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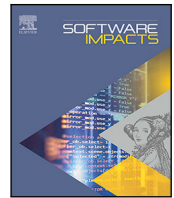
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Original software publication

X-ray computed tomography data structure tensor orientation mapping for finite element models — STXAE

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ABSTRACT

Accurate modelling of fibre reinforced composites requires anisotropic material models. Structure tensor analysis of X-ray 3D images has been shown to provide fast and robust estimation of local structural orientations in fibre reinforced composites. We present two mapping algorithms which can be used to map estimated local orientations onto finite element models for more accurate material modelling. The two functions allow for element-wise and integration point-wise mapping, respectively, and have been implemented using Python in a Jupyter notebook. Together with the previously published structure tensor code, these two functions demonstrate the concept of Structure Tensor X-ray computed tomography Aided Engineering (STXAE) (Phonetics: [steksei:]).

Code metadata

Current code version	v01.0
Permanent link to code/repository used for this code version	https://github.com/SoftwareImpacts/SIMPAC-2021-183
Permanent link to Reproducible Capsule	https://codeocean.com/capsule/3494546/tree/v1
Legal Code License	MIT License (MIT)
Code versioning system used	none
Software code languages, tools, and services used	Python, Jupyter
Compilation requirements, operating environments & dependencies	Microsoft Windows, Linux
If available Link to developer documentation	
Support email for questions	robaue@chalmers.se

1. Structure tensor X-ray computed tomography aided engineering

Structure tensor X-ray computed tomography aided engineering (STXAE) is a new method for simplifying the creation of finite element models of anisotropic materials based on X-ray computed tomography image data. The method can be implemented as a part of the X-ray computed tomography aided engineering (XAE) process [1]. Along with this paper, we provide an implementation of STXAE method in a Jupyter notebook. The notebook is based on the structure tensor implementation and notebooks by Jeppesen and Dahl [2,3]. This implementation has been previously used in [4,5]. These studies focus on the

analysis of fibre orientation in glass-fibre reinforced composites imaged using 3D X-ray computed tomography. It uses structure tensor analysis to estimate the fibre orientation at each voxel position, which serves as the basis for STXAE.

In our notebook, we present two novel mapping functions. The first assigns the local material orientations element-wise onto a finite element mesh, while the second one assigns the local material orientations integration point-wise (see Fig. 1). The mapping functions work for continuum (2D, 3D) and structural (beam, shell,...) elements for first and second order element formulations. The implemented mapping functions support the Abaqus™ syntax. For the element-wise mapping,

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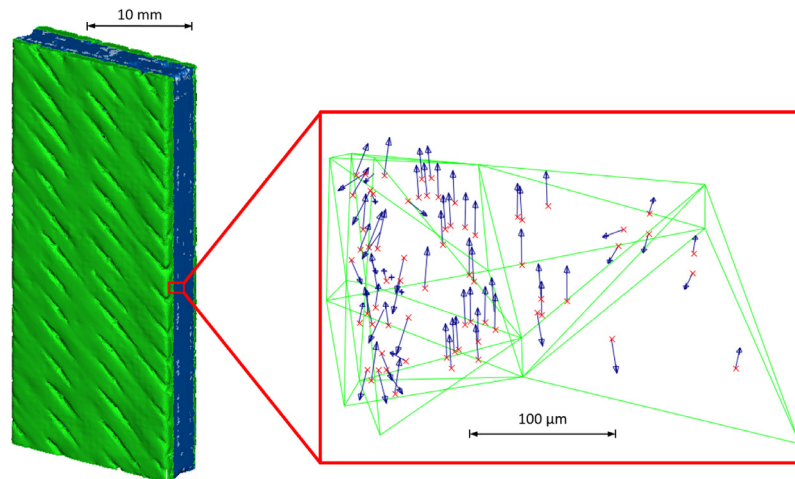


Fig. 1. Integration point-wise material orientation mapping for second order tetrahedral elements depicted for a few elements of a full finite element model. The blue arrows indicate the main fibre orientation in the domain around the integration point. The material orientation analysis and mapping process are created by *STXAE* [6].

the Abaqus™ mesh INP-file is sufficient as input. The integration point-wise mapping on the other hand requires an Abaqus™ DAT-file with the coordinates of all integration points. For elements with more than one integration point, the integration point-wise mapping allows for a more precise material orientation modelling, as it has more mapping destination points than the element-wise mapping.

The output of the mapping function depends on the chosen mapping scheme. For the integration point-wise scheme, a Fortran 77 file is created, which serves as input for the Abaqus™ ORIENT subroutine during simulation. For the element-wise mapping, an Abaqus™ INP-file is created that contains the original Abaqus™ INP-file enhanced by the estimated local material orientation for all elements in Abaqus™ syntax. Even though the mapping demonstrated in the notebook is designed for the Abaqus™ syntax, it can be easily adapted to other finite element solvers, e.g., LS-Dyna™.

2. Impact overview

3D X-ray computed tomography image data reveals information about the material state inside of the scanned sample by imaging the local material density. With modern image acquisition technologies, terabytes of data can be easily acquired. Therefore, efficient, accurate, and cheap image analysis and model creation methods are required. For modelling of anisotropic materials such as fibre reinforced composites, a material orientation assignment is essential. Standard material orientation analysis of fibre reinforced composites uses single fibre tracking [7], which requires high resolution images. Structure tensor-based estimation of local structural orientations does not track individual fibres. Instead, it estimates the dominant structural orientation in an area around specific positions. This approach requires much less computational power than individual fibre tracking. Furthermore, it is more robust for analysis of lower resolution images compared to individual fibre tracking methods [8].

The structure tensor method used for *STXAE* has been tested in several studies. Jeppesen et al. [4] introduced the structure tensor method implementation for analysis of fibre orientations in a non-crimp fabric glass fibre reinforced composite. In another study Jeppesen et al. [5] tested the structure tensor method on pultruded and pre-preg carbon fibre reinforced composites, and on a non-crimp fabric glass fibre reinforced composite. With this analysis they characterised the fibre misalignment induced by different manufacture techniques. Salling et al. [9] compared individual fibre tracking with the structure tensor

method on unidirectional glass fibre reinforced thermoset composite and an air-textured glass fibre reinforced composite. Both segmentation approaches showed no significant differences in fibre inclinations. Those studies underline the excellence of the structure tensor method and justify the choice for using this method in combination with the novel material orientation mapping.

In [6] *STXAE* was used to analyse the mechanical stress distribution and elastic modulus of a non-crimp fabric reinforced glass fibre composite under tensile loading. *STXAE* has shown its accuracy and robustness even for low resolution image data. Although single fibres with an average diameter of $17\ \mu\text{m}$ could not be resolved at a voxel size of $64\ \mu\text{m}$, acceptable finite element simulation results were attained. More specifically this means while 99.8% of the original image data was removed, the elastic modulus was only underestimated by 3.9% compared to the simulation results based on the original voxel size of $8\ \mu\text{m}$. Those results would allow for larger model size in the range of two orders of magnitude.

Further studies are necessary to support those findings. Here in particular different fibre types, e.g., carbon or natural fibres, and fibre layouts, e.g., pultruded or injection moulded, in combination with different load cases, e.g., compression, are currently under investigation. Especially, compression failure of unidirectional carbon fibre composites is known to be extremely sensitive to small fibre misalignment. Until now, this load case has primarily been addressed more generically [10] and in 2D [11]. *STXAE* gives an applicable method to model and predict the influence of the actual 3D distribution of the fibre orientations on the compression strength in specific material samples. Furthermore, we believe that the approach is widely applicable for any anisotropic material where X-ray computed tomography can produce reasonable quality image data.

The current version of the code is not capable of directly creating a finite element model based on the 3D X-ray computed tomography data. The user has to create the mesh in a finite element pre-processor. The reason for this detour is that not even commercial pre-processors can automate the meshing task of the complex fibre composite structures that have been investigated in [6]. However, we aim to update the code to be able to handle simpler meshing tasks to allow for a fully automated XAE process in one Jupyter notebook.

The advantages of *STXAE* can be summarised as:

- (a) Highly robust and fast fibre orientation analysis
- (b) Applicable for image data of different anisotropic material types

- (c) Few parameters need to be set
- (d) Integration point-wise mapping scheme

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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