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Statistical reconstruction of two-phase random media

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ABSTRACT

A robust and efficient algorithm is proposed to reconstruct two-phase composite materials with random morphology, according to given samples or given statistical characteristics. The new method is based on nonlinear transformation of Gaussian random fields, where the correlation of the underlying Gaussian field is determined explicitly rather than through iterative methods. The reconstructed media can meet the binary-valued marginal probability distribution function and the two point correlation function of the reference media. The new method, whose main computation is completed using fast Fourier transform (FFT), is highly efficient and particularly suitable for reconstructing large size random media or a large number of samples. Its feasibility and performance are examined through a series of practical examples with comparisons to other state-of-the-art methods in random media reconstruction.

1. Introduction

Multi-phase random media such as rocks, concrete, alloy and composite materials are ubiquitous in the natural environment and engineering. Their mechanical, thermal and electrical etc. properties exhibit a strong random nature with discontinuities on the interfaces between different phases. The responses of multi-phase random media subjected to force, thermal or other type of loading are often of great interest to engineers and researchers, and such responses should be analyzed in the sense of statistics due to the inherent heterogeneity. At present, Monte Carlo methods remain the most popular and versatile approach for simulating the randomness of multi-phase random media and estimating their stochastic responses. The effectiveness of Monte Carlo methods relies largely on rapid reconstruction of large amounts of samples that can accurately represent the diversity and variation of the practical random media under simulation.

The main focus of this work is on the reconstruction of two-phase composite materials with random morphology, based on statistical characteristics derived from a few measured samples. The proposed reconstruction method is general and applicable to other types of random media as well, and instead of using the term "composite", we will use the general term "random media" for the remainder of the paper.

For a two-phase (black & white) random medium D, the indicator function $I(\boldsymbol{x})$, $\forall \boldsymbol{x} \in D$ is defined as

$$I(x) = \begin{cases} 0, & \text{if the material at } \boldsymbol{x} \text{ is in black phase} \\ 1, & \text{if the material at } \boldsymbol{x} \text{ is in white phase} \end{cases}. \quad (1)$$

Due to the random nature of phase distribution, the indicator function is often treated in the context of probability as a binary valued random field, denoted by $I(\boldsymbol{x}, \omega)$ where ω indicates a basic random event.

In practice, the random field $I(\boldsymbol{x}, \omega)$ is often assumed to be stationary (also termed as statistically homogeneous in [1–3]) up to the second order, so that its mean μ and variance σ^2 are invariant when shifted in space. In addition, the autocorrelation function between points $\boldsymbol{x}$ and $\boldsymbol{x}+\boldsymbol{\tau}$ depends only on the relative position $\boldsymbol{\tau}$ of the two points, i.e.

$$R_I(\boldsymbol{\tau}) = \frac{E[(I(\boldsymbol{x},\omega)-\mu)(I(\boldsymbol{x}+\boldsymbol{\tau},\omega)-\mu)]}{\sigma^2}, \quad \forall \boldsymbol{x}, \quad (2)$$

where $E()$ is the expectation operator. The range of $R_I(\boldsymbol{\tau})$ is $-1 \leqslant R_I(\boldsymbol{\tau}) \leqslant 1$ (Schwarz inequality).

Another assumption of $I(\boldsymbol{x}, \omega)$ is ergodicity. That is, the ensemble average of statistical parameters can be derived by the space average of these parameters over a sufficiently large sample.

Given a few, or even only one, realizations of the random media, the task of reconstruction is to extract statistical parameters (μ, σ^2 and $R_I(\boldsymbol{\tau})$ etc.) regarding the random field $I(\boldsymbol{x}, \omega)$ and generate samples that obey the same statistics as the reference realizations.

2. Overview

2.1. Related work

Over the past few decades, random media reconstruction has attracted growing attention from both academia and industry, in

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particular in the fields of composite materials, geostatistics and computational mechanics. To date, there are four main categories of reconstruction methods: the random set method, the stochastic optimization method, the maximum entropy method and the iterative nonlinear transformation method.

The random set method [4–6] is based on Boolean operations (union, intersection, dilation, erosion, et al. [7]) of random sets. This method is fast but it is limited to a few types of random media with relatively simple morphology, e.g. composites with sphere or polygon inclusions or Voronoi cell structure. For example, if the inclusion phase is spheres, their centers can be generated following a Poisson distribution; the radius can be similarly assumed to obey certain probability distribution; and adjacent spheres need to be trimmed if they overlap. However, for composites with complicated structures, e.g. amorphous phases, the random set objects are difficult to locate and operate, leading to deterioration in efficiency. In short, the random set method is fast and effective for certain types of random media, but is not a universal method.

Yeong and Torquato [1,8] introduced a simulated annealing method for generating digitalized random media realizations. Given a scanned image of the target random medium, this method starts from an initial configuration satisfying the volume fraction, and for the simulated image it successively performs random exchanges of pixels with different colors to minimize certain "energy" that measures the difference in correlation function, two-point cluster function [9] or n-point correlation function [10] etc. between the reference image and the simulated image. If the energy decreases after the exchange, the new configuration is considered superior to the old one, and the exchange is accepted. If the energy increases after the exchange, the new configuration is considered possible to be a transitional state from "local optimum" to "global optimum", and hence the exchange is accepted with a probability, which depends on the energy of the old and the new configurations and the annealing temperature [1]. Recently, several other stochastic optimization approaches were developed to overcome the low efficiency of the simulated annealing method, including genetic algorithm, Tabu-list and hybrid optimization methods [3,11]. The stochastic optimization method is perhaps the most flexible method for reconstructing random media samples, and it allows a wide range of statistical characteristics to be incorporated in sample generation. Its disadvantage is the expensive computational burden when large samples (either in size or in number) are required.

In the maximum entropy method [10,12,13], random media are modeled as Markov random fields. The joint probability distribution of Markov random fields is the Gibbs distribution [14], which is exactly the probability distribution that maximizes the entropy under expectation-type confinements (e.g. μ, σ^2, $R_l(\boldsymbol{\tau})$, etc) [15,16]. The explicit formation of the Gibbs distribution cannot be obtained because it is an infinite dimensional function. Thus, Markov chain Monte Carlo (MCMC) methods [17] are employed to sample from the Gibbs distribution, for which the Metropolis–Hastings algorithm [18,19] (a random walk MCMC method) has been a popular choice. Similar to the stochastic optimization method, which can be viewed as a special type of the Metropolis–Hastings algorithm [19,20], a large number of random walk steps are often required to achieve the equilibrium distribution status of the Markov chain. For practical use, the maximum entropy method is criticized to be even slower than the stochastic optimization method, and not suitable for large size problems [3].

The nonlinear transformation of Gaussian fields has been extensively used in modeling multivariate distributions [21,22]. The marginal distribution of the non-Gaussian field is met exactly, and the covariance of the underlying Gaussian field is computed numerically to satisfy the two point covariance requirement of the non-Gaussian field. This approach has been employed to model two-phase random media [2,23,24]. However, the relationship between the covariance of the non-Gaussian field and that of the Gaussian field is ignored in [23,24], while using an iterative algorithm the covariance function of the underlying Gaussian field is calculated in [2]. The most costly part of the nonlinear transformation approach is to determine the nonnegative definite covariance function (nonnegative definite covariance matrix in the discrete case) of the underlying Gaussian field. In most of the literature [2] and [25–28], the Gaussian field is constructed from an initial power spectral density (PSD) structure and an iterative algorithm is adopted to repeatedly update the PSD of the Gaussian field in order to make the PSD of the non-Gaussian field meet the target, and this can be a very slow process for practical problems. Another limitation of this method is that the marginal distribution and the covariance of the non-Gaussian field need to satisfy a compatibility relation in advance [29].

In this paper, the relationship between the correlation of the binary field and that of the Gaussian field is derived explicitly to avoid the costly iteration procedure commonly employed in existing nonlinear transformation approaches. The compatibility relation between the marginal distribution and the autocorrelation of binary valued fields are also rigorously investigated, and proved to be not a critical restriction. These new developments significantly improve the efficiency of sample generation, allowing thousands of large samples to be generated within a few minutes. The main limitation of the method is that it does not utilize other statistical characteristics (e.g. n-point correlation and lineal-path function). However, numerical examples demonstrate that the new method is suitable for a variety of types of two-phase random media, as two-point correlation contains considerable information on random morphology.

2.2. Preliminary knowledge: spectral decomposition of stationary random fields

The Wiener–Khinchin theorem [30,31] states that the PSD $f(\boldsymbol{X})$ of a stationary second-order random field $a(\boldsymbol{x}, \omega)$ is the Fourier transform of the corresponding autocorrelation function $R(\boldsymbol{\tau})$. If $a(\boldsymbol{x}, \omega)$ is a periodical stochastic process [32,33] with a period of $2N$, i.e. $a(x_1,\ldots,x_n,\omega) = a(x_1+2N_1,\ldots,x_n+2N_n,\omega)$, the discrete version of the Wiener–Khinchin theorem can be written as [34,35]:

$$f(X_1,\ldots X_n) = \sum_{\tau_1=-N_1+1}^{N_1} \cdots \sum_{\tau_n=-N_n+1}^{N_n} R(\tau_1,\ldots,\tau_n) e^{-\sum_{j=1}^{n} \frac{\pi i}{N_j} X_j \tau_j},$$
$$X_j = [-N_j+1, N_j] \tag{3}$$

$$R(\tau_1,\cdots,\tau_n) = \frac{1}{\prod_j (2N_j)} \sum_{X_1=-N_1+1}^{N_1} \cdots \sum_{X_n=-N_n+1}^{N_n} f(X_1,\cdots X_n) e^{\sum_{j=1}^{n} \frac{\pi i}{N_j} X_j \tau_j},$$
$$\tau_j = [-N_j+1, N_j] \tag{4}$$

where i is the imaginary unit, N_j are positive integers, the integer coordinates $\tau_1,\ldots,\tau_n$ denote the space domain, the integer coordinates $X_1,\ldots X_n$ denote the frequency domain, and $f(X_1,\ldots X_n)$ is real and nonnegative valued due to the nonnegative definite property of $R(\tau_1,\ldots,\tau_n)$.

Then, $a(\boldsymbol{x}, \omega)$ can be represented by an orthogonal increment process: