Variance reduction approaches in stochastic homogenization

Frédéric Legoll

ENPC (Navier) and INRIA (MICMAC team-project)

Joint work with William Minvielle (ENPC and INRIA)

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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 } D, \quad u^\varepsilon = 0 \text{ on } \partial D.

Thermal diffusion, . . .
Outline of the talk

- Some background materials on random homogenization
- Variance reduction by the control variate approach
- 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
Random homogenization
\[ -\text{div} \left[ A_{\text{per}} \left( \frac{x}{\varepsilon} \right) \nabla u^\varepsilon \right] = f \quad \text{in } D, \quad u^\varepsilon = 0 \quad \text{on } \partial D, \quad A_{\text{per}} \text{ is } \mathbb{Z}^d\text{-periodic.} \]
Homogenization 1.0.1: the periodic setting

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

When \( \varepsilon \to 0 \), \( u^\varepsilon \) converges to \( u^* \) solution to

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

The effective matrix \( A^* \) is given by

\[
[A^*]_{ij} = \int_{Q} e^T_i A_{\text{per}}(y) \left( e_j + \nabla w_{e_j}(y) \right) \, dy, \quad Q = \text{unit cube } = (0, 1)^d,
\]

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

\[- \text{div} \left[ A_{\text{per}}(y) \left( p + \nabla w_p \right) \right] = 0, \quad w_p \text{ is } \mathbb{Z}^d\text{-periodic.}\]
Homogenization 1.0.1: the periodic setting

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

When \( \epsilon \to 0 \), \( u^\epsilon \) converges to \( u^* \) solution to

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

The effective matrix \( A^* \) is given by

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

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

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

\( \rightarrow \) The corrector problem is set on the bounded domain \( Q \): easy!
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 $k \in \mathbb{Z}^d$,

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

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

There is some order in the randomness.
Periodic case: for any $F_{\text{per}} \in L^\infty(\mathbb{R}^d)$ that is $\mathbb{Z}^d$-periodic,

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

Stochastic case: for any $F \in L^\infty(\mathbb{R}^d, L^1(\Omega))$ that is statistically homogeneous (i.e. random ergodic stationary),

$$F \left( \frac{x}{\varepsilon}, \omega \right) \xrightarrow{\varepsilon \to 0} \mathbb{E} \left( \int_Q F(y, \cdot) \, dy \right) \quad \text{in} \quad L^\infty(\mathbb{R}^d), \quad \text{almost surely.}$$
Stochastic homogenization: result

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

\[u^\varepsilon (\cdot, \omega) \text{ converges (a.s.) to } u^* \text{ solution to}\]

\[-\text{div} \left[ A^* \nabla u^* \right] = f \quad \text{in} \ D, \quad u^* = 0 \quad \text{on} \ \partial D, \]
Stochastic homogenization: result

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

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

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

where the homogenized matrix \(A^*\) is given by

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

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

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:

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

- This yields an approximate (apparent) homogenized matrix

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

Due to numerical truncation, \(A_N^*\) is random!

- Bourgeat & Piatnitski, 2004:

\[
\lim_{N \to \infty} A_N^*(\omega) \to A^* \text{ a.s.}
\]
\[ A(x, \omega) = \sum_{k \in \mathbb{Z}^2} 1_{Q+k}(x) a_k(\omega) \text{Id}_2, \quad a_k \text{ independent identically distributed} \]

\[ a_k = \alpha \text{ or } \beta \text{ with equal probability.} \]
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 $A^*_N,m(\omega)$.

Approximate $\mathbb{E}(A^*_N)$ by

$$I_M = \frac{1}{M} \sum_{m=1}^{M} A^*_N,m(\omega).$$
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 \( A^*_{N,m}(\omega) \).

Approximate \( \mathbb{E}(A^*_N) \) by

\[
I_M = \frac{1}{M} \sum_{m=1}^{M} A^*_{N,m}(\omega).
\]

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

\[
\left| \mathbb{E}([A^*_N]_{ij}) - [I_M]_{ij} \right| \leq 1.96 \frac{\sqrt{\text{Var}([A^*_N]_{ij})}}{\sqrt{M}}.
\]
In practice, on a typical example

$\bar{I}_M \approx \mathbb{E}(A_{N}^{*})_{11}$ (along with confidence intervals) for a given number $M$ of realizations, and several sizes for $Q_N$. 

![Graph showing the relationship between number of cells in $Q_N$ and the expected value of $A_{N}^{*}$](image-url)
Objective

\[ A^* - A_N^*(\omega) = A^* - \mathbb{E}[A_N^*] + \mathbb{E}[A_N^*] - A_N^*(\omega) \]

systematic error  
statistical error

- several studies on convergence rates wrt \( N \):
  - Yurinskii 1986, Bourgeat & Piatniski 2004
  - Naddaf & Spencer 1998
  - Gloria & Otto 2011-13

- this is NOT the question we want to address here.

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

Central Limit Theorem (CLT):

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

- Can we reduce the prefactor in the CLT? For the same \( M \) (same cost), get a smaller confidence interval?
Variance reduction using control variate

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

Later, we will take $X(\omega) = [A_N^*(\omega)]_{ij}$ for some $1 \leq i, j \leq d$. 
Estimating $\mathbb{E}(X)$

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

$$I_{MC}^M = \frac{1}{M} \sum_{m=1}^{M} X(\omega_m)$$

that satisfies

$$\left| \mathbb{E}(X) - I_{MC}^M \right| \leq 1.96 \frac{\sqrt{\text{Var}(X)}}{\sqrt{M}}$$
Estimating $\mathbb{E}(X)$

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

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

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

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

where $\rho$ is a **deterministic** parameter.

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

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

- **Accuracy gain** iff $\text{Var}(C) < \text{Var}(X)$. 

F. Legoll, CEMRACS 2013 seminar, 7 August 2013 – p. 15
Choice of the control variate $X_{\text{app}}(\omega)$

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

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

Extreme cases:

- $X_{\text{app}}$ is deterministic: then $C(\omega) = X(\omega)$ and no gain!

- $X_{\text{app}} = X$: for $\rho = 1$, $C$ is deterministic (hence small variance!), but the algorithm requires $\mathbb{E}[X_{\text{app}}] = \mathbb{E}(X)$, which is what we are looking for! Not practical!

In general, we need something in-between (problem-dependent).
Choice of the deterministic parameter $\rho$

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

We wish to minimize the variance of $C$.

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

  $$\rho_{\text{opt}} = \frac{\text{Cov}(X, X_{\text{app}})}{\text{Var}(X_{\text{app}})}$$

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

- For this optimal choice of $\rho$,

  $$\frac{\text{Var}(C)}{\text{Var}(X)} = 1 - \left( \frac{\text{Cov}(X, X_{\text{app}})}{\text{Var}(X) \text{ Var}(X_{\text{app}})} \right)^2 < 1$$

  The more $X$ and $X_{\text{app}}$ are correlated, the better!
A weakly stochastic case:
Rare defects in a periodic structure

A. Anantharaman and C. Le Bris,
– SIAM MMS 9 (2011)

Our aim wrt variance reduction: build a surrogate model close to $A_N^*(\omega)$.
A defect model (A. Anantharaman and C. Le Bris, CRAS 2010)

\[ A_{\text{per}}: \text{fiber} \]
\[ A_{\text{per}} + C_{\text{per}} = \text{Id} : \text{no fiber (defect)} \]

\[ A(x, \omega) = A_{\text{per}}(x) + b_\eta(x, \omega)C_{\text{per}}(x) \]

where \( A_{\text{per}} \) and \( C_{\text{per}} \) are both \( \mathbb{Z}^d \)-periodic, and
\[ b_\eta(x, \omega) = \sum_{k \in \mathbb{Z}^d} 1_{Q+k}(x) B^k_\eta(\omega), \quad Q = (0,1)^d, \]

where \( \{B^k_\eta\}_{k \in \mathbb{Z}^d} \) are i.i.d. random variables:
\[ \mathbb{P}(B^k_\eta = 1) = \eta, \quad \mathbb{P}(B^k_\eta = 0) = 1 - \eta. \]

When \( \eta \) is a small parameter, \( A = A_{\text{per}} \) “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 $B^n_k$ ($0$: fiber; $1$: no fiber = defect) in each cell $k$ of $Q_N$. 
Genericity of the setting

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

Then

\[ A(x, \omega) = A_{\text{per}}(x) + b \eta(x, \omega) C_{\text{per}}(x) \]

with

\[ A_{\text{per}}(x) = \alpha, \quad A_{\text{per}}(x) + C_{\text{per}}(x) = \beta, \quad \eta = 1/2. \]
Homogenized matrix expansion (Anantharaman Le Bris, CRAS 2010)

- Approximate homogenized matrix:

\[
A_N^*(\omega)p = \frac{1}{|Q_N|} \int_{Q_N} A(y, \omega) \left( \nabla w^N_p(y, \omega) + p \right) \, dy
\]

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

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

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

\[
\mathbb{E}[A_N^*] = \sum_{\omega \text{ s.t. 0 defect}} A_N^*(\omega)\mathbb{P}(\omega) + \sum_{\omega \text{ s.t. 1 defect}} A_N^*(\omega)\mathbb{P}(\omega) + \ldots
\]

\[
= (1 - \eta)^{N^d} A^*_\text{per} + \sum_{k \in I_N} \eta(1 - \eta)^{N^d - 1} A_N^*(1 \text{ defect in } k) + \ldots
\]

\[
= A^*_\text{per} + \eta A^{*,N}_1 + \eta^2 A^{*,N}_2 + O(\eta^3)
\]
\[ E[A_N^*] = A_{\text{per}}^* + \eta A_{1}^{*,N} + \eta^2 A_{2}^{*,N} + \cdots \]

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

\[ -\text{div} \left[ A_{\text{per}} \left( p + \nabla w_0^p \right) \right] = 0, \quad w_0^p \text{ is } Q\text{-periodic} \]

and

\[ A_{\text{per}}^* p = \int_Q A_{\text{per}}(\nabla w_0^p + p). \]
\[ E[A_N^*] = A_{\text{per}}^* + \eta \overline{A}_{1}^{*,N} + \eta^2 \overline{A}_{2}^{*,N} + \cdots \]

\[
\overline{A}_{1}^{*,N} p = \frac{1}{|Q_N|} \sum_{k \in I_N} \left[ \int_{Q_N} A_1^k (\nabla w_{p,k}^1 + p) - \int_{Q_N} A_{\text{per}} (\nabla w_0^p + p) \right]
\]

\[
= \frac{1}{|Q_N|} \sum_{k \in I_N} A_1^{1,\text{def}} p
\]

where \(w_0^p\) is the periodic corrector (no defect) and \(w_{p,k}^1\) is the corrector associated to

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

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

\(w_{p,k}^1\) is \(Q_N\)-periodic.

Remark: here, due to periodic BC, \(A_1^{1,\text{def}}\) independent of \(k\).
\[ \mathbb{E}[A^*_N] = A^*_\text{per} + \eta A^*_{1,N} + \eta^2 A^*_{2,N} + \cdots \]

\[ A^*_{1,N} \mathcal{P} = \frac{1}{|Q_N|} \sum_{k \in I_N} A^\text{1\,def}_k \mathcal{P} \]

where \( A^\text{1\,def}_k \) is the marginal contribution of a single defect in \( k \).
\[ \mathbb{E} [A_N^*] = A_{\text{per}}^* + \eta A_1^{*,N} + \eta^2 A_2^{*,N} + \cdots \]

\[
A_1^{*,N} p = \frac{1}{|Q_N|} \sum_{k \in I_N} A_{k}^{1 \text{def}} p
\]

where \( A_{k}^{1 \text{def}} \) is the marginal contribution of a single defect in \( k \).

Similar expression for second order:

\[
A_2^{*,N} p = \frac{1}{2|Q_N|} \sum_{k \neq \ell} A_{k,\ell}^{2 \text{def}} p
\]

Marginal contribution from pairs of defects.
\( \mathbb{E} [A_N^*] = A_{\text{per}}^* + \eta A_{1}^{*,N} + \eta^2 A_{2}^{*,N} + \cdots \)

\[
A_{1}^{*,N} p = \frac{1}{|Q_N|} \sum_{k \in I_N} A_{1}^{\text{def},k} p
\]

where \( A_{1}^{\text{def},k} \) is the marginal contribution of a single defect in \( k \).

Similar expression for second order:

\[
A_{2}^{*,N} p = \frac{1}{2|Q_N|} \sum_{k \neq \ell} A_{2}^{\text{def},k,\ell} p
\]

Marginal contribution from pairs of defects.

Possible to use a Reduced Basis approach to compute \( w_{2,k,\ell}^P \), corrector associated to

\[
A_{2}^{k,\ell} = A_{\text{per}} + \mathbf{1}_{Q+k} C_{\text{per}} + \mathbf{1}_{Q+\ell} C_{\text{per}}.
\]

C. Le Bris and F. Thomines, CAM 2012.
A control variate approach

Joint work with W. Minvielle.

Our aim: at any given $N$, compute $\mathbb{E}(A_N^*)$ more efficiently.
Control variate - 1

\[ \mathbb{E} [A^*_N] = A^*_\text{per} + \eta A^*_{1,N} + \eta^2 A^*_{2,N} + \cdots \]

where

\[ \eta A^*_{1,N} = \eta \frac{\eta}{|Q_N|} \sum_{k \in I_N} A_k^{1,\text{def}} \]

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

We see that

\[ \eta A^*_{1,N} = \mathbb{E} [A^*_{1,N}] \]

where

\[ A^*_{1,N} (\omega) = \frac{1}{|Q_N|} \sum_{k \in I_N} B_k^\eta (\omega) A_k^{1,\text{def}} \]

where \( B_k^\eta = 1 \) if defect in cell \( Q + k \) (which happens with probability \( \eta \)).
\[ \mathbb{E} [A^*_N] = A^*_{\text{per}} + \eta A^{*,N}_1 + \eta^2 A^{*,N}_2 + \cdots \]

We introduce
\[ A^*_{\text{app}}(\omega) := A^*_{\text{per}} + A^{*,N}_1(\omega) \quad \text{with} \quad A^{*,N}_1(\omega) := \frac{1}{|Q_N|} \sum_{k \in I_N} B_k^\eta(\omega) \ A_k^{1,\text{def}}, \]

notice that
\[ \mathbb{E} [A^*_N] = \mathbb{E} [A^*_{\text{app}}] + \eta^2 A^{*,N}_2 + \cdots \]

and think of \( A^*_{\text{app}}(\omega) \) as a good approximation of \( A^*_N(\omega) \).

This is confirmed by the fact that, for any function \( \varphi \),
\[ \mathbb{E} [\varphi (A^*_N)] = \mathbb{E} [\varphi (A^*_{\text{app}})] + O(\eta^2). \]
Control variate - 3

Procedure:

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

$$C^*_N(\omega) = A^*_N(\omega) - \rho \left( A^*_\text{per} + A^*_1,N(\omega) - \mathbb{E} \left[ A^*_\text{per} + A^*_1,N(\omega) \right] \right)$$

with $A^*_1,N(\omega) = \frac{1}{|Q_N|} \sum_{k \in I_N} B^k_\eta(\omega) A_k^{1,\text{def}}$ (expectation analyt. computable).
\[ C_N^*(\omega) = A_N^*(\omega) - \rho \left( A_{\text{per}}^* + A_{1,N}^*(\omega) - \mathbb{E} \left[ A_{\text{per}}^* + A_{1,N}^*(\omega) \right] \right) \]

- Expect \( A_{\text{app}}^*(\omega) = A_{\text{per}}^* + A_{1,N}^*(\omega) \) to be a good approx. of \( A_N^*(\omega) \) (at least for \( \eta \ll 1 \)).

- Observe that \( \mathbb{E} \left[ A_N^*(\omega) \right] = \mathbb{E} \left[ C_N^*(\omega) \right] \)

- **IDEA:** approximate \( \mathbb{E} \left[ A_N^*(\omega) \right] = \mathbb{E} \left[ C_N^*(\omega) \right] \) by

\[
J_M = \frac{1}{M} \sum_{m=1}^{M} C_N^*(\omega_m) \quad \left[ \text{Confidence interval: } \text{Var} \ C_N^* \right]
\]
Control variate - 4

\[ C^*_N(\omega) = A^*_N(\omega) - \rho \left( A^*_{\text{per}} + A^{*,N}_1(\omega) - \mathbb{E} \left[ A^*_{\text{per}} + A^{*,N}_1(\omega) \right] \right) \]

- Expect \( A^*_{\text{app}}(\omega) = A^*_{\text{per}} + A^{*,N}_1(\omega) \) to be a good approx. of \( A^*_N(\omega) \) (at least for \( \eta \ll 1 \)).

- Observe that \( \mathbb{E} [A^*_N(\omega)] = \mathbb{E} [C^*_N(\omega)] \)

- IDEA: approximate \( \mathbb{E} [A^*_N(\omega)] = \mathbb{E} [C^*_N(\omega)] \) by

\[ J_M = \frac{1}{M} \sum_{m=1}^{M} C^*_N(\omega_m) \quad \left[ \text{Confidence interval: } \mathbb{V} \text{ar } C^*_N \right] \]

Optimal \( \rho \) that minimizes the variance of (an entry of the matrix) \( C^*_N \):

\[ \rho_{\text{opt}} = \frac{\text{Cov}(A^*_N, A^{*,N}_1)}{\text{Var}(A^{*,N}_1)} \quad \text{well approx. by empirical mean} \]

F. Legoll, CEMRACS 2013 seminar, 7 august 2013 – p. 30
Control variate based on second order approximation - 1

\[ \mathbb{E}[A_N^*] = A_{\text{per}}^* + \eta A_{1,N}^* + \eta^2 A_{2,N}^* + \cdots \]

where

\[ \eta^2 A_{2,N}^* = \frac{\eta^2}{2|Q_N|} \sum_{k \neq \ell} A_{2,\text{def}}^{k,\ell} \]

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

\[ \eta^2 A_{2,N}^* = \mathbb{E}[A_{2,N}^*] \]

where

\[ A_{2,N}^*(\omega) = \frac{1}{2|Q_N|} \sum_{k \neq \ell} B_{\eta}^k(\omega) B_{\eta}^\ell(\omega) A_{2,\text{def}}^{k,\ell} \]

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

\[ A_{\text{app}}^*(\omega) := A_{\text{per}}^* + A_{1,N}^*(\omega) + A_{2,N}^*(\omega) \]

is such that \( \mathbb{E}[A_N^*] = \mathbb{E}[A_{\text{app}}^*] + O(\eta^3) \).
Second order control variate approach:

\[
C_N^*(\omega) = A_N^*(\omega) - \rho \left( A_{\text{per}}^* + A_1^{*,N}(\omega) - \mathbb{E} [...]\right) - \rho_2 A_2^{*,N}(\omega) - \mathbb{E} [...]
\]

For any entry \(1 \leq i, j \leq d\), optimal parameters \(\rho\) and \(\rho_2\) by minimizing \(\text{Var}(C_N^*_{ij})\) (inverse a \(2 \times 2\) 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:

\[
C_N^*(\omega) = A_N^*(\omega) - \rho \left( A_{\text{per}}^* + A_1^{*,N}(\omega)\right) - \rho_2 A_{2, \text{ wrt } \eta=0}^{*,N}(\omega)
- \rho_3 A_{2, \text{ wrt } \eta=1}^{*,N}(\omega) - \mathbb{E} [...]
\]
Numerical test case

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

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

Not always clear to decide who is the defect / background (e.g. when \( \eta = 1/2 \)).
Small contrast test case: \((\alpha, \beta) = (3,23)\) - Homogenized coefficient

Blue curve: standard Monte Carlo estimator

\[ I_M^{MC} = M^{-1} \sum_{m=1}^{M} A_N^*(\omega_m) \]

Black curves: weakly stochastic approximation (expansion wrt \(\eta = 0\) or \(\eta = 1\)): inaccurate when \(0.4 \leq \eta \leq 0.7\).
**Ratios** \( \frac{\text{Var}(A_N^*)}{\text{Var}(C_N^*)} \equiv \text{CPU time gain} \)

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: $(\alpha, \beta) = (3, 23)$ - Efficiency at $\eta = 1/2$

\[ C_N^*(\omega) = A_N^*(\omega) - \rho \left( A_{\text{per}}^* + A_{1, N}^*(\omega) - \mathbb{E} [... \right) \]

- $\rho_2 \left( A_{2, \text{wrt. } \eta=0}^* N(\omega) - \mathbb{E} [... \right) - \rho_3 \left( A_{2, \text{wrt. } \eta=1}^* N(\omega) - \mathbb{E} [... \right) \]

Control variate using first order approximation ($\rho_2 = \rho_3 = 0$):
- variance ratio = 6
- computing the control variate is inexpensive, hence
  \[ \text{CPU time gain} = \text{Variance ratio} = 6 \]

Control variate using second order approximation (optimal $\rho$, $\rho_2$ and $\rho_3$):
- variance ratio = 44
- using a RB approach (Le Bris & Thomines, 2012), computing the control variate is inexpensive:
  \[ \text{CPU time gain} = \text{Variance ratio} = 44 \]
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: \((\alpha, \beta) = (3, 103)\) - Homogenized coefficient

Blue curve: standard Monte Carlo estimator

\[ I^\text{MC}_M = M^{-1} \sum_{m=1}^{M} A^*_N(\omega_m) \]

Black curves: weakly stochastic approximation (with \(\alpha\) or \(\beta\) 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 $\mathbb{E}[A^*_N]$:

- **Standard Monte Carlo** approach with $M$ realizations:
  
  Error $\approx$ statistical error $\propto \sqrt{\text{Var}(A^*_N)/M} \propto \sqrt{\eta/M}$
Quantitative estimation of the variance reduction ($\eta \ll 1$)

Three approaches to compute $\mathbb{E}[A_N^\ast]$:

- **Standard Monte Carlo** approach with $M$ realizations:

  \[
  \text{error} = \text{statistical error} \propto \sqrt{\text{Var}(A_N^\ast)/M} \propto \sqrt{\eta/M}
  \]

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

  \[
  \text{error} = \text{statistical error} \propto \sqrt{\text{Var}(C_N^\ast)/M} \propto \sqrt{\eta^2/M}
  \]

At equal cost, more accurate than Monte Carlo.
Quantitative estimation of the variance reduction \((\eta \ll 1)\)

Three approaches to compute \(\mathbb{E}[A_N^*]\):

- **Standard Monte Carlo** approach with \(M\) realizations:
  
  \[
  \text{error} = \text{statistical error} \propto \sqrt{\text{Var}(A_N^*)/M} \propto \sqrt{\eta/M}
  \]

- **Control Variate** approach (first order) with \(M\) realizations:
  
  \[
  \text{error} = \text{statistical error} \propto \sqrt{\text{Var}(C_N^*)/M} \propto \sqrt{\eta^2/M}
  \]

  At equal cost, more accurate than Monte Carlo.

- **Expansion** of \(\mathbb{E}[A_N^*]\) (Anantharaman / Le Bris) using the same information as the Control Variate approach:
  
  \[
  \mathbb{E}[A_N^*] = A_{\text{per}}^* + \eta \overline{A}_1^* + O(\eta^2), \quad \text{error} = \text{systematic error} \propto \eta^2.
  \]

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

Regime of interest for our CV approach: \(\eta\) neither close to 0 nor 1.
Conclusions

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

- When none of the phase dominates ($\eta \approx 1/2$), the defect model becomes inaccurate per se, but remains useful as a control variate. In a nutshell: use a weakly stochastic model to improve efficiency for fully stochastic cases.

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

- Review article:
  Anantharaman, Costaouec, Le Bris, L., Thomines, in *Lecture Notes Series*, National University of Singapore 2011.

- Variance reduction using antithetic variables:

- Multi-Level Monte Carlo approach:
  Efendiev, Kronsbein, L., arXiv 1301.2798

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