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Sample-based synthesis of two-scale structures with anisotropy☆

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ABSTRACT

A vast majority of natural or synthetic materials are characterized by their anisotropic properties, such as stiffness. Such anisotropy is effected by the spatial distribution of the fine-scale structure and/or anisotropy of the constituent phases at a finer scale. In design, proper control of the anisotropy may greatly enhance the efficiency and performance of synthesized structures.

We propose a sample-based two-scale structure synthesis approach that explicitly controls anisotropic effective material properties of the structure on the coarse scale by orienting sampled material neighborhoods at the fine scale. We first characterize the non-uniform orientations distribution of the sample structure by showing that the principal axes of an orthotropic material may be determined by the eigenvalue decomposition of its effective stiffness tensor. Such effective stiffness tensors can be efficiently estimated based on the two-point correlation functions of the fine-scale structures. Then we synthesize the two-scale structure by rotating fine-scale structures from the sample to follow a given target orientation field. The effectiveness of the proposed approach is demonstrated through examples in both 2D and 3D.

1. Introduction

1.1. Motivation and goals

Anisotropy of material refers to the dependence of material's properties on direction. Anisotropy should not be confused with heterogeneity, which is the property of being location dependent. A material can be homogeneous on the coarse scale and have its fine-scale structures being anisotropic at the same time, as is the case, for example, with carbon fiber sheets in composite manufacturing. Similar to heterogeneity, anisotropy is a property of scales, depending on the effective material property of the associated neighborhood. Many nature and man-made materials exhibit various degrees of anisotropy. For example, crystalline materials are generally anisotropic, as many of their physical properties depend on the direction of the crystal. Wood is anisotropic with a high percentage of grains parallel to the tree trunk. The fine scale structures of bones are anisotropic with internal architecture of the trabeculae adapting to the loads, making bones more efficient given the competing constraints in nature.

The term anisotropy is overloaded in the context of material structures. Depending on how it is measured, it could refer to **geometry anisotropy**, where the statistics of the structural geometry is anisotropic; it could also refer to **property anisotropy**, where the physical properties of the material are anisotropic. It is widely accepted that the latter is the result of the former combined with the third type of anisotropy: the material anisotropy of the constituent phases of the fine scale material structure, which can be regarded as the property anisotropy from a finer scale. This also suggests that property anisotropy at the course scale can be controlled locally by rotation of the fine-scale structure, which is the orientation control mechanism adopted in the present work.

Mankind has relied on and benefited from material anisotropy for many centuries, from using the ancient combination of straw and mud to form brick for building construction to modern day prestressed concrete and fibrous composites [1]. Even though the mechanism is straightforward, most of the fine-scale structures controlling the property anisotropy of the man-made materials to date can be reasonably characterized as one-dimensional, e.g. rebar in the concrete, fiber in the composite. This is partly due to the difficulties involved in the characterization of property anisotropy of 3D material structures (see Section 2.1), and partly due to inherent complexity of the design and manufacturing of three-dimensional multiscale structures [2]. The rapid advancement of additive manufacturing technologies eliminates many of the geometric restrictions in traditional subtractive manufacturing processes, enabling the fabrication of three-dimensional multiscale structures in place of traditional solid parts. The goal of this paper is to propose a computational framework that facilitates the design of

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two-scale material structures with anisotropic properties at coarse scale controlled by geometric synthesis at the fine scale.

1.2. Contributions and outline

We propose a sample-based approach to synthesis of two-scale structures while controlling the spatial orientation of the anisotropic material properties at the coarse scale (see Fig. 1). After reviewing the related work on material anisotropy characterization and texture synthesis for fine-scale structure modeling in Section 2, an automatic way to determine the orientation of the material property anisotropy directly from the elasticity tensor of an orthotropic material is proposed in Section 3.4 (Fig. 1c). This is done by first converting the 4th-rank elasticity tensor into the 6 by 6 matrix form with Mandel notation and calculating the eigenvalues and eigenvectors of the matrix with the commonly available tools. We then compute the principal strains of the dominant strain vector with another eigenvalue decomposition after converting the strain vector back into the tensor form. We prove that resultant directions of principal strains are the principal axes of the orthotropic material.

For sample structures with non-uniform orientations, multiple boundary value problems may need to be solved for the coarse scale effective material properties to characterize the spatial orientation distribution of material anisotropy. In Section 4, we efficiently estimate the effective elasticity tensors of fine-scale structures based on their two-point correlation functions (Fig. 1b). A significant speed-up is observed without sacrificing the accuracy of the spatial orientation distribution of the fine-scale structures.

In Section 5, we develop and implement texture synthesis techniques to generate the two-scale structures whose material anisotropies follow target orientation fields prescribed on the coarse scale. First, the principal axes of the fine-scale structures in the sample are aligned with directions of the image lattice grid (Fig. 1d). This step is a necessary addition to the traditional texture synthesis algorithms where the orientation of the sample structure is often assumed to be constant. Then the new two-scale structure is synthesized by rotating these fine-scale structures to align with the target orientation field (Fig. 1e). Gaussian pyramid and correction subpasses are engaged to parallelize the algorithm. The effectiveness of the proposed approach is demonstrated through examples. Section 6 concludes with discussions.

2. Related works

2.1. Material anisotropy characterization

Most existing methods characterize material anisotropy by the geometry of fine-scale structures of material. One common way to characterize the geometry anisotropy is to measure the directional variations of average chord lengths, where a chord is a segment of an infinite straight line fully contained in a single phase [3]. The method is often referred as mean intercept lengths (MIL) in the literature. Such characterization has been widely adopted for the studies of trabecular bones [4–7]. The distribution of cord lengths is found to have the shapes of ellipses (ellipsoidal in three dimensions) indicating the trabecular bones are orthotropic according to these measures.

Minkowski tensors [8], which are the tensorial generalization of Minkowski functionals [9], have also been used to characterize the geometry anisotropy. Measures of anisotropy have been proposed based on eigenvalue ratios of Minkowski tensors [10]. Minkowski tensors have been used in the anisotropy analysis of the shape of neuronal cells [11] and galaxies [12].

Fourier transforms have been applied to characterize the geometry anisotropy of various structures, including electrodeposited patterns [13], trabecular bone [14], and fiber systems [15]. The approach is based on the observation that major structural direction lines in the spatial domain image correspond to high values of frequency components in the frequency domain [15]. The wavelet transform has also been used to characterize the anisotropy in paper structure [16]. One problem with all frequency domain approaches is that they measure the boundaries of structures rather than the structures themselves, which may lead to the loss of important anisotropic information [17].

To use the material anisotropy in design, the relationship between the geometry anisotropy and the anisotropy of the physical property of interest also needs to be established. Huber and Gibson [18] associated anisotropy of chord lengths with anisotropy of Young's modulus through an axisymmetric unit cell model proposed in [19]. Good agreements are found between experimental results and the proposed formula for polyurethane foams. However, the model is tailored for low-density axisymmetric foams and does not apply to general fine scale material structures. In addition, the possible anisotropy of the constituent phases is often left out in such relations. The geometry-based characterization will cease to work for polycrystalline, where each individual crystal inside has its own orientation. As an alternative, a new approach to characterize anisotropy directly from the effective elasticity tensor of the material is proposed in Section 3.4.

2.2. Texture synthesis for fine-scale structure modeling

Texture synthesis in the field of computer graphics and computer vision has matured during the last two decades [20–24]. Texture synthesis aims to create large non-repetitive images from a small input texture. The term "texture" generally refers to images containing repeated patterns with a certain amount of randomness. During the synthesis process, the new texture is synthesized based on an existing sample such that the resulting pattern and existing sample appear to be generated by the same underlying stochastic process [20].

Texture synthesis techniques have recently been adopted for fine-scale material structure modeling by several researchers. For example, Holdstein et al. [25] designed the bone scaffold as the complement of the missing bone structures generated by volumetric texture synthesis. The mechanical property of the designed scaffold is later modified by morphological operations to match the performance of the original bone structure. Liu and Shapiro [26] demonstrated that texture synthesis can be used to reconstruct a variety of periodic and random heterogeneous structures while preserving their geometric, topological, and physical properties. Machine Learning approaches such as classification trees and convolutional deep belief networks have been proposed to accelerate the reconstruction process [27,28]. The reconstruction of 3D material structures from 2D cross-sectional images has been studied in [26,29,30]. Acar and Sundararaghavan [31] modeled the spatio-temporal evolution of microstructures with a movie of microstructure evolution over a small sample window as the sample input. Liu and Shapiro [32] proposed the design and reconstruction of functionally graded material (FGM) structure by representing and controlling material properties of FGM at macro scale using the notion of material descriptors which include common geometric, statistical, and topological measures, such as volume fraction, correlation functions, and Minkowski functionals. The proposed algorithm to generate a two-scale structure with fine-scale structures from the sample rotated to aligned with the given coarse scale orientation field is inspired by results in [23,33]. To the best of our knowledge, such techniques have not been applied to the two-scale material structure modeling.

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