

Multiscale shape–material modeling by composition

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ABSTRACT

We propose a formal framework for modeling multiscale material structures by recursive composition of two-scale material structures. The framework comprises three components: (1) single scale shape–material models, supported by single scale queries, to represent the geometry and spatial distribution of material property on each coarse and fine scales, (2) mechanisms to link the scales by establishing an explicit relationship between shape–material properties at fine scale and material properties at the coarse scale, and (3) multiscale queries abstracting fundamental multiscale operations by recursive composition. While the first component is consistent with classical solid heterogeneous material modeling, the second component manifests itself as a pair of conceptually new upscaling and downscaling functions. We show that classical solid modeling queries, exemplified by point membership testing, distance computation, and material evaluation, generalize to the corresponding multiscale queries that support implicit representations of multiscale structures as a composition of distinct single scale solid material models. The concept of neighborhood is indispensable in all three components. The framework provides a formal and consistent extension of solid modeling framework that underlies most commercial systems in use today, encompasses the variety of different approaches to multiscale modeling, identifies open issues and research problems with existing two-scale modeling methods, and provides foundations for next-generation systems by identifying key objects, classes, representation schemes, and API queries.

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1. Introduction

1.1. Motivation

Current computer-aided design (CAD) systems are widely adopted by the industry, replacing manual drawings with intuitive user interfaces, robust three-dimensional modeling, and the automatic generation of engineering drawings. The inherent limitations of traditional subtractive manufacturing processes also shield CAD systems from the need to model mechanical components with complex internal geometries and heterogeneous material compositions. This status quo is challenged by the rapid development of advanced manufacturing technologies, creating a critical demand for computer models to facilitate the design, analysis, and manufacturing planning of complex structures. A diverse body of examples includes, but is not limited to, laminated and composite objects, such as airplane wings and ship hulls, embedded sensors and actuators for active structures, mechanical components made of polycrystalline, porous, insulating materials and complex structures enabled by additive manufacturing.

The complexity of such structures is often distinctly characterized by the apparent presence of multiple length scales (see Fig. 1). The length scale is loosely defined as the smallest interval where a notable change of material property or physical phenomenon of interest can be observed or measured. The presence of multiple scales significantly changes the characteristics of a structure, in particular, its surface area. For example, metal foams with 5% relative density may have a surface area density up to 10,000 m²/m³, which is several orders of magnitude larger than that in traditional homogeneous solids. Heavily relying on the boundary representation (BRep), current CAD systems do not scale well with and often break down in the face of such geometric and material complexities.

Over the last decade, several methods have been developed for design and modeling of fine scale structures, ranging from periodic lattice infills to stochastically generated structures in materials. For example, material descriptors such as correlation functions [2] and nearest neighbor distribution [3] have been used to represent and reconstruct random heterogeneous materials. Metal foams are commonly modeled by various construction procedures, such as Boolean model [4] and Voronoi cells [5,6], defined over stochastic distribution of points. Periodic lattice structures may be efficiently represented by composing periodic functions with implicitly [7]

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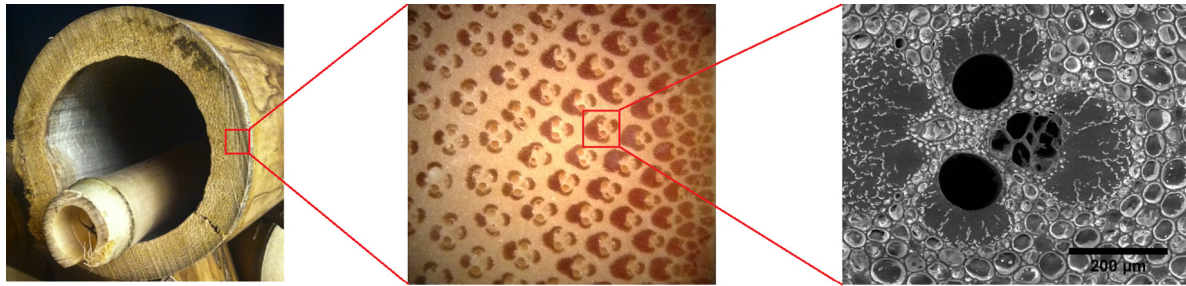


Fig. 1. Multiscale structures of bamboo. The complexity of the structure is distinctly characterized by the apparent presence of multiple length scales. SEM micrograph image courtesy of [1].

or parametrically [8] defined shapes. Unit cell approaches decompose the coarse-scale shape into disjoint regions that are filled by unit cells with predefined shapes and material properties [9–11]. The sample-based approach is most versatile among all methods, capable of modeling a wide range of material structures while fulfilling the requirement of effective material properties on the coarse scale [12]. We briefly review these methods in Section 2.2.

Some of these methods led to new commercial tools, such as nTopology and Autodesk Within, where periodic or Voronoi-based lattice structures are used to create light-weight infills. However, despite the abundance of new methods for modeling fine scale structures, few of them are supported by legacy commercial CAD systems. The lack of a common mathematical model to compare and categorize these methods leads to the rising difficulty in the composition and interoperability with other two-scale modeling methods and classical solids. This, in turn, leads to the proliferation of ad hoc approaches and dependence on specific software/hardware architectures that may not be extendable. The lack of a unified framework of modeling the multiscale structure stands out as a key issue that is addressed by this paper.

1.2. Contributions and outline

In this paper, we propose a formal framework for modeling multiscale structures. It is based on recursive application of a two-scale shape–material model. Each two-scale model includes the following components: (1) two single-scale shape–material models to represent the geometry and spatial distribution of material property on coarse and fine scales, respectively, each abstracted by single scale queries; (2) mechanisms to link the coarse and fine scales, such that homogenized shape and material properties of the structures on the fine scale correspond to those on the coarser scale; and (3) multi-scale queries that generalize single-scale queries to their multi-scale counterparts.

In the first component, each scale is self-contained shape–material model that supports all classical single scale queries and analyses. The single scale shape–material model and queries are consistent with classical solid and heterogeneous material modeling, and are briefly reviewed in Section 2.1. We note that the material properties on the finest scale are assumed to be well-defined, i.e. they are achievable by a single material or an idealized mixture of multiple materials, as is usually assumed in the heterogeneous material modeling literature.

The second component, mechanisms to link coarse and fine scales, is the focus of Section 3. The mechanism to link the scales manifests itself in terms of upscaling or downscaling operations, where upscaling estimates the coarse scale shape–material model of a given fine-scale structure and downscaling generates the fine-scale structure that refines the shape–material model at the coarse scale. The correspondence in mechanical behavior between the scales is expressed in term of effective material properties computed by homogenization of neighborhoods at each scale.

Multi-scale queries, the third ingredient of the formulated framework, is discussed in Section 4. We start by redefining the single-scale queries explicitly in terms of neighborhood scale to support the multiscale operations. The redefined single scale queries reduce to their classical form when neighborhoods become infinitesimal. We then formulate multiscale queries to return scale dependent results. For example, a point may be inside the shape on the coarse scale while outside the structure on some finer scale; material properties are also different on different scales. When the upscaling or downscaling algorithms support localized computations, the multiscale queries are implemented recursively based on the local evaluation of neighborhoods. Localized multi-scale queries hold the key to efficient multi-scale modeling operations. In particular, they support on-demand streaming and local evaluation of multiscale structures that may be defined implicitly and/or procedurally, eliminating the need for complete evaluation of models at all scales.

Section 5 showcases a reference implementation to demonstrate the generalities and capabilities of the proposed framework and multiscale queries. Examples of three different implementations of fine-scale structures with the same coarse scale material properties but different representations are shown to demonstrate the interchangeability enabled by the proposed query-based framework. Another example demonstrates the design of a three-scale structure by the recursive application of the proposed framework. Section 6 concludes with a brief summary and discussion of open research issues.

2. Background and related work

2.1. Single scale shape–material model and queries

Single scale shape–material models combine the classical results of solid modeling in shape and heterogeneous material representations. For decades modeled solids were generally assumed to have a homogeneous interior, dividing space into three point-sets: the interior of the solid, its boundary, and the exterior of the solid. With advances in manufacturing, modeling of material composition became a major research issue in solid modeling. The material properties are usually represented by a collection of scalar or vector fields defined over a decomposition of the geometric domain. Over the years, a great variety of shape and heterogeneous material representations have been developed. Readers are referred to [13] and [14] for comprehensive reviews on heterogeneous solid modeling.

The various representations have been evolved and refined to respond to the specific needs of the applications using them. If a multiscale modeling framework is to realize its full potential, the various representations used for different scales and phases (see Section 3) have to be integrated. Conventional wisdom relies on a data-centric approach which focuses on either specific format or representation conversions. Recently, we saw a departure

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