Stochastic homogenization: Study of fluctuations

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Outline

Introduction to stochastic homogenization

The goal is to solve efficiently the following problem:

Oscillating problem

$$\begin{cases} -\operatorname{div}[A(\frac{\cdot}{\varepsilon},\omega)\nabla u_\varepsilon(\cdot,\omega)] = f \quad \text{in} \quad D \\ u_\varepsilon(\cdot,\omega) \in H_0^1(D) \end{cases}$$

where D is a regular bounded domain in $\mathbb{R}^d$ ($\varepsilon \ll diam(D)$), $f \in L^2(D)$ and the matrix A is random, elliptic, bounded and stationary.

Main issues to solve numerically with standard FE methods:

- Need to discretize D at scale ε to get an accurate solution
- The coefficients are random so many realizations are necessary to estimate the law of the solution u_ε

Question: How to approximate the solution when $\varepsilon \ll diam(D)$?

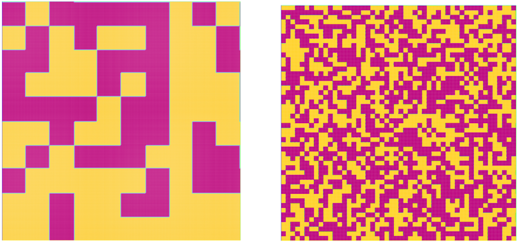


Figure: Two checkerboard random realizations: $\varepsilon = \frac{1}{10}$(left) and $\frac{1}{50}$(right)

Theorem (Stochastic homogenization)

If A is bounded, elliptic and stationary then:

$$u_\varepsilon(\cdot,\omega) \underset{\varepsilon\to 0}{\overset{L^2(D)}{\longrightarrow}} u^\star \ a.s$$

$$\nabla u_\varepsilon(\cdot,\omega) \underset{\varepsilon\to 0}{\overset{L^2(D)^d}{\rightharpoonup}} \nabla u^\star \ a.s$$

with $u^\star$ solution of the following deterministic PDE with constant coefficients:

$$\begin{cases} -\operatorname{div}[A^\star \nabla u^\star] = f \ \text{ in } D, \\ u^\star \in H_0^1(D). \end{cases}$$

The homogenized matrix $A^\star$ is defined by

$$A^\star_{i,j} = \mathbb{E}[\int_Q (\nabla w_i(\cdot,\omega) + e_i) \cdot A(\cdot,\omega)(\nabla w_j(\cdot,\omega) + e_j)]$$

where $Q = (0,1)^d$ and w_i is the corrector in the e_i direction, solution to:

Corrector problem

$$\begin{cases} -\operatorname{div}[A(\cdot,\omega)(\nabla w_i(\cdot,\omega) + e_i)] = 0 \quad \text{in } \mathbb{R}^d \\ \nabla w_i \quad \text{stationary} \\ \mathbb{E}[\int_Q \nabla w_i] = 0 \end{cases}$$

How to compute $A^\star$

- The corrector equation is defined on $\mathbb{R}^d$: impossible to solve numerically and no analytic expression
- Numerical approximation w_i^N on the truncated domain $Q_N = (-N, N)^d$ solution to:

$$\begin{cases} -\operatorname{div}[A(\cdot,\omega)(\nabla w_i^N(\cdot,\omega) + e_i)] = 0 \quad \text{in } Q_N \\ w_i^N \quad Q_N\text{-periodic} \end{cases}$$

$A^\star$ is approximated by the following formula:

$$\boxed{{A^\star}_{i,j}^N(\omega) = \frac{1}{|Q_N|} \int_{Q_N} (\nabla w_i^N(\cdot,\omega) + e_i) \cdot A(\cdot,\omega)(\nabla w_j^N(\cdot,\omega) + e_j)}$$

Question: Knowing $u_\varepsilon(\cdot,\omega)$ is random, what is its law? How does $u_\varepsilon(\cdot,\omega)$ fluctuate around its mean behavior?

Study of fluctuations : Theoretical framework

First, we consider the problem

$$-\operatorname{div}_{\varepsilon}[A(\frac{\cdot}{\varepsilon},\omega)\nabla_{\varepsilon}u_{\varepsilon}(\cdot,\omega)] = f \quad \text{in } \mathbb{R}^d$$

for some appropriate f, where ∇_{ε} is a finite difference operator. In contrast to our problem, this problem is a discrete PDE posed in $\mathbb{R}^d$.

Our quantity of interest is:

$$\boxed{I^{\varepsilon}(g) = \varepsilon^{-\frac{d}{2}} \int_{\mathbb{R}^d} (u_{\varepsilon}(\cdot,\omega) - \mathbb{E}[u_{\varepsilon}])g}$$

For some given g, $I^{\varepsilon}(g)$ allows to study the fluctuations of u_{ε} locally around its mean.

It can be shown that the fluctuations of I^ε depend on:

- The corrected energy density function $\rho_{i,j}$:
  $\rho_{i,j} = (\nabla w_i + e_i) \cdot A(\nabla w_j + e_j) - \nabla w_i \cdot A^\star e_j - \nabla w_j \cdot A^\star e_i$
- $u^\star$ and $v^\star$, the solutions of the homogenized problem with right-hand side f and g respectively.

Denoting $Q_L = (-L, L)^d$, a fourth order tensor $\mathcal{Q}$, that governs the fluctuations and is independent from f and g, can be computed from ρ:

$$\mathcal{Q}_{i,j,k,l} = \lim_{L \to \infty} \mathcal{Q}^L_{i,j,k,l}$$

$$\mathcal{Q}^L_{i,j,k,l} = \mathrm{Cov}\left(\int_{Q_L} \rho_{i,j}, \frac{1}{|Q_L|} \int_{Q_L} \rho_{k,l} \right)$$

Theorem (for discrete PDE's, Duerinckx et al, 2016)

For $d \geq 2$, $I^\varepsilon(g)$ converges in law, when $\varepsilon \to 0$, towards a Gaussian r.v.:

$$I^\varepsilon(g) \xrightarrow[\varepsilon \to 0]{\mathcal{L}} \mathcal{N}(0, \sigma^2)$$

with the variance σ^2 defined by:

$$\sigma^2 = \int_{\mathbb{R}^d} (\nabla u^\star \otimes \nabla v^\star) : \mathcal{Q} : (\nabla u^\star \otimes \nabla v^\star)$$

and $\mathcal{Q}$ defined by:

$$\mathcal{Q}_{i,j,k,l} = \lim_{L \to \infty} \mathrm{Cov}\left(\int_{Q_L} \rho_{i,j}, \frac{1}{|Q_L|} \int_{Q_L} \rho_{k,l} \right)$$

Theorem's consequences

Knowing $\mathcal{Q} \implies$ knowing the fluctuations of I^{ε} for all f and g

But some questions arise:

1. How to compute $\mathcal{Q}$ efficiently? $\mathcal{Q}$ is indeed very challenging to compute:
   - w_i and $A^{\star}$ not computable so need to approximate them by w_i^N and $A_N^{\star}(\omega)$
   - Need a lot of realizations to compute the covariance accurately
2. Theoretical result for discrete PDE's posed on $\mathbb{R}^d$. Extension of this result to continuous PDE's posed on bounded domains?

The multi-dimension case: a perturbative setting

We consider the problem $-\operatorname{div}[A(\frac{\cdot}{\varepsilon},\omega)\nabla u_\varepsilon(\cdot,\omega)] = f$ in D with A such as:

- $A(x,\omega) = A_{per}(x) + \eta \sum_{k\in\mathbb{Z}^d} \mathbb{1}_{Q+k}(x) X_k(\omega) I_d$, with $\eta \ll 1$ and X_k centered i.i.d

We then expand our values of interest in power of η:

$$\begin{cases} I^\varepsilon(g) = \varepsilon^{-\frac{d}{2}} \int_D (u_\varepsilon - \mathbb{E}[u_\varepsilon])g = \eta I_1^\varepsilon(g) + h.o.t \\ \rho_{i,j} = \rho_{i,j}^{per} + \eta\rho_{i,j}^1 + h.o.t. \\ \mathcal{Q}_{i,j,k,l}^L = \mathrm{Cov}\left(\int_{Q_L} \rho_{i,j}, \frac{1}{|Q_L|}\int_{Q_L} \rho_{k,l}\right) = \eta^2 \mathcal{Q}_{i,j,k,l}^{L,1} + h.o.t. \\ \sigma_L^2 = \int_D (\nabla u^\star \otimes \nabla v^\star) : \mathcal{Q}^L : (\nabla u^\star \otimes \nabla v^\star) = \eta^2 \sigma_{L,1}^2 + h.o.t \end{cases}$$

The multi-dimension case: a perturbative setting

Theorem

If we are in the perturbative case, then:

$$I^{\varepsilon}(g) = \eta I_1^{\varepsilon}(g) + h.o.t, \quad \sigma_L^2 = \eta^2 \sigma_{L,1}^2 + h.o.t$$

and

$$I_1^{\varepsilon}(g) \xrightarrow[\varepsilon \to 0]{\mathcal{L}} \mathcal{N}(0, \sigma_1^2)$$

$$\sigma_1 = \lim_{L \to \infty} \sigma_{L,1}$$

At the leading order in η the result of Duerinckx et al. again holds.

Numerical results

Numerical results

Goal : Find an estimate of the localized fluctuations of u_ε without solving the oscillating problem for any right-hand side f.

Main steps of the approach

1. Compute an estimate of $A^\star$ and $\mathcal{Q}$
2. Choose the relevant localization function g
3. Approximate the variance of I_ε with the variance

$$\sigma^2_{priori} = \int_D \nabla u^\star \otimes \nabla v^\star : \mathcal{Q} : \nabla u^\star \otimes \nabla v^\star$$

Challenges to estimate $\mathcal{Q}$:

- $\rho_{i,j}$ depends on $A^\star$, w_i and w_j random functions $\Longrightarrow$ approximate with truncated corrector w_i^N.
- Compute covariance $\Longrightarrow$ many realizations of $\int_{Q_L} \rho_{i,j}$.

Approach to estimate $\mathcal{Q}$

Main steps to approximate $\mathcal{Q}$:

1. Choose the truncated domain Q_N, the integration domain $Q_L \subset Q_N$ and the number of realizations M
2. Solve in parallel $w_i^N(\cdot, \omega_m)$ for $1 \leq m \leq M$
3. Compute in parallel $\displaystyle\int_{Q_L} \rho_{i,j}^N(x, \omega_m) dx$ for $1 \leq m \leq M$
4. Compute $\mathcal{Q}_M^{N,L} = \widehat{\mathrm{Cov}}_M \left(\int_{Q_L} \rho_{i,j}^N, \frac{1}{|Q_L|} \int_{Q_L} \rho_{k,l}^N \right)$

As a result $\mathcal{Q}$ is approximated by $\mathcal{Q}_M^{N,L}$

2D full stochastic case: random checkerboard

$D = (0,1)^2$, A is chosen to be a random checkerboard: for each square of size ε, $A = 0.2 I_2$ and $A = 1.8 I_2$ with probability $\frac{1}{2}$.

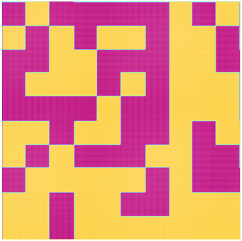
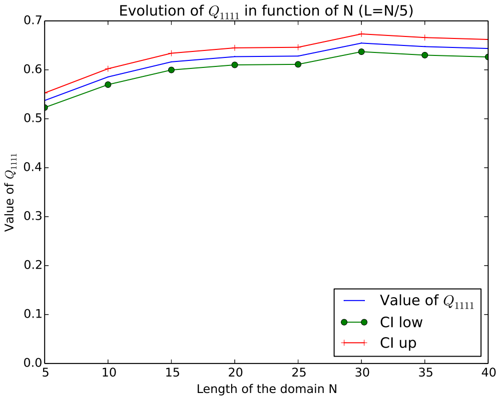


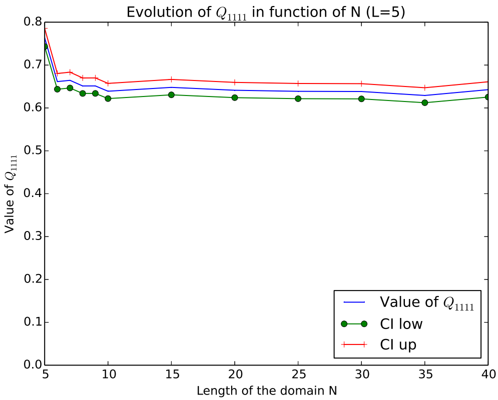
Figure: Two realizations of the checkerboard with $\varepsilon = \frac{1}{10}$ (left), $\frac{1}{50}$ (right)

Evolution of the approximation $\mathcal{Q}_M^{N,L}$ $(N = 5L,\ M = 10^4)$



With N significantly larger than L $(N = 5L)$ the approximation is stable for $N \geq 30$

Evolution of the approximation $\mathcal{Q}_M^{N,L}$ $(L = 5,\ M = 10^4)$



If L is fixed, the approximation $\mathcal{Q}_M^{N,L}$ is stable for $N \geq 3L$

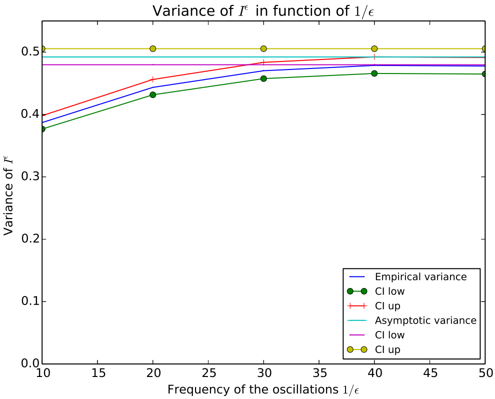
Verification of the approach

The approach has been rigorously proved in the weakly stochastic setting. We here consider a full stochastic case and numerically check that $\mathrm{Var}(I^\varepsilon) \underset{\varepsilon \to 0}{\longrightarrow} \sigma^2$

Procedure:

1. Choose g and f
2. Compute many realizations of I^ε by solving the PDE for u_ε
3. Build the corresponding empirical variance estimator σ^ε_{emp}
4. Estimate $\mathcal{Q}$ with $\mathcal{Q}^{N,L}_M$ for large N, L and M
5. Compute $\sigma^{N,L}_M$
6. Compare σ^ε_{emp} and $\sigma^{N,L}_M$

Results for Dirichlet BC



Empirical and Asymptotic values quite close for $\varepsilon \leq \frac{1}{40}$

Conclusion and future work

Numerical part:

- $\sigma_M^{N,L}$ is a good approximation of $\sigma_{emp}^{\varepsilon}$ when $N,L,M \gg 1$ and $\varepsilon \ll 1$ even in a full stochastic case.
- $\mathcal{Q}$ is accurately approximated by $\mathcal{Q}_M^{N,L}$ for affordable L and N; currently the appropriate value for M is too large.

Theoretical part:

- Study carried out in the 1D and weakly random (for $d \geq 2$) cases
- Understand how to choose the different numerical parameters (N, L and M) in relation to one another

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