Abstracts

Characterizing fluctuations in stochastic homogenization

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(joint work with Mitia Duerinckx)

Let $\boldsymbol{a}$ be a uniformly elliptic random coefficient field, which is stationary and ergodic. Given a macroscopic r.h.s. $f = \hat{f}(\frac{\cdot}{L})$, $\hat{f} \in C_0^\infty(\mathbb{R}^d)^d$ deterministic, we consider the equation

$$\nabla \cdot (\boldsymbol{a}\nabla u + f) \,=\, 0 \qquad \text{in } \mathbb{R}^d, \tag{1}$$

and we study macroscopic observables of the form $\int g \cdot \nabla u$ with $g = \hat{g}(\frac{\cdot}{L})$, $\hat{g} \in C_0^\infty(\mathbb{R}^d)^d$ deterministic. Qualitative homogenization theory states that almost surely $L^{-d}\int g\cdot\nabla u - L^{-d}\int g\cdot\nabla\bar{u} \to 0$ as $L \uparrow \infty$, where $\bar{u}$ solves the (deterministic) homogenized equation

$$\nabla \cdot (\bar{\boldsymbol{a}}\nabla \bar{u} + f) \,=\, 0 \qquad \text{in } \mathbb{R}^d,$$

where the homogenized coefficient $\bar{\boldsymbol{a}} \in \mathbb{R}^{d\times d}$ is given by $\bar{\boldsymbol{a}}e_i = \mathbb{E}\left[\boldsymbol{a}(e_i + \nabla\varphi_i)\right]$ in terms of the corrector φ, that is, the solution of $\nabla\cdot\boldsymbol{a}(e_i+\nabla\varphi_i) = 0$ in $\mathbb{R}^d$. A natural concept in homogenization is to compare u to its "two-scale expansion" $(1+\varphi_i\partial_i)\bar{u}$ (using Einstein's summation convention), which captures the oscillations of u to order $O(L^{-1})$, in the sense that the difference between the gradients is of (relative) order $O(L^{-1})$. Such expansions can be pursued to higher order: while φ is characterized by $(1+\varphi_i\partial_i)\bar{\ell}$ being $\boldsymbol{a}$-harmonic for all affine functions $\bar{\ell}$, the second-order corrector φ' (throughout the talk, a prime denotes a second-order object) is characterized by the property that $(1+\varphi_i\partial_i+\varphi'_{ij}\partial^2_{ij})\bar{q}$ is $\boldsymbol{a}$-harmonic for all $\bar{\boldsymbol{a}}$-harmonic quadratic polynomials $\bar{q}$. The second-order two-scale expansion $(1+\varphi_i\partial_i+\varphi_{ij}\partial^2_{ij})\bar{u}'$ then captures the oscillations of u at order $O(L^{-2})$, where $\bar{u}' := \bar{u}+\tilde{u}'$ with $\tilde{u}'$ given by $\nabla\cdot(\bar{\boldsymbol{a}}\nabla\tilde{u}'+\bar{\boldsymbol{a}}'_i\nabla\partial_i\bar{u}) = 0$ and where $\bar{\boldsymbol{a}}'_i \in \mathbb{R}^{d\times d}$ is the second-order homogenized coefficient, see below for a definition. While these error estimates are classical in the periodic setting, they also hold in the random setting for large enough dimension: $O(L^{-1})$ for $d>2$, when φ is stationary; and $O(L^{-2})$ for $d>4$, when φ' is stationary [3]. Here and in the following we assume that $\boldsymbol{a}$ has integrable correlations.

Periodic homogenization is about understanding the oscillations of u by means of two-scale expansions, random homogenization means in addition studying the random fluctuations of the macroscopic observable $\int g\cdot\nabla u$. It was recently shown that the rescaled observable $L^{-d/2}\int g\cdot(\nabla u-\mathbb{E}[\nabla u])$ converges in law to a Gaussian. We may naturally look for a finer description of this convergence by means of a two-scale expansion. As first observed in [2], however, the limiting variance of $L^{-d/2}\int g\cdot\nabla u$ generically differs from that of $L^{-d/2}\int g\cdot\nabla(1+\varphi_i\partial_i)\bar{u}$: when it comes to fluctuations, the two-scale expansion cannot be applied naively. In [1], we unravelled the mechanism behind this observation by means of the "homogenization commutator", which led to a new pathwise theory of fluctuations (see also the pathwise heuristics in [2]). In the present talk we explain how this approach naturally extends to higher orders, in parallel with the known theory of oscillations. For simplicity of exposition, we focus on second order, which is the relevant order for dimension $d = 3$.

Key is the homogenization commutator, which on first-order level takes the form

$$\Xi_k[u] := e_k \cdot (\boldsymbol{a} - \bar{\boldsymbol{a}})\nabla u.$$

This expression is natural: H-convergence is equivalent to convergence of $L^{-d} \int g \cdot \Xi[u]$ to 0. This is made quantitative with help of the flux corrector, a skew-symmetric matrix field σ_i with $\boldsymbol{a}(e_i + \nabla\varphi_i) = \bar{\boldsymbol{a}}e_i + \nabla \cdot \sigma_i$. Indeed, Leibniz' rule yields $\Xi_k[u] = -\nabla \cdot ((\varphi_k^* \boldsymbol{a}^* + \sigma_k^*)\nabla u)$ for any $\boldsymbol{a}$-harmonic u, where φ_k^*, σ_k^* are the correctors for the pointwise transpose field $\boldsymbol{a}^*$. As the r. h. s. is in divergence form and φ_k^*, σ_k^* are stationary for $d > 2$, it is of order $O(L^{-1})$ with g. For a higher-order theory, we need a second-order extension of Ξ:

$$\Xi_k'[u] := e_k \cdot (\boldsymbol{a} - \bar{\boldsymbol{a}})\nabla u + \bar{\boldsymbol{a}}_k^{*\prime} e_l \cdot \nabla\partial_l u,$$

which, for $\boldsymbol{a}$-harmonic u, indeed satisfies the corresponding identity $\Xi_k'[u] = \partial_l \nabla\big((\varphi_{kl}^{*\prime}\boldsymbol{a}^* + \sigma_{kl}^{*\prime})\nabla u\big)$, where the r.h.s. is now of order $O(L^{-2})$ for dimension $d > 4$, when also $\varphi^{*\prime}, \sigma^{*\prime}$ are stationary. The identity follows from the characterizing property of φ', σ', and $\bar{a}'$, namely $(\phi_i a - \sigma_j)e_j = \bar{\boldsymbol{a}}_i' e_j - \boldsymbol{a}\nabla\varphi_{ij}' + \nabla \cdot \sigma_{ij}'$, which also yields $\bar{\boldsymbol{a}}_i' e_j = \mathbb{E}\left[(\phi_i a - \sigma_j)e_j + \boldsymbol{a}\nabla\varphi_{ij}'\right]$. Next, we define suitable two-scale expansions of these objects. For the first order, we simply inject the first-order two-scale expansion of ∇u into $\Xi[\cdot]$ and set

$$\Xi_k^\circ[\bar{u}] := e_k \cdot (\boldsymbol{a} - \bar{\boldsymbol{a}})(e_i + \nabla\varphi_i)\partial_i \bar{u},$$

which alternatively is characterized by $\Xi^\circ[\bar{u}](x) = \Xi[(1 + \varphi_i\partial_i)T_x\bar{u}](x)$, where $T_x\bar{u}$ denotes the first-order Taylor polynomial of $\bar{u}$ at x. For the second order, we similarly define

$$\Xi^{\circ\prime}[\bar{u}'](x) := \Xi[(1 + \varphi_i\partial_i + \varphi_{ij}\partial_{ij})T_x'\bar{u}'](x),$$

where $T_x'\bar{u}'$ is the second-order Taylor polynomial of $\bar{u}'$ at x. The above defined $\Xi[\cdot]$ and $\Xi^\circ[\cdot]$ (resp. $\Xi'[\cdot]$ and $\Xi^{\circ\prime}[\cdot]$) are viewed as a first-order (resp. second-order) differential operators with (distributional) stationary random coefficients.

Theorem. *It holds*

$$\mathrm{Var}\left[L^{-\frac{d}{2}}\int g \cdot \nabla u - L^{-\frac{d}{2}}\int \nabla\bar{v}' \cdot \Xi'[u]\right]^{\frac{1}{2}}$$

$$+\,\mathrm{Var}\left[L^{-\frac{d}{2}}\int g \cdot \Xi'[u] - L^{-\frac{d}{2}}\int g \cdot \Xi^{\circ\prime}[\bar{u}']\right]^{\frac{1}{2}} \lesssim_{\hat{f},\hat{g}} \begin{cases} L^{-\frac{3}{2}}\log L & : d = 3; \\ L^{-2}\log L & : d = 4; \\ L^{-2} & : d > 4; \end{cases}$$

where $\bar{v}' := \bar{v} + \tilde{v}'$ *with* $\nabla \cdot (\bar{\boldsymbol{a}}^*\nabla\bar{v} + g) = 0$ *and* $\nabla \cdot (\bar{\boldsymbol{a}}^*\nabla\tilde{v}' + \bar{\boldsymbol{a}}_i^{*\prime}\nabla\partial_i\bar{v}) = 0$.

The above result splits into two parts: 1) The fluctuations of macroscopic observables can be recovered from those of $\Xi'[\cdot]$ by a suitable Helmholtz-type projection with an error of order $O(L^{-\frac{d}{2}})$ up to logarithmic corrections (the stated estimate saturates at $d=4$, starting from $d>4$, third-order correctors should be taken into account and so forth). 2) The second-order two-scale expansion $\Xi^{\circ\prime}[\cdot]$ of the homogenization commutator $\Xi'[\cdot]$ is accurate in the fluctuation scaling at order $O(L^{-\frac{d}{2}})$. We focus here on the second part, the first part follows from a direct computation. Combining the two parts leads to a second-order pathwise theory of fluctuations: the fluctuations of all macroscopic observables are almost surely determined up to order $O(L^{-\frac{d}{2}}\log L)$ (here only for $d\le 4$) by the fluctuations of the new intrinsic quantity $\Xi^{\circ\prime}[\cdot]$. In dimension $d=3$, the above yields a full pathwise description of the fluctuations of $L^{-d}\int g\cdot\nabla u$ with accuracy $O(L^{-d}\log L)$, that is, the square of the CLT scaling! In upcoming work we establish this result in any dimension, and that fluctuations of $\Xi^{\circ\prime}[\cdot]$ are asymptotically Gaussian.

For the proof, we focus on the model setting $\boldsymbol{a}(x):=h(G(x))$ for some smooth map h and Gaussian random field G with integrable covariance function, in which case a Malliavin calculus is available on the probability space and substantially simplifies the analysis. In particular, for any random variable X, a Poincaré inequality holds in the form $\mathrm{Var}\,[X]\le C\mathbb{E}\left[\int|\delta X/\delta\boldsymbol{a}|^2\right]$, where $\delta X/\delta\boldsymbol{a}$ denotes the functional (Malliavin) derivative of X with respect to $\boldsymbol{a}$. Key is a representation formula for the infinitesimal variation of the two-scale expansion error $\Xi'[u]-\Xi^{\circ\prime}[\bar u']$. We start with the infinitesimal variation of $\Xi'[u]$:

$$\text{(2)}\quad \delta\Xi_k'[u] = (e_k+\nabla\varphi_k^*)\cdot\delta\boldsymbol{a}\nabla u-\partial_l\big((\varphi_k^*e_l+\nabla\varphi_{kl}^{*\prime})\cdot\delta\boldsymbol{a}\nabla u\big) + \partial_l\nabla\cdot\big((\varphi_{kl}^{*\prime}\boldsymbol{a}+\sigma_{kl}^{*\prime})\nabla\delta u\big)+\partial_l\nabla\cdot\big(\varphi_{kl}^{*\prime}\delta\boldsymbol{a}\nabla u\big).$$

We argue that the last two terms lead to a contribution of order $O(L^{-2})$. First note that (1) yields $\nabla\cdot(\boldsymbol{a}\nabla\delta u+\delta\boldsymbol{a}\nabla u)=0$, so that $\nabla\delta u$ essentially behaves like $\delta\boldsymbol{a}\nabla u$, and hence we may focus on the last term in (2). Applying Poincaré's inequality to $X:=L^{-d/2}\int g\cdot\Xi'[u]$, the contribution of it is estimated by $L^{-d}\mathbb{E}\left[\int|\nabla^2 g|^2|\varphi^{*\prime}|^2|\nabla u|^2\right]$. Using the stationarity of the corrector $\varphi^{*\prime}$ for $d>4$ and the equation for u, this is essentially estimated by $L^{-d}\int|\nabla^2 g|^2|f|^2\lesssim_{\hat f,\hat g}(L^{-2})^2$ as claimed. The only important terms in (2) are thus the first two. Next, applying identity (2) to the two-scale expansions $(1+\varphi_i\partial_i)\bar\ell$ and $(1+\varphi_i\partial_i+\varphi_{ij}'\partial_{ij})\bar q$ with first- and second-order polynomials $\bar\ell$ and $\bar q$, and suitably arranging the terms, we find

$$\delta\Xi_k^{\circ\prime}[\bar u'] = (e_k+\nabla\varphi_k^*)\cdot\delta\boldsymbol{a}\nabla(1+\varphi_i\partial_i+\varphi_{ij}'\partial_{ij})\bar u' - \partial_l\big((\varphi_k^*e_l+\nabla\varphi_{kl}^{*\prime})\cdot\delta\boldsymbol{a}\nabla(1+\varphi_i\partial_i)\bar u\big)+O(L^{-2}).$$

Subtracting this identity from (2), and recognizing the two-scale errors $\nabla u-\nabla(1+\varphi_i\partial_i)\bar u=O(L^{-1})$ and $\nabla u-\nabla(1+\varphi_i\partial_i+\varphi_{ij}'\partial_{ij})\bar u'=O(L^{-2})$, the conclusion follows in the form $\mathrm{Var}\left[L^{-d/2}\int g\cdot(\Xi'[u]-\Xi^{\circ\prime}[\bar u'])\right]\lesssim_{\hat f,\hat g}(L^{-2})^2$.

References

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[3] P. Bella, B. Fehrman, J. Fischer, F. Otto, *Stochastic homogenization of linear elliptic equations: higher-order error estimates in weak norms via second-order correctors*, SIAM J. Math. Analysis, **49**, 2016.

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