RECOVERY OF 3D ANISOTROPY DATA FROM CT SCANS OF 3D WOVEN COMPOSITES BY PRINCIPAL COMPONENT ANALYSIS

Gadoury, P[1]*, Gitman, I M[2], Smith, A I[1], Scaife, R[1]
[1] AMRC Composites, University of Sheffield, Sheffield, UK
[2] Mechanical Engineering, University of Sheffield, Sheffield, UK
* Corresponding author (p.gadoury@sheffield.ac.uk)

Keywords: *Design and Analysis, Textile Composites, Material Characterization and Testing*

ABSTRACT

A set of tools were developed with the aim of facilitating the design and qualification of 3D woven composite materials. Specifically, software tools facilitating the recovery of multi-scale structures from computer tomography (CT) scans have been developed with the aim of generating suitable inputs into finite element analysis (FEA) solvers and ground truth for computational preform geometry generation models.

While it is currently easy to recover volume fractions from a CT scan voxel array, a means of recovering fibre orientations within the reconstructed image is lacking to properly characterize the anisotropic properties of fibre reinforced composites. Following existing research in the recovery of anisotropy data from micrographs using 2D Fast Fourier Transforms (FFT), a generalization in 3D is presented in this paper, similar in theme to Principal Component Analysis. The method consists of calculating the multivariate covariance matrix of the 3D FFT of the CT scan sample. Boundary effects were mitigated by applying isotropic multivariate Gaussian and radial Heaviside window functions in the spatial and spectral domains, respectively. Strategies to mitigate the effects of noise are also presented. Average fibre orientations are thereby recovered from the raw voxel representation of the CT scan.

As case studies, the method is applied to a range of simulated data, and then finally to a scan of an infused 3D woven fibre reinforced composite, proving the suitability of the method for NDT and materials characterization and as a useful tool in computational model validation.

1 INTRODUCTION

The ability to recover the principal axes of orthotropy from CT scans has many applications, especially in the field of composites. The highly orthotropic material properties of fibre reinforced composites are a result of preferential orientations of their constituent fibres. As such, to properly qualify such materials, not only must a local fibre volume fraction be ascertained, but a measure of the mean orientation and degree of alignment of the fibres is also critical. An impartial analysis of parts for quality assurance or model validation therefore calls for a means of evaluating these quantities.

An exact measurement of material orthotropy can be tricky even for simple preform architectures such as laminates consisting of unidirectional plies, and the difficulty is compounded in the case of 3D woven composites, which are intricate and highly variable throughout their thickness. To start, obtaining the input data typically involves some form non-destructive testing. Of course, for parts where the orientations vary throughout the thickness, 3D scans are needed. As such 3D NDT methods are typically employed such as x-ray Computer Tomography (CT) or ultrasound.

Following some post-processing, these methods yield a voxel array representing the mean sampled image response of the material for the given imaging technique. This response is then correlated to a mean volume fraction for each voxel. This may be sufficient in a gross quality control or damage assessment application. For a more in-depth analysis, the traditional workflow then involves the generation of isosurfaces representing general features such as yarns or layers from these opacities. Finite element meshes could then manually be created and populated with orientation data and estimations to predict the material's behaviour.

The steady improvement of CT scan resolutions and computer power presents attractive opportunities to supplement or replace these last manual steps. Notably, it is now practical to generate CT scans capturing individual carbon or glass fibres for small parts such as test coupons and to evaluate their micro-scale properties through the application of high resolution finite element models. Without recovering the local fibre orientations, however, such simulations must assume the constituents behave isotropically – an assumption which may hold for glass fibres, but not for carbon fibres, for instance. Furthermore, the acquisition and analysis of such dense data over anything much larger than a small test coupon is impossible or at least impractical. For the purpose of inline quality assurance, damage and repair analysis and in order to facilitate the creation of efficient multi-scale finite element meshes, a means of recovering fibre orientations and generating an interpolation scheme would be a boon. Thus, such an approach is being developed and the current progress is outlined in this paper.

2 METHODOLOGY

2.1 Overview

Current state of the art CT scan analysis software packages such as Synopsys *Simpleware* and Brucker *Skyscan* reconstruction software offer a means to generate average volume fraction voxel data or isocontour meshes. Though these methods present a useful starting point towards conformal mesh generation for FEA, a means of generating the complementary fibre orientation vector field is also needed. Indeed, Skyscan replicates the desired results through the use of a Mean Intercept Length (MIL) algorithm [2], and Synopsis' *Simpleware* package goes some way towards achieving this through the use of "principal coordinate axes" [1]. However, the former approach requires several expensive ray-casting operations and may not return accurate results is the objects are too few or too small, and the latter approach is not laid out in detail, so little can be said about its efficacy. This paper will therefore focus on developing a FFT-based material orthotropy measure not unlike MIL in some respects, but which is fast, robust and requires little or no human intervention.

The recovery of anisotropy data from micrographs is subject of ongoing research in the fields of metallurgy to quantify grain microstructure, as was presented by Holota and Něměček [3], and further applied to nonwoven fibrous materials by Jeddi et al [4]. Both approaches examine histogram data of the 2D Fast Fourier Transform (FFT) of the original micrographs and recover a measure of angle and magnitude of the anisotropy of the examined structure. An extension of this method to 3D is presented which aims to robustly generate mean orientation vectors as sampled over an arbitrary unstructured grid within a CT scan voxel array whereby the Principal Component Analysis (PCA) of the FFT spectrum of a local windowed sample effectively determines the best fit for orthotropic axes, as well as to quantify the degree of orthotropy along each axis.

2.2 *Fast Fourier Transform and Image Processing*

The Fast Fourier Transform algorithm recovers the complex Fourier coefficients defined in the frequency domain from a set of uniformly spaced samples in the spatial domain. These frequencies and amplitudes are encoded as a set of complex coefficients:

$$F(\mathrm{k}) = \mathrm{FFT}[k](f) \equiv \sum_{n=0}^{N-1} \mathrm{f}_n \mathrm{e}^{-2\,\pi\, i\, k\, n\,/\,N} \tag{1}$$

where $F(k)$ is the k^{th} complex Fourier coefficient of the sampled series f and N represents the number of samples. This transform readily generalises to d-dimensions:

$$F(\mathbf{k}) = \mathrm{FFT}[\boldsymbol{k}](f) \equiv \sum_{\boldsymbol{n}=\mathbf{0}}^{\boldsymbol{N}-1} \mathrm{f}_{\boldsymbol{n}} \mathrm{e}^{-2\,\pi\, i\; \boldsymbol{n}\cdot\boldsymbol{k}\,/\,\boldsymbol{N}} \tag{2}$$

where bolded terms represent d-dimensional vectors and the division $\boldsymbol{k}\,/\,\boldsymbol{N}$ is defined as:

$$(\frac{n_1}{N_1}, \frac{n_2}{N_2}, \dots, \frac{n_d}{N_d})$$

for d-dimensions. The magnitude of each coefficient in the spectrum represents the amplitude of the sinusoid at a given frequency, whereas the complex argument represents its phase.

An intuitive description of how FFT can be used to recover material orthotropy axes can be constructed as follows. As per the MIL algorithm, if on average several fluctuations occur in the amplitude of an orthotropic scalar field along a given path, then this path is likely along a more transverse direction. Conversely, should very few fluctuations occur along a given path, then this path coincides with a longitudinal direction. One should therefore see large spectral amplitudes even into the high frequencies along the transverse direction owing to the repeated fibre crossings, and a very compact spectral distribution in the longitudinal direction as the amplitudes stays mostly constant. This effect is illustrated for 2 dimensions in Figure 1, with the calculated principal components overlaid.

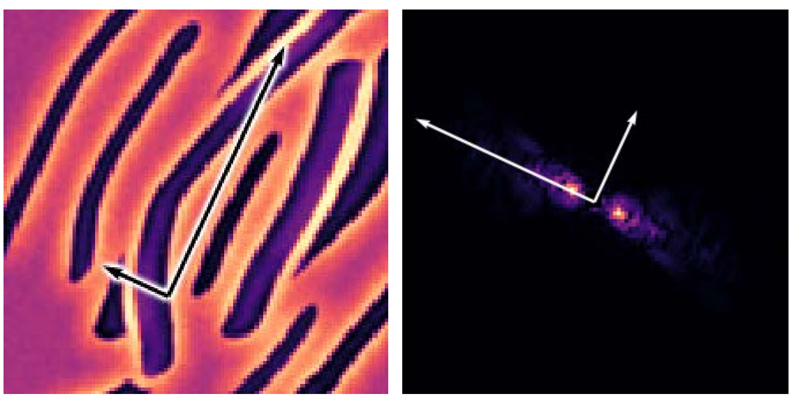

Figure 1a) 2D simulacrum of fibres, and; b) its convoluted FFT with central coefficients masked, both with superimposed orthogonal vectors following the full treatment described in this section

Few fibres are crossed in the longitudinal direction denoted by the long arrow, resulting in a very narrow spectrum distribution in the spectral domain. Conversely, several fibres are crossed in the transverse direction, resulting in a wide spectrum distribution in that direction.

To obtain the principal fibre directions at chosen sampling points, each sampled neighbourhood is first multiplied by a convolution kernel corresponding to a radially symmetric Gaussian:

$$\mathcal{N}(\boldsymbol{\xi};\ C_0) = \exp(-\frac{1}{2}\boldsymbol{\xi}^T C_0^{-1}\,\boldsymbol{\xi}) \tag{3}$$

where C_0 is the covariance matrix, in this case corresponding to the identity matrix multiplied by a scalar variance (or inverse falloff) parameter s, and $\boldsymbol{\xi}$ represents some distance offset from the sampling neighbourhood centre. The kernel is shown for the 2D case in Figure 2.

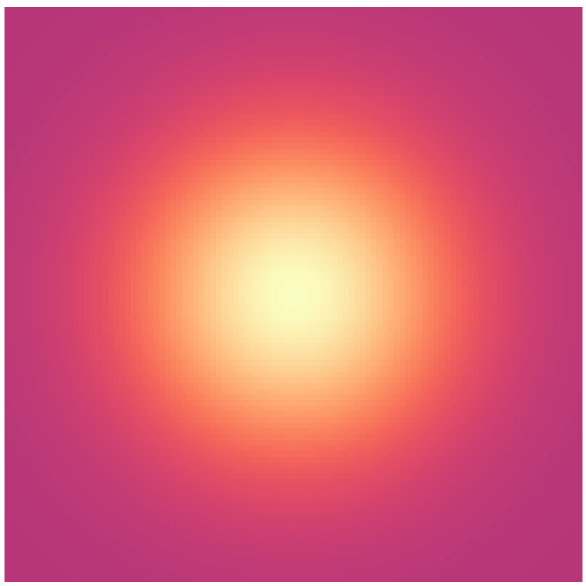

Figure 2: Gaussian kernel

From the FFT convolution property, this initial operation ensures that spurious high frequency noise is removed (this multiplication corresponds to a Gaussian blur in the spectral domain). More importantly the application of a radial convolution kernel mitigates the edge and corner effects on the angular reconstruction, as the Gaussian kernel approaches zero away from its centre. The variance and size of the kernel (its falloff and support) can be adjusted to result in more or less noise reduction with a tradeoff on minimum detail resolution.

$$F(\mathbf{k}) = \text{FFT}[\boldsymbol{k}](\mathcal{N}(\boldsymbol{\xi} - \boldsymbol{x_n})\cdot f(\boldsymbol{x_n})) \tag{4}$$

The result of the ensuing FFT resembles that shown in Figure 1b) for a given sampling neighbourhood. In the 3D case, the magnitude of the Fourier spectrum for a mostly unidirectional anisotropic scalar field resembles a flat disc whose normal is oriented along the principal fibre direction. The low magnitude components below some threshold value can be discarded, yielding a series of high magnitude coefficients and their corresponding coordinates in the frequency domain. To determine the primary axes describing their distribution and magnitude, these points and weights are then fed into the principal component analysis.

2.3 Principal Component Analysis

PCA is a method or recovering the underlying orthogonal basis set of a set of punctual observations. This powerful analysis technique has applications in statistics and in machine learning, but its use in CT scan analysis will be made clear as follows: a geometric interpretation of PCA consists of fitting an n-ellipsoid to the data. In the case of normally distributed data, the PCA recovers the orthogonal singular vectors of the covariance matrix describing that distribution.

The technique involves calculating the estimated covariance of a set of samples (in this case the truncated subset of spectral coordinates weighted by their corresponding set of Fourier coefficient magnitudes):

$$\mathrm{C} = \sum_{m=\mathbf{0}}^{M-1} (\boldsymbol{k}_m - \mu)\ (\boldsymbol{k}_m - \mu)^{\mathrm{T}} \frac{\|F(\mathbf{k}_m)\|}{\sum\|F(\mathbf{k}_m)\|} \tag{5}$$

where $\boldsymbol{k}_n$ represents the n-th sampled spectral coordinate $\|F(\mathbf{k}_m)\|$ represents complex magnitude of the m-th corresponding Fourier coefficient acting as a weight, $\sum\|F(\mathbf{k}_m)\|$ is the sum of all these Fourier magnitudes and μ represents the mean of these coordinates weighted by their Fourier coefficients:

$$\mu = \sum_{\boldsymbol{m}=0}^{M-1} \boldsymbol{k}_n \frac{\|F(\mathbf{k}_m)\|}{\sum\|F(\mathbf{k}_m)\|} \tag{6}$$

As the $d \times d$ covariance matrix recovered from the d-dimensional weighted sample set, C encodes the orthogonal basis of the distribution. To extract that information, it is necessary to apply an eigendecomposition, or equivalently a Singular Value Decomposition (SVD):

$$\mathrm{C} = \mathrm{U\ S\ V}^{T} \tag{7}$$

where, since C is square, U is a $d \times d$ matrix containing d orthogonal left-singular column vectors, and similarly V is a $d \times d$ matrix containing d orthogonal right-singular row vectors. S is a diagonal matrix containing d singular (or Eigen) values.

Specifically, the singular vector corresponding to the smallest singular value corresponds to the prevailing fibre direction. Vectors corresponding the second and third (and so on for higher dimensions) are aligned along the remaining prevailing orthogonal directions, in order of relative scaling. The ratio of the largest singular value to the smallest singular value of the covariance SVD, also known as its condition number is a measure of the degree of anisotropy.

2.4 Derivatives

Optionally chain rule derivatives can be calculated at each step in order to feed the result forward into gradient-based optimizers such that the position of interpolation nodes can be optimized to the most anisotropic regions, for instance. In this section. a subscript preceded by a comma (e.g. $a_{,b}$) represents a derivative with regards to the subscript.

In order, the gradient of the FFT of the product of the convolution kernel and the sampled neighbourhood with regards to its centre can be simplified by precomputing a gradient convolution kernel:

$$\mathcal{N}_{,\xi}(\boldsymbol{x};\, \boldsymbol{\xi}, s) = \, 2(\boldsymbol{x} - \,\boldsymbol{\xi})\left(C_0 + \, C_0^{\mathrm{T}}\right)^{-1} \mathcal{N}(\boldsymbol{x};\, \boldsymbol{\xi}, s) \tag{8}$$

A visualisation of the gradient convolution kernel along ξ_0 (the vertical direction) is shown in Figure 3.

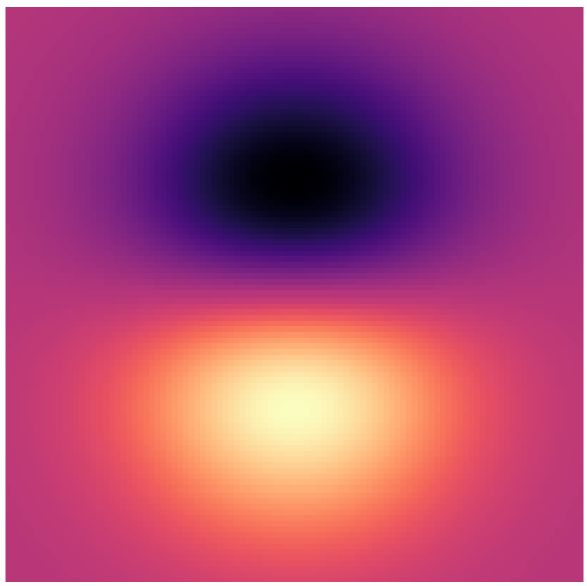

Figure 3: Gaussian gradient kernel along the vertical direction

These gradient kernels can be applied in the same manner as the Gaussian kernel prior to the FFT to yield the gradient of the transform with regards to analysis region placement.:

$$F(\boldsymbol{k}) = \, \mathrm{FFT}[\boldsymbol{k}](\mathcal{N} \cdot f)_{,\xi} = \mathrm{FFT}[\boldsymbol{k}](\mathcal{N})_{,\xi} * \, \mathrm{FFT}[\boldsymbol{k}](f) \, = \mathrm{FFT}[\boldsymbol{k}](\mathcal{N}_{,\xi} \, \cdot f) \tag{9}$$

The gradient of a complex magnitude corresponds to :

$$\|F(\mathbf{k}_m)\|_{,F(\mathbf{k}_m)} = \mathrm{sgn}\big(F(\mathbf{k}_m)\big)\, F(\mathbf{k}_m)_{,\mathbf{k}_m} \tag{10}$$

Next, the weighted mean’s derivative with regards to the Fourier coefficient complex magnitude:

$$\mu_{,\|F(\mathbf{k}_m)\|} = \frac{\boldsymbol{k} - \mu}{M - 1} \tag{11}$$

Using the derivative of the mean w.r.t. a given Fourier coefficient complex magnitude, the derivative of the covariance w.r.t. that magnitude can be expressed as:

$$\mathrm{C}_{,\|F(\mathbf{k}_m)\|} = (\boldsymbol{k}_m - \mu)(\boldsymbol{k}_m - \mu)^{\mathrm{T}} \frac{1}{\sum\|F(\mathbf{k}_m)\|} - \sum_{p=\mathbf{0}}^{P-1} \left(\mu_{,\|F(\mathbf{k}_m)\|}\right) \left(\boldsymbol{k}_p - \mu\right)^{\mathrm{T}} + \left(\boldsymbol{k}_p - \mu\right)\left(\mu_{,\|F(\mathbf{k}_m)\|}\right)^{\mathrm{T}} \frac{\left\|F(\mathbf{k}_p)\right\|}{\sum\left\|F(\mathbf{k}_p)\right\|} \tag{12}$$

Finally, the derivative of each component of the SVD (the left singular vectors, the singular values and the right singular vectors) is described in [5].

All of these quantities and their gradients were coded in python using the numpy/scipy libraries and tested using finite difference to ensure stability.

3 Results

As a first trial of the recovery capabilities of the subroutines, a synthetic dataset of 100 voxels cubed was generated consisting of a completely orthotropic quadratically distributed noise source random in two directions and constant along the third. Unsurprisingly, the software was able to determine the principal orientations to within machine epsilon.

The trial was incremented by rotating the extruded noise source along some arbitrary vector. Again, the software is able to recover the orientations to within a few degrees, limited it seems by the aliasing caused by the rotation operation and by the Nyquist limit on interpolation and Fourier Transform. Isotropic noise was then progressively added until it accounted for 93.75% of the input signal, with little effect on the accuracy of the PCA, likely due to the noise correcting properties of the Gaussian convolution kernel and the wide support. The condition number indicating the degree of orthotropy dropped, intimating that the samples were more isotropic, which is to be expected since, again, the added noise was uniform. 100 trials were conducted for each noise level to iron out inconsistencies. Figure 4 shows the effect of noise on the angular error and condition number.

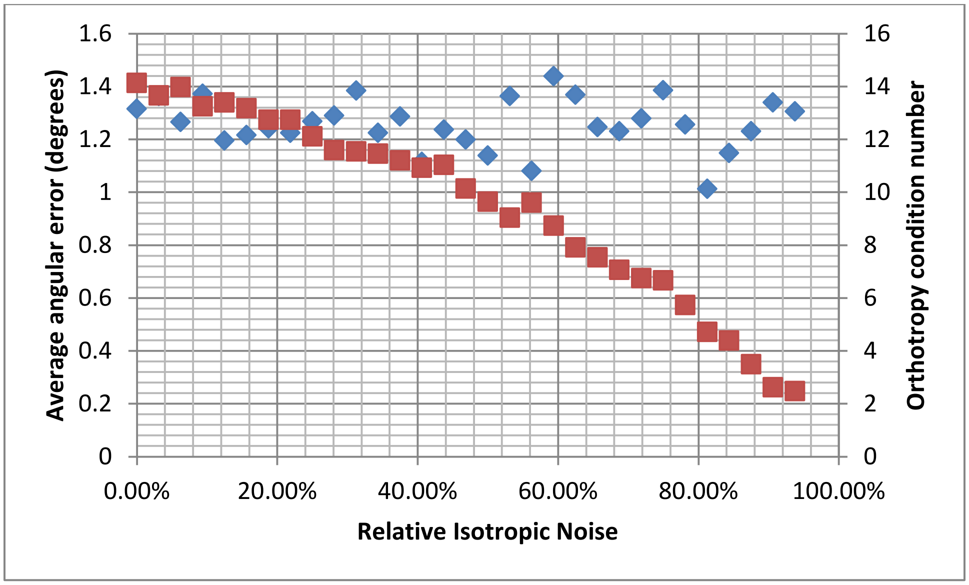

Figure 4 Average angular error and condition number w.r.t. isotropic noise

The final and ongoing testing consists of extracting fibre orientation from actual CT scans. Figure 5 shows a subset of a 3D orthogonal weave vector field where the length and colourscale of the vectors corresponds to the degree of orthotropy, and their directions correspond to the principal orientation of the vectors. As might be intimated by this figure, current difficulties specifically include dataset visualization and validation, as well as computational efficiency working with extremely large voxel arrays. Indeed full scale high resolution reconstructions can take several hours on a relatively high performance consumer PC. Some sample placement optimization testing is also ongoing, but it was discovered that with the orientation gradients being as highly sensitive to small changes in node placement, the optimizer tends to fall into local minima, or take a very long time indeed to converge.

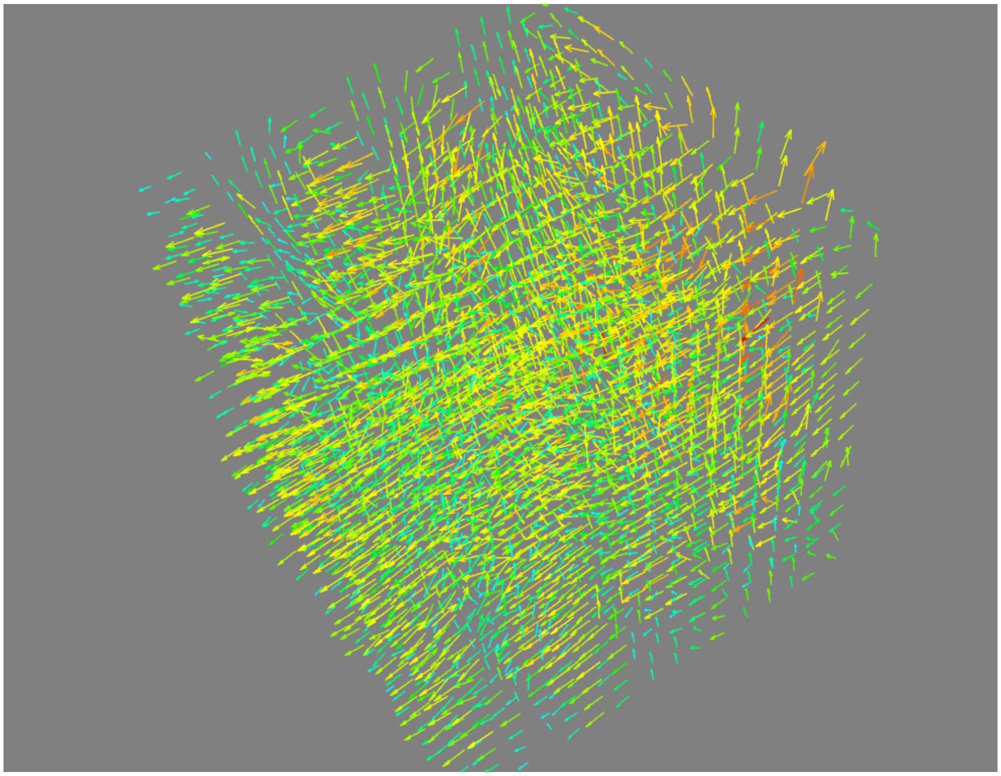

Figure 5 Reconstructed fibre orientation vector field of an orthogonal 3D woven composite section

4 ONGOING WORK

The next steps in this programme consist of refining the CT scan reconstruction algorithm to allow it to better handle large datasets, to implement more efficient visualization tools, and to integrate it with a FEA solver. It is hoped that the ability to generate efficient conformal meshes will integrate well with isogeometric and harmonic basis function elements currently being developed in parallel.

As it stands, the means to robustly and automatically isolate a measure of fibre orthotropy over an arbitrary region shows great promise for the modelling, validation and quality assurance of fibre reinforced composites.

5 REFERENCES

[1] The Synopsis Simpleware physics modules technical data sheet. Technical report, 2009.

[2] Morphometric parameters measured by Skyscan (TM) CT analyser software. Technical report, 2016.

[3] Radek Holota and Stanislav Nemecek. Recognition of oriented structures by 2d Fourier transform.

[4] Ali AA Jeddi, HS Kim, and B Pourdeyhimi. Measurement of fiber orientation in nonwovens: optical Fourier transform. *Int Nonwoven J*, 10:10–16, 2001.

[5] Théodore Papadopoulo and Manolis IA Lourakis. Estimating the Jacobian of the singular value decomposition: Theory and applications. In *European Conference on Computer Vision*, pages 554–570. Springer, 2000.