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ScienceDirect
Comput. Methods Appl. Mech. Engrg. 338 (2018) 275–298
Computer methods in applied mechanics and engineering
www.elsevier.com/locate/cma

New algorithms for virtual reconstruction of heterogeneous microstructures

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Received 18 February 2018; received in revised form 15 April 2018; accepted 17 April 2018
Available online 26 April 2018

Highlights

- Explicit representation of material interfaces during microstructure reconstruction using NURBS.
- New packing algorithm relying on bounding box representation of geometry.
- New algorithm specialized for packing randomly-shaped fibers.
- Efficient optimization phase to replicate all target statistical microstructural descriptors.
- High integration with mesh generation algorithms to facilitate subsequent finite element analysis.

Abstract

A new set of algorithms is introduced for the virtual reconstruction of heterogeneous material microstructures, in which morphologies of embedded particles/fibers are explicitly represented. As a pre-processing phase, a shape library containing morphologies of heterogeneities, parameterized in terms of Non-Uniform Rational B-Splines (NURBS), is extracted from digital data such as micro-computed tomography images. Two packing algorithms are then introduced to reconstruct an initial (raw) periodic microstructure: In the first approach, a set of hierarchical bounding boxes approximating particle shapes are employed to check for overlap. The second approach, which is specialized for fibrous microstructures, uses the NURBS representation of fiber centerlines during the packing process. An optimization phase is applied to build the final microstructural model, relying either on the Genetic Algorithm to selectively eliminate some of the inclusions or their sequential relocation within the raw microstructure. The objective functions of this optimization phase are designed to replicate the target statistical microstructural descriptors such as the volume fraction, size distribution, and spatial arrangement of inclusions. Several example problems are presented to show the

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https://doi.org/10.1016/j.cma.2018.04.030

application of these algorithms for synthesizing various heterogeneous microstructures, as well as their finite element modeling and simulation.

Keywords: Microstructure reconstruction; NURBS; Heterogeneous material; Packing algorithm; Mesh generation; CISAMR

1. Introduction

The computational design of composite materials requires predicting the micromechanical behavior of multiple repeating unit cells (RUCs) of the material with various microstructural features. One of the main challenges involved in this process is the creation of realistic geometrical models of the microstructure and more importantly virtually changing its characteristics such as the volume fraction and spatial arrangement of embedded particles/fibers throughout the design process. To accomplish this, one could convert digital data such as Scanning Electron Microscopy (SEM) or micro-computed tomography (micro-CT) images into geometrical models [1,2]. For example, the characterization and direct reconstruction of 3D microstructures of a fiber-reinforced polymer from micro-CT data are presented in [3]. However, in addition to the fact that the preparation of imaging data (specially in 3D) is time-consuming and expensive, several challenges are often encountered during the image processing phase due to difficulty in identifying material interfaces, which emanates from low contrast between different phases or their close proximity [4]. More importantly, direct microstructure reconstruction from imaging data can only provide a single microstructural model of an existing material, which would not be useful for the computational design of a new materials system.

Alternatively, one can implement a reconstruction algorithm [5] to virtually create realistic microstructures of composite materials. Significant research has been conducted to address the need for synthesizing material microstructures based on geometrical and statistical data extracted from 2D/3D imaging data. Such methods can be categorized into two main groups: descriptor-based methods [5–7] and correlation function-based techniques [8–11]. In the former approach, the goal is to replicate descriptor functions such as those describing the spatial arrangement of heterogeneities (e.g., nearest neighbor distance function), their morphologies, and the volume fraction. Optimization algorithms such as the Genetic Algorithm (GA) [12,13] and Simulated Annealing (SA) [14–16] are often utilized during the dispersion reconstruction phase to replicate the desired spatial distribution of inclusions. However, using such iterative algorithms often lead to a computationally demanding reconstruction process for synthesizing complex 3D microstructures.

Correlation function-based approaches such as N-point statistics [9] have also been implemented to reconstruct virtual microstructures for a wide array of heterogeneous materials [14,17,18]. Various techniques have been adopted for creating the virtual microstructure in these methods, among which we can mention the random sequential adsorption (RSA) [19–21], nearest neighbor algorithm (NNA) [22,23], Voronoi tessellations (VT) [24–27], and random field-based methods [11,28–30]. Unlike NNA and VT, RSA cannot reconstruct microstructures with high volume fractions of embedded inclusions due to the jamming limit [31]. However, all three algorithms are not capable of handling arbitrary-shaped heterogeneities. Further, none of these methods alone can replicate all desired correlation functions, in particular when the spatial arrangement of embedded heterogeneities in the domain is nonuniform [6]. This can be compensated by implementing stochastic optimization techniques such as the Monte-Carlo methods [32–34], pixel switching [35,36], and the mass–spring mutation operator [8,37]. Note that some of these techniques overlook the periodicity of the resulting microstructure, which is of significant importance for imposing appropriate boundary conditions in numerical homogenization and multiscale simulations. Further, the elimination of overlapping inclusions during the optimization phase could lead to a high computational cost and a low convergence rate.

In this article, a set of integrated reconstruction algorithms are presented that relies on Non-Uniform Rational B-Splines (NURBS) for the explicit representation of morphologies of arbitrary-shaped heterogeneities. As the first step, particles/fibers are virtually packed inside the domain to build an initial (raw) periodic model of the microstructure. Two algorithms are introduced to perform this packing process: In the first approach, a set of hierarchical bounding boxes (BBoxes) are defined to approximate the morphology and determine overlaps between