

*From microscopic structures  
to models at the macroscopic scale:  
a mathematical and numerical perspective*

Claude Le Bris

ENPC and INRIA

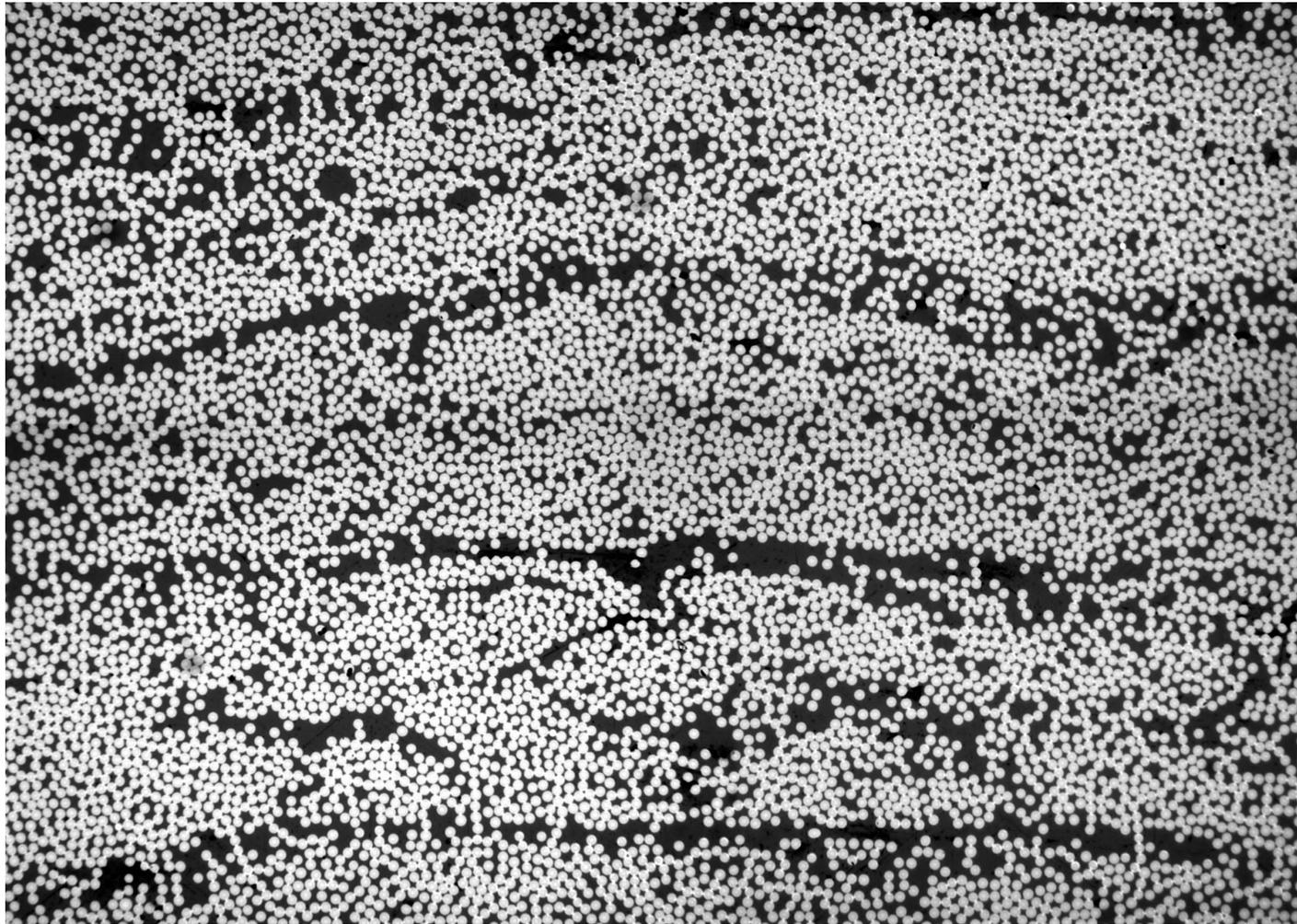
<http://cermics.enpc.fr/~lebris>

based on a series of joint works with

X. Blanc (CEA), PL. Lions (Collège de France)

A. Anantharaman, R. Costaouec, F. Legoll and F. Thomines (ENPC and INRIA)

*Real composite material*



Courtesy M. Thomas and EADS

Common denominator of many of the works presented:

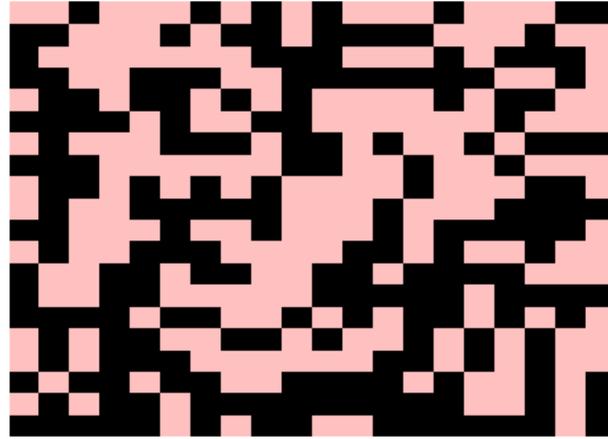
- go beyond the idealistic setting of periodic materials
- do not treat fully general random materials (fine theoretically, but too expensive to treat practically);
- consider materials that are, in a sense to be made precise, random **perturbations** of periodic materials;
- and adapt the modelling and the numerical approach.

Even more broadly,

**Make mechanics of random materials practical**

Work on the simplest possible equation  $-\operatorname{div} \left( a \left( \frac{\cdot}{\varepsilon} \right) \nabla u^\varepsilon \right) = f$ .

# Bounds

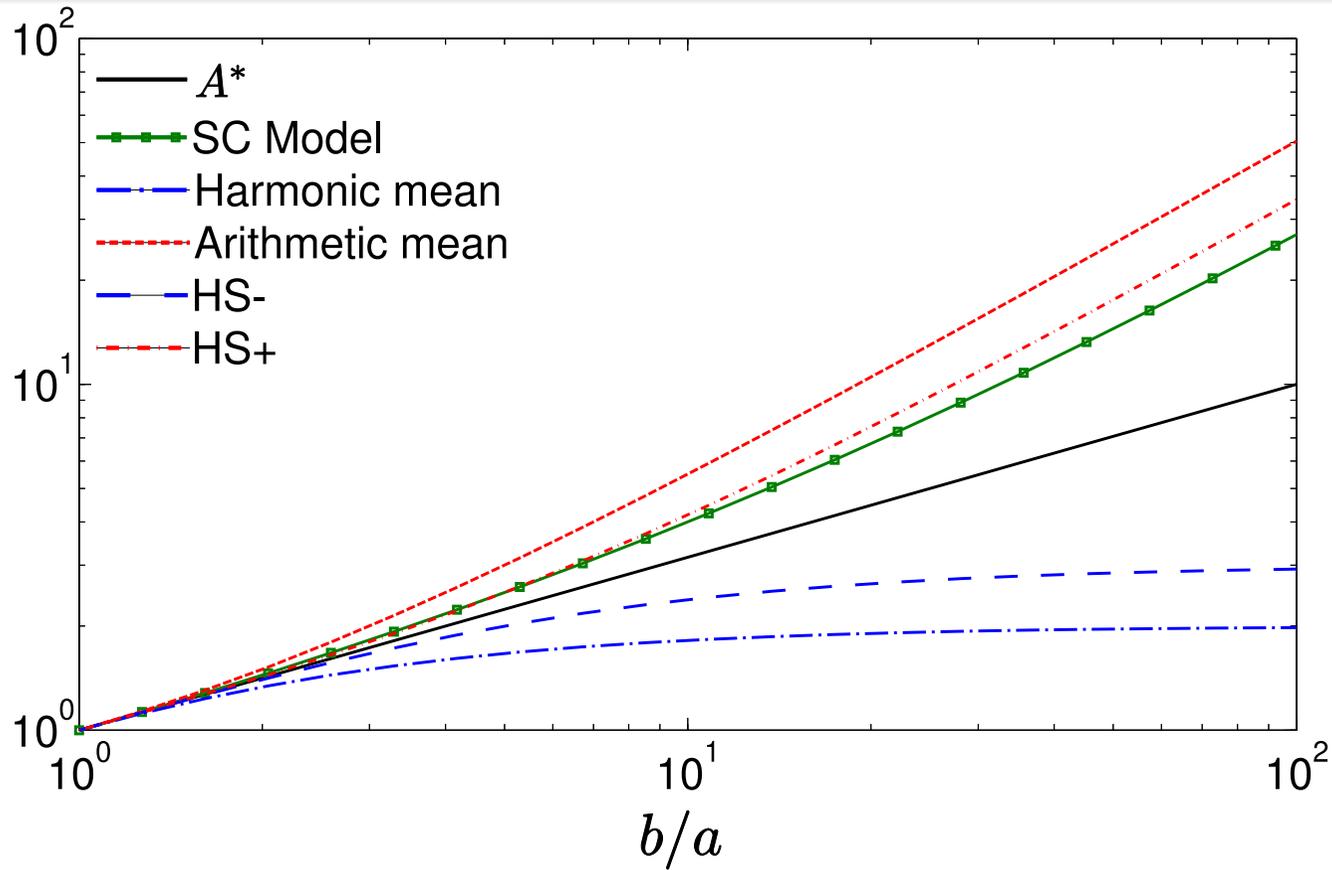


$$A(x, \omega) = \sum_{k \in \mathbb{Z}^2} 1_{Q+k}(x) a_k(\omega) \text{Id}_2, \quad a_k \text{ i.i.d.}, \mathbb{P}(a_k = a) = \mathbb{P}(a_k = b) = 1/2$$

$$A^* = a^* \text{Id}_2 = \sqrt{ab} \text{Id}_2.$$

Set  $a = 1$ , and check the accuracy of some classical bounds for various  $b$ .

# Hashin-Shtrikman bounds - 2



Case  $a = 1, b = 10$ :

Harmonic (Reuss)	HS-	$A^*$	SC Model	HS+	Arithmetic (Voigt)
1.81	2.38	3.16	4.00	4.19	5.50

Error is larger than 25 %.

$$-\operatorname{div} \left( a \left( \frac{x}{\varepsilon} \right) \nabla u^\varepsilon \right) = f, \quad a \text{ periodic}$$

$$-\operatorname{div} \left( a \left( \frac{x}{\varepsilon}, \omega \right) \nabla u^\varepsilon \right) = f \quad a \text{ stationary}$$

$$-\operatorname{div} \left( a \left( \Phi^{-1} \left( \frac{x}{\varepsilon}, \omega \right) \right) \nabla u^\varepsilon \right) = f \quad a \text{ periodic, } \nabla \Phi \text{ stationary}$$

$$-\operatorname{div} \left( a \left( \Phi^{-1} \left( \frac{x}{\varepsilon}, \omega \right), \omega' \right) \nabla u^\varepsilon \right) = f \quad a \text{ stationary, } \nabla \Phi \text{ stationary}$$

$$-\operatorname{div} \left( a \left( \frac{x}{\varepsilon} \right) \nabla u^\varepsilon \right) = f \quad a \text{ belongs to a general, abstract, algebra}$$

## Homogenization 1.0.1: the periodic setting

$$-\operatorname{div} \left[ A_{\text{per}} \left( \frac{x}{\varepsilon} \right) \nabla u^\varepsilon \right] = f \quad \text{in } \mathcal{D}, \quad u^\varepsilon = 0 \quad \text{on } \partial\mathcal{D},$$

with  $A_{\text{per}}$  symmetric and  $\mathbb{Z}^d$ -periodic:  $A_{\text{per}}(x + k) = A_{\text{per}}(x)$  for any  $k \in \mathbb{Z}^d$ .

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When  $\varepsilon \rightarrow 0$ ,  $u^\varepsilon$  converges to  $u^*$  solution to

$$-\operatorname{div} [A^* \nabla u^*] = f \quad \text{in } \mathcal{D}, \quad u^* = 0 \text{ on } \partial\mathcal{D}.$$

The effective matrix  $A^*$  is given by

$$[A^*]_{ij} = \int_Q (e_i + \nabla w_{e_i}(y))^T A_{\text{per}}(y) e_j dy, \quad Q = \text{unit cube} = (0, 1)^d$$

with, for any  $p \in \mathbb{R}^d$ ,  $w_p$  solves the so-called corrector problem:

$$-\operatorname{div} [A_{\text{per}}(y) (p + \nabla w_p)] = 0 \quad \text{in } \mathbb{R}^d, \quad w_p \text{ is } \mathbb{Z}^d\text{-periodic}.$$

Note that  $u_p(y) = p \cdot y + w_p(y)$  satisfies  $\langle \nabla u_p \rangle = p$ .

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Note that  $u_p(y) = p \cdot y + w_p(y)$  satisfies  $\langle \nabla u_p \rangle = p$ .

→ Solve  $d$  PDEs (for  $p = e_i$ ,  $1 \leq i \leq d$ ) on the bounded domain  $Q$ : easy!

## Some simple cases

$$-\operatorname{div} \left[ A_{\text{per}} \left( \frac{x}{\varepsilon} \right) \nabla u^\varepsilon \right] = f$$

- in the 0D case (remove differential operators):

$$-a_{\text{per}} \left( \frac{x}{\varepsilon} \right) u^\varepsilon(x) = f(x)$$

Then  $u^\varepsilon(x) = -f(x) a_{\text{per}}^{-1} \left( \frac{x}{\varepsilon} \right) \rightharpoonup -f(x) \langle a^{-1} \rangle$ , because a highly oscillatory **periodic** function weakly converges to its average. Hence  $u^\varepsilon \rightharpoonup u^*$  with

$$-a^* u^*(x) = f(x) \quad \text{with} \quad a^* = \langle a_{\text{per}}^{-1} \rangle^{-1} \quad (\text{harmonic average})$$

- in the 1D case: analytical expression for  $u^\varepsilon$ , pass to the limit,

$$-\frac{d}{dx} \left[ a^* \frac{du^*}{dx} \right] = f \quad \text{with again} \quad \frac{1}{a^*} = \int_0^1 \frac{1}{a_{\text{per}}(y)} dy.$$

# Stochastic homogenization setting

We consider statistically homogeneous **random** materials:

$$-\operatorname{div} \left[ A \left( \frac{x}{\varepsilon}, \omega \right) \nabla u^\varepsilon \right] = f \quad \text{in } \mathcal{D}$$

The tensor  $A(x, \omega)$  is such that

- $A(x, \omega)$  and  $A(x + k, \omega)$  share the **same** probability distribution, for any  $k \in \mathbb{Z}^d$ . For a given realization of the randomness, properties may be different. But, on average, they are identical: the material is **statistically homogeneous**.
- $x \mapsto \mathbb{E}(A(x, \cdot))$  is a **periodic** function.
- Ergodicity property: space average  $\sim$  average over realizations:

$$\frac{1}{|Q_N|} \int_{Q_N} A(x, \omega) dx \xrightarrow{N \rightarrow \infty} \mathbb{E} \left[ \int_Q A(x, \cdot) dx \right]$$

with  $Q = (0, 1)^d$  and  $Q_N = (-N, N)^d$ .

## Stochastic homogenization

$$-\operatorname{div} \left[ A \left( \frac{x}{\varepsilon}, \omega \right) \nabla u^\varepsilon \right] = f \quad \text{in } \mathcal{D}, \quad u^\varepsilon = 0 \text{ on } \partial\mathcal{D}.$$

$u^\varepsilon(\cdot, \omega)$  converges to  $u^*$  solution to

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where the effective matrix  $A^*$  is given by

$$[A^*]_{ij} = \mathbb{E} \left( \int_Q (e_i + \nabla w_{e_i}(y, \cdot))^T A(y, \cdot) e_j dy \right),$$

where  $w_p$  solves

$$\begin{cases} -\operatorname{div} [A(y, \omega) (p + \nabla w_p(y, \omega))] = 0 & \text{in } \mathbb{R}^d, \quad p \in \mathbb{R}^d, \\ \nabla w_p \text{ is statist. homog.}, \quad \mathbb{E} \left( \int_Q \nabla w_p(y, \cdot) dy \right) = 0. \end{cases}$$

The corrector problem is set on  $\mathbb{R}^d$ . Theoretically, the RVE is infinite.

# A variant of the classical homogenization setting

## A variant of classical stochastic homogenization

Classical stochastic homogenization:

$$-\operatorname{div} \left[ A \left( \frac{x}{\varepsilon}, \omega \right) \nabla u^\varepsilon(x, \omega) \right] = f(x) \text{ in } \mathcal{D}, \quad u^\varepsilon = 0 \text{ on } \partial\mathcal{D}$$

where the matrix  $A$  is **stationary**.

We consider here a variant:

$$-\operatorname{div} \left[ A_{\text{per}} \left( \Phi^{-1} \left( \frac{x}{\varepsilon}, \omega \right) \right) \nabla u^\varepsilon(x, \omega) \right] = f(x) \text{ in } \mathcal{D}, \quad u^\varepsilon = 0 \text{ on } \partial\mathcal{D}$$

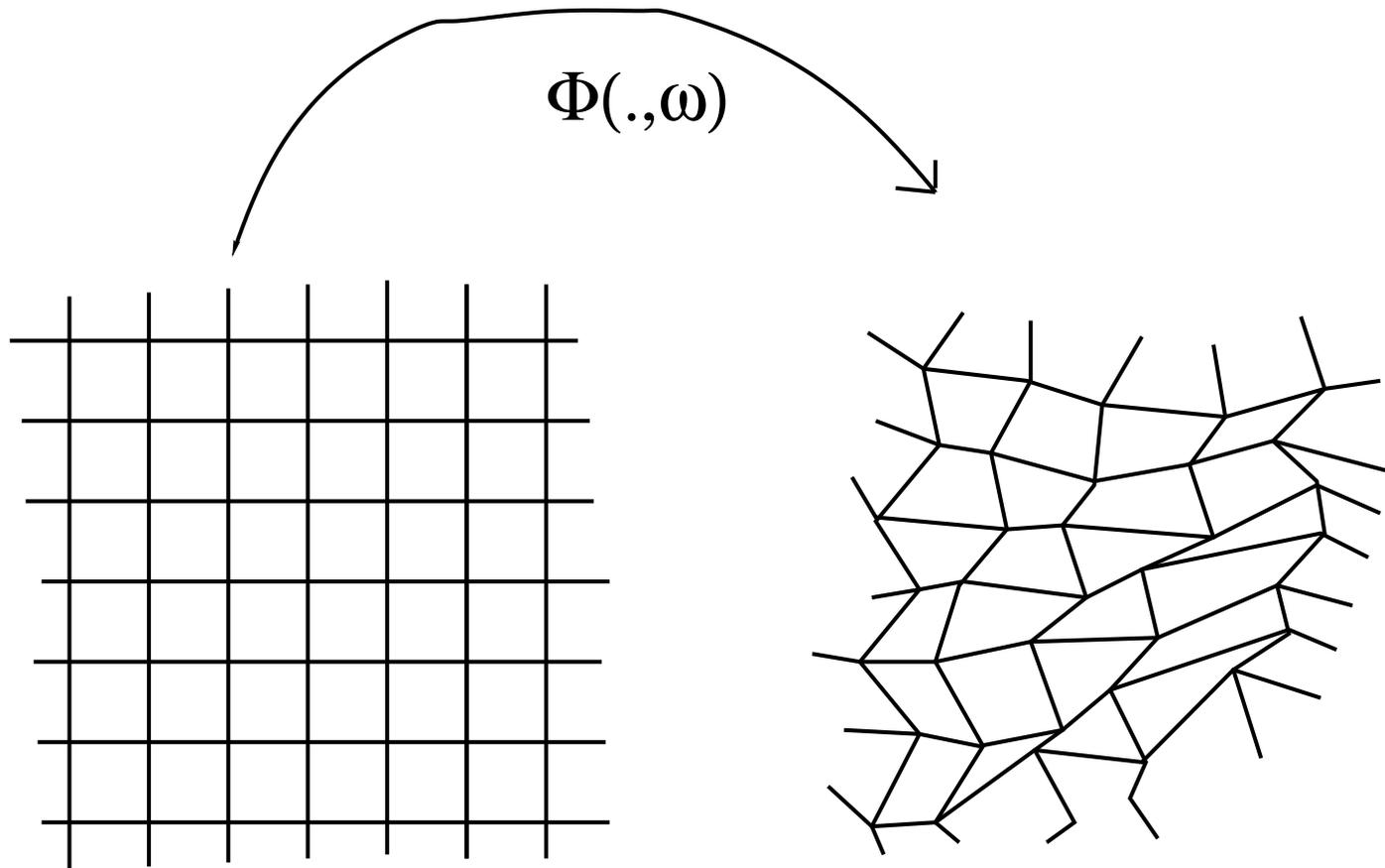
for a **periodic** matrix  $A_{\text{per}}$  and a **random diffeomorphism**  $\Phi$ , with  $\nabla\Phi$  stationary.

In general,  $A_{\text{per}} \circ \Phi^{-1}$  is NOT stationary.

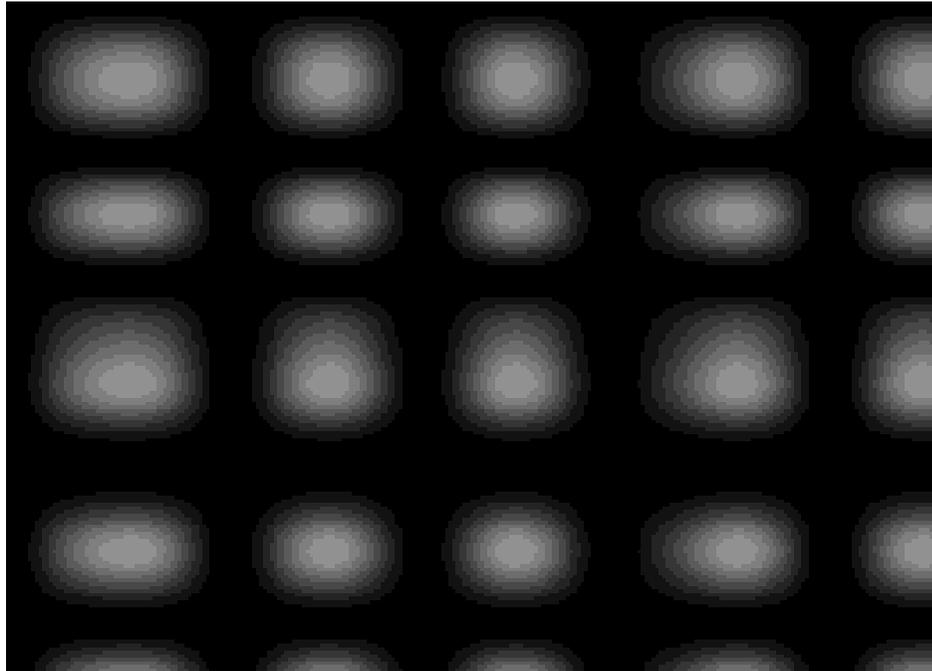
X. Blanc, CLB and P.-L. Lions, C. R. Acad. Sci., 2006.

X. Blanc, CLB and P.-L. Lions, J. Math. Pures et Appliquées, 2007.

# Random diffeomorphism



A 'real' material  $\equiv$  a random deformation of a reference periodic material  
Up to (more or less) random glasses, the material is periodic!



Deformed structure

The periodic structure corresponds to identical fibers set on a  $\mathbb{Z}^2$  lattice.

## Discrete stationary setting

Let  $(\tau_k)_{k \in \mathbb{Z}^d}$  be a group action that preserves the measure  $\mathbb{P}$  and is ergodic:

$$\forall k \in \mathbb{Z}^d, \quad \forall B \in \mathcal{F}, \quad \mathbb{P}(\tau_k B) = \mathbb{P}(B)$$

$$\forall B \in \mathcal{F}, \quad (\tau_k B = B \text{ for any } k \in \mathbb{Z}^d) \implies \mathbb{P}(B) = 0 \text{ or } 1.$$

A function  $F$  is said **stationary** if,

$$\forall k \in \mathbb{Z}^d, \quad F(x + k, \omega) = F(x, \tau_k \omega) \quad \text{a.e., a.s.}$$

Only **discrete** shifts are allowed.

Ergodic theorem:

$$F\left(\frac{x}{\varepsilon}, \omega\right) \xrightarrow[\varepsilon \rightarrow 0]{*} \mathbb{E} \left( \int_Q F(x, \cdot) dx \right) \text{ in } L^\infty(\mathbb{R}^d), \text{ a.s.}$$

$$-\operatorname{div} \left[ A_{\text{per}} \left( \Phi^{-1} \left( \frac{x}{\varepsilon}, \omega \right) \right) \nabla u^\varepsilon(x, \omega) \right] = f(x) \text{ in } \mathcal{D}, \quad u^\varepsilon = 0 \text{ on } \partial \mathcal{D}$$

Assumptions:

- the map  $\Phi(\cdot, \omega)$  is almost surely a **diffeomorphism** from  $\mathbb{R}^d$  to  $\mathbb{R}^d$ , with

$$\operatorname{EssInf}_{\omega \in \Omega, x \in \mathbb{R}^d} (\det(\nabla \Phi(x, \omega))) = \nu > 0,$$

$$\operatorname{EssSup}_{\omega \in \Omega, x \in \mathbb{R}^d} |\nabla \Phi(x, \omega)| = M < +\infty,$$

- $\nabla \Phi(x, \omega)$  is **stationary**:

$$\forall k \in \mathbb{Z}^d, \quad \nabla \Phi(x + k, \omega) = \nabla \Phi(x, \tau_k \omega)$$

Why do we need  $\nabla \Phi$  to be stationary?

## A simple 0D computation

Consider  $b(x, \omega) = b_{\text{per}}(\Phi^{-1}(x, \omega))$ . Let us compute its **average**,

$$\frac{1}{R} \int_0^R b(x, \omega) dx = \frac{1}{R} \int_0^R b_{\text{per}}(\Phi^{-1}(x, \omega)) dx$$

With the change of variables  $y = \Phi^{-1}(x, \omega)$ , we have

$$\frac{\int_0^R b(x, \omega) dx}{R} = \frac{\frac{1}{\Phi^{-1}(R, \omega) - \Phi^{-1}(0, \omega)} \int_{\Phi^{-1}(0, \omega)}^{\Phi^{-1}(R, \omega)} b_{\text{per}}(y) \Phi'(y, \omega) dy}{\frac{1}{\Phi^{-1}(R, \omega) - \Phi^{-1}(0, \omega)} \int_{\Phi^{-1}(0, \omega)}^{\Phi^{-1}(R, \omega)} \Phi'(y, \omega) dy}$$

Our assumptions on  $\Phi$  imply that  $\Phi^{-1}(R, \omega) - \Phi^{-1}(0, \omega) \geq M^{-1}R$  a.s.

Thus, **if  $\Phi'(y, \omega)$  is stationary, this converges to**

$$\left[ \mathbb{E} \int_0^1 \Phi'(y, \omega) dy \right]^{-1} \mathbb{E} \int_0^1 b_{\text{per}}(y) \Phi'(y, \omega) dy.$$

## Homogenization result (X. Blanc, CLB, P.-L. Lions, 2006)

$$-\operatorname{div} \left[ A_{\text{per}} \left( \Phi^{-1} \left( \frac{x}{\varepsilon}, \omega \right) \right) \nabla u^\varepsilon(x, \omega) \right] = f(x) \text{ in } \mathcal{D}, \quad u^\varepsilon = 0 \text{ on } \partial\mathcal{D}$$

$u^\varepsilon(\cdot, \omega)$  converges (weakly in  $H^1$  and strongly in  $L^2$ ) to  $u_\star$  almost surely, with

$$-\operatorname{div} [A^\star \nabla u_\star(x)] = f(x) \text{ in } \mathcal{D}, \quad u_\star = 0 \text{ on } \partial\mathcal{D}$$

with the **homogenized** matrix

$$A_{ij}^\star = \det \left[ \mathbb{E} \left[ \int_Q \nabla \Phi(y, \cdot) dy \right] \right]^{-1} \mathbb{E} \left[ \int_{\Phi(Q, \cdot)} (e_i + \nabla w_{e_i}(y, \cdot))^T A_{\text{per}}(\Phi^{-1}(y, \cdot)) e_j dy \right]$$

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where, for all  $p \in \mathbb{R}^d$ ,  $w_p$  is the corrector defined by

$$\left\{ \begin{array}{l} -\operatorname{div} [A_{\text{per}}(\Phi^{-1}(x, \omega)) (p + \nabla w_p(x, \omega))] = 0 \text{ in } \mathbb{R}^d, \\ w_p(x, \omega) = \tilde{w}_p(\Phi^{-1}(x, \omega), \omega), \quad \nabla \tilde{w}_p \text{ is stationary,} \\ \mathbb{E} \left( \int_{\Phi(Q, \cdot)} \nabla w_p(y, \cdot) dy \right) = 0. \end{array} \right.$$

Going further

$$-\operatorname{div} \left[ A_{\text{per}} \left( \Phi^{-1} \left( \frac{x}{\varepsilon}, \omega \right) \right) \nabla u^\varepsilon(x, \omega) \right] = f(x) \text{ in } \mathcal{D}, \quad u^\varepsilon = 0 \text{ on } \partial\mathcal{D}$$

The **corrector** problem is set on  $\mathbb{R}^d$ :

$$\begin{cases} \mathcal{L}(w_p) = 0 \text{ in } \mathbb{R}^d, \\ \nabla w_p \text{ is stationary} \end{cases}$$

In practice, need to introduce **truncation**: introduce  $Q_N = (-N, N)^d$  and approximate  $w_p$  by  $w_p^N$  with

$$\begin{cases} \mathcal{L}(w_p^N) = 0 \text{ on } Q_N, \\ w_p^N(\cdot, \omega) \text{ is } Q_N\text{-periodic} \end{cases}$$

and compute  $A_N^*(\omega)$  from there: **large domain** ( $N \gg 1$ ), **random output**, ...

Very expensive!

## Perturbations of identity - 1

Assume the diffeomorphism  $\Phi$  is close to the identity:

$$\Phi(x, \omega) = x + \eta\Psi(x, \omega) + O(\eta^2),$$

for  $\eta$  small. Then

$$w_p(x, \omega) = w_p^0(x) + \eta w_p^1(x, \omega) + O(\eta^2),$$

with

$$-\operatorname{div} (A_{\text{per}} (p + \nabla w_p^0)) = 0, \quad w_p^0 \text{ is } \mathbb{Z}^d\text{-periodic},$$

and

$$\begin{cases} -\operatorname{div} [A_{\text{per}} (\nabla w_p^1 - \nabla\Psi\nabla w_p^0) + (\nabla\Psi^T - (\operatorname{div}\Psi)\operatorname{Id}) A_{\text{per}} (p + \nabla w_p^0)] = 0, \\ \mathbb{E} \left( \int_Q \nabla w_p^1 \right) = \mathbb{E} \left( \int_Q (\nabla\Psi - (\operatorname{div}\Psi)\operatorname{Id}) \nabla w_p^0 \right), \quad \nabla w_p^1 \text{ stationary.} \end{cases}$$

However, to compute  $A^*$ , only the **expectation** of  $w_1^p$  is needed!

$$A_{ij}^* \sim \mathbb{E} \left[ \int (e_i + \nabla w_{e_i}(y, \cdot))^T A_{\text{per}} (\Phi^{-1}(y, \cdot)) e_j dy \right]$$

## Perturbations of identity - 2

Taking the expectation and setting  $\overline{w}_p^1 = \mathbb{E}(w_p^1)$ ,

$$\begin{cases} -\operatorname{div} [A_{\text{per}} \nabla \overline{w}_p^1] = \text{RHS} (A_{\text{per}}, \mathbb{E}(\nabla \Psi), \nabla w_p^0), \\ \int_Q \nabla \overline{w}_p^1 = \int_Q (\mathbb{E}(\nabla \Psi) - \mathbb{E}(\operatorname{div} \Psi) \operatorname{Id}) \nabla w_p^0, \quad \nabla \overline{w}_p^1 \text{ periodic.} \end{cases}$$

Eventually,

$$A^* = A^0 + \eta A^1 + O(\eta^2),$$

with

$$A_{ij}^0 = \int_Q (e_i + \nabla w_{e_i}^0)^T A_{\text{per}} e_j$$

$$A_{ij}^1 = \int_Q \text{fct} [\mathbb{E}(\nabla \Psi), A^0, \nabla w^0, A_{\text{per}}] + \int_Q (\nabla \overline{w}_{e_i}^1 - \mathbb{E}(\nabla \Psi) \nabla w_{e_i}^0)^T A_{\text{per}} e_j.$$

Two periodic computations instead of an expensive stochastic one.

## After space truncation and discretization

In practice, the corrector problem is solved on  $Q_N = (-N, N)^d$ , using e.g. FEM.

→ We do not compute  $A^*$ , but some  $A_{N,h}^*(\omega)$ .

Yet, a similar result holds (R. Costea, CLB, F. Legoll, CRAS 2010):

$$A_{N,h}^*(\omega) = A_h^0 + \eta A_{N,h}^1(\omega) + O(\eta^2)$$

where

- $A_h^0$  is the Finite Element approximation of  $A^0$ , obtained by periodic homogenization of  $A_{\text{per}}$ .
- $\overline{A}_h^1 := \mathbb{E} \left[ A_{N,h}^1 \right]$  is independent of  $N$ , and is easy to compute.

## Numerical illustration (2D)

$$\Phi_\eta(x, \omega) = x + \eta \Psi(x, \omega) \quad \text{with} \quad \Psi(x, \omega) = \begin{pmatrix} \psi_A(x_1, \omega) \\ \psi_B(x_2, \omega) \end{pmatrix}$$

with

$$\psi_A(x, \omega) = \sum_{k \in \mathbb{Z}} 1_{[k, k+1)}(x) \left( \sum_{q=0}^{k-1} 2A_q(\omega) + A_k(\omega) \int_k^x \sin^2(2\pi t) dt \right)$$

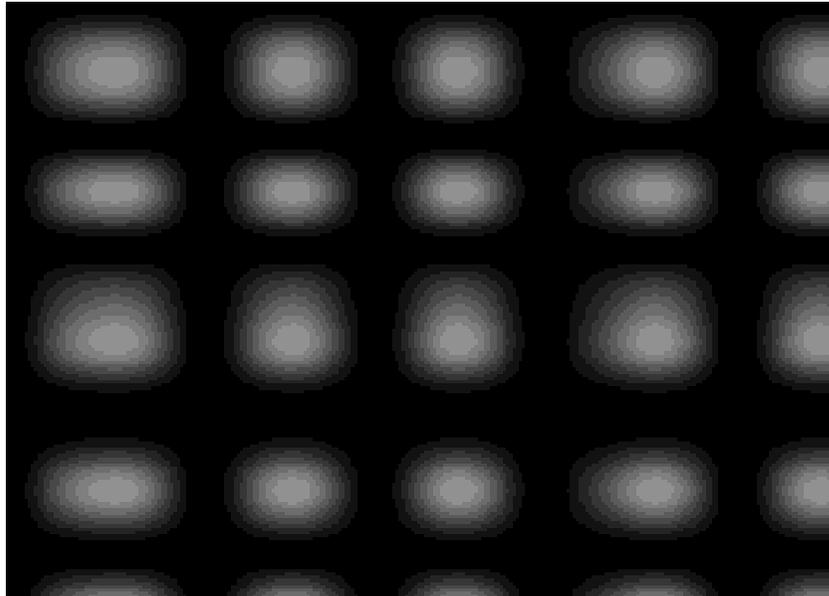
where  $(A_k)_{k \in \mathbb{Z}}$  and  $(B_k)_{k \in \mathbb{Z}}$  are all i.i.d. uniform random variables.

Take as periodic reference structure

$$A_{\text{per}}(x) = a_{\text{per}}(x) \text{ Id}$$

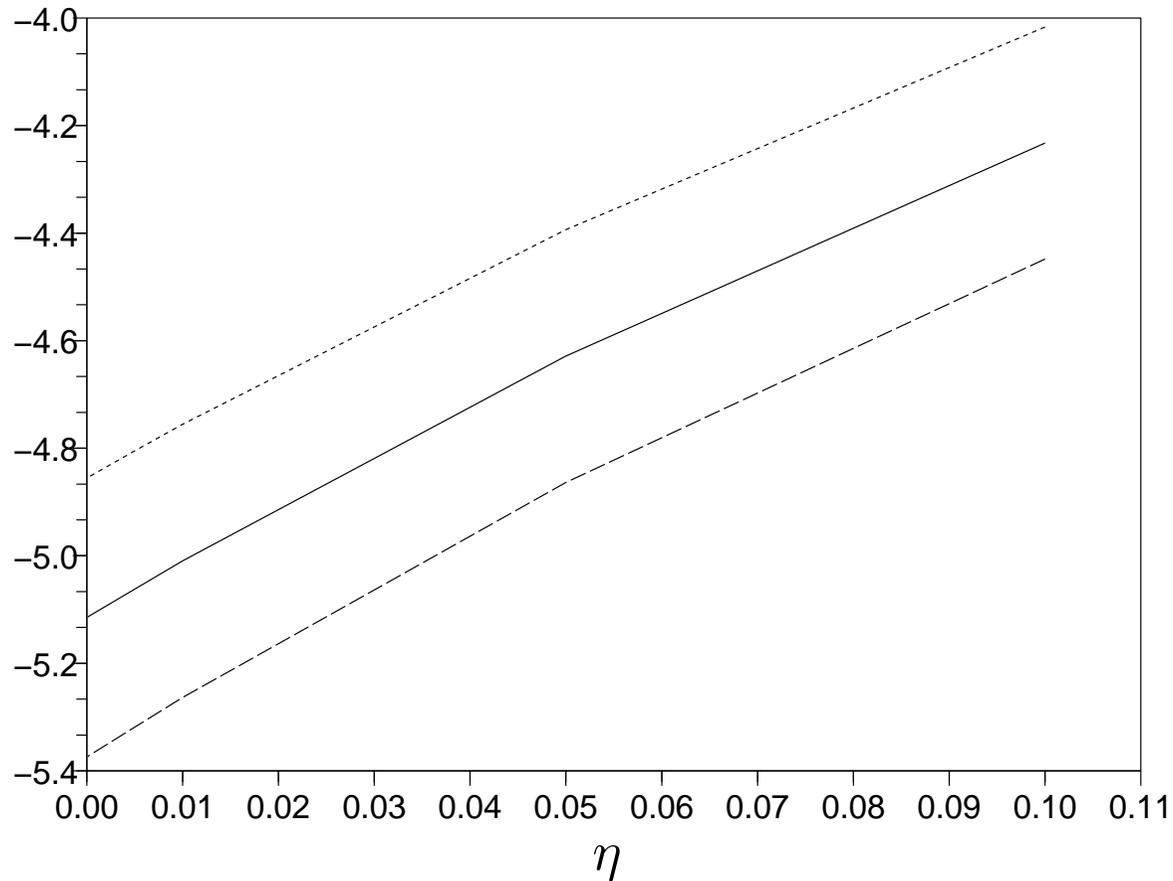
with

$$a_{\text{per}}(x) = \beta + (\alpha - \beta) \sin^2(\pi x) \sin^2(\pi y) \in C^\infty(\mathbb{R}^2)$$

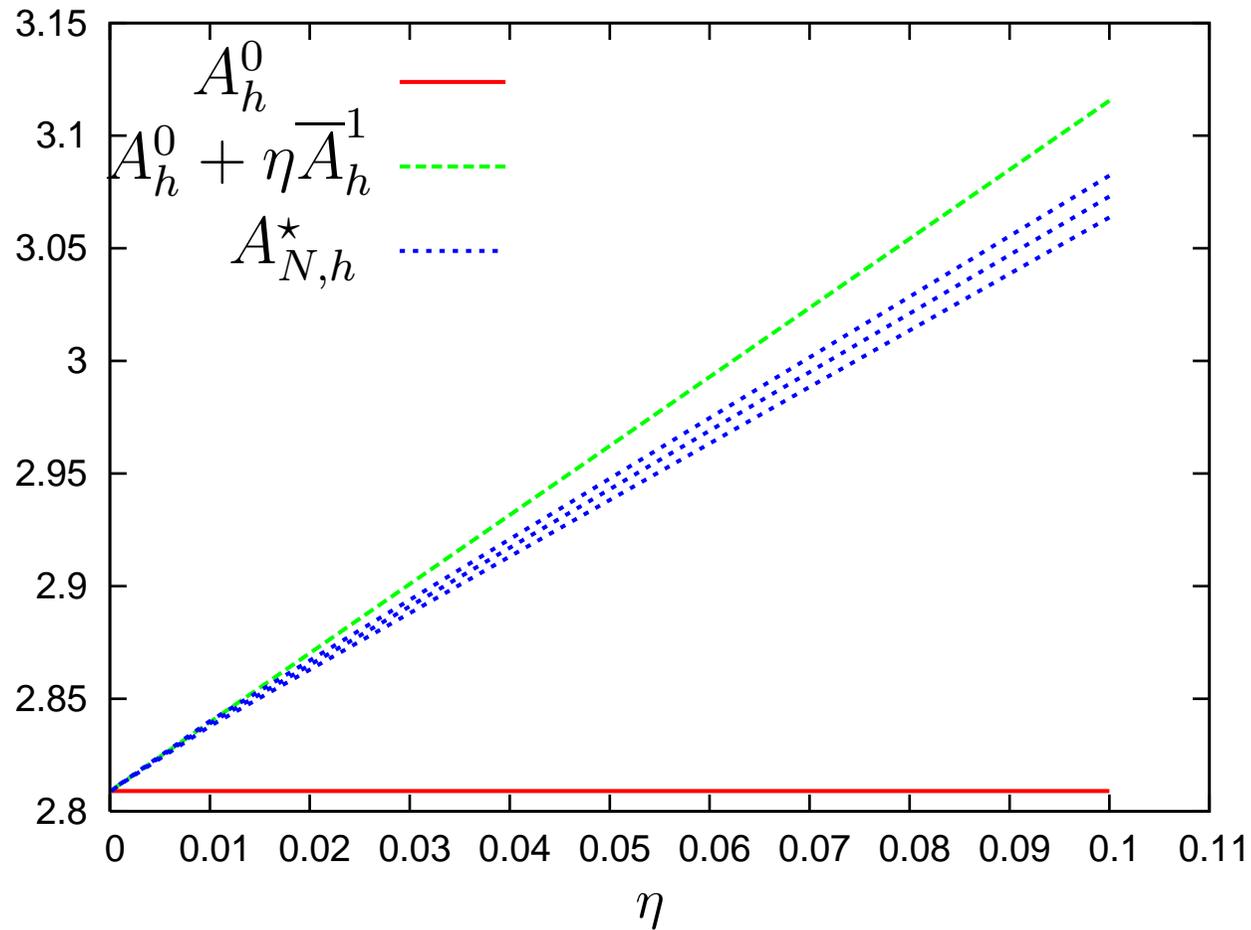


Deformed structure in  $Q_N$ , with  $N = 5$  and  $\eta = 0.05$

# Error at order $\eta^2$



Relative error:  $\frac{A_{N,h}^*(\omega) - A_h^0 - \eta A_{N,h}^1(\omega)}{\eta^2}$  for  $h = 1/3, N = 20$



$$h = 1/3, N = 20$$

$$A_{N,h}^*(\omega) = A_h^0 + \eta A_{N,h}^1(\omega) + O(\eta^2) \quad \text{and} \quad \bar{A}_h^1 := \mathbb{E} [A_{N,h}^1]$$

## **Further extension: more randomness!**

Define a random “perturbation” in a different topology and provide an efficient approach to compute the homogenized coefficients

Joint work with A. Anantharaman.

C. R. Acad. Sc., 348 (2010) 529-534.

SIAM MMS, 9, 2 (2011) 513-544,

Comm. Comp. Phys., 11 (2011), pp. 1103-1143.

In the previous setting, we have considered  $a_{per}(\Phi^{-1}(x, \omega))$  with

$$\Phi_\eta(x, \omega) = x + \eta\Psi(x, \omega) + \dots,$$

and  $\eta$  a small scalar. We can alternately consider

$$\Phi_\eta(x, \omega) = x + b_\eta(x, \omega)\Psi(x, \omega) + \dots,$$

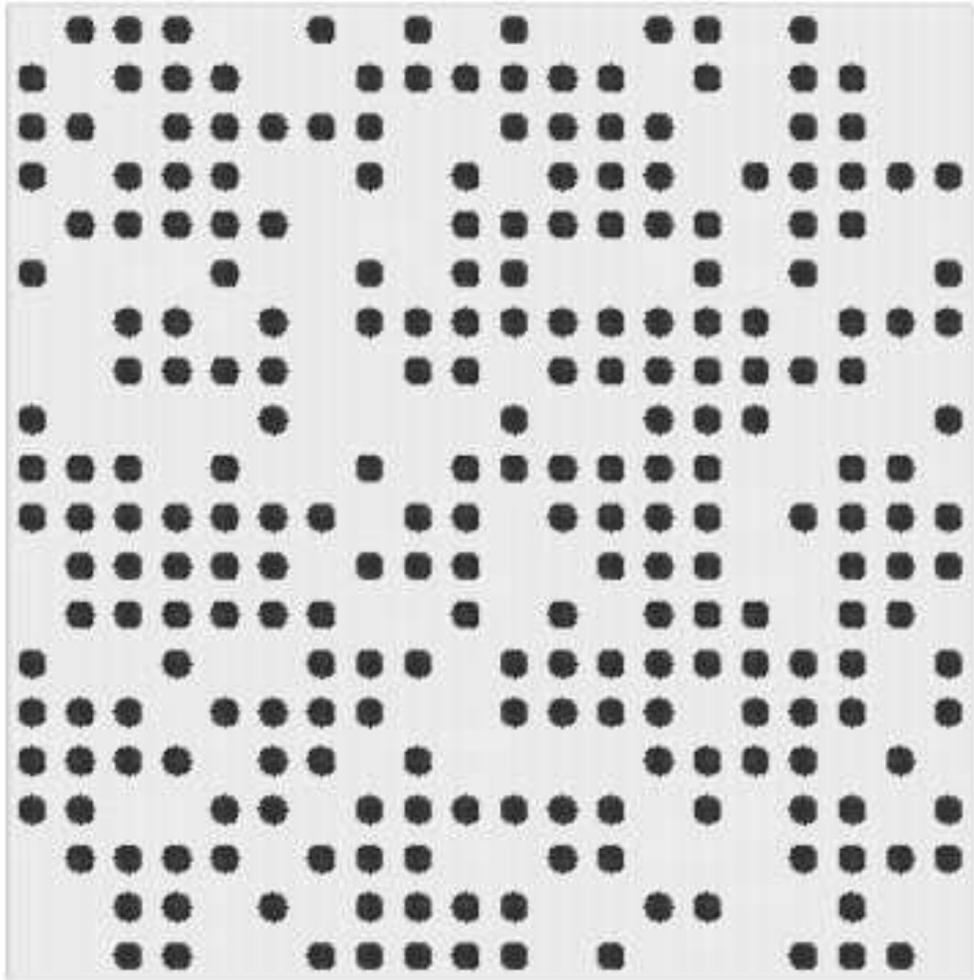
with  $b_\eta$  small in some appropriate (random) norm.

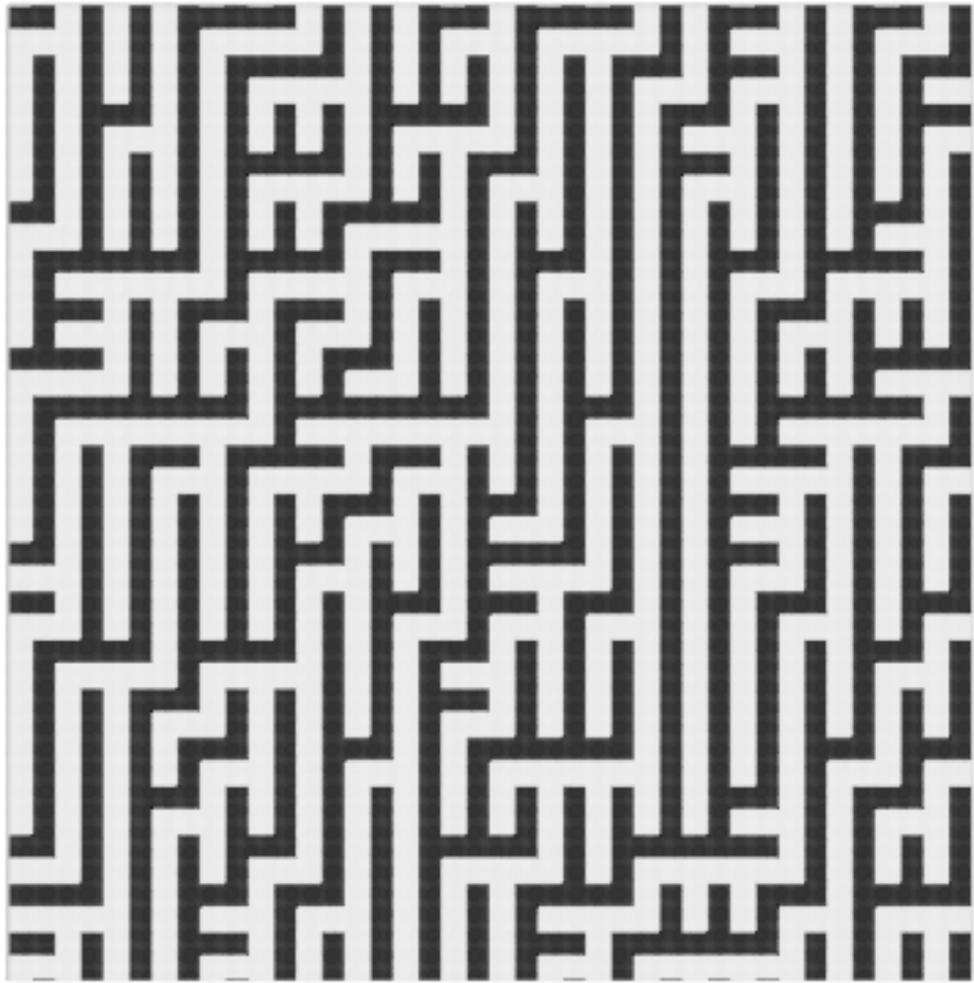
To keep things simple, let us assume

$$a(x, \omega) = a_{per}(x) + b_\eta(x, \omega) c_{per}(x).$$

The most interesting case is typically  $b_\eta(x, \omega)$  a Bernoulli random variable.

Random  $\eta$  (Anantharaman/LB)





Law of the material:

$$\delta_a + \eta (\delta_c - \delta_a)$$

on each cell. Cells are independent from one another. Product. Expand at first order in  $\eta$ :

$$\prod_{k=1}^N \delta_a(\text{cell } k) + \eta N \left[ \delta_c(\text{cell } k = 1) \prod_{k=2}^N \delta_a(\text{cell } k) - \prod_{k=1}^N \delta_a(\text{cell } k) \right].$$

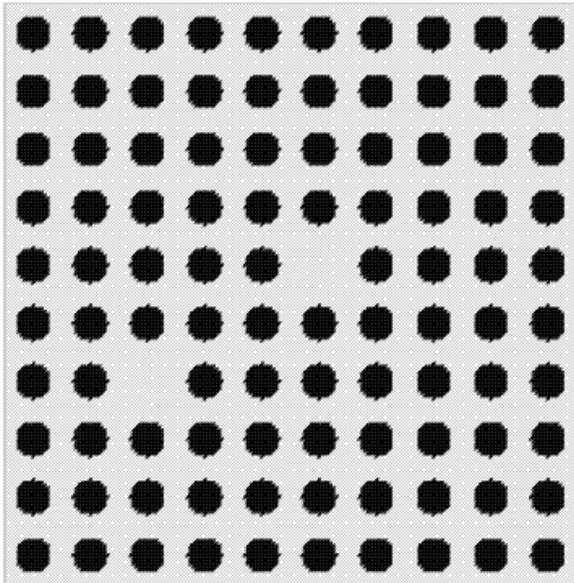
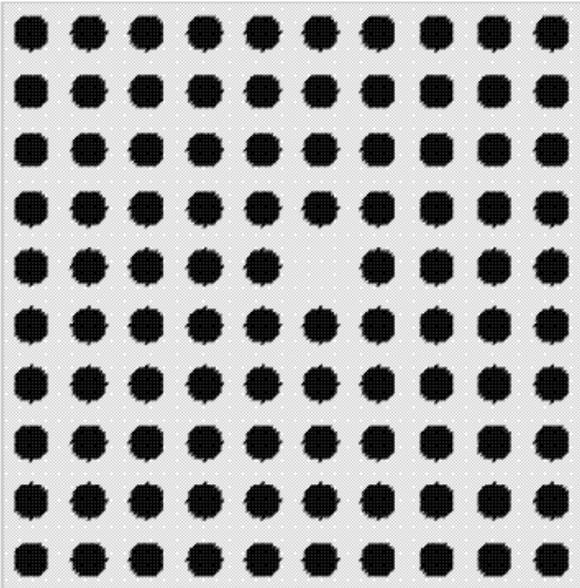
Think of a jellium model in Physics, or, otherwise stated, of a model for [defects](#).

Next remark that in  $-\text{div}(A(x, \omega)(p + \nabla w(x, \omega))) = 0$ , the only source of randomness is in  $A$ . Otherwise stated,  $w$  is a deterministic function of  $A$ . Thus, formally

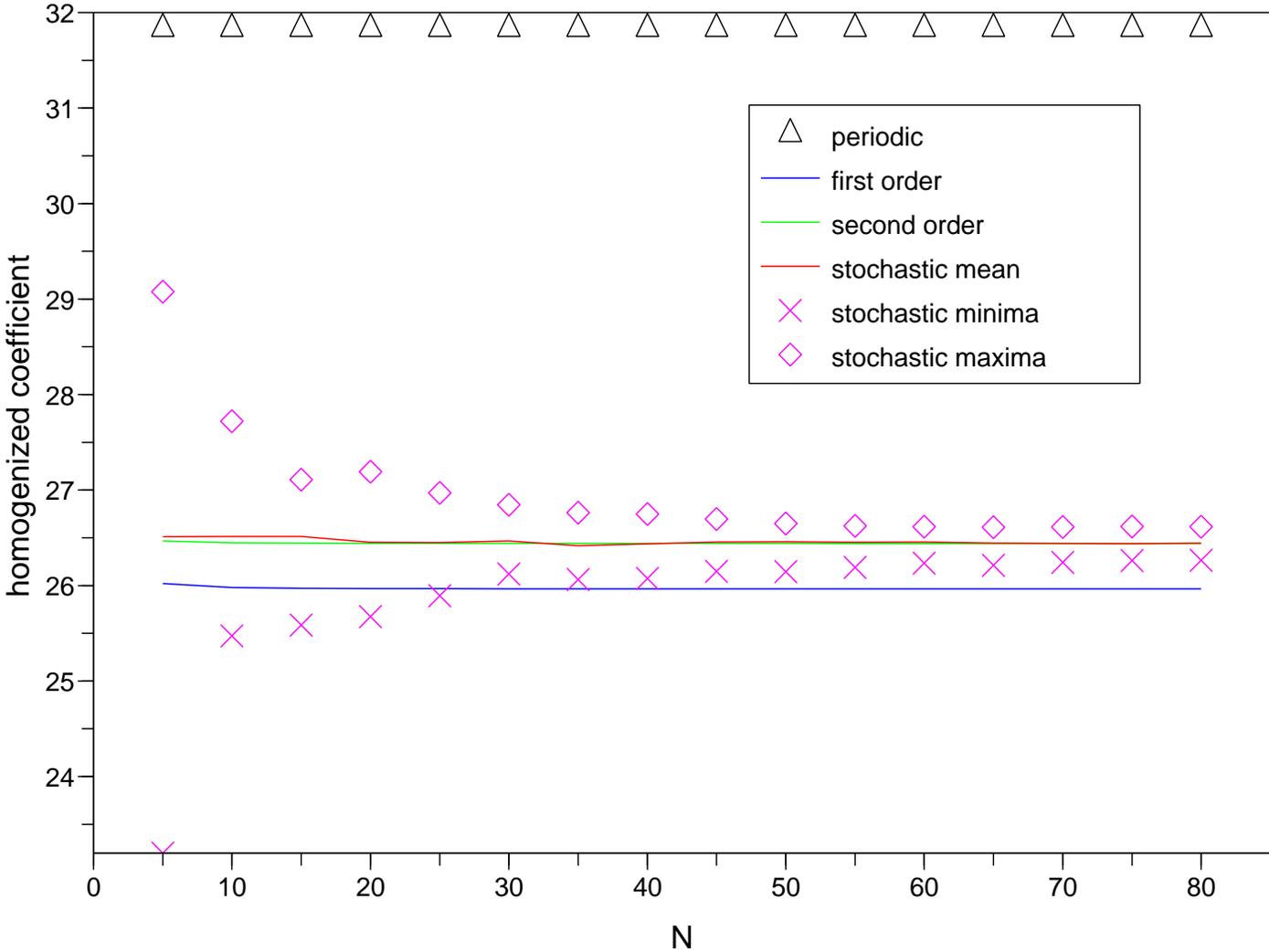
$$A_{ij}^* = \int \int (e_i + \nabla w_{e_i}(A, y))^T A(y) e_j dy \rho(A) dA.$$

$$A^* = A_0 + \eta A_1 + \dots$$

No proof of the expansion.  $A_0, A_1$  (and  $A_2, \dots$ ) finite..

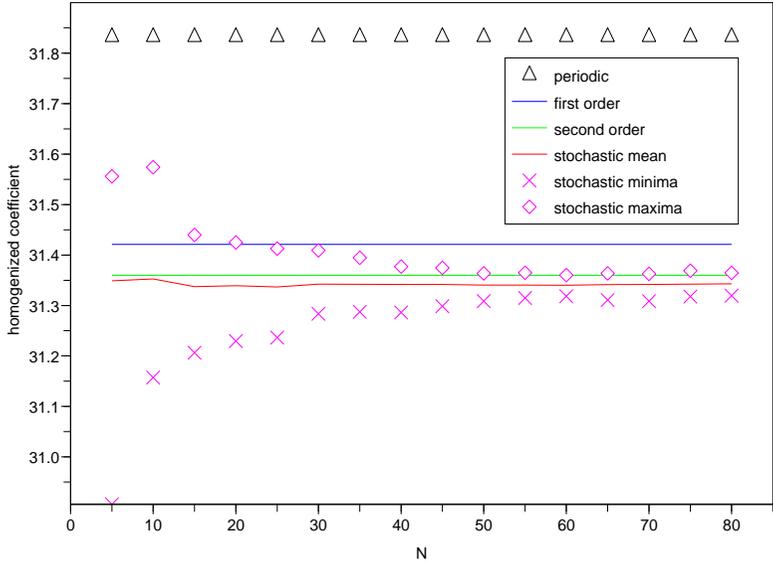


Inclusions – eta=0.4

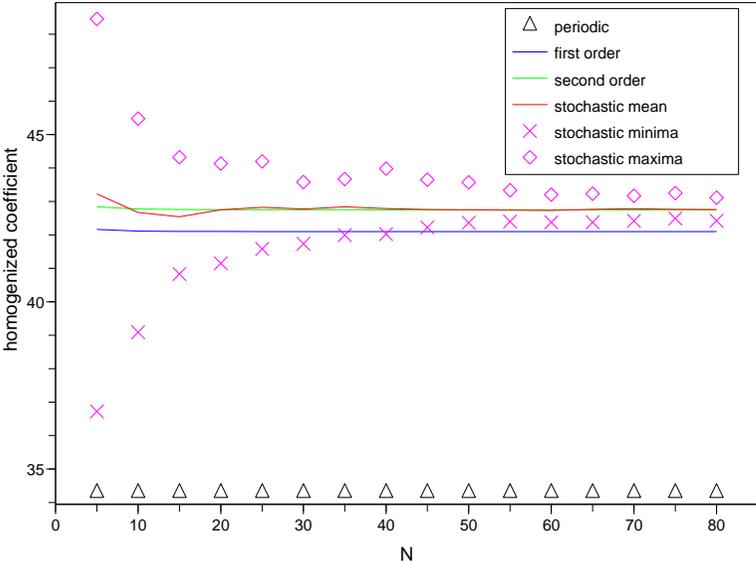


# Random $\eta$ (Anantharaman/LB)

Inclusions – Gaussian perturbation – eta=0.2



Laminate – eta=0.3



Left: Gaussian law; Right: Bernoulli and laminate.

# What if the material is “fully” stochastic?

We go back to the standard setting:

$$-\operatorname{div} \left[ A \left( \frac{x}{\varepsilon}, \omega \right) \nabla u^\varepsilon \right] = f \quad \text{in } \mathcal{D}, \quad u^\varepsilon = 0 \quad \text{on } \partial\mathcal{D}$$

with  $A$  stationary.

R. Costaouec, CLB, F. Legoll, Bol. Soc. Esp. Mat. Apl., 2010.

X. Blanc, R. Costaouec, CLB, F. Legoll, MPRF, 2012.

X. Blanc, R. Costaouec, CLB, F. Legoll, Lect. Notes Comp. Sci. Eng., vol 82, 2011.

## Standard stochastic homogenization

We go back to the standard setting:

$$-\operatorname{div} \left[ A \left( \frac{x}{\varepsilon}, \omega \right) \nabla u^\varepsilon \right] = f \quad \text{in } \mathcal{D}, \quad u^\varepsilon = 0 \quad \text{on } \partial \mathcal{D}$$

with  $A$  stationary. Then the effective matrix  $A^*$  is given by

$$[A^*]_{ij} = \mathbb{E} \left( \int_Q (e_i + \nabla w_{e_i}(y, \cdot))^T A(y, \cdot) e_j dy \right),$$

where  $w_p$  solves

$$\begin{cases} -\operatorname{div} [A(y, \omega) (p + \nabla w_p(y, \omega))] = 0 & \text{in } \mathbb{R}^d, \\ \mathbb{E} \left( \int_Q \nabla w_p(y, \cdot) dy \right) = 0, & \nabla w_p \text{ stationary} \end{cases}$$

This corrector problem is set on  $\mathbb{R}^d$ . Some approximation is in order to get to a tractable problem.

- Solve the corrector problem on a **truncated domain**:

$$\begin{cases} -\operatorname{div} [A(y, \omega) (p + \nabla w_p^N(y, \omega))] = 0 & \text{in } \mathbb{R}^d, \\ w_p^N \text{ is } Q_N\text{-periodic, } & Q_N = (-N, N)^d \end{cases}$$

- This yields an approximate effective matrix

$$[A_N^*]_{ij}(\omega) = \frac{1}{|Q_N|} \int_{Q_N} (e_i + \nabla w_{e_i}^N(y, \cdot))^T A(y, \omega) e_j dy$$

- Solve the corrector problem on a **truncated domain**:

$$\begin{cases} -\operatorname{div} [A(y, \omega) (p + \nabla w_p^N(y, \omega))] = 0 & \text{in } \mathbb{R}^d, \\ w_p^N \text{ is } Q_N\text{-periodic, } & Q_N = (-N, N)^d \end{cases}$$

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Due to numerical truncation,  $A_N^*$  is **random**!

When  $N \rightarrow \infty$ , we have  $A_N^* \rightarrow A^*$  a.s. (Bourgeat/Piatnitski, 2004).

$$[A_N^*]_{ij}(\omega) = \frac{1}{|Q_N|} \int_{Q_N} (e_i + \nabla w_{e_i}^N(y, \omega))^T A(y, \omega) e_j dy$$

At fixed  $N$ ,

$$A^* - A_N^*(\omega) = \underbrace{A^* - \mathbb{E}[A_N^*]}_{\text{(small) systematic error}} + \underbrace{\mathbb{E}[A_N^*] - A_N^*(\omega)}_{\text{(large) statistical error}}$$

Can we reduce the statistical error? Can we compute more accurately  $\mathbb{E}[A_N^*]$ ?

[Related works by Gloria and Otto]

## Understanding the truncation in the 1D case

Assume that  $a(x, \omega) = \sum_{k \in \mathbb{Z}} 1_{[k-1, k)}(x) a_k(\omega)$  with  $a_k$  i.i.d.

The effective coefficient is the harmonic average:

$$a^* = \left[ \mathbb{E} \left( \int_0^1 a^{-1}(x, \cdot) dx \right) \right]^{-1} = \left[ \mathbb{E} \left( \frac{1}{a_0} \right) \right]^{-1}$$

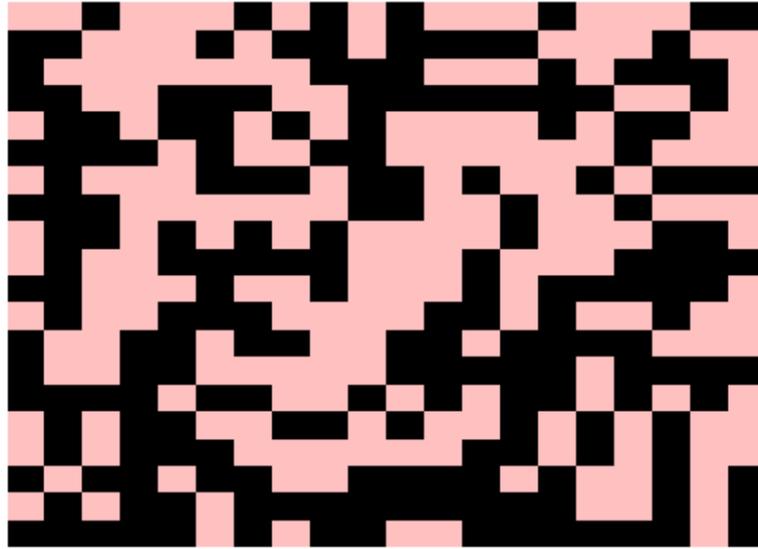
After truncation, we obtain the approximation

$$a_N^*(\omega) = \left[ \frac{1}{N} \int_0^N a^{-1}(x, \omega) dx \right]^{-1} = \left[ \frac{1}{N} \sum_{k=1}^N \frac{1}{a_k(\omega)} \right]^{-1}$$

By law of large numbers,  $\lim_{N \rightarrow \infty} a_N^*(\omega) = a^*$ .

But, at any  $N$ ,  $\mathbb{E}(a_N^*) \neq a^*$  (bias), and  $a_N^*$  is random (variance).

For finite  $N$ , the approximation  $a_N^*(\omega)$  is random.



$$A(x, \omega) = \sum_{k \in \mathbb{Z}^2} 1_{Q+k}(x) a_k(\omega) \text{Id}_2, \quad a_k \text{ independent identically distributed}$$

$a_k = \alpha$  or  $\beta$  with equal probability.

- Consider  **$2M$  realizations**  $A^m(y, \omega)$ , compute for each of these
  - the corrector  $w_p^{N,m}$ , solution to

$$-\operatorname{div} [A^m(y, \omega) (p + \nabla w_p^{N,m}(y, \omega))] = 0, \quad w_p^{N,m} \text{ is } Q_N\text{-periodic,}$$

- and the approximate homogenized matrix

$$[A_{N,m}^*]_{ij}(\omega) = \frac{1}{|Q_N|} \int_{Q_N} (e_i + \nabla w_{e_i}^{N,m}(y, \cdot))^T A^m(y, \omega) e_j dy.$$

- Approximate  $\mathbb{E}(A_N^*)$  by  $I_{2M} = \frac{1}{2M} \sum_{m=1}^{2M} A_{N,m}^*(\omega)$ .

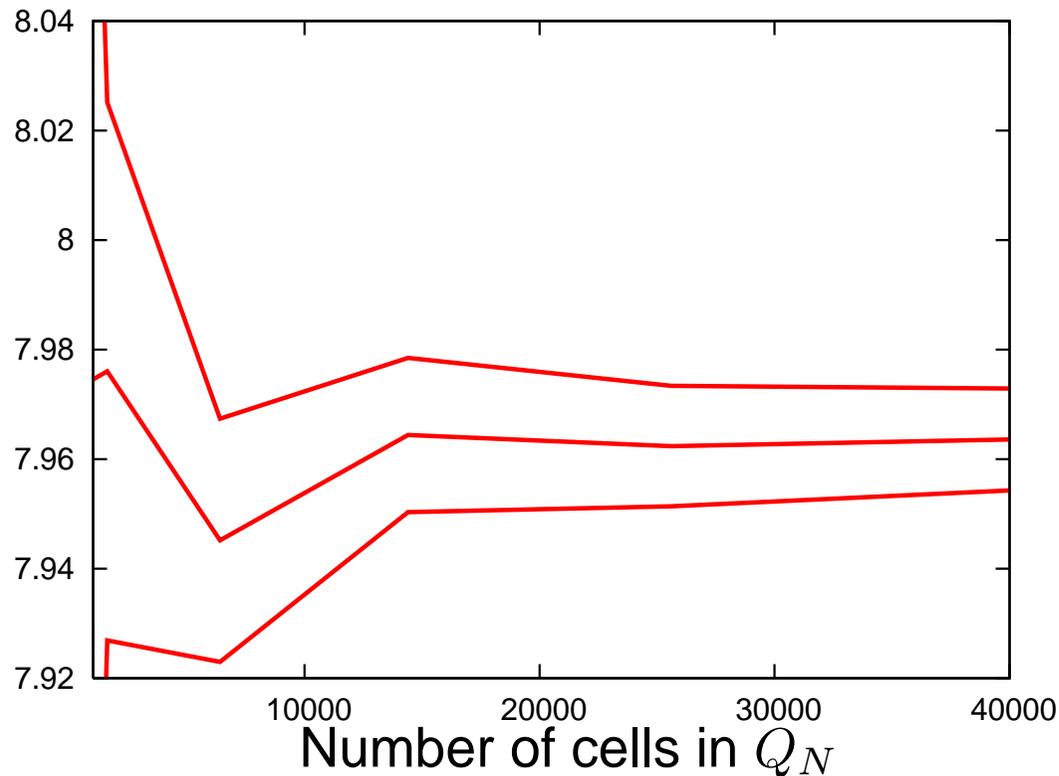
Classical confidence interval:

$$\left| \mathbb{E}([A_N^*]_{ij}) - [I_{2M}]_{ij} \right| \leq 1.96 \frac{\sqrt{\operatorname{Var}([A_N^*]_{ij})}}{\sqrt{2M}}$$

The accuracy of  $I_{2M}$  is directly linked with the variance of  $A_N^*$ .

## *In practice, on a 2D example ...*

$I_{2M} \approx \mathbb{E}([A_N^*]_{11})$  (along with confidence intervals) for a given number  $2M$  of realizations, and several sizes for  $Q_N$ .



For moderate  $N$ , the statistical error  $\gg$  systematic error

Our aim: compute  $\mathbb{E}(A_N^*)$  more efficiently, for any given  $N$ .

Goal: compute  $\mathbb{E}(f(U))$ , with  $U$  a random variable uniformly distributed in  $[0, 1]$ .

- Basic Monte Carlo method: using  $2M$  independent realizations of  $U(\omega)$ ,

$$I_{2M}(\omega) = \frac{1}{2M} \sum_{m=1}^{2M} f(U_m(\omega))$$

- Alternative approximation:

$$\bar{I}_{2M}(\omega) = \frac{1}{M} \sum_{m=1}^M \frac{1}{2} \left( f(U_m(\omega)) + f(1 - U_m(\omega)) \right)$$

$1 - U(\omega)$  has the same law as  $U(\omega)$ :

$I_{2M}$  and  $\bar{I}_{2M}$  both converge to  $\mathbb{E}(f(U))$

At fixed  $M$ ,

- both estimators have the **same cost** (same number of evaluations of  $f$ )
- accuracy?

## When does it work?

$$I_{2M}(\omega) = \frac{1}{2M} \sum_{m=1}^{2M} f(U_m(\omega))$$

$$\bar{I}_{2M}(\omega) = \frac{1}{M} \sum_{m=1}^M \frac{1}{2} \left( f(U_m(\omega)) + f(1 - U_m(\omega)) \right)$$

Let's compare the variance:

$$\text{Var } \bar{I}_{2M} = \text{Var } I_{2M} + \frac{1}{2M} \text{Cov}(f(U), f(1 - U))$$

$\bar{I}_{2M}$  is a better estimator than  $I_{2M}$   $\iff \text{Cov}(f(U), f(1 - U)) \leq 0$

Lemma: assume that  $f : [0, 1] \mapsto \mathbb{R}$  is **non-decreasing**. Then

$$\text{Cov}(f(U), f(1 - U)) \leq 0.$$

## Back to the homogenization context

We will apply the exact same idea to homogenization, with

$$\text{input} \equiv U(\omega) \sim A(x, \omega)|_{x \in Q_N}, \quad \text{output} \equiv f(U) \sim A_N^*(\omega)$$

Any time a random structure is considered, we will also make the computations with the antithetic structure.

Example: each time we see

$$A(x, \omega) = \sum_{k \in \mathbb{Z}^d} 1_{Q+k}(x) a_k(\omega) \text{Id}, \quad a_k(\omega) \text{ are i.i.d.}$$

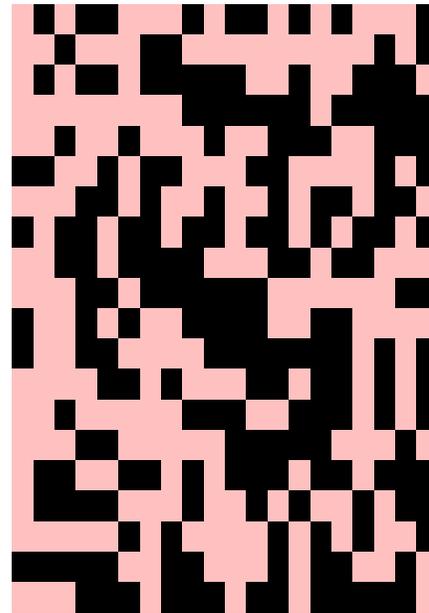
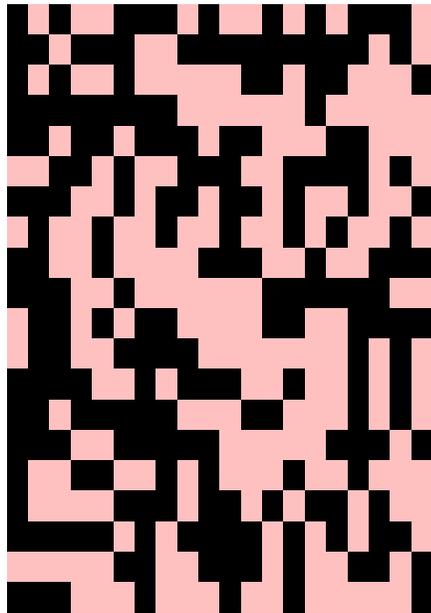
we also do the computations with the antithetic field:

$$B(x, \omega) = \sum_{k \in \mathbb{Z}^d} 1_{Q+k}(x) b_k(\omega) \text{Id}$$

where  $b_k(\omega)$  is antithetic to  $a_k(\omega)$ .

At each point  $x$ , we replace the local microstructure by the antithetic microstructure.

$$A(x, \omega) = \sum_{k \in \mathbb{Z}^d} 1_{Q+k}(x) a_k(\omega) \text{Id} \quad \longrightarrow \quad B(x, \omega) = \sum_{k \in \mathbb{Z}^d} 1_{Q+k}(x) b_k(\omega) \text{Id}$$



If  $a_k = \alpha$  or  $\beta$  with equal probability, then set  $b_k(\omega) = \beta$  whenever  $a_k(\omega) = \alpha$ .

If  $a_k$  is uniformly distributed in  $[\alpha, \beta]$ , then set  $b_k(\omega) = \alpha + \beta - a_k(\omega)$ .

- consider  $2M$  independent realizations  $A^m(x, \omega)$ , the associated correctors  $w_p^{N,m}$  and effective matrices  $A_{N,m}^*(\omega)$ , and the estimator

$$I_{2M} = \frac{1}{2M} \sum_{m=1}^{2M} A_{N,m}^*(\omega).$$

- consider  $2M$  independent realizations  $A^m(x, \omega)$ , the associated correctors  $w_p^{N,m}$  and effective matrices  $A_{N,m}^*(\omega)$ , and the estimator

$$I_{2M} = \frac{1}{2M} \sum_{m=1}^{2M} A_{N,m}^*(\omega).$$

- consider  $M$  independent realizations  $A^m(x, \omega)$ ,
  - build the  $M$  antithetic fields  $B^m(x, \omega)$ ,
  - for each of these  $B^m(x, \omega)$ , compute the associated corrector

$$-\operatorname{div} [B^m(y, \omega) (p + \nabla v_p^{N,m}(y, \omega))] = 0 \text{ in } \mathbb{R}^d, \quad v_p^{N,m} \text{ is } Q_N\text{-periodic.}$$

$$\text{Set } B_{N,m}^*(\omega) = \frac{1}{|Q_N|} \int_{Q_N} (e_i + \nabla v_{e_i}^{N,m}(y, \cdot))^T B^m(y, \omega) e_j dy.$$

- $\bar{I}_{2M} = \frac{1}{M} \sum_{m=1}^M \frac{1}{2} (A_{N,m}^*(\omega) + B_{N,m}^*(\omega)).$

$$I_{2M} = \frac{1}{2M} \sum_{m=1}^{2M} A_{N,m}^*(\omega)$$

$$\bar{I}_{2M} = \frac{1}{M} \sum_{m=1}^M \frac{1}{2} (A_{N,m}^*(\omega) + B_{N,m}^*(\omega))$$

- **Equal cost:** for both estimators,  $2M$  corrector problems need to be solved.

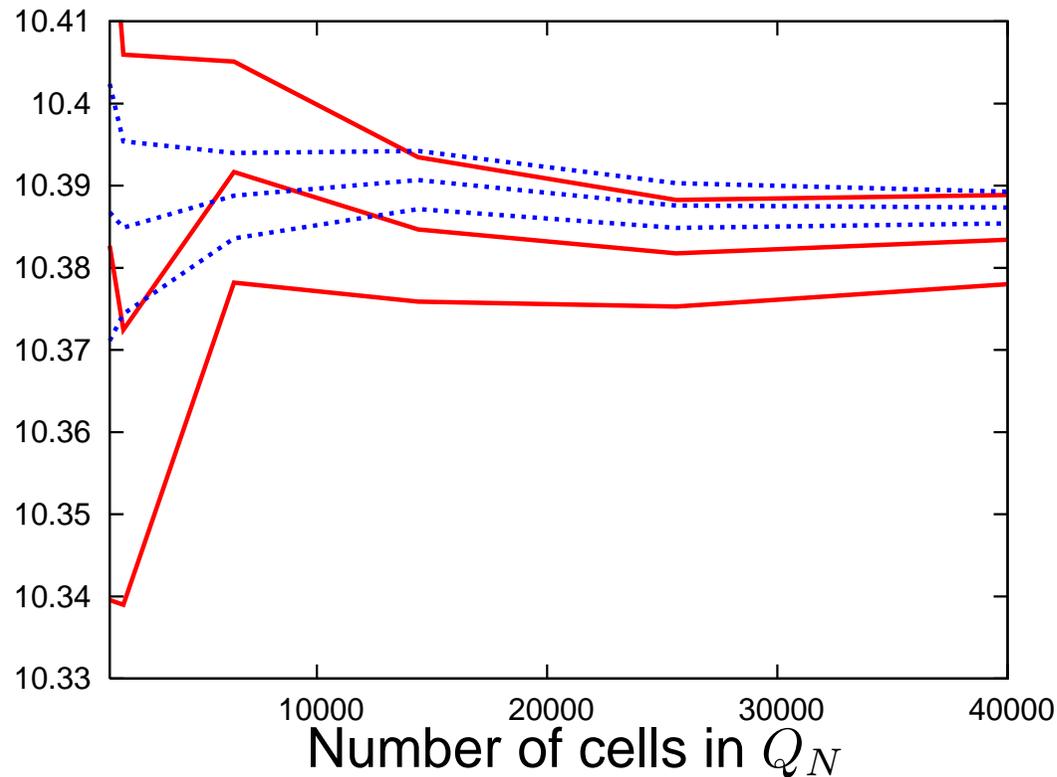
- **Convergent:**

$$I_{2M} \text{ and } \bar{I}_{2M} \text{ both converge to } \mathbb{E}(A_N^*)$$

- **Efficiency:** let's see numerically!

# Numerical experiments

$$A(x, \omega) = \sum_{k \in \mathbb{Z}^2} 1_{Q+k}(x) a_k(\omega) \text{Id}_2, \quad a_k \text{ i.i.d.}, \quad a_k \sim \mathcal{U}[\alpha, \beta]$$



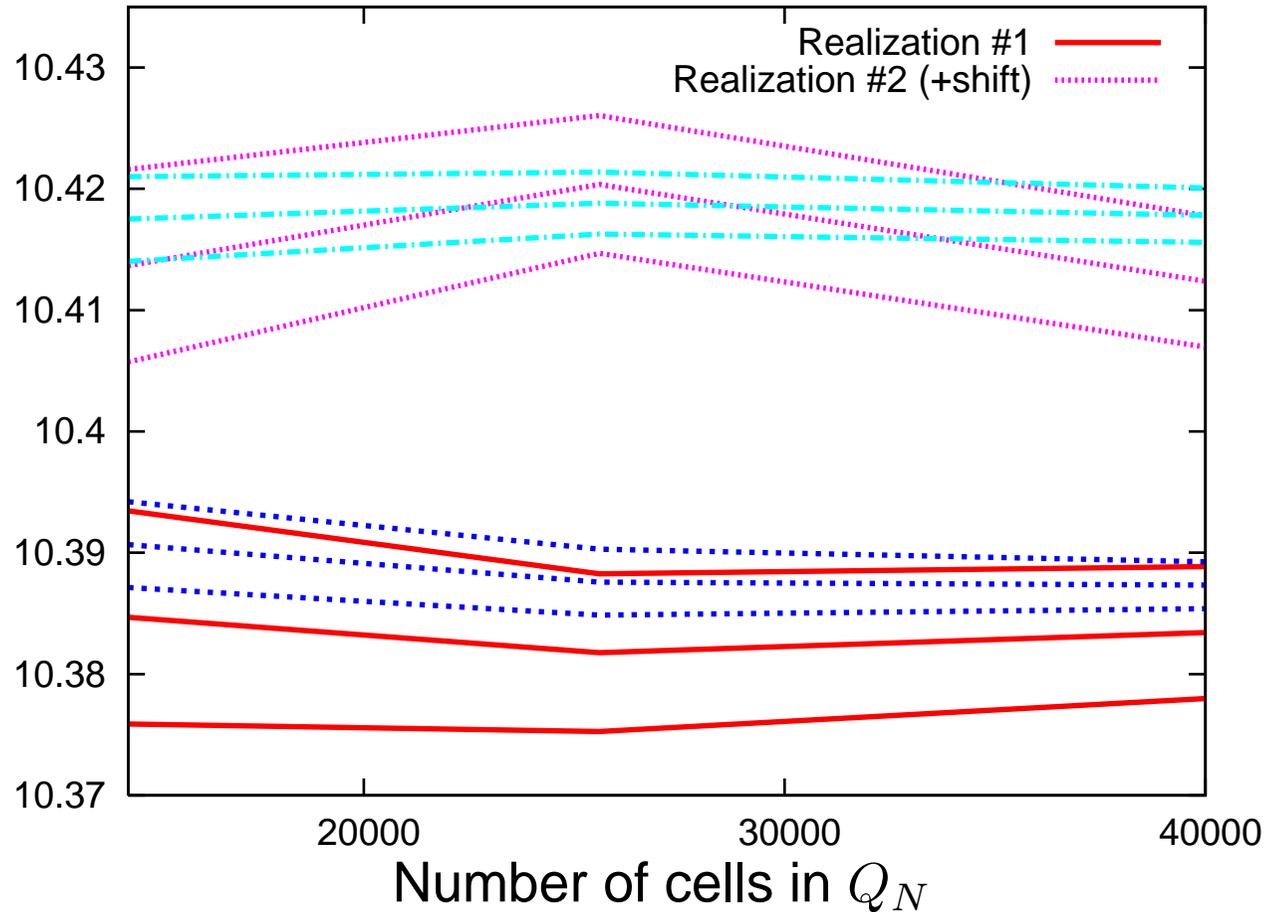
$I_{2M}$  and  $\bar{I}_{2M}$  (and confidence interval),  $\alpha = 3, \beta = 20$ .

Accuracy gain  $\geq \sqrt{6}$  (e.g. CPU time gain of 6 for equal accuracy).

Approach efficient even if  $N$  is not large!

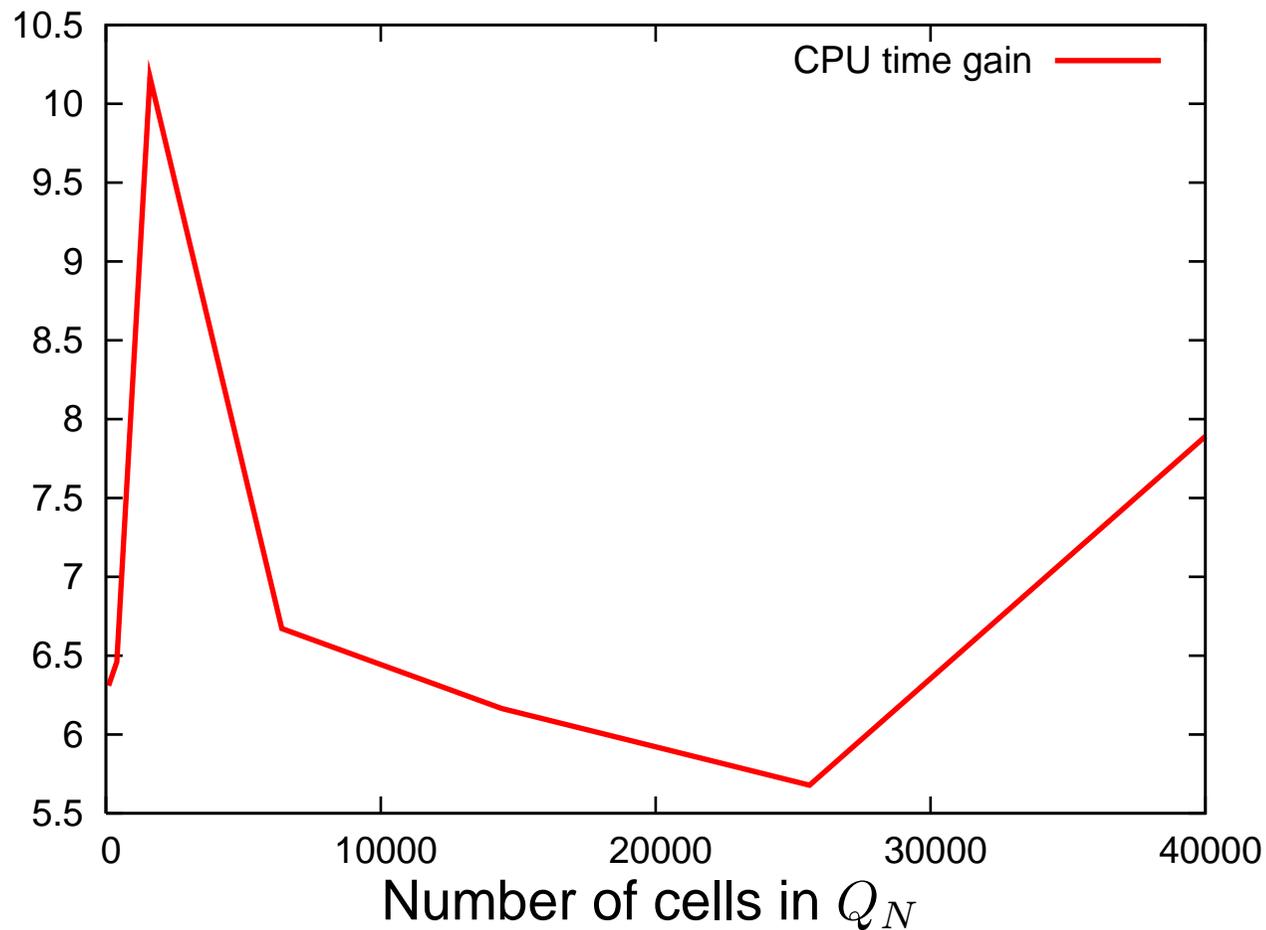
## Different realizations: no systematic bias

$$A(x, \omega) = \sum_{k \in \mathbb{Z}^2} 1_{Q+k}(x) a_k(\omega) \text{Id}_2, \quad a_k \text{ i.i.d.}, \quad a_k \sim \mathcal{U}[\alpha, \beta]$$



In addition, the CPU gain is roughly insensitive to the size of  $Q_N$ .

$$A(x, \omega) = \sum_{k \in \mathbb{Z}^2} 1_{Q+k}(x) a_k(\omega) \text{Id}_2, \quad a_k \text{ i.i.d.}, \quad a_k \sim \mathcal{U}[\alpha, \beta]$$



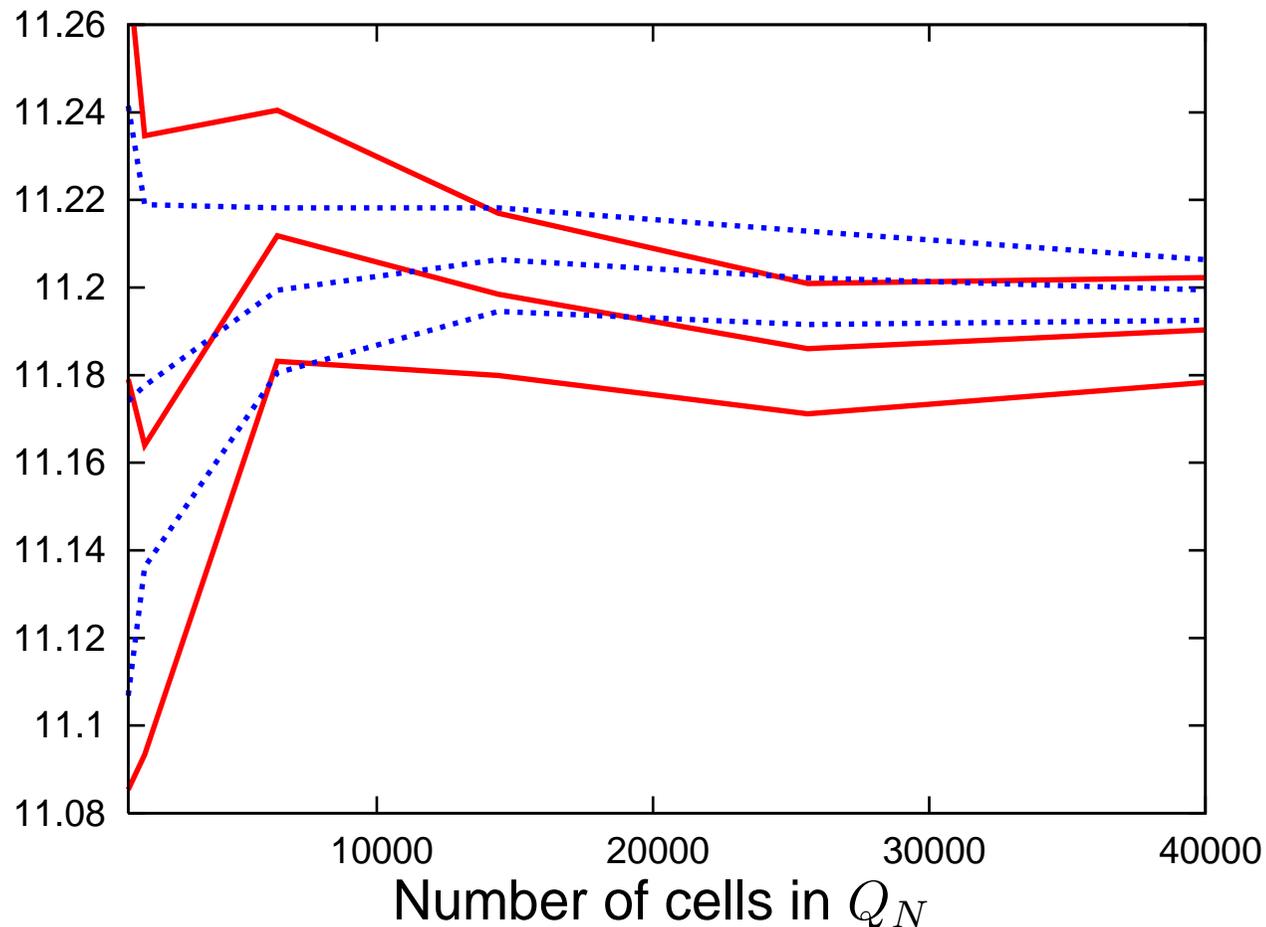
The CPU time gain (ratio of variances) is roughly insensitive to the size of  $Q_N$ .

## Numerical experiments - 2: non equidistributed case

$$A(x, \omega) = \sum_{k \in \mathbb{Z}^2} 1_{Q+k}(x) a_k(\omega) \text{Id}_2, \quad a_k \text{ i.i.d.}, \quad \mathbb{P}(a_k = \alpha) = 1/3, \quad \mathbb{P}(a_k = \beta) = 2/3$$

In practice:  $a_k = \phi(u_k) = \alpha 1_{0 \leq u_k \leq 1/3} + \beta 1_{1/3 \leq u_k \leq 1}$ , with  $u_k \sim \mathcal{U}[0, 1]$ .

Take  $b_k = \phi(1 - u_k)$ .



Good variance reduction on  $A_N^*$  for many input fields:

- **Correlated** fields:  $A(x, \omega)|_{Q+k}$  is possibly correlated with  $A(x, \omega)|_Q$ . The underlying uncorrelated structure is **known**:

$$A(x, \omega) = \sum_{k \in \mathbb{Z}^2} 1_{Q+k}(x) \left[ \frac{1}{2} a_k(\omega) + \frac{1}{16} \sum_{|q|=1} a_{k+q}(\omega) \right] \text{Id}_2$$

with  $a_k$  i.i.d. and  $a_k \sim \mathcal{U}[\alpha, \beta]$ .

$$B(x, \omega) = \sum_{k \in \mathbb{Z}^2} 1_{Q+k}(x) \left[ \frac{1}{2} b_k(\omega) + \frac{1}{16} \sum_{|q|=1} b_{k+q}(\omega) \right] \text{Id}_2$$

with  $b_k$  antithetic to  $a_k$ : here,  $b_k(\omega) = \alpha + \beta - a_k(\omega)$ .

$N$	40	60	80	100
Variance reduction on $[A_N^*(\omega)]_{11}$	31.17	39.89	25.43	45.52

## Robustness of the numerical results - 2

Good variance reduction on  $A_N^*$  for many input fields:

- **Anisotropic** fields:

$$A(x, \omega) = \sum_{k \in \mathbb{Z}^2} 1_{Q+k}(x) A_k(\omega) \text{ with } A_k(\omega) = \begin{pmatrix} \alpha_k(\omega) & \gamma_k(\omega) \\ \gamma_k(\omega) & \beta_k(\omega) \end{pmatrix},$$

where  $\{\alpha_k\}_{k \in \mathbb{Z}^2}$ ,  $\{\beta_k\}_{k \in \mathbb{Z}^2}$  and  $\{\gamma_k\}_{k \in \mathbb{Z}^2}$  are three independent families of independent random variables.

$$B(x, \omega) = \sum_{k \in \mathbb{Z}^2} 1_{Q+k}(x) B_k(\omega) \text{ with } B_k(\omega) = \begin{pmatrix} \bar{\alpha}_k(\omega) & \bar{\gamma}_k(\omega) \\ \bar{\gamma}_k(\omega) & \bar{\beta}_k(\omega) \end{pmatrix}$$

where  $\bar{\alpha}_k$  is antithetic to  $\alpha_k$ , ...

$N$	40	60	80	100
Variance reduction on $[A_N^*(\omega)]_{11}$	49.44	30.54	34.39	28.55

Variance reduction not only for  $A_N^*$ , but also for

- its **eigenvalues**
- the **eigenvalues**  $\lambda_k$  of the operator ( $\sim$  vibration frequencies):

$$-\operatorname{div} [A_N^*(\omega) \nabla u_k(\omega)] = \lambda_k(\omega) u_k(\omega)$$

- the **solution** of the (approximated) homogenized problem:  
 $A(x, \omega) \rightarrow$  homogenized matrix  $A_N^*(\omega)$ , and then solve

$$-\operatorname{div} [A_N^*(\omega) \nabla u_N^*(\omega)] = f$$

$A(x, \omega) \rightarrow$  antithetic field  $B(x, \omega), \dots, -\operatorname{div} [B_N^*(\omega) \nabla v_N^*(\omega)] = f$

$$\inf_{x \in \mathcal{D}} \frac{\operatorname{Var} u_N^*(x)}{\operatorname{Var} \left[ \frac{1}{2} (u_N^*(x) + v_N^*(x)) \right]} \approx 9 = \text{CPU time gain at equal accuracy}$$

- The method has been tested in several 2D situations:
  - various input fields,
  - various outputs
- It has been proved to reduce the variance in 1D, for 2D weakly random settings, and for some truly random 2D problems.

Behind the scene:  $-\operatorname{div} [a(x, \omega) \nabla u(x, \omega)] = f(x, \omega)$

# MsFEM approaches for weakly stochastic materials

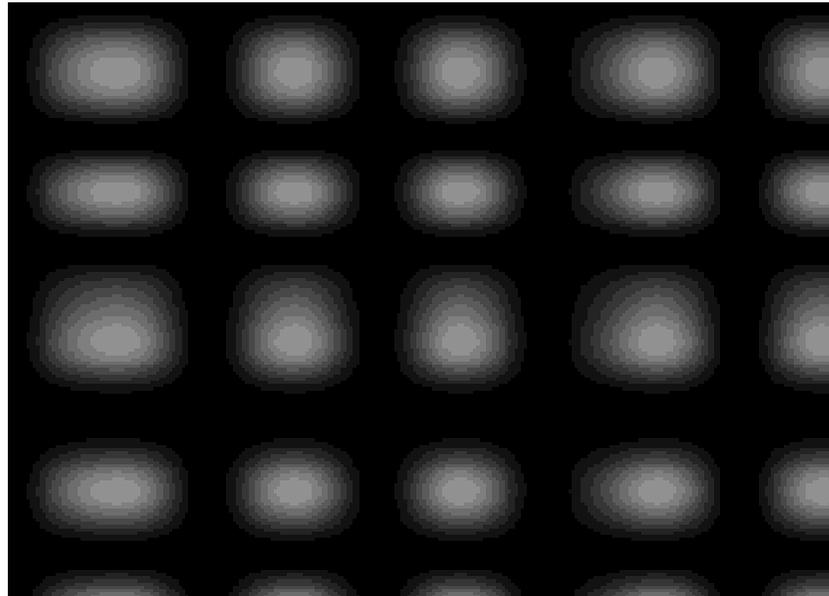
Keep  $\varepsilon$  at its small fixed value

MsFEM approach: introduced by Efendiev, Hou and Wu (subsequent large literature: Aarnes, Allaire & Brizzi, Dostert, Ginting, Chen et al . . . )

Joint work with F. Legoll and F. Thomines.

M2AN, submitted

Asymptotic Analysis, in press.



Not all materials are fully stochastic!

An interesting case: stochastic **perturbations** of deterministic materials.

Several ways to formalize this.

$$-\operatorname{div}(A^\varepsilon(x)\nabla u^\varepsilon(x)) = f(x) \text{ in } \mathcal{D}, \quad u^\varepsilon = 0 \text{ on } \partial\mathcal{D}.$$

where  $A^\varepsilon$  is not necessarily periodic.

Variational formulation: find  $u^\varepsilon$  such that

$$\forall v \in H_0^1(\mathcal{D}), \quad \mathcal{A}_\varepsilon(u^\varepsilon, v) = b(v),$$

where

$$\mathcal{A}_\varepsilon(u, v) = \int_{\mathcal{D}} (\nabla v)^T A^\varepsilon \nabla u \quad \text{and} \quad b(v) = \int_{\mathcal{D}} f v \, dx.$$

Idea: introduce an approximation with **suitably chosen basis functions**.

We introduce a classical P1 discretization of the domain  $\mathcal{D}$ , with  $L$  nodes, and denote  $\phi_i^0$  the basis functions.

- One possible definition (many have been proposed: Allaire, Hou, Efendiev):

$$\begin{cases} -\operatorname{div}(A^\varepsilon(x)\nabla\phi_i^{\varepsilon,\mathbf{K}}) & = 0 \quad \text{in } \mathbf{K} \\ \phi_i^{\varepsilon,\mathbf{K}} & = \phi_i^0|_{\mathbf{K}} \quad \text{on } \partial\mathbf{K}. \end{cases}$$

These problems, indexed by  $\mathbf{K}$ , are all **independent** from one another.

- Introduce the finite dimensional space

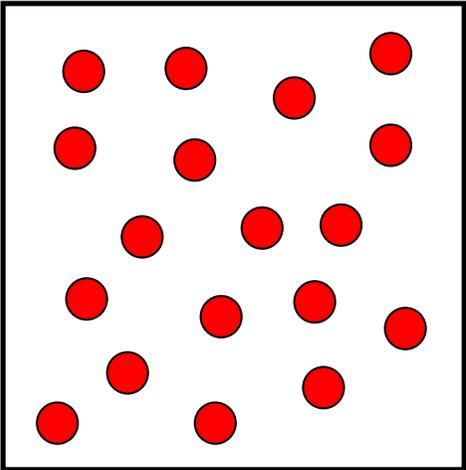
$$\mathcal{W}_h := \operatorname{span} \{ \phi_i^\varepsilon, i = 1, \dots, L \},$$

where  $\phi_i^\varepsilon$  is such that  $\phi_i^\varepsilon|_{\mathbf{K}} = \phi_i^{\varepsilon,\mathbf{K}}$  for all  $\mathbf{K}$ , and proceed with a standard Galerkin approximation using  $\mathcal{W}_h$ :

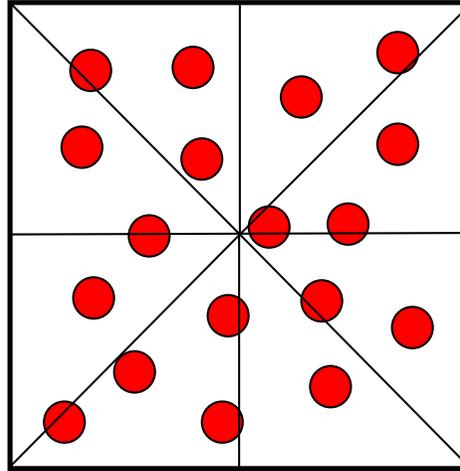
$$\text{Find } u_h^\varepsilon \in \mathcal{W}_h \text{ such that, } \forall v \in \mathcal{W}_h, \mathcal{A}_\varepsilon(u_h^\varepsilon, v) = b(v).$$

This only involves a **limited** number of degrees of freedom.

*A three step method*

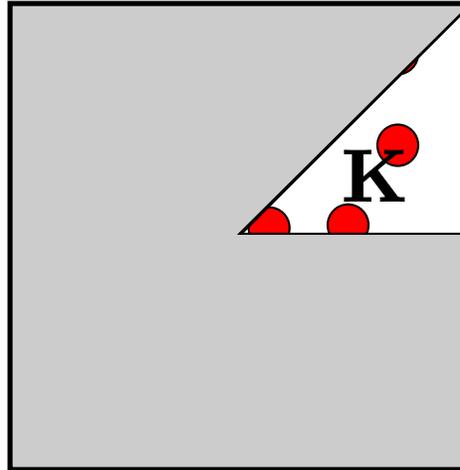


## A three step method



- **Coarse mesh** with a P1 Finite Element basis functions  $\phi_i^0$ .

# A three step method



- **Coarse mesh** with a P1 Finite Element basis functions  $\phi_i^0$ .

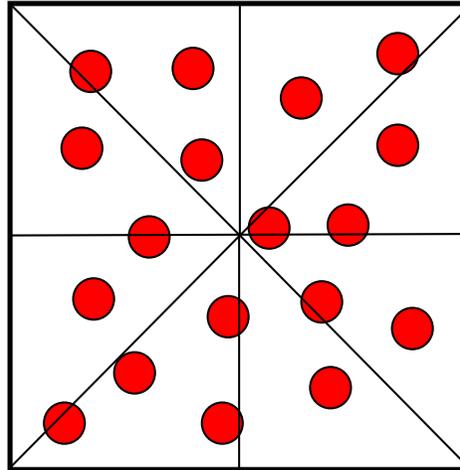


- **MsFEM basis**

$$\left\{ \begin{array}{ll} -\operatorname{div}(A^\varepsilon(x)\nabla\phi_i^{\varepsilon,\mathbf{K}}) = 0 & \text{in } \mathbf{K} \\ \phi_i^{\varepsilon,\mathbf{K}} = \phi_i^0|_{\mathbf{K}} & \text{on } \partial\mathbf{K} \end{array} \right.$$

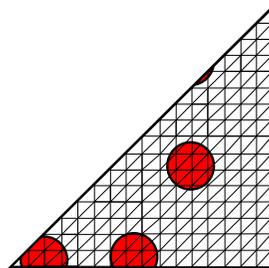
and glue them together:  $\phi_i^\varepsilon$  such that  $\phi_i^\varepsilon|_{\mathbf{K}} = \phi_i^{\varepsilon,\mathbf{K}}$  for all  $\mathbf{K}$ . The MsFEM functions are computed **independently** (in **parallel**) over each  $\mathbf{K}$ .

# A three step method



- **Coarse mesh** with a P1 Finite Element basis functions  $\phi_i^0$ .

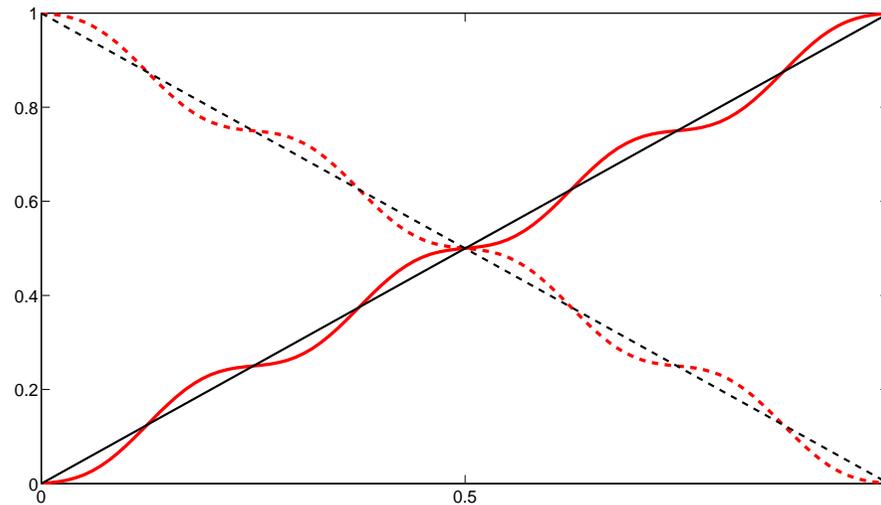
- **MsFEM basis**



$$\left\{ \begin{array}{ll} -\operatorname{div}(A^\varepsilon(x)\nabla\phi_i^{\varepsilon,\mathbf{K}}) = 0 & \text{in } \mathbf{K} \\ \phi_i^{\varepsilon,\mathbf{K}} = \phi_i^0|_{\mathbf{K}} & \text{on } \partial\mathbf{K} \end{array} \right.$$

and glue them together:  $\phi_i^\varepsilon$  such that  $\phi_i^\varepsilon|_{\mathbf{K}} = \phi_i^{\varepsilon,\mathbf{K}}$  for all  $\mathbf{K}$ . The MsFEM functions are computed **independently** (in **parallel**) over each  $\mathbf{K}$ .

- Solve the **macro problem** with MsFEM basis functions  $\phi_i^\varepsilon$ .



FEM basis vs **MsFEM basis**

The MsFEM method is accurate even with a coarse mesh, because the basis functions **encode the specific fast oscillations** of the problem.

$$-\operatorname{div}(A^\varepsilon(x)\nabla\phi_i^{\varepsilon,\mathbf{K}}) = 0 \quad \text{in } \mathbf{K} \quad \text{with} \quad \phi_i^{\varepsilon,\mathbf{K}} = \phi_i^0|_{\mathbf{K}} \quad \text{on } \partial\mathbf{K}$$

$$w := \phi_i^{\varepsilon,\mathbf{K}} - \phi_i^0|_{\mathbf{K}}$$

$$-\operatorname{div}(A^\varepsilon(x)(\nabla\phi_i^0 + \nabla w)) = 0 \quad + \text{Dirichlet BC: } \sim \text{corrector problem}$$

# Simple elements of numerical analysis

Recall the classical argument for the approximation

$$a(u, v) = L(v), \quad \forall v \in V$$

by

$$a(u_h, v_h) = L(v_h), \quad \forall v_h \in V_h.$$

Infer from

$$a(u - u_h, u - u_h) = a(u - u_h, v) = a(u - u_h, u - v_h), \quad \forall v_h \in V_h$$

that (Céa's Lemma)

$$\|u - u_h\|_{H^1} \leq (i.e. =) \inf_{v_h \in V_h} \|u - v_h\|_{H^1}.$$

Next, use the interpolant  $R_h(u)$  to majorize

$$\|u - u_h\|_{H^1} \leq \inf_{v_h \in V_h} \|u - v_h\|_{H^1} \leq \|u - R_h(u)\|_{H^1} \leq Ch \|D^2 u\|_{L^2}.$$

If  $u$  oscillates, we are doomed ....

# Simple elements of numerical analysis

Solve now (say) the one-dimensional equation  $Lu := -(\eta u')' + \alpha u = f$  with possibly highly oscillatory coefficients  $\eta$  and  $\alpha$ , using

$$V_H = \{v_H \text{ continuous, } Lu_H = 0 \text{ on each } [kH, (k+1)H]\}.$$

Using the classical argument, and the energy norm,

$$\|u - u_H\|_E = \inf_{v_H \in V_H} \|u - v_h\|_E \leq \|u - R_h(u)\|_E.$$

But, on each interval  $[kH, (k+1)H]$ ,  $L(u - R_H(u)) = 0$  and  $u - R_H(u)$  vanishes on the boundary, thus

$$\begin{aligned} \|u - R_H(u)\|_E^2 &= (L(u - R_H(u)), (u - R_H(u))) \leq \|f\|_{L^2} \|u - R_H(u)\|_{L^2} \\ &\leq \|f\|_{L^2} C H \|u - R_H(u)\|_{H^1} \end{aligned}$$

using the Poincaré inequality on each interval to get the rightmost majoration. Therefore,

$$\|u - u_H\|_E \leq C H \|f\|_{L^2}.$$

Consider the stochastic problem

$$\begin{cases} -\operatorname{div}(A^\varepsilon(x, \omega) \nabla u^\varepsilon(x, \omega)) & = f(x) \text{ in } \mathcal{D}, \\ u^\varepsilon & = 0 \text{ on } \partial\mathcal{D}, \end{cases}$$

and assume that we wish to build an estimate of the mean  $\mathbb{E}(u^\varepsilon(x, \cdot))$  using a Monte-Carlo simulation method.

Then, for **each realization** of  $A^{\varepsilon, m}(x, \omega)$ ,

- first construct a (**random**) MsFEM basis  $\phi_i^{\varepsilon, m}(x, \omega)$
- and next solve the macroscale problem to compute  $u^{\varepsilon, m}(x, \omega)$ .

Eventually,  $\mathbb{E}(u^\varepsilon(x, \cdot)) \approx \frac{1}{M} \sum_{m=1}^M u^{\varepsilon, m}(x, \omega)$ .

This is extremely expensive.

## Weakly stochastic setting

$$A^\varepsilon(x, \omega) \equiv A_\eta^\varepsilon(x, \omega) = A_0^\varepsilon(x) + \eta A_1^\varepsilon(x, \omega),$$

where  $A_0^\varepsilon$  is a deterministic matrix, and  $\eta$  is a **small** parameter, uniquely determined by  $\left\| \frac{A_1^\varepsilon}{A_0^\varepsilon} \right\|_{L^\infty} = 1$ .

Alternative MsFEM method:

- compute the MsFEM basis functions only **once**, with the **deterministic part** of the matrix  $A_\eta^\varepsilon$ :

$$-\operatorname{div}(A_0^\varepsilon(x) \nabla \phi_i^{\varepsilon, \mathbf{K}}) = 0 \quad \text{in } \mathbf{K}, \quad \phi_i^{\varepsilon, \mathbf{K}} = \phi_i^0|_{\mathbf{K}} \quad \text{on } \partial \mathbf{K}.$$

**Deterministic** approximation space

$$\mathcal{W}_h := \operatorname{span} \{ \phi_i^\varepsilon, i = 1, \dots, L \},$$

- next perform Monte-Carlo realizations only for the macro scale problem:

$$\forall v \in \mathcal{W}_h, \quad \int_{\mathcal{D}} (\nabla v(x))^T A_\eta^{\varepsilon, m}(x, \omega) \nabla u^m(x, \omega) dx = \int_{\mathcal{D}} f v.$$

## Numerical illustration ( $\varepsilon = 0.025$ , $\mathcal{D} = [0, 1]^2$ , $f = 1$ )

$$A_\eta^\varepsilon(x, y, \omega) = A_0^\varepsilon(x, y) + \eta \sum_{(k, \ell) \in \mathbb{Z}^2} \mathbf{1}_{(k, k+1]}(\frac{x}{\varepsilon}) \mathbf{1}_{(\ell, \ell+1]}(\frac{y}{\varepsilon}) X_{k, \ell}(\omega) A_0^\varepsilon(x, y)$$

where  $(X_{k, \ell})_{(k, \ell) \in \mathbb{Z}^2}$  are i.i.d. scalar random variables,  $X_{k, \ell} \sim \mathcal{U}[0, 1]$ , and  $A_0^\varepsilon(x, y)$  is a classical test case of the literature.

- We build the deterministic basis functions by locally solving  $-\operatorname{div}(A^\varepsilon(x) \nabla \phi_i^\varepsilon) = 0$ .
- For each realization  $A_\eta^{\varepsilon, m}(x, y, \omega)$ , solve for  $u^m(x, \omega) = \sum_i U_i^m(\omega) \phi_i^\varepsilon(x)$ .

Compare three functions:

- $u_{\text{ref}}$ : reference solution
- $u_M$ : approximation by the general MsFEM approach
- $u_{w-S}$ : approximation by the weakly-stochastic MsFEM approach

## Errors ( $u_M$ : general MsFEM; $u_{w-S}$ : weakly-stochastic MsFEM)

Relative error in % (here, with  $H^1$  norm; similar conclusion with  $L^2$  norm, although errors are 10 times smaller):

$\eta$	$e(u_M, u_{\text{ref}})$	$e(u_{w-S}, u_{\text{ref}})$	$e(u_{w-S}, u_M)$
1	$8.12 \pm 0.19$	$17.37 \pm 0.78$	$15.51 \pm 0.87$
0.1	$7.17 \pm 0.02$	$7.62 \pm 0.07$	$2.56 \pm 0.10$
0.01	$7.15 \pm 0.002$	$7.28 \pm 0.007$	$1.39 \pm 0.002$

- when  $\eta$  is small (here,  $\eta \leq 0.1$ ),  $u_{w-S}$  is an approximation of  $u_{\text{ref}}$  as accurate as  $u_M$ , and is obtained for a much smaller cost (the MsFEM basis has only been computed once!)
- as expected, when  $\eta$  is not small (say  $\eta \approx 1$ ), the accuracy of the solution  $u_{w-S}$  computed with the alternative approach proposed here decreases.

CLB, F. Legoll, F. Thomines,

<http://arxiv.org/abs/1110.5206> and [/1111.1524](http://arxiv.org/abs/1111.1524).

**“General” but “explicit” deterministic problems**

Joint work with X. Blanc, P.L. Lions.

What is the most general property that allows homogenization while keeping formulae explicit and staying deterministic?

Based on previous works (CPDE 2002, JMPA 2007, Milan Journal of Maths 2012) and ongoing works.

Consider a set of points  $\{X_i\}_{i \in \mathbf{N}}$  s.t.

$$(H1) \quad \sup_{x \in \mathbf{R}^3} \#\{i \in \mathbf{N} \mid |x - X_i| < 1\} < +\infty,$$

$$(H2) \quad \exists R_0 > 0, \inf_{x \in \mathbf{R}^3} \#\{i \in \mathbf{N}, |x - X_i| < R_0\} > 0,$$

(H3) the following limit exists in  $L^\infty(\mathbf{R}^n)$ :

$$\lim_{R \rightarrow \infty} \frac{1}{|B_R|} \#\left\{ (i_0, i_1, \dots, i_n) \in \mathbf{N}^{n+1}, \right. \\ \left. |X_{i_0}| \leq \delta_0 R, \quad |X_{i_0} - X_{i_1} - h_1| \leq \delta_1, \dots, |X_{i_0} - X_{i_n} - h_n| \leq \delta_n \right\}.$$

(H3) may also be written as follows: for any  $n \in \mathbb{N}$ , the following limit exists

$$\lim_{R \rightarrow \infty} \frac{1}{|B_R|} \sum_{X_{i_0} \in B_R} \cdots \sum_{X_{i_n} \in B_R} \delta_{(X_{i_0} - X_{i_1}, \dots, X_{i_0} - X_{i_n})}(h_1, \dots, h_n) = l^n(h_1, \dots, h_n),$$

and is a non-negative uniformly locally bounded measure.

Condition (H3) (originally designed for thermodynamic limit problems) has to be strengthened into [(H3')] for any  $n \in \mathbb{N}$ , the following limit exists

$$\lim_{\varepsilon \rightarrow 0} \mu^n \left( \frac{x}{\varepsilon}, h_1, \dots, h_n \right) = \nu^n(h_1, \dots, h_n),$$

where

$$\mu^n(y, h_1, \dots, h_n) = \sum_{i_0 \in \mathbb{Z}^d} \sum_{i_1 \in \mathbb{Z}^d} \cdots \sum_{i_n \in \mathbb{Z}^d} \delta_{(X_{i_0}, X_{i_0} - X_{i_1}, \dots, X_{i_0} - X_{i_n})}(y, h_1, h_2, \dots, h_n).$$

(H3') differs from (H3) in the sense it allows for averages on balls not only centered at 0 (or at a point bounded independently of the radius  $R$  of the ball) but also at all points  $|x_R| = O(R)$ .

(H3') allows to have a weak-\* limit of all rescaled functions of the algebra, which in addition is constant:

$$f \left( \frac{x}{\varepsilon} \right) \xrightarrow[\varepsilon \rightarrow 0]{*} \langle f \rangle.$$

Also, we may assume: (H3'') for any  $n \in \mathbb{N}$ , the following limit exists

$$\begin{aligned} \lim_{\varepsilon \rightarrow 0} \sum_{i_0 \in \mathbb{Z}^d} \sum_{i_1 \in \mathbb{Z}^d} \cdots \sum_{i_n \in \mathbb{Z}^d} \delta_{(X_{i_0}, X_{i_0} - X_{i_1}, \dots, X_{i_0} - X_{i_n})} \left( \frac{x}{\varepsilon}, h_1, h_2, \dots, h_n \right) \\ = \nu^n(x, h_1, \dots, h_n). \end{aligned}$$

which allows to have a non necessarily constant weak-\* limit of all rescaled functions of the algebra. E.g.,

$$\sum_{i_1 \in \mathbb{N}} \sum_{i_2 \in \mathbb{N}} \varphi \left( \frac{x}{\varepsilon} - X_{i_1}, \frac{x}{\varepsilon} - X_{i_2} \right) \rightharpoonup \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} \varphi(y, y + h_1) \nu^1(x, h_1) dy dh_1.$$

## Non stochastic problems

With  $\{X_i\}$  now defined, we introduce, for all  $\varphi \in \mathcal{D}(\mathbf{R}^{3n})$ , the functions (for  $\varphi \in \mathcal{D}(\mathbf{R}^{3n})$ )

$$f(x) = \sum_{i_1 \in \mathbf{N}} \cdots \sum_{i_n \in \mathbf{N}} \varphi(x - X_{i_1}, \dots, x - X_{i_n})$$

Assumptions (Hi) allow these functions to have averages

$$\langle f \rangle = \int_{\mathbf{R}^3} \int_{\mathbf{R}^{3(n-1)}} \varphi(x, x - h_1, \dots, x - h_{n-1}) dl^{n-1}(h_1, \dots, h_{n-1}) dx.$$

Definition: Set  $\mathcal{A}^{k,p}(\{X_i\})$  the closure, for  $\|\cdot\|_{W_{\text{unif}}^{k,p}}$ , of the vector space generated by

$$f(x) = \sum_{i_1 \in \mathbf{N}} \sum_{i_2 \in \mathbf{N}} \cdots \sum_{i_n \in \mathbf{N}} \varphi(x - X_{i_1}, x - X_{i_2}, \dots, x - X_{i_n}), \quad (1)$$

with  $\varphi \in \mathcal{D}(\mathbf{R}^{3n})$ . It is also the closure for the same norm of the algebra generated by the

$$f(x) = \sum_{i \in \mathbf{N}} \varphi(x - X_i), \quad \varphi \in \mathcal{D}(\mathbf{R}^3).$$

The question is homogenization for

$$-\operatorname{div} \left( a \left( \frac{x}{\varepsilon} \right) \nabla u^\varepsilon \right) = f,$$

where  $a$  is a function of the algebra, for instance

$$a(y) = 1 + \sum_{i \in \mathbf{N}} \varphi(x - X_i).$$

Homogenization does hold (because the case falls under the setting of, say, H-convergence). But the issue we examine is the existence of an explicit expression for the limit (thus the uniqueness, and the convergence without considering extractions).

A general theory by N'Guetseng covers (for (H3')) our setting, but the formulae are not sufficiently explicit (averages, etc...):

$$\forall v \in \mathcal{A}, \quad \langle A(\nabla w_p + p) \nabla v \rangle = 0,$$

$$a_{ij}^* = \langle a_{ij} + a_{ik} \partial_k w_{e_j} \rangle,$$

## Examples of sets $\{X_i\}$

Examples of sets  $\{X_i\}$ :

Compactly perturbed periodic systems:  $\{X_i\}_{i \in \mathbb{N}\mathbb{N}}$  is a periodic set, except for a finite number of points. For instance,  $\mathbf{Z}^3 \setminus \{0\}$ .

$$\mathcal{A}^p(\{X_i\}) = L_{\text{per}}^p(\mathbf{Z}^3) + L_0^p(\mathbf{R}^3), \quad (2)$$

where  $L_0^p(\mathbf{R}^3) = \{f \in L_{\text{loc}}^p(\mathbf{R}^3), \lim_{|x| \rightarrow \infty} \|f\|_{L^p(B+x)} = 0\}$ . The algebra consists of periodic functions up to local perturbations. Note that  $\langle |\cdot| \rangle$  is not a norm!

Two semi-crystals:

$$\mathcal{A}^p(\{X_i\}) = \left( L_{\text{per},1}^p((\mathbf{Z}^3)_-), L_{\text{per},2}^p((\mathbf{Z}^3)_+) \right) + L_0^p(\mathbf{R}^3).$$

Deformed periodic lattices:

Set  $X_i(\omega) = \Phi(i, \omega)$  where  $\Phi$  is a stationary diffeomorphism, and consider the associated algebra. Then  $A = B(\Phi^{-1})$  where  $B$  is stationary and we may apply the results of our theory.

## A motivation

$$-\frac{d}{dx} \left( (a_{per}(x/\varepsilon)) + b(x/\varepsilon) \frac{d}{dx} u_\varepsilon \right) = f$$

where  $b$  is a compact perturbation of the periodic function  $a_{per}$ . It homogenizes into  $-a^*(u^*)'' = f$  with  $a^* = a_{per}^* = (\langle a_{per}^{-1} \rangle)^{-1}$ . Using the corrector  $w'_{per}(y) = -1 + a_{per}^* (a_{per})^{-1}(y)$  solution to

$$-\frac{d}{dx} \left( a_{per}(y) \left( 1 + \frac{d}{dy} w_{per}(y) \right) \right) = 0$$

we note that (for  $F(x) = \int_0^x f$  and appropriate integration constants)

$$\begin{aligned} [u'_\varepsilon - (1 + w'_{per}(\cdot/\varepsilon)) (u^*)'] (x) &= (a_{per} + b)^{-1}(x/\varepsilon) (F(x) + c_\varepsilon) - (a_{per})^{-1}(x/\varepsilon) (F(x) + c^*) \\ &= \left[ (a_{per} + b)^{-1} - (a_{per})^{-1} \right] (x/\varepsilon) (F(x) + c_\varepsilon) \\ &\quad + (a_{per})^{-1}(x/\varepsilon) (c_\varepsilon - c^*) \end{aligned}$$

Consider  $\varepsilon x$  instead of  $x$  (that is, micro instead of macro scale), the r.h.s. does not vanish (because of the first term of the r.h.s.).

It however does in the perfect periodic case...

## A motivation

Consider now:

$$-\frac{d}{dy} \left( (a_{per} + b)(y) \left( 1 + \frac{d}{dy} w(y) \right) \right) = 0$$

that is  $w'(y) = -1 + a_{per}^* (a_{per} + b)^{-1}(y)$ , then:

$$[u'_\varepsilon - (1 + w'(\cdot/\varepsilon)) (u^*)'] (x) = (a_{per} + b)^{-1}(x/\varepsilon) (c_\varepsilon - c^*)$$

Bingo!

The "quality" of the approximation is identical to that obtained in the perfect periodic case: one can accurately approximate  $u^\varepsilon$  close to the defects.

## Example: periodic lattice with a defect

$1/\varepsilon$	$\delta_{per}^\varepsilon$	$\delta^\varepsilon$
3	0.198112	0.0850091
5	0.191952	0.0425306
10	0.183784	0.0266084
20	0.175248	0.0139564

Relative errors using the periodic corrector (left column) and the corrector adapted to the case with defect (right column).

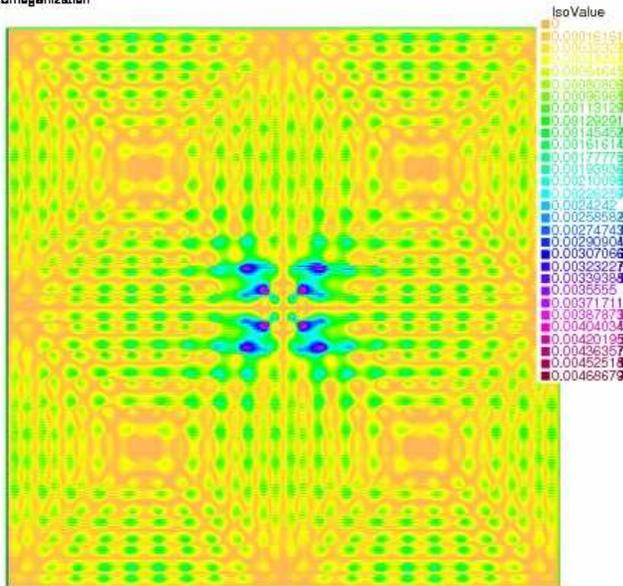
$$\delta_{per}^\varepsilon = \frac{\left\| \nabla u^\varepsilon (\varepsilon \cdot) - \nabla u_{per}^{\varepsilon,1} (\varepsilon \cdot) \right\|_{L^2(\Omega)}}{\left\| \nabla u^\varepsilon (\varepsilon \cdot) \right\|_{L^2(\Omega)}}, \quad \delta^\varepsilon = \frac{\left\| \nabla u^\varepsilon (\varepsilon \cdot) - \nabla u^{\varepsilon,1} (\varepsilon \cdot) \right\|_{L^2(\Omega)}}{\left\| \nabla u^\varepsilon (\varepsilon \cdot) \right\|_{L^2(\Omega)}}.$$

$$-\operatorname{div} ((a_{per}(x/\varepsilon) + b(x/\varepsilon)) \nabla u_\varepsilon) = f.$$

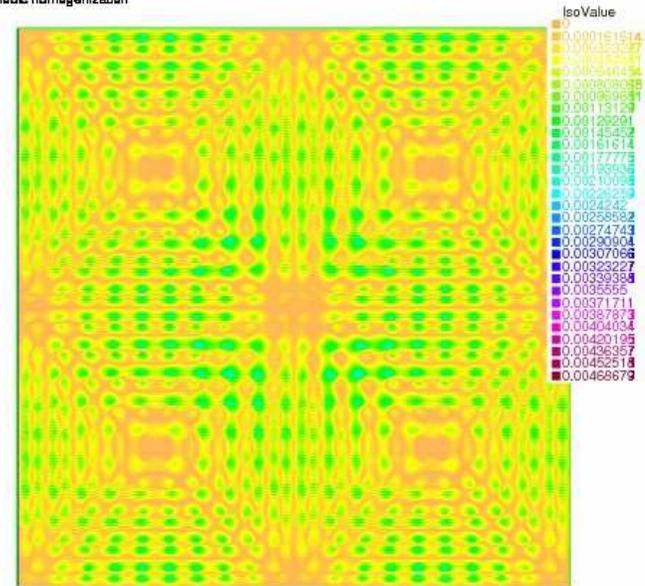
$$-\operatorname{div} ((a_{per}(y) + b(y)) (p + \nabla w_p)) = 0$$

# Ongoing work

Periodic homogenization



Non periodic homogenization



Blanc/LB/Lions, Milan Journal of Maths (in press), and in preparation.

Objective: Generalize this to other specific cases, to the general case, in one dimension and in dimensions higher than one.

Current difficulty (work in progress – Blanc-LB-Lions–): show that the corrector problem is well posed in the algebra, that is, if  $a \in \mathcal{A}$  then the corrector problem

$$-\operatorname{div} (a(y) (p + \nabla w_p)) = 0$$

is uniquely solvable for  $\nabla w_p \in \mathcal{A}$  and  $\langle \nabla w_p \rangle = 0$ .

**Passage from Atomistic to Continuum for non periodic materials**

Joint work with X. Blanc, PL. Lions.

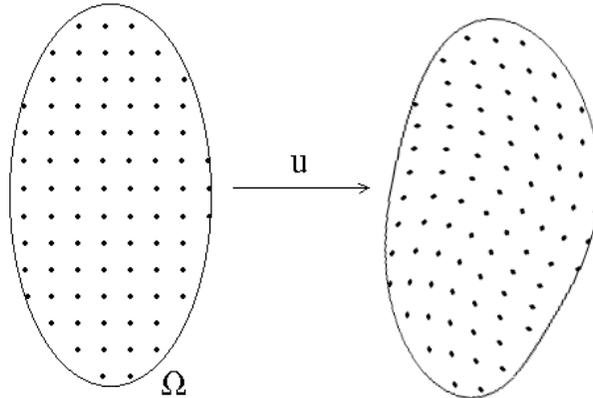
Understand the passage from the atomistic scale to the continuum scale when the microstructure of the material has some random character.

Extend the theory essentially based on the periodic setting to the random (ergodic stationary) case.

Series of joint works with X. Blanc and P-L. Lions.

- **From molecular models to continuum mechanics**, Archive for Rational Mechanics and Analysis, 2002.
- **Discrete to continuum limit for some models of stochastic lattices of atoms**, Note aux Comptes Rendus de l'Académie des Sciences, 2006.
- **The energy of some microscopic stochastic lattices**, Archive for Rational Mechanics and Analysis, 2007.
- **Stochastic homogenization and random lattices**, Journal de Mathématiques Pures et Appliquées, 2007

# Change of scales in crystalline materials



- At the atomic scale, the energy is defined through a (possibly quantum) model  $\mathcal{E}_\mu = \mathcal{E}_\mu(\{X_i\})$ , where  $\{X_i\}_{1 \leq i \leq N}$  denote the positions of atoms .
- At the macroscale, the energy is given by a density of mechanical energy  $\mathcal{E}_M(u) = \int_\Omega F(u)(x) dx$  where  $u$  denotes the deformation.

## *With a view to defining macroscopic energies from microscale*

We first perform a limiting process for a **periodic** arrangement of sites, and then we ask ourselves

What is the most general geometrical property that allows for such a change of scale ?

In fact, also:

- what is the most general geometrical property of an infinite set of particles that allows for the **definition of the energy** per unit particle?
- what is the most general property of functions that allows for **homogenization theory** to apply?

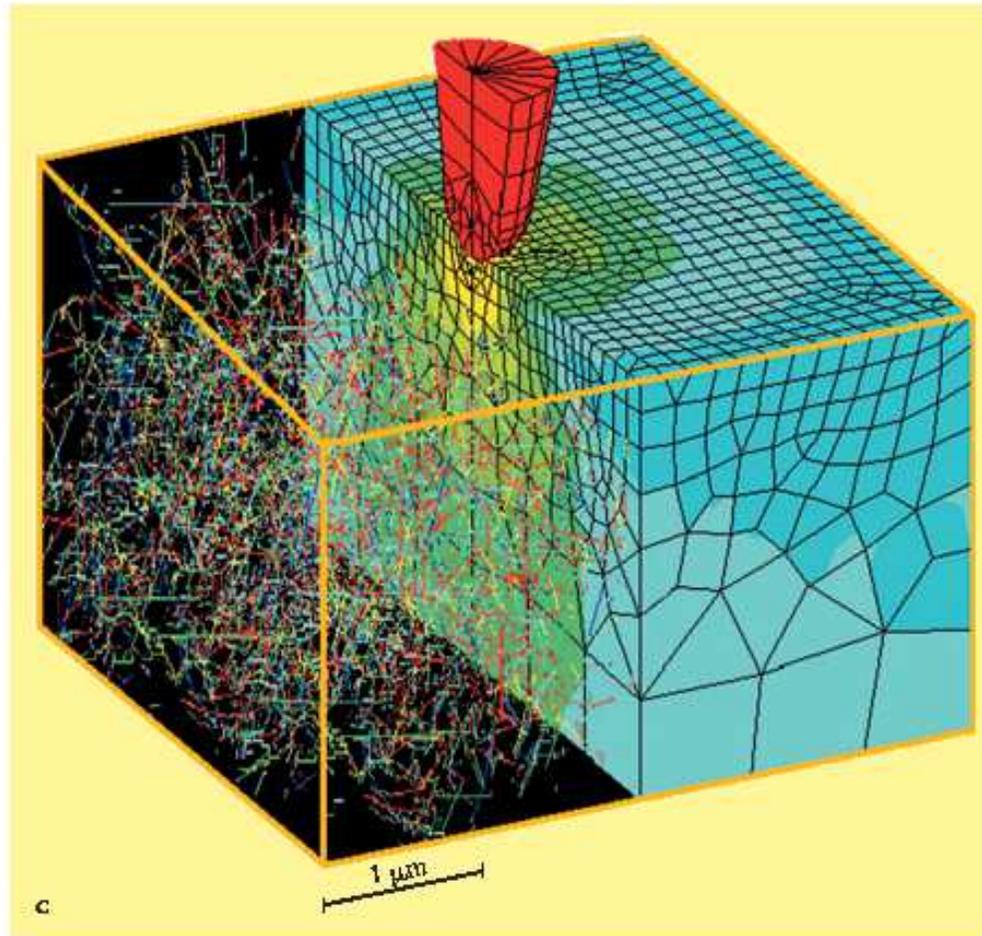
Assumptions :

- ▶ The atoms are **periodically** arranged (or ...):  $\{X_i^0\}_{1 \leq i \leq N} = \varepsilon \mathbf{Z}^3 \cap \Omega$ .
- ▶ The deformation is mapped from the macro onto the microscale :  $X_i = u(X_i^0)$ . (variants with Gamma-limit techniques, other authors)

$$\mathcal{E}_\mu^\varepsilon(u) = \frac{1}{N} \mathcal{E}_\mu \left( u(\varepsilon \mathbf{Z}^3 \cap \Omega) \right) \xrightarrow{\varepsilon \rightarrow 0} \mathcal{E}_M(u) \quad ?$$

Another viewpoint yielding the same question : practical computation of

$$\sum_{i=1}^{10^{23}} \sum_{j=1}^{10^{23}} V(X_i - X_j)$$



Nanoindentation simulation, **Courtesy Marc Fivel (INPG).**

We do this in two steps

► **First step** : go from a molecule (finite number of particles) to a crystal (infinitely many particles)

**“Thermodynamic limit problem”** : take  $I_N$  the energy of a molecule of size  $N$ ,  $\rho_N$  the ground state; let  $N$  go to infinity as the nuclei fill a periodic infinite lattice, does  $\frac{I_N}{N}$  converge ? to  $I_{per}$  a minimization problem on the unit cell ? does  $\rho_N$  converge ? to the minimizing  $\rho_{per}$  ?

► **Second step**: let the micro size go to zero, and reach the continuum

**“Change of scale”** can we deduce the functional  $F$  in  $\int_{\Omega} F(\nabla u(x))dx$  from the one  $\mathcal{E}_{\mu}$  at the atomic scale ?

## Step 1: thermodynamic limit

- ▶ Two-body potentials :

$$\mathcal{E}_\mu(\{X_i\}) = \frac{1}{2} \sum_{i \neq j} V(X_i - X_j), \quad \left( W_0(x) = \frac{1}{|x|^{12}} - \frac{1}{|x|^6} \right),$$

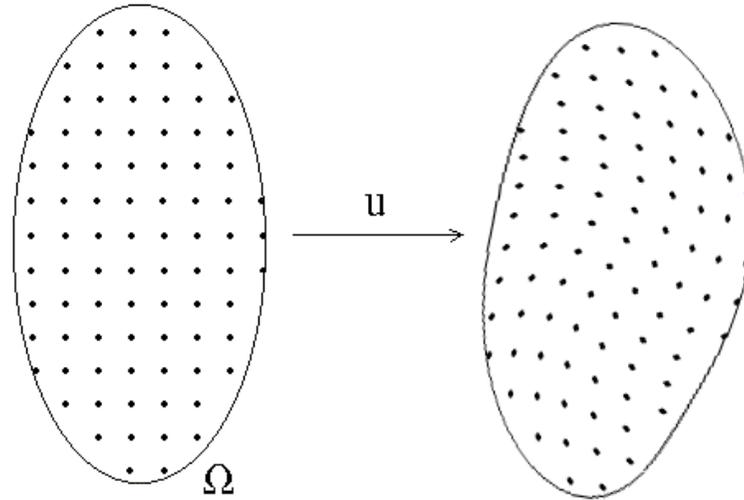
In the limit where  $\{X_i\} \longrightarrow \mathbb{Z}^3$ ,

$$\frac{1}{N} \mathcal{E}_\mu(\{X_i\}) \longrightarrow \frac{1}{2} \sum_{X_i \neq 0 \in \mathbb{Z}^3} V(X_i)$$

- ▶ Other classical interactions, Quantum models

## Step 2: Change of scale

Now, we change the scale... (Blanc/LB/Lions, ARMA, 2002)



$$\inf \left\{ \int_{\Omega} F(u)(x) dx - \int_{\Omega} f u - \int_{\partial\Omega} g u \mid u \text{ satisfies b.c.} \right\},$$

Two-body potential:

$$\frac{1}{2N^3} \sum_{\bar{x}_i \in \mathcal{D} \cap \mathbb{Z}^3} \sum_{\bar{x}_j \neq \bar{x}_i \in \mathcal{D} \cap \mathbb{Z}^3} V\left(\frac{u(\frac{\bar{x}_i}{N}) - u(\frac{\bar{x}_j}{N})}{\frac{1}{N}}\right).$$

Notice that

$$\frac{u(\frac{\bar{x}_i}{N}) - u(\frac{\bar{x}_j}{N})}{\frac{1}{N}} = N(u(\frac{\bar{x}_i}{N}) - u(\frac{\bar{x}_j}{N})) \approx \nabla u(\frac{\bar{x}_j}{N}) \cdot (\bar{x}_i - \bar{x}_j) = \nabla u(\frac{\bar{x}_j}{N}) \cdot (\bar{x}_k)$$

and denote by

$$\Psi(x) = \frac{1}{2} \sum_{\bar{x}_k \neq 0 \in \mathbb{Z}^3} V(\nabla u(x) \cdot \bar{x}_k),$$

Next observe that this is of the form

$$\lim_{\text{card}\{y_j\} \rightarrow +\infty} \frac{1}{\text{card}\{y_j\}} \sum_{y_j} \Psi(y_j),$$

where the points  $y_j$  form a grid in a unit volume, and thus is a Riemann sum, that converges as  $N \rightarrow +\infty$  to

$$\frac{1}{2} \int_{\mathcal{D}} \sum_{\overline{x}_k \neq 0 \in \mathbb{Z}^3} V(\nabla u(x) \cdot \overline{x}_k) dx$$

At the macroscopic level, our density of mechanical energy therefore reads

$$W(\nabla u(x)) = \frac{1}{2} \sum_{\overline{x}_k \neq 0 \in \mathbb{Z}^3} V(\nabla u(x) \cdot \overline{x}_k)$$

## Beyond the periodic setting: stochastic lattices

A notion of **stationary ergodic stochastic lattices** On the probability space  $(\Omega, \mathcal{F}, \mathbb{P})$ , we consider a random variable  $\ell$  valued in  $(\mathbb{R}^d)^{\mathbb{Z}^d}$  :

$$\begin{aligned} \ell : \Omega &\longrightarrow (\mathbb{R}^d)^{\mathbb{Z}^d} \\ \omega &\longmapsto \ell(\omega) = \{\overline{x}_i, i \in \mathbb{Z}^d\}. \end{aligned}$$

and a group action  $(\tau_k)_{k \in \mathbb{Z}^d}$  on  $\Omega$ , that preserves  $\mathbb{P}$ , and that is assumed ergodic:

$$\left( \tau_k A = A, \forall k \in \mathbb{Z}^d \right) \text{ implies } \mathbb{P}(A) = 0 \text{ or } 1.$$

The lattice  $\ell$  is said a *stationary ergodic stochastic lattice* if

$$\ell(\tau_k \omega) = \ell(\omega) - k, \quad \forall k \in \mathbb{Z}^d.$$

(Blanc/LB/Lions, ARMA, 2006)

Three simple examples of such lattices are:

a) a periodic lattice

$$\ell(\omega) = \{k, \quad k \in \mathbb{Z}^d\},$$

b) a perturbation of a periodic lattice

$$\ell(\omega) = \{k + X_k(\omega), \quad k \in \mathbb{Z}^d\}$$

by independent identically distributed random variables  $X_k(\omega)$   
and c) the same perturbation but by stationary random variables

$$X_k(\omega) = X_0(\tau_k \omega),$$

## Beyond the periodic setting: stochastic lattices

$$\frac{1}{\#(\ell(\omega) \cap \mathcal{D})} \sum_{\bar{x}_i \in \ell(\omega) \cap N\mathcal{D}} \sum_{\bar{x}_j \in (\ell(\omega) \cap N\mathcal{D}) \setminus \{\bar{x}_i\}} V \left( \frac{u(\frac{\bar{x}_i}{N}) - u(\frac{\bar{x}_j}{N})}{1/N} \right)$$

is approximately

$$\frac{1}{\#(\ell(\omega) \cap \mathcal{D})} \sum_{\bar{x}_i \in \ell(\omega) \cap N\mathcal{D}} \sum_{\bar{x}_j \in (\ell(\omega) \cap N\mathcal{D}) \setminus \{\bar{x}_i\}} V \left( \nabla u \left( \frac{\bar{x}_i}{N} \right) (\bar{x}_i - \bar{x}_j) \right)$$

and thus converges almost surely (by the ergodic theorem) to

$$\frac{1}{2\mathbb{E}(\#(\ell(\omega) \cap Q))} \frac{1}{|\mathcal{D}|} \int_{\mathcal{D}} \mathbb{E} \left( \sum_{\bar{x}_i \in \ell(\omega) \cap Q} \sum_{\bar{x}_j \in \ell(\omega) \setminus \{\bar{x}_i\}} V(\nabla u(x)(\bar{x}_i - \bar{x}_j)) \right) dx,$$

where  $Q = [0, 1[{}^d$ .

## Beyond the periodic setting: stochastic lattices

Pedagogic illustration : assume  $\ell(\omega)$  is an i.i.d. perturbation of a periodic lattice, that is

$$\bar{x}_i(\omega) = i + X_i(\omega),$$

with  $X_i(\omega)$  i.i.d.

Then

$$\begin{aligned} \frac{u\left(\frac{i+X_i(\omega)}{N}\right) - u\left(\frac{j+X_j(\omega)}{N}\right)}{1/N} &\approx \nabla u\left(\frac{j+X_j(\omega)}{N}\right)(i-j+X_i(\omega)-X_j(\omega)) \\ &= \nabla u\left(\frac{j+X_j(\omega)}{N}\right)(k+X_{j+k}(\omega)-X_j(\omega)) \\ &\approx \nabla u\left(\frac{j}{N}\right)(k+X_{j+k}(\omega)-X_j(\omega)) \end{aligned}$$

## Beyond the periodic setting: stochastic lattices

Thus we have

$$\sum_{i,j} V \left( \frac{u\left(\frac{i+X_i(\omega)}{N}\right) - u\left(\frac{j+X_j(\omega)}{N}\right)}{1/N} \right) \approx \sum_j \sum_k V \left( \nabla u\left(\frac{j}{N}\right) (k + X_{j+k}(\omega) - X_j(\omega)) \right)$$

which, once renormalized, converges (**Riemann sum** and **Strong law of large numbers**) to

$$\int \mathbb{E} \left( \sum_k V (\nabla u(\mathbf{x})(k + X_k(\omega) - X_0(\omega))) \right) d\mathbf{x}$$

Rk: further simplification : NN model in 1-d

$$\frac{1}{N} \sum_j V \left( \nabla u\left(\frac{j}{N}\right) (1 + X_{j+1}(\omega) - X_j(\omega)) \right) \longrightarrow \int \mathbb{E} (V (\nabla u(\mathbf{x})(1 + X_1(\omega) - X_0(\omega)))) d\mathbf{x}$$

The arguments and results carry over to the case of

- other interaction potentials
- quantum models
- abstract stochastic setting (measure defining the lattice)
- lattice with stationary increments

$$\Phi : \mathbb{R}^3 \longrightarrow \mathbb{R}^3, \quad \Phi(x + k, \omega) = \Phi(x, \tau_k \omega) + \Phi(k, \omega)$$

Plus many relations with general deterministic settings (see Blanc/LB/Lions, CPDE 2003)

Formally differentiate w.r.t.  $x$ :

$$\nabla_x \Phi(x + k, \omega) = \nabla_x \Phi(x, \tau_k \omega)$$

and find our assumptions for homogenization!

The macroscopic properties of crystals are often directly related to the presence of defects

- Mechanical behavior: e.g. dislocation and plasticity
- Electronic/optical properties: e.g. impurities and conductivity/color

The electronic structure of crystals is difficult to model for crystals contain an infinite number of electrons

Recent progress have been accomplished in the modelling on crystals in the framework of the Density Functional Theory (DFT)

- Catto, CLB and Lions (1998-2001): thermodynamic limit for perfect crystals
- Cancès, Deleurence and Lewin (2008-): crystals with local defects
- E and Lu (2010-): smoothly deformed crystals

Within DFT, electronic states are described by density matrices

- For finite systems (molecules and clusters), the ground state density matrix  $\gamma$  is a self-adjoint trace-class operator on  $L^2(\mathbb{R}^3)$

$$\rho_\gamma(x) := \gamma(x, x) \text{ electronic density,} \quad \text{Tr}(\gamma) = \int_{\mathbb{R}^3} \rho_\gamma = \text{number of electrons}$$

- For perfect crystals, the ground state density matrix  $\gamma_{\text{per}}$  is an infinite-rank orthogonal projector on  $L^2(\mathbb{R}^3)$  which commutes with the translations of the lattice; it can be computed using Bloch-Floquet theory
- For crystals with local defects,  $\gamma = \gamma_{\text{per}} + Q$ . As a consequence of the **long-range of the Coulomb interaction**, the operator  $Q$  is not trace-class in general but nevertheless possesses a density  $\rho_Q$  and a generalized trace  $\text{Tr}_0(Q)$

$$\text{"bare" charge of the defect} = \text{Tr}_0(Q) \neq \int_{\mathbb{R}^3} \rho_Q = \text{"renormalized" charge}$$

Macroscopic counterpart: **dielectric permittivity** of the host crystal

**Passage from the Newton equation to the wave equation**

Joint work with X. Blanc, P.L. Lions.

We prove that, in some simple situations at least, the one-dimensional wave equation is the limit as the microscopic scale goes to zero of some time-dependent Newton type equation of motion for atomistic systems.

We address both some linear and some nonlinear cases.

Follow-up on our work on similar issues in the static setting (see ARMA 2002 and other publications)

**We emphasize we work in 1D, on simple cases!**

Berezhnyy/Berlyand, E/Ming, Ortner/Theil (2012).

$$\frac{d^2 X_i}{dt^2} = - \sum_{j \neq i} \nabla V(i - j + X_i - X_j)$$

Assuming that  $X_i(t) = N\phi\left(\frac{i}{N}, \frac{t}{N}\right)$  and considering a macroscopic time  $\tau = t/N$ ,

$$\frac{1}{N} \frac{\partial^2 \phi}{\partial \tau^2} \left( \frac{i}{N}, \frac{t}{N} \right) = - \sum_{j \neq i} \nabla V \left[ i - j + N \left( \phi \left( \frac{i}{N}, \frac{t}{N} \right) - \phi \left( \frac{j}{N}, \frac{t}{N} \right) \right) \right].$$

As  $N \rightarrow \infty$ , we remark

$$N \left( \phi \left( \frac{i}{N}, \frac{t}{N} \right) - \phi \left( \frac{j}{N}, \frac{t}{N} \right) \right) \approx \nabla \phi \left( \frac{i}{N}, \frac{t}{N} \right) \cdot (i - j) - \frac{1}{N} D^2 \phi \left( \frac{i}{N}, \frac{t}{N} \right) (i - j, i - j).$$

Assuming that  $i/N \rightarrow x$ , a fixed macroscopic point, we obtain

$$\frac{\partial^2 \phi}{\partial \tau^2} (x, \tau) - \div [D_A E(\nabla \phi)] = 0,$$

where

$$E(A) = \sum_{k \in \mathbb{Z}^d \setminus \{0\}} V(k + Ak),$$

## Simplest possible case: NN

$$\frac{d^2 X_i}{dt^2} = -V'(1 + X_i - X_{i+1}) - V'(1 + X_i - X_{i-1})$$

with the convention that  $X_0 = 0$ ,  $X_{N+1} = 0$ , Convergence to

$$\frac{\partial^2 \phi}{\partial \tau^2}(x, \tau) - \frac{\partial}{\partial x} \left[ V' \left( 1 + \frac{\partial \phi}{\partial x}(x, \tau) \right) \right] = 0.$$

The linear wave equation is obtained for the specific interaction potential  $V(x) = \frac{1}{2}(x - 1)^2$ .

Easy for linear, or nonlinear convex. What about nonlinear nonconvex?

## Proposition

Let  $(\phi^0, \phi^1) \in [H^4(0, 1)]^2$  be such that  $\phi^0(0) = 0$  and  $\phi^0(1) = 1$ . Define, for all  $N \in \mathbb{N}$ , and for all  $1 \leq i \leq N$ ,

$$X_i^0 = N\phi^0\left(\frac{i}{N}\right), \quad V_i^0 = \phi^1\left(\frac{i}{N}\right).$$

Let  $X_i(t)$  be the unique solution to the NN-linear Newton equation, with the convention  $X_0 = 0$ ,  $X_{N+1} = 0$ , and let  $\phi \in L^\infty(\mathbb{R}^+, H^1(0, 1))$  be the unique solution of linear-NN wave equation. Then, we have the convergences

$$\forall \tau > 0, \quad \sup_{1 \leq i \leq N} \left| \frac{1}{N} X_i(N\tau) - \phi\left(\frac{i}{N}, \tau\right) \right| \xrightarrow{N \rightarrow \infty} 0,$$

and

$$\forall \tau > 0, \quad \left[ \sup_{1 \leq i \leq N} \left| \frac{dX_i}{dt}(N\tau) - \frac{\partial \phi}{\partial \tau}\left(\frac{i}{N}, \tau\right) \right| \right] \xrightarrow{N \rightarrow \infty} 0.$$

Proving the result amounts to proving convergence of a finite difference scheme.

For a function  $\Phi$ , we denote by

$$D_\varepsilon \Phi(x) = \varepsilon^{-1}(\Phi(x + \varepsilon/2) - \Phi(x - \varepsilon/2)),$$

where, of course,  $\varepsilon$  plays the role of  $1/N$ . This discrete differentiation can be iterated:

$$D_\varepsilon^2 \Phi = \varepsilon^{-2}(\Phi(x + \varepsilon) - 2\Phi(x) + \Phi(x - \varepsilon)).$$

Using this notation, proving (after renormalization in time) the convergence of the solution to the Newton equation to the solution to the wave equation basically amounts to proving (if we omit the truncation error terms) that the solution  $\Phi_\varepsilon$  to

$$\frac{\partial^2 \Phi_\varepsilon}{\partial t^2} - D_\varepsilon^2 \Phi_\varepsilon = 0,$$

with suitable (vanishing) initial and boundary conditions, vanishes with  $\varepsilon$ . This is an immediate consequence of the fact that  $\Phi_\varepsilon$  satisfies the energy equality

$$\frac{d}{dt} \left( \left\| \frac{\partial}{\partial t} \Phi_\varepsilon \right\|^2 + \|D_\varepsilon \Phi_\varepsilon\|^2 \right) = 0.$$

## Nonlinear but convex: easy!

Same NN case, but now with a non necessarily quadratic but convex potential:

The main idea of the proof is to introduce the following energy

$$E_i(\tau) = V(1 + X_{i+1}(N\tau) - X_i(N\tau)) - V \left[ 1 + N\phi \left( \frac{i+1}{N}, \tau \right) - N\phi \left( \frac{i}{N}, \tau \right) \right] \\ - NV' \left[ 1 + N\phi \left( \frac{i+1}{N}, \tau \right) - N\phi \left( \frac{i}{N}, \tau \right) \right] (\delta_{i+1} - \delta_i), \quad (3)$$

where the presence of the last term, the first order derivative, basically allows to proceed as *if* the potential  $V$  were quadratic, and therefore reduces the proof, up to technicalities, to the proof performed for the linear case in the previous slide.

## First non immediate case: linear NNN nonconvex

$$\frac{d^2 X_i}{dt^2} = c_1(X_{i+1} - 2X_i + X_{i-1}) + c_2(X_{i+2} - 2X_i + X_{i-2})$$

with "only"  $c_1 + 4c_2 > 0$  and not the trivial case ( $c_1 > 0, c_2 > 0$ ).

The limit expected (and indeed proven) reads:

$$\frac{\partial^2 \phi}{\partial \tau^2}(x, \tau) - (c_1 + 4c_2) \frac{\partial^2 \phi}{\partial x^2}(x, \tau) = 0,$$

which, precisely since  $c_1 + 4c_2 > 0$ , is well-posed.

$$\frac{\partial^2 \Phi_\varepsilon}{\partial t^2} - c_1 D_\varepsilon^2 \Phi_\varepsilon - 4 c_2 D_{2\varepsilon}^2 \Phi_\varepsilon = 0,$$

Elementary manipulations yields the energy estimate

$$\frac{d}{dt} \left( \left\| \frac{\partial}{\partial t} \Phi_\varepsilon \right\|^2 + c_1 \|D_\varepsilon \Phi_\varepsilon\|^2 + 4 c_2 \|D_{2\varepsilon} \Phi_\varepsilon\|^2 \right) = 0.$$

When both  $c_1$  and  $c_2$  are nonnegative, we immediately observe (cf. above) that this imposes that  $\Phi_\varepsilon$  vanishes in the limit. Use now:

$$4 D_\varepsilon^2 \Phi = 4 D_{2\varepsilon}^2 \Phi - \varepsilon^2 D_\varepsilon^4 \Phi.$$

and rewrite Eqn as

$$\frac{\partial^2 \Phi_\varepsilon}{\partial t^2} - (c_1 + 4c_2) D_\varepsilon^2 \Phi_\varepsilon + c_2 \varepsilon^2 D_\varepsilon^4 \Phi_\varepsilon = 0.$$

The corresponding energy estimate reads

$$\frac{d}{dt} \left( \left\| \frac{\partial}{\partial t} \Phi_\varepsilon \right\|^2 + (c_1 + 4c_2) \|D_\varepsilon \Phi_\varepsilon\|^2 - c_2 \varepsilon^2 \|D_\varepsilon^2 \Phi_\varepsilon\|^2 \right) = 0.$$

## Linear NNN nonconvex (ct'd)

We readily observe that if  $c_1 + 4c_2 > 0$  and  $c_2 \leq 0$  we again “formally” obtain convergence.

This can be easily formalized rigorously. The only interesting case is thus the case  $c_1 + 4c_2 > 0$  and  $c_2 \leq 0$ .

Proof 1: use spectral decomposition of  $(c_1 + 4c_2)D_\varepsilon^2 + c_2\varepsilon^2 D_\varepsilon^4$ . **Difficulty: no generality, because it exploits too much the simple form of the operator (and the fact it has constant coefficients).**

Proof 2: Proof by "weak convergence + energy conservation". **Interest: transferable!**

## Proof by weak convergence

$$\frac{\partial^2 \Phi_\varepsilon}{\partial t^2} - (c_1 + 4c_2) D_\varepsilon^2 \Phi_\varepsilon + c_2 \varepsilon^2 D_\varepsilon^4 \Phi_\varepsilon = 0.$$

Energy estimate:

$$\frac{d}{dt} \left( \left\| \frac{\partial}{\partial t} \Phi_\varepsilon \right\|^2 + (c_1 + 4c_2) \|D_\varepsilon \Phi_\varepsilon\|^2 - c_2 \varepsilon^2 \|D_\varepsilon^2 \Phi_\varepsilon\|^2 \right) = 0.$$

Differentiate  $k$  times the equation and obtain a similar energy estimate

$$\frac{d}{dt} \left( \left\| D_\varepsilon^k \frac{\partial}{\partial t} \Phi_\varepsilon \right\|^2 + (c_1 + 4c_2) \|D_\varepsilon^{k+1} \Phi_\varepsilon\|^2 - c_2 \varepsilon^2 \|D_\varepsilon^{k+2} \Phi_\varepsilon\|^2 \right) = 0.$$

for each differentiation order  $k$ . In order to “eliminate” the nonpositive contribution of the last term, we now weight and combine all these estimates so as to obtain

$$\frac{d}{dt} \sum_{k=1}^{+\infty} \delta^{2k} \left( \left\| D_\varepsilon^k \frac{\partial}{\partial t} \Phi_\varepsilon \right\|^2 + (c_1 + 4c_2) \|D_\varepsilon^{k+1} \Phi_\varepsilon\|^2 - c_2 \varepsilon^2 \|D_\varepsilon^{k+2} \Phi_\varepsilon\|^2 \right) = 0.$$

for some parameter  $\delta$ .

## *Proof by weak convergence (ct'd)*

This parameter  $\delta$  is next adjusted, in function of  $\varepsilon$ , so as to cancel the series of the two right-most terms by making it a telescopic series. We therefore conclude that some norm of the form

$$\sum_{k=1}^{+\infty} \delta^{2k} \left\| D_{\varepsilon}^{k+1} \Phi_{\varepsilon} \right\|^2$$

remains bounded over time.

Up to an extraction, we may assume  $\Phi_{\varepsilon}$  is weakly convergent, and it remains to deduce that the convergence is strong.

This will be a consequence of the preservation of the energy by the equation, and the fact that strong convergence holds at initial time.

## Difficult nonlinear cases: linearized regimes

We introduce a parameter  $\gamma \in (0, 1)$  and modify the (say NN) Newton equation as follows:

$$\frac{d^2 X_i}{dt^2} = N^\gamma \left[ V' \left( 1 + \frac{X_{i+1} - X_i}{N^\gamma} \right) - V' \left( 1 + \frac{X_i - X_{i-1}}{N^\gamma} \right) \right]$$

Then we can prove that the corresponding limit is

$$\frac{\partial^2 \phi}{\partial \tau^2}(x, \tau) - V''(1) \frac{\partial^2 \phi}{\partial x^2}(x, \tau) = 0$$

Likewise in the NNN case...

**Remark: We have no clue on the nonlinear nonconvex non-linearized case.**

Formal idea:

$$\frac{\partial^2 \Phi_\varepsilon}{\partial t^2} - \varepsilon^{\gamma-1} D_\varepsilon \nabla V(\varepsilon^{1-\gamma} D_\varepsilon \Phi_\varepsilon) = 0,$$

When  $\gamma \in (0, 1)$ , we observe that, still formally,  $\Phi_\varepsilon$  converges to the solution  $\Phi$  to

$$\frac{\partial^2 \Phi}{\partial t^2} - \nabla V(0).D^2 \Phi = 0.$$

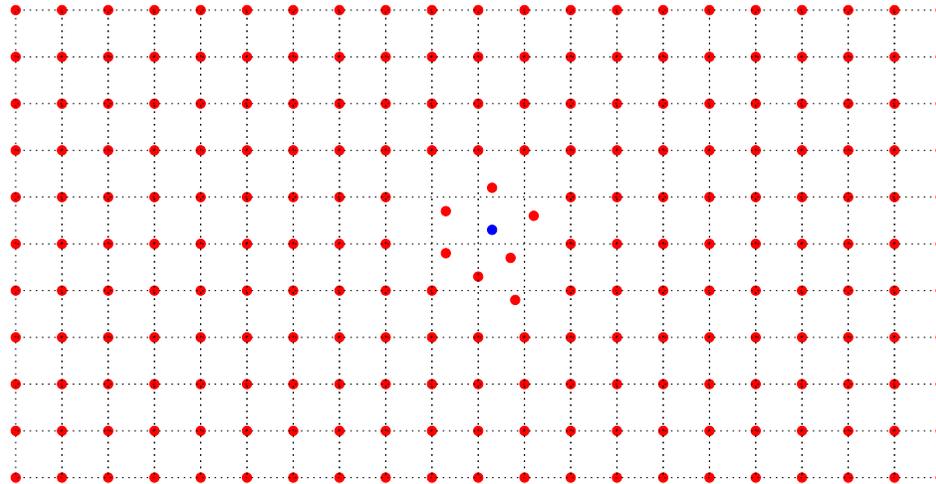
Proof using our "weak convergence + energy conservation" technique.

It is beyond our reach, without assuming convexity and thus simply using weak convergence arguments, to determine the limit of a term like  $D_\varepsilon \nabla V(D_\varepsilon \Phi_\varepsilon)$  unless  $\nabla V$  is linear. This explains why, in the present state of our understanding, we need to resort to the specific normalization using  $\gamma \in (0, 1)$ .

Blanc/LB/Lions, *From the Newton equation to the wave equation in some simple cases*, Networks and Heterogeneous Media, Vol. 7, N. 1, 2012, pp 1-41.

## Future research directions

- time-dependent models (TDDFT, random phase approximation)
- optimal control of electronic wave packets
- defects on surfaces, extended defects (dislocations, junctions)
- nuclear relaxation, positive temperature, electron-phonon interactions
- interaction between defects, **stochastic distributions of defects**
- excited states



<http://www-rocq.inria.fr/MICMAC/>



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