Méthodes de réduction de variance en homogénéisation aléatoire

Frédéric Legoll

ENPC et INRIA

En collaboration avec W. Minvielle (ENPC et INRIA)

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Setting

Homogenization of random materials often leads to very expensive computations, and thus many practical difficulties.

Simplify the situation from the theoretical viewpoint: consider the simple scalar linear PDE

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

Thermal diffusion, ...

Outline of the talk

- Some background materials on random homogenization

- Variance reduction by the control variate approach (generalities)
- A weakly stochastic model (rare defects) due to A. Anantharaman and C. Le Bris
- Use this model to build a surrogate model and design a control variate approach to reduce the variance

In a nutshell: use a weakly stochastic model to improve efficiency for fully stochastic cases.

Random homogenization

Homogenization 1.0.1: the periodic setting

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

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When $\varepsilon \to 0$, u^ε converges to $u^\star$ solution to

$$-\text{div}\left[A^\star \nabla u^\star\right] = f \ \text{ in } \mathcal{D}, \qquad u^\star = 0 \ \text{ on } \partial\mathcal{D}.$$

The effective matrix $A^\star$ is given by

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

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

$$-\text{div}\left[A_{\rm per}(y)\left(p + \nabla w_p\right)\right] = 0, \qquad w_p \text{ is } \mathbb{Z}^d\text{-periodic.}$$

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$\rightarrow$ The corrector problem is set on the bounded domain Q: easy!

Stochastic homogenization: setting

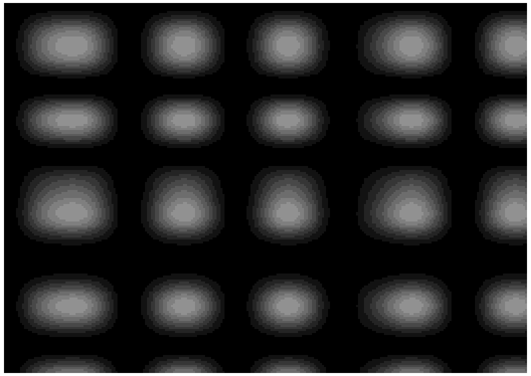
We consider statistically homogeneous random materials:

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

The tensor $A(x,\omega)$ is such that, for any $k \in \mathbb{Z}^d$,

$A(x,\omega)$ and $A(x+k,\omega)$ share the same probability distribution.

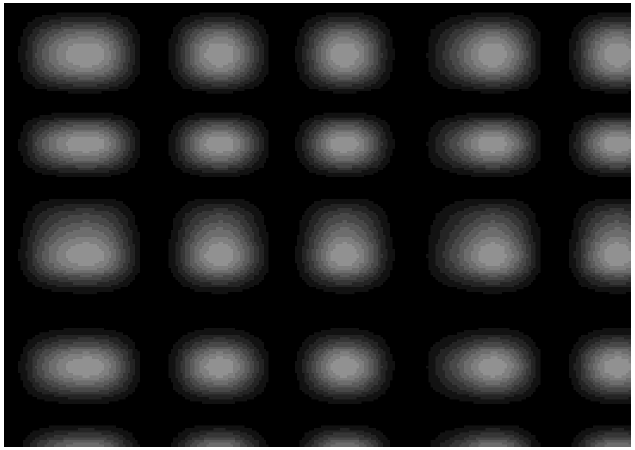
For a given realization of the randomness, properties may be different.
But, on average, they are identical: the material is statistically homogeneous (and $\mathbb{E}\left[A(x,\cdot)\right]$ is $\mathbb{Z}^d$ periodic).



There is some order in the randomness.

Stochastic homogenization: a typical example

$A(x, \omega)$ and $A(x+k, \omega)$ share the same probability distribution.



A typical example of statistically homogeneous function:

$$A(x, \omega) = \sum_{k \in \mathbb{Z}^d} 1_{Q+k}(x) \; B_{\rm per}(x) \; X_k(\omega), \qquad Q = (0,1)^d,$$

where X_k are i.i.d. random variables and $B_{\rm per}$ is $\mathbb{Z}^d$ periodic.

Formalization

Structure on the probability space $(\Omega, \mathcal{F}, \mathbb{P})$:

- there exists a group action $(\tau_k)_{k \in \mathbb{Z}^d}$ on Ω, that preserves the probability measure:

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

- the action τ is ergodic: for any $B \in \mathcal{F}$,

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

A function F is statistically homogeneous (or stationary) if

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

If F does not depend on ω, recover the periodic case.

Averaging theorems

- Periodic case: for any $F_{\rm per} \in L^\infty\left(\mathbb{R}^d\right)$ that is $\mathbb{Z}^d$-periodic,

$$F_{\rm per}\left(\frac{x}{\varepsilon}\right) \underset{\varepsilon\to 0}{\overset{*}{\rightharpoonup}} \int_Q F_{\rm per}(y)\,dy \quad \text{in } L^\infty(\mathbb{R}^d), \qquad Q = (0,1)^d.$$

- Stochastic case: for any $F \in L^\infty\left(\mathbb{R}^d, L^1(\Omega)\right)$ that is statistically homogeneous,

$$F\left(\frac{x}{\varepsilon},\omega\right) \underset{\varepsilon\to 0}{\overset{*}{\rightharpoonup}} \mathbb{E}\left(\int_Q F(y,\cdot)\,dy\right) \quad \text{in } L^\infty(\mathbb{R}^d), \text{ almost surely.}$$

Stochastic homogenization: result

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

$u^\varepsilon(\cdot,\omega)$ converges (a.s.) to $u^\star$ solution to

$$-\text{div}\left[A^\star \nabla u^\star\right] = f \quad \text{in} \quad \mathcal{D}, \qquad u^\star = 0 \text{ on } \partial\mathcal{D},$$

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where the homogenized matrix $A^\star$ is given by

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

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

In contrast to the periodic case, the corrector problem is set on $\mathbb{R}^d$.

Standard discretization

- Solve the corrector problem on a truncated domain:

$$\begin{cases} -\text{div}\left[A(y,\omega)\left(p + \nabla w_p^N(y,\omega)\right)\right] = 0, \\ w_p^N \quad \text{is } Q_N\text{-periodic}, \quad Q_N = (-N,N)^d. \end{cases}$$

- This yields an approximate (apparent) homogenized matrix

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

Due to numerical truncation, $A_N^\star$ is random!

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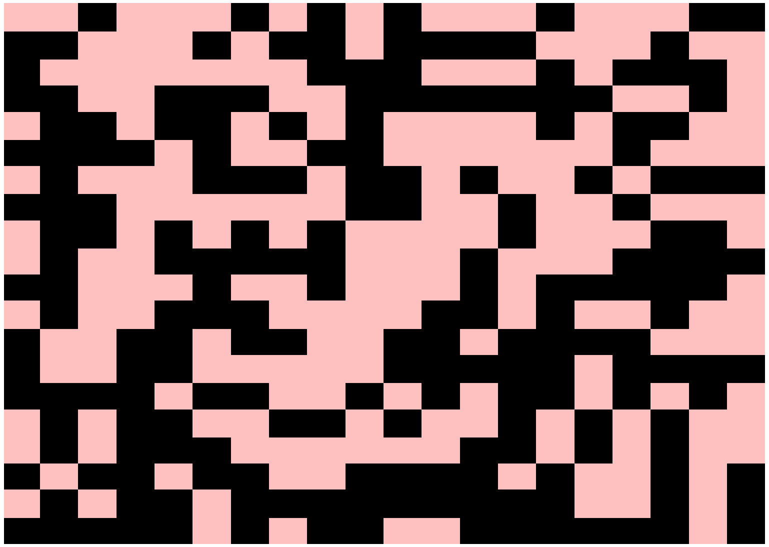
  Due to numerical truncation, $A_N^\star$ is random!

- We have $\lim_{N\to\infty} A_N^\star(\omega)\to A^\star$ a.s. (Bourgeat/Piatnitski, 2004).
- In practice, N is finite (and possible not large!):

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

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

An academic random material



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

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

Monte Carlo approximation

- Consider M independent realizations $A^m(y,\omega)$, compute for each
  - the corrector $w_p^{N,m}$ on Q_N:

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

  - and the approximate homogenized matrix

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

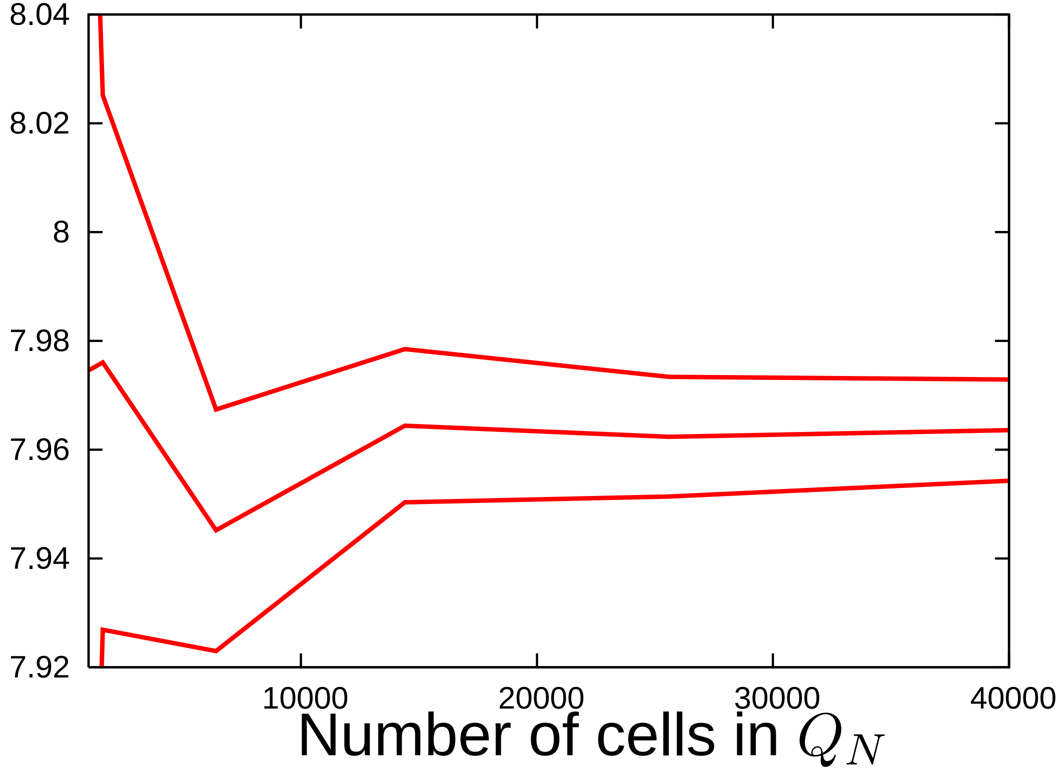
- Approximate $\mathbb{E}(A^\star_N)$ by $\quad I_M=\dfrac{1}{M}\displaystyle\sum_{m=1}^{M} A^\star_{N,m}(\omega)$.

Classical confidence interval: with a probability equal to 95 %,

$$\left|\mathbb{E}([A^\star_N]_{ij})-[I_M]_{ij}\right|\le 1.96\frac{\sqrt{\mathbb{V}\text{ar}([A^\star_N]_{ij})}}{\sqrt{M}}$$

The accuracy of I_M is directly linked with the variance of $A^\star_N$.

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



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

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

Variance reduction using control variate

Let $X(\omega)$ be a scalar random variable. We want to compute $\mathbb{E}(X)$.

Later, we will take $X(\omega) = [A_N^\star(\omega)]_{ij}$.

Estimating $\mathbb{E}(X)$

- standard Monte Carlo method: generate M independent realizations of $X(\omega)$, and approximate $\mathbb{E}(X)$ by

$$I_M^{\rm MC} = \frac{1}{M} \sum_{m=1}^M X(\omega_m) \quad \text{that satisfies} \quad \left| \mathbb{E}(X) - I_M^{\rm MC} \right| \leq 1.96 \frac{\sqrt{\mathbb{V}{\rm ar}(X)}}{\sqrt{M}}$$

- control variate method: consider $X_{\rm app}(\omega)$ a random variable "close" to $X(\omega)$, s.t. $\mathbb{E}\left[X_{\rm app}\right]$ is analytically computable, and introduce

$$C(\omega) = X(\omega) - \rho \Big(X_{\rm app}(\omega) - \mathbb{E}\left[X_{\rm app}\right] \Big)$$

  where ρ is a deterministic parameter.

  Approximate $\mathbb{E}(X) = \mathbb{E}(C)$ by

$$I_M^{\rm CV} = \frac{1}{M} \sum_{m=1}^M C(\omega_m) \quad \text{that satisfies} \quad \left| \mathbb{E}(X) - I_M^{\rm CV} \right| \leq 1.96 \frac{\sqrt{\mathbb{V}{\rm ar}(C)}}{\sqrt{M}}$$

- Accuracy gain iff $\mathbb{V}{\rm ar}(C) < \mathbb{V}{\rm ar}(X)$.

Choice of the control variate $X_{\rm app}(\omega)$

$$C(\omega) = X(\omega) - \rho\Big(X_{\rm app}(\omega) - \mathbb{E}\left[X_{\rm app}\right]\Big), \quad \rho \text{ deterministic parameter}$$

$$I_M^{\rm CV} = \frac{1}{M}\sum_{m=1}^{M} C(\omega_m) \quad \text{satisfies} \quad \left|\mathbb{E}(X) - I_M^{\rm CV}\right| \leq 1.96\frac{\sqrt{\mathbb{V}\mathrm{ar}(C)}}{\sqrt{M}}$$

Extreme cases:

- $X_{\rm app}$ is deterministic: then $C(\omega) = X(\omega)$ and no gain!
- $X_{\rm app} = X$: for $\rho = 1$, C is deterministic (hence small variance!), but the algorithm requires $\mathbb{E}\left[X_{\rm app}\right] = \mathbb{E}(X)$, which is what we are looking for! Not practical!

In general, we need something in-between (problem-dependent).

Choice of the deterministic parameter ρ

$$C(\omega) = X(\omega) - \rho\Big(X_{\rm app}(\omega) - \mathbb{E}\left[X_{\rm app}\right]\Big), \quad \rho \text{ deterministic parameter}$$

We wish to minimize the variance of C.

- For any choice of $X_{\rm app}(\omega)$, there exists an optimal ρ that minimizes the variance of C:

$$\rho_{\rm opt} = \frac{\mathbb{C}{\rm ov}(X, X_{\rm app})}{\mathbb{V}{\rm ar}(X_{\rm app})}$$

  Not exactly computable in practice, but can be well enough approximated by an empirical mean.

- For this optimal choice of ρ,

$$\frac{\mathbb{V}{\rm ar}(C)}{\mathbb{V}{\rm ar}(X)} = 1 - \frac{\Big(\mathbb{C}{\rm ov}(X, X_{\rm app})\Big)^2}{\mathbb{V}{\rm ar}(X)\,\mathbb{V}{\rm ar}(X_{\rm app})} < 1$$

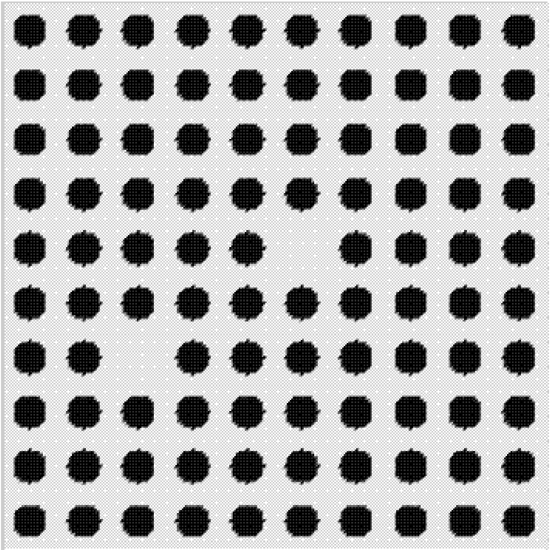
  The more X and $X_{\rm app}$ are correlated, the better!

A weakly stochastic case:
Rare defects in a periodic structure

A. Anantharaman and C. Le Bris,
– C. R. Acad. Sciences 348 (2010)
– SIAM MMS 9 (2011)
– Comm. Comp. Phys. 11 (2012)

Our aim wrt variance reduction: build a surrogate model close to $A_N^\star(\omega)$.

A defect model (A. Anantharaman and C. Le Bris, CRAS 2010)



$A_{\rm per}$: fiber

$A_{\rm per} + C_{\rm per} = \mathrm{Id}$: no fiber (defect)

$$A(x,\omega) = A_{\rm per}(x) + b_\eta(x,\omega)\, C_{\rm per}(x)$$

where $A_{\rm per}$ and $C_{\rm per}$ are both $\mathbb{Z}^d$-periodic, and

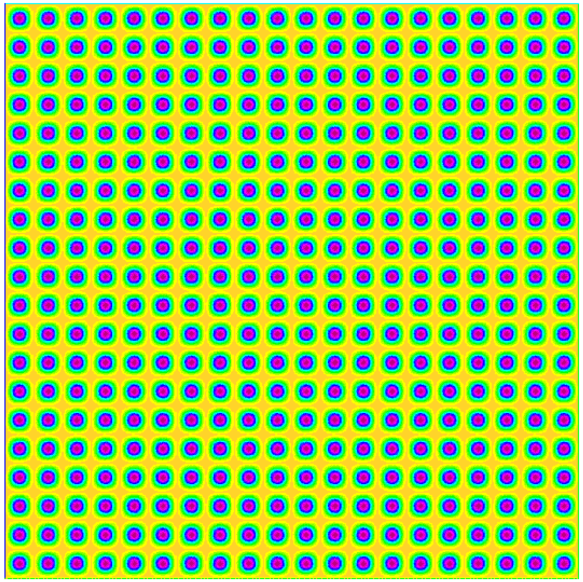
$$b_\eta(x,\omega) = \sum_{k \in \mathbb{Z}^d} 1_{Q+k}(x)\, B_\eta^k(\omega), \quad Q = (0,1)^d,$$

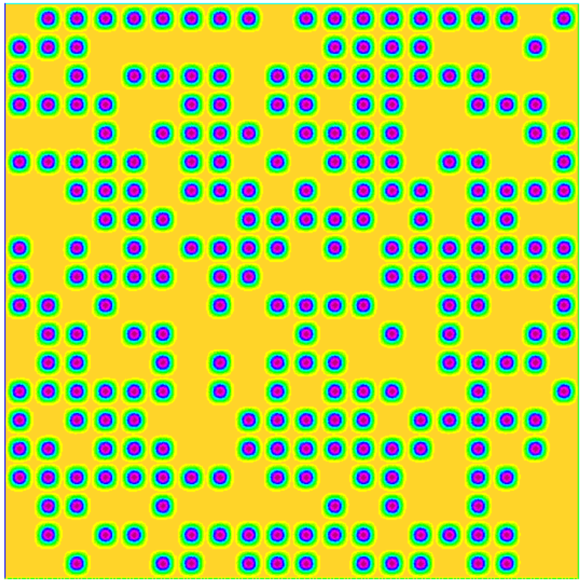
where $\left\{ B_\eta^k \right\}_{k \in \mathbb{Z}^d}$ are i.i.d. random variables:

$$\mathbb{P}(B_\eta^k = 1) = \eta, \quad \mathbb{P}(B_\eta^k = 0) = 1 - \eta.$$

When η is a small parameter, $A = A_{\rm per}$ “most of the time”.

Defects may be not so rare!



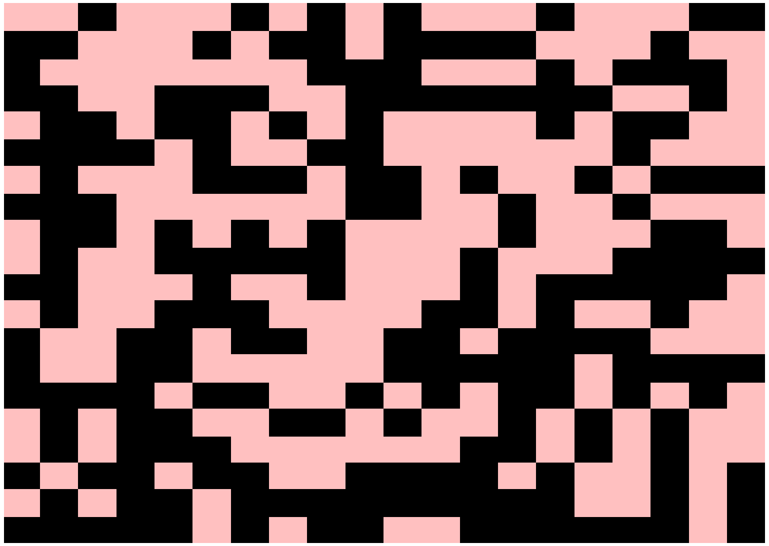


Left: perfect (periodic) material: $\eta = 0$.

Right: a realization of the material with defects of probability $\eta = 0.4$.

When $\eta = 1/2$, defects are as frequent as non-defects!

A realization of the matrix A on Q_N is determined by the collection of the B_k^η (0: fiber; 1: no fiber = defect) in each cell k of Q_N.



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

Then $\quad A(x,\omega) = A_{\rm per}(x) + b_\eta(x,\omega)\, C_{\rm per}(x)$

with $A_{\rm per}(x) = \alpha$, $A_{\rm per}(x) + C_{\rm per}(x) = \beta$ and $\eta = 1/2$.

Homogenized matrix expansion (Anantharaman Le Bris, CRAS 2010)

- Approximate homogenized matrix:

$$A_N^\star(\omega)p = \frac{1}{|Q_N|}\int_{Q_N} A\,(y,\omega)\,\left(\nabla w_p^N(y,\omega)+p\right)\,dy$$

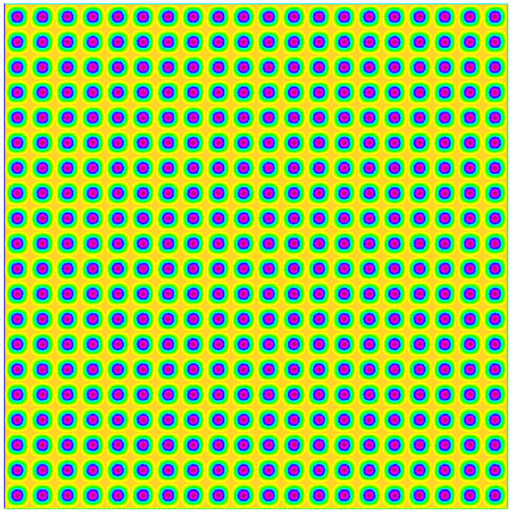
where we solve the corrector problem on $Q_N = (-N,N)^d$:

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

- By enumerating all possible realizations of $A(x,\omega)$ on Q_N, we obtain an expansion of $\mathbb{E}\left[A_N^\star\right]$ in powers of η:

$$\begin{aligned}
\mathbb{E}\left[A_N^\star\right] &= \sum_{\omega \text{ s.t. 0 defect}} A_N^\star(\omega)\mathbb{P}(\omega) + \sum_{\omega \text{ s.t. 1 defect}} A_N^\star(\omega)\mathbb{P}(\omega) + \dots \\
&= (1-\eta)^{N^d} A_{\rm per}^\star + \sum_{k\in I_N} \eta(1-\eta)^{N^d-1} A_N^\star(\text{1 defect in } k) + \dots \\
&= A_{\rm per}^\star + \eta \overline{A}_1^{\star,N} + \eta^2 \overline{A}_2^{\star,N} + O(\eta^3)
\end{aligned}$$

$\mathbb{E}\left[A_N^\star\right] = A_{\rm per}^\star + \eta \overline{A}_1^{\star,N} + \eta^2 \overline{A}_2^{\star,N} + \cdots$



Leading order term given by the periodic (no defect!) situation:

$$-\text{div}\left[A_{\rm per}\left(p + \nabla w_p^0\right)\right] = 0, \quad w_p^0 \text{ is } Q\text{-periodic}$$

and

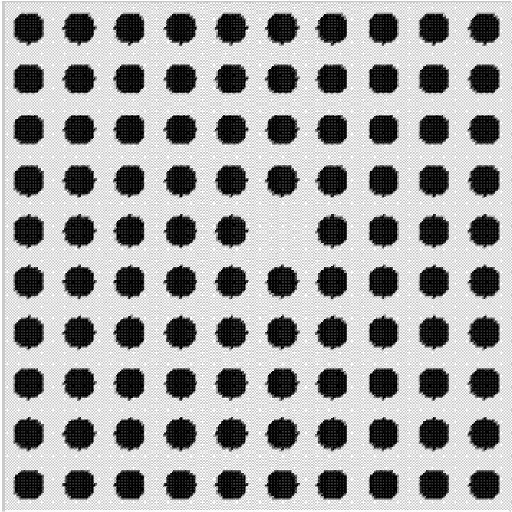
$$A_{\rm per}^\star p = \int_Q A_{\rm per}(\nabla w_p^0 + p).$$

$\mathbb{E}\left[A_N^\star\right] = A_{\rm per}^\star + \eta \overline{A}_1^{\star,N} + \eta^2 \overline{A}_2^{\star,N} + \cdots$

$$\begin{aligned} \overline{A}_1^{\star,N} p &= \frac{1}{|Q_N|} \sum_{k \in I_N} \left[\int_{Q_N} A_1^k (\nabla w_p^{1,k} + p) - \int_{Q_N} A_{\rm per} (\nabla w_p^0 + p) \right] \\ &= \frac{1}{|Q_N|} \sum_{k \in I_N} \mathcal{A}_k^{1\,\rm def} p \end{aligned}$$

where w_p^0 is the periodic corrector (no defect) and $w_p^{1,k}$ is the corrector associated to

$$A_1^k = A_{\rm per} + \mathbf{1}_{Q+k} C_{\rm per} \quad \text{(material with a single defect in } Q+k\text{)}$$



$$-\text{div}\left[A_1^k \left(p + \nabla w_p^{1,k} \right) \right] = 0$$

$w_p^{1,k}$ is Q_N-periodic.

Remark: here, due to periodic BC, $\mathcal{A}_k^{1\,\rm def}$ independent of k.

$$\overline{A}_1^{\star,N} p = \frac{1}{|Q_N|} \sum_{k \in I_N} \mathcal{A}_k^{1\,\rm def} p$$

where $\mathcal{A}_k^{1\,\rm def}$ is the marginal contribution of a single defect in k.

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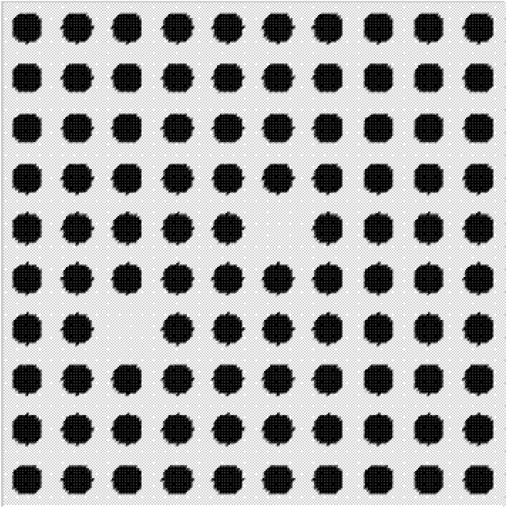

Similar expression for second order:

$$\overline{A}_2^{\star,N} p = \frac{1}{2|Q_N|} \sum_{k \neq \ell} \mathcal{A}_{k,\ell}^{2\,\rm def} p$$

Marginal contribution from pairs of defects.

$\mathbb{E}\left[A_N^\star\right] = A_{\mathrm{per}}^\star + \eta \overline{A}_1^{\star,N} + \eta^2 \overline{A}_2^{\star,N} + \cdots$

$$\overline{A}_1^{\star,N} p = \frac{1}{|Q_N|} \sum_{k \in I_N} \mathcal{A}_k^{1\,\mathrm{def}} p$$

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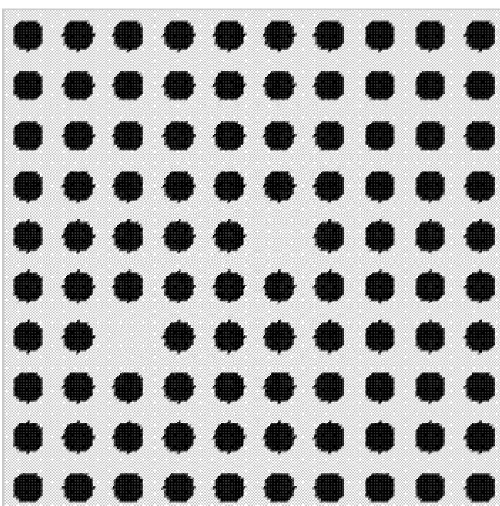

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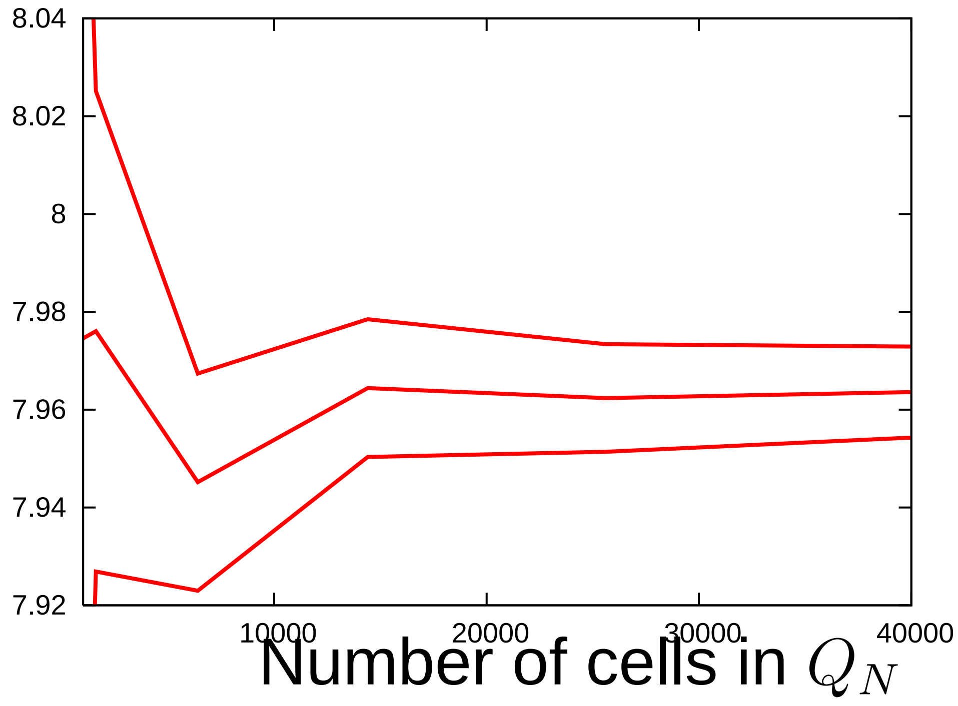
Marginal contribution from pairs of defects.

Possible to use a Reduced Basis approach to compute $w_p^{2,k,\ell}$, corrector associated to $A_2^{k,\ell} = A_{\mathrm{per}} + \mathbf{1}_{Q+k} C_{\mathrm{per}} + \mathbf{1}_{Q+\ell} C_{\mathrm{per}}$.
C. Le Bris and F. Thomines, CAM 2012.

A control variate approach

Joint work with W. Minvielle.



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

Control variate based on first order approximation - 1

$$\mathbb{E}\left[A^\star_N\right] = A^\star_{\rm per} + \eta \overline{A}_1^{\star,N} + \eta^2 \overline{A}_2^{\star,N} + \cdots$$

where

$$\eta \overline{A}_1^{\star,N} = \frac{\eta}{|Q_N|} \sum_{k \in I_N} \mathcal{A}_k^{1\,\rm def}$$

is the contribution to the homogenized matrix due to all the defects in the system, considered isolated one from each other.

We see that

$$\eta \overline{A}_1^{\star,N} = \mathbb{E}\left[A_1^{\star,N}\right]$$

where

$$A_1^{\star,N}(\omega) = \frac{1}{|Q_N|} \sum_{k \in I_N} B^k_\eta(\omega)\ \mathcal{A}_k^{1\,\rm def}$$

where $B^k_\eta = 1$ if defect in cell $Q + k$ (which happens with probability η).

Heuristics: $A^\star_{\rm per} + A_1^{\star,N}(\omega)$ good approx. of $A^\star_N(\omega)$.

Control variate based on first order approximation - 2

$$\mathbb{E}\left[A^\star_N\right] = A^\star_{\rm per} + \eta \overline{A_1}^{\star,N} + \eta^2 \overline{A_2}^{\star,N} + \cdots$$

We introduce

$$A^\star_{\rm app}(\omega) := A^\star_{\rm per} + A_1^{\star,N}(\omega) \quad \text{with} \quad A_1^{\star,N}(\omega) := \frac{1}{|Q_N|} \sum_{k \in I_N} B^k_\eta(\omega)\, \mathcal{A}_k^{1\,\rm def},$$

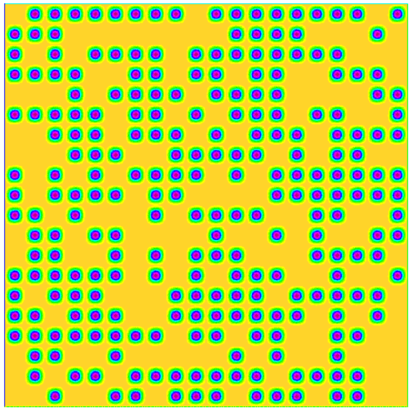
notice that

$$\mathbb{E}\left[A^\star_N\right] = \mathbb{E}\left[A^\star_{\rm app}\right] + \eta^2 \overline{A_2}^{\star,N} + \cdots$$

and infer that $A^\star_{\rm app}(\omega)$ is a good approximation of $A^\star_N(\omega)$.

This is confirmed by the fact that, for any function φ,

$$\mathbb{E}\left[\varphi\left(A^\star_N\right)\right] = \mathbb{E}\left[\varphi\left(A^\star_{\rm app}\right)\right] + O\left(\eta^2\right).$$



Procedure:

- draw $B_\eta^k(\omega)$ in each cell $Q+k$ (defect or not?). This determines the field $A(x,\omega)$ on Q_N.
- compute the associated $A_N^\star(\omega)$ (corrector pb on Q_N)
- build the control variate (ρ deterministic parameter)

$$C_N^\star(\omega) = A_N^\star(\omega) - \rho \left(A_{\rm per}^\star + A_1^{\star,N}(\omega) - \mathbb{E}\left[A_{\rm per}^\star + A_1^{\star,N}(\omega) \right] \right)$$

with $A_1^{\star,N}(\omega) = \dfrac{1}{|Q_N|} \displaystyle\sum_{k \in I_N} B_\eta^k(\omega)\, \mathcal{A}_k^{1\,\rm def}$ (expectation analyt. computable).

Control variate based on first order approximation - 4

$$C_N^\star(\omega) = A_N^\star(\omega) - \rho\left(A_{\rm per}^\star + A_1^{\star,N}(\omega) - \mathbb{E}\left[A_{\rm per}^\star + A_1^{\star,N}(\omega)\right]\right)$$

- Expect $A_{\rm per}^\star + A_1^{\star,N}(\omega)$ to be a good approx. of $A_N^\star(\omega)$ (at least for $\eta \ll 1$).
- Observe that $\mathbb{E}\left[A_N^\star(\omega)\right] = \mathbb{E}\left[C_N^\star(\omega)\right]$
- IDEA: approximate $\mathbb{E}\left[A_N^\star(\omega)\right] = \mathbb{E}\left[C_N^\star(\omega)\right]$ by

$$J_M = \frac{1}{M}\sum_{m=1}^{M} C_N^\star(\omega_m) \quad \left[\text{Confidence interval: } \mathbb{V}\mathrm{ar}\, C_N^\star\right]$$

Control variate based on first order approximation - 4

$$C_N^\star(\omega) = A_N^\star(\omega) - \rho\left(A_{\rm per}^\star + A_1^{\star,N}(\omega) - \mathbb{E}\left[A_{\rm per}^\star + A_1^{\star,N}(\omega)\right]\right)$$

- Expect $A_{\rm per}^\star + A_1^{\star,N}(\omega)$ to be a good approx. of $A_N^\star(\omega)$ (at least for $\eta \ll 1$).
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Optimal ρ that minimizes the variance of (an entry of the matrix) $C_N^\star$:

$$\rho_{\rm opt} = \frac{\mathbb{C}\text{ov}(A_N^\star, A_1^{\star,N})}{\mathbb{V}\text{ar}(A_1^{\star,N})}$$ well approx. by empirical mean, $\rho_{\rm opt} \underset{\eta\to 0}{\to} 1$

Control variate based on second order approximation - 1

$$\mathbb{E}\left[A_N^\star\right] = A_{\rm per}^\star + \eta \overline{A}_1^{\star,N} + \eta^2 \overline{A}_2^{\star,N} + \cdots$$

where

$$\eta^2 \overline{A}_2^{\star,N} = \frac{\eta^2}{2|Q_N|} \sum_{k \neq \ell} \mathcal{A}_{k,\ell}^{2\,\rm def}$$

is the contribution to the homogenized matrix due to all pairs of defects in the system, located at k and ℓ. We see that

$$\eta^2 \overline{A}_2^{\star,N} = \mathbb{E}\left[A_2^{\star,N}\right]$$

where

$$A_2^{\star,N}(\omega) = \frac{1}{2|Q_N|} \sum_{k \neq \ell} B_\eta^k(\omega)\, B_\eta^\ell(\omega)\, \mathcal{A}_{k,\ell}^{2\,\rm def}$$

where $B_\eta^k = 1$ if defect in cell $Q + k$ (which happens with probability η).

Control variate based on second order approximation - 2

- Second order control variate approach:

$$C_N^\star(\omega) = A_N^\star(\omega) - \rho \left(A^\star_{\rm per} + A_1^{\star,N}(\omega) - \mathbb{E}\left[\dots\right] \right) - \rho_2 \left(A_2^{\star,N}(\omega) - \mathbb{E}\left[\dots\right] \right)$$

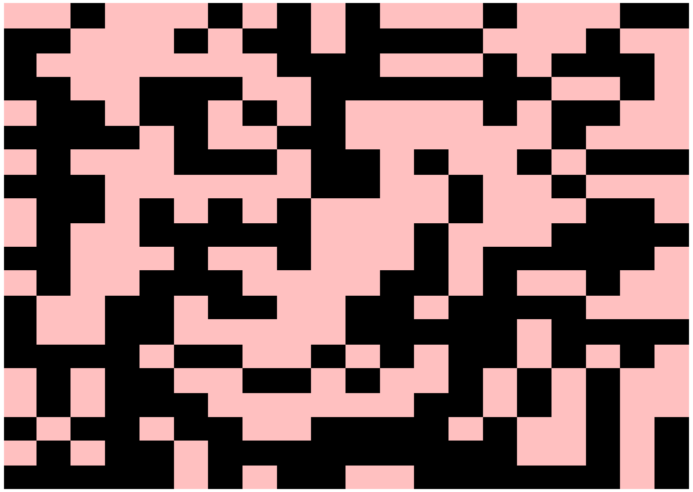
  For any entry $1 \leq i,j \leq d$, optimal parameters ρ and ρ_2 by minimizing $\mathbb{V}{\rm ar}([C_N^\star]_{ij})$ (inverse a 2×2 matrix).

- Here, we systematically refer to the situation “no defect”, $\eta \ll 1$. It is also possible to refer to the situation “all defects”, $1 - \eta \ll 1$.

  The first order correction turns out to be the same, but not the second order correction:

$$C_N^\star(\omega) = A_N^\star(\omega) - \rho \left(A^\star_{\rm per} + A_1^{\star,N}(\omega) \right) - \rho_2 A^{\star,N}_{2,\ {\rm wrt}\ \eta=0}(\omega) - \rho_3 A^{\star,N}_{2,\ {\rm wrt}\ \eta=1}(\omega) - \mathbb{E}\left[\dots\right]$$

Numerical test case

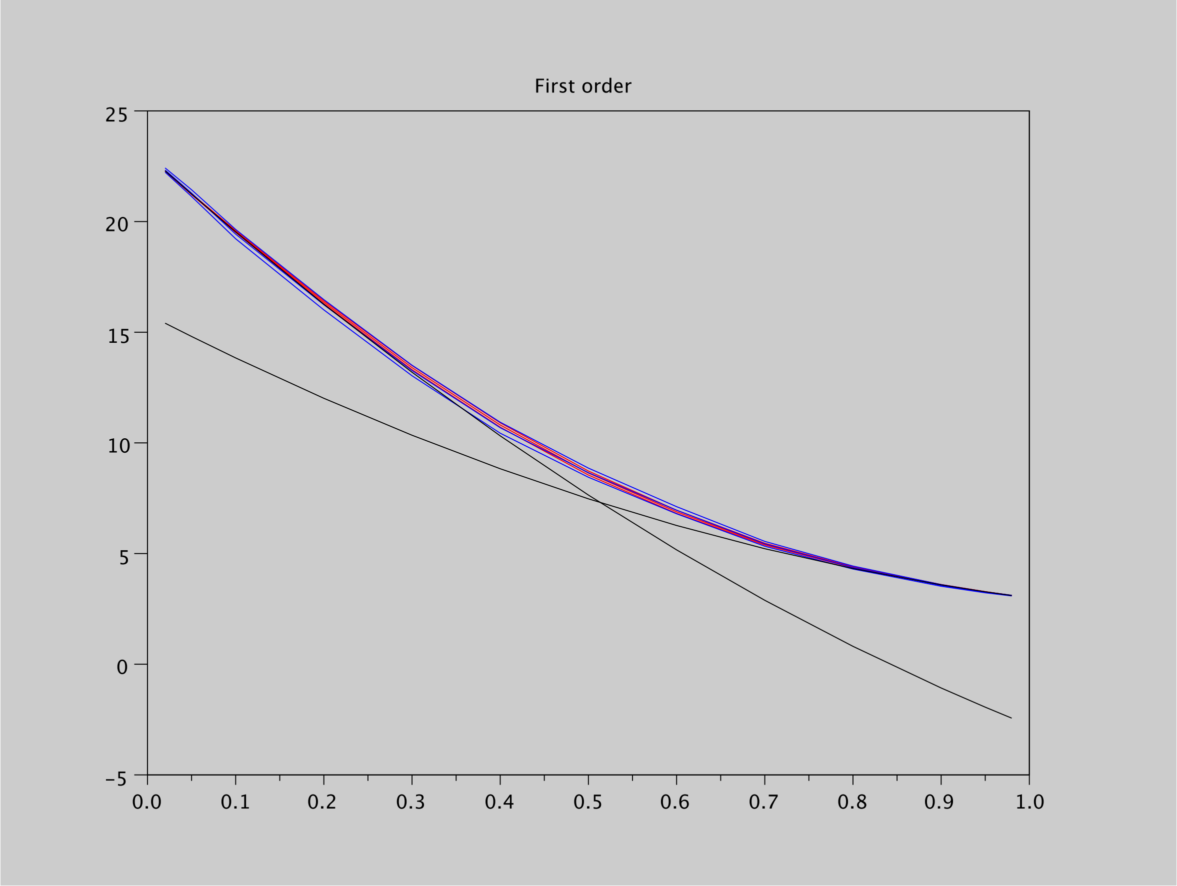


$$A(x,\omega) = \sum_{k \in \mathbb{Z}^2} 1_{Q+k}(x)\, a_k(\omega)\, \mathrm{Id}_2, \quad a_k \text{ independent identically distributed}$$

$$\mathbb{P}(a_k = \alpha) = \eta, \quad \mathbb{P}(a_k = \beta) = 1 - \eta.$$

Not always clear to decide who is the defect / background (e.g. when $\eta = 1/2$).

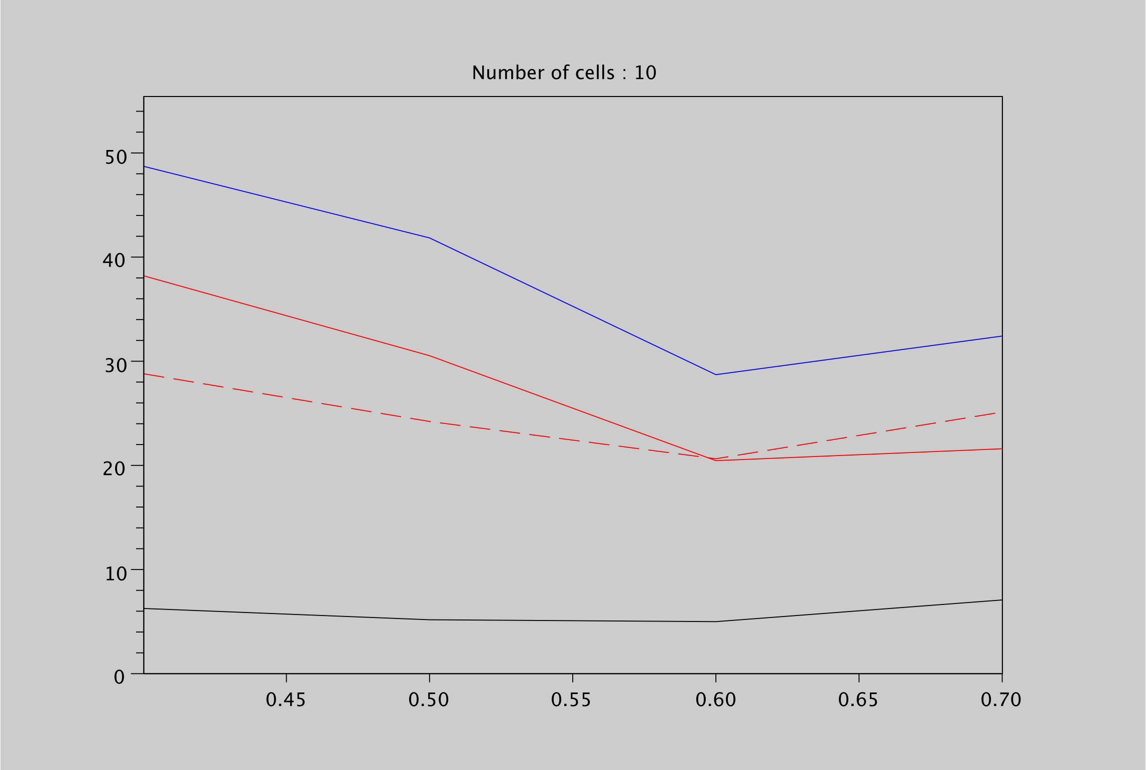
Small contrast test case: (α, β) *= (3,23) - Homogenized coefficient*



Blue curve: standard Monte Carlo estimator $I_M^{\mathrm{MC}} = M^{-1} \sum_{m=1}^{M} A_N^\star(\omega_m)$

Black curves: weakly stochastic approximation (expansion wrt $\eta = 0$ or $\eta = 1$): inaccurate when $0.4 \leq \eta \leq 0.7$.

Ratios $\mathbb{V}\mathrm{ar}(A_N^\star)/\mathbb{V}\mathrm{ar}(C_N^\star) \equiv$ *CPU time gain*



Black curves: control variate approach using *first order* approximation.

Red curves: control variate approach using second order approximation (wrt $\eta = 0$ OR $\eta = 1$).

Blue curve: control variate approach simultaneously using first and second order approximations at both ends ($\eta = 0$ AND $\eta = 1$).

Small contrast test case: (α,β) *= (3,23) - Efficiency at* $\eta = 1/2$

$$C_N^\star(\omega) = A_N^\star(\omega) - \rho\left(A^\star_{\rm per} + A_1^{\star,N}(\omega) - \mathbb{E}\left[\dots\right]\right)$$
$$- \rho_2\left(A^{\star,N}_{2,\ \mathrm{wrt.}\ \eta=0}(\omega) - \mathbb{E}\left[\dots\right]\right) - \rho_3\left(A^{\star,N}_{2,\ \mathrm{wrt.}\ \eta=1}(\omega) - \mathbb{E}\left[\dots\right]\right)$$

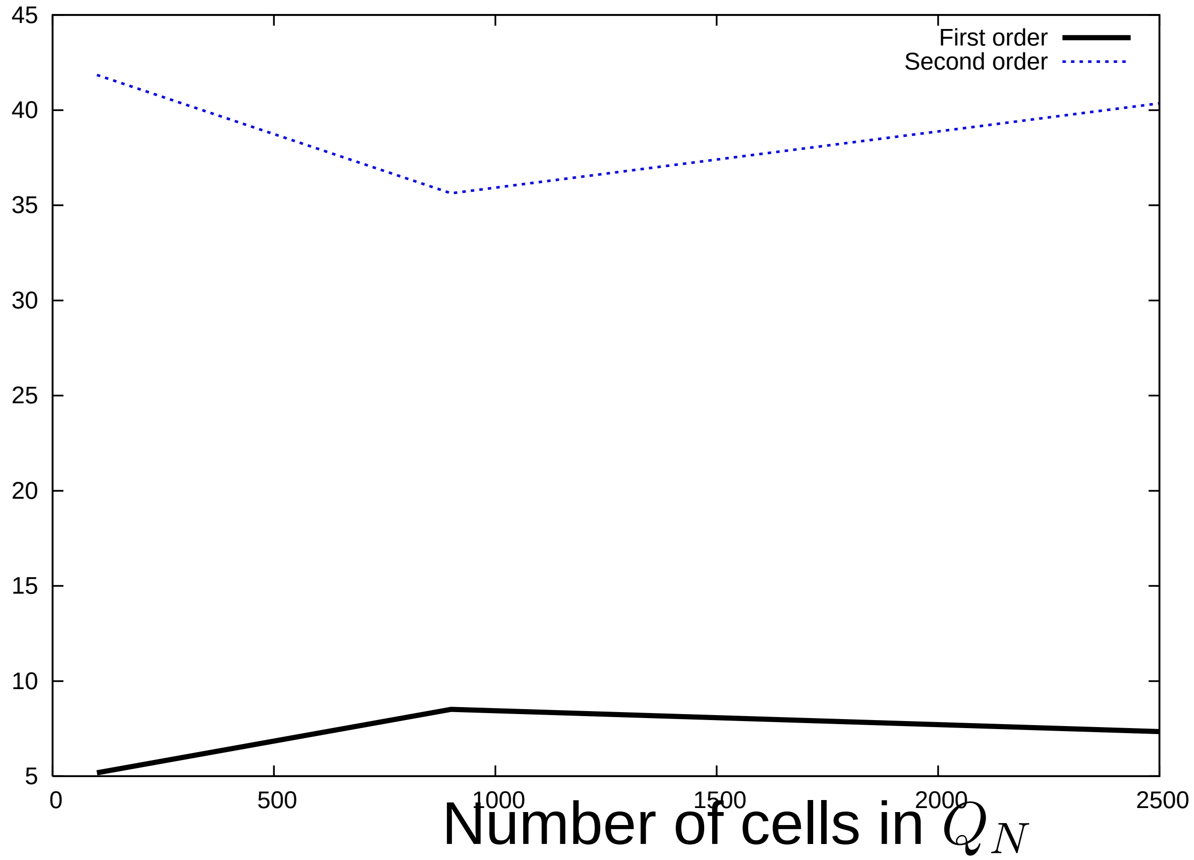
- Control variate using *first order* approximation ($\rho_2 = \rho_3 = 0$):
  - variance ratio = 6
  - computing the control variate is inexpensive, hence

CPU time gain = Variance ratio = 6

- Control variate using second order approximation (optimal ρ, ρ_2 and ρ_3):
  - variance ratio = 44
  - using a RB approach (Le Bris & Thomines, 2012), computing the control variate is inexpensive:

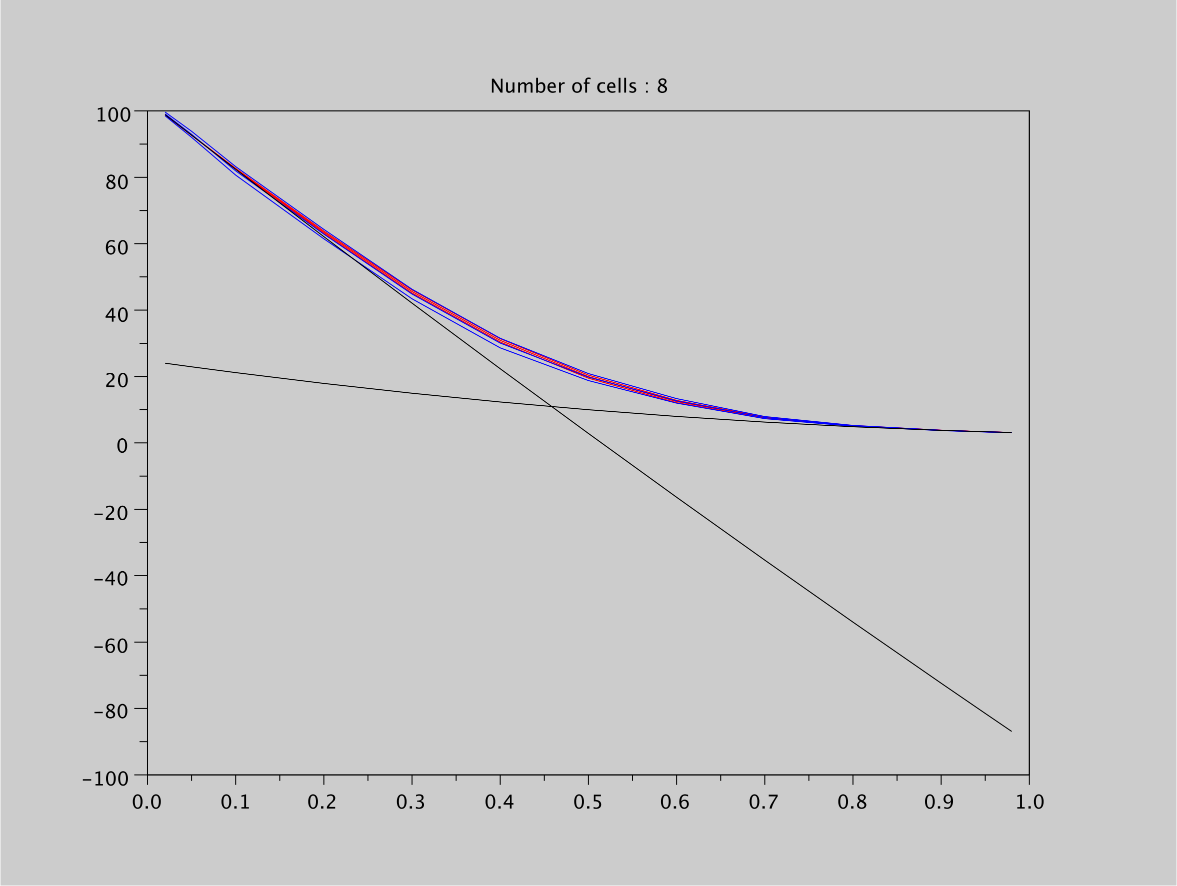
CPU time gain = Variance ratio = 44

Robustness ($\eta = 1/2$) wrt supercell size



Variance reduction ratio (*first order* or second order approximation): insensitive to the supercell size.

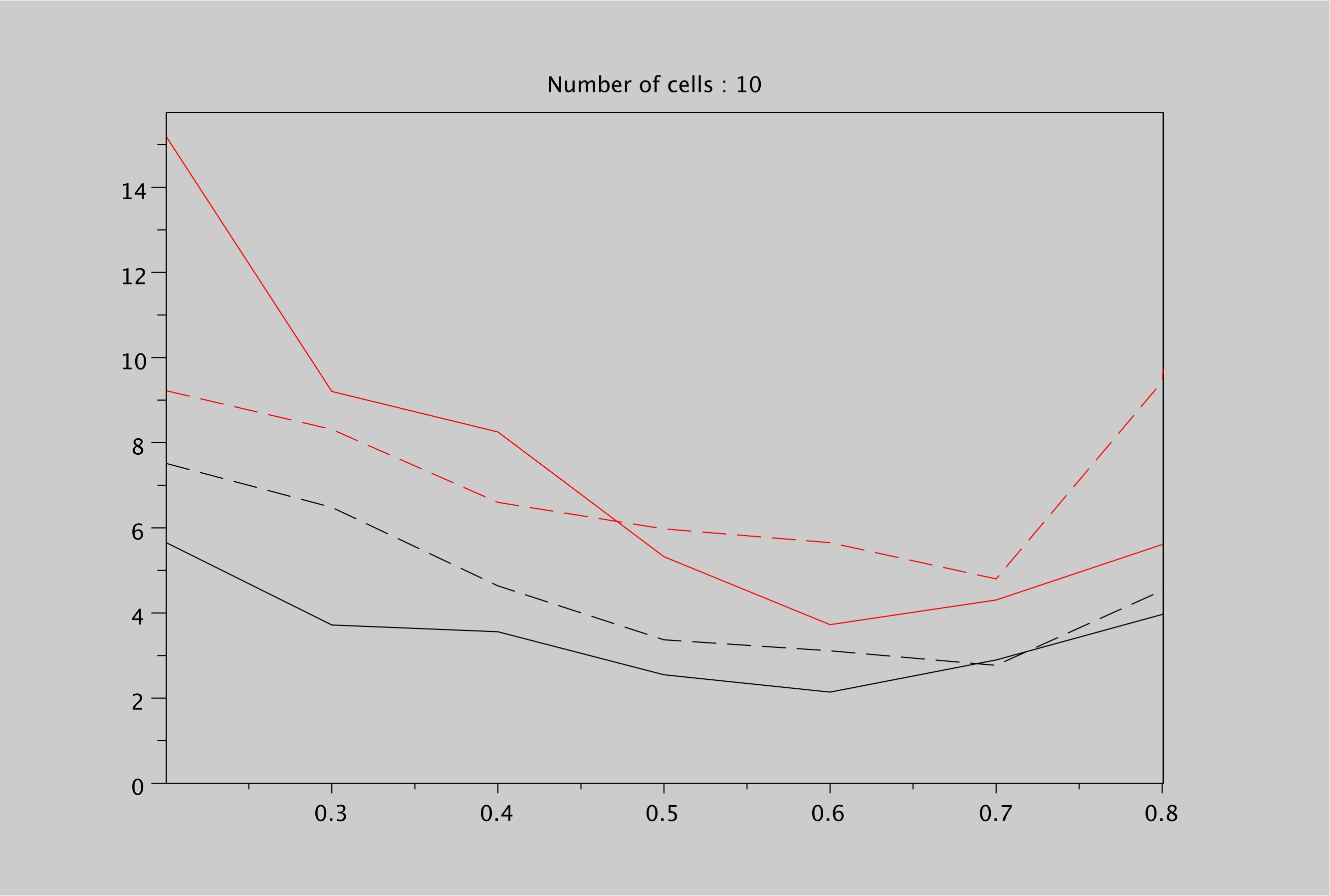
Large contrast test case: (α, β) = (3,103) - Homogenized coefficient



Blue curve: standard Monte Carlo estimator $I_M^{\mathrm{MC}} = M^{-1} \sum_{m=1}^{M} A_N^\star(\omega_m)$

Black curves: weakly stochastic approximation (with α or β as background): inaccurate when $0.3 \leq \eta \leq 0.7$.

Variance ratios (CPU time gain)



Black curves: control variate approach using *first order approximation*

Red curves: control variate approach using second order approximation (wrt $\eta = 0$ OR $\eta = 1$).

Quantitative estimation of the variance reduction ($\eta \ll 1$)

Three approaches to compute $\mathbb{E}\left[A_N^\star\right]$:

- Standard Monte Carlo approach with M realizations:

$$\text{error} = \text{statistical error} \propto \sqrt{\mathbb{V}\text{ar}(A_N^\star)/M} \propto \sqrt{\eta/M}$$

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- Control Variate approach (first order) with M realizations:

$$\text{error} \;=\; \text{statistical error} \;\propto\; \sqrt{\mathbb{V}\text{ar}(C_N^\star)/M} \;\propto\; \sqrt{\eta^2/M}$$

  At equal cost, more accurate that Monte Carlo.

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  At equal cost, more accurate that Monte Carlo.

- Expansion of $\mathbb{E}\left[A_N^\star\right]$ (Anantharaman / Le Bris) using the same information as the Control Variate approach:

$$\mathbb{E}\left[A_N^\star\right] = A_{\rm per}^\star + \eta \overline{A_1^{\star,N}} + O(\eta^2), \quad \text{error} = \text{systematic error} \propto \eta^2.$$

  CV approach needs $M \propto 1/\eta^2 \gg 1$ to reach a similar accuracy.

Regime of interest for our CV approach: η neither close to 0 nor 1.

Conclusions

- We have proposed a control variate approach based on a defect-type model to better compute $\mathbb{E}\left[A_N^\star\right]$.

- When none of the phase dominates ($\eta \approx 1/2$), the defect model becomes inaccurate per se, but remains useful as a control variate.

- For the moment, all computations have been done with the exact $A_2^{\star,N}(\omega)$. If we indeed use the RB approach, what impact on the variance reduction?
  Up to what can we degrade the surrogate model?

- This approach seems to yield a ($\sim$ 10 times) better variance reduction than the antithetic variable approach, which is a generic (and simple) variance reduction approach (less fitted to the homogenization context).

Some references

- Review article:

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  - R. Costaouec, C. Le Bris, F.L., Boletin Soc. Esp. Mat. Apl. 2010.
  - X. Blanc, R. Costaouec, C. Le Bris, F.L., Markov Processes and Related Fields 2012 and Lect. Notes Comput. Sci. Eng. 2012.
  - F.L., W. Minvielle, arXiv 1302.0038 (nonlinear case).

- Multi-Level Monte Carlo approach:

  Y. Efendiev, C. Kronsbein, F.L., arXiv 1301.2798

- Control variate approach: F.L., W. Minvielle, in preparation.