratory (AFRL) under prime contract FA8650-13-C-5213 (Dr. George Jefferson, program monitor) through a subcontract from the United Technologies Research Center (UTRC), Subcontract # UTC PSA-1205265, PO 2603158. The materials presented were published in [58], which has been approved by the AFRL for public release, Case # 88ABW-2016-3072.
1.4.1.2 Aggregate reinforced concrete

The material family of particle reinforced composites is represented by concrete composed of limestone aggregates and Portland cement, which was used for the construction of pre-stressed reinforced girders. The material system was consisted of a special mixture designed to ensure that the concrete was placed correctly without voids or honeycombs. Mixture’s design was also dictated by early strength requirements, according to which concrete had to achieve 80% of the minimum specified compressive strength (f’c) in 12 hours. This was accomplished by using aggregates with maximal size of 15 mm, which resulted in a minimum slump \(^2\) of 20 cm. The unique concrete requirements resulted in the fabrication of a non-standard concrete both in composition and mechanical properties. Material (see Fig. 1.4) and experimental data for this study were provided by the Moyeda Construction Company \[63\].

![CT views of the concrete sample, generated using 3DSlicer© \[64, 65\]: (a) - top view, (b) - three dimensional view, (b) - front view, and (d) - right view.](image)

\(^2\)Empirical test for concrete, intended to examine the shear stress induced material flow \[62\]
1.4.1.3 Fiber reinforced concrete

A sample of fiber reinforced concrete represented the fiber reinforced composite family. Straight and hooked fibers were embedded in a cement matrix of the material sample (see Fig. 1.5)\(^3\). The material sample on which the classification and separation process was implemented in this work, was first studied in [66, 67] in the context of energy dissipation mechanisms. Due to the high degree of contact and overlapping between the fibers, isolating individual fibers proved to be most challenging.

![Figure 1.5: 3D reconstruction of the fiber reinforced concrete sample with (a) and without (b) the cement matrix, along with a representative sample of the reinforcement fibers (c).](image)

However, before analyzing the geometric parameters of the fibers, it was necessary to separated and identified individual fibers. The need for automatic separation of intersecting fibers led to the study of machine vision and learning, object identification, segmentation, separation, recognition and classification. The work done in this area is presented in chapter 3.

\(^3\)Figures courtesy of Ms. Lauren S. Flanders and Prof. Eric N. Landis [66].
1.4.2 Outline

Data collection, data analysis and implementation are the three stages of this research. These stages are reflected in the organization and structure of this dissertation. Visual data in the form of micrograph images, CT scans etc. was the base for gathering structural data. The processing, analysis and registration of the visual data are explained in chapter 2.

Chapter 3 describes a methodology for unsupervised segmentation and classification of objects in 3D which was developed in order to separate and individually identify intersecting structural elements in 3D imaging.

The analysis of geometric information extracted from visual data, proceeds in chapter 4 with the statistical characterizations of structural elements and ends with the process of creating and exploring the implementation of statistically equivalent representative volume elements (SERVEs).
2. Image Processing & Analysis

2.1 Introduction

Advanced image acquisition methods which were limited to medical applications, are becoming more accessible and common in other areas of research. Creating models of material systems using imaging techniques is a well established approach. Methods of generating material models with complex micro-structures have become widely used thanks to imaging tools such as micrographs, X-ray tomography, computed tomography (CT) and computed micro-tomography (µCT).

Automated methods for modeling complex meso-scale structures, using these image acquisition methods, have been developed and extended to generating a FE models and meshes [68]. Improved imaging resolution plays a vital role in characterizing complex micro-structures [11, 28, 31] and in understating failure mechanisms [69–71]. An accurate and intricate modeling of material micro-structure requires an even more complicated and strenuous computational work.

This chapter discusses the methods used for image processing and analysis in the context of structural modeling of material systems and presents the processes implemented on the studied materials: ceramic matrix composite, aggregate reinforced concrete and fiber reinforced concrete. The main drivers and limitations for the processes described in this chapter were induced by the raw imaging data that was available for this study and its quality.
2. Image Processing & Analysis

2.2 Image processing

2.2.1 Image processing in 2D

The structural characteristics of the SiC/SiNC material system were identified and studied based on 2D images. Six cross-sectional optical micrographs of SiC/SiNC samples were made available for this work (Fig. 2.1). All 6 images had a resolution of 600x495 pixels and were on a scale of 0.005in (shown in the lower right corner of each micrograph in Fig. 2.1).

For this material system structural characterization was done by focusing on typical defect structures, which were identified and registered based on the available imaging data. The provided micrographs were processed and analyzed using MATLAB™ image processing toolbox. All six micrographs were processed in the following way:

(i) Histogram equalization method was used for image enhancement [72, 73].
(ii) Background surrounding the material sample was removed (Fig. 2.2b).
(iii) Gray scale image was separated to 3 binary masks (matrix, tows and defects). Tows and defects masks were determined based on the pixels’ values (see Table 2.1). Matrix mask was produced by excluding the two other masks and the image background (Fig. 2.2c).
(iv) Tow phase was separated again to longitudinal and transverse phases. This distinction was done based on the size of the area of the objects in the binary image. Objects with area larger than 10 connected pixels were classified as longitudinal tow and objects with continues area of less than five pixels were classified as transverse tow (Fig. 2.2d).
(v) Binary images of the different phases underwent erosion and dilation in order to filter noises and smooth objects in the images.
Figure 2.1: Optical micrographs of the six polished cross-section samples. Image scale: 0.005in. Image resolution: 600x495 pixels.
Figure 2.2: Optical micrographs image processing: (a) original image; (b) enhanced gray scale image; (c) masks separation; (d) longitudinal-transverse tow separation.

Table 2.1: Micrographs image threshold values for CMC (in pixels).

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<thead>
<tr>
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<th>Min</th>
<th>Max</th>
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<tbody>
<tr>
<td>Defects</td>
<td>1</td>
<td>65</td>
</tr>
<tr>
<td>Matrix</td>
<td>66</td>
<td>219</td>
</tr>
<tr>
<td>Tows</td>
<td>220</td>
<td>255</td>
</tr>
</tbody>
</table>
2.2.2 Image processing in 3D

The work on the particle reinforced material family was done using material system of aggregate reinforced concrete which represented the structural characteristics this family. Computed tomography (CT) scans of several cylindrical concrete samples (see Fig. 2.3), showing aggregates and defect structures in the samples and experimental data of these samples were accessible thanks to the Moyeda Construction Company [63].

![CT views of the concrete sample](image)

Figure 2.3: CT views of the concrete sample: (a) - top view and (b) - front view. See Table 2.2 for pixel intensity threshold values of the different phases.

The CT data was processed and analyzed using MATLAB™ image processing toolbox as well. A preliminary examination of the CT images was done in order to determine pixels’ value threshold ranges for the aggregates, mortar and defects (see Table 2.2). A circular cross section of the cylindrical sample was recognized. The radios and center of the sample’s cross section were obtained for each slice and averaged. Once the preliminary image processing was done, the CT images were processed in the following way (similar to that presented in subsection 2.2.1):
2. Image Processing & Analysis

(i) Background surrounding material sample was removed based on pre-determined thresholds and circular geometric information (Fig. 2.4b).

(ii) Linear gradient based correction was applied to CT images in order to account for beam hardening effect (Fig. 2.5a).

(iii) Each gray scale CT image was separated to 3 binary masks based on pixels’ ranges (aggregates, mortar and defects). After producing aggregates and defects masks mortar mask was generated by excluding the other two masks (Fig. 2.5b).

(iv) Erosion and dilation were applied to the masks for smoothing and noise filtering (Fig. 2.5c).

<table>
<thead>
<tr>
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<th>Min</th>
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<tbody>
<tr>
<td>Aggregates</td>
<td>240</td>
<td>255</td>
</tr>
<tr>
<td>Mortar</td>
<td>150</td>
<td>200</td>
</tr>
<tr>
<td>Defects</td>
<td>0</td>
<td>100</td>
</tr>
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Table 2.2: CT image threshold values for concrete (pixels intensity).

Figure 2.4: Original CT image of concrete sample (a) and a cleared background image (b).

Image processing in 3D was part of the work done on fiber reinforced material family, which was represented by high performance fiber reinforced concrete. A reconstructed 3D image of material sample was available for structural characterization. The reconstruction of the 3D image from CT images was performed and presented in [74].
As a preliminary step to the separation and classification process, a few image processing measures were carried out in order to filter and smooth the raw 3D imaging data. It is worth mentioning that images were in gray-scale to begin with, or converted to that format. Initial image processing was done in a similar way to that presented in subsections 2.2.1 and 2.2.2. First, histogram equalization method was used for image enhancement [72, 73], this was followed by applying threshold to the image. Image threshold process was chosen based on the input quality and characteristics. Lastly, morphological opening was done for the purpose of smoothing the image. The complex 3D geometry required more rigorous image processing, analysis, separation, classification and registration procedures. Chapter 3 provides detailed descriptions of the methods and tools developed in order to identify individual structural objects in the 3D image for this material system.

2.3 Image analysis

2.3.1 Object registration: CMC

Once the micrographs were processed and separated to different masks, material discontinuities represented in defects mask were approximated as ellipses with equivalent geometric properties.
The first moment of the area provided the center of the defect, denoted as \( X_c \) and \( Y_c \). Geometric parameters of an ellipse with the same normalized second central moment as the defect were extracted: major axis, minor axis and orientation, denoted as \( a \), \( b \) and \( \theta \) respectively (see Fig. 2.6). Defects were divided into categories according to their dimensions: pores, cracks (including micro-cracks and micro voids) voids and large voids [3, 70, 75–77] (see Table 2.3). Aside from the small number of large defects, which was insufficient for statistical analysis, larger defects were excluded from any further analysis since they were attributed to fibers that were removed form the samples during the polishing process. The defects that were considered, in the longitudinal tows and transverse tows, can be seen in Fig. 2.7.

Figure 2.6: Geometric parameters of the approximated defects.

### 2.3.2 Object registration: Aggregate reinforced concrete

The binary masks of the processed CT images were used to generate a 3D volumetric representation of the cylindrical concrete sample. The reconstructed 3D volume included the aggregates and defects embedded in the mortar. Image processing, selected parameters (such as minimum volume) and chosen threshold values led to the identification and registration of 648
aggregates and 320 defects. The aggregates and defects (objects) in the reconstructed sample were approximated as ellipsoids with equivalent geometric properties.

The first moment of the volume provided the center of the objects, denoted as $X_c$, $Y_c$ and $Z_c$. The geometric parameters of an ellipsoid with the same normalized second central moment as the object were extracted: major axis, middle axis, minor axis and rotation with respect to the z, y and x axes, denoted as $a$, $b$, $c$, $\phi$, $\theta$ and $\psi$ respectively (see Figs. 2.8 and 2.9).
2.3.3 Object registration: Fiber reinforced concrete

The geometric characteristics of the fiber reinforced material system led to the following structural simplifications which can be applied for fiber reinforced-like materials:

(i) The cylindrical like geometry of the fibers resulted in simplified geometry of straight lines.

(ii) Low width-to-length ratio \( w/l < R_{max} \), reflecting a difference of approximately one order of magnitude \( R_{max} = 0.2 \)

(iii) Maximal acceptable width \( w_{max} \), where \( w_{max} = 15[\text{voxels}] \).
Once the objects separation process described in chapter 3 was completed, 31,500 fibers were identified (see Fig. 4.13). Only the fibers location (coordinates of the center) and direction vectors (or orientation vectors, see Fig. 4.14) were registered since their length and width were assumed to be the same in all fibers.
3. Unsupervised Classification

3.1 Introduction

The fiber reinforced concrete material sample reconstructed 3D image posed a challenge in identifying individual fibers for the purpose of structural characterization. As mention previously, this challenge expanded the scope of this work in order to develop the required image analysis tools.

Identifying structural elements in 2D and 3D imaging has become a common practice in many fields as imaging technology availability grows. In micro-structural material modeling and analysis, computed tomographic (CT), micro-computed tomographic (μCT) imaging, and other imaging techniques are often used for structural reconstruction and analysis [78, 79]. Moreover, these imaging techniques become a valuable tool for analyzing failure processes such as fracture, creep and other damage mechanisms [74, 80, 81].

Spatial descriptors of objects, originated in information extracted from images, enable to identify objects and associate different instances to various classes. Prior to recognition objects must be segmented through the process of segmentation, in which an image is partitioned to different regions of interest based on their characteristics (gray levels for example) [82]. A widely used segmentation methodology includes clustering based segmentation methods where regions
in images are segmented based on clusters of distinct features (such as color, pixel intensity or texture).

Many studies in the field of machine vision have focused on the challenges in object recognition and image segmentation, covering different aspects, both in 2D and 3D. A technique for analyzing complex multi-mode features, called feature space analysis, was introduced in [83]. In feature space analysis, densities of image subsets, estimated with the mean shift method, received parametric representations in the parameter space. Significant features in the image could then be identified based on the density distribution in the parameter space, which corresponds to the image features. Segmentation based on the mean shift method was extended in [84, 85] to the temporal dimension. Spatial-temporal filtering and segmentation of magnetic resonance images (MRI), resulted in segmentation and tracking of multiple sclerosis (MS) lesions.

Probability distribution based segmentation was explored in [86] for the purpose of segmenting skeletal fiber tracts. The spatial information for tracts segmentation was provided by combining diffusion maps and a probability density based metric. Measuring tract similarity, this metric was obtained from the affinity between multivariate Gaussian probability densities, which represented fiber tracts. A similar approach was taken in [87], where a different probabilistic measure for clustering fiber tracts into bundles was suggested. Expanding 2D fiber tracts segmentation, a framework for 3D classification of fiber tracts based on curvature points was developed in [88].

The work presented in [89] yielded a simple clustering based segmentation method, which incorporated spatial position constraint of pixels. After the image was partitioned to blocks and their descriptors were extracted, the blocks were clustered using K-means algorithm. An automatic segmentation using Constrained Parametric Min-Cuts (CPMC) was developed in [90]. The segmentation process included two steps, first the target image was partitioned to sub-regions that were segmented and ordered according to their alignment with the image contours. In the second step, the sub-regions were ranked based on the probability of similarity to real-world
3. Unsupervised Classification

objects. The highest ranked object hypotheses were then evaluated and compared against the original image. This method was further developed in [91] by combining it with Unsupervised Discriminant Clustering (UDC). Segment hypotheses with high percentage of object regions were clustered together with the purpose of obtaining shape segmentation with higher accuracy.

Classification or recognition of objects or patterns are the most common applications to follow the segmentation process. Fiber dye classification method was presented in [92]. Fibers reflectance spectra dimensionality was reduced using Principal Component Analysis (PCA), and fiber dyes were identified based on the nearest neighbor classification of their principal components. A scheme developed in [93] suggested a two steps process for unsupervised classification of large dimensionality hyper-spectral imaging. Fit parameters associated with image features were clustered based on their histograms, after sets of basis functions were generated based on the relevant fit parameters.

The problem of recognizing an object class based on a small number of unsegmented images was addressed in [94] using a learning model. Learning Objects Classes with Unsupervised Segmentation (LOCUS) was employed in learning the shape of a representative objects, by inferring object segmentation throughout the learning process. Recognizing objects in a point cloud was a subject of interest in several studies, such as [95] for example. A pipeline for computing a recognition threshold was proposed, by extracting key point feature of the point cloud and matching them with descriptors of segmented objects.

For the purpose of tracking objects in space in the context of robotic sensing, [96] applied object recognition to thermal imaging in, by mapping thermal data to a point cloud, and recognizing objects by their heat radiation. Objects tracking was also discussed in [97], where a framework for vehicle tracking was developed. In the proposed framework object detection and segmentation were followed by camera self calibration and vehicle modeling. The final stage of the framework employed adaptive segmentation in order to deal with problem of objects merging, caused by poor segmentation due to color similarities between objects. Although image segmentation and object recognition are key challenges in machine vision, and despite the
numerous studies and different methodologies dedicated to the subject [72, 73, 82], as pointed out in [98], the problem of separating merged or overlapping objects still poses a great challenge.

In this chapter a methodology for unsupervised separation and classification of merged objects in 3D is presented. The foundation on which this methodology was built upon, is one of the central ideas in learning - Boosting. By incorporating several ”weak classifiers” to form a ”committee”, boosting methods produce a robust classifier [99, 100]. Although the suggested methodology was developed for structural characterization of fiber reinforced concrete, it was also implemented on another structural composite material - ceramic matrix composite arranged in an eight-harness weave architecture.

3.2 Methodology

3.2.1 Initial Volume Based Segmentation

In the first stage of the volume segmentation, 3D processed images are further analyzed in order to find and label connected volumetric objects. First, the elements of the 3D array, representing the voxels in 3D image, were scanned. If an unlabeled voxel was identified, the voxel and all connected voxels were assigned a new label using a flood-fill algorithm [101]. Voxels connectivity was based on the 6 nearest neighbors to a certain voxel (for example, the nearest neighbors of \( v_{i,j,k} \) were \( v_{i-1,j,k}, v_{i+1,j,k}, v_{i,j-1,k}, v_{i,j+1,k}, v_{i,j,k-1} \) and \( v_{i,j,k+1} \)). This process was repeated until all voxels were labeled.

3.2.2 Plane Based Segmentation

A single connected object was in fact composed of several intersecting, overlapping or tangent objects - a bundle of fibers for example. In order to separate connected objects, the following assumption was made: All points of a convex body in \( \mathbb{R}^n \) belong to the same sub-body in \( \mathbb{R}^m \), where \( m < n \). In other words: All points of a 3D convex objects belong to the same 2D convex object, in
any cutting plane. It is important to point out that this approach was based on the boosting concept, in the sense that an improved classification (or connectivity) of voxels in a higher dimension was achieved by combining the output of ”weak” classifiers in a lower dimension.

2D connectivity in cross-sectional planes was determined using an efficient *run-length* implementation of *local table method* [82, 101]. The process included the following stages:

(i) Encoding the image using *run-length encoding* - A list of pixel runs was generated. Each run recorded the location of the start pixel and the length of the run (the term *run* refers to a sequence of pixels in 1D).

(ii) Preliminary labeling and label equivalency - Each run was assigned a preliminary label, adjacent runs were aggregated to an equivalent class label and their labels were recorded as well (adjacent runs were then determined as equivalent).

(iii) Determining class equivalency - Different classes containing equivalent runs were merged into a single class.

(iv) Relabeling - The merged classes were relabeled where each merged class contained all the equivalent runs. An illustrated example of the runs and classes appears in Fig. 3.1.

2D connectivity in consecutive slices was used to determine 3D connectivity in a process conceptually similar to that of the *run-length* implementation. To this end, the equivalencies of merged classes in neighboring slices were evaluated. Equivalent classes were grouped into global classes (volumetric classes) and merged. The merged global classes were then relabeled and resulted in 3D connectivity based on 2D cross-sectional connectivity.

Classes equivalency in different slices was determined in the manner described below, where *local labels* were labels of merged classes in 2D and *global labels* were labels of merged global classes in 3D. The process described here is also illustrated in Fig. 3.2. While advancing from one slice to another in a specific direction, local and global labels of all pixels in the *i*-th slice were recorded in an equivalency table. Several scenarios of local and global labeling were possible:

(i) A class with a local label but without a global label.

(ii) A class with a local label but only a subset of the class had a global label.
3. Unsupervised Classification

(iii) A class with a single local label and subset of that class with different global labels.

(iv) Several classes with different local labels but with common global labels.

Examining each local label in the $i$-th slice yielded three possible events:

(i) Non of the pixels in the class had a global label - in this case all pixels were assigned the same new global label.

(ii) Some of the pixels in the class had the same global label - here the unlabeled pixels were assigned the global label of the other pixels in that class.

(iii) Some of (or all) the pixels in the class had different global labels - this event occurred when two objects (or more) from previous slices merged into a single object.

Unlabeled pixels were iteratively assigned global labels using a nearest neighbor based hierarchical algorithm hereafter referred to as the conflict resolution algorithm (for which further details are provided below).

After each voxel in the $i$-th slice was assigned a global label, slice was checked for disconnected global labels. This was the fourth possible event, in which a single object from previous slices was split to two or more objects. In this case, new global labels were assigned to disconnected areas with the same global label, and backward adjustment correction was performed in all related previous slices using the conflict resolution algorithm.

In order to determine voxel labeling where the same global label appeared in different local classes or where different global labels appeared in the same local class, the conflict resolution algorithm was employed. First, all pixels in question were assigned global label based on $K$ nearest neighbors, where the number of nearest neighbors was set to be $K = 8$. This number of neighbors was chosen after providing the best results for the cases considered herein. If unlabeled pixels where to be found, after the initial assignment, another iteration was performed with $K = k - 1$ nearest neighbors. The process continued until all pixels were labeled or until $K$ was reduced to zero. In case unlabeled pixels remained, a problem flag was raised. This did not happen in the present studies.

Once all classes that had local labels were assigned global labels as well, global labels were
projected to the next slice, and the process advanced onwards to the \((i + 1)-\)th slice. Otherwise, the voxels with local labels but without a global one in \((i + 1)\) were examined and assigned global labels separately. Global labels were projected to the next slice based on the following principle: if a voxel with a global label in \(i\), had a parallel non-empty voxel in \(i + 1\) with a local label, the voxel in \(i + 1\) was assigned the same global label as its parallel voxel in \(i\).

Figure 3.1: Connectivity and labeling implementation in 2D and its 3D linkage.
3. Unsupervised Classification

Figure 3.2: Secondary classification procedure in merging segmented fibers.

3.2.3 Linking Different Segmentations

The process described above, yielding a plane based 3D voxels connectivity, was executed again as necessary (according to the structural complexity), each time in different direction. A voxels
global labels table was then constructed, in which each row corresponded to a certain voxel, and contained the voxel’s global labels from the plane based segmentations in the different directions.

Unique rows in the global labels table, which represented unique combinations of global labels (from the different directions), were identified, and voxels were grouped to 3D super classes based on these unique combinations of global labels. Finally, new labels were assigned to all super classes, which represented the separated and segmented volumetric objects. In some cases the process described above resulted in over segmentation, where continuous objects were represented by several different smaller objects. An example of over segmentation is given in the following section 3.3. Additional ad hoc steps, which are described below, were taken in order address the distinct challenges resulted from the different characteristics of the case studies.

3.3 Implementation

3.3.1 CMC: Eight harness weave

The eight-harness weave (8HW) of a ceramic matrix composite (CMC) that was described in section 1.4 was also considered here to illustrate the implementation of the approach described above. A geometric model of the material, which was generated as part of the work presented in [58], is shown in Fig. 3.3. The relatively simple geometry of the problem, required a plane based volume segmentation in only one direction. Two directional segmentations are presented herein in order to highlight the similarities and differences between them. Due to the contacts and intersections of the warp and waft tows, the initial volume segmentation, which was determined based on six nearest neighbors connectivity, yielded a single volumetric object, merging the tows.

The initial volume based segmentation was followed by determining the 2D connectivity of the cross-sectional planes. The final tows separation of the 8HW is presented in Fig. 3.4. Furthermore, the resulting connectivities in the y direction and in the x direction are illustrated in Fig. 3.4a and Fig. 3.4b respectively.
3. Unsupervised Classification

Figure 3.3: Longitudinal (orange) and transverse (blue) tows (a); and separated tows (b).

Figure 3.4: Eight harness weave plane based segmentation in the transverse direction (a) and the longitudinal direction (b), resulting in bundle separation and classification (c).
Linking different cross-sectional connectivities in the y direction using the methods described above, led to the determination that the tow labeled as $\alpha$ in Fig. 3.5a included the areas labeled as A1, A2 and A4, as well as subareas in the areas labeled as A3 and A7. Similarly, the tow labeled as $\gamma$ in Fig. 3.5b included the areas labeled as B2 and B4, as well as subareas in the areas labeled as B3 and B6.

The subareas in the merged areas A3, A7, B3 and B6 in Fig. 3.5 were determined based on neighboring slices according to the methods previously discussed. Another approach for detecting subareas in this case would involve exploring the overlaps between cross-sectional connectivities in several directions. For example, the union between A3 and B2, B3, B4 and B6 would result in detecting the tow labeled as $\gamma$ in Fig. 3.5c.
3.3.2 Fiber reinforced concrete

In the fiber reinforced concrete material system straight and hooked fibers were embedded in a cement matrix (see Fig. 3.6). As mentioned in section 1.4, the material sample at hand was previously studied in [66, 66]. Due to the high degree of contact and overlapping between the fibers, isolating individual fibers proved to be most challenging.

![Figure 3.6: 3D reconstruction of the fiber reinforced concrete sample with the cement matrix.](image)

Figure 3.6: 3D reconstruction of the fiber reinforced concrete sample with the cement matrix.

The original sample, measured $1513 \times 1513 \times 2843$ pixels (see Fig. 3.7a), was partitioned to manageable sub-volumes. One of the sub-volumes, measured $250 \times 250 \times 500$ pixels (see Fig. 3.7b), was considered to illustrate the implementation of the proposed segmentation approach. Initial volume segmentation of the original sample, using six nearest neighbors connectivity, yielded 131486 connected objects of any volume. However, less than 7000 objects remained, after excluding smaller objects with volumes ranging from 500 to 1500 voxels.

A representative sample of six objects, shown in Fig. 3.8, illustrates the problematic nature of fibers interactions. Cross intersection and tangential contact of fibers, as well as merging of separate fibers and splitting of fibers, led to an intricate geometric space for analysis and segmentation.

The first steps of the segmentation process in this case, were similar to those employed in the segmentation of the eight harness weave model. Since the initial volume analysis identified more than one object, the plane based segmentation stage which followed was executed separately for each of the registered objects. In order to deal with the geometric complexity, the plane based
3. Unsupervised Classification

Figure 3.7: 3D reconstruction of the fiber structure in original sample (a) and in the analyzed sub-volume (b).

Figure 3.8: A representative sample six objects, demonstrating the variability of bundles of merged fibers.

segmentation was performed in three different directions: x, y and z.

Implementing the plane based segmentation on object #3 in Fig. 3.8, led to three different subdivisions of the connected fibers in the object of interest. Each voxel was assigned three labels based on the distinctive partitioning in the x, y and z directions. The plane based segmentation produced different morphologies and subsegments: the x, y and z directional segmentations yielded
3. Unsupervised Classification

38, 8 and 7 partitioned volumetric segments, respectively (shown in Fig. 3.9a, 3.9b and 3.9c).

Figure 3.9: The resulting plane based segmentation of object number 3 in the x (a), y (b) and z (c) directions.

Once analysis was completed in all three directions, directional segmentations were combined by identifying unique sequences of directional labels. Each of the 60 unique sequences obtained for object #3, were assigned a new global label. Bearing in mind that object #3 consisted of only three fibers, the process yielded an over segmented output which required further processing specifically designed for this geometry. Due to the resulting over segmentation, merging and joining of segments motivated additional handling.

Breaking away from the general directional segmentation process in order to focus on fiber reinforced-like materials in general, and high performance concrete studied herein in particular, provided the necessary justification for making several simplifications and assumptions pertaining the geometry in question. The following assumptions were made regarding the objects that were to be identified:

(i) Fibers had a cylindrical like geometry that was simplified as straight lines.

(ii) Fibers had a low width-to-length ratio \(w/l < R_{max}\), reflecting a difference of approximately one order of magnitude \(R_{max} = 0.2\).
(iii) Fibers had a maximal acceptable width $w_{\text{max}}$, where $w_{\text{max}}$ was set as $w_{\text{max}} = 15$ [voxels].

The first stage of merging over segmented objects to fibers included two parts which are illustrated in Fig 3.10. In the first part, after small objects and objects with $w/l$ higher than the predetermined threshold were excluded, geometric characterizations of remaining objects were established. Geometric characteristics included object’s center, axis (start and end points of the axis) and direction vector. In order to determine the latter two (axis and direction vector), Principal Components Analysis (PCA) [102] was employed in conjunction with Orthogonal Regression through the object’s voxels [101], resulting in a line in space (the object’s axis).

Serving as an input for the second part of the first stage, the geometric characteristics were used to identify parallel objects. Pairwise angles between unlabeled and labeled objects were calculated and pairs of objects with $\alpha < \alpha_{\text{max}}$ were categorized as parallel ($\alpha_{\text{max}}$ was set as $\alpha_{\text{max}} = 7.5^\circ$). Pairs of parallel labeled and unlabeled objects, for which the shortest distance between their edge points (axis start and end points) was less than $d_{\text{max}}$, were merged ($d_{\text{max}}$ was set as $d_{\text{max}} = 15$ [voxels], similar to $w_{\text{max}}$).

A secondary classification procedure was executed in the second stage of the merging process (see Fig 3.11). The second stage, similarly to the first one, consisted of two parts. Some of the measures taken in the first stage were repeated, modified or accompanied by new ones. A bounding box was obtained for each unlabeled object, and its edges and shortest-longest edges ratio were examined. Objects with at least one edge longer than $w_{\text{max}}$ or objects with $w_{\text{sort}}/w_{\text{long}} > R_{\text{max}}$ were ignored in the first part. Each unlabeled object was paired with a labeled object and all the pairing combinations were examined as followed:

(i) Three angles between the unlabeled object and the labeled objects were calculated:

(a) Angle between the axes (or direction vectors) of the two objects.

(b) Angle between the axis of the labeled object and the vector connecting the centers of the two objects.

(c) Angle between the axis of the unlabeled object and the vector connecting the centers of the two objects.
(ii) For each object in a pair (denoted as object A), three distances were measured with respect to the axis of its paired object (denoted as object B): start point (object A) - axis (object B), center point (object A) - axis (object B) and end point (object A) - axis (object B). Unlabeled objects of pairs in which all angles were smaller than $\alpha_{\text{max}}$ and all distances were shorter than $d_{\text{max}}$, were merged with their paired labeled object.

This concluded the first part of the second stage of the merging process.

Figure 3.10: Process illustration of the first stage in merging over segmented fibers.

In the second part of the second stage (the final portion of the merging process), each unlabeled voxel was considered separately. All labeled objects, for which the voxel in question was inside their bounding box, were identified, and distances between the voxel and their axes were calculated. The voxel was then assigned the label of the object with the nearest axis. Illustrating for object #3, the input and output of the aforementioned process are presented in Fig. 3.12. Inputting the over segmented result of applying plane based segmentation on object #3 (Fig. 3.12a), produced the desired fiber segmentation output for object #3 (Fig. 3.12b).
3. Unsupervised Classification

Figure 3.11: Secondary classification procedure in merging over segmented fibers.

Figure 3.12: Object #3 prior to the merging procedure (a), and the final separated fibers (b).
4. SERVE

Statistically Equivalent Representative Volume Element

4.1 Introduction

The formulation of a SERVE involved several stages. The first stage was a statistical characterization of the structural parameters of interest. In the second stage, structural elements were generated and embedded in a representative volume element (RVE). Finally, the statistical characteristics of the generated RVE were compared with those of the original material sample to evaluate its statistical equivalency. The statistical characterization stage was implemented on all three materials discussed before, while the other two stages were implemented on the CMC and aggregate reinforced concrete only. The resultant SERVEs were then incorporated in numerical simulations which were later compared with experimental results.

The chapter is organized according to the process described above. Section 4.2 focuses on statistical characterization of structural elements in the material systems. Section 4.3 describes the SERVE generation and discusses the statistical equivalency evaluation in the generated SERVEs. Finally, numerical simulations and experiments are presented and compared in section 4.4.
4.2 Statistical characterization

4.2.1 CMC: Eight harness weave

In order to obtain a more robust collection of data, the small defects (cracks and pores) were grouped together into one data set. This simplification was made as a result of the similar distributions of the geometric parameters in the two groups (see Fig. 4.1). The first step in the statistical analysis was to determine whether there was a dependency between the geometric parameters and to characterize it in case there was one. Covariance matrix and correlation coefficient matrix (denoted as $CCM$) of the data were used to identify correlations between the different parameters. The most significant correlation ($R = 0.689$) was observed between the major axis and the minor axis of the elliptical defects (see Eq. 4.1). Weaker correlations ($R = 0.230$ and $R = 0.214$) were found between the orientation angle and the axes as well. It is worth mentioning that the results presented in this section refer to defects in all three phases: longitudinal tow (LT), transverse tow (TT) and matrix (M). Similar results obtained when the defects were separated to the three phases.

Figure 4.1: Normalized frequencies of $X_c$ (a) and the major axis (b) in cracks (top) and pores (bottom).
4. SERVE: Statistically Equivalent Representative Volume Element

\[
CCM = \begin{pmatrix}
X_c & Y_c & a & b & \theta \\
X_c & 1 & -0.061 & -0.017 & -0.006 & -0.027 \\
Y_c & -0.061 & 1 & 0.037 & -0.033 & 0.015 \\
a & -0.017 & 0.037 & 1 & 0.689 & -0.230 \\
b & -0.006 & -0.033 & 0.689 & 1 & -0.214 \\
\theta & -0.027 & 0.015 & -0.230 & -0.214 & 1 \\
\end{pmatrix}
\] (4.1)

4.2.1.1 Univariate analysis

The probability density functions of all the geometric parameters (dependent and independent) were estimated using a kernel distribution (all parameters were treated as independent at this stage). A kernel distribution is a distribution estimator based on smooth kernel functions [103–106]. The smoothness of the kernel estimator is determined by the smoothing function \(K(\cdot)\), which is a probability density function, and its bandwidth \(h\) (see Eq. 4.2). The kernel estimator uses the sample data to determine the shape of the curve used in the probability density function estimation. Since the kernel distribution is non parametric, it can be used to approximate the distribution of data that does not fit a specific parametric distribution. Instead of using a parametric distribution in the statistical model, based on assumptions - e.g. assuming normal distribution with unknown mean and standard deviation - with the piecewise kernel these assumptions were not needed. The kernel distribution takes the form of Eq. 4.2, where \(n\) is the size of the sample.

\[
f_h(u) = \frac{1}{nh} \sum_{i=1}^{n} K\left(\frac{u - u_i}{h}\right) \tag{4.2}
\]

Various kernel smoothing function can be used for the probability density estimation of the geometric parameters. Here normal, Epanechnikov [107], uniform (box) and triangle probability density functions were compared in order to obtain the best density estimation (see Table 4.1). The kernel bandwidth, which minimizes the asymptotic mean squared error, was determined
based on an optimization formula (Eq. 4.3, where $\sigma$ is the standard deviation of the sample) [106, 108]. The bandwidth optimization formula resulted in very good approximations of the normalized frequencies, except for the orientation angle parameter (Eq. 4.2). This can be explained by the high frequency at the edge of the support range (where $\theta$ was close to $\pi$). The bandwidth for the orientation angle which provided the best kernel approximation was $h = 0.3$.

**Table 4.1: Kernel probability density distributions**

<table>
<thead>
<tr>
<th>Distribution</th>
<th>Kernel Function</th>
</tr>
</thead>
<tbody>
<tr>
<td>Normal</td>
<td>$K(u) = \frac{1}{\sqrt{2\pi}} e^{-\frac{1}{2}u^2}$</td>
</tr>
<tr>
<td>Epanechnikov</td>
<td>$K(u) = \frac{3}{4}(1-u^2), for{</td>
</tr>
<tr>
<td>Box</td>
<td>$K(u) = \frac{1}{2}, for{</td>
</tr>
<tr>
<td>Triangle</td>
<td>$K(u) = (1-</td>
</tr>
</tbody>
</table>

$h = \left(\frac{4}{3n}\right)^{1/5} \sigma$ \hspace{1cm} (4.3)

The nature of the distribution of the geometric parameters, combined with the CCM, led to the following assumption:

(i) The $x$ and $y$ coordinates of the center of a defect were independent and uniformly distributed.

(ii) The distribution of the orientation angle was approximated using a normal kernel smoothing function with a bandwidth of $h = 0.3$.

(iii) The major axis and minor axis of the defects were jointly distributed and had a bivariate normal probability density function.

### 4.2.1.2 Multivariate analysis

Since normal distributions fit the univariate analysis of the major axis and minor axis data, a bivariate normal distribution was used to approximate the joint distribution of these parameters. As a generalization of the univariate normal distribution, the bivariate normal distribution was
parameterized in Eq. 4.4 using the mean vector of the random variables (denoted as $\mu$) and their covariance matrix (denoted as $\Sigma$) [108, 109]. A normalized histogram and the compatible bivariate normal distribution are presented in Fig. 4.2.

$$f(Q, \mu, \Sigma) = \frac{1}{\sqrt{\Sigma(2\pi)^2}} e^{-\frac{1}{2}(Q-\mu)^T \Sigma^{-1}(Q-\mu)}$$ (4.4)

Where $Q$ is the vector or random variables and $\rho$ is the correlation between $a$ and $b$:

$$Q = \begin{pmatrix} a \\ b \end{pmatrix}; \quad \mu = \begin{pmatrix} \mu_a \\ \mu_b \end{pmatrix}; \quad \Sigma = \begin{pmatrix} \sigma_a^2 & \rho \sigma_a \sigma_b \\ \rho \sigma_a \sigma_b & \sigma_b^2 \end{pmatrix}$$

Figure 4.2: Jointly distributed parameters: bivariate histogram (a) and bivariate normal distribution (b) of the major axis and minor axis (axes length in pixels).

### 4.2.2 Aggregate reinforced concrete

The geometric parameters of the aggregates and defects were first tested for statistical dependency. Such dependency was observed in the covariance matrix and correlation coefficients.
matrix (denoted as CCM). Similarly to the results presented in subsection 4.2.1, the most substantial statistical dependency was detected between the ellipsoids axes. For the aggregates, correlations of $R = 0.885$, $R = 0.857$ and $R = 0.9$ were found between the major and middle axes, the major and minor axes and the middle and minor axes respectively (see Eq. 4.5). Similar correlations were found in the ellipsoids represented the defects: $R = 0.932$, $R = 0.892$ and $R = 0.949$ for the major and middle axes, the major and minor axes and the middle and minor axes respectively (see Eq. 4.6 and Figs. 4.3, 4.4). Less significant correlations, ranging from $R = -0.112$ to $R = 0.112$ were observed between the centroid coordinates and the rotation angles.

\[
CCM_{agg} = \begin{pmatrix}
X_c & Y_c & Z_c & a & b & c & \phi & \theta & \psi \\
X_c & 1 & 0.027 & 0.030 & -0.008 & -0.008 & -0.014 & -0.018 & 0.017 & 0.039 \\
Y_c & 0.027 & 1 & -0.008 & -0.038 & -0.063 & -0.074 & 0.018 & -0.017 & 0.037 \\
Z_c & 0.030 & -0.008 & 1 & -0.016 & -0.009 & 0.002 & -0.017 & -0.041 & 0.005 \\
a & -0.008 & -0.038 & -0.016 & 1 & 0.885 & 0.857 & 0.070 & 0.069 & -0.019 \\
b & -0.008 & -0.063 & -0.009 & 0.885 & 1 & 0.900 & 0.040 & 0.064 & -0.020 \\
c & -0.014 & -0.074 & 0.002 & 0.857 & 0.900 & 1 & 0.049 & 0.049 & -0.020 \\
\phi & -0.018 & 0.018 & -0.017 & 0.070 & 0.040 & 0.049 & 1 & 0.112 & -0.009 \\
\theta & 0.017 & -0.017 & -0.041 & 0.069 & 0.064 & 0.049 & 0.112 & 1 & 0.040 \\
\psi & 0.039 & 0.037 & 0.005 & -0.019 & -0.020 & -0.020 & -0.009 & 0.040 & 1
\end{pmatrix} \tag{4.5}
\]

\[
CCM_{def} = \begin{pmatrix}
X_c & Y_c & Z_c & a & b & c & \phi & \theta & \psi \\
X_c & 1 & 0.010 & 0.037 & 0.077 & 0.070 & 0.057 & 0.034 & 0.099 & 0.038 \\
Y_c & 0.010 & 1 & 0.104 & -0.064 & -0.078 & -0.068 & 0.062 & 0.018 & -0.052 \\
Z_c & 0.037 & 0.104 & 1 & -0.031 & -0.048 & -0.044 & 0.009 & 0.014 & 0.047 \\
a & 0.077 & -0.064 & -0.031 & 1 & 0.932 & 0.892 & -0.069 & 0.026 & 0.005 \\
b & 0.070 & -0.078 & -0.048 & 0.932 & 1 & 0.949 & -0.092 & 0.075 & 0.056 \\
c & 0.057 & -0.068 & -0.044 & 0.892 & 0.949 & 1 & -0.112 & 0.051 & 0.037 \\
\phi & 0.034 & 0.062 & 0.009 & -0.069 & -0.092 & -0.112 & 1 & 0.026 & -0.108 \\
\theta & 0.099 & 0.018 & 0.014 & 0.026 & 0.075 & 0.051 & 0.026 & 1 & 0.078 \\
\psi & 0.038 & -0.052 & 0.047 & 0.005 & 0.056 & 0.037 & -0.108 & 0.078 & 1
\end{pmatrix} \tag{4.6}
\]
4. SERVE: Statistically Equivalent Representative Volume Element

Figure 4.3: Scatter plots of the geometric parameters - aggregates.

Figure 4.4: Scatter plots of the geometric parameters - defects.
4.2.2.1 Univariate analysis

Continuous probability distributions considered to characterize the statistical behavior of the parameters (all parameters treated as independent at this stage). In order to find the model that best fits the data set, the following distributions were considered: normal, log-normal, inverse Gaussian, generalized extreme value (GEV) and kernel. Normal and log-normal distributions [110] shown in Eq. 4.7 and Eq. 4.8, where $\mu$ and $\sigma$ are mean and standard deviation respectively.

\[
f(u) = \frac{1}{\sigma \sqrt{2\pi}} \exp \left\{ -\frac{(u - \mu)^2}{2\sigma^2} \right\} \tag{4.7}
\]

\[
f(u) = \frac{1}{u \sigma \sqrt{2\pi}} \exp \left\{ -\frac{(\ln u - \mu)^2}{2\sigma^2} \right\} \tag{4.8}
\]

The inverse Gaussian distribution [111], used in modeling time distribution for Brownian motion, can also be used in modeling nonnegative data which skews from the Gaussian distribution. The inverse Gaussian distribution takes the form of Eq. 4.9, where $\mu$ is the mean and $\lambda$ is the shape parameter - for $\lambda \to \infty$, the inverse Gaussian takes the form of the normal Gaussian distribution.

\[
f(u) = \sqrt{\frac{\lambda}{2\pi u^3}} \exp \left\{ -\frac{\lambda}{2\mu^2 u} (u - \mu)^2 \right\} \tag{4.9}
\]

When examining the tail properties of a statistical distribution the extreme value theory is a useful tool, particularly for evaluating the probability of extreme events occurrence [112]. The generalized extreme value distribution (see Eq. 4.10) integrates the Gumbel, Fréchet and Weibull distributions into a combined formulation. Applying the combined formulation results in one of three cases, each relates to one of the three base distributions, that best characterizes the data set.

\[
f(u) = \begin{cases} 
\frac{1}{\sigma} \exp \left\{ - \left[ 1 + k \frac{(u - \mu)}{\sigma} \right]^{-\frac{1}{k}} \right\} \left\{ 1 + k \frac{(u - \mu)}{\sigma} \right\}^{-1 - \frac{1}{k}}, & \text{for } 1 + k \frac{(u - \mu)}{\sigma} > 0 \\
\frac{1}{\sigma} \exp \left\{ - \exp \left[ -\frac{(u - \mu)}{\sigma} - \frac{(u - \mu)}{\sigma} \right] \right\}, & \text{for } k = 0
\end{cases} \tag{4.10}
\]
A kernel distribution estimator [103–106], combined with a normal probability density function as the smoothing function, was used to generate a non parametric distribution (see Eq. 4.11 and Eq. 4.12). The generated non parametric distribution approximated the distribution of the data set (the process was similar to that detailed in subsection 4.2.1).

\[ f_h(u) = \frac{1}{nh} \sum_{i=1}^{n} K \left( \frac{u - u_i}{h} \right) \]  

(4.11)

\[ K(u) = \frac{1}{\sqrt{2\pi}} \exp \left\{ -\frac{1}{2} u^2 \right\} \]  

(4.12)

The fitted distributions of the geometric parameters are shown in Figs. 4.5 and 4.6. Since the rotation angles included negative values, the inverse Gaussian and the log-normal models were not fitted for these parameters. Based on the CCM and the fit of the suggested distributions, the following assumptions were made:

(i) The x, y and z coordinates of the center of the ellipsoidal objects (aggregates and defects) were considered as independent and uniformly distributed.

(ii) The rotation angles of the ellipsoidal objects were independent and their distribution was approximated using a kernel distribution estimator combined with normal kernel smoothing function.

(iii) The major middle and minor axes of the ellipsoidal objects were jointly distributed and had a trivariate distribution, which is explored and characterized in the following section.

4.2.2.2 Multivariate analysis

Of the five statistical models that were used in the univariate analysis, the models that resulted in the best fit for the major axis, middle axis and minor axis were the log-normal distribution, the generalized extreme value distribution and the inverse Gaussian distribution. The assumption according to which the three axes of the ellipsoidal objects were jointly distributed was expanded
4. SERVE: Statistically Equivalent Representative Volume Element

by characterizing the trivariate distribution of the ellipsoidal axes, as a log-normal trivariate probability density function. The bivariate analysis presented in section 4.2.1 was extended to a trivariate analysis by extending the two parameters formulation to three parameters (see Eq. 4.13 and Eq. 4.14).

The major axis, middle axis and minor axis (denoted as \(a\), \(b\) and \(c\)) are converted to their logarithmic form: \(a_L = \ln(a)\), \(b_L = \ln(b)\) and \(c_L = \ln(c)\). Converting the variables to their logarithmic form simplifies the statistical analysis since the log-normal trivariate
4. SERVE: Statistically Equivalent Representative Volume Element

Figure 4.6: Normalized frequencies and fitted distribution for the geometric parameters of the ellipsoidal defects: $X_C$ (a), $Y_C$ (b), $Z_C$ (c), $a$ (d), $b$ (e), $c$ (f), $\phi$ (g), $\theta$ (h), $\psi$ (i).

distribution of $a$, $b$ and $c$ becomes the normal trivariate distribution of $a_L$, $b_L$ and $c_L$.

$$f(Q, \mu, \Sigma) = \frac{1}{\sqrt{\Sigma(2\pi)^3}} \exp \left\{ -\frac{1}{2} (Q - \mu)^T \Sigma^{-1} (Q - \mu) \right\}$$  \hspace{1cm} (4.13)

Where $Q$ is the vector or random variables, $\mu$ is the mean vector, $\Sigma$ is the covariance matrix and $\rho_{ij}$ is the correlation between the logarithm of the major axis, middle axis and minor axis.
(denoted as $a_L$, $b_L$ and $c_L$):

$$
Q = \begin{pmatrix}
    a_L \\
    b_L \\
    c_L 
\end{pmatrix} ;
\mu = \begin{pmatrix}
    \mu_{aL} \\
    \mu_{bL} \\
    \mu_{cL} 
\end{pmatrix} ;
\Sigma = \begin{pmatrix}
    \sigma_{aL}^2 & \rho_{aLbL} \sigma_{aL} \sigma_{bL} & \rho_{ac} \sigma_{aL} \sigma_{cL} \\
    \rho_{aLbL} \sigma_{aL} \sigma_{bL} & \sigma_{bL}^2 & \rho_{bc} \sigma_{bL} \sigma_{cL} \\
    \rho_{ac} \sigma_{aL} \sigma_{cL} & \rho_{bc} \sigma_{bL} \sigma_{cL} & \sigma_{cL}^2
\end{pmatrix} (4.14)
$$

The first stage of the multivariate analysis of the major axis, middle axis and minor axis, included a bivariate characterization of the distribution of these parameters. Since normal and log-normal distributions approximated the axes univariate distributions quite well, their bivariate forms were selected to model the bivariate behavior of pairs of ellipsoids axes for both aggregates and defects. Bivariate normal probability density functions, with the same means and covariances as the original data, were generated. In a similar way, bivariate log-normal probability density functions were generated using the means and covariances of the original data (in its logarithmic form).

Normal probability density functions and their compatible bivariate histograms, for the pairs of ellipsoids axes in aggregates, are shown Fig. 4.7 and an equivalent illustration of the log-normal form is presented in Fig. 4.8. For defects, an identical illustration of the normal and log-normal probability density functions and their compatible histograms, for the pairs of ellipsoids axes, are displayed in Figs. 4.9 and 4.10 respectively.

A comparison between the bivariate normal and log-normal models revealed that the log-normal models captured the bivariate behaviors of the original data more accurately and provided better approximations to the original data (for both aggregates and defects).

In the second stage of the multivariate analysis, trivariate analysis followed the bivariate one in characterizing the statistical behavior and dependencies between the three ellipsoidal axes for aggregates and defects. Probability densities of the original data, based on frequency of observations, were compared with trivariate probability density functions with the same means.
Figure 4.7: Bivariate normal probability density functions with the same mean and covariance as the original data (a), (b) and (c). Bivariate histograms for the pairs of the aggregates axes (d), (e) and (f).

Figure 4.8: Bivariate histograms for the pairs of the logarithmic form of the aggregates axes (a), (b) and (c). Bivariate normal probability density functions with the same mean and covariance as the logarithmic form of the original data (d), (e) and (f).
Figure 4.9: Bivariate normal probability density functions with the same mean and covariance as the original data (a), (b) and (c). Bivariate histograms for the pairs of the defects axes (d), (e) and (f).

Figure 4.10: Bivariate histograms for the pairs of the logarithmic form of the defects axes (a), (b) and (c). Bivariate normal probability density functions with the same mean and covariance as the logarithmic form of the original data (d), (e) and (f).

and covariances as the original data. Theses are illustrated in Figs. 4.11 and 4.12 for the aggregates and defects respectively.
For the three ellipsoidal axes of the aggregates, frequency based trivariate density (Fig. 4.11a) and trivariate normal probability density function (Fig. 4.11b), were compared with frequency based trivariate density of the logarithmic form of the data (Fig. 4.11c) and trivariate log-normal probability density (Fig. 4.11d). The same process was applied for the defects data, where frequency based trivariate density (Fig. 4.12a) and trivariate normal probability density function (Fig. 4.12b) were compared with the frequency trivariate density function of the logarithmic form of the data (Fig. 4.12c) and trivariate log-normal probability density function (Fig. 4.12d). The trivariate analysis provided insights that were consistent with those provided by the bivariate analysis. The log-normal model was able to capture the statistical behavior of the ellipsoidal axes much better than the normal model.
Figure 4.11: Aggregates: Trivariate density (a) and normal probability density (b). Trivariate density of the logarithmic form (c) and log-normal probability density (d).

Figure 4.12: Defects: Trivariate density (a) and normal probability density (b). Trivariate density of the logarithmic form (c) and log-normal probability density (d).
4.2.3 Fiber reinforced concrete

A process similar to those presented in 4.2.1 and in 4.2.2 was used for statistical characterization of the fiber reinforced concrete sample. The matrix consistency and uniform fiber length led to the assumption according to which the randomness in the fiber reinforced concrete was a result of the random nature of fibers orientation. Therefore, in order to characterize the statistical properties of the material system at hand, the statistical behavior of the fibers orientation had to be captured first. An illustration of the identified fibers is presented in Fig 4.13. The direction cosines and their respective angles with the axes are depicted in Fig. 4.14. The direction cosines were considered for the fibers orientation analysis, where $\alpha = \cos(a)$, $\beta = \cos(b)$ and $\gamma = \cos(c)$.

The statistical analysis indicated that center coordinates were independent and uniformly distributed. A moderate correlation existed between the direction cosines (see Fig. 4.15 and Eq. 4.15). $\alpha$ and $\beta$ (the x and y direction cosines respectively) appeared to be independent of each other with a normal-like distribution, however both of them were correlated with $\gamma$ (the z direction cosine). The $\alpha - \gamma$ and the $\beta - \gamma$ correlation were $R_{\alpha-\gamma} = 0.469$ and $R_{\beta-\gamma} = -0.361$ respectively. The bivariate histograms in Fig. 4.16 and Fig. 4.17 illustrate the dependencies between the direction cosines (and therefore the orientation angles).
4. SERVE: Statistically Equivalent Representative Volume Element

Figure 4.15: Scatter plots of the geometric parameters - fibers.

\[
CCM = \begin{bmatrix}
X_c & Y_c & Z_c & \alpha & \beta & \gamma \\
X_c & 1 & -0.015 & 0.031 & -0.102 & -0.169 & 0.079 \\
Y_c & -0.015 & 1 & -0.008 & 0.110 & -0.117 & -0.072 \\
Z_c & 0.031 & -0.008 & 1 & 0.013 & -0.106 & 0.051 \\
\alpha & -0.102 & 0.110 & 0.013 & 1 & 0.011 & -0.469 \\
\beta & -0.169 & -0.177 & -0.106 & 0.011 & 1 & -0.361 \\
\gamma & 0.079 & -0.072 & 0.051 & -0.496 & 0.361 & 1
\end{bmatrix}
\] (4.15)
4. SERVE: Statistically Equivalent Representative Volume Element

Figure 4.16: Direction cosines scatters and their marginal histograms.

Figure 4.17: Bivariate histograms for pairs of direction cosines in the x-y (a), x-z (a) and y-z (a) directions.

The direction analysis indicated that fiber had a preferred orientation in the z direction (see Fig. 4.18). The x and y direction cosines had moderate negative correlations to the z direction cosine ($R = -0.469$ and $R = -0.361$ respectively). A preliminary analysis of the z direction cosines indicated that the generalized extreme value distribution or a non-parametric distribution would provide a good fit to the data. This will be further analyzed in the near future. Furthermore the x and y direction cosines which were independent and not correlated ($R = 0.01$) to each other. The normal-like distributions of the x and y direction cosine (Fig. 4.17) was attributed to the size of the data set ($\sim 31,500$ fibers).
4. SERVE: Statistically Equivalent Representative Volume Element

4.3 Generating Statistically equivalent RVE

4.3.1 CMC: Eight harness weave

4.3.1.1 Defect-free representative volume element

A defect-free representative volume element (DFRVE) of an eight-harness weave, was the base for the generated SERVE model. This model was based on a single lamina of the material system discussed in [57, 59]. After the geometry of the model was imported into MATLAB™, three binary 3D masks were created for the longitudinal tows, transverse tows and matrix (Fig. 4.19).

4.3.1.2 Embedding defects in the defects free RVE

Three dimensional ellipsoids were introduced to the defect-free model using a Monte-Carlo simulation. The justification for generating 3D defects based on data from 2D material samples,
was provided by the material symmetry. Assuming that there was a symmetry between the longitudinal and transverse directions (regarding the geometry of the defects), it was possible to make an educated assumption about the third dimension. It is important to point out that the use of the material symmetry required a separate statistical analysis for the longitudinal tows, transverse tows and matrix.

A Monte-Carlo simulation for introducing the ellipsoidal defects to the DFRVE was performed in several stages. First, defects were added to the longitudinal tows in the following way:

(i) Centroid coordinates - the \(x\), \(y\) and \(z\) coordinates of a centroid \((X_c, Y_c \text{ and } Z_c)\) were generated separately from a uniform distribution of the possible coordinates inside the LT phase.

(ii) Ellipsoid axes - the first and second ellipsoid axes \((a \text{ and } b)\) were generated from the bivariate normal distribution of the LT - \(f_{LT}^{ab}(a, b)\) (see subsection 4.2.1); the third ellipsoid axis \((c)\) was then generated from the conditional TT bivariate normal distribution, using the generated second axis as an input - \(f_{TT}^{cb}(c|b)\).

(iii) Rotation angles - the first and second rotation angles \((\theta \text{ and } \phi)\) were generated from the kernel distribution of the TT and the LT orientation angle respectively; the third angle \((\psi)\) was assumed to have the same distribution as the TT orientation angle and was generated accordingly.
After all nine geometric parameters were obtained the ellipsoid was either rejected or added to longitudinal phase based on the following criteria:

(i) The first, second and third axes were in a decreasing order (i.e. $c < b < a$).
(ii) The entire ellipsoid had to be inside the longitudinal phase region.
(iii) The ellipsoid did not overlap or had contact with any of the existing ellipsoids.

The first stage was completed once the volume fraction of the defects reached the same volume fraction found in the original material samples ($VF = 0.03$). In the second stage, defects were added to the transverse tows in the same way they were added to the longitudinal tows. This was done based on the observed symmetry of the material in the longitudinal and transverse direction. A similar process was used for the third stage, in which defects were added to the matrix phase. However since the material symmetry did not apply for the matrix phase several modifications were made:

(i) Ellipsoid axes - the first and second ellipsoid axes ($a$ and $b$) were generated from the bivariate normal distribution of the $M$; the third ellipsoid axis ($c$) was then generated from uniform distribution, ranging between zero to $b$.
(ii) Rotation angles - all three rotation angles were generated from the kernel distribution of the $M$.

4.3.1.3 Generated defects structure

Cross sections of the model with the embedded defects are shown in Fig. 4.20. In order to evaluate the statistical equivalency between the generated model and the original material specimen, the geometric parameters of the generated defects were gathered and their statistical characteristics were analyzed. When the CCM of the nine geometric parameters of the generated ellipsoids (Eq. 4.16) was compared with the CCM of the five geometric parameters of the approximated ellipses from the 2D micrographs (Eq. 4.1), a similar set of dependencies was observed. The correlation between the major axis and the middle axis was the most significant one ($R = 0.624$). This correlation was also very close to that between the major axis and minor
axis in the 2D ellipses \((R = 0.689)\). As expected, the correlation between the middle axis and the minor axis was significant as well \((R = 0.585)\). A less powerful correlation was found between the major axis and minor axis \((R = 0.385)\). This could be explained by the indirect relation between the major axis and minor axis, through the middle axis. Furthermore, based on the assumptions made for the defects generation process, inconsequential correlations (less than \(R = 0.04\)) were observed between the other six parameters (centroid coordinates and rotation angles).

\[
CCM = \begin{pmatrix}
X_c & Y_c & Z_c & a & b & c & \theta & \phi & \psi \\
X_c & 1 & 0.012 & 0.008 & 0.006 & 0.005 & 0.002 & -0.009 & 0.012 & -0.011 \\
Y_c & 0.012 & 1 & -0.016 & -0.004 & -0.012 & -0.005 & -0.007 & 0.008 & 0 \\
Z_c & 0.008 & -0.016 & 1 & 0.014 & 0.015 & 0.010 & 0.008 & -0.014 & 0.002 \\
a & 0.006 & -0.004 & 0.014 & 1 & 0.624 & 0.385 & 0.007 & 0.037 & 0.003 \\
b & 0.005 & -0.012 & 0.015 & 0.624 & 1 & 0.585 & 0.020 & 0.018 & 0.007 \\
c & 0.002 & -0.005 & 0.010 & 0.385 & 0.585 & 1 & 0.027 & 0.025 & 0.022 \\
\theta & -0.009 & -0.007 & 0.008 & 0.007 & 0.020 & 0.027 & 1 & 0.018 & -0.001 \\
\phi & 0.012 & 0.008 & -0.014 & 0.037 & 0.018 & 0.025 & 0.018 & 1 & -0.006 \\
\psi & -0.011 & 0 & 0.002 & 0.003 & 0.007 & 0.022 & -0.001 & -0.006 & 1 \\
\end{pmatrix}
\]

Histograms of the normalized frequencies of the centroid coordinates of the defects in the \(x\) and \(y\) directions are shown in Fig. 4.21. Despite the differences in the ranges of the centroid coordinates in \(x\) and \(y\) directions between the defects in the micrographs (Fig. 4.21a and Fig. 4.21b) and the generated defects (Fig. 4.21c and Fig. 4.21d), which were a result of the differences between the dimensions of the micrographs and the dimensions of the model, there were similarities between the distributions of the geometric parameters of the generated defects and the defects in the micrographs. The generated \(X_c\) and \(Y_c\) coordinates were uniformly distributed over the possible range of coordinates. The agreement between the distribution of the orientation angle of the defects in the micrographs and the first orientation angle of the generated defects can be seen in Fig. 4.22. Since the Monte-Carlo simulation for generating the orientation angle was based on the smoothed kernel approximation, the generated orientation angle
(Fig, 4.22b) had a smoother distribution than that of the original orientation angle (Fig. 4.22a). Finally, the approximated bivariate normal distribution of the major axis and minor axis of the 2D ellipse (from the original material samples), was compared with the normalized bivariate histogram of the first two axes of the generated 3D ellipsoid (major axis and middle axis). This was done since the major axis and middle axis are in the 3D ellipsoids were the equivalent parameters of the major and minor axis in the 2D ellipses (Fig. 4.23).

![Five sequential cross sections of the model with defects in the longitudinal tows, transverse tows and matrix (orange, yellow and green respectively).](image)

Figure 4.20: Five sequential cross sections of the model with defects in the longitudinal tows, transverse tows and matrix (orange, yellow and green respectively).

4.3.2 Aggregate reinforced concrete

4.3.2.1 Generating volume element

A simple cube shaped representative volume element was the base for the generated models of the aggregate reinforced concrete. The 3D cubic geometry (measuring 45x45x45 in pixels) was constructed as a 3D array in MATLAB™. Aggregates and defects, simplified as ellipsoids, were introduced to the representative volume element using a Monte-Carlo simulation which included several steps. First ellipsoidal aggregates were added to the model in the following way:

(i) Centroid coordinates - $X_c$, $Y_c$ and $Z_c$ were separately generated from uniform distributions (within the limits of the cubic model - ranging from 0 to 45).

(ii) Ellipsoid axes - $a_L$, $b_L$ and $c_L$ were randomly generated from a trivariate normal distribution
Figure 4.21: Normalized frequencies of the centroid coordinates of the defects in the micrographs (top) and the generated defects (bottom).

and then converted back from the logarithmic form to their conventional form: \( a = \exp(a_L) \), \( b = \exp(b_L) \) and \( c = \exp(c_L) \).

(iii) Rotation angles - \( \phi \), \( \theta \) and \( \psi \) were generated from the compatible kernel distribution.

Once all nine geometric parameters of an ellipsoidal aggregate were generated, the ellipsoid was constructed and embedded in the representative volume element. An ellipsoidal aggregate which did not meet the following criteria was rejected:

(i) Major axis, middle axis and minor axis were in a decreasing order (i.e. \( a > b > c \)).

(ii) Major axis, middle axis and minor axis were within the determined range (see Table 4.2).

(iii) The entire ellipsoid was inside the volume element.
(iv) There was no overlapping or contact between the generated ellipsoid and any of the existing ellipsoids in the volume element.

Ellipsoidal aggregates were added to the unit cell until their volume fraction reached 11% (the same volume fraction as that of the original concrete sample).

After the ellipsoidal aggregates were embedded in the representative volume element, a similar
process was employed for embedding ellipsoidal defects in the representative volume element. For each ellipsoidal defect nine geometric parameters were also randomly generated from their respective trivariate and univariate probability distributions. Each ellipsoidal defect had to meet the criteria described above. Once the ellipsoidal defects volume fraction in the representative volume element reached the volume fraction of the defects in the original sample - 0.37%, no more ellipsoidal defects were added and a representative volume element model was complete.

Table 4.2: Major axis, middle axis and minor axis ranges (pixels).

<table>
<thead>
<tr>
<th></th>
<th>Major axis</th>
<th>Middle axis</th>
<th>Minor axis</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Max</td>
<td>Min</td>
<td>Max</td>
</tr>
<tr>
<td>Aggregates</td>
<td>20</td>
<td>2</td>
<td>10</td>
</tr>
<tr>
<td>Defects</td>
<td>10</td>
<td>1</td>
<td>6</td>
</tr>
</tbody>
</table>

4.3.2.2 From a representative volume element to a finite element model

The process described above resulted in two sets of geometric parameters for ellipsoidal aggregates and defects. In order to generate a CAD model and later a finite element model of RVE further steps were taken. A Gmsh© script was written to create the CAD geometry of the representative volume element [42, 113]. For each ellipsoidal object (aggregates and defects) the script included its vertices, curves and surfaces which formed together the ellipsoid’s volume. Six vertices of the ellipsoid were computed, and used to construct 12 curves that framed the ellipsoid. Groups of 3 curves, closing a loop, formed a section of the ellipsoid surface ($\frac{1}{8}$ of the outer surface). Eight connected surfaces framed created a closed outer surface of the ellipsoid, that framed its volume. After all ellipsoidal objects were generated, the representative volume element was completed by bounding them using periodic surfaces.

The second step included generating a periodic mesh for the representative volume element. Since the RVE was designed for homogenization of the fine-scale structure of a unit cell, the
model was assumed to be locally periodic [7]. Geometry Gmsh© file was used as an input for Gmsh© meshing. Surface periodicity was imposed on the outer surfaces of the volume element. Each surface in pairs of parallel surfaces was defined as either a master surface or a slave surface. Periodic surfaces constraint in the geometric model resulted in periodic mesh of the representative volume element. The mesh was then converted from a Gmsh© file an ABAQUS input file (see Fig. 4.24). Four nodes first order tetrahedron elements were used for the finite element models in ABAQUS, mostly due to the intricate geometry and to the Gmsh© - ABAQUS interaction. Elements who reached their maximal load (determined in the different phased based on experimental data) stopped carrying loads and contributed to the damage evolution. Maximal load was defined as the averaged maximal principal stress in the element.

![Figure 4.24: FE model of a concrete RVE. (a) cement, (b) aggregates, (c) embedded aggregates.](image)

### 4.3.2.3 Multiple RVEs

The process described above generated only a single realization of the RVE. In order to obtain the effective material properties of a material system, a large ensemble of realizations of the representative volume elements have been considered. By repeating the process, a total of 1000 Monte-Carlo simulations were performed for generating 1000 realizations of a representative volume element. Number of elements in the RVE realizations ranged between 23071 to 93823, with an average of 38545 elements.
4.3.2.4 Generated concrete samples

Each of the 1000 aggregate reinforced concrete models contained between 83 to 287 aggregates (133 on average) and between 11 to 32 defects (19 on average). Frequencies of the number of objects (aggregates and defects) in the 1000 models are shown in Fig. 4.25. The geometric parameters of the generated aggregates and defects were grouped in order to evaluate the statistical equivalency between the generated and original aggregates and defects.

Similarity between the univariate distributions of the generated and original geometric parameters was observed in the probability histograms (see Fig. 4.26). The coordinates of the ellipsoids centers in the generated and original ellipsoids also demonstrated similarity in their statistical behavior, however they were omitted due to the different support ranges.

![Figure 4.25](image)

Figure 4.25: Number of generated aggregates (a) and defects (b) in the concrete models.

Comparing the CCM of the major axis, middle axis and minor axis of the generated (denoted as Gen.) ellipsoidal aggregates and defects with the CCM of the original (denoted as Or.) geometric parameters (Eq. 4.17 and 4.18 respectively) shows very good agreement between the correlation coefficients of these parameters. The correlations between the couples of axes (major-middle, major-minor and middle minor) were the most significant ones, indicating that the
Figure 4.26: Univariate histograms of the original and generated geometric parameters of aggregates: (a) \(a\), (b) \(b\), (c) \(c\), (d) \(\phi\), (e) \(\theta\), (f) \(\psi\).

generated ellipsoids were statistically equivalent to those which approximated the aggregates and defects in the physical material sample \(R_{\text{Agg}}^{ab} = 0.862, R_{\text{Agg}}^{ac} = 0.739\) and \(R_{\text{Agg}}^{bc} = 0.843\) for the aggregates and \(R_{\text{Def}}^{ab} = 0.803, R_{\text{Def}}^{ac} = 0.789\) and \(R_{\text{Def}}^{bc} = 0.914\) for the defects respectively.

Insignificant correlations ranging between \(R = 0.005\) to \(R = -0.006\) and between \(R = 0.016\) to \(R = -0.019\) were found between the rest of the generated geometric parameters for the aggregates and defects respectively.

\[
\begin{align*}
\text{CCM}^{\text{Gen.}}_{\text{Agg}} &= \begin{pmatrix} a & b & c \\ a & 1 & 0.862 & 0.739 \\ b & 0.862 & 1 & 0.843 \\ c & 0.739 & 0.843 & 1 \end{pmatrix}, \\
\text{CCM}^{\text{Or.}}_{\text{Agg}} &= \begin{pmatrix} a & b & c \\ a & 1 & 0.885 & 0.857 \\ b & 0.885 & 1 & 0.900 \\ c & 0.857 & 0.900 & 1 \end{pmatrix} \quad (4.17)
\end{align*}
\]
4. SERVE: Statistically Equivalent Representative Volume Element

\[
CCM_{\text{Gen.}}^{\text{Def.}} = \begin{pmatrix}
    a & b & c \\
    a & 1 & 0.803 & 0.789 \\
    b & 0.803 & 1 & 0.914 \\
    c & 0.789 & 0.914 & 1
\end{pmatrix}; \quad CCM_{\text{Or.}}^{\text{Def.}} = \begin{pmatrix}
    a & b & c \\
    a & 1 & 0.932 & 0.892 \\
    b & 0.932 & 1 & 0.949 \\
    c & 0.802 & 0.949 & 1
\end{pmatrix}
\] (4.18)

The trivariate behavior of the axes of the generated ellipsoids was examined in comparison to that of the original ellipsoids (for both aggregates and defects). This was done by comparing the trivariate probabilities of the axes (in the logarithmic form). For the aggregates, the trivariate probability of the original data, in its logarithmic form (Fig. 4.27a), was compared with the trivariate probability of the generated data, in its logarithmic form (Fig. 4.27b). For the defects, the trivariate probability of the original data, in its logarithmic form (Fig. 4.28a), was compared with the trivariate probability of the generated data, in its logarithmic form (Fig. 4.28b).

Considering the aggregates - the evident similarity between the trivariate probabilities of the original and generated data can be observed in Fig. 4.27. As for the defects, although the CCM for the geometric parameters of the generated ellipsoidal defects was in agreement with that of the original ellipsoidal defects, their trivariate probabilities behaved slightly different (see Fig. 4.28). This can be attributed to several factors, the first is the relatively low number of registered defects - 320 defects versus 648 aggregates. The small number of defects in the generated models provides another explanation for the differences in the statistical behaviors of the original and generated data. Generated models contained an average of 133.11 aggregates and 19.38 defects, limiting the statistical equivalency of the defects in the generated RVEs.
4. SERVE: Statistically Equivalent Representative Volume Element

Figure 4.27: Trivariate probabilities of axes for the original (a) and generated (b) aggregates.

Figure 4.28: Trivariate probabilities of axes for the original (a) and generated (b) defects.
4.3 SERVE: Statistically Equivalent Representative Volume Element

4.4 Simulation and experiments

4.4.1 CMC: Eight harness weave

4.4.1.1 Finite element models

Elements in the 8HW DFRVEs were categorized as tow or matrix according to their location (Fig. 4.29). Phases were assumed to be isotropic and non-linear behavior was modeled using a bilinear damage model [114] (Fig. 4.30). The constitutive model was implemented using a user material subroutine (UMAT). Another FE model with the generated defects was created. Defects were embedded in the defect free model by deleting elements which were labeled as defects. Displacement boundary conditions and quasi-static displacement controlled load were applied to the models.

4.4.1.2 Finite element simulations results

Experimental results of uniaxial mechanical testing performed on specimens of the material of interest were available for this study [115]. Experimental procedures were similar to those detailed in [60]. The material and FE model parameters of the defect free configuration were calibrated based on the experimental results and were then used for the configuration with defects. The resulted stress-strain curves are shown in Fig. 4.31. Homogenized elastic modulus and strength were calculated for the defect free and for the defected models (Table 4.3). The elastic modulus was reduce by 4.74% in the defected model. A 7.87% reduction in strength was observed in the defected model with respect to the defect free model.

The two models resulted in different element damage evolution processes. The matrix and weave damage evolution are illustrated in Figure 4.32 and Figure 4.33 respectively. Damage initiation at a lower load was observed in the defected model. Furthermore the damage in the defected model begins near the structural defects while in the defect free model damage begins
near the constrained edges. The observed damage evolution processes in the two models, although different in magnitude, are similar in their progress and damage patterns.
4.4.2 Aggregate reinforced concrete

4.4.2.1 Material properties assignment

Mechanical testings results of the aggregate reinforced concrete were available for this study, thanks to the Moyeda Construction Company [63]. These results provided the base for assigning material properties for the aggregates and mortar phases in the FE model. 3 cement samples, 3 limestone samples and 2 concrete samples were tested in compression until failure (see Fig. 4.34d and Table 4.4). Limestone sample number 3 displayed a non-physical mechanical response that was attributed to experimental errors and was excluded from the analysis.
Figure 4.31: Experimental and FE results.

Table 4.4: Limestone, cement and concrete samples.

<table>
<thead>
<tr>
<th>Material</th>
<th>Number of Samples</th>
<th>Samples Age [Days]</th>
<th>Sample Area ([cm^2])</th>
</tr>
</thead>
<tbody>
<tr>
<td>Limestone</td>
<td>3</td>
<td>6</td>
<td>72.42</td>
</tr>
<tr>
<td>Cement</td>
<td>3</td>
<td>6</td>
<td>78.54</td>
</tr>
<tr>
<td>Concrete</td>
<td>2</td>
<td>6</td>
<td>78.54</td>
</tr>
</tbody>
</table>

The limestone samples displayed brittle material behavior and therefore linear elastic material properties were assigned to the aggregates in the FE model. The ductile plastic characteristics of the cement’s mechanical response, were modeled by the modified Gurson yield criterion \([116, 117]\). Although the modified Gurson yield criterion is mostly used to model metal plasticity, it has been previously used to model inelastic behavior of concrete \([118, 119]\). Assigned material properties of the phases are shown in Table 4.5.
Figure 4.32: Damage evolution in the defect free (left) and the defected models (right).
Figure 4.33: Damage evolution (tows) in the defect free (left) and the defected models (right).
4. SERVE: Statistically Equivalent Representative Volume Element

![Graphs showing load-displacement and stress-strain curves for different samples](image)

Figure 4.34: Load-displacement experimental results for cement (a), limestone (b) and concrete (c) samples and averaged results (d).

Table 4.5: Limestone and cement material properties assignment.

<table>
<thead>
<tr>
<th>Material Behavior</th>
<th>Modulus of Elasticity [GPa]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Limestone</td>
<td>Linear Elastic 61.3</td>
</tr>
<tr>
<td>Cement</td>
<td>Elastic-Plastic (Gurson) 29.5</td>
</tr>
</tbody>
</table>

4.4.2.2 Loading and boundary conditions

The 45x45x45 cubic representative volume element was constrained using symmetric boundary conditions on the $x - y$, $y - z$ and $x - z$ planes. Negative prescribed displacement in the $x$ direction was applied on the right $y - z$ plane to provide compressive loading similar to that applied during
the experiments (see Fig. 4.35). These loading and boundary conditions were applied to each of
the 1000 realizations of the representative volume element.

![Symmetric Boundary Constraint](image)

![Displacement Controlled Loading](image)

Figure 4.35: Boundary conditions and loading in the FE simulations.

### 4.4.3 Finite element simulations results

Each of the 1000 models provided different mechanical response. The stress-strain response
values of the models, though different, varied within a very small range with a maximal difference
of 2.3%. The range of variation of the stresses in the different models are illustrated in Fig. 4.36,
which also depicts the stress distribution and variation at three strain sample points.

The mechanical responses of the generated models were compared with experimental results
from uniaxial compression test in Fig. 4.37. The generated models were able to capture very well
the non linear behavior of the tested concrete samples. Moreover, for each model the maximal axial
stress (in the loading direction) was calculated and analyzed. The ensemble of the maximal stresses
produced a mean maximal stress of $\sigma_{\text{mean}}^{\max} = 381\,[\text{MPa}]$. The ensemble’s most frequent value (the
ensemble’s mode) was slightly higher than it’s mean - $\sigma_{\text{mode}}^{\max} = 390\,[\text{MPa}]$ (see Fig. 4.38). When
compared with the experimental maximal stress, the mean and mode of the stresses ensemble were
only 1.8% and 4.2% different from the latter, respectively.
Figure 4.36: Mechanical response variation in the generated models and stress distributions.
4. SERVE: Statistically Equivalent Representative Volume Element

Figure 4.37: Mechanical response of the generated models vs. mechanical testing results.

Figure 4.38: Maximal stress distribution.
5. Summary & Conclusions

The primary goal of the work presented in this monograph was to study the effects of random phenomena and stochastic processes on the mechanical behavior of composite material systems and to confront the difficulty of incorporating those effects in multi-scale structural modeling. A secondary goal in area of machine vision and learning had emerged from the efforts towards achieving the primary goal. Structural characterization of fiber reinforced concrete required the separation, identification and classification of connected objects in 3D.

A framework for a reliable prediction of mechanical behavior of material systems with random structural attributes was developed. The suggested frameworks is based on generating a representative volume element which integrates significant random attributes in a way that yields equivalency between the representative volume element and the modeled material system, an equivalency in the statistical sense. The framework can be divided to 3 central phases: image processing and analysis, statistical characterization and finally generating a statistically equivalent representative volume element (SERVE).

Three material systems, which represented three families of composite materials, were considered in developing the framework: ceramic matrix composite, Sic/SiNC (S-200H), aggregate reinforced concrete and high performances fiber reinforced concrete. Structural imaging of the material systems were processed and analyzed in order to register structural
5. Summary & Conclusions

elements which contributed to micro-structural and meso-structural randomness. Defects and their geometry were identified as the random elements in the ceramic matrix composite (CMC), while aggregates and defects were selected for in the aggregate reinforced concrete. Attention was focused on fibers orientation in the fiber reinforced concrete as result of its characteristics.

Two-dimensional micrographs of the CMC were used for characterizing the statistical behavior of micro-scale material discontinuities. The 2D micrographs provided most of the necessary geometric information, however 3D images would have resulted in a full 3D reconstruction of the material system and a complete geometric characterization of the discrete defects. The information gap regarding the 3D geometry was bridged using the material symmetry and complimentary assumptions.

The analysis of defects, showed negligible correlations between the geometric parameters of the ellipses approximation, except between the ellipse axes. A univariate analysis of the independent parameters and a bivariate analysis of the dependent parameters provided a non-parametric approximation of the distributions of the parameters. Volumetric defects were generated and embedded in a defect free model using a Monte-Carlo simulation based on the inferred statistical properties. The resulting model was analyzed and the statistical properties of the generated defects were compared with those of the defects in the original material samples.

CT images were available for the aggregate reinforced concrete material system, which enabled a full 3D reconstruction, processing and analysis of the material in order to identify and register aggregates and defects. The aggregates and defects were approximated as ellipsoids and their geometric parameters were registered and statistically characterized. The results were then used to generate a large ensemble of RVEs of concrete, with the same statistical properties as the material sample. Generated models were used in a nonlinear finite element simulation, where they were loaded in compression until failure. Finally, the results of all the models and their distribution were analyzed and compared with experimental results.

Analysis of a 3D image of fiber reinforced concrete inspired a novel methodology for separation of intersecting objects in 3D imaging based on unsupervised classification. The
boosting concept from the field of statistical learning motivated grouping several 2D classifiers for the purpose of assembling a 3D classifier. Separated fibers were identified and registered for statistical characterization of fibers orientation.

5.1 Conclusions

Statistical properties of geometric parameters of the ellipsoidal defects in the CMC model were equivalent to those of geometric parameters of the elliptical approximation of the observed defects in the original CMC material samples, thus achieving the goal of producing a SERVE for this material system. The most significant correlation was observed between the first two ellipsoid axes ($R = 0.624$), corresponding to the correlation between the ellipse axes ($R = 0.689$). Furthermore, the univariate and bivariate distributions of the geometric parameters of the generated defects were almost identical to those of the observed defects.

Numerical simulations of the CMC SERVE resulted in a reduction in the homogenized mechanical properties of the unit cell once the micro-structural defects were considered. The similarity between the damage evolution patterned suggests that the fabric weave and tow structure are the main factors that effected damage patterns while the presence of defects effected damage initiation and magnitude.

The geometric analysis of the aggregates and defects in the aggregate reinforced concrete, demonstrated a strong correlation between the ellipsoidal axes. This dependency led to characterize the statistical behavior of the dependent variables using trivariate log-normal distribution, while univariate uniform and normal kernel distributions were used for the independent variables.

A Monte-Carlo simulation, combined with the statistical characterization of the aggregates and defects, were used to generate an ensemble of SERVEs. 1000 models of SERVEs of concrete were generated by embedding ellipsoidal aggregates and defects in a cement matrix. Geometric parameter of the generated ellipsoidal aggregates resulted in the equivalent statistical behavior to that obtained from the CT reconstruction of the concrete sample.
Numerical simulations of the 1000 SERVEs resulted in mechanical response which closely followed the mechanical response of the tested material samples. Mechanical properties of the different phases, which were based on experimental data, produced accurate predictions of the macroscopic mechanical response of the SERVEs. Moreover, the 1000 simulations provided a range of mechanical responses, which had a normal-like distribution. The average maximal stress had only 1.8% difference in comparison to the experimental maximal stress.

Structural statistical characterization of the high performance fiber reinforced concrete material system was done through the analysis of fibers direction (direction cosines). Moderate negative correlations were found between the direction cosines in the x and z directions ($R = -0.469$) and between the direction cosines in the y and z directions ($R = -0.361$). Weak correlation ($R = 0.01$) was observed between the direction cosines in the x and y directions. The direction cosines analysis indicated that the z direction was the predominant direction in the material sample in question. The analysis also indicated that the statistical behavior of the z direction cosines followed a generalized extreme value distribution, which will be the subject of future research.

5.2 Future work

As mentioned previously, future work will focus on completing the statistical characterization of the fibres orientation in high performance fiber reinforced concrete. This will be followed by a process similar to that implemented on the CMC and the aggregate reinforced material systems. Namely, the results of the orientation statistical analysis will be used as a base for generating SERVEs of the fiber reinforced concrete material system, which will then be incorporated in numerical simulation for validation.
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[119] V. Kafka, “Concrete under complex loading: mesomechanical model of deformation and of cumulative