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Correlating structure topological metrics with bulk composite properties via neural network analysis

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ABSTRACT

Given a database of any quantifiable set of cause and effect, machine learning methods can be trained to predict future effects based upon an assumed set of causes. In this paper, neural networks are trained to predict the bulk Young's modulus and electrical conductivity of a two-phase composite with high material property contrast, based upon a sample's microstructure. Various structure metrics are used to quantify the topological connectivity and disorder of analytically generated heterogeneous samples. The neural network is trained to predict the Young's modulus and coefficient of electrical conductivity based upon values calculated for a training set of samples using a finite element model. By repeating the process with various subset of structure metrics we can determine which metrics—or combination of metrics—have the strongest influence in accurately predicting bulk material properties. Not only are neural net predictions of bulk properties in good agreement with calculated values for the 2D two-phase composites, but the insights into which metrics most strongly correlate with these properties (in this case, the connectivity metrics) may help focus the development of improved structure–property relations.

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1. Introduction

Composites composed of two or more constituent materials are studied extensively in materials science and engineering. Homogenizing the locally heterogeneous properties and structure to arrive at global properties for such a material is a common goal [1–6]. Understanding how the microstructure of a heterogeneous material influences its bulk properties (such as Young's modulus and electrical conductivity) may ultimately allow the microstructure of the material to be designed and fabricated in such a way as to produce specifically desired bulk properties in the material [7–9].

Exact solutions for the homogenization of spheres, ellipsoids, and other geometries of a material deposited within a matrix of a second material have been determined analytically ([1,2]). However, not all material arrangements have an analytical solution describing homogenized behavior. To gain better understanding of these materials, theories have been developed to predict bulk material properties as well as possible ranges of values. *Effective medium theory* is one such theory that works well in predicting the homogenization values of a sample whose constituent materials have material property values similar to each other [10]. Effective medium theory becomes less accurate for homogenization as the constituent material properties become more and more dissimilar. For samples composed of dramatically different constituent materials *percolation theory* is a more appropriate tool to determine bulk properties [11–13]. Furthermore, various theories exist for providing bounds on the range of possible values of homogenized physical properties for a heterogeneous material [14–17].

Homogenization methods can often produce an accurate estimation of bulk properties under certain conditions, but each falls short in pinpointing exact values consistently. This may be due as much to insufficiency of structure information in the structure metrics that are input to the models as it is to the overall failings of the model itself to capture underlying physics. Typical descriptors of structural arrangement include n-point statistics [2,8], clustering [18] and percolation metrics [10,12,19,20]. More recently, interest has risen in more esoteric structure metrics, such as homology [21–23] and geometrical entropy [24,25]. The aim of this paper will be to assemble a variety of different structure metrics that describe connectivity, entropy, etc. and feed these into a machine learning environment to determine which structure descriptors have the strongest influence on the global properties, and to determine whether an accurate prediction of homogenized properties is possible using the full set of metrics.

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2. Materials and methods

In order to assess the structure–property relations of a range of 2D heterogeneous material samples, two-phase composites are created on a simple square lattice that is 128 by 128 pixels using Matlab [26]. These two dimensional samples may be referred to as plates. The size of the plates was chosen to enable numerous computations to be undertaken in a reasonable amount of time, while also providing samples that are at least close to being representative of a bulk material geometry. In our investigation, all samples are 50% matrix (black) and 50% particulate (white). The contrast between the properties of the two material phases is high for both stiffness and electrical conductivity. The matrix has values of Young's modulus and electrical conductivity of $E_1 = 10^7$ Pa, and $\sigma_1 = 10^5$ S/m, respectively. The particles have the properties $E_2 = 7 * \text{Pa}$, and $\sigma_2 = 10^9$ S/m. These properties represent a typical order of magnitude contrast that might be found in common composite materials.

Three different sample-generating algorithms are employed so that a variety of geometrical arrangements can be analyzed. These algorithms employ different methods for clustering particles. The first algorithm creates microstructures that exhibited chains of approximately spherical particles that are "strung" together, thus the name, "stringy clusters". In this algorithm, particles are seeded by randomly selecting center points until 10% of the desired volume fraction is reached. Then, as the additional particles are placed, they are moved some percentage closer to their nearest neighbor. The second algorithm creates microstructures that feature clusters that are circular in nature called "circle clusters". In this algorithm, particles are randomly placed into a virtual circle, which represented a cluster, until a specified volume fraction is reached. The cluster was then randomly placed in the sample space. This process continues until the desired sample volume fraction is reached. Clusters never have a diameter more than half the height of the sample plate (64 pixels). The third and final algorithm for generating sample plates is to randomly assign each pixel of our lattice to be either matrix or particle material. Fig. 1 shows examples of plates generated from these algorithms. The volume fraction of each of these algorithms is adjustable; more details regarding these algorithms are given in Ref. [27].

3. Calculation

3.1. Microstructure metrics

The constituent materials of any heterogeneous sample can form into an essentially infinite number of geometric arrangements. Attempting to describe the precise geometric layout of material phases is impractical, and may even be impossible. However, there are topological and large-scale behaviors that can easily be described in a quantitative manner.

In this analysis nine metrics of the composite structure are used. These metrics relate to the connectivity/percolative nature, the homology and the entropy of the system. In the list of them, below, the first six are measures of topological connectivity related to homology; the last two are geometric measures; and the remaining metric, entropy, is a measurement of disorder. We also include the range of values observed in this study. See the Appendix for more details regarding the individual definitions, and examples of metric values for particular structures.

1. Betti zero: the number of disconnected pieces of particulate material. $\beta_0(\chi)$ [1,291].
2. Betti one: the number of independent interior loops within particle clusters. $\beta_1(\chi)$ [0,1100].
3. Betti zero/Betti one: $\beta_0(\chi)/\beta_1(\chi)$. [0.00658, 65535]; the peak value is capped when $\beta_1(\chi)$ is zero.
4. Relative Betti zero homology: the Betti zero number for the plate with top and bottom edges of plate acting as particulate material. $\beta_0(\chi, T+B)$ [0, 263].
5. Relative Betti one homolgy: the Betti one number for the plate with top and bottom edges of plate acting as particulate material. $\beta_1(\chi, T+B)$ [0, 1156].
6. Percolation: equates to one if percolation occurs across the particles, else zero. (P) [0, 1].
7. Entropy: the disorder of the materials within the sample plate. (e) (see Appendix) [183.3, 5700.66].
8. Maximum cluster height: the height of the cluster of particulates. (h_{max}) [33, 128].
9. Mean cluster height: the arithmetic mean height of all clusters of particulates. (h_{avg}) [2.94, 126].

3.2. Finite element analysis

The bulk properties are calculated using finite element software ANSYS [28]. The two material properties that we examine, Young's modulus and electrical conductivity, are calculated only in the vertical direction (see Fig. 2). Material one (black) has a Young's modulus of $E_1 = 1.0 * 10^7$ Pa, and conductivity of $\sigma_1 = 1.0 * 10^5$ S/m material two (white) has a Young's modulus of $E_2 = 7.0 * 10^9$ Pa, and conductivity of $\sigma_2 = 1.0 * 10^9$ S/m.

To calculate Young's modulus for a 2-D plate, the bottom nodes are prevented from moving in the y-direction. The top nodes are displaced by an equal distance in the y-direction to produce a sample strain of 0.01, thus keeping the top edge of the sample flat; the side nodes are free to move in x and y. The overall required force to produce the strain is used to calculate Young's modulus for the entire plate. Similarly, conductivity is found by applying a voltages

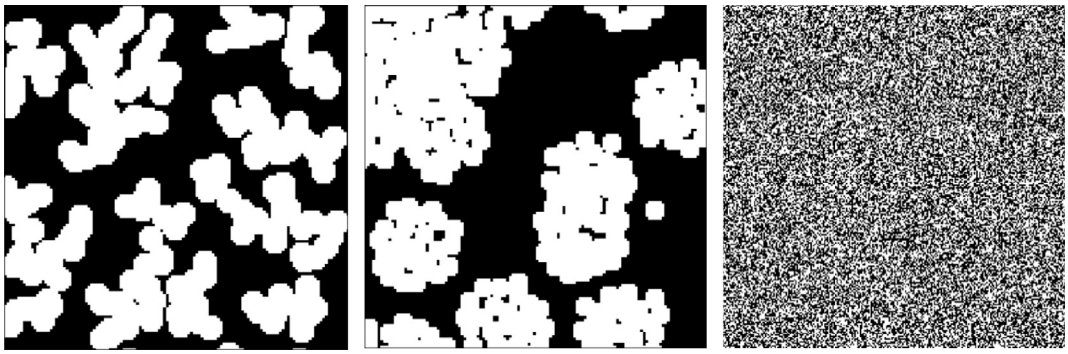

Fig. 1. Three different examples of geometrical arrangements of samples that might be used. *Left:* stringy cluster algorithm. *Middle:* circle cluster algorithm. *Right:* random placement.

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