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Original software publication

Three-dimensional finite element modeling of anisotropic materials using X-ray computed micro-tomography data (?)

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ABSTRACT

Keywords: Structure tensor analysis Fiber-reinforced polymers Fiber orientation distribution Constitutive behavior A complete software package is developed for finite element modeling of anisotropic materials with orientation information estimated from X-ray μ CT scans. The method is demonstrated for a carbon fiber-reinforced epoxy pultruded profile where fiber orientations are estimated using structure tensor analysis. A finite element model is automatically generated with the same dimensions as the X-ray μ CT volume and with orientation information stored at the integration points of the mesh. A static tensile simulation is executed in AbaqusTM, and results are exported to a Python program for post-processing and analysis of the mechanical response.

Code metadata

Current code version	V01.0
Permanent link to code/repository used for this code version	https://github.com/SoftwareImpacts/SIMPAC-2023-173
Permanent link to reproducible capsule	https://codeocean.com/capsule/9342448/tree/v1
Legal code license	MIT License (MIT)
Code versioning system used	Git
Software code languages, tools and services used	Python, Linux, Fortran
Compilation requirements, operating environments and dependencies	Microsoft Windows, Linux
If available, link to developer documentation/manual	
Support email for questions	olen@dtu.dk

1. Introduction

Finite element simulation of anisotropic materials is often idealized to engineering constants where variations in the internal structure are neglected. Materials such as fiber-reinforced polymers used in the wind turbine industry are sensitive to variations in fiber orientation, where the constitutive behavior and ultimate failure may be affected. The present method provides a complete package for quantifying the effect of material orientation variation on the bulk mechanical response of anisotropic materials. The method is demonstrated in a Jupyter Notebook for a carbon fiber-reinforced epoxy pultruded profile and is based on the X-ray computed micro-tomography (X-ray µCT) data available in [1]. The Jupyter Notebook is a precompiled version of the complete package. The complete package is available in [2] where some parts are dependent on a license for the commercial Finite Element (FE) software, Abaqus $^{\rm m}.$

The method comprises three major steps for quantifying the mechanical response, as presented in Fig. 1.

First, the volumetric material orientations are estimated from an X-ray μ CT scan using the image processing method, structure tensor analysis (see Fig. 1a and b). The work is based on the method presented by Jeppesen et al. [3,4], where the structure tensor analysis is used for quantifying the internal material orientations of glass and carbon fiber-reinforced polymers. The method provides a dominant material orientation at every voxel position in the X-ray μ CT volume based on the gradient information in the volumetric grayscale image.

Secondly, the estimated material orientations and the dimensions of the X-ray μ CT volume are used as input for the automatic generation of a FE model in Abaqus[™]. Volumetric material orientations

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are mapped to the integration points of the mesh through pointwise interpolation, like the method presented by Auenhammer in [5]. The Abaqus^M user-subroutine, ORIENT, is subsequently used to rotate the local coordinate systems of all integration points based on the mapped material orientation information (see Fig. 1c).

Finally, the FE simulation is solved in Abaqus^M, where the results are exported and used for post-processing in a Python program. Here the bulk mechanical response and field variables are used for studying the behavior of anisotropic materials with material orientation variations (see Fig. 1d).

2. Impact overview

The method is demonstrated for a simple static tensile test of the entire X-ray μ CT volume in a common fiber direction (x-axis). The model can equally well be used for studying alternative loading conditions where variations in material orientations impact the material stiffness and ultimate failure.

The compressive strength of unidirectional fiber-reinforced polymers is notoriously sensitive to off-axis fiber orientations and has been shown to cause significant strength reduction relative to the tensile strength [6]. The large reduction in compressive strength has been related to the strain localization mechanism, kink band formation. Some of the first kink band prediction models were based on idealized uniform fiber orientation distributions in 2D. Later, non-uniformity was introduced to study the effect of different imperfection parameters [7, 8]. Although representative for fiber-reinforced polymers with periodic fiber orientation distribution, these models do not account for realistic orientation distributions, which are more randomly distributed. A 2D model accounting for realistic fiber orientation distributions based on optical microscopy images was presented for non-crimp fabrics in [9]. Like the idealized models, this method is applicable for materials where fiber orientation distributions are considered constant through the depth of the sample, i.e., local imperfections are neglected or considered constant. The method presented in this paper enables the analysis of fiber orientation distributions in three dimensions. It has been used in combination with a user-subroutine in Abaqus™, capable of describing the elastic-plastic behavior of fiber-reinforced polymers [10]. The model is used for compressive strength predictions associated with kink band initiation and is in good agreement with the constitutive behavior of experimental results. The predictions are based on the same X-ray μ CT scan data as presented in the Jupyter Notebook and compared with experimental compression test samples from the same material used in the X-ray scan.

Modeling the influence of imperfections, such as wrinkles, on the fiber orientation distribution in large composite structures is often associated with complex meshing strategies based on observations from the material layup [11]. The method presented in this paper may be used for modeling three-dimensional imperfections in fiber-reinforced composite structures with a simple mesh setup where orientation information related to the imperfection is stored in the integration points. The process of modeling the constitutive behavior of materials with imperfections would thus be simplified. Finally, the method would also enable the analysis of imperfections with three-dimensional fiber orientation distributions where assumptions about constant depth can be avoided.

The Jupyter Notebook demonstration is based on, but not limited to, a uniform load case for a simple cuboid model. More complex structures with non-uniform load cases may be studied using this method, provided that a dataset for quantifying material orientations is available or can be generated. Compared with idealized FE models of complex structures, a model considering realistic material orientation distributions would enable more accurate simulations of the structural behavior and, potentially, capture local effects which are detrimental to the global response.



Fig. 1. Finite element simulation of carbon fiber-reinforced epoxy pultruded profile based on material orientations estimated from X-ray μ CT data. (a) Volumetric image of X-ray μ CT data presented as a grayscale image. (b) Fiber orientation color plot on top of X-ray μ CT image, where ϕ is the fiber orientation deviation from the global x-axis. (c) Fiber orientations, ϕ , mapped to integration points in the FE mesh. (d) In-plane shear stress results at integration points from uniaxial tension simulation with applied displacement in the x-direction found at an applied uniaxial stress of $\sigma_{11} = 1100$ MPa.

3. Future work and updates

The present method considers the material orientation distribution in anisotropic materials. In the case of modeling fiber-reinforced composites, stress distribution through the volume is affected by the distribution of material constituents i.e., fiber and resin distribution. A method for quantifying the fiber-resin distribution is presented in [12] based on high-resolution scanning electron microscopy images. A similar method can be used in this framework for modeling the constituent behavior and analysis of stress distribution in fiber-reinforced composites. This update would improve the analysis of materials with local imperfections in terms of fiber volume fractions with large deviations from the global mean.

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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