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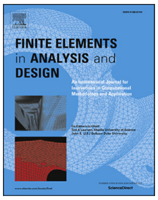

Virtual microstructure generation using thermal growth: Case study of a plain-weave Kevlar fabric

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ABSTRACT

Generating realistic 3D yarn-level finite element models of textile weaves and impregnated textile composites poses a challenge because of the complexity of the 3D architecture and the need for achieving high quality finite elements and non-intersecting yarn volumes. A common approach is to sweep a constant yarn cross-sectional shape along a smooth and continuous centerline that repeats over a unit cell length. This approach breaks down with tight and complex weave architectures. Moreover, actual microstructures of dry fabrics and textile composites are often aperiodic and non-deterministic. In this work, a new method to generate realistic virtual microstructures of woven fabrics and textile composites using a “thermal growth” approach is presented. This involves a series of mechanics-driven orthotropic volumetric expansions and shrinkages of the yarn cross-sections and centerlines that are artificially induced by prescribed thermal loads, along with mechanics-driven yarn deformations in order to “grow” or “form” the yarns into their final realistic configurations within the weave. Contact-pairs are defined between interlacing yarn surfaces to prevent yarn inter-penetrations. The final virtual microstructures are generated through a series of finite element simulations executed using LS-DYNA®. This process is demonstrated by considering the case study of a plain-weave Kevlar fabric used in body armor. Movies of the thermal growth process in action are available in the *Supplementary Files* section. The virtual microstructures are characterized using ImageJ®-based image analysis and then validated against experimental microstructures. Relatively fine microstructural features are accurately reproduced. The process is amenable to any textile weave architecture.

1. Introduction

High-fidelity finite element analysis (FEA) of woven fabrics and impregnated textile composites utilize yarn-level models wherein each yarn (also referred to as a tow or fiber bundle) is individually modeled as an anisotropic 3D homogenous continuum. The local longitudinal material axis of these yarns is aligned with their undulating centerlines. Orthotropic and transversely isotropic material models are typically utilized to represent the local homogenized yarn behavior with the correct local orientation. The yarns can be meshed with 3D hexahedral or tetrahedral elements or using voxel-based approaches [1–3].

There are several available textile preprocessors (e.g. TexGen [4], WiseTex [5]) that are capable of generating yarn-level geometric models of 2D and 3D woven fabrics, as well as braids and knits. Geometric representations include CAD, STL, and IGES formats. After cleaning up the geometry and removing any yarn inter-penetrations, the individual yarns can be discretized using various commercial meshing software (e.g. Hypermesh®, TrueGrid®, Abaqus/CAE®) and then exported to commercial finite element solvers (e.g. ABAQUS®, ANSYS®, LS-DYNA®) to run linear and non-linear simulations of the structural and thermal response of the woven fabric. TexGen also has the capability to discretize the textile geometry and directly export an inputfile to ABAQUS.

When analyzing a textile composite that includes a polymeric or ceramic matrix in addition to the yarns, then the additional steps of generating the matrix geometry and mesh are required. This is not necessarily a trivial task as the odd-shaped matrix regions at the yarn interstitials and the small sliver-like matrix regions between interlacing yarns can cause meshing problems, moreover enforcing coincident nodes between the yarn surface mesh and the matrix surface mesh is not trivial. These challenges have been previously well recognized, leading to investigations of voxel-based meshing approaches [2,3,6]. Other software (e.g. pcGINA [7], mmTexLam [8]) allow the user to define a customized weave based on a pre-defined, parameterized, internal library of 2D and 3D idealized weave architectures and then the software computes the effective orthotropic elastic and thermal properties of the composite model using various analytical (e.g. micromechanics) and hybrid-FEA techniques.

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A common approach to generating textile architectures relies on sweeping a constant yarn cross-section along a centerline trajectory: these approaches are referred to as "geometry-driven". A disadvantage of this idealized approach is that it can result in large intersections or penetrations between yarn volumes, particularly as the weave architecture gets tighter, the overall fiber volume fraction (FVF) increases, and the yarn undulations increase. In contrast, "mechanics-driven" preprocessors utilize a motive force (viz. An external stimuli) to drive interactions between the modeled constituents of the textile geometry in order to determine the equilibrium shapes and final positions of these constituents. The motive force may comprise a tensile pre-strain, a thermal load, or a fluid flux. The constituents depend on the modeling resolution used, for e.g. individual fibers or individual homogenized yarns. The interactions are typically contact-based, i.e. two entities come into contact with each other resulting in translation, rotation, and/or deformation of one or both contacting entities. For example, Digital Fabric Mechanics Analyzer (DFMA) [9] and Virtual Textile Morphology Suite (VTMS) [10] use a tensile pre-strain along with static relaxation and strain energy minimization techniques to pack individual fibers within a yarn and to allow these fiber bundles to deform into their final positions and shapes within the weave preform. The circular-shaped fibers are modeled with 1D elements or 'digital-elements' with contact definitions between them. The fiber-level yarns can then be converted into homogenized 3D yarns for FE simulations. However this process can result in uneven yarn surfaces and yarn interpenetrations, which need to be remediated before the model can be used in a FEA simulation. Other approaches [11,12] very similar to this digital-element method use a temperature drop to contract the binder yarn lengths in order to compact the preform to its target thickness, after which the bundle of 1D element chains are converted into a TexGen representation of 3D yarns. Another interesting approach [13] models yarns as initially-slender inflatable tubes with contact defined between them, which are then expanded under a fluid flux until their desired volume fraction is reached.

Other preprocessor techniques utilize Monte Carlo algorithms based on Markov Chain operators to generate virtual textile composite structures, both 1D yarn loci and 3D yarn volumes, that possess the same statistical characteristics as the micro-CT scan data of the specimens [14,15]. Most textile preprocessors generate either a representative volume element (RVE) or a flat-panel of finite in-plane dimensions. Recently, a 1D weave modeler [16] capable of generating large, complex structures such as distance-weave sandwich preforms and airfoils was developed, where the weave architecture is defined by sets of bounded integers, and simple algorithms based on topological ordering rules are used to generate the weave models. Each yarn is discretized using 1D finite elements (e.g. truss, beam). The 1D weave model is then converted into a Binary Model [17–19] ('slave' 1D yarns embedded in a 'master' 3D effective medium) in order to run thermostructural simulations of the textile composite.

In this paper, an innovative method of generating realistic deterministic and stochastic virtual microstructures of dry fabrics and textile composites using a "thermal growth" technique is presented, wherein a series of controlled mechanics-driven orthotropic volumetric expansions and contractions of the yarn cross-sections and yarn centerlines coupled with mechanics-driven yarn deformations are used to generate 2D, 2.5D, and 3D weave architectures. The output is a high-quality, ready-to-use finite element mesh of the textile weave with each yarn individually modeled in 3D. The framework is implemented as a series of thermostructural simulations executed using LS-DYNA. The case study of a plain-weave Kevlar fabric (Style 706) used in body armor is considered. The virtual microstructures of the finite element model are extensively validated against experimental microstructures obtained from optical microscopy characterization and ImageJ-based image analysis of the material specimens. The thermal growth approach described herein can also be applied to textile composites, in which case the matrix is also subjected to controlled volumetric expansions and contractions.

2. Virtual microstructure generation using thermal growth

2.1. Case study material

The selected case study is based on a greige Kevlar S706 fabric. This plain-weave architecture fabric has an areal density of 183.43 g/m^2, a thickness of 0.282 mm, and a yarn span of 0.747 mm in the warp and fill directions. The nominal denier of the warp and fill Kevlar KM2 yarns is 600. Each yarn comprises 400 approximately circular fibers of nominal diameter 12 μm and density 1.44 g/cm^3. Fig. 1 displays optical micrographs of the warp and fill yarn cross-sections of the Kevlar S706 fabric.

2.2. Setup of the initial finite element model of the weave architecture

2.2.1. Generating the starting yarn volumes and mesh

The process begins with generating the 1D yarn centerlines of the weave architecture. For simple 2D weave architectures, the centerlines may be represented by smooth, continuous mathematical functions that repeat over the dimension of the weave unit cell. For example, the yarn centerlines of a plain-weave fabric can be represented by sinusoidal functions as follows:

$$y_i^{warp} = +\frac{t^{warp}}{2}\cos\left(\frac{\pi x_i^{warp}}{s^{fill}}\right) \tag{1}$$

$$y_i^{fill} = -\frac{t^{fill}}{2}\cos\left(\frac{\pi z_i^{fill}}{s^{warp}}\right) \tag{2}$$

Here, 't' represents the yarn thickness, 's' represents the yarn span (i.e. yarn spacing or the distance between two yarns). The warp yarn centerlines are along the X axis and the fill yarn centerlines are along the Z axis. The Y axis represents the fabric thickness direction. 'x_i' and 'z_i' represent discrete points along the 1D yarn centerlines between the origin and the fabric length and width respectively. Following this sinusoidal 1D centerline representation, the profiles of the 2D yarn cross-sections are given by:

$$y_i^{warp} = \frac{t^{warp}}{2}\cos\left(\frac{\pi z_i^{warp}}{s^{warp}}\right) \tag{3}$$

$$y_i^{fill} = \frac{t^{fill}}{2}\cos\left(\frac{\pi x_i^{fill}}{s^{fill}}\right) \tag{4}$$

Here, 'z_i' represents a set of discrete points about the origin between $-w^{warp}/2$ and $+w^{warp}/2$ (i.e. spans the warp yarn width) while 'x_i' similarly represents a set of discrete points between $-w^{fill}/2$ and $+w^{fill}/2$ (i.e. spans the fill yarn width) with 'w' representing the yarn width. Both the upper and lower profiles of the 2D yarn cross-section follow these equations (i.e. horizontal line of symmetry), thus the yarn cross-sectional shapes are also 'sinusoidal' (note, this is somewhat similar to a 'lenticular' shape). These 2D yarn cross-sections are swept along the 1D yarn centerlines to generate the 3D textile weave architecture. Equations (1)–(4) also indicate that the warp yarn cross-sectional shapes are governed by the fill yarn centerlines and vice-versa.

Another possible representation for plain-weave fabric architectures with elliptical yarn cross-sections utilizes a combination of ellipses and tangential connecting lines for the yarn centerlines [20]. For more complex weave architectures such as 2.5D angle-interlocks and layer-to-layer interlocks as well as 3D orthogonals and stepped-orthogonals, 1D yarn loci generators such as Cox et al. [16] can be employed. However, it should be noted that the starting 1D yarn centerlines only need be approximate representations of the actual centerline paths (i.e. an approximate representation of the overall topology of the textile architecture) because the mechanics-driven component of the thermal growth microstructure generation