Stochastic homogenization: Study of fluctuations

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Outline

1. Introduction to stochastic homogenization
2. Theoretical study
3. Numerical results
The goal is to solve efficiently the following problem:

\[
\begin{cases}
- \text{div} [A(\cdot, \omega) \nabla u_{\varepsilon}(\cdot, \omega)] = f \quad \text{in} \quad D \\
u_{\varepsilon}(\cdot, \omega) \in H^1_0(D)
\end{cases}
\]

where \( D \) is a regular bounded domain in \( \mathbb{R}^d \) (\( \varepsilon \ll \text{diam}(D) \)), \( f \in L^2(D) \) 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 $\varepsilon$ to get an accurate solution
- The coefficients are random so many realizations are necessary to estimate the law of the solution $u_\varepsilon$

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

**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:

$$u_\varepsilon(\cdot, \omega) \xrightarrow[\varepsilon \to 0]{L^2(D)} u^* \text{ a.s}$$

$$\nabla u_\varepsilon(\cdot, \omega) \xrightarrow[\varepsilon \to 0]{L^2(D)^d} \nabla u^* \text{ a.s}$$

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

$$\begin{cases}
-\text{div}[A^* \nabla u^*] = f \text{ in } D, \\
u^* \in H^1_0(D).
\end{cases}$$
The homogenized matrix $A^*$ is defined by

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

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

**Corrector problem**

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

- The corrector equation is defined on $\mathbb{R}^d$: impossible to solve numerically and no analytic expression

- Numerical approximation $w^N_i$ on the truncated domain $Q_N = (-N, N)^d$ solution to:

$$\begin{cases} 
- \text{div}[A(\cdot, \omega)(\nabla w^N_i(\cdot, \omega) + e_i)] = 0 & \text{in } Q_N \\
 w^N_i & \text{$Q_N$-periodic}
\end{cases}$$

$A^*$ is approximated by the following formula:

$$A^*_{i,j}^N(\omega) = \frac{1}{|Q_N|} \int_{Q_N} (\nabla w^N_i(\cdot, \omega) + e_i) \cdot A(\cdot, \omega)(\nabla w^N_j(\cdot, \omega) + e_j)$$

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

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

for some appropriate \( f \), where \( \nabla_{\varepsilon} \) is a finite difference operator. In contrast to our problem, this problem is a \textit{discrete} PDE posed in \( \mathbb{R}^d \).

Our quantity of interest is:

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

For some given \( g \), \( I^{\varepsilon}(g) \) allows to study the fluctuations of \( u_{\varepsilon} \) locally around its mean.
It can be shown that the fluctuations of $I^c$ depend on:

- The corrected energy density function $\rho_{i,j}$:
  $$\rho_{i,j} = (\nabla w_i + e_i) \cdot A(\nabla w_j + e_j) - \nabla w_i \cdot A^* e_j - \nabla w_j \cdot A^* e_i$$

- $u^*$ and $v^*$, the solutions of the homogenized problem with right-hand side $f$ and $g$ respectively.

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

$$Q_{i,j,k,l} = \lim_{L \to \infty} Q_{L}^{i,j,k,l}$$

$$Q_{L}^{i,j,k,l} = \text{Cov} \left( \int_{Q_L} \rho_{i,j}, \frac{1}{|Q_L|} \int_{Q_L} \rho_{k,l} \right)$$
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.:

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

with the variance \(\sigma^2\) defined by:

\[
\sigma^2 = \int_{\mathbb{R}^d} \left( \nabla u^* \otimes \nabla v^* \right) : Q : \left( \nabla u^* \otimes \nabla v^* \right)
\]

and \(Q\) defined by:

\[
Q_{i,j,k,l} = \lim_{L \to \infty} \text{Cov} \left( \int_{Q_L} \rho_{i,j}, \frac{1}{|Q_L|} \int_{Q_L} \rho_{k,l} \right)
\]
Knowing $Q \implies$ knowing the fluctuations of $I^ε$ for all $f$ and $g$

But some questions arise:

1. How to compute $Q$ efficiently? $Q$ is indeed very challenging to compute:
   - $w_i$ and $A^*$ not computable so need to approximate them by $w_i^N$ and $A^*_N(\omega)$
   - 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

\[- \text{div} [A(\cdot, \omega) \nabla u_\varepsilon(\cdot, \omega)] = f \text{ in } D\]

with \(A\) such as:

\[A(x, \omega) = A_{\text{per}}(x) + \eta \sum_{k \in \mathbb{Z}^d} 1_{Q+k}(x) X_k(\omega) l_d,\]

with \(\eta \ll 1\) and \(X_k\) centered i.i.d.

We then expand our values of interest in power of \(\eta\):

\[
\begin{align*}
I_\varepsilon(g) &= \varepsilon^{-\frac{d}{2}} \int_D (u_\varepsilon - \mathbb{E}[u_\varepsilon])g = \eta I_{1\varepsilon}(g) + h.o.t \\
\rho_{i,j} &= \rho_{i,j}^{\text{per}} + \eta \rho_{i,j}^1 + h.o.t. \\
Q_{i,j,k,l}^L &= \text{Cov} \left( \int_{Q_L} \rho_{i,j}, \frac{1}{|Q_L|} \int_{Q_L} \rho_{k,l} \right) = \eta^2 Q_{i,j,k,l}^{L,1} + h.o.t. \\
\sigma_L^2 &= \int_D (\nabla u^* \otimes \nabla v^*) : Q^L : (\nabla u^* \otimes \nabla v^*) = \eta^2 \sigma_{L,1}^2 + h.o.t
\end{align*}
\]
The multi-dimension case: a perturbative setting

**Theorem**

*If we are in the perturbative case, then:*

\[ I^\varepsilon(g) = \eta I_1^\varepsilon(g) + h.o.t, \quad \sigma^2_L = \eta^2 \sigma_{L,1}^2 + h.o.t \]

*and*

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

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

At the leading order in \( \eta \) the result of Duerinckx et al. again holds.
Numerical results
Numerical results

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

Main steps of the approach

1. Compute an estimate of $A^*$ and $Q$
2. Choose the relevant localization function $g$
3. Approximate the variance of $I_\varepsilon$ with the variance

$$\sigma^2_{\text{prior}} = \int_D \nabla u^* \otimes \nabla v^* : Q : \nabla u^* \otimes \nabla v^*$$

Challenges to estimate $Q$:

- $\rho_{i,j}$ depends on $A^*$, $w_i$ and $w_j$ random functions $\Rightarrow$ approximate with truncated corrector $w_i^N$.
- Compute covariance $\Rightarrow$ many realizations of $\int_{Q_l} \rho_{i,j}$. 
Approach to estimate $Q$

Main steps to approximate $Q$:

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 $\int_{Q_L} \rho_{i,j}^N(x, \omega_m) dx$ for $1 \leq m \leq M$

4. Compute $Q_{M}^{N,L} = \text{Cov}_M \left( \int_{Q_L} \rho_{i,j}^N, \frac{1}{|Q_L|} \int_{Q_L} \rho_{k,l}^N \right)$

As a result $Q$ is approximated by $Q_{M}^{N,L}$
2D full stochastic case: random checkerboard

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

Figure: Two realizations of the checkerboard with \( \varepsilon = \frac{1}{10} \) (left), \( \frac{1}{50} \) (right).
With $N$ significantly larger than $L$ ($N = 5L$) the approximation is stable for $N \geq 30$
Evolution of the approximation $Q_{N,L}^{N,L} (L = 5, M = 10^4)$

If $L$ is fixed, the approximation $Q_{N,L}^{N,L}$ 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 $\text{Var}(I_\varepsilon) \xrightarrow{\varepsilon \to 0} \sigma^2$

Procedure:

1. Choose $g$ and $f$

2. Compute many realizations of $I_\varepsilon$ by solving the PDE for $u_\varepsilon$

3. Build the corresponding empirical variance estimator $\sigma_{emp}^\varepsilon$

4. Estimate $Q$ with $Q_{N,L}^{N,L}$ for large $N$, $L$ and $M$

5. Compute $\sigma_{M}^{N,L}$

6. Compare $\sigma_{emp}^\varepsilon$ and $\sigma_{M}^{N,L}$
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.

- $Q$ is accurately approximated by $Q_{M}^{N,L}$ 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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