Mathematical Morphology
Random sets and Porous Media

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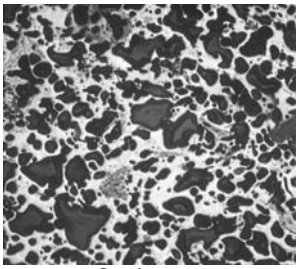
Origin – Motivations
G. Matheron, 1967



L = 1 mm

- **Characterization of the morphology** of a heterogeneous medium?
- **Prediction of the macroscopic behaviour** of a porous medium (composition of permeabilities)?
- **Representation** of a heterogeneous medium by a model?

Introduction

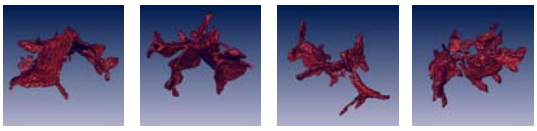
- Extraction of quantitative information on microstructures (3D images, measurements)
- Models of random sets and simulation of microstructures
- Theory of random sets and tools to solve homogenization problems

Characterization of a random structure

- 3D Images
- Morphological Criteria
- Probabilistic Criteria

3D Images of Intermetallic particles in Al alloys

- X ray microtomography performed at the ESRF (ID 19 line)
- 3D measurements
- High resolution (0.7µm)
- 3D complex shapes of particles (morphological parameters, local curvature) (E. Parra-Denis PhD)



ZnO by Nanotomography

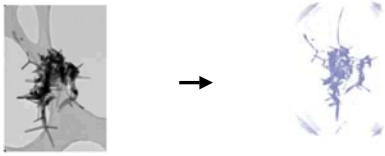
ZnO needles after sublimation in the solair oven
PROMES Laboratory (CNRS Odeillo)

Application : ionic conduction

Acquisition : -42° à +37° with 1° increments

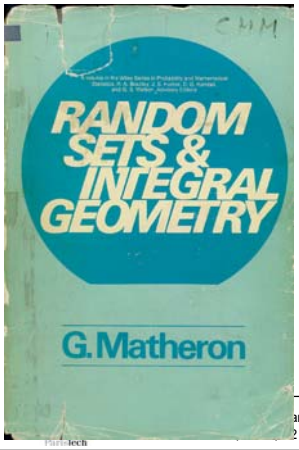
Resolution of images : x12000
2 nm ↔ 1 voxel

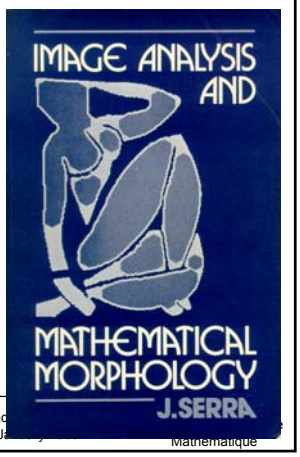
Arnaud GROSJEAN
Dominique JEULIN
Maxime MOREAUD
Alain THOREL



ZnO by Nanotomography

Resolution : 2 nm ↔ 1 voxel





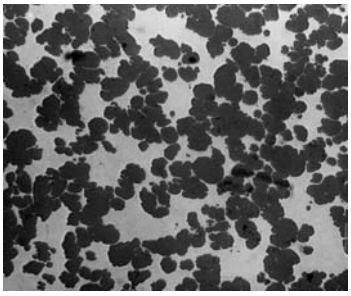
Characterization of a random structure: Main Criteria

- **Morphological criteria**
  - Size
  - Shape
  - Distribution in space (Clustering, Scales, Anisotropy)
  - Connectivity
- **Probabilistic criteria**
  - Probability laws (n points, $\sup_K$)
  - Moments

Characterization of a random set

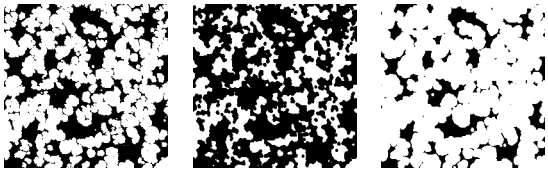
- Models derived from the ***theory of Random Sets by G. MATHERON***
- For a random closed set A (RACS), characterization by the ***CHOQUET capacity*** *T(K)* defined on the compact sets *K*
  $T(K) = P\{K \cap A \neq \Phi\} = 1 - P\{K \subset A^c\} = 1 - Q(K)$
- In the euclidean space R^n, CHOQUET capacity and ***dilation operation*** $T(K_x) = P\{x \in A \oplus K\}$

Binary Morphology (Fe-Ag)



L = 250 µm

Basic Operations of MM



Erosion hexagonal (2)

Dilation hexagonal (2)

Morphological interpretation

- ***Experimental estimation*** of *T(K)* by image analysis, using realizations of *A*, and dilation operation.
- General case: ***several realizations*** and estimation for every point *x*
- For a ***stationary random set***, $T(K_x) = T(K)$;
- For an ***ergodic random set***, *T(K)* estimated from a single realization by measurement of a volume fraction
- Every compact set *K* (points, ball...) brings its ***own information*** on the random set *A*

Calculation of the CHOQUET capacity

For a given model, the functional *T* is obtained:

- by **theoretical calculation**
- by **estimation**
  - on simulations
  - on real structures (possible estimation of the parameters from the "experimental" *T* , and tests of the validity of assumptions).

Models of Random Structures

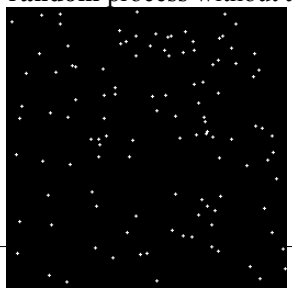
Point Processes

Most simple kind of random structure: very small defects isolated in a matrix

- Particular RACS: ***Choquet capacity*** *T(K)*
- ***Probability generating function*** $G_K(s)$ of the random variable *N(K)* (number of points of the process contained in *K)*

Poisson Point Process

Prototype **random** process without any order



Random sets and Random Functions Models

Starting from a point process, more general models, called **grain** models:

- The ***Boolean model***
- ***The dead leaves model***
- ***Random function models***

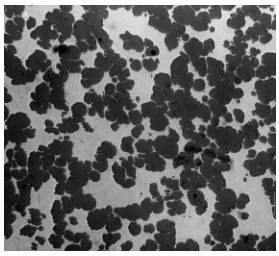
Boolean Model

- The Boolean model (G. Matheron) is obtained by implantation of random primary grains *A'* (with possible overlaps) on Poisson points x_k with the intensity q:

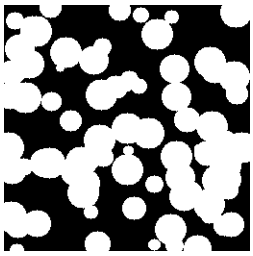
$$A = \bigcup x_k A'_{xk}$$

- Any shape (convex or non convex, and even non connected) can be used for the grain *A'*

Boolean Model (G. Matheron, 1967)



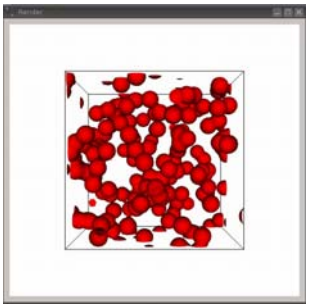
Fe-Ag Alloy



Boolean Model of Spheres (0.5)

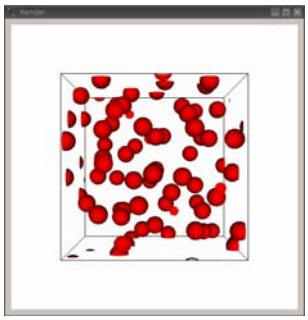
Boolean Model of Spheres 3D Simulation

D. Jeulin
M. Faessel
(CMM)



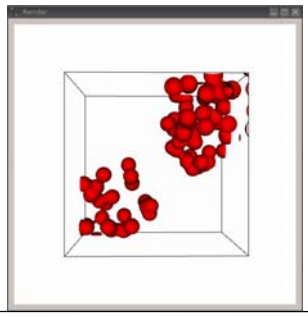
Hard Spheres 3D Simulation

D. Jeulin
M. Faessel
(CMM)



2 scales Cox Boolean model of Spheres 3D Simulation

D. Jeulin
M. Faessel
(CMM)



Boolean Model

WC Co (J.L. Chermant, M. Coster, J.L. Quennec 'h et D. Jeulin) L = 40 µm

Poisson Boolean Model (P. Delfiner)

Boolean Model

- Choquet capacity, with $q = P\{x \in A^c\}$

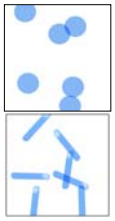
$$T(K) = 1 - Q(K) = 1 - \exp\left(-\theta\,\mu_n(A' \oplus K)\right) = 1 - q^{\frac{\mu_n(A' \oplus K)}{\mu_n(A')}}$$

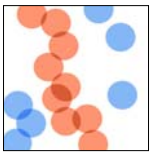
- Ex: contact distribution (ball), covariance
- **Percolation threshold** obtained **from simulations**: 0:2895 +- 0:0005 for spheres with a single diameter
- Percolation threshold related to the zeroes of $N_V - G_V(p)$

Percolation threshold

- **Materials made of components with a high contrast of properties: strong effect on the macroscopic properties when a given phase (e.g. the pores) percolates through the structure (connected paths in the samples of the medium)**
- **For a given model, estimation of the critical percolation threshold ρc (volume fraction above which a component percolates)**

Percolation of random structures



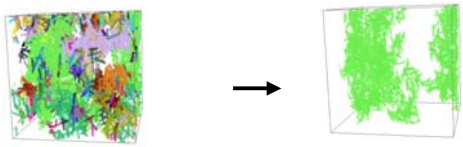


No percolation : no path connects two opposite faces

Percolation: one aggregate connects two opposite faces

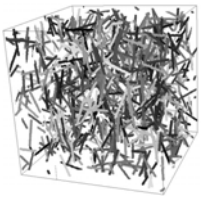
How to estimate a percolation threshold?

Labelisation of aggregates allows easy extraction of aggregates connecting two opposite faces



Percolation threshold ρc = volume fraction of objects when 50% of the realizations have aggregates connecting two opposite faces

Carbon nanotubes composite materials



Outstanding mechanical, electrical or chemical properties, mainly due to their low percolation threshold

Percolation of a Boolean model of spheres

[*] Jeulin D., Moreaud M. Multi-scale simulation of random spheres aggregates – application to nanocomposites, Proc. 9th European Congress on Stereology and Image Analysis, Zakopane, Poland, May 10-13 2005, Vol. I p. 341-348.

Volume : 2000^3

sphere radius : 10

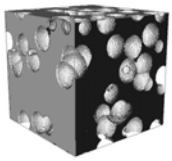
Average Nb. of simulated spheres	Average computation time for one realization	Percolation threshold
about 5 000 000	48 s.	0.2897±0.0004

PC PIV 2.6GHz RAM 768 Mo

(*) 0.2895±0.005
M.D. Rintoul et S. Torquato, Precise determination of the critical threshold and exponents in a three-dimensional continuum percolation model, J. Phys. A: Math. Gen. 30, L585-L592, 1997

Percolation of a Boolean model of spheres (complementary set)

Estimation of the percolation threshold of the complementary random set of a boolean model of spheres (constant radius)

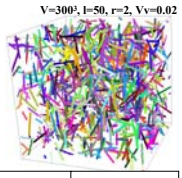


ρc = 0.0540±0.005

Percolation of a Boolean model of sphero-cylinders with uniform orientations

One scale simulation
Periodic simulations along axis x and y (50 realizations)

AR=l / r

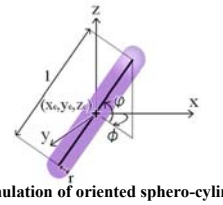


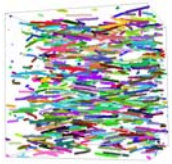
Aspect ratio l/r	3000	500	100	10
ρ_c	0.00037	0.00232	0.01145	0.09780

Jeulin D., Moreaud M. Percolation of multi-scale fiber aggregates, Proc. 6th International Conference on Stereology, Spatial Statistics and Stochastic Geometry, Czech Republic, June 26-26, 2006.

Percolation of oriented sphero-cylinders

Materials like papers or carbon nanotubes enhanced elastomers are composed of oriented fibers





V=300³, l=50, r=2, Vv=0.02, x=± 15°

Simulation of oriented sphero-cylinders: Φ uniformly distributed, φ limited between –x and +x

Percolation of oriented sphero-cylinders

φ between –x and +x

Aspect ratio	1000	Volume = (10 x AR)³		
x	5	15	40	60
ρ_c Z	0.0018	0.0015	0.0013	0.0012
ρ_c XY	0.0015	0.0013	0.0012	0.0012
Aspect ratio	**100**	**Volume = (10 x AR)³**		
x	5	15	40	60
ρ_c Z	0.0250	0.0197	0.0149	0.0140
ρ_c XY	0.0192	0.0165	0.0138	0.0132
Aspect ratio	**10**	**Volume = (10 x AR)³**		
x	5	15	40	60
ρ_c Z	0.1612	0.1556	0.1325	0.125
ρ_c XY	0.1294	0.1275	0.1175	0.12

More oriented the fibers are, higher ρc is in the two directions (axis Z and plane XY)

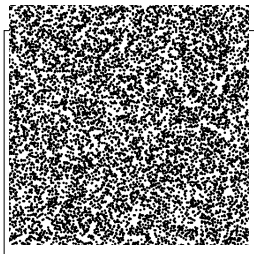
Combination of basic random sets

- Starting from the basic models, more complex structures, such as ***superposition of scales***, or fluctuations of the local volume fraction *p* of one phase
- ***Union or intersection*** of independent random sets

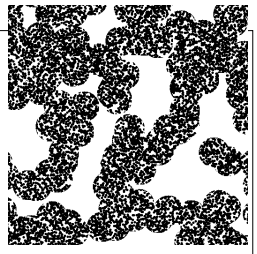
$$A = A_1 \cap A_2$$

$$P(K) = P\{K \subset (A_1 \cap A_2)\} = P\{K \subset A_1\}\ P\{K \subset A_2\}$$

Intersection of random sets

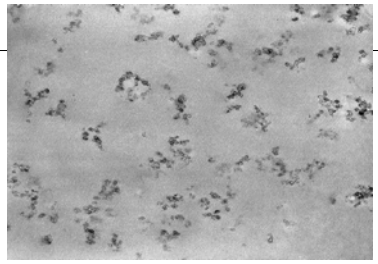


P = 0.49



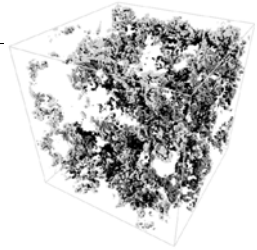
P = 0.49 ($P_1 = P_2 = 0.7$)

Nanocomposite carbon black - polymer (TEM)



Transmission micrographs (L. Savary, D. Jeulin, A. Thorel)

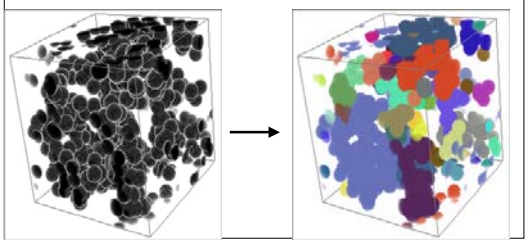
Simulation of a Carbon black Nanocomposite



Intersection of 3 scales Boolean models of spheres (identification from thick sections)

Percolation of multiscale aggregates

- Cox Boolean model



Simulation — Labeling of aggregates

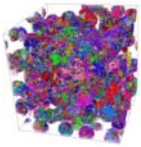
Percolation multiscale spherical aggregates

- **Two scales of spheres**

Volume : 2000^3

∅ sphères : 10

∅ aggregates : 300



s^2= 0.0838 (s: ρc SB spheres)

ρc = 0.085±0.003

- **Critical percolation threshold lower than for the Boolean model of spheres (0.2895)**

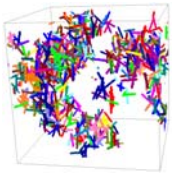
[*] Jeulin D., Moreaud M. Multi-scale simulation of random spheres aggregates – application to nanocomposites, Proc. 9th European Congress on Stereology and Image Analysis, Zakopane, Poland, May 10-13 2005, Vol. I p. 341-348.

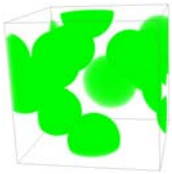
Percolation of multi-scale distributions of sphero-cylinders

•Two-scale simulation, with sphero-cylinders randomly located into inclusion spheres according to a Cox point process

•Dichotomic research used to estimate ρc with 20 realizations for each volume fraction **ρc = 0.05%**

$V=300^3$, l=30, r=2, Vv=0.05





$V=300^3$, r=60, Vv=0.3

Percolation of multi-scale distributions of sphero-cylinders

Aspect ratio AR	**1000** Volume dimensions = $(5 \times D)^3$		
Diameter of spheres D	2 x AR		
Vv of spheres	0.51	0.44	0.34
ρ_c	0.00051	0.00047	0.00049

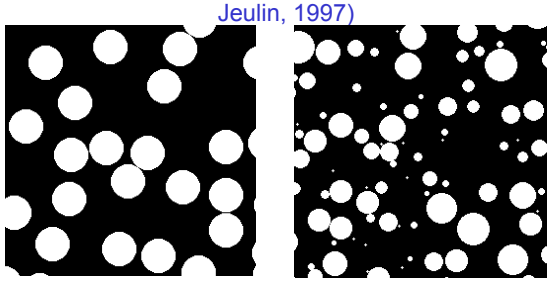
Aspect ratio AR	**50** Volume dimensions = $(5 \times D)^3$					
Diameter of spheres D	2 x AR			5 x AR		
Vv of spheres	0.51	0.42	0.35	0.5	0.43	0.35
ρ_c	0.014	0.016	0.019	0.014	0.012	0.012

• ρc lower than for a homogenous distribution

• lowest ρc obtained for a large diameter of spheres and a low volume fraction of spheres

Color dead leaves (D. Jeulin, 1979)

Color dead leaves: non overlaping grains (D. Jeulin, 1997)



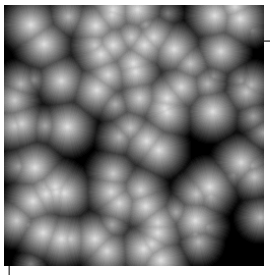
Size distribution (initial – intact); single symmetric convex grain in R^n for homogeneous model: $V_V <= 1 / 2^n$

Random Functions Models

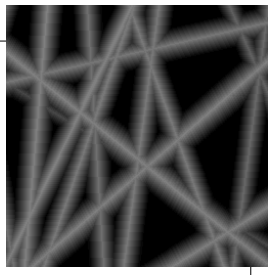
Continuous version of random sets models

- ***Boolean RF***: random implantation of primary random functions on points of a Poisson point process.
- The *U* operation for overlapping grains is replaced by the supremum or by the infimum
- ***Change of support*** by Sup or by Inf (Extreme Values)

Boolean random functions

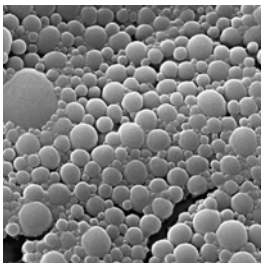


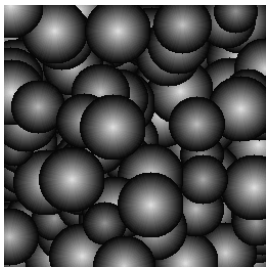
Cone Primary grains



Boolean Variety

Powders and dead leaves

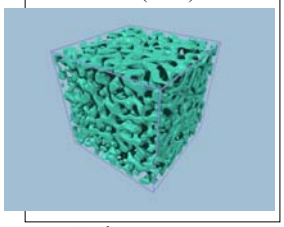




D. Jeulin, CALGON L = 15.5 µm

Reaction-Diffusion Models

Reaction-Diffusion Thesis
L. Decker (1999)



Turing texture

Simulation of connected media

Change of scale in random media (Physics-Texture)

49

From Nano to Macro

Homogenization

50

- Heterogeneous Medium (composite, porous medium, metalli polycristal, rocks, biological medium, rough surfaces …)

↓

- Eqyuvalent Homogeneous Medium?
- Prediction of the « effective» properties

Examples of homogenization problems

51

- **Thermal conductivity** of a two-component medium (thermal insulation)
- **Transport properties of porous media**
- **Elastic Moduli** of heterogeneous medium
- **Wave Propagation** in heterogeneous medium (electromagnetic, acoustic…)
- **Optical Properties** of a heterogeneous medium or of a rough surface

Examples of Physical Properties

52

Problem			Property
Thermal conduction	Heat Flux	Temperature Gradient	Thermal Conductivity
Electrostatics	Dielectric Displacement	Electric Field	Dielectric Permittivity
Elasticity	Stress	Srain	Elastic Moduli
Fluid Flow in porous media	Velocity	Pressure Gradient	Permeability

Homogenization

53

- **Bounds** of macroscopic properties (order 3: multicomponent random sets and functions)
- **Optimal random Microstructures**
- ***Probabilistic Definition of the RVE for numerical simulations***

Change of scale

54

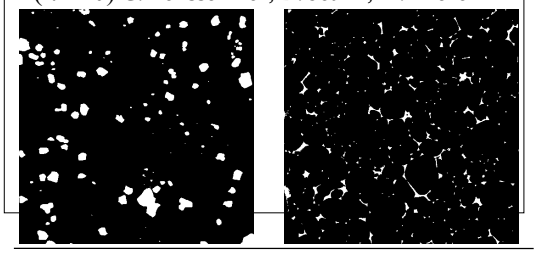
Applications of the models of random media to the prediction of the macroscopic behavior of a physical system from its microscopic behavior.

- ***Estimation of the effective properties*** (overall properties of an equivalent homogeneous medium) of random heterogeneous media from their microstructure (Homogenization)
  - From variational principles, bounds of the effective properties for linear constitutive equations.
  - Estimation of the effective behaviour from numerical simulations on random media.
- ***Fracture statistics models***

55

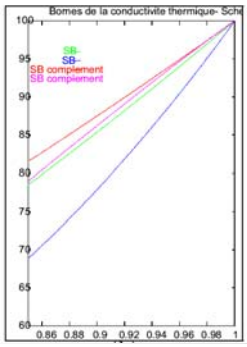
Thermal Conductivity of Ceramics (Use of Bounds for the Boolean Model)

- Textures AlN (λ=100) with a Y rich binder (λ= 10) *C. Pélissonnier, D. Jeulin, A. Thorel*



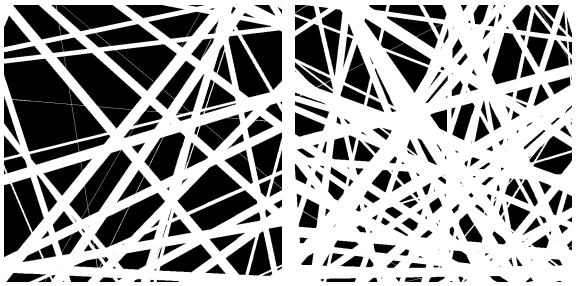
56

Thermal Conductivity of Ceramics: 3rd Order Bounds of the Boolean model



57

Random Composite with optimal effective properties



58

Digital Materials

59

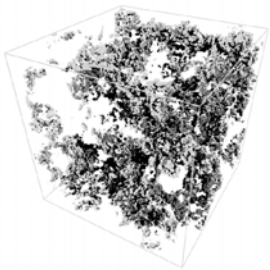
Digital Materials

- Input of 3D images
  - Real images (confocal, microtomography)
  - Simulations from a random model
- Use of a computational code (Finite Elements, Fast Fourier Transform, PDE numerical solver)
- Homogenization
- Representative Volume Element?

60

Homogenization and Simulation

- Prediction of the effective properties by 3D FFT
- *Nano Composites Carbon Black - polymer*: permittivity, from a multi-scale random model (PhD *A. Delarue, 2001 M. Moreaud, 2007, D. Jeulin, A. Thorel*, DGA, EADS)
- *Charged Elastomers:* ***elastic behaviour*** (PhD A. Jean, Michelin, 2006-2009 (19 February))



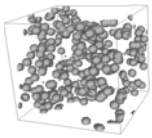
61

Homogenization and Simulation

Method:

Properties of components

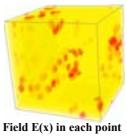
+



Iterative algorithm based on Fourier tansform, to solve the Gauss equation of electrostatics, derived from the Maxwell equations

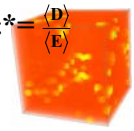
Periodic boundary conditions

Field D(x) in each point



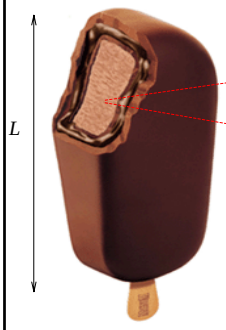
Field E(x) in each point

$$\varepsilon^* = \frac{\langle D \rangle}{\langle E \rangle}$$

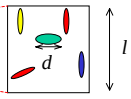


62

Ice cream: mechanical behavior (Unilever)



Three scales of observation



$d \ll l \ll L$

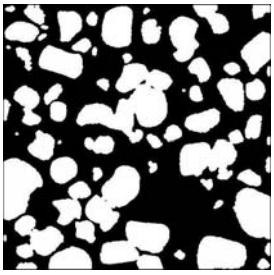
(thesis T. Kanit, 2003, S. Forest)

RVE

63

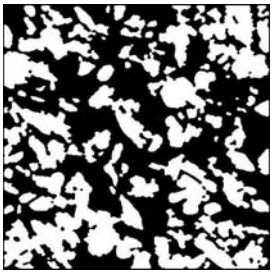
Morphology and effectives properties

***Heterogeneities in 2D**



100 µm

Coarse microstructure

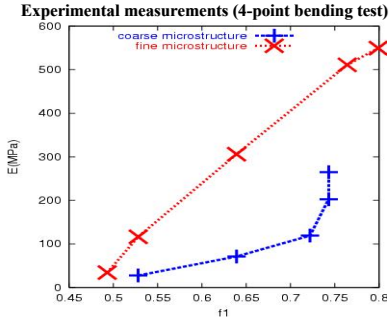


Fine microstructure

64

Morphology and Young's modulus

Experimental measurements (4-point bending test)



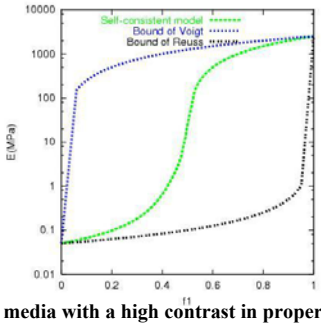
How to predict the Young's modulus for different microstructures ?

65

Analytical models: bounds and estimations

*** Bounds : very large.**

***Estimation : does not really take the morphology into account.**



Not really useful for media with a high contrast in properties

66

Principle of Homogenization Theory

- Two-phase heterogeneous material with elastic tensors C_1 and C_2
- Homogeneous equivalent material with the macroscopic elastic tensor C^{eff}
- We have:
- With the spatial averages $\underset{\sim}{\Sigma} = C^{eff} \underset{\sim}{E}$
- Where $\underset{\sim}{\Sigma} = \langle \underset{\sim}{\sigma} \rangle \qquad \underset{\sim}{E} = \langle \underset{\sim}{\varepsilon} \rangle$

$$\langle P \rangle = \frac{1}{V} \int_V P(x)\, dx$$

$\underset{\sim}{\sigma}$ and $\underset{\sim}{\varepsilon}$ are the local stress and strain tensors

67

Principle of Homogenization Theory

- Two-phase heterogeneous material with elastic tensors C_1 and C_2
- Average elastic energy (Hill-Mandel lemma) of a specimen V submitted to one of the following boundary conditions:
- **KUBC : kinematic (strain) uniform boundary conditions**
- **SUBC : static (stress) uniform boundary conditions**
- **PERIODIC : periodic boundary conditions**

$$<\underset{\sim}{\sigma}:\underset{\sim}{\varepsilon}>=<\underset{\sim}{\varepsilon}:\underset{\sim}{C}:\underset{\sim}{\varepsilon}>=\Sigma:E=<\underset{\sim}{\varepsilon}>C^{eff}<\underset{\sim}{\varepsilon}>$$

$\underset{\sim}{\sigma}$ and $\underset{\sim}{\varepsilon}$ are uncorrelated

RVE and Integral Range

- $P(x)$: local random property (indicator function, Young's modulus, …) in the domain V.
- Local variance of P: $D^2[P(x)]$
- Mean value of P in V: $<P>=\frac{1}{V}\int_V P(x)dx$
- Variance of the mean: $D^2[<P>]=D^2[P(x)]\frac{A_3}{V}$
- A_3 is the Integral Range of P (giving the size of a RVE for P)
- If $A_3 << V$, V may be subdivided into $N = V/A_3$ subdomains with uncorrelated properties P_i

69

Integral Range and Covariance

- Fluctuations of the average values $<P>$ of $P(x)$ (stationary RF) in the domain V, as a function of the centred covariance $\overline{W}_2(h)$
- $\overline{W}_2(h)=E\{(P(x+h)-E(P))(P(x)-E(P)\}$

$$D_P^2(V)=\frac{1}{V^2}\int_V\int_V \overline{W}_2(x-y)\,dxdy$$

70

Integral Range and Covariance

- For large specimens ($V >> A_3$), where A_3 is the integral range, asymptotic formula for the variance:

$$D_P^2(V) = D_P^2\frac{A_3}{V}$$

$$\text{with } A_3 = \frac{1}{D_P^2}\int_{R^3}\overline{W}_2(h)\,dh$$

where D^2_P is the point variance of P(x)

71

Set Covariance

- Covariance $C(h)$ of a random set A

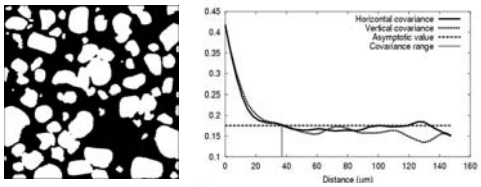
$$C(x,x+h) = P\{x \in A, x+h \in A\}$$

- For a stationary random set, $C(x,x+h) = C(h)$
- For an ergodic random set, $C(h)$ is estimated by the volume fraction of $A \cap A_{-h}$

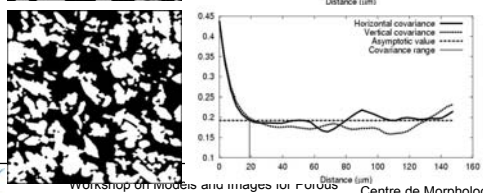
72

Microstructure and Covariance

without AFP



with AFP



73

Set Covariance and field Covariance

- Connexion between the two?
- Generally, no direct link!!
- The Covariance of fields depends on all « sets » moments with *n* points…

74

Determination of the integral range and of the RVE

- Start from realisations of the microstructure (images or simulations)
- Use appropriate Boundary Conditions (Periodic,…) to estimate the effectives properties of every realisation
- Estimate the average and the variance of effectives properties as a function of the volume of specimens
- Estimate A_3, the RVE and the number of fields to simulate as a function of the wanted precision

75

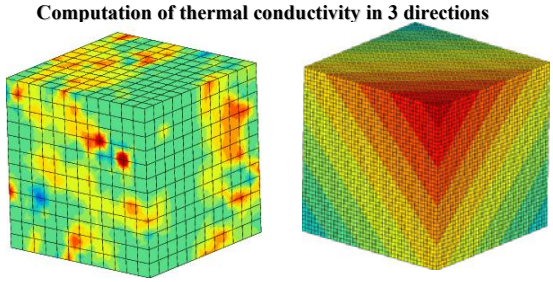
Elastic Moduli and Thermal Conductivity of the 3D Voronoï Mosaïc

- 3D Voronoï space tessellation: zones of inluence of random Poisson points
- Independent random coloration of each Voronoï polyhedron: Poisson mosaïc (approximation of some real two-phase textures)
- Finite element calculations on finite volume realizations of Voronoï mosaïc in *V*

76

Thermal computation on Voronoï mosaïc

70% ice, contrast = 100 in thermal conductivity
Computation of thermal conductivity in 3 directions



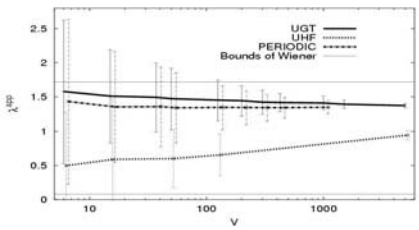
map of the flux in direction (z) with periodic b. c. (8281 d.o.f.)

map of the temperature with UGT b. c. (312481 d.o.f. on 20 pc)

77

Results for the Voronoï mosaïc

*** Fluctuations of the thermal conductivity**
-volume fraction = 70% of hard phase (ice)
-contrast in thermal conductivity = 100
-UGT : uniform temperature gradient at the boundary
-UHF : uniform heat flux at the boundary
-PERIODIC : periodic boundary conditions



78

Results for the Voronoi mosaïc

Minimal number of realizations for periodic boundary conditions
Example: RVE for unbiased volume = 125 grains

	$\varepsilon_{relative} = 1\%$	$\varepsilon_{relative} = 5\%$
	number of RVE	number of RVE
thermal conductivity	765	30

Integral range (volume fraction *P*)

	0.5	1.178
P =	0.7	1.111
	0.9	1.177

Gilbert (1962): 1.179

Integral range (elastic moduli)

$E_1 \,/\, E_2 = 100$

K (P = 0.7)	KUBC	2.088
μ (P = 0.7)	KUBC	1.863
μ (P = 0.5)	Périodic	1.637

Integral range (thermal conductivity)

$P = 0.7;\ \lambda_1 / \lambda_2 = 100$

	UGT	2.335
λ	UHF	2.036
	Périodic	2.619

Integral Range and Representative Volume Element for the estimation of the Elastic Moduli of the Boolean Model of Spheres

(joint work with F. Willot)

Elastic Fields solved by the Fourier transform (FFT)

Algorithm based on the Lippmann-Shwinger equations (Moulinec, Suquet, 1994). Introduction of a homogeneous elastic tensor $L^{(0)}$ (reference medium) and of the corresponding Green function $G^{(0)}$

- Iterations in the Fourier space (Green function) and in the real space. For $G^{(0)}$ with zeo mean:

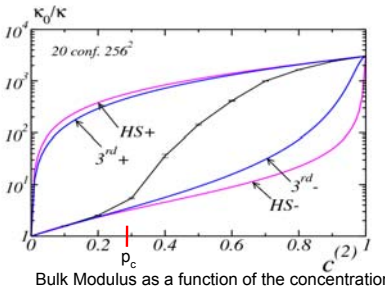
$$\varepsilon_{ij}(\mathbf{x}) = \varepsilon^0_{ij} + \int d^3\mathbf{y}\, G^0_{ij,kl}(\mathbf{x}-\mathbf{y})\,\tau_{kl}(\mathbf{y}), \qquad \tau_{ij}(\mathbf{x}) \equiv \sigma_{ij}(\mathbf{x}) - L^{(0)}_{ij,kl}\varepsilon_{kl}(\mathbf{x})$$

- **Periodic boundary conditions. Operation on images, without any mesh**
- Convergence for an infinite contrast with the improved algorithm "*increased Lagrangien* (Moulinec, Suquet + Moulinec, 2001)

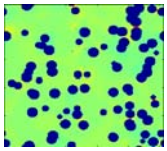
For an isotropic medium, in the Fourier space:

$$G^0_{khij}(\mathbf{q}) = \frac{\lambda_0+\mu_0}{\mu_0(\lambda_0+2\mu_0)} q_i q_j q_k q_h - \frac{1}{4\mu_0}(\delta_{ki}q_h q_j + \delta_{hi}q_k q_j + \delta_{kj}q_h q_i + \delta_{hj}q_k q_i),$$

Effective Bulk Modulus of the Boolean model of spheres



	κ	μ
matrice	1/3	½
inclusions	1000	1000



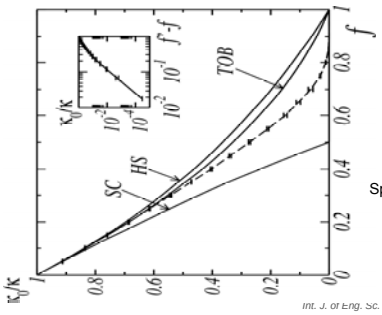
Bulk Modulus as a function of the concentration of the rigid phase and HS, Beran bounds

f=0,2

Effective Bulk Modulus of the Boolean model of spheres pores

85

Non compressible matrix (Poisson coeff. ~ 0,4999)

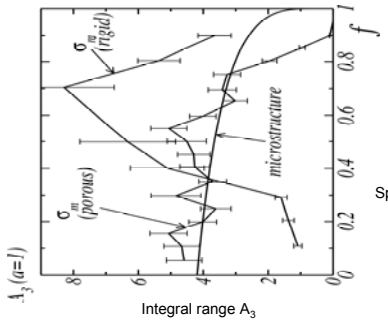


Sphere V_V

Bulk Modulus

Integral Range for different properties

86



Sphere V_V

Integral range A_3

Representative Volume Element

87

- The RVE depends on:
  - The morphology
  - The physical property (elastic moduli, thermal conductivity, dielectric permittivity, …)
  - The contrast between properties of components
  - The type of boundary conditions (uniform, periodic,;..)

Conclusion

88

- **Random models of structures**, to simulate the complex morphology of microstructures
- Approach, based on **measurements** obtained by image analysis: **test and select appropriate models**, estimate their parameters
- Physical and Morphological Modelling « **Which textures for which properties?** »
- Possible use in the **synthesis of textures**
- Many **domains of application**: Materials, Nano composites, Porous media, Biology, Food, Surfaces, Vision...

To learn more

89

- Courses ENSMP, 60 Bd Saint-Michel, Paris
  - Physics and Mechanics of Random Media (30 March - 3 April 2009)
  - Models of Random Structures (November 2009)
- ***Groupe de Travail MECAMAT*** « Approches probabilistes en Mécanique des Milieux Hétérogènes » (Bordeaux, 14-15 May 2009)

http://cmm.ensmp.fr/