Sample-based synthesis of two-scale structures with anisotropy

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A R T I C L E   I N F O

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A B S T R A C T

A vast majority of natural or synthetic materials are characterized by their anisotropic properties, such as stiffness. Such anisotropy is affected 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.

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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 coarse 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
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 anisotopic information [17].

To use the material anisotropy in design, the relationship between the geometry anisotropy and the anisotropy of the physical property of interest 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.
3. Orientation of an anisotropic material

In this section, we identify the orientation of a material directly from its elasticity tensor — the material property of interest in the present paper. We note that the proposed method also applies to other tensorial properties, such as thermal and electrical conductivity. We define the orientation of a material by the directions of its principal axes. For orthotropic material, principal axes of material are defined as the three orthogonal directions where three planes of symmetry meet [34]. We generalize the definition of principal axes to other anisotropic materials in Section 3.4. To find the principal axes of a material, the following conjecture is made:

The principal axes of an orthotropic material coincide with the principal directions of the strain, which is the dominant eigentensor (eigentensor associated with the largest eigenvalue) of the material’s elasticity tensor if such principal directions are uniquely defined.

The eigentensor of a fourth-rank tensor is defined by Mehrabadi and Cowin [35]: “The eigenvectors of the 3-dimensional fourth-rank anisotropic elasticity tensor, considered as a second-rank tensor in a 6-dimensional space, are called eigentensor when projected back into the 3-dimensional space”.

We say the principal directions of a strain tensor are uniquely defined when the strain is not isotropic or transverse isotropic, i.e. the three principal strains all have different numeric values. We choose Mandel notation as $6 \times 6$ matrix representation of the fourth-rank elasticity tensor. The advantage of Mandel notation over Voigt notation is explained in [36]. We include a brief discussion on the Eigen decomposition of the elasticity tensor before proving the conjecture in 2D. The discussion may be obvious to some researchers and unknown to others, and therefore is included.

3.1. Eigen decomposition of the elasticity tensor

Eigen decomposition of elasticity tensor was first studied by Lord Kelvin [37], who determined the eigentensor of a fourth-rank tensor in 3-dimensional space by the eigenvectors of the second-rank tensor in 6-dimensional space. Since the eigenvectors of elasticity tensor in Mandel notation are strains, we refer to them as strain eigentensor and to corresponding stress vector as stress eigentensor. The properties of strain and stress eigentensors follow the general properties of eigenvectors regardless of the material symmetry. For example, the strain and stress can be decomposed into a sum of six or fewer eigentensors. And the stress eigentensor is proportional to its strain eigentensor. We also note that dominant strain eigentensor is the unit strain that maximize the strain energy, hence the efficiency, of the material.

Kelvin determined the eigenstrains for many material symmetries and summarized his results in Encyclopaedia Britannica. We give a brief summary of his results here. Readers may refer [35] for a detailed review. For materials with isotropic and cubic symmetries, only two and three distinct eigenvalues were found, respectively. Four different eigenvalues were found for materials with transverse isotropic and hexagonal symmetries. Five different eigenvalues exist for materials with tetragonal symmetry. Only materials with orthotropic symmetry and no general symmetries have all six different eigenvalues. We observe that the largest eigenvalue of the elasticity tensor always has the multiplicity of one, meaning the eigentensor maximizing the strain energy is uniquely defined unless the strain is isotropic or transverse isotropic. In the latter case, the number of strains to maximize the strain energy is infinite. Next, we will discuss how to predict the principal orientation of the material based on the largest eigenvalue and corresponding strain eigentensor with the assumption of orthotropic symmetry.

3.2. Proof of the conjecture in 2D

The proof of the conjecture consists of two steps. In the first step, we study the optimal orientation of the material for a given unit strain. We first calculate the strain energy which is a function of the relative orientation between the material and the given strain. We then show that the alignment of the principal orientation of material and principal directions of the given strain is one of the potential stationary points when maximizing or minimizing
the strain energy. This first step is inspired by the work of Cheng and Pedersen [38].

In the second step, we show that other potential stationary points will not become actual stationary points when the given strain eigentensor has the potential to maximize the strain energy among all possible unit strain tensors. Therefore the principal orientation of the material is aligned with the principal directions of the dominant eigentensor.

The following is the detailed proof of the conjecture in 2D. The elasticity tensor of 2D orthotropic material, when its principal orientation coincides with the reference coordinate system, takes the form:

\[
\mathbf{C} = \begin{bmatrix}
C_{11} & C_{12} & 0 \\
C_{12} & C_{22} & 0 \\
0 & 0 & C_{33}
\end{bmatrix}.
\]

For a given strain \(\epsilon\), let \(\theta\) be the angle between the principal orientation of the orthotropic material and the principal directions of the strain. The rotation matrix in Mandel notation is:

\[
\mathbf{R} = \begin{bmatrix}
c^2 & -s^2 & -\sqrt{2}cs \\
s^2 & c^2 & \sqrt{2}cs \\
\sqrt{2}cs & -\sqrt{2}cs & -2s^2
\end{bmatrix},
\]

where \(c = \cos(\theta)\) and \(s = \sin(\theta)\). For different relative orientations \(\theta\), the strain energy is calculated as:

\[
U = \epsilon^T \mathbf{R} C \mathbf{R}^T \epsilon
\]

\[
= \epsilon_1^2 c^2 + \epsilon_2^2 s^2 c^2 + \epsilon_2^2 e_1^2 c^2 + 2\epsilon_1 \epsilon_2 e_1^2 e_2^2 c_1 c_2 + 2c_2^2 (\epsilon_1 - \epsilon_2)^2 c_3^2
\]

where \(\epsilon = (\epsilon_1, \epsilon_2, 0)^T\) is the given strain in its principal directions.

To maximize or minimize the strain energy, we shall evaluate its derivatives. The partial derivative of \(U\) for a given strain with respect to \(\theta\) is:

\[
\frac{\partial U}{\partial \theta} = \epsilon^T \frac{\partial \mathbf{R}}{\partial \theta} \mathbf{R}^T \epsilon + \epsilon^T \mathbf{R} \frac{\partial \mathbf{R}^T}{\partial \theta} \epsilon = 2 \epsilon^T \frac{\partial \mathbf{R}}{\partial \theta} \mathbf{R}^T \epsilon
\]

\[
= -2s(2\theta) [\epsilon_1^2 - \epsilon_2^2] \cos(2\theta) [\epsilon_1 - \epsilon_2] c_1 c_2
\]

\[
+ c_2^2 (2 - c_3^2) + c_1 (\epsilon_1 + \epsilon_2) - 2c_2 (\epsilon_1 - \epsilon_2)].
\]

Let \(\partial U/\partial \theta = 0\), we have the following solutions:

\[
\theta = 0^\circ \text{ or } 90^\circ
\]

\[
\theta = \pm \frac{1}{2} \arccos \left( \frac{c_1 (\epsilon_1 + \epsilon_2) - c_2 (\epsilon_1 - \epsilon_2)}{\epsilon_1 - \epsilon_2} \right) \text{ or } \frac{1}{2} \arccos \left( \frac{1}{c_1 - 2c_2 + c_3} \right)
\]

where the first solution (Eq. (1)) implies alignment of the principal strain and the principal orientation of orthotropic material, the second solution (Eq. (2)) is a non-trivial high shear case and is not always feasible [38]. It is straightforward to show that the \(0^\circ\) alignment renders a higher strain energy than the \(90^\circ\) alignment. However, it is less straightforward to show the existence of the second solution and when it maximizes or minimizes the strain energy. Of course, none of these would matter if the given strain were isotropic and the derivative of \(U\) were always 0.

Nonetheless, to prove our conjecture, we only need to show that the second solution is not feasible when the given strain is the dominant strain eigentensor of the material’s elasticity tensor. Recall that the largest eigenvalue of the elasticity tensor does not repeat itself, meaning that the unit strain to maximize the strain energy is always uniquely defined (except for the isotropic strain, as shown both in the third solution and in Table 1). Since \(U\) is an even function of \(\theta\), the two results in the second solution inevitably lead to the same strain energy, which contradicts the uniqueness of the largest eigenvalue. As a result, the second solution is not feasible when the given strain is the dominant eigentensor and therefore the principal orientation of an orthotropic material coincides with the principal directions of the given strain. This concludes the proof in 2D.

### 3.3. Discussion for 3D cases

Due to the number of terms involved, we were not able to give a close form solution of the relative orientation to maximize or minimize the strain energy in 3D as we did in 2D. However, we were able to verify that \(\alpha, \beta, \gamma \in \{0^\circ, 90^\circ\}\). Tait–Bryan angles representing the relative orientations between the principal directions of the given strain and principal axes of the orthotropic material, are stationary points for the strain energy.

The elasticity tensor of 3D orthotropic material, when its principal orientation coincides with the reference coordinate system, takes the form:

\[
\begin{bmatrix}
C_{11} & C_{12} & C_{13} & 0 & 0 & 0 \\
C_{12} & C_{22} & C_{23} & 0 & 0 & 0 \\
C_{13} & C_{23} & C_{33} & 0 & 0 & 0 \\
0 & 0 & 0 & C_{44} & 0 & 0 \\
0 & 0 & 0 & 0 & C_{55} & 0 \\
0 & 0 & 0 & 0 & 0 & C_{66}
\end{bmatrix}.
\]

Just like in 2D case, the strain energy may be calculated for different relative orientations:

\[
U = \epsilon^T \mathbf{R} C \mathbf{R}^T \epsilon
\]

where \(\mathbf{R}\) is the rotation matrix in Mandel notation mapped from the tensor notation with the form:

\[
\begin{bmatrix}
1 & 0 & 0 & 0 & \cos(\beta) & 0 \\
0 & \cos(\gamma) & -\sin(\gamma) & 0 & \sin(\beta) & 0 \\
0 & \sin(\gamma) & \cos(\gamma) & 0 & -\sin(\beta) & 0 \\
\end{bmatrix}
\]

It is easy to verify in MATLAB that \(\alpha, \beta, \gamma \in \{0^\circ, 90^\circ\}\) are indeed stationary points for the strain energy. These observations, together with the proof in 2D, lead us to conjecture that the proposed method is also applicable in 3D.

### 3.4. Principal axes of an anisotropic material

Most anisotropic materials are not perfectly orthotropic: some materials are only approximately orthotropic while others may share other type of material symmetry, e.g. triclinic, or no symmetry at all. Yet the proposed method to identify the three orthogonal axes still applies as the Eigen decomposition of the elasticity tensor does not assume any material symmetries. We define these three orthogonal axes as the principal axes of the material, which represent the principal directions of the unit strain maximizing the strain energy. This generalization allows us to define the orientation of anisotropic materials.

Fig. 2 shows the principal axes of the effective elasticity tensors of the sample materials. Young’s modulus and Poisson’s ratio, \(E = 1\) MPa, \(\nu = 0.3\) and \(E = 0.02\) MPa, \(\nu = 0.3\) are assigned to the white and black phases, respectively. Our efficient method of estimating effective elasticity tensors will be discussed in the next section. What is worth to note is that the orientation of Fig. 2(c) does not correspond to the pattern in the structure by direct visual examination. However, the pattern becomes clear if lines parallel to the predicted major axis are drawn over the sample material.

Fig. 3 shows two examples of the algorithm in 3D. Same as the 2D examples, Young’s modulus and Poisson’s ratio, \(E = 1\) MPa, \(\nu = 0.3\) and \(E = 0.02\) MPa, \(\nu = 0.3\) are assigned to the white and black phases, respectively. In the first example, the major and minor axes align with the directions with most and least cross-section areas, therefore the stiffest and softest directions, respectively. In the second example, the major axis aligns with the direction of the pore and the directions of the minor and median axes capture the shape of the pore.
3.5. Limitation

One limitation of the algorithm is that the principal axes of the material cannot be completely determined if the directions of the principal strain or stress are not fully determined, i.e. two or more of the principal strains or stresses are identical. Table 1 shows effective stiffness, its largest eigenvalue and dominant eigenvector of the same material structure rotated at 0, 30, and 45°. Ignoring the discretization errors, every strain tensor maximizing the strain energy having identical principal strains in X–Y plane demonstrates that the proposed algorithm cannot detect the principal axes for this particular material structure. Young’s modulus and Poisson’s ratio, $E = 1$ MPa, $\nu = 0.3$ and $E = 0.02$ MPa, $\nu = 0.3$ are assigned to the white and black phases, respectively.

![Table 1](image)

### Table 1

<table>
<thead>
<tr>
<th>Material structure</th>
<th>Effective stiffness tensor</th>
<th>Largest eigenvalue</th>
<th>Eigenvector</th>
</tr>
</thead>
<tbody>
<tr>
<td><img src="image" alt="Square" /></td>
<td>$\begin{bmatrix} 0.1982 &amp; 0.0706 &amp; 0.0806 &amp; 0 &amp; 0 &amp; 0 \ 0.0706 &amp; 0.1982 &amp; 0.0806 &amp; 0 &amp; 0 &amp; 0 \ 0.0806 &amp; 0.0806 &amp; 0.2421 &amp; 0 &amp; 0 &amp; 0 \ 0 &amp; 0 &amp; 0 &amp; 0.1200 &amp; 0 &amp; 0 \ 0 &amp; 0 &amp; 0 &amp; 0 &amp; 0.1200 &amp; 0 \ 0 &amp; 0 &amp; 0 &amp; 0 &amp; 0 &amp; 0.0058 \end{bmatrix}$</td>
<td>0.5283</td>
<td>0.5281</td>
</tr>
<tr>
<td><img src="image" alt="Diamond" /></td>
<td>$\begin{bmatrix} 0.1874 &amp; 0.0814 &amp; 0.0806 &amp; 0 &amp; 0 &amp; -0.0087 \ 0.0814 &amp; 0.1873 &amp; 0.0806 &amp; 0 &amp; 0 &amp; 0.0087 \ 0.0806 &amp; 0.0806 &amp; 0.2421 &amp; 0 &amp; 0 &amp; 0 \ 0 &amp; 0 &amp; 0 &amp; 0.1199 &amp; 0 &amp; 0 \ 0 &amp; 0 &amp; 0 &amp; 0 &amp; 0.1200 &amp; 0 \ -0.0087 &amp; 0.0087 &amp; 0 &amp; 0 &amp; 0 &amp; 0.1174 \end{bmatrix}$</td>
<td>0.5282</td>
<td>0.5282</td>
</tr>
<tr>
<td><img src="image" alt="Square" /></td>
<td>$\begin{bmatrix} 0.1832 &amp; 0.0848 &amp; 0.0804 &amp; 0 &amp; 0 &amp; 0 \ 0.0848 &amp; 0.1832 &amp; 0.0804 &amp; 0 &amp; 0 &amp; 0 \ 0.0804 &amp; 0.0804 &amp; 0.2412 &amp; 0 &amp; 0 &amp; 0 \ 0 &amp; 0 &amp; 0 &amp; 0.1196 &amp; 0 &amp; 0 \ 0 &amp; 0 &amp; 0 &amp; 0 &amp; 0.1196 &amp; 0 \ 0 &amp; 0 &amp; 0 &amp; 0 &amp; 0 &amp; 0.1242 \end{bmatrix}$</td>
<td>0.3691</td>
<td>0.3645</td>
</tr>
</tbody>
</table>

4. Spatial orientation of the sample material structure

The orientation of material properties can, and often will, vary from point to point. To characterize the coarse scale orientation field of the sample structure, we first need to evaluate the effective material properties of neighborhoods in the sample material at the fine scale. The process to calculate the effective material property is commonly referred as homogenization [39]. One popular strategy for homogenizing a material structure numerically is through Finite Element Method (FEM) where six independent periodic boundary conditions are imposed [40]. Though being effective, the FEM approach may become computationally too expensive to evaluate multiple fine-scale structures in the sample. Facing this challenge, the effective material properties are often estimated through various homogenization theories, including the Gibson model for cellular materials [41]. Voigt–Ruess bounds, Hashin–Strikman bounds [42], Green’s function based method [43,44], and power law [45] which is frequently used in SIMP-based topology optimization [46]. Many of these homogenization theories rely on the rotation invariant volume fraction as the sole characterization of the material structure, therefore, failing to capture the important anisotropic structural information of the material.

Instead, we propose to use the two-point correlation function of the material structure to efficiently estimate the effective property of the material. A two-point correlation function is a special case of an $n$-point correlation function which can be defined as a probability that all vertices of a randomly tossed $n$-vertex polyhedron fall into the same phase of a material structure [47]. For a heterogeneous material, the indicator function $I^i(x)$ is defined as:

$$f^0(x) = \begin{cases} 1, & \text{if } x \text{ lies in phase } i, \\ 0, & \text{otherwise} \end{cases}$$

and the $n$-point correlation of phase $i$ is formulated mathematically as:

$$S_n^i(x_1, x_2, \ldots, x_n) = I^i(x_1) I^i(x_2) \ldots I^i(x_n).$$

The first moment of $n$-point correlation function

$$S_1^i(x) = I^i(x)$$

is just the volume fraction $\phi$. The second moment is two-point correlation function

$$S_2^i(x_1, x_2) = I^i(x_1) I^i(x_2)$$

which can be described as the probability that a randomly tossed line segment having both of its ends fall into phase $i$ (either material phase or void phase for a porous material).

To estimate the effective material property from its two-point correlation function, we start from the Lippmann–Schwinger
and black phases, respectively. (For interpretation of the reference to colour in this figure legend, the reader is referred to the web version of this article.)

Fig. 2. The principal axes of the effective elasticity tensors of 2D sample material structures. Red and blue arrows represent the major and minor axes, respectively. The median axes are represented in blue arrows. Young’s modulus and Poisson’s ratio, E = 1 MPa, ν = 0.3 and E = 0.02 MPa, ν = 0.3 are assigned to the white and black phases, respectively. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

Green’s function which is the impulse response of homogeneous reference material \( C^0 \), and \( ΔC \) is the difference between the elasticity tensors of the fine scale material structure and the reference homogenization material. The effective elasticity tensor may be derived by eliminating \( ϵ \) and \( ϵ^0 \) (see Appendix A for details):

\[
C_{\text{eff}} = C^0 + (ΔC(x)) - \left( \int_{Ω} δC(x)Γ(x, x')δC(x') \, dx' \right) \\
+ \left( \int_{Ω} \int_{Ω} δC(x)Γ(x, x')δC(x') \, Γ(x', x'')δC(x'') \, dx'' \, dx' \right) - \cdots \\
\tag{4}
\]

where \( ⟨. . .⟩ \) is the expectation of a function. Clearly, the integrands bear the form of correlation functions. We estimate the effective elasticity tensor of the material by truncating after the first line of this equation, which is informationally equivalent to the two-point correlation function of the material.

To make this more explicit, let us assume heterogeneous material has two phases and \( C^0 = C_1 \) is the material property of phases 1 in a two-phase material, so that \( δC(x) = I^{(1)}(x)(C_2 - C_1) \). Eq. (4) becomes

\[
C_{\text{eff}} = C_1 + (C_2 - C_1)(S^{(1)}(x)) \\
- (C_2 - C_1)^2 \left( \int_{Ω} Γ(x, x')S^{(1)}(x, x') \, dx' \right) \\
+ (C_2 - C_1)^3 \left( \int_{Ω} \int_{Ω} Γ(x, x')Γ(x', x'')S^{(1)}(x, x', x'') \, dx'' \, dx' \right) \\
- \cdots \\
\tag{5}
\]

which represents the elasticity tensor by a series expansion of all orders of correlation functions. The assumption may be relaxed for material to have more than two phases, but the equation will have significantly more terms.

Eqs. (4) and (5) allow the proposed method to take two different forms of inputs: (1) we may be given the detailed image of the material structure and our method only using information that is equivalent to the two-point correlation function, (2) or we may be given the correlation function of the material structure as the input to Eq. (5). The two different types of the input will result in the same estimation of the effective elasticity tensor.

Fig. 4 shows the spatial variation of principal axes within sample materials. The second and third columns of Fig. 4 compare the principal axes calculated from the effective elasticity tensors estimated from all terms (therefore, full field estimation) in Eq. (4) and terms equivalent to two-point correlation functions, respectively. Each set of principal axes is calculated from the effective elasticity tensor of a neighborhood in the sample material. The effects of different neighborhood sizes are discussed in the conclusion section.

Comparison of computation time between full field homogenization and the proposed two-point correlation function based method. Time is in seconds.

<table>
<thead>
<tr>
<th>Material</th>
<th>Full field</th>
<th>Correlation</th>
<th>Speed-up (times)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fig. 2(a)</td>
<td>542.25</td>
<td>54.62</td>
<td>9.93×</td>
</tr>
<tr>
<td>Fig. 2(b)</td>
<td>6028</td>
<td>53.43</td>
<td>112.82×</td>
</tr>
<tr>
<td>Fig. 4(a)</td>
<td>51.20</td>
<td>2.07</td>
<td>24.73×</td>
</tr>
<tr>
<td>Fig. 4(b)</td>
<td>80.91</td>
<td>5.48</td>
<td>14.76×</td>
</tr>
<tr>
<td>Fig. 4(c)</td>
<td>31.68</td>
<td>2.69</td>
<td>11.78×</td>
</tr>
<tr>
<td>Fig. 4(d)</td>
<td>106.27</td>
<td>6.73</td>
<td>15.79×</td>
</tr>
</tbody>
</table>

Table 2

Fig. 3. The principal axes of the effective elasticity tensors of 3D sample material structures. Red and blue arrows represent the major and minor axes, respectively. Young’s modulus and Poisson’s ratio, \( E = 1 \) MPa, \( ν = 0.3 \) and \( E = 0.02 \) MPa, \( ν = 0.3 \) are assigned to the white and black phases, respectively. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

The computation time and the relative speed-ups are reported in Table 2. An average of 16 times decrease in computation time is observed for 2D materials. The time to estimate each individual neighborhood by the correlation function based method depends only on the size of the neighborhood. As a result, the time to estimate effective elasticity tensors of the two material structures in Fig. 2 are nearly identical since they are discretized with the same resolution.

\[
ε(x) = ε^0 \cdot \int_{Ω} Γ(x, x')δC(x'x)dx', \\
\tag{3}
\]

where \( ε \) is the strain distribution of material structure under the constant strain \( ε^0 \) on the coarse scale, \( Γ \) is the second derivative of the equation, whose derivation may be found in the appendix of [44]:
5. Synthesis with rotated neighborhoods

Texture synthesis techniques are used to generate structures with non-uniform orientations from the sample material. Our implementation is inspired by results in [23,33] with the difference that our sample material may have non-uniform orientations predicted by the method proposed in the previous section. To address this issue, we first rotate its neighborhoods to align their principal axes with the lattice grid of the image. During the synthesis, we may rotate every neighborhood in the sample material to align...
with the target orientation field; or equivalently, we may rotate the neighborhood window of the synthesized structure and leave the input material sample intact. The latter approach is adopted in our implementation given its computational efficiency. Gaussian pyramid and correction subpasses are used to make the algorithm parallel (Fig. 5). The Gaussian pyramid is a stack of series of images which are smoothed (blurred) by a Gaussian kernel and then down-sampled. After finishing the sampling at the lower resolution, the result will be up-sampled to be the template of sampling at the higher resolution. The sampling will be determined by sites sampled at the lower resolution. The benefit of using Gaussian Pyramid is twofold: firstly, it alleviates the computational burden without jeopardizing the actual size of the neighborhood by using a much smaller window size for comparison at different levels of resolution. Secondly, lower level Gaussian Pyramid can be seen as a good initial guess to guide the sampling and therefore eliminate the dependency on sampling order. In this process, closer sites gain more weight than sites further apart.

Since the material structures are synthesized with neighborhoods upsamplied from a lower level of the image pyramid, these neighborhoods do not accurately represent the material at the current level of the MRF. Additional passes of sampling are required by using the neighborhoods from the current level of resolution. However, the concurrent resampling of all sites may lead to slow convergence or even cyclic changes because the neighborhoods of a site are also updating. To address this issue, we perform multiple resampling subpasses where only one site within a neighborhood is resampled in a single subpass.

Fig. 6 shows the design of two-scale structures with Fig. 4(d) as the sample input. The top row of Fig. 6 shows the relative density distribution of cantilever beams designed by SIMP-based topology optimization [48,49] with fixtures at the left edge and downward loads at the lower right corner. The objective of the optimization is to minimize the structure's compliance (total strain energy, a measure of global deformation). SIMP employs power law as the material interpolation scheme to relate the relative density \( \rho \) and Young's modulus of the material:

\[
E = E_{\min} + \rho^p (E_0 - E_{\min}), \quad \rho \in [0, 1]
\]

where \( E_0 \) and \( E_{\min} \) are Young's moduli of the solid and void materials, respectively. \( E_{\min} \) is non-zero to avoid singularity of the finite element stiffness matrix. Power \( p \) penalizes intermediate relative density and driving the structure towards a black-and-white design on the coarse scale.

The top row images on the left and right are optimization results with penalty factors \( p \) equal 3 and 1, respectively. Images on the second row represent the principal stress field inside the cantilever beams under the same boundary conditions as the optimization. The target orientation of the material structure is generated to follow the direction of major principal stress. Images on the third row show the sampling of design space without any rotation of the neighborhoods. These structures are generated to contrast with structures on the last row, which are designed material structures whose orientations follow the directions of major principal stress.

The compliance of the structures generated with and without the rotation of the neighborhoods is reported in Table 3. Stress concentrations near the boundary conditions may cloud the significance of the results. To remove such effects, we refine the generated structure by making the area near boundary conditions solid. Volume fractions and compliance of the refined structure, as well as their relative difference, are also reported in Table 3. The results clearly demonstrate the effectiveness of the proposed method by decreasing the total compliances of the synthesized structures by roughly 60% and 40%, respectively. It is also worth noting that Fig. 6(g) results in a smaller compliance than Fig. 6(f) with only about the half of its volume fraction.

### Table 3

<table>
<thead>
<tr>
<th>Structure</th>
<th>Volume fraction</th>
<th>Compliance</th>
<th>Relative difference</th>
</tr>
</thead>
<tbody>
<tr>
<td>e</td>
<td>0.240</td>
<td>5280.3557</td>
<td>60.51%</td>
</tr>
<tr>
<td>g</td>
<td>0.231</td>
<td>2085.2674</td>
<td>0.01%</td>
</tr>
<tr>
<td>f</td>
<td>0.438</td>
<td>2378.2289</td>
<td>0.00%</td>
</tr>
<tr>
<td>h</td>
<td>0.412</td>
<td>1431.6915</td>
<td>0.00%</td>
</tr>
</tbody>
</table>

### 6. Conclusion and discussion

We proposed a sample-based two-scale structures synthesis approach that explicitly controls the spatial orientations of the anisotropic effective properties on the coarse scale. An automatic way to characterize the material anisotropy is proposed by directly determining the principal axes of the fine scale structure from its effective elasticity tensor. The expensive numerical homogenization process for the effective elasticity tensor is replaced by a much more efficient two-point correlation function based method with minimum impacts on accuracy. The proposed method extends naturally other tensorial material properties, including electrical and thermal conductivity.

The current implementation infers the target orientation field from the principal stress field of a cantilever beam designed by
SIMP-based topology optimization method. This is heuristics for two reasons. Firstly, the material is assumed isotropic during the SIMP iteration and therefore does not provide the optimal material property distribution for the beam that will subsequently be made from anisotropic two-scale structures. For a better integration of the two scales, the constraints imposed by the sample materials could be included in the optimization iterations to concurrently update both isotropic and anisotropic aspects of the coarse scale effective material properties. Secondly, the alignment of the principal axes of material and the principal direction of the stress only guarantee to maximize the strain energy only when the material is orthotropic and the stress is not high shear (see Eq. (1)). The direction to maximize the efficiency of a general anisotropic material is still an open issue for a given arbitrary stress.

Another open issue in the present work is the size of the neighborhood for the evaluation of material properties. Fig. 7 shows the effects of different neighborhood size on orientations of neighborhoods. It is evident that orientations from larger neighborhood render smoother and more continuous variation while ones from the smaller neighborhood are more sensitive to local variations of the material structures. In our implementation, we opt for the larger neighborhood size to capture the general trend within the sample material structure. Albeit requiring a longer time to evaluate, a larger neighborhood can potentially improve the computational efficiency by interpolating the distribution of principal axes from a few sampling neighborhoods due to the relative smoothness of the field.

Acknowledgments

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Appendix A. Effective elasticity tensor by correlation functions

In this section, we derive relationship between correlation functions and effective elasticity tensor from Neumann series expansion of the Lippmann–Schwinger equation. We first eliminate strain $\epsilon$ from Eq. (3). Rearrange $\epsilon$ and $\epsilon^0$ and multiple $C$ on the both sides of Eq. (3):

$$\epsilon = [I + \Gamma \delta C]^{-1} \epsilon^0$$

(A.1)

$$\sigma = (C^0 + \delta C)[I + \Gamma \delta C]^{-1} \epsilon^0.$$  

(A.2)

Take the average on both side of Eq. (A.1) and Eq. (A.2)

$$\tau = (I + \Gamma \delta C)^{-1} \epsilon^0$$

(A.3)

$$\sigma = (C^0 + \delta C)[I + \Gamma \delta C]^{-1} \epsilon^0.$$  

(A.4)

Combine Eq. (A.3) and Eq. (A.4) to eliminate $\epsilon^0$

$$\sigma = (C^0 + \delta C)[I + \Gamma \delta C]^{-1} \xi$$

By the definition of effective elastic tensor

$$C^{\text{eff}} = ([C^0 + \delta C][I + \Gamma \delta C]^{-1})^{-1}$$

(A.5)

If both bodies of the same domain are subject to the same displacement boundary condition, they share the same mean strain, i.e. $\epsilon^0 = \tau$. Eq. (A.1) becomes

$$\tau = (I + \Gamma \delta C)^{-1} \tau.$$  

(A.6)

Multiply Eq. (A.6) on both sides of Eq. (A.5)

$$\sigma = C^{\text{eff}} \tau = C^0 \tau + \langle \delta C[I + \Gamma \delta C]^{-1} \xi$$

$$C^{\text{eff}} = C^0 + \langle \delta C[I + \Gamma \delta C]^{-1}.$$  

(A.7)

Use Neumann series (generalized geometric series) to expand the right side of Eq. (A.7)

$$C^{\text{eff}} = C^0 + \langle \delta C \rangle - \langle \delta C \Gamma \delta C \rangle + \langle \delta C \Gamma \delta C \Gamma \delta C \rangle - \cdots$$

$$= C^0 + \langle \delta C \rangle - \langle \delta C \xi \rangle - \langle \delta C \rangle \int_{\Omega} \Gamma(x, x') \delta C(x') \, dx'$$

$$+ \langle \delta C \rangle \int_{\Omega} \Gamma(x, x') \delta C(x') \, dx' \int_{\Omega} \Gamma(x, x') \delta C(x') \, dx' \cdots$$

where $C^0$ is the constant reference material property and $\delta C(x) = C(x) - C^0$. Combine the integrals and move $\delta C(x)$ inside:

$$C^{\text{eff}} = C^0 + \langle \delta C \rangle - \int_{\Omega} \delta C(x) \Gamma(x, x') \delta C(x') \, dx'$$

$$+ \int_{\Omega} \delta C(x) \Gamma(x, x') \delta C(x') \, dx' \int_{\Omega} \Gamma(x, x') \delta C(x') \, dx' \cdots$$

References


