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To cite this article: Dominique Jeulin 2011 *J. Phys.: Conf. Ser.* **319** 012013

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Multi-scale random sets: from morphology to effective properties and to fracture statistics

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Abstract. Complex microstructures in materials often involve multi-scale heterogeneous textures, modelled by random sets derived from Mathematical Morphology. Starting from 2D or 3D images, a complete morphological characterization by image analysis is performed, and used for the identification of a model of random structure. From morphological models, simulations of realistic microstructures are introduced in a numerical solver to compute appropriate fields (electric, elastic stress or strain, ...) and to estimate the effective properties by numerical homogenization, accounting for scale dependent statistical fluctuations of the fields. Our approach is illustrated by various examples of multi-scale models: Boolean random sets based on Cox point processes and various random grains (spheres, cylinders), showing a very low percolation threshold, and therefore a high conductivity or high elastic moduli for a low volume fraction of a second phase. Multiscale Cox point processes are also a source of instructive models of fracture statistics, such as multiscale weakest link models.

1. Introduction

In the context of many materials, such as nanocomposites, it is common to encounter a non-homogeneous dispersion of a charge in a matrix [1]. For instance arrangement of aggregates (like carbon black) appear at different scales. This multiscale arrangement has implications on the prediction of the effective properties of such composites (like the conductivity, the dielectric permittivity or the elastic moduli), from the properties of the two components (charge and matrix), and their spatial distribution. Similarly, in the context of fracture statistics, crack initiation can occur on random defects with a multiscale distribution.

In this paper, we introduce a general methodology for modelling these situations [2]. It is based on the theory of random sets [3, 4, 5, 6]. The morphology is summarized and simulated by multi-scale random models accounting for the heterogeneous distribution of aggregates. Identification of the model is made from image analysis.

In the next sections, we develop the following points:

- Principle of random structure modeling
- Models of multi scale random sets, simulation of microstructures, and percolation
- Prediction of effective properties by numerical simulations
- Multi-scale and multi-criteria Fracture Statistics models

2. Principle of random structure modeling

The heterogeneity of materials can be handled through a probabilistic approach, which enables us to generate models and simulation of the microstructures.

When considering two-phase materials (for instance a set of particles A embedded in a matrix A^c), we use a model of random closed set (RACS) A [3, 4, 5, 6], fully characterized from a probabilistic point of view by its Choquet capacity $T(K)$ defined on the compact sets K , from (1) below, where P denotes a probability:

$$T(K) = P(K \cap A \neq \emptyset) = 1 - Q(K) = 1 - P(K \subset A^c). \quad (1)$$

In practice, $T(K)$ can be estimated by area fraction measurements on 2D images, or from volume fraction estimation on 3D images (from true microstructures, or from simulations), after a morphological dilation of the set A by the set K [3, 4, 5, 6], noted $A \oplus K$, or calculated for a given theoretical model. Equation (1) is used for the identification of a model (estimation of its parameters, and test of its validity). Particular cases of morphological properties deduced from (1) are the volume fraction V_v , the covariance (a useful tool to detect the presence of scales or anisotropies), the distribution of distances of a point in A^c to the boundary of A . The access to 3D images of microstructures by means of X-ray microtomography [7] makes it possible to use 3D compact sets K (like balls $B(r)$ with various radii r) to characterize the random set.

3. One scale models

The archetype of random structure model is a random point process. It represents the most simple kind of random structure, like small defects isolated in a matrix. As a particular case of RACS, a random point process is characterized by its Choquet capacity $T(K)$. For a locally finite point process, use can be made of the probability generating function $G_K(s)$ of the random variable $N(K)$ (random number of points of the process contained in K). We have

$$G_K(s) = E\{s^{N(K)}\} = \sum_{n=0}^{\infty} P_n(K) s^n,$$

where $P_n(K) = P\{N(K) = n\}$, P being a probability. From this definition, we have $1 - T(K) = G_K(0) = P\{N(K) = 0\}$. For example, a typical model is the Poisson point process. It is the prototype of random point process without any order, since the numbers of points of the process contained in any pair of sets without intersection are independent random variables. For the homogeneous Poisson point process with intensity θ (i.e. average number of points per unit volume in 3D), we have, $\mu(K)$ being the Lebesgue measure (volume in 3D) of the compact set K :

$$P_n(K) = \frac{(\theta\mu(K))^n}{n!} \exp(-\theta\mu(K)) \text{ and } G_K(s) = \exp(\theta\mu(K)(s-1))$$

Starting from a point process, more general models, called grain models, can be generated, like the Boolean model, multi-scale models from intersection of random sets, or the multi-scale Cox Boolean model.

3.1. Boolean model

Some materials (like porous media or composite materials) can be simulated by means of a basic random set model, namely by distributions of overlapping objects. A random set model, the Boolean model, was proposed by G. Matheron [3, 4] to reproduce this situation. First, we consider a location of centres of grains by means of a Poisson point process with intensity θ . In this condition, a volume V contains a random number of centres N following a Poisson

distribution with average value θV . Then a random set is obtained by the union of random grains (any compact set). For this model, the Choquet capacity is given by (2), where $\bar{V}(A' \oplus \check{K})$ is the average volume of the random primary grain A' , dilated by K :

$$T(K) = 1 - \exp -\theta \bar{V}(A' \oplus \check{K}) \quad (2)$$

As a particular case, the volume fraction V_V of the grains, is given by (3):

$$q = 1 - V_V = 1 - \exp -\theta \bar{V}(A'). \quad (3)$$

Using for K a pair of points, 3 points, or a ball with radius r gives access to the covariance, the third order moment, and to the spherical contact distribution (namely the distribution of the distance of a random point in A^c to the boundary of A). For a given population of random grains, these morphological functions are theoretically available from (2). In the special case of spherical grains, the distribution function of the spheres radii can be estimated from the covariance [8], and therefore the model can be identified from the two points statistics, which is a one-dimensional information. For more general situations, the population of grains requires higher order moments for the identification of the model.

3.2. Percolation of the Boolean model

For materials made of components with a high contrast of properties, like for instance carbon black in a polymeric matrix, there is a strong effect on the macroscopic properties when a given phase percolates through the structure, inducing connected paths in the samples of the medium. Analytical estimations of the percolation of Boolean models of cylinders are available with the excluded volume model [9]. More recent analytical estimates of the percolation threshold of isotropic Boolean models with convex grains are based on the zeroes of the connectivity number [8, 10, 11]. They give an estimate of the percolation threshold of the grains p_c^1 and of A^c . These two percolation thresholds are different, as a result of the fact that the two sets A and A^c are non-symmetrical. The percolation threshold can also be estimated on simulations of the microstructure. It appears that a Boolean model with anisotropic primary grains (for instance spherocylinders) shows a much lower percolation threshold (0.01145 for an aspect ratio $l/r = 100$ [9]) than for isotropic grains (0.2895 for spheres [12, 13]). This can explain the expected outstanding mechanical, electrical or chemical properties of composites containing carbon nanotubes, mainly due to their shape, giving a low percolation threshold. The percolation of the complementary set of a Boolean model of spheres obtained analytically from the connectivity number and by simulations are given by 0.05698 and 0.0540 ± 0.005 respectively [14].

4. Models of multi-scale random sets, simulation of microstructures, and percolation

4.1. Combination of independent random sets to generate multi-scale random media

Starting from the basic models, more complex structures, such as superposition of scales, or fluctuations of the local volume fraction p of one phase can be generated in a simple way by a combination of various random sets, considering independent realizations. A convenient construction of multi-scale models makes use of the union or intersection of independent random sets A_i with different scales. In the case of intersections, $A = \cap_i A_i$, and it is easy to show that we have:

$$P(K) = P\{K \subset (\cap_i A_i)\} = \prod_i P\{K \subset A_i\}. \quad (4)$$

The result (4) is exact without any approximation, whatever the independent random sets A_i and their scales. For instance the overall volume fraction is the product of the volume fractions

of the A_i . Similarly the binary covariance $C(h) = P\{x \in A, x+h \in A\}$, and more generally the n points probabilities are obtained as a product of the corresponding individual n points probabilities. A lower bound of the corresponding percolation threshold p_c can be estimated by the products of percolation thresholds p_c^i when the scales are widely separated: $p_c \simeq \prod_i p_c^i$. This model was used to simulate the random distribution of carbon black in composites by means of the intersection of three Boolean models of spheres at different scales, reproducing the carbon black particles, aggregates, and zones of exclusion in the matrix [15]. The identification of the model is made from the measurement of the overall binary covariance on $C(h)$ images obtained by transmission electron microscope on thin sections of the material.

4.2. The multi-scale Cox Boolean model

In another way to account for a non homogeneous distribution of random grains, it is possible to replace the Poisson point process by a Cox point process [16]. Consider a positive random function (RF) giving a non homogenous intensity $\theta(x)$. For any realization of this RF, a Poisson point process with intensity $\theta(x)$ is generated. For any realization, the number of points in a domain D follows a Poisson distribution with average $\theta(D) = \int_D \theta(dx)$:

$$P_n(D) = P\{N(D) = n\} = \frac{\theta(D)^n}{n!} \exp(-\theta(D)).$$

Furthermore, for each realization, the number of points falling in any family of domains without any intersection are independent random variables. This is not anymore the case when considering the ensemble of realizations of the random intensity.

If $\varphi_K(\lambda)$ is the Laplace transform of the positive random variable $E_{A'}\{\theta(\check{A}' \oplus K)\}$, where $E_{A'}$ states for the mathematical expectation with respect to the random set A' , and E_θ the mathematical expectation with respect to the random function $\theta(x)$, we have:

$$T(K) = 1 - E_\theta\{\exp(-E_{A'}\{\theta(\check{A}' \oplus K)\})\} = 1 - \varphi_K(1). \quad (5)$$

An interesting particular case is obtained by means of a constant intensity θ inside a first random set A . For instance A is a Boolean model of spheres with a large radius R . We then keep the points of a Poisson point process contained in A , as germs for centers of spheres with a smaller radius r [12]. The random measure becomes $\theta(dx) = \theta 1_A(x)dx$, where $1_A(x)$ is the indicator function of the set A ($1_A(x) = 1$ if $x \in A$ and $1_A(x) = 0$ if $x \in A^c$). We have

$$T(K) = 1 - \Phi_K(\theta), \quad (6)$$

where $\Phi_K(\lambda)$ is the Laplace transform of the random variable $E_{A'}\{V((\check{A}' \oplus K) \cap A)\}$ obtained on the realizations of the random set A , after averaging over the realizations of the primary grain A' . As a particular case for a deterministic grain A' the Choquet capacity of the Boolean Cox model is deduced from the distribution of the change of support of the set A over the compact set $\check{A}' \oplus K$ (or probability law of $V((\check{A}' \oplus K) \cap A)$). It is usually difficult to access to this law for any random set A , but it can be easily estimated from simulations. We can therefore estimate the theoretical covariance (or higher order moments) of the model.

In the case of a large separation of scales between the two sets A and A' we can obtain an approximation of the $T(K)$ and then of $P(K)$ when assuming that $V(\check{A}' \oplus K) \rightarrow 0$. Therefore, the covariance and the three points probability are asymptotically equal to the corresponding theoretical values (4) given for the intersection of independent random sets. This result is valid for any n points probability, giving an approximation of the corresponding moments for this Cox Boolean model. It can be obtained as follows, to first order in $V((\check{A}' \oplus K))$, writing $P_1(K) = P\{K \subset A\}$, $Q_1(K) = P\{K \subset A^c\}$:

$$\Phi_K(\lambda) \simeq P_1(\check{A}' \oplus K) \exp(-\lambda V(\check{A}' \oplus K)) + Q_1(\check{A}' \oplus K)$$

and therefore, noting A_2 the standard Boolean model made of the union of grains A' located on Poisson points with intensity θ , $P_2(K) = P\{K \subset A_2\}$, $Q_2(K) = P\{K \subset A_2^c\}$

$$\begin{aligned} Q(K) &\simeq P_1(\check{A}' \oplus K) \exp(-\theta V(\check{A}' \oplus K)) + 1 - P_1(\check{A}' \oplus K) \\ P(K) &\simeq 1 - Q(K) \simeq P_1(\check{A}' \oplus K)(1 - Q_2(K)) \simeq P_1(\check{A}' \oplus K)P_2(K) \\ &\simeq P_1(K)P_2(K) \end{aligned}$$

For thin sections in electron microscopy, we can notice that the available experimental information is a projection of the set A through the thickness e , and therefore we can estimate $T(K \oplus e)$, from which the model can be identified, after replacing the primary grain A' by $A' \oplus e$.

For carbon black nanocomposites, it is usual to model the distribution of carbon black particles by means of a three scale model [15, 12, 1]: spherical carbon particles (with a possible distribution of radii $f_1(r)$) are located on Poisson points inside inclusion zones (Boolean model of spheres with a distribution of radii $f_2(r)$) and outside of exclusion zones (Boolean model of spheres with a distribution of radii $f_3(r)$). The identification of the parameters of the model is made by means of an iterative optimization process, minimizing the difference between probabilistic properties of simulations and of images of the material: in [1], the multi-scale model is identified from measurements of the covariance, the third order moment, and of the area fraction after 2D closings on transmission electron images.

4.3. Percolation of the Cox Boolean model

As expected, the generation of aggregates produces random media with a lower percolation threshold: for a large separation of scales in a two scales model, the lower bound of the overall percolation threshold p_c is given by the product $p_c^1 p_c^2$ of the corresponding thresholds, as in the case of the intersection of independent random sets. Models involving iteration of scales generate microstructure with a very low percolating threshold, and therefore with improved macroscopic properties when the percolating component presents the higher property (e.g. conductivity or elastic moduli). It shows that a typical homogeneous distribution of grains in space (like for the standard Boolean model) does not produce a medium with optimal properties. The percolation threshold of various multi-scale models was estimated in various situations [12, 17, 14]. In [14], we get $p_c = 0.0849$ for a scale factor equal to 30 in a two scale Cox Boolean model of spheres, close to $0.2897^2 = 0.0839$. In [17] the percolation threshold of spherocylinders (aspect ratio $l/r = 100$) with centres located in a primary Boolean model of spheres (with $V_v = 0.32$) percolates for $p_c = 0.0056$. Again, considering the case of aggregates of carbon nanotubes, high performances are expected from such a microstructure for a very low volume fraction of charge, due to the presence of clusters.

5. Prediction of effective properties by numerical simulations

An efficient way to solve the problem of homogenization of physical properties, for instance to predict the dielectric permittivity or the effective mechanical properties of heterogeneous media, makes use of numerical solutions of the corresponding partial differential equations (PDE) solutions, before estimating the effective properties by spatial averaging of the solution. This requires the input of 3D images (real images, as obtained by confocal microscopy, or by X-ray microtomography) or simulations, so-called digital materials. In a second step a computational code (Finite Elements, Fast Fourier Transform, PDE numerical solver) is implemented.

We use a method derived from [18, 19], to estimate the equivalent macroscopic dielectric constant ε^* from the structure of a material and the properties of its constituents [20]. The numerical solution is obtained by means of the Green function of a homogeneous reference medium for the corresponding PDE for the electrical field or for the elastic field problem. For this, we determine the polarization field $P(x)$ inside the material knowing the local dielectric

permittivity $\varepsilon(x)$, by application of a constant electric field E_0 , and of periodic boundary conditions. An iterative calculation in the Fourier space is used to estimate $P(x)$, giving ε^* by means of a spatial average $\langle \cdot \rangle$. We have

$$\varepsilon^* = \frac{\langle D \rangle}{\langle E \rangle} = \frac{\langle (\varepsilon(x) - \varepsilon_0)^{-1} \varepsilon(x) P(x) \rangle}{\langle (\varepsilon(x) - \varepsilon_0)^{-1} P(x) \rangle} \quad (7)$$

ε_0 being the dielectric permittivity of a reference medium used for the iterative solution, and D the electric displacement ($D(x) = \varepsilon(x)E(x)$).

Using the FFT approach is very versatile and does not require any meshing of the microstructure, in contrast with other numerical methods such as Finite Elements. In elasticity, stress and strain field maps are obtained on the scale of microstructure, to get a detailed study of the effect of the microstructure on the local fields. With the Morph-Hom code developed by F. Willot [21, 22] images of large sizes (up to 1500^3) can be handled for any contrast of properties, and therefore the electrostatic or elastic behavior of porous media or of rigid media could be successfully studied by numerical techniques. This was applied to the Boolean model of spheres with any volume fractions [21] and to two-scales and three-scales Cox Boolean models of spheres [22]. The reinforcing effect of the iteration of scales with a large separation is clearly observed in the case of a very high conductivity or of a rigid phase, as a result of a lower percolation threshold. In the case of porous media, the reverse effect is observed, as would appear in the case of a damage at the interface between clusters of rigid particles and the matrix. A similar approach was applied to a microtomographic image of a mortar material [23]. A detailed study of the local enhancement of the stress field by the microstructure was made by means of image analysis of the maps obtained by FFT. This is a promising approach to study the sensitivity of microstructural elements on damage.

Finally, when working on images of a material or on realizations of a random medium, a natural question arises [24, 25]: what is the representativeness of the effective property estimated on a bounded domain of a microstructure? In other words, what is the size of a so-called "Representative Volume Element" RVE. We address this problem by means of a probabilistic approach giving size-dependent intervals of confidence, initially developed in the framework of the homogenization of the elastic moduli of random media [26], and based on the size effect of the variance of the effective properties of simulations of random media.

6. Multi-scale and multi-criteria Fracture Statistics models

Fracture Statistics models are necessary in order to predict the probability of fracture according to the microstructure, the size of specimens and the applied stress field. These models are of major importance for engineering purpose.

In a medium with heterogeneities at different scales, several populations of defects may exist in various sub-volumes V_i inside a domain with volume V (with $V = \sum_{i=1}^{i=r} V_i$).

We propose for this type of situation theoretical models based on the weakest link model. After a recall of the weakest link model, connected to the Poisson points process, we introduce multi-criteria and multi-scale weakest link models. This is illustrated by some continuum models.

6.1. Recall of the weakest link model

The standard weakest link model is based on the assumption that fracture in a brittle material is initiated on the most critical defect, that controls the full fracture process. For this model, it means that when there is at least one point x in a specimen where the applied principal stress component $\sigma(x)$ is larger than the local critical stress $\sigma_c(x)$, the specimen is broken. Usually it is assumed that the occurrence or absence of critical defects (generating fracture) of any volume elements generate a set of independent events. After a decomposition of the volume V into

links v_i and assuming that there is a fracture of the volume V when a single link v_i is broken, a classical computation for independent events gives:

$$P\{\text{Non fracture}\} = \prod_i P\{\text{Non fracture of } v_i\}$$

For $v_i \rightarrow 0$

$$P\{\text{Non fracture of } V\} = \exp\left(-\int_V \Phi(\sigma(x))dx\right) = \exp(-V\Phi(\sigma_{eq}))$$

where the equivalent stress is defined from

$$\Phi(\sigma_{eq}) = \frac{1}{V} \int_V \Phi(\sigma(x))dx$$

This assumption is equivalent to a distribution of point defects in a matrix with $\sigma_c = \infty$, according to a Poisson point process in space, with intensity $\Phi(\sigma)$, where $\Phi(\sigma)$ is the average number per unit volume of defects with a critical stress σ_c lower than σ . For the Weibull model, the function $\Phi(\sigma)$ is power law in σ .

For a homogeneous applied stress field $\sigma(x) = \sigma$,

$$P\{\text{Non fracture of } V\} = \exp(-V\Phi(\sigma))$$

6.2. Multi-criteria and multi-scale weakest link model

We consider now r populations of defects and a decomposition of the specimen V in various sub-volumes $V_i : V = \cup_{i=1}^r V_i$, with $V = \sum_{i=1}^r V_i$. Every sub-volume V_i contains a sub-class of Poisson defects with intensity $\Phi_i(\sigma)$. In what follows, no specific assumption on the type of $\Phi_i(\sigma)$ is made (it should increase monotonously with the loading [27, 24]), and therefore possible mixing of various kinds of point defects are considered, like Weibull models for power laws, with different moduli. The sub-volumes generate a family of random variables summing to V , with a multivariate Laplace transform $\phi(\lambda_1, \lambda_2, \dots, \lambda_r)$:

$$\phi(\lambda_1, \lambda_2, \dots, \lambda_r) = E\left\{\exp\left(-\sum_{i=1}^r \lambda_i V_i\right)\right\}$$

Applying the weakest link assumption to each sub-volume, the fracture probability of volume V is given by:

- For fixed volumes V_i , in the case of a homogeneous applied stress:

$$1 - P\{\text{fracture}\} = \exp\left(-\sum_{i=1}^r V_i \Phi_i(\sigma)\right) \quad (8)$$

- Taking the mathematical expectation of expression (8) with respect to V_i , we obtain the fracture probability:

$$1 - P\{\text{fracture}\} = \phi(\Phi_1(\sigma), \Phi_2(\sigma), \dots, \Phi_r(\sigma)) \quad (9)$$

For a non homogeneous applied stress field $\sigma(x)$, equation (8) becomes, when the V_i are given:

$$1 - P\{\text{fracture}\} = \exp\left(-\sum_{i=1}^r V_i \Phi_i(\sigma_{eq}^i(V_i))\right) \quad (10)$$

noting

$$V_i \Phi_i(\sigma_{eq}^i(V_i)) = \int_{V_i} \Phi_i(\sigma(x)) dx \quad (11)$$

Taking the mathematical expectation with respect to the random variables $V_i \Phi_i(\sigma_{eq}^i(V_i))$, the fracture probability is expressed by means of the Laplace transform of these variables, noted:

$$\phi_H(\lambda_1, \lambda_2, \dots, \lambda_r) = E\left\{\exp\left(-\sum_{i=1}^{i=r} \lambda_i V_i \Phi_i(\sigma_{eq}^i(V_i))\right)\right\}$$

$$1 - P\{\text{fracture}\} = \phi_H(1, 1, \dots, 1) \quad (12)$$

For very large samples, compared to the microstructure, modelled by a stationary multi-component random set, with components A_i , every $\Phi_i(\sigma_{eq}^i(V_i))$ can be replaced by

$$\Phi_i(\sigma_{eq}^i) = \frac{1}{V} \int_V \Phi_i(\sigma(x)) dx,$$

after substitution of the average in a random V_i by the overall average in the total volume V . With this approximation, the fracture probability is given by (9), replacing each $\Phi_i(\sigma)$ by $\Phi_i(\sigma_{eq}^i)$:

$$1 - P\{\text{fracture}\} = \phi(\Phi_1(\sigma_{eq}^1), \Phi_2(\sigma_{eq}^2), \dots, \Phi_r(\sigma_{eq}^r)) \quad (13)$$

6.3. Continuous model with two modes of fracture

We consider a random set A (and its complementary set A^c), with $p = P\{x \in A\}$. We assume that the random set A contains Poisson point defects with intensity $\Phi_1(\sigma)$, and A^c contains Poisson point defects with intensity $\Phi_2(\sigma)$. The probability of fracture can be deduced from the bivariate distribution of the random volumes V_1 and V_2 (with $V_1 + V_2 = V$) of A and A^c in the domain with volume V .

This bivariate distribution is not known in general, but can be assumed to be deduced from the Beta distribution. Let X be the random variable giving the proportion of A in a sample. The pdf $f(x)$ of the random variable X ($0 \leq X \leq 1$) is assumed to follow a Beta distribution, with parameters α and β as for a Poisson sequence generated on a line in a 1D process:

$$f(x) = \frac{\Gamma(\alpha + \beta)}{\Gamma(\alpha)\Gamma(\beta)} x^{\alpha-1} (1-x)^{\beta-1} \quad (14)$$

The average and the variance of this distribution are given by:

$$E(X) = \frac{\alpha}{\alpha + \beta}$$

$$Var(X) = \frac{\alpha\beta}{(\alpha + \beta)^2(\alpha + \beta + 1)}$$

For a random set A with volume fraction p and with centred covariance $\overline{W}_2(h)$, we have

$$E(X) = p \quad (15)$$

$$Var(X) = \frac{1}{V^2} \int_V \int_V \overline{W}_2(x-y) dx dy$$

For large volumes, when $V \gg A_n$ (A_n being the integral range deduced from the integral of the covariance), the variance becomes

$$Var(X) = p(1-p)\frac{A_n}{V} \quad (16)$$

The parameters α and β are expressed as a function of p and of $Var(X)$ or of A_n for large specimens, that are microstructural properties. We have:

$$\begin{aligned} \frac{\alpha}{\alpha + \beta} &= p \\ \frac{\alpha\beta}{(\alpha + \beta)^2(\alpha + \beta + 1)} &= \frac{\alpha}{\alpha + \beta} \frac{\beta}{\alpha + \beta} \frac{A_n}{V} \end{aligned}$$

and

$$\begin{aligned} \alpha &= p\left(\frac{V}{A_n} - 1\right) \\ \beta &= (1-p)\left(\frac{V}{A_n} - 1\right) \end{aligned}$$

The Laplace transform of the bivariate distribution of variables XV and $(1-X)V$ is defined by:

$$\begin{aligned} \phi(\lambda_1, \lambda_2) &= E\{\exp(-\lambda_1 VX - \lambda_2 V(1-X))\} \\ &= \exp(-\lambda_2 V) E\{\exp(-VX(\lambda_1 - \lambda_2))\} \\ &= \phi((\lambda_1 - \lambda_2)V) \exp(-\lambda_2 V) \end{aligned} \quad (17)$$

where $\phi(\lambda)$ is the Laplace transform of the Beta distribution (14). We have:

$$\phi(\lambda) = \frac{\Gamma(\alpha + \beta)}{\Gamma(\alpha)} \sum_{k=0}^{k=\infty} \frac{(-1)^k \lambda^k}{k!} \frac{\Gamma(\alpha + k)}{\Gamma(\alpha + \beta + k)} \quad (18)$$

and

$$\begin{aligned} \frac{\Gamma(\alpha + \beta)}{\Gamma(\alpha)} \frac{\Gamma(\alpha + k)}{\Gamma(\alpha + \beta + k)} &= \frac{(\alpha + k - 1) \dots (\alpha + 1) \alpha}{(\alpha + \beta + k - 1) \dots (\alpha + \beta)} \\ &= \frac{(p(\frac{V}{A_n} - 1) + k - 1) \dots p(\frac{V}{A_n} - 1)}{(\frac{V}{A_n} - 1 + k - 1) \dots (\frac{V}{A_n} - 1)} \end{aligned} \quad (19)$$

The probability of fracture is obtained by replacing (19) in (17, 18). Replacing the term V by $V(\check{A}' \oplus K)$ in 19, we obtain an estimation of the Choquet capacity of a Cox Boolean random set from equation (6), when the random variable $V((\check{A}' \oplus K) \cap A)$ introduced in section 4.2 follows a Beta distribution. This can occur for sets $\check{A}' \oplus K$ that cannot be considered as negligible with respect to A , while a large separation of scales was considered previously.

For very large samples ($V \rightarrow \infty$), the term in (19) becomes p^k and $\phi(\lambda) = \exp(-p\lambda)$. Then,

$$\phi(\lambda_1, \lambda_2) = \exp(-\lambda_2 V) \exp -pV(\lambda_1 - \lambda_2) = \phi(\lambda_1, \lambda_2) = \exp -V(p\lambda_1 + (1-p)\lambda_2)$$

and the fracture probability is given by:

$$1 - P\{\text{rupture}\} = \exp -V(p\Phi_1(\sigma) + (1-p)\Phi_2(\sigma))$$

6.4. Multi-scale weakest link model

We can specialize the previous results to a single population of defects $\Phi(\sigma) = \Phi_1(\sigma)$, using $\Phi_2(\sigma) = 0$ in the previous developments. This corresponds to a multi-scale model, where the defects are located in a random set A . We have, using the Laplace transform of the Beta distribution $\phi(\lambda)$ and equation (17):

$$1 - P\{\text{fracture}\} = \phi(\Phi(\sigma)V)$$

For very large samples ($V \rightarrow \infty$), the term in (19) becomes p^k and $\phi(\lambda) = \exp(-p\lambda)$. Then $1 - P\{\text{fracture}\} = \exp -V(p\Phi(\sigma))$. Therefore, very large scale effects of this model are similar to the standard model, but different scale effects are obtained at a very small scale and at intermediary scales.

As in [27], this approach can be generalized to fracture controlled by a critical density of defects. The fracture probability is then worked out from the probability $P\{N \text{ defects} = k\}$ available for the multi-scale models, from its generator function $G_V(s) = E\{s^N\}$:

$$G_V(s) = \phi((s-1)\Phi(\sigma)V) \quad (20)$$

The probability to find k critical defects in a domain with volume V is deduced from (20) by use of the appropriate Laplace transform ϕ (for instance the Laplace transform of the Beta distribution).

6.5. Continuous model with r modes of fracture

The previous model can be generalized to the case of r modes of fracture, the Beta distribution being replaced by a multivariate Dirichlet distribution with parameters $\alpha_1, \alpha_2, \dots, \alpha_r$. We have

$$f(x_1, x_2, \dots, x_r) = \frac{\Gamma(\alpha_0)}{\prod_{i=1}^r \Gamma(\alpha_i)} \prod_{i=1}^r x_i^{\alpha_i-1}$$

with $\alpha_0 = \sum_{i=1}^r \alpha_i$ and $x_r = 1 - \sum_{i=1}^{r-1} x_i$.

Each random variable X_i follows a Beta distribution with parameters α_i and $\alpha_0 - \alpha_i$, with average $E(X_i) = \frac{\alpha_i}{\alpha_0}$ and variance $Var(X_i) = \frac{\alpha_i(\alpha_0 - \alpha_i)}{(\alpha_0)^2(\alpha_0 + 1)}$. For illustration we consider a random mosaic built on a random tessellation of space, by affecting independently to each class (or cell) the mode of fracture i with the probability p_i . On a large scale for a random mosaic, $Var(X_i) = p_i(1 - p_i) \frac{A_n}{V}$ (the Dirichlet distribution implies that the integral range A_n does not depend on the mode i).

For this model we have $\alpha_0 = 1 - \frac{V}{A_n}$ and $\alpha_i = p_i(1 - \frac{V}{A_n})$.

The expansion of the multivariate Laplace transform $\phi(\lambda_1, \lambda_2, \dots, \lambda_r)$ depends on the moments $\mu_{k_1 \dots k_r}$:

$$\mu_{k_1 \dots k_r} = E\left\{\prod_{j=1}^r X_j^{k_j}\right\} = \frac{\Gamma(\sum_{i=1}^r \alpha_i)}{\prod_{i=1}^r \Gamma(\alpha_i)} \prod_{i=1}^r \frac{\Gamma(\alpha_i + k_i)}{\Gamma(\sum_{i=1}^r (\alpha_i + k_i))}$$

The Laplace transform of the Dirichlet distribution is obtained from:

$$\phi(\lambda_1, \lambda_2, \dots, \lambda_r) = \sum_{n=0}^{\infty} \frac{(-1)^n}{n!} \left(\sum_{k_1 + \dots + k_r = n} \lambda_1^{k_1} \dots \lambda_r^{k_r} \mu_{k_1 \dots k_r} \right) \quad (21)$$

The fracture probability is given by replacing in (21) the λ_i by $V\Phi_i(\sigma)$. In practice, the expansion can be stopped after a finite rank n .

7. Conclusion

Multi-scale models of random media provide a wide variety of morphologies to simulate complex microstructures for application to real materials. These models are able to capture phenomena like the observation of very low percolation thresholds, explaining the enhancement of some effective properties for a low volume fraction of additions in a matrix. Our approach is based on measurements obtained by image analysis, to test and select appropriate models, and to estimate their parameters. Combined to predictive models, by analytical means, or more generally by numerical simulations, the multi-scale models give access to the optimization of microstructures with respect to the required properties. They are also the source of new fracture statistics behavior in multi-scale distributions of defects, that would be helpful for the explanation of the observed behavior of very heterogeneous materials [28]. This approach can be used in many domains of application, like materials, nanocomposites, porous media, or biological media.

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