Modeling of random media and stochastic homogenization for elliptic equations

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Outline

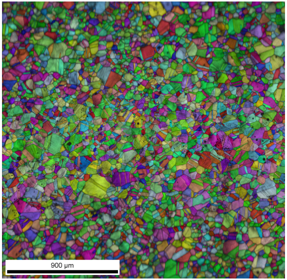
1. Modeling of random media
   - Examples of disordered media
   - Generation of samples of disordered media

2. Periodic homogenization (elliptic equations)
   - General principle
   - Multi-scale homogenization
   - Numerical approximation and bounds

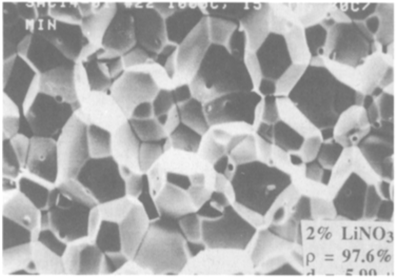
3. Stochastic homogenization (elliptic equations)
   - Energy method
   - Periodic-Stochastic comparison
   - Numerical simulation of homogenized coefficients
   - Quasi-periodic media

Outline

Examples of discrete disordered media



(a) Polycrystalline Material [1]



(b) Cell material [2]

- The information is very rich : what parameter (connectivity, "grain" size, correlation of properties between two grains, ...) do you want your model to enforce ?
- When (many) different samples are available, stationarity and ergodicity hypotheses can be checked
- Experimentally, one can measure the statistics of the different possible quantities of interest, often assuming ergodicity

$$\overline{\kappa} = \int_D \kappa(\boldsymbol{x})d\boldsymbol{x}, \quad C_\kappa(\boldsymbol{y}) = \int_D \kappa(\boldsymbol{x})\kappa(\boldsymbol{y}-\boldsymbol{x})d\boldsymbol{x}$$

1. P. Mu. "Study of crack initiation in low-cycle fatigue of an austenitic stainless steel". Thèse de doct. France : École Centrale de Lille, 2011
2. S. Kumar et al. "Properties of a three-dimensional Poisson-Voronoi tesselation : a Monte Carlo study". In : J. Stat. Phys. 67.3-4 (1992), p. 523-551. DOI : 10.1007/BF01049719

Examples of continuous complex recordings

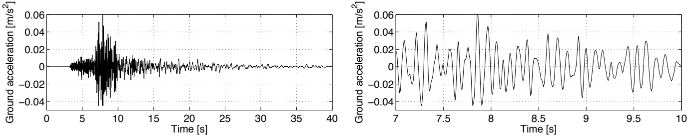


FIGURE – Example of a seismic record (right : zoom on the coda).

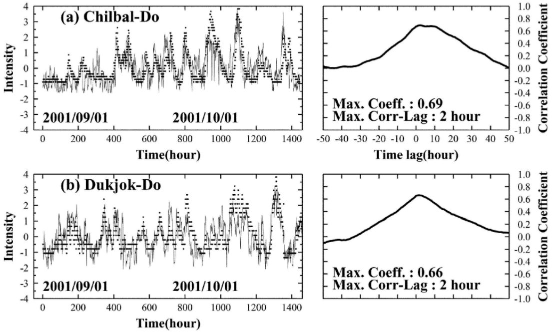
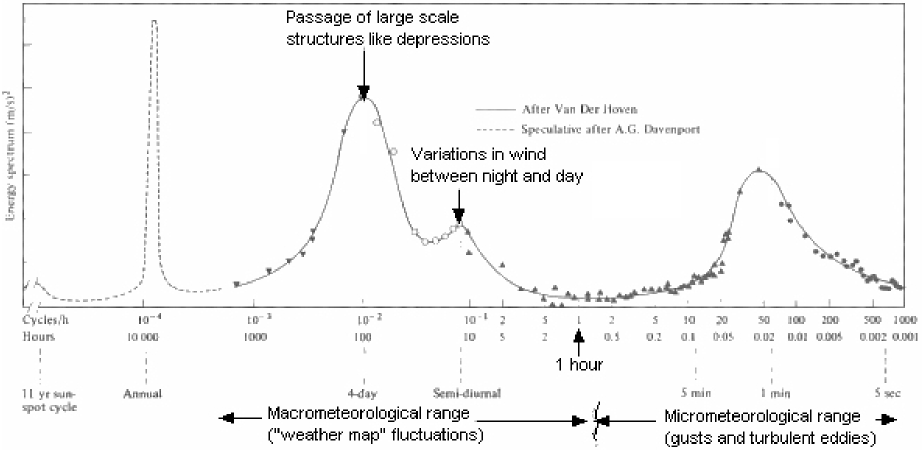


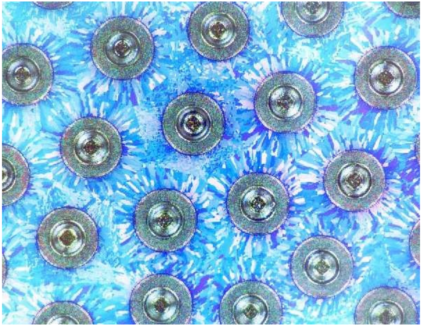
FIGURE – Correlation between wind speed and wave height in the Yellow Sea

Examples of power spectral density

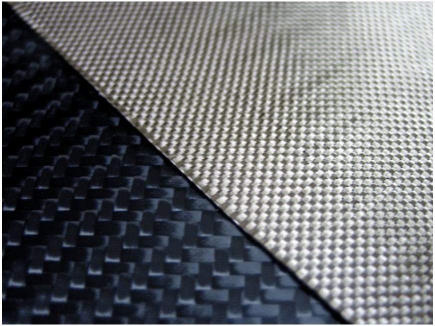


Energy spectrum of wind speed at 100 metres above the ground.
(Van der Hoven at Brooklyn, NY, USA)
From *Wind Forces on Buildings and Structures* by E.L.Houghton and N.B.Carruthers
Edward Arnold 1976

Examples of quasi-periodic structures



(a) Silicon carbide fibres in a titanium matrix (© ONERA)

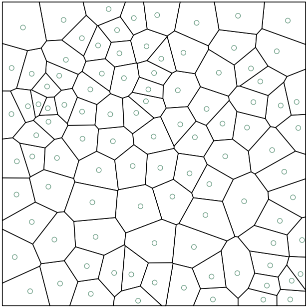


(b) Carbon fibres woven material

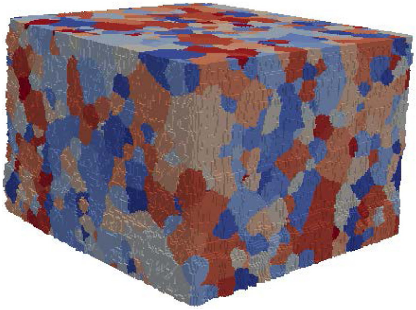
- Man-made material can potentially be "almost" periodic
- How much does the influence of small deviations from periodicity influence the final design ?

Outline

Generation of samples of discrete random media



(a) 2D model of a polycrystalline material [3]



(b) 3D model of a polycrystalline material [4]

1. Draw n points (for instance uniformly in space) $(\boldsymbol{x}_k)_{1 \leq k \leq n} \in \mathbb{R}^d$
2. Generate the Voronoi tesselation, that is, for each $1 \leq k \leq n$,

$$V(\boldsymbol{x}_k) = \left\{ \boldsymbol{x} \in \mathbb{R}^d, |\boldsymbol{x} - \boldsymbol{x}_k| < |\boldsymbol{x} - \boldsymbol{x}_j|, j \neq k \right\}$$

3. Draw (following appropriate probability law) realizations of the mechanical parameter associated to each $V(\boldsymbol{x}_k)$.

3. C. Talischi et al. "PolyMesher : a general-purpose mesh generator for polygonal elements written in Matlab". In : *Struct. Multidisc. Optim.* 45 (2012), p. 309-328. DOI : 10.1007/s00158-011-0706-z

4. K. Teferra et L. Graham-Brady. "Tesselation growth models for polycrystalline microstructures". In : *Comp. Mat. Sci.* 102 (2015), p. 57-67. DOI : 10.1016/j.commatsci.2015.02.006

Generation of samples of discrete random media

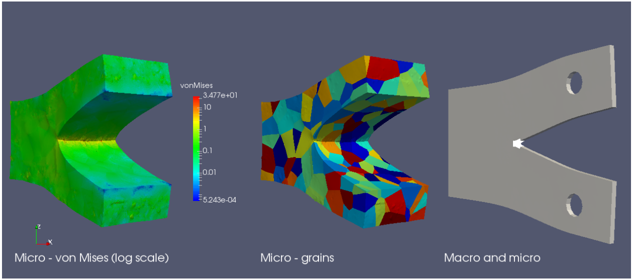


FIGURE – Simulation of the influence of grains at the tip of a fracture [5]

- Once generated (for instance using point processes), it is possible to obtain (at least numerically) statistics of the continuous fields of mechanical parameters

$$(\kappa^*)^{-1} = \frac{1}{N}\sum_{j=1}^{N}\int_D \kappa_j^{-1}(\boldsymbol{x})d\boldsymbol{x}, \quad C_\kappa(\boldsymbol{y}) = \frac{1}{N}\sum_{j=1}^{N}\int_D \kappa(\boldsymbol{x})\kappa_j(\boldsymbol{y}-\boldsymbol{x})d\boldsymbol{x}$$

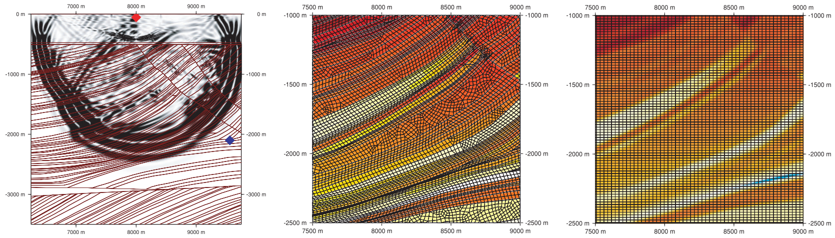
- Samples can be generated (contrarily to experiments), so stationarity or ergodicity can be checked.

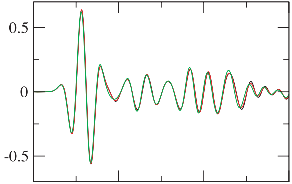
5. T. Milanetto-Schlittler et R. Cottereau. "Fully scalable implementation of a volume coupling scheme for the modeling of polycrystalline materials". In : *Comp. Mech.* 60.5 (2017), p. 827-844. DOI : 10.1007/s00466-017-1445-9

Raining technique

- Check the statistics ! ! !

Discrete or continuous random fields ?





- Discrete or continuous heterogeneity is often a modeling assumption more than a "fact"
- *wink* : homogenization is useful ! !

Generation of samples of a continuous random field

Realizations of a continuous Gaussian random field with expectation a_0 and power spectral density $S(k)$ can be generated using the following spectral representation formula[6] :

$$A(x) = a_0 + 2\sum_{j=1}^{N} \sqrt{S(k_j)\delta k}\zeta_j \cos(k_j x + \phi_j)$$

where $k_j = j\delta k$, and the $\{\zeta_j\}_{1\leq j\leq N}$ et $\{\phi_j\}_{1\leq j\leq N}$ are families of independent random variables, respectively with average 0 and variance 1 (any probability density), and uniform on $[-\pi, \pi]$.

- The only control on the field is on its expectation and covariance (in particular, all the marginal laws are Gaussian).
- Can be easily (but not necessarily cheaply) generalized to multidimensional fields
- Very efficient FFT scheme.
- Other techniques exist (see Olivier's talk ?)

6. M. Shinozuka et G. Deodatis. "Simulation of stochastic processes by spectral representation". In : *Appl. Mech. Rev.* 44.4 (1991), p. 191-205. DOI : 10.1115/1.3119501

Large scale generation of random fields : overlap and merge [7]

Issue

- N increases with the total size of the generation domain even for fixed correlation length
- We are performing a sum of functions correlated over the entier to retrieve a function correlated only over a correlation length

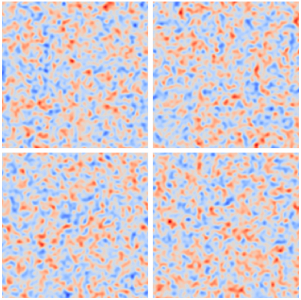
Idea

- Generate independent random fields $u_j(x)$ over each domain for an overlapping partition P
- Assemble the field through partition of unity functions $\psi_j(x)$

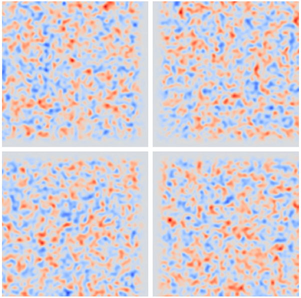
$$u(x) = \sum_{j \in P} \sqrt{\psi_j(x)} u_j(x)$$

7. L. de Carvalho Paludo, V. Bouvier et R. Cottereau. "Scalable parallel scheme for sampling of Gaussian random fields over large domains". In : *Int. J. Numer. Meth. Engr.* 117.8 (2019), p. 845-859. DOI : 10.1002/nme.5981

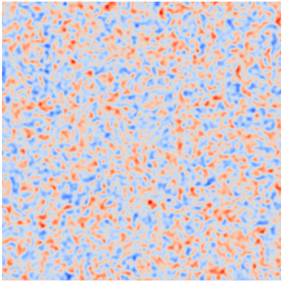
Illustration in 2D



Generate independent fields
(u_i)



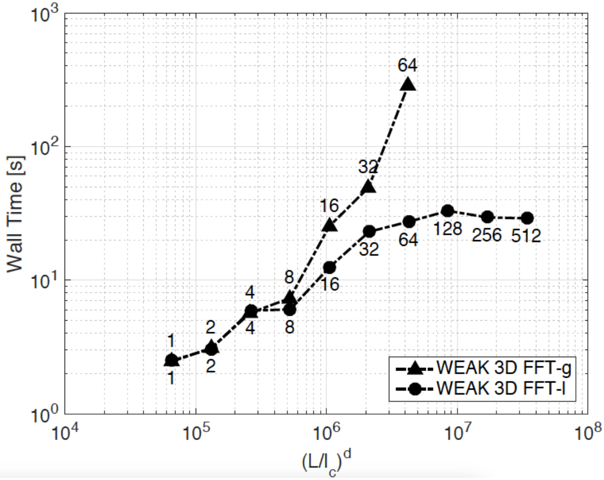
Multiplicate each field by the square root of a partition of unity
($u_i\sqrt{\psi_i}$)



Sum all the fields
($\sum u_i\sqrt{\psi_i}$)

Weak scalability of local scheme (versus global scheme)

on Igloo (SGI machine with 800 Intel Xeon X5650 cores at Châtenay-Malabry, France)

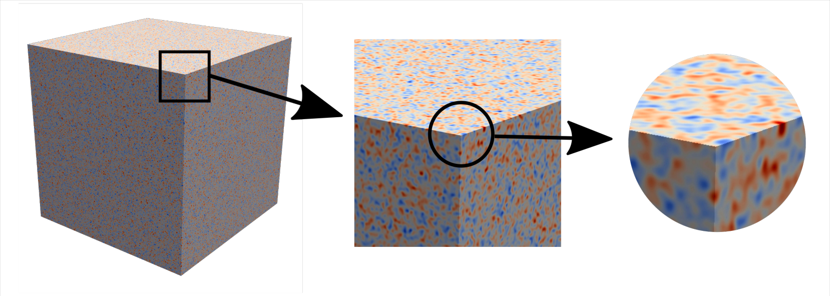


on each processor : 8×10^6 DOFs, $30 \times 30 \times 60\ \ell_c^3$

overlap $= 5\ell_c$ (in overlapping technique)

Random field generation over large cluster

Generation over $300\ell_c \times 300\ell_c \times 300\ell_c$ in 116 s (walltime) over 512 processors



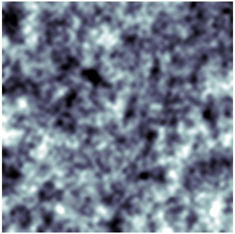
Development of an open-source library for large-scale generation of random fields

https://github.com/cottereau/randomField

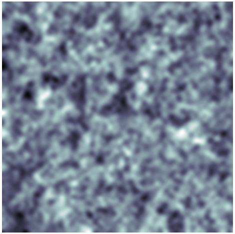
(based on MPI, pHDF5, FFTW)

Comparison of power spectral density models

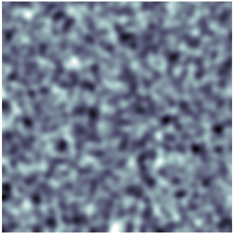
Centered Gaussian fields with $\tau_c = 1$ et $\sigma^2 = 1$ (in 2D)



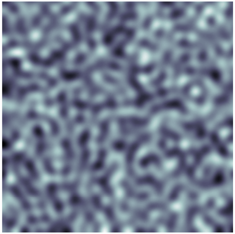
(a) Exponential



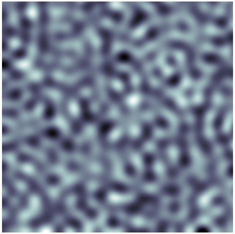
(b) Power law



(c) Gaussian



(d) Triangular



(e) Truncated white noise

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Outline

Objectives of homogenization

Example of a diffusion problem (elliptic equation)

Micro-scale problem

$$-\nabla \cdot A\left(\frac{x}{\epsilon}\right)\nabla u_\epsilon\left(x, \frac{x}{\epsilon}\right) = f(x), \quad \text{in } D$$

$$u_\epsilon = 0, \quad \text{on } \partial D$$

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$$u_\epsilon = 0, \quad \text{on } \partial D$$

Macro-scale problem

$$\mathcal{L}(u^*(x), x; f(x)) = 0, \quad \text{in } D$$

$$u^* = 0, \quad \text{on } \partial D$$

How to find the homogenized equation (and does it exist ?) and its coefficients ?

Objectives of homogenization

Example of a diffusion problem (elliptic equation)

Micro-scale problem

$$-\nabla \cdot A\left(\frac{x}{\epsilon}\right) \nabla u_\epsilon \left(x, \frac{x}{\epsilon}\right) = f(x), \quad \text{in } D$$

$$u_\epsilon = 0, \quad \text{on } \partial D$$

Macro-scale problem

$$-\nabla \cdot A^* (x) \nabla u^*(x) = f(x), \quad \text{in } D$$

$$u^* = 0, \quad \text{on } \partial D$$

How to find the homogenized equation (and does it exist ?) and its coefficients ?

General principle of multi-scale homogenization

Description of the micro-scale problem

- Sequence of problems indexed on ϵ : Find $u_\epsilon \in H_0^1(D)$ such that

$$-\nabla \cdot A\left(\frac{x}{\epsilon}\right)\nabla u_\epsilon\left(x, \frac{x}{\epsilon}\right) = f(x), \quad \text{in } D$$

$$u_\epsilon = 0, \quad \text{on } \partial D$$

- If $f \in L^2(D)$, then the problem is well posed : there exists a unique solution $u_\epsilon \in H_0^1(D)$ and

$$\|u_\epsilon\|_{H_0^1(D)} \leq C\|f\|_{L^2(D)}$$

- Study of the convergence of $u_\epsilon \to u^*$

Outline

- Expanding the solution using a separation of scales assumption $\epsilon \ll 1$

$$u_\epsilon(x) = \sum_{k=0}^{+\infty} \epsilon^k u_k \left(x, y = \frac{x}{\epsilon}\right)$$

- Introduction of the *ansatz* in the diffusion equation (micro)
- Modification of the derivation operator

$$\nabla = \epsilon^{-1} \nabla_y + \nabla_x$$

using the relation, valid for functions $v_\epsilon(x) = v(x, x/\epsilon)$,

$$\nabla v_\epsilon(x) = \left[\frac{1}{\epsilon} \nabla_y v(x,y) + \nabla_x v(x,y)\right]_{y=\frac{x}{\epsilon}}$$

- A sequence of problems is obtained for each power of ϵ

This part follows G. Allaire's course notes [8]. The classical book [9] is extremely clear, and treats both periodic and stochastic cases.

8. G. Allaire. "Introduction to homogenization theory". In : *Multiscale methods – 32nd Computational Fluid Dynamics*. Sous la dir. de H. Deconinck. Von Karman Institute Lecture Series. Von Karman Institute, 2002

9. A. Bensoussan, J.-L. Lions et G. Papanicolaou. *Asymptotic analysis for periodic structures*. Studies in Mathematics and its Applications 5. North Holland, 1978

Two-scale homogenization

General expansion

$$
\begin{aligned}
&-\epsilon^{-2}\left[\nabla_y \cdot A \nabla_y u_0\right]\left(x, \frac{x}{\epsilon}\right) \\
&-\epsilon^{-1}\left[\nabla_y \cdot A(\nabla_x u_0 + \nabla_y u_1) + \nabla_x \cdot A \nabla_y u_0\right]\left(x, \frac{x}{\epsilon}\right) \\
&-\epsilon^{0}\left[\nabla_y \cdot A(\nabla_x u_1 + \nabla_y u_2) + \nabla_x \cdot A(\nabla_x u_0 + \nabla_y u_1)\right]\left(x, \frac{x}{\epsilon}\right) \\
&-\sum_{k=1}^{+\infty} \epsilon^{k}\left[\nabla_x \cdot A(\nabla_x u_k + \nabla_y u_{k+1}) + \nabla_y \cdot A(\nabla_x u_{k+1} + \nabla_y u_{k+2})\right]\left(x, \frac{x}{\epsilon}\right) \\
&= f(x)
\end{aligned}
$$

Two-scale homogenization

- Cancellation of ϵ^{-2} order term

$$-\nabla_y \cdot A(y)\nabla_y u_0(x,y) = 0$$

- The leading-order term is the solution of the homogenized problem

$$u_0(x,y) = u(x)$$

Two-scale homogenization

- Cancellation of ϵ^{-1} order term

$$-\nabla_y \cdot A(y)\nabla_y u_1(x,y) = \nabla_y \cdot A(y)\nabla_x u(x)$$

- Proportionality of $u_1(x,y)$ and $\nabla_x u(x)$:

$$u_1(x,y) = \boldsymbol{w}(y) \cdot \nabla_x u(x) = \sum_{k=1}^{d} (w_k(y)\boldsymbol{e}_k) \cdot \nabla_x u(x)$$

- Defines the corrector problems with periodic boundary conditions :

$$-\nabla_y \cdot A(y)\nabla_y w_k(y) = \nabla_y \cdot A(y)\boldsymbol{e}_k$$

Two-scale homogenization

- Cancellation of ϵ^0 order term

$$-\nabla_y \cdot A(y)\nabla_y u_2(x,y) = \nabla_y \cdot A(y)\nabla_x u_1 + \nabla_x \cdot A(y)(\nabla_y u_1 + \nabla_x u) + f(x)$$

Theorem 1 (Fredholm alternative)

Let $f(y) \in L^2_\#(Y)$ be a periodic function. There exists a solution in $H^1_\#(Y)$ of

$$-\nabla_y \cdot (A(y)\nabla_y w(y)) = f(y)$$

if and only if $\int_Y f(y)dy = 0$. The solution is unique up to an additive function.

Two-scale homogenization

- Cancellation of ϵ^0 order term

$$-\nabla_y \cdot A(y)\nabla_y u_2(x,y) = \nabla_y \cdot A(y)\nabla_x u_1 + \nabla_x \cdot A(y)(\nabla_y u_1 + \nabla_x u) + f(x)$$

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- Using $\int_Y \nabla_y \cdot \alpha(x,y)dy = 0$ for α Y-periodic, this yields :

$$\begin{aligned} \left(\frac{1}{|Y|}\int_Y -\nabla_x \cdot A(y)\left(\nabla_y u_1 + \nabla_x u\right) dy\right) &= f(x) \\ -\nabla_x \cdot \left(\frac{1}{|Y|}\int_Y A(y)\left(I + \nabla_y \mathbf{w}(y)\right) dy\right)\nabla_x u &= f(x) \end{aligned}$$

- This equation is the homogenized equation and

$$A^* = \frac{1}{|Y|}\int_Y A(y)\left(I + \nabla_y \mathbf{w}(y)\right) dy = \frac{1}{|Y|}\int_Y (I + \nabla_y \mathbf{w}(y))^T A(y)(I + \nabla_y \mathbf{w}(y))dy$$

Corrector problem

For each basis vector $\boldsymbol{e}_i$ (canonical basis of $\mathbb{R}^d$), find $w_i \in H^1_{\#}(Y)$ such that

$$-\nabla_y \cdot A(y)(\boldsymbol{e}_i + \nabla_y w_i(y)) = 0, \quad \text{in } Y.$$

Macro-scale problem

Find $u^* \in H^1_0(D)$ such that

$$-\nabla \cdot A^*(x)\,\nabla u^*(x) = f(x), \text{ in } D, \text{ et } \quad u^* = 0, \text{ on } \partial D$$

with

$$A^* = \frac{1}{|Y|}\int_Y (I + \nabla_y \boldsymbol{w}(y))^T A(y)(I + \nabla_y \boldsymbol{w}(y))dy.$$

Homogenized solution

$$u_\epsilon \approx u(x) + \epsilon\, \boldsymbol{w}(y) \cdot \nabla_x u(x)$$

The approach described before is very efficient at providing the "correct" homogenized solution but other methods are often needed to prove that it is indeed correct (energy method, ...).

Outline

Numerical approximations

Corrector problem

For each basis vector $\boldsymbol{e}_i$, find $w_i \in H^1_\#(Y)$ such that

$$-\nabla_y \cdot A(y)(\boldsymbol{e}_i + \nabla_y w_i(y)) = 0, \quad \text{in } Y$$

- provides micro-scale information on the reaction of the medium to macro-scale excitations
- must (in general) be approximated numerically
- the problem is set on a cell (much cheaper numerically than the micro-scale problem) ...
  NB : this will not be true anymore in stochastics ...

Functional characterization of the homogenized tensor

- Homogenized tensor

$$A^* = \frac{1}{|Y|} \int_Y (I + \nabla_y \boldsymbol{w}(y)) \cdot A(y)(I + \nabla_y \boldsymbol{w}(y)) dy$$

- Redefining the homogenized problem as a minimization problem

$$A^*_{jj} = \frac{1}{|Y|} \min_{w(y) \in H^1_\#(Y)} \int_Y (\boldsymbol{e}_j + \nabla_y w_j) \cdot A(\boldsymbol{e}_j + \nabla_y w_j) dy$$

Voigt and Reuss bounds

Voigt (upper) bound

For $w(y) = \mathrm{cst}$

$$A^*_{jj} \leq \boldsymbol{e}_j \cdot \left(\frac{1}{|Y|} \int_Y A \, dy \right) \boldsymbol{e}_j$$

Reuss (lower) bound

By increasing the space over which minimization is performed

$$A^*_{jj} \geq \min_{\zeta(y) \in (L^2_\#(Y))^d, \int_Y \zeta dy = 0} \int_Y (\boldsymbol{e}_j + \zeta_j) \cdot A(\boldsymbol{e}_j + \zeta_j) dy = \boldsymbol{e}_j \cdot \left(\frac{1}{|Y|} \int_Y A^{-1} dy \right)^{-1} \boldsymbol{e}_j$$

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Some preliminary notations

- $\mathcal{H} = L^2(\Theta, \mathcal{T}, \mathbb{P})$ is the Hilbert space of square integrable functions on Θ with

$$\mathbb{E}\left[gh\right] = \int_\Theta g(\theta)h(\theta)\mathbb{P}(d\theta)$$

- $H = L^2(D, \mathcal{H})$ is the Hilbert space of square integrable functions on D with values in $\mathcal{H}$ with

$$(u, v) = \int_D \mathbb{E}[u(x)v(x)]dx = \int_D \int_\Theta u(x,\theta)v(x,\theta)\mathbb{P}(d\theta)dx$$

- $H^1 = H^1(D, \mathcal{H})$ is the Hilbert space of $\mathcal{H}$-valued functions over D whose derivatives are square integrable with

$$(u, v)_1 = (u, v) + \sum_{k=1}^{d} \left(\frac{\partial u}{\partial x_k}, \frac{\partial v}{\partial x_k} \right)$$

- $H_0^1 = H_0^1(D, \mathcal{H})$ is the Hilbert space of $\mathcal{H}$-valued functions with square integrable derivatives and such that $u = 0$ on ∂D

This part follows Papanicolaou and Varadhan's paper [10]

10. G. C. Papanicolaou et S. R. S. Varadhan. "Boundary value problems with rapidly oscillating random coefficients". In : *Proceedings of the Conference on Random Fields*. Sous la dir. de J. Fritz et J. L. Lebowitz. T. 2. Seria Colloquia Mathematica Societatis Janos Bolyai 27. North Holland, 1981, p. 835-873

Hypotheses on the diffusion tensor

Diffusion tensor

We consider a strictly stationary matrix-valued continuous random field of diffusion tensor $A(y,\theta) = a_{ij}(y,\theta)\boldsymbol{e}_i \otimes \boldsymbol{e}_j$ bounded and coercive

- the probability measure $\mathbb{P}$ is invariant with respect to the translation group $\tau_x : \Theta \to \Theta$ defined by

$$(\tau_x\theta)(y) = \theta(y-x), \quad \forall x, y \in \mathbb{R}^d.$$

For stationary random fields, we introduce the notation

$$\tilde{A}_{ij}(\theta) = A_{ij}(0,\theta), \quad \text{such that} \quad A_{ij}(x,\theta) = \tilde{A}_{ij}(\tau_x\theta)$$

The translation group is also assumed ergodic : the only sets that are invariant are such that $\mathbb{P}(A) = 0$ or 1.

- the continuity is such that

$$\lim_{h\to 0} \mathbb{P}\left[|A(y+h,\theta) - A(y,\theta)| > \delta\right] = 0, \quad \forall \delta > 0, y \in \mathbb{R}^d$$

- $\exists a_0 > 0$ such that

$$a_0|\xi|^2 \leq \xi \cdot A(y,\theta) \cdot \xi \leq a_0^{-1}|\xi|^2, \quad \forall y, \xi \in \mathbb{R}^d, \forall \theta \in \Theta$$

General setting

- We consider a strictly stationary continuous random field $A(y)$ bounded and coercive ...
- ... and a sequence of problems parameterized by ϵ : Find $u_\epsilon(x,\theta) \in H_0^1$ such that

$$\int_D \int_\Theta \left(A\left(\frac{x}{\epsilon}, \theta\right) \nabla u_\epsilon(x,\theta) \right) \cdot \nabla \phi(x,\theta) \mathbb{P}(d\theta) dx = \int_D \int_\Theta f(x) \phi(x,\theta) \mathbb{P}(d\theta) dx, \quad \forall \phi \in H_0^1 \tag{1}$$

where $f(x) \in L^2(D, \mathbb{R})$ is a given deterministic function
- Each problem has a unique solution (by Lax-Milgram), which is bounded

$$(u_\epsilon, u_\epsilon)_1 \leq C \int_D |f(x)|^2 dx$$

Weak convergence theorem

Theorem 2 (Weak convergence)

The solution $u_\epsilon \in H_0^1$ *converges weakly in* H_0^1 *to the solution* $u(x) \in H_0^1(D, \mathbb{R})$ *of the deterministic variational problem*

$$\int_D (A^* \nabla u(x)) \cdot \nabla \phi(x) dx = \int_D f(x)\phi(x) dx, \quad \forall \phi(x) \in H_0^1(D, \mathbb{R})$$

Here, the homogenized matrix A^* *is a constant matrix defined by*

$$A^* = \mathbb{E}\left[\tilde{A}\left(I + \tilde{\psi}\right)\right],$$

where the corrector strains $\tilde{\psi}$ *are stationary and defined below (Theorem 3)*

- Weak convergence means

$$\lim_{\epsilon \to 0} (u_\epsilon, \phi)_1 = (u, \phi)_1, \quad \forall \phi \in H_0^1$$

- The homogenized problem is no longer stochastic

Corrector problem

Theorem 3 (Correctors)

There exist functions $\tilde{\psi}^k \in \mathcal{H}^d$, $1 \leq k \leq d$, *such that*

$$\mathbb{E}\left[\tilde{A}(\boldsymbol{e}_k + \tilde{\psi}^k) \cdot \nabla\tilde{\phi}\right] = 0, \quad \forall\tilde{\phi} \in \mathcal{H}^1$$

Furthermore, there exist uniquely defined random fields $\boldsymbol{w} = (w_k(x,\theta))_{1\leq k\leq d}$ *that are not stationary, but whose gradients are stationary, and such that* $\boldsymbol{w}(0,\theta) = 0$ *and*

$$\nabla w_k(x,\theta) = \psi^k(x,\theta) = \tilde{\boldsymbol{\psi}}^k(\tau_{-x}\theta).$$

We denote $\tilde{\boldsymbol{\psi}} = \{\tilde{\psi^k}\}_{1\leq k\leq d}$.

Proof : see [11]

11. G. C. Papanicolaou et S. R. S. Varadhan. "Boundary value problems with rapidly oscillating random coefficients". In : *Proceedings of the Conference on Random Fields*. Sous la dir. de J. Fritz et J. L. Lebowitz. T. 2. Seria Colloquia Mathematica Societatis Janos Bolyai 27. North Holland, 1981, p. 835-873

Steps of the proof of Theorem 2 (energy method)

- Issue : the product of two weakly converging sequences $A(x/\epsilon)$ and ∇u_ϵ does not necessarily converge to the product of the limit (but $\xi^\epsilon = A(x/\epsilon)\nabla u^\epsilon(x)$ does)
- Solution : use a particular test function (oscillating function) ϕ_ϵ that allows to pass to the limit

$$\phi_\epsilon(x) = \phi(x) + \epsilon \sum_{j=1}^{d} w_j^*(x/\epsilon) \frac{\partial \phi(x)}{\partial x_j}$$

where w_k^* is solution to the adjoint corrector problem (with diffusion matrix A^T loaded in direction $\boldsymbol{e}_k$). Note that

$$\nabla \phi_\epsilon(x) = \sum_{j=1}^{d} \frac{\partial \phi(x)}{\partial x_j} \left(\boldsymbol{e}_j + \nabla_y w_j^*(x/\epsilon) \right) + \epsilon \sum_{j=1}^{d} w_j^*(x/\epsilon) \nabla \frac{\partial \phi(x)}{\partial x_j}$$

- In the weak formulation

$$(A(x/\epsilon)\nabla u_\epsilon, \nabla \phi_\epsilon) = (f, \nabla \phi_\epsilon)$$

$$-\left(u_\epsilon, \nabla \cdot \left(A^T(x/\epsilon) \sum_{j=1}^{d} \frac{\partial \phi(x)}{\partial x_j} \left(\boldsymbol{e}_j + \nabla_y w_j^*(x/\epsilon) \right) \right) \right) + \epsilon C = (f, \nabla \phi_\epsilon)$$

$$-\sum_{j=1}^{d} \left(u_\epsilon, \left(\nabla \frac{\partial \phi(x)}{\partial x_j} \right) \left(A^T(x/\epsilon) \left(\boldsymbol{e}_j + \nabla_y w_j^*(x/\epsilon) \right) \right) \right) + \epsilon C = (f, \nabla \phi_\epsilon)$$

Strong convergence theorem

Theorem 4 (Strong convergence)

Let $u_\epsilon \in H^1$ be the solution of (1) and $u \in H^1(\mathbb{R}^d, \mathbb{R})$ be the solution of the deterministic variational problem

$$\int_D (A^* \nabla u(x)) \cdot \nabla \phi(x) dx = \int_D f(x)\phi(x)dx, \quad \forall \phi(x) \in H_0^1(\mathbb{R}^d, \mathbb{R}),$$

where the homogenized matrix A^* is defined as earlier. Then

$$\lim_{\epsilon \to 0} \int_{\mathbb{R}^d} \int_\Theta |u_\epsilon(x,\theta) - u(x)|^2 \, \mathbb{P}(d\theta)dx = 0$$

and

$$\lim_{\epsilon \to 0} \int_{\mathbb{R}^d} \int_\Theta \left\| \nabla u_\epsilon(x,\theta) - \nabla u(x) - \sum_{k=1}^{d} \psi^k \left(\frac{x}{\epsilon}, \theta \right) \frac{\partial u(x)}{\partial x_k} \right\|^2 \mathbb{P}(d\theta)dx = 0$$

where the corrector strains ψ^k were defined earlier (Theorem 3)

Proof : see [12]

12. G. C. Papanicolaou et S. R. S. Varadhan. "Boundary value problems with rapidly oscillating random coefficients". In : *Proceedings of the Conference on Random Fields*. Sous la dir. de J. Fritz et J. L. Lebowitz. T. 2. Seria Colloquia Mathematica Societatis Janos Bolyai 27. North Holland, 1981, p. 835-873

Outline

Periodic-Stochastic comparison

- Stationarity of the material random field replaces periodicity in the deterministic case.
- The physical "averaging" phenomena are the same and the ingredients of the theoretical proofs are (mostly) the same
- In the stochastic case, the corrector problem is posed on the entire (space) domain rather than on the periodic cell. The corrector problem is therefore *a priori* as expensive to approximate as the full-scale problem.
- When using the alternative formulation of the homogenized tensor, convergence is obtained for very large sizes $N \to +\infty$, even when multiple Monte Carlo realizations are considered. Approaches can be developed to improve that convergence

Outline

Numerical simulation of homogenized coefficients

Alternative formulation of the corrector problem

There exist uniquely defined functions $w_k(x,\theta)$, $1 \leq k \leq d$, whose gradients are stationary, and such that, if B_N is a cube of side $2N$ in $\mathbb{R}^d$, centered at the origin,

$$\lim_{N\to+\infty} \frac{1}{(2N)^d} \int_{B_N} (A(x,\theta)(\boldsymbol{e}_k + \nabla w_k(x,\theta))) \cdot \nabla\phi(x,\theta) dx = 0,$$

$$\forall \phi \in H^1_S(\mathbb{R}^d, \mathcal{H}), \quad \mathbb{P} - \text{almost everywhere}$$

The gradients of w_k have mean zero and

$$A^* = \lim_{N\to+\infty} \frac{1}{(2N)^d} \int_{B_N} A(x,\theta)(I + \nabla \mathbf{w}(x,\theta)) dx, \quad \mathbb{P} - \text{almost everywhere}$$

Numerical simulation of homogenized coefficients

Neumann and Dirichlet homogenized tensors

$$\check{a}_{N,\mathrm{M}} = \frac{1}{\mathrm{M}(2N)^d} \sum_{i=1}^{\mathrm{M}} \int_{B_N} A(x,\theta_i) \left(I + \nabla w_N^i(x) \right) dx, \quad w_N^i(x) \text{ computed with KUBC}$$

$$\hat{a}_{N,\mathrm{M}} = \left(\frac{1}{\mathrm{M}} \sum_{i=1}^{\mathrm{M}} \left(\frac{1}{(2N)^d} \int_{B_N} A(x,\theta_i) \left(I + \nabla w_N^i(x) \right) dx \right)^{-1} \right)^{-1}, \ w_N^i(x) \text{ computed with SUBC}$$

Theorem 5 (Convergence of approximate homogenized tensors [13])

$$\lim_{N\to\infty} \check{a}_{N,\mathrm{M}} = \lim_{N\to\infty} \hat{a}_{N,\mathrm{M}} = a^*$$

The following hierarchy can be shown [14],

$$\hat{a}_{N,\mathrm{M}} \leq a^* \leq \check{a}_{N,\mathrm{M}}$$

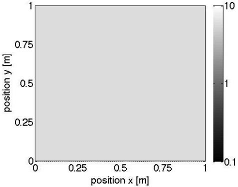
Except for particular situations, for finite size N,

$$\lim_{\mathrm{M}\to\infty} \hat{a}_{N,\mathrm{M}} \neq \lim_{\mathrm{M}\to\infty} \check{a}_{N,\mathrm{M}} \neq a^*$$

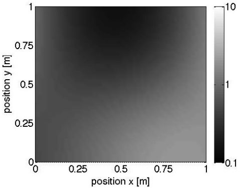
13. A. Bourgeat et A. Piatnitski. “Approximations of effective coefficients in stochastic homogenization”. In : *Ann. Inst. Henri Poincaré* 40 (2004), p. 153-165. DOI : 10.1016/j.anihpb.2003.07.003

14. C. Huet. “Application of variational concepts to size effects in elastic heterogeneous bodies”. In : *J. Mech. Phys. Solids* 38.6 (1990), p. 813-841. DOI : 10.1016/0022-5096(90)90041-2

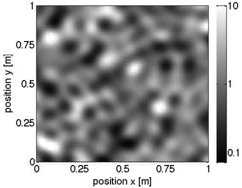
Numerical illustration of convergence of estimates of homogenized tensors [15]



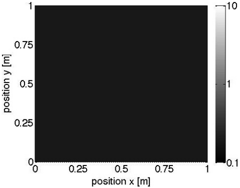
(f) $N = \ell_c/10$, Sample 1



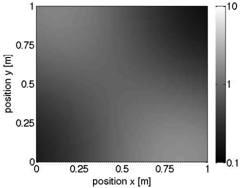
(g) $N = \ell_c$, Sample 1



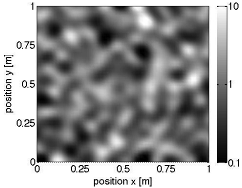
(h) $N = 10\ell_c$, Sample 1



(i) $N = \ell_c/10$, Sample 2



(j) $N = \ell_c$, Sample 2

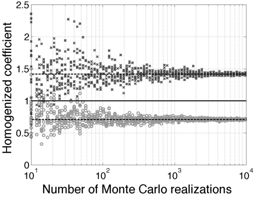


(k) $N = 10\ell_c$, Sample 2

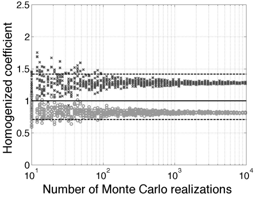
FIGURE – Map of parameter $A(x, \theta_i)$ (in logarithmic scale) for two realizations of each of the box sizes.

15. R. COTTEREAU. "Numerical strategy for the unbiased homogenization of random materials". In : *Int. J. Numer. Meth. Engr.* 95.1 (2013), p. 71-90. DOI : 10.1002/nme.4502

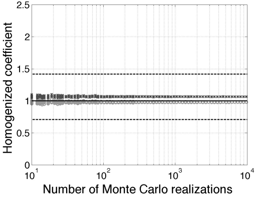
Numerical illustration of convergence of estimates of homogenized tensors



(a) $N = \ell_c/10$



(b) $N = \ell_c$



(c) $N = 10\ell_c$

FIGURE – Convergence of the homogenized coefficients $\check{a}_{N,\mathrm{M}}$ (dark grey crosses) and $\hat{a}_{N,\mathrm{M}}$ (light grey circles) for different box sizes N as a function of the numbers of Monte Carlo trials M. The dashed lines indicate the values of the arithmetic average $\mathrm{E}[\boldsymbol{k}_\epsilon]$ and of the harmonic average $\mathrm{E}[\boldsymbol{k}_\epsilon^{-1}]^{-1}$. The solid lines indicate the value of $a^* = 1$.

Outline

Quasi-periodic media [16]

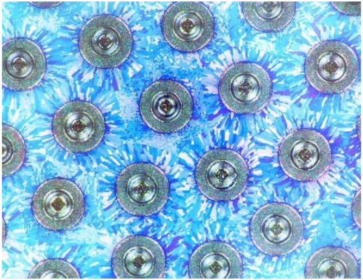


FIGURE – Silicon carbide fibres in a titanium matrix (© ONERA)

we consider a particular medium, of the type

$$A\left(\frac{x}{\epsilon},\theta\right) = A_{\mathrm{per}}\left(\Phi^{-1}\left(\frac{x}{\epsilon},\theta\right)\right)$$

where $A_{\mathrm{per}}(x) \in L^2_\#([0,1]^d)$ is a deterministic periodic material parameter field, and $\Phi(x,\theta)$ is a random diffeomorphism, whose gradient $\nabla\Phi$ is assumed stationary in the sense that there exists an ergodic group action τ such that, $\forall k \in \mathbb{Z}^d$,

$$\nabla\Phi(x+k,\theta) = \nabla\Phi(x,\tau_k\theta), \quad \text{almost surely, almost everywhere in x}$$

16. X. BLANC, C. LE BRIS et P.-L. LIONS. "Stochastic homogenization and random lattices". In : *Journal Mathématiques Pures Appliquées* 88.1 (2007), p. 34-63. DOI : 10.1016/j.matpur.2007.04.006

The particular case of perturbations of the identity

- we are particularly interested in the case when (for a "small" ϵ)

$$\Phi(y,\theta) = y + \epsilon\Psi(y,\theta) + \mathcal{O}\left(\epsilon^2\right)$$

In that case the matrix $A_{\rm per}(\Phi^{-1}(y,\theta))$ is formally close to a periodic matrix $A_{\rm per}(y)$.

- The corrector is expanded $\boldsymbol{w} = \boldsymbol{w}_0 + \epsilon\boldsymbol{w}_1 + \mathcal{O}\left(\epsilon^2\right)$ and both $\boldsymbol{w}_0$ and $\overline{\boldsymbol{w}}_1 = \mathbb{E}[\boldsymbol{w}_1]$ are shown to be solutions to deterministic periodic corrector problems (NB : tedious computations)

$$-\nabla\cdot\left(A_{\rm per}(y)\left(\mathbf{I}_d + \nabla\boldsymbol{w}_0\right)\right) = 0$$

and

$$\begin{aligned} -\nabla\cdot\left(A_{\rm per}(y)\nabla\overline{\boldsymbol{w}}_1\right) &= -\nabla\cdot\left(A_{\rm per}(y)\left(\mathbb{E}\left[\nabla\Psi\right]\nabla\boldsymbol{w}_0\right)\right) \\ &\quad - \nabla\cdot\left(\left(\mathbb{E}\left[\nabla\cdot\Psi\right]\mathbf{I}_d - \mathbb{E}\left[\nabla\Psi\right]^T\right)A_{\rm per}(y)\left(\mathbf{I}_d + \nabla\boldsymbol{w}_0\right)\right) \end{aligned}$$

- The approximation of the homogenized matrix $A^* = A_0^* + \epsilon A_1^* + \mathcal{O}\left(\epsilon^2\right)$ only requires the knowledge of $\boldsymbol{w}_0$ and $\overline{\boldsymbol{w}}_1$ (NB : tedious computations)

$$A_0^* = \int_Y A_{\rm per}(y)\left(\mathbf{I}_d + \nabla\boldsymbol{w}_0\right)dy,$$

and

$$\begin{aligned} A_1^* = -A_0^*\int_Y \mathbb{E}\left[\nabla\cdot\Psi\right]dy + \int_Y \mathbb{E}\left[\nabla\cdot\Psi\right]A_{\rm per}(y)\left(\mathbf{I}_d + \nabla\boldsymbol{w}_0\right)dy \\ + \int_Y A_{\rm per}(y)\left(\nabla\overline{\boldsymbol{w}}_1 - \mathbb{E}\left[\nabla\Psi\right]\nabla\boldsymbol{w}_0\right)dy \end{aligned}$$

Modeling of random media and stochastic homogenization for elliptic equations

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