The RVE method for random sets and homogenization problems

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Outline

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Introduction

Context and motivation

- The mechanical properties of materials are strongly influenced by their microstructure. A key issue in materials science consists in studying and describing material microstructures by quantitative rigorous means.
- Experimental imaging is a straightforward method to probe material microstructure.
- Yet, a mathematically-rigorous approach must also be considered : that of probabilistic models of structures , a.k.a. as stochastic materials.
- In this lecture, our aim is to introduce basic notions on random set theory and methods, applications that allow one to characterize experimental materials and structures, and tools for studying the representativity of material images with respect to their apparent properties.

Example : inclusions in a matrix

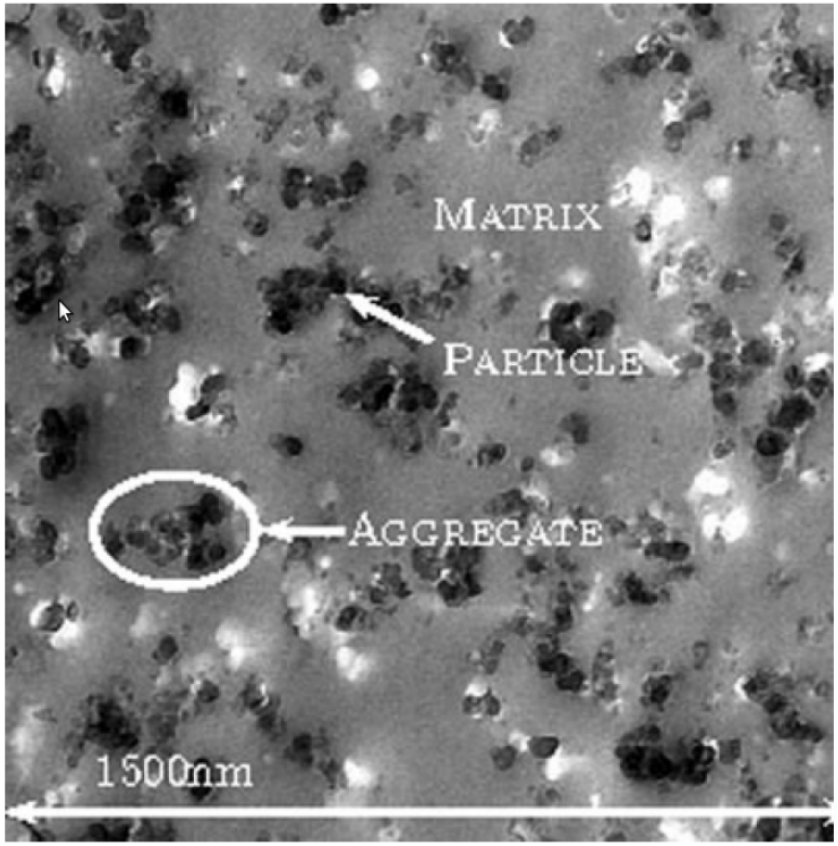


FIGURE – Inclusion of black carbon particles in a rubber matrix (Jean et al., Journal of microscopy, 2011).

Example : Coldspray film

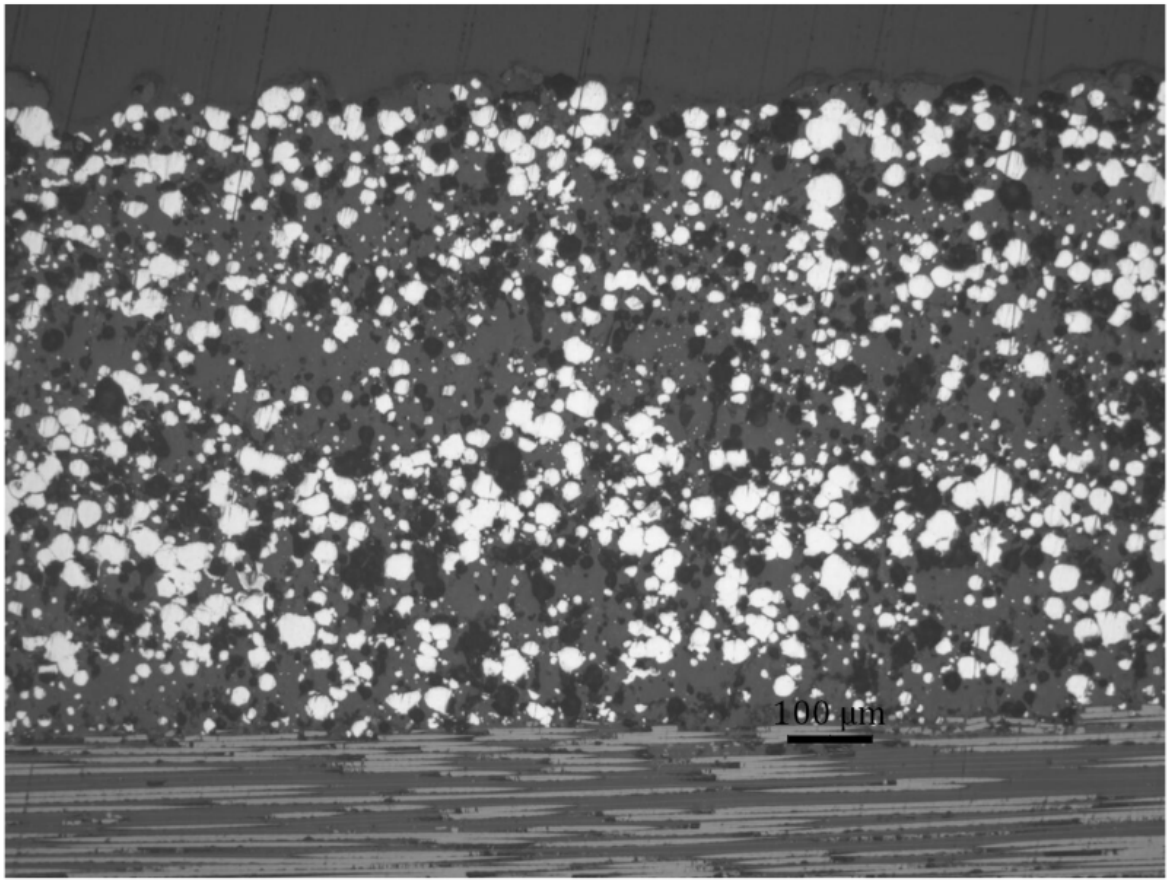
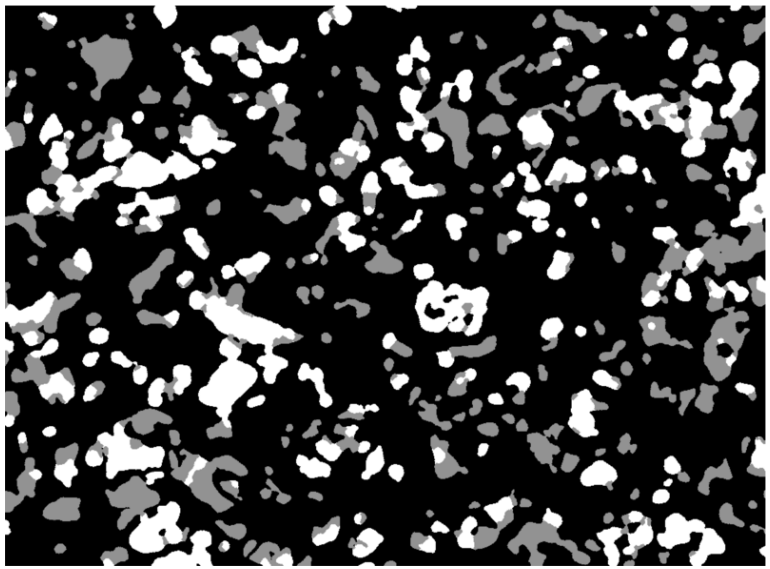
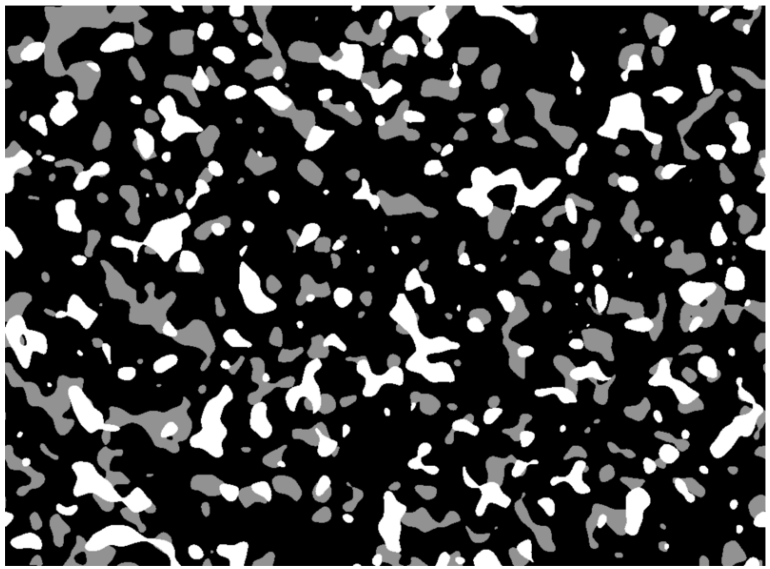


FIGURE – Coating made from a coldsprayed thin film (Bortolussi et al., 2018).

Example : fuel cell



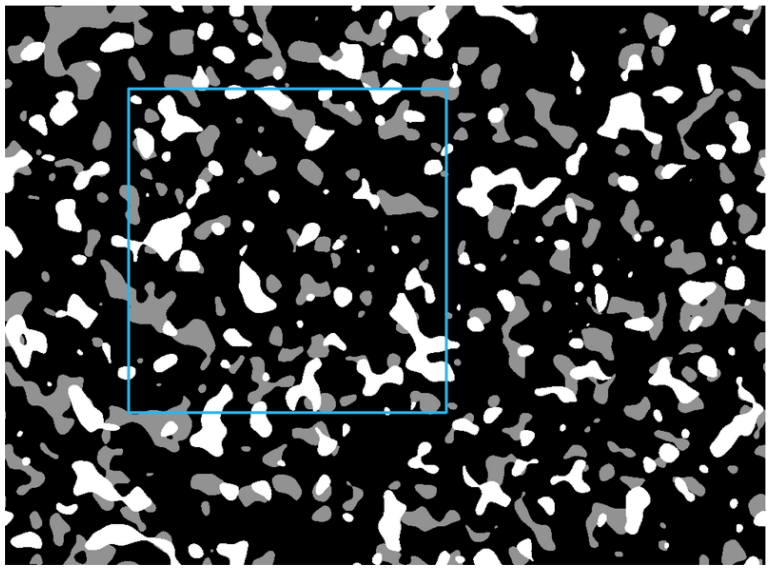
SEM image (segmented)

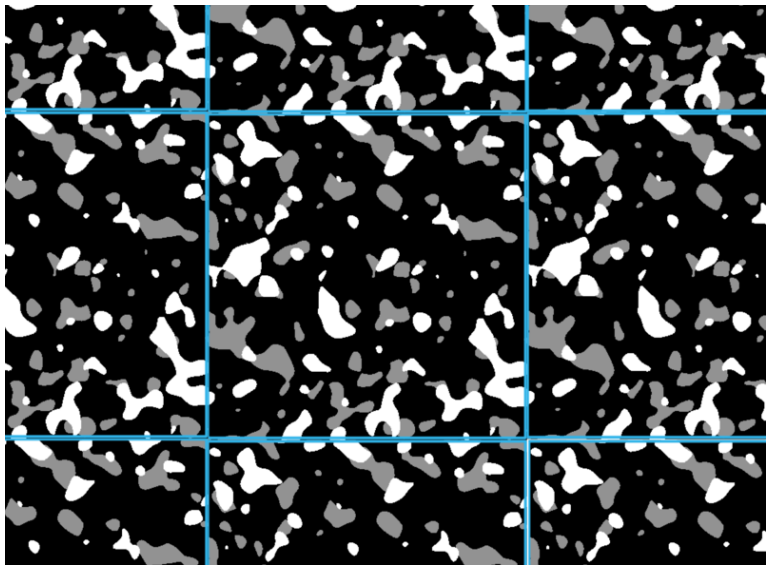


Model

FIGURE – Multi-phasic anode material from cold-spray (Abdallah et al., 2016).

Example : fuel cell





Compute the physical response on many subvolumes assuming periodic boundary conditions (as in FFT). Does the mean apparent property tends to the effective property as the number of subvolumes $\rightarrow \infty$?

Models of random structures

- Microstructure models must be able to account for a wide range of geometries
- They must enable the study of various physical and mechanical properties
- These models are interesting in that they rely on strong mathematical foundations

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Models of random structures

- Random set theory : modern developments originate in the works of Choquet (1954), Matheron (1965) and Kendall (1974). It aims to quantify and simulate the morphology of heterogeneous media by probabilistic means.
- A random set is usually a stochastic model whose realizations are closed subsets of $\mathbb{R}^d$ ($d = 2$ or 3 is the dimension). More generally, scalar or tensorial functions on $\mathbb{R}^d$ (or on a manifold).
- Random sets based on a *rigorous* definition theorized by G. Matheron, defined as random variables in an appropriate metric space. The probability distribution function of a random set is completely specified by a probability measure defined on a σ-algebra, that is, a space containing $\mathbb{R}^d$, the empty set, and which is stable by a countless number of unions and intersections and by complement. This algebra is used to define measures on sets of $\mathbb{R}^d$.

Models of random structures

Early attempts on specific models (Rice, S.O., 1944 ; Miles, R.E., 1964). The general theory and modern understanding was initiated by Matheron and Kendall.
References :

- Matheron, G. (1975). Random Sets and Integral Geometry, Wiley, New York.
- Kendall, D. (1974). Foundations of a theory of random sets.
- Serra, J. (1983). Image Analysis and Mathematical Morphology. Academic Press, Cambridge.
- Lantuéjoul (2002). Geostatistical Simulation : Models and Algorithms. Springer, Berlin, Chapter 2.
- Schneider, R., Weil, W. (2008). Stochastic and Integral Geometry. Springer-Verlag, Berlin, Heidelberg.

Models of random structures

The theory of random sets originate in image analysis (or mathematical morphology), i.e. the interest in finding criteria for characterizing random sets.
Usually, this is achieved in two steps : (i) a transformation of the set ; (ii) a measure on the transformed set. Mathematical morphology considers trasnformations that involve comparing two sets, one of them called the "structuring element".

Models of random structures

The fundamental theoretical tool for characterizing random sets is the Choquet capacity (Choquet, 1954) :

$$T(K) = P\{X \cap K \neq \varnothing\}, \tag{1}$$

The Choquet capacity satisfies :

i) $0 \leqslant T(K) \leqslant 1$ for any compact subset K, and $T(\varnothing) = 0$, $T(\mathbb{R}^d) = 1$,

ii) $T(K) \leqslant T(K \cup K')$ all compact subsets K and K',

iii) If K_n is a sequence of decreasing compact subsets (for inclusion) in $\mathbb{R}^d$, with limit $\mathcal{K}$, then

$$\lim_{n\to\infty} T(K_n) = T(\mathcal{K}).$$

Models of random structures

The "hitting functional" T "Choquet capacity" plays the same role for random sets with inclusion as that of the cumulative distribution function for random scalar variables with order relation $<$ (Matheron, 1975).This interpretation is justified by the following theorem (Choquet 1954 ; Kendall 1974 ; Matheron 1975) :

Theorem Let T be a functional defined on the set of compact subsets $\mathbb{K}$ of $\mathbb{R}^d$. Then a single probability measure P defined on the σ-algebra $\mathbb{F}_K$ exists such that :

$$P(\mathbb{F}_K) = T(K),$$

if, and only if, T is a Choquet capacity verifying (i), (ii) and (iii) in the previous slide.

Models of random structures

The σ-algebra $\mathbb{F}_K$ is then the smallest σ-algebra containing the closed sets that meet the compact subsets of $\mathbb{R}^d$:

$$\mathbb{F}_K = \{F \in \mathbb{F} : \ F \cap K \neq \varnothing\}, \qquad K \in \mathbb{K},$$

where $\mathbb{F}$ is the set of the closed subsets of $\mathbb{R}^d$ and $\mathbb{K}$ the set of compact subsets.
This property allows one to define random structures, but also to characterize them.

Models of random structures

Stationarity : a random set is stationary iff its Choquet capacity is translation-invariant : $T(K) = T(K_{\boldsymbol{x}})$ for all $\boldsymbol{x}$.

Isotropy : the Choquet capacity is rotation-invariant.

Ergodicity : all realizations of the random set model have the same Choquet capacity. There are other definitions of ergodicity, see Heinrich, 1992.

Models of random structures

Example : the Boolean random set with homogeneous Poisson point process $\mathcal{P}$ of intensity θ and primary grain G.

$$T(K) = 1 - \mathrm{e}^{-\theta \overline{\mu}_d(G \oplus \check{K})}$$

where $\check{K} = \{-\boldsymbol{x} | \boldsymbol{x} \in K\}$, $\oplus$ is the Minkowski addition :
$G \oplus \check{K} = \{\boldsymbol{x} | K_{\boldsymbol{x}} \cap G \neq \varnothing\}$ $(K_x = \{\boldsymbol{x} + \boldsymbol{y} | \boldsymbol{y} \in K\})$.
This capacity is that of realizations of the Boolean model (Serra, 1981) :

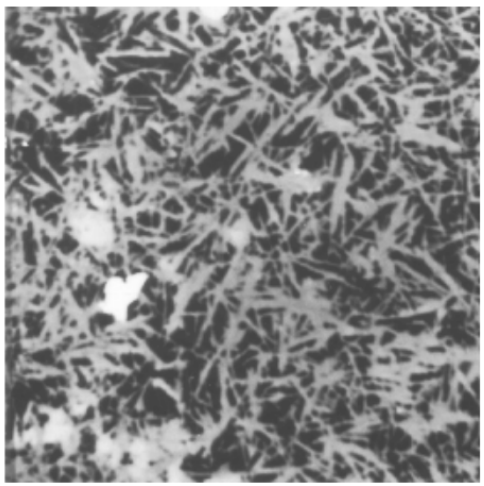
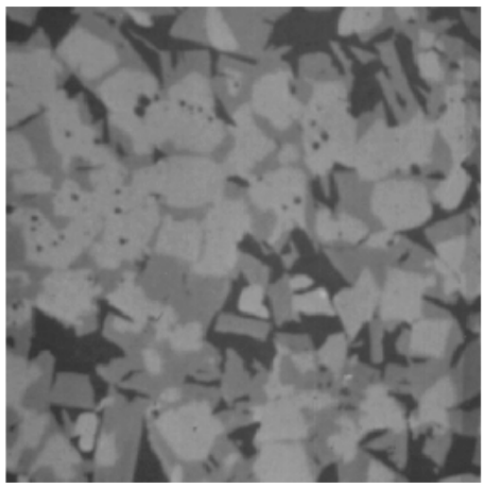
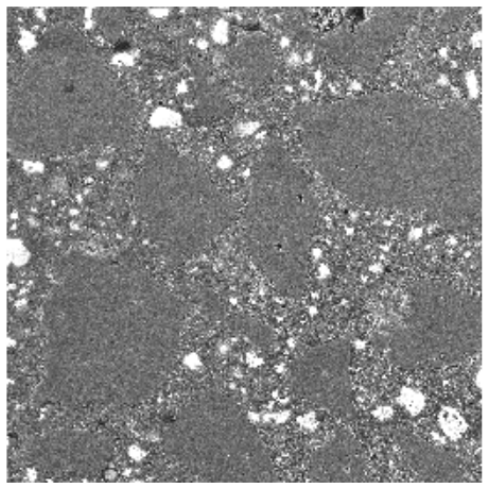
$$X = \bigcup_{x \sim \mathcal{P}} G_x$$

The set X is stationary and ergodic.

Boolean models can be considered to play the same role as the normal distribution for random sets with addition replaced by union. There exists the equivalent of a central limit theorem for random sets, where unions of i.i.d. random sets asymptotically tend to Boolean sets (Serra, 1981).

Models of random structures

Random media (microstructures) that fit with Boolean model

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Covariance

Probe the microstructure with compact sets. Spatial law : set of points $K = \{\boldsymbol{x}_1, \boldsymbol{x}_2, ..., \boldsymbol{x}_n\}$ $(n \geqslant 1)$.
Examples :

- $K = \{\boldsymbol{x}\}$. Then : $T(K) = P\{\boldsymbol{x} \in X\}$.
- Linear erosion : $K = \{\boldsymbol{x} + s(\boldsymbol{y} - \boldsymbol{x}) | 0 \leqslant s \leqslant 1\}$.
- Covariance : $K = \{\boldsymbol{x}, \boldsymbol{y}\}$. Then :
  $T(K) = P\{\boldsymbol{x} \in X \text{ and } \boldsymbol{y} \in X\} = C(\boldsymbol{x}, \boldsymbol{y})$.

Covariance

Useful properties of the covariance function :

- For stationary media, the covariance depends onlyon $\boldsymbol{h} = \boldsymbol{x} - \boldsymbol{y}$: $C(\boldsymbol{h}) = C(\boldsymbol{x}, \boldsymbol{y})$.
- For isotropic random sets, $C(h) = C(\boldsymbol{x}, \boldsymbol{y})$ where $h = |\boldsymbol{x} - \boldsymbol{y}$ is a one-dimensional function.
- $C(0) = V(X)$ the mean d-dimensional volume fraction of X.
- $\lim_{h \to \infty} C(h) = C(0)^2$
- $C(X; h) = 1 - 2C(X^c; 0) + C(X^c; h)$ where X^c is X's complementary set
- $C(h)$ is periodic if the set X is periodic
- If $C(h)$ admits the Taylor expansion $C(h) = C(0) - c_0 h + O(h^2)$, c_0 is the specific surface area in dimension 3, or specific perimeter, in dimension 2, of the set X.
- $C(h) - C(0) \sim h^\nu$ $(0 < \nu < 1)$ for a fractal set X of Hausdorff dimension $d_h = 3 - \nu$ (Matheron, 1989).
- Anti-correlation phenomena, mean length of cords, angular points, cusp are some of the geometrical properties that ca be related to covariances (e.g. Emery and Lantuéjoul, 2011)

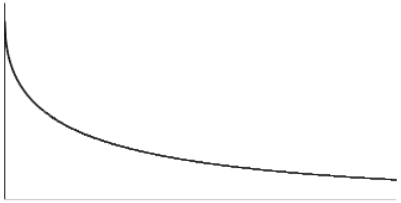
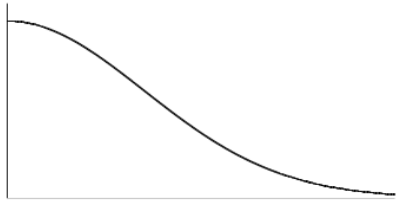
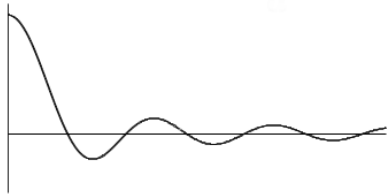
Covariance examples

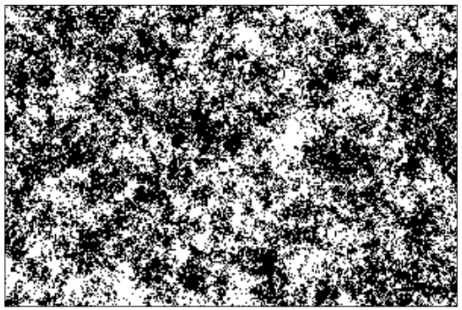
Any function does not define a covariance. Covariances are definite positive :

$$\sum_{\alpha,\beta=1}^{n} \lambda_\alpha \lambda_\beta C(h_\alpha - h_\beta) \geqslant 0, \qquad \lambda_\alpha, h_\alpha \in \mathbb{R}.$$

Some exact covariances.

Stable	Gaussian	Cardinal sine
$C(h) = \mathrm{e}^{-\sqrt{\lvert h\rvert/a}}$	$C(h) = \mathrm{e}^{-\lvert h\rvert^2/a^2}$	$C(h) = \frac{\sin(\lvert h\rvert/a)}{\lvert h\rvert/a}$



Covariance examples

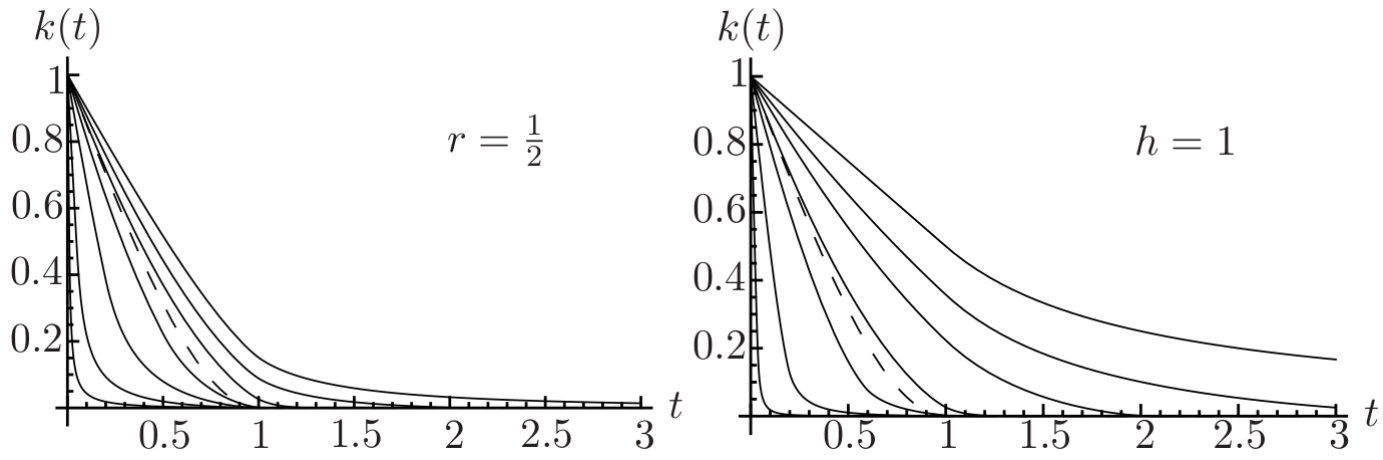
For a Boolean model of primary grains G,

$$C(h) = 2p - 1 + (1-p)^{2-k(h)/k(0)}$$

with k the covariogram :

$$k(h) = \langle |G \cap G_{\boldsymbol{h}}| \rangle_{|\boldsymbol{h}|=h}$$

where the mean is taken over all directions.
Ex : covariogram of cylinders with varying aspect ratio (first obtained by Gille, 1987)



Integral range

The integral range, homogeneous to a d-dimensional volume, is by definition :

$$A_d = \int_{h \in \mathbb{R}^d} \mathrm{d}^d \boldsymbol{h} \frac{C(\boldsymbol{h}) - C(0)^2}{C(0)[1 - C(0)]}$$

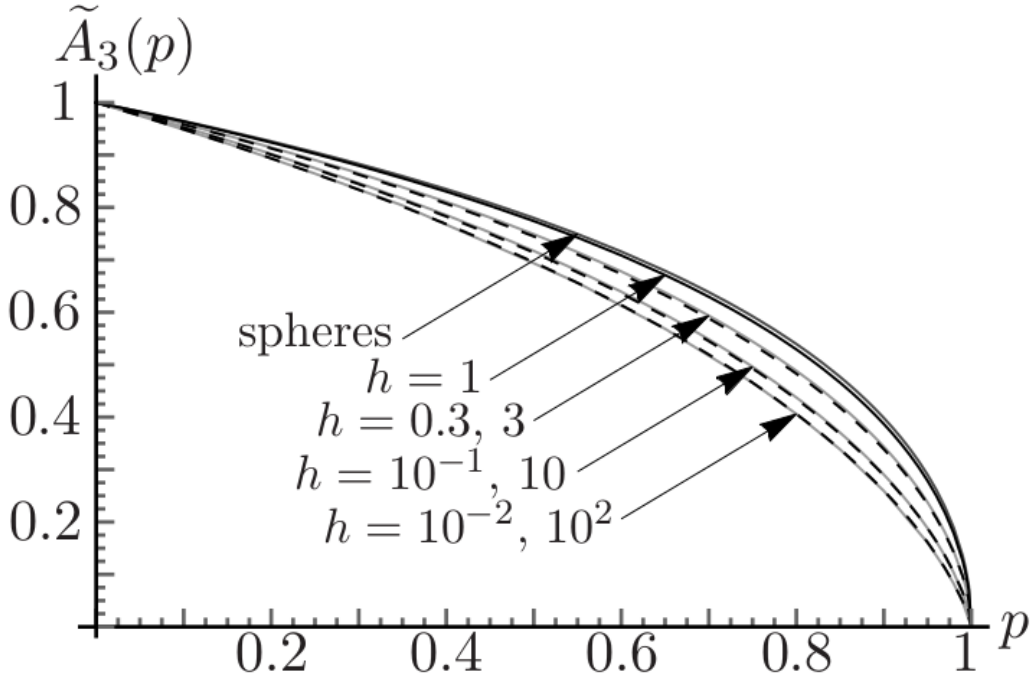
where $p = C(0)$ is the density of X.
For isotropic models :

$$A_d = \frac{1}{p(1-p)} \int_{h=0}^{\infty} S_d \mathrm{d}h [C(h) - p^2]$$

where S_d is the surface of the d-dimensional sphere.

Integral range

Example : integral range of Boolean models of cylinders vs. density p (in units of primagry grain volume).



Varying aspect ratios (Willot, 2017)

Representative volume element

Variance $D_X^2(V)$ of the apparent density of a stationary random set X, computed on d-dimensional domain Ω of volume V :

$$D_X^2(V) = \left\langle \left(\overline{p} - \frac{1}{V} \int_\Omega \mathrm{d}^d \boldsymbol{x} \chi_X(\boldsymbol{x}) \right)^2 \right\rangle$$

computed over random realizations of X, where $\overline{p}$ is the observed mean density, computed over all realizations and χ_X the characteristic function of X. For ergodic media, the mean can be computed over subvolumes "sufficiently" far from each other.

Representative volume element

For $N \gg 1$ we have $\overline{p} \longrightarrow p$ and :

$$D_X^2(V) = \frac{1}{NV^2} \sum_{i=1}^{N} \int_{\boldsymbol{x},\boldsymbol{y}\in\Omega} \mathrm{d}^d\boldsymbol{x}\mathrm{d}^d\boldsymbol{y} \left[\chi x(\boldsymbol{x})\chi x(\boldsymbol{y}) - p^2\right].$$

Property : when $V \gg A_d$:

$$D_X^2(V) = p(1-p)\frac{A_d}{V} + o(1/V).$$

Representative volume element

Proof :

$$D_X^2(V) = \frac{1}{NV^2} \sum_{i=1}^{N} \int_{\boldsymbol{x},\boldsymbol{y}\in\Omega} \mathrm{d}^d\boldsymbol{x}\mathrm{d}^d\boldsymbol{y} \left[\chi x(\boldsymbol{x})\chi x(\boldsymbol{y}) - p^2\right].$$

Use the variable change $\boldsymbol{t} = \boldsymbol{x} - \boldsymbol{y}$.

Representative volume element

Interpretation of the relation :

$$D^2_X(V) = p(1-p)\frac{A_d}{V} + o(1/V).$$

When $V \gg A_d$,

$$D^2_X(V) \sim \frac{\text{var}(\chi(0))}{V/A_d}$$

where $\text{var}(\chi(0))$ is the point variance and $n = V/A_d$ is the volume size, expressed in units of integral range.
The $D^2_X(V) = \text{var}(\chi(0))/n$ represents the variance of a mean of n independent observations. This is as if the domain V had been divided into n independent domains of the same size A_d. A_d must then be interpreted as the scale of the phenomenon (see Lantuéjoul, 1991).

Representative volume element

Special case : when $A_d = 0$ (possible when anti-correlations are present), the variance displays "super-convergence", i.e. goes to 0 faster than $1/V$.

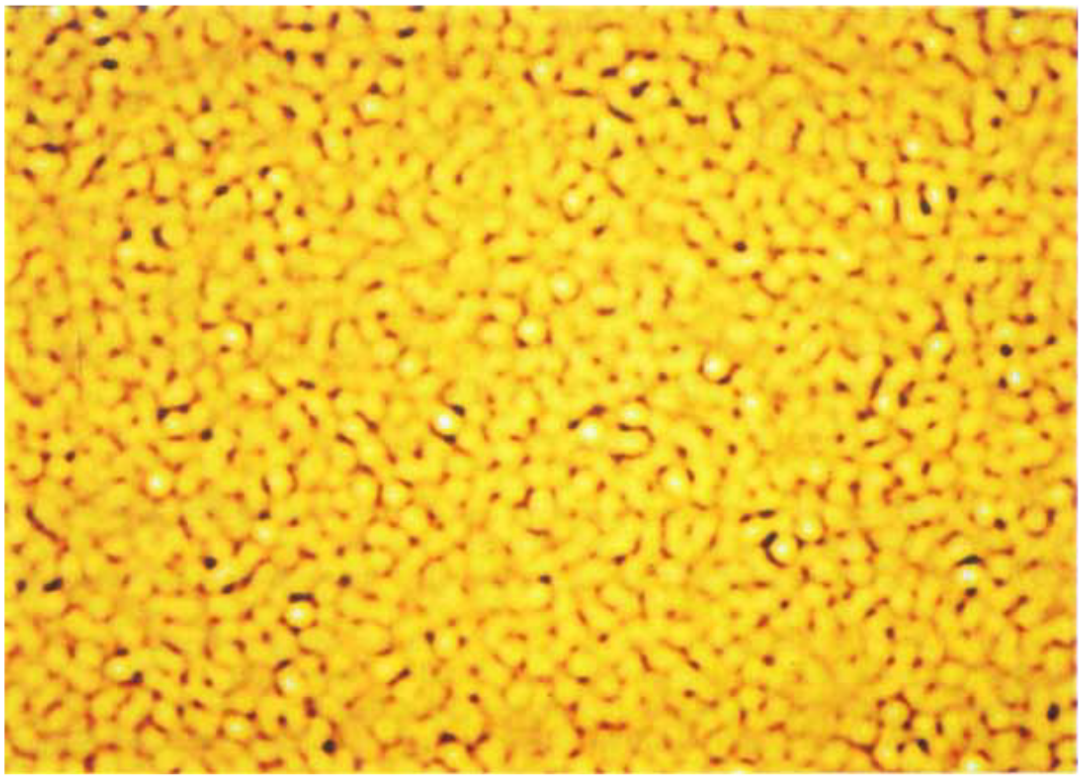


Fig. 7. Realization of an SERF with a zero integral range (dilution random function).

From Lantuéjoul (1991). Dilution function : $\sum_{\boldsymbol{y} \in \mathcal{P}} f(\boldsymbol{x} - \boldsymbol{y})$ with $\langle f \rangle = 0$.

Representative volume element

Extensions and properties.

Miles-Lantuéjoul correction for subvolumes V of a larger volume V_0 (Lantuéjoul, 1991) :

$$D_X^2(V) = p(1-p)\frac{A_d}{V}\left(1 - \frac{V}{V_0}\right) + o(1/V).$$

Interpretation : the mean of the values computed on subvolumes is biased (equal to that in V_0), hence there are two sources for the variance, that of "regular" domains of volume V and that for V_0.

Due to the central limit theorem, the distribution of the mean is asymptotically Gaussian (Legoll, 2014).

Representative volume element

The absolute and relative errors for n samples of volume V are defined as :

$$\varepsilon_{\text{abs}} = \frac{2D_X(V)}{\sqrt{n}}, \qquad \varepsilon_{\text{rela}} = \frac{\varepsilon_{\text{abs}}}{p} = \frac{2D_X(V)}{p\sqrt{n}}$$

The RVE size for a given relative precision $\varepsilon_{\text{rela}}$ is then :

$$V_{\text{RVE}} = \frac{4\text{var}(\chi(0))A_d}{n\varepsilon_{\text{rela}}^2 p^2}$$

Note the $\varepsilon_{\text{rela}}^2$ term. This is because ε is proportional to the standard deviation. Hence, one additional digit of precision requires in general $100\times$-larger volume size.

Representative volume element

The precision of a given prediction can conversely be computed as :

$$\varepsilon_{\text{rela}} = \frac{2\text{std}(\chi(0))\sqrt{A_d}}{p\sqrt{nV_{\text{RVE}}}}$$

In terms of absolute error :

$$V_{\text{RVE}} = \frac{4\text{var}(\chi(0))A_d}{n\varepsilon_{\text{abs}}^2}$$

$$\varepsilon_{\text{abs}} = \frac{2\text{std}(\chi(0))\sqrt{A_d}}{\sqrt{nV_{\text{RVE}}}}$$

Representative volume element

Example : Voronoi tesselation of space (Kanit et al, 2003) Every cell colored at random.

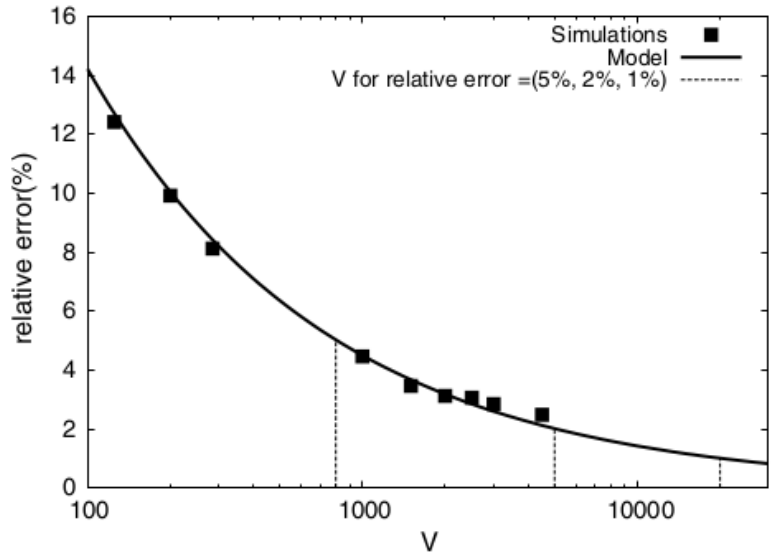


Fig. 14. Relative precision $\varepsilon_{\text{rela}}$ for volume fraction $P = 70\%$ and $n = 1$ realization: It decreases when the size of the domain increases.

RVE for random fields

Straightforward extension of the theory to random functions, i.e. *scalar fields*. Spatial distribution of an ergodic, stationary random function $Z(\boldsymbol{x})$:

$$F_{\boldsymbol{x}_1,\ldots,\boldsymbol{x}_n}(z_1,\ldots,z_n) = P\{Z(\boldsymbol{x}_i) < z_i\}$$

The spatial distribution can be extended to a unique probability measure on a σ-algebra (Kolmogorov, 1933 ; Neveu, 1965).
Covariogram :

$$K(\boldsymbol{h}) = \int_{\mathbb{R}^d} \mathrm{d}\boldsymbol{x} Z(\boldsymbol{x}) Z(\boldsymbol{x}+\boldsymbol{h})$$

Covariance : $C(\boldsymbol{h}) = \mathrm{Cov}(Z(\boldsymbol{x}), Z(\boldsymbol{x}+\boldsymbol{h})) = K(\boldsymbol{h}) - p^2$ where $p = \int_{\mathbb{R}^d} \mathrm{d}\boldsymbol{x} Z(\boldsymbol{x})$
Interal range :

$$A_d = \int_{\mathbb{R}^d} \mathrm{d}\boldsymbol{h} \left[C(\boldsymbol{h}) - C(0)^2\right] = \lim_{V\to\infty} \frac{V D_Z^2(V)}{\mathrm{var}(Z(\boldsymbol{x}))}$$

Extensions to vectorial (Jeulin, 1990) and tensorial fields are delicate.

Contents

The RVE method in homogenization

To apply Matheron's formula to random fields from stochastic homogenization one need to solve two problems :

- (i) The random fields are NOT stationary when boundary conditions are applied on a volume element ;
- (ii) Unknown correlations length.

Solution for these two issues :

- Problem (i) can be solved by considering the solutions of auxiliary problems with stationary fields that approximate (in a way that can be controlled) the fields of interest.
- Problem (ii) can be tracted for certain problems by applying Matheron's techniques on the auxiliary fields. Correlation length are provided by the Green operator.

The RVE method in homogenization

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Solution for these two issues for elliptic problems :

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- Problem (ii) can be tracted for certain problems by applying Matheron's techniques on the auxiliary fields. Correlation length are provided by the Green operator.

Main results obtained by Yurinskii (Sibirsk Mat. Zh. ; 1986), Naddaf and Spencer (1998) and the theory subsequently developed by Gloria and Otto (2011). More general results by Kozlov (1979), Papanicolaou and Varadhan (1981) and Künnemann (1983) in the continuum and discrete case, with ergodic hypothesis.

The RVE method in homogenization

Consider the simple case of a d-dimensional lattice $\mathbb{Z}^d$ with random conductivity $a(\boldsymbol{x}, \boldsymbol{x})$ along each bond connecting $\boldsymbol{x}$ and $\boldsymbol{y} = \boldsymbol{x} + \mathrm{e}_i$.
"Conductivity" problem with macroscopic loading ξ for the gradient field :

$$-\nabla^* \cdot [A(\xi + \nabla\Phi)](\boldsymbol{x}) = \sum_{|\boldsymbol{x}-\boldsymbol{y}|=1} = a(\boldsymbol{x}, bmy)[\phi(\boldsymbol{x}) - \phi(\boldsymbol{y})] = 0.$$

Hypothesis :

- Uniform ellipticity :

$$0 < \alpha \leqslant a(\boldsymbol{x}, bmy) \leqslant \beta$$

  for some α, $\beta < \infty$.
- The $a(\boldsymbol{x}, bmy)$ are independently and identically distributed ;

The RVE method in homogenization

Homogenized conductivity defined by :

$$\xi \cdot A_{\text{hom}}\xi = \langle (\xi + \nabla\phi) \cdot A(\xi + \nabla\phi) \rangle$$

where the mean is evaluated over random configurations (at any given point, since the model is stationary).
Since the corrector field ϕ is ergodic :

$$\sum (\xi + \nabla\phi) \cdot A(\xi + \nabla\phi)\eta_L \to \xi \cdot A_{\text{hom}}\xi$$

as $L \to \infty$ where η_L is an averaging function so that $\text{supp}(\eta_L) \subset \{|x| \leqslant L\}$, $|\eta_L| \lesssim L^{-d}$, $\sum \eta_L = 1$.
Convergence rate w.r.t. L ?

The RVE method in homogenization

Main problem : the field ϕ has to be solved on the whole space $\mathbb{Z}^d$ (for a single realization).
It is natural to replace the field ϕ by the field ϕ_R solution of :

$$\begin{aligned} -\nabla^* \cdot [A(\xi + \nabla \Phi_R)] = 0 \quad & \text{in } \mathbb{Z}^d \cap \{|\boldsymbol{x}| < R\}, \\ \Phi_R = 0 \quad & \text{in } \mathbb{Z}^d \cap \{|\boldsymbol{x}| \geqslant R\}, \end{aligned}$$

where $R \gg L$.
However ϕ_R is not stationary anymore.

The RVE method in homogenization

The main idea in a nutshell : replace the elliptic PDE for the conductivity problem by :

$$\frac{1}{T}\phi_T - \nabla^* \cdot [A(\xi + \nabla\Phi_T)] = 0$$

the field solution (Φ_T) is
The zero-order term introduces a characteristic length $\sim \sqrt{T}$ in ϕ_T.
In a second step, one replaces the above PDE with :

$$\begin{aligned} \tfrac{1}{T}\phi_T - \nabla^* \cdot [A(\xi + \nabla\Phi_{T,R})] = 0 \quad & \text{in } \mathbb{Z}^d \cap \{|\boldsymbol{x}| < R\}, \\ \Phi_{T,R} = 0 \quad & \text{in } \mathbb{Z}^d \cap \{|\boldsymbol{x}| \geqslant R\}, \end{aligned}$$

with unknown $\Phi_{T,R}$.
With suitable choice of R and L, $\phi_{T,R}$ (which can be computed) is a very good approximation of ϕ_T which is a very good approximation of ϕ as $T \to \infty$.

The RVE method in homogenization

Error we make when replacing :

$$\xi \cdot A_{\text{hom}} \xi \rightarrow \sum (\xi + \nabla \phi_T) \cdot A(\xi + \nabla \phi_T) \eta_L$$

Two sources of error : finite-size effects ($L \neq \infty$) and that related to the cut-off length-scale T :

$$\left\langle \left| \sum (\xi + \nabla \phi_T) \cdot A(\xi + \nabla \phi_T) \eta_L - \xi \cdot A_{\text{hom}} \xi \right|^2 \right\rangle = \left\langle \left| \sum (\xi + \nabla \phi_T) \cdot A(\xi + \nabla \phi_T) \eta_L - \langle (\xi + \nabla \phi) \cdot A(\xi + \nabla \phi) \rangle \right|^2 \right\rangle$$

$$= \underbrace{\text{var}\left[\sum (\xi + \nabla \phi_T) \cdot A(\xi + \nabla \phi_T) \eta_L \right]}_{\sim L^{-d} \text{ in the low-limit contrast}} + \underbrace{\left| \left\langle \sum (\xi + \nabla \phi_T) \cdot A(\xi + \nabla \phi_T) \eta_L \right\rangle - \langle (\xi + \nabla \phi) \cdot A(\xi + \nabla \phi) \rangle \right|^2}_{\left\langle (\nabla \phi_T - \nabla \phi) \cdot A(\nabla \phi_T - \nabla \phi) \right\rangle \text{ stationarity of } \phi, \phi_T \atop \sim T^{-d} \text{ in the low-contrast limit}}$$

The RVE method in homogenization

The choice $L \sim \sqrt{T} \sim R$ is "optimal" in the sense that errors due to the cut-off can then be neglected and finite-size effects are the leading order term, which scales as :

$$\mathrm{var}\left[\sum(\xi + \nabla\phi_T) \cdot A(\xi + \nabla\phi_T)\eta_L\right] \lesssim L^{-d}$$

except for $d = 2$:

$$\mathrm{var}\left[\sum(\xi + \nabla\phi_T) \cdot A(\xi + \nabla\phi_T)\eta_L\right] \lesssim L^{-d}(\log L)^{q(\alpha,\beta)}$$

In the above, an additional assumption on the smoothness of η_L is made : $|\nabla\eta_L| \lesssim L^{-d-1}$.
Proof in Gloria and Otto (2011), Annex A. Consider the low-contrast regime. In that setting, the Lippman-Schwinger equation gives an exact solution to first-order in the contrast, and depends only on the statistics of $A - \langle A \rangle$. Variations are given by derivatives w.r.t. $a(\boldsymbol{x})$, and the Green identity results in terms $\eta_L^2 \sim L^{-d}$.

The RVE method in homogenization

This leads to the scaling-law (Kozlov, Math. Sb, 1979) :

$$|\langle A_L \rangle - A_{\text{hom}}| \sim \begin{cases} C(\alpha,\beta) L^{-1} (\log L)^{q(\alpha,\beta)} & \text{if } d = 2, \\ C(\alpha,\beta) L^{-3/2} & \text{if } d = 3, \\ C(\alpha,\beta) L^{-2} \log L & \text{if } d = 4, \\ C(d,\alpha,\beta) L^{-2} & \text{if } d \geqslant 5. \end{cases}$$

with $d = 4$ the critical dimension. Different from the result of random fields with finite correlation length.
Results have been extended to the continuum (Gloria and Otto, 2018).

The RVE method in homogenization

The same result holds for periodic boundary conditions (Gloria, ESAIM, 2012) :

$$|\langle A_{L,\#}\rangle - A_{\text{hom}}| \sim \begin{cases} C(\alpha,\beta)L^{-1}\left(\log L\right)^{q(\alpha,\beta)} & \text{if } d=2, \\ C(\alpha,\beta)L^{-3/2} & \text{if } d=3. \end{cases}$$

For Dirichlet and Neuman boundary conditions :

$$|\langle A_{L,\#}\rangle - A_{\text{hom}}| \sim \begin{cases} C(\alpha,\beta)L^{-1/2} & \text{if } d=2, \\ C(\alpha,\beta)L^{-1} & \text{if } d=3. \end{cases}$$

In general, the fields are disturbed in a region along the surface with a width of the same order as the charatcertic length in the microstructure. See Gloria and Mourrat (2012).

Representative volume element

Example : stress field in multi-scale rigidly-reinforced Boolean models in elasticity (Willot and Jeulin, 2010)

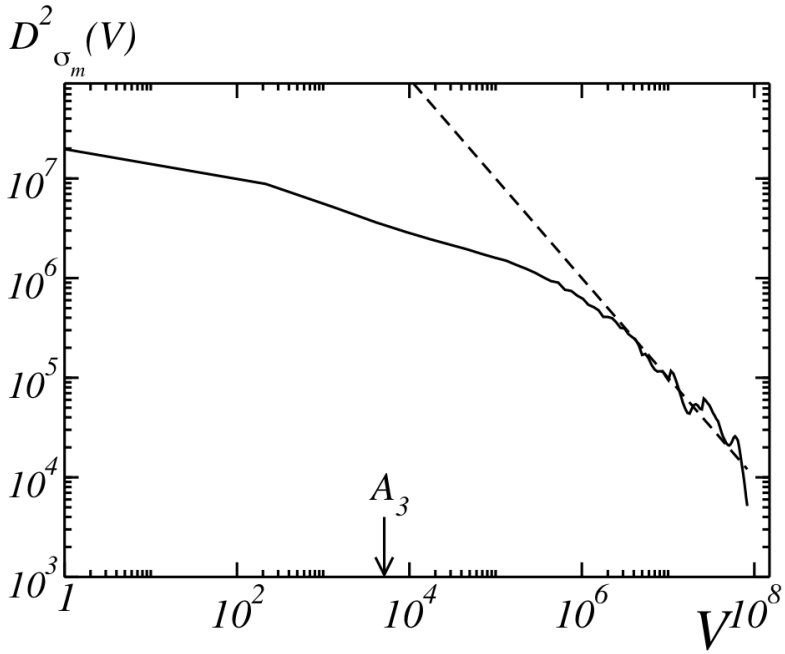
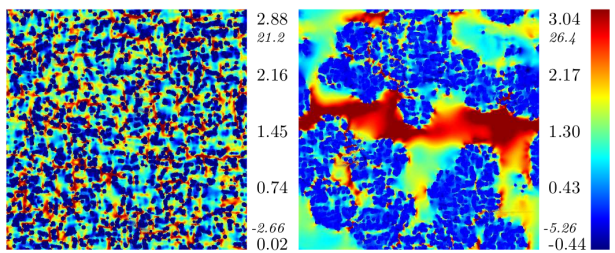


FIG. 10.7. *Variance of the mean average stress field $\langle\sigma_m\rangle$, proportional to the material apparent bulk-modulus, as computed on volumes of size V, as a function of the volume size, for two-scales iterated Boolean model (IB) with quasi rigid inclusions, at $f = 0.7$ (solid line). The dotted line represents a fit of the variance $D^2_{\sigma_m}(V)$ with Eq. 9.2, which holds for volumes much larger than the integral range, i.e. $V \gg A_3$.*



Representative volume element

Comparison between finite element and FFT computations (Jean et al, 2009). Elasticity.

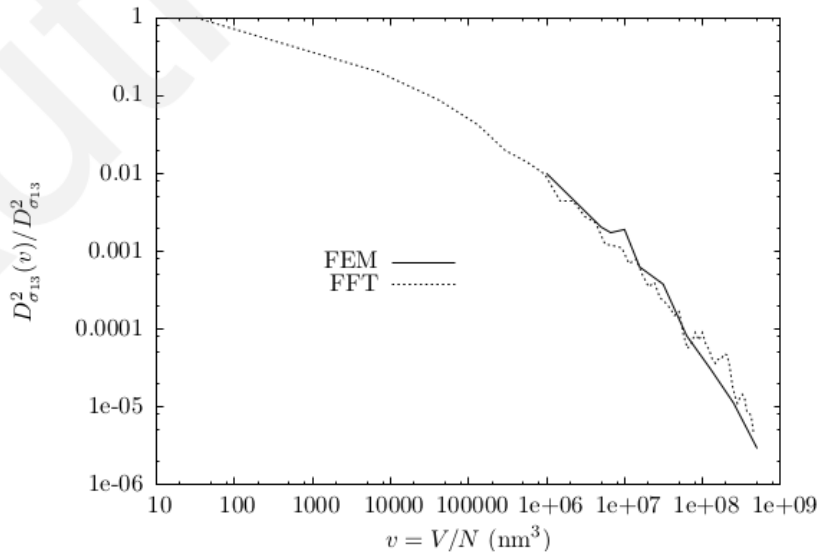
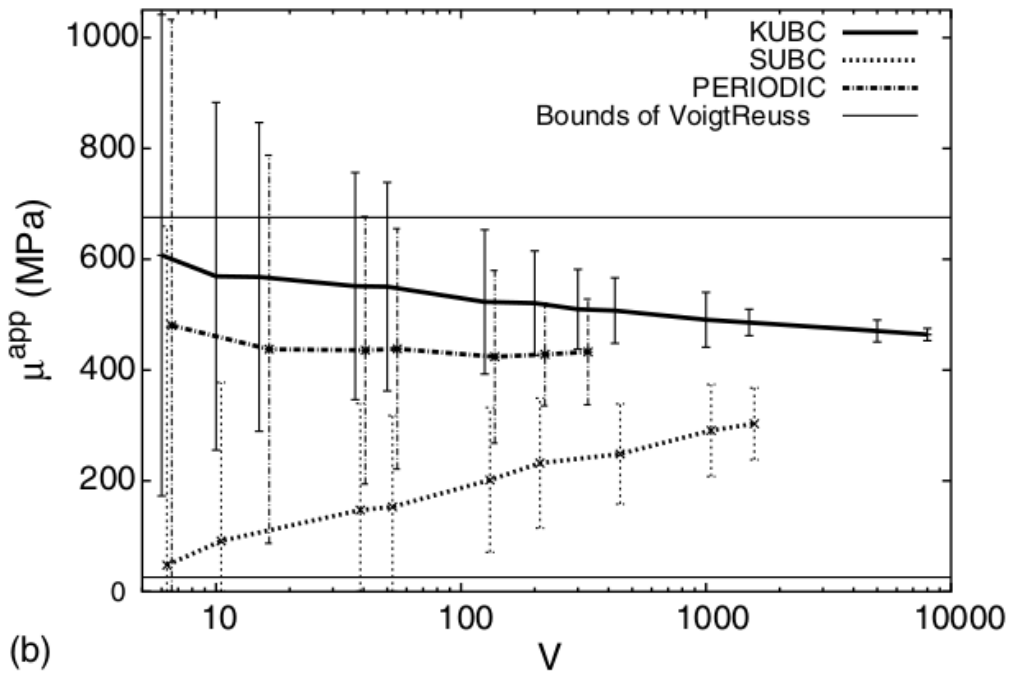


FIG. 17: Variance of apparent mechanical properties on punctual variance as a function of volume of subdomains.

Representative volume element

Example : effect of boundary conditions (Kanit et al, 2003), unifrm (static, kinematic) and periodic.



As expected, $\mathbb{C}_{\text{app}}^{\text{subc}} \leqslant \mathbb{C}^{\text{hom}} \leqslant \mathbb{C}_{\text{app}}^{\text{kubc}}$. Yet, huge size effects are observed for uniform boundary conditions, particularly SUBC (porous media).

The RVE method in homogenization

Some references related to RVEs for physical properties :

- Elasticity in concrete (Escoda et al, 2011).
- Elasticity and thermal conductivity in fibrous media (Altendorf et al, 2011). Role of the shape of the RVE.
- Multiscale RVEs (Willot and Jeulin, 2011).
- Optics in electrostatics for deposit models (Azzimonti et al, 2013). Singular scaling laws due to surface effects (in 3D) induced by deposit models.
- Acoustics (Peyrega et al, 2009)
- Plasticity (Dirrenberger et al, 2016)
- Mesoporous alumina (Wang et al, 2014)
- Permeability (Abdallah et al, 2016)
- Schneider et al, 2021.

Contents

Conclusion

- The size of the representative volume element depends in general on the property sought for and on the required precision.
- For the density of random sets, its scaling law can be derived in the limit of a large RVE as a Taylor expansion. In the absence of large-scale correlation, this results in a Taylor expansion.
- The scaling law obeys that of random independent, identically-distributed scalar variables where the number of i.i.d. variables is the voluem size, expressed in integral-range unit-size
- The integral range is the integral of the correlation function. Accordingly, singular behavior occur when the integral range is infinite (correlation at infinite length) or zero.

Conclusion (II)

- Elliptic PDEs (for the simple conductivity problems, with finite contrast) follow the same trend, up to logarithmic corrections, provided one uses periodic boundary conditions.
- The theory may be applied to any self-averaging quantity, e.g. the field fluctuations, or local fields in one given phase of a composite.
- Do consider several samples when doing numerical mechanics ! In most cases, the standard dviation decreases as $1/\sqrt{n}$ so you gain a lot at the beginning.
- Mechanics.