GAMM-workshop in UQ, TU Dortmund

Characterization of fluctuations in stochastic homogenization

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Random medium ...

symmetric coefficient field a = a(x) on *d*-dimensional space $\lambda |\xi|^2 \leq \xi \cdot a(x)\xi \leq |\xi|^2$ for all points x and vectors ξ

 \rightsquigarrow uniformly elliptic operator $-\nabla\cdot a\nabla u$

Ensemble $\langle \cdot \rangle$ of such coefficient fields a

Example of ensemble $\langle \cdot \rangle$: points Poisson distributed with density 1, union of balls of radius $\frac{1}{4}$ around points, a = id on union, $a = \lambda id$ on complement,



Stationarity: a and $a(y + \cdot)$ have same distribution under $\langle \cdot \rangle$

 \dots = elliptic operator with random stationary coefficient field

Plan for talk

1) Error in Representative Volume Element (RVE) Method: Scaling of random and systematic contribution in terms of RVE-size

2) Fluctuations of macroscopic observables: leading-order pathwise characterization RVE method for extraction

Representative Volume Element method to extract effective tensor \bar{a} : Scaling of random and systematic error in RVE size Gloria, Neukamm

Goal: Extract effective behavior \bar{a} from $\langle \cdot \rangle$...

Recall example of ensemble $\langle \cdot \rangle$: points Poisson distributed with density 1, union of balls of radius $\frac{1}{4}$ around points, a = id on union, $a = \lambda id$ on complement,



ensemble $\langle \cdot \rangle$ \rightsquigarrow effective conductivity \overline{a} $\begin{cases}
\text{density of points 1} \\
\text{radius of inclusions } \frac{1}{4} \\
\text{conductivity in pores } \lambda
\end{cases} \quad \Rightarrow \quad \overline{a} = \begin{pmatrix} \overline{a}_{11} & \overline{a}_{12} \\ \overline{a}_{21} & \overline{a}_{22} \end{pmatrix} = \overline{\lambda} \text{ id}$ $3 \text{ numbers} \quad \rightsquigarrow \quad 1 \text{ number}$

... via Representative Volume Element (RVE)

Representative Volume Element method

Introduce artificial period L

Periodized ensemble $\langle \cdot \rangle_L$ points Poisson distributed with density 1, on *d*-dimensional torus $[0, L)^d$ union of balls of radius $\frac{1}{4}$ around points, a = id on union, $a = \lambda id$ on complement,



Given coordinate direction $i = 1, \dots, d$ seek *L*-periodic φ_i with

$$-\nabla \cdot a(e_i + \nabla \varphi_i) = 0$$
 on $[0, L)^d$.

Spatial average $\int_{[0,L)^d} a(e_i + \nabla \varphi_i)$ of flux $a(e_i + \nabla \varphi_i)$ as approximation to $\overline{a}e_i$ for $L \gg 1$;

 φ_i is approximate corrector, e_i unit vector in *i*-th coordinate direction

Solving d elliptic equations $-\nabla \cdot a(e_i + \nabla \varphi_i) = 0$...

direction e_1 potential $x_1 + \varphi_1$ flux $a(e_1 + \nabla \varphi_1)$





direction e_2 potential $x_2 + \varphi_2$

flux $a(e_2 + \nabla \varphi_1)$ simulations by R. Kriemann (MPI)





average flux $f a(e_1 + \nabla \varphi_1)$ $= \begin{pmatrix} 0.49641 \\ -0.02137 \end{pmatrix}$ $\approx \overline{a}e_1$

average flux $f a(e_2 + \nabla \varphi_2)$ $= \begin{pmatrix} -0.02137 \\ 0.53240 \end{pmatrix}$ $\approx \overline{a}e_2$

... gives approximation \bar{a}_L

Random error: approx. \bar{a}_L depends on realization

realization 1 potential, current

realization 2 potential, current



realization 3 potential, current







 $\bar{a}_L = \begin{pmatrix} 0.45101 & 0.01104 \\ 0.01104 & 0.45682 \end{pmatrix}$

 $\overline{a}_L = \left(\begin{array}{c} 0.56213 & 0.00857 \\ 0.00857 & 0.60043 \end{array} \right)$

... and thus fluctuates is random

Fluctuations of \bar{a}_L decrease with increasing L



... scaling of variance $var(\bar{a}_L)$ in L?

Systematic error, decreases with increasing L

Also expectation $\langle \bar{a}_L \rangle_L$ depends on Lsince from $\langle \cdot \rangle$ to $\langle \cdot \rangle_L$ statistics are altered by artificial long-range correlations



Scaling of both errors in L ...

Pick *a* according to $\langle \cdot \rangle_L$, solve for φ (period *L*), compute spatial average $\bar{a}_L e_i := \int_{[0,L)^d} a(e_i + \nabla \varphi_i)$

Take random variable \bar{a}_L as approximation to \bar{a}

$$\langle \operatorname{error}^2 \rangle_L = \operatorname{random}^2 + \operatorname{systematic}^2$$
:
 $\langle |\overline{a}_L - \overline{a}|^2 \rangle_L = \operatorname{var}_{\langle \cdot \rangle_L} [\overline{a}_L] + |\langle \overline{a}_L \rangle_L - \overline{a}|^2$

Qualitative theory yields:

 $\lim_{L\uparrow\infty} \operatorname{var}_{\langle\cdot\rangle_L}[\bar{a}_L] = 0, \quad \lim_{L\uparrow\infty} \langle \bar{a}_L \rangle_L = \bar{a}$

... why rate is of interest?

Number of samples N vs. artificial period L

Take **N** samples, i. e. independent picks $a^{(1)}, \dots, a^{(N)}$ from $\langle \cdot \rangle_L$. Compute empirical mean $\frac{1}{N} \sum_{n=1}^{N} f_{[0,L)d} a^{(n)} (e_i + \nabla \varphi_i^{(n)})$

 $\langle \text{total error}^2 \rangle_L = \frac{1}{N} \text{random error}^2 + \text{systematic error}^2$

L ↑ reduces systematic error and random error

N ↑ reduces only effect of random error



An optimal result

Let $\langle \cdot \rangle_L$ be ensemble of *a*'s with period *L*, with $\langle \cdot \rangle_L$ suitably coupled to $\langle \cdot \rangle$

For *a* with period *L* solve $\nabla \cdot a(e_i + \nabla \varphi_i) = 0$ for φ_i of period *L*. Set $\bar{a}_L e_i = \int_{[0,L)^d} a(e_i + \nabla \varphi_i)$.

Theorem [Gloria&O.'13, G.&Neukamm&O. Inventiones'15]

Random error² = $\operatorname{var}_{\langle \cdot \rangle_L} [\bar{a}_L] \leq C(d,\lambda) L^{-d}$ Systematic error² = $|\langle \bar{a}_L \rangle_L - \bar{a}|^2 \leq C(d,\lambda) L^{-2d} \ln^d L$

Gloria&Nolen '14: (random) error approximately Gaussian Fischer '17: variance reduction

State of art in quantitative stochastic homogenization ...

Yurinskii '86 : suboptimal rates in L for mixing $\langle \cdot \rangle$

Naddaf & Spencer '98, & Conlon '00: optimal rates for small contrast $1 - \lambda \ll 1$, for $\langle \cdot \rangle$ with spectral gap

Gloria & O. '11, & Neukamm '13, & Marahrens '13: optimal rates for all $\lambda > 0$ for $\langle \cdot \rangle$ with spectral gap, Logarithmic Sobolev (concentration of measure)

Armstrong & Smart '14, & Mourrat '14, & Kuusi '15, Gloria & O. '15

optimal stochastic integrability for finite range $\langle \cdot \rangle$

Gaussianity of error: Biskup & Salvi & Wolf '14, Rossignol '14, Nolen '14

... of linear equations in divergence form

Homogenization error on macroscopic observables Characterization of leading-order variances via a pathwise characterization of leading-order fluctuations Duerinckx, Gloria

Macroscopic r. h. s. and observable ...

solution u of $\nabla \cdot a \nabla u = \nabla \cdot f$, where r. h. s. $f(x) = \hat{f}(\frac{x}{L})$ deterministic macroscopic observable $\int g \cdot \nabla u$, where $g(x) = L^{-d} \hat{g}(\frac{x}{L})$ deterministic



Marahrens & O.'13: $\operatorname{var}(\int g \cdot \nabla u) = O(\frac{1}{L^d})$

Goal: Characterize limiting variance $\lim_{L\uparrow\infty} L^d \operatorname{var}(\int g \cdot \nabla u)$

Naive approach via two-scale expansion

Goal: Characterize limiting variance $\lim_{L\uparrow\infty} L^d \operatorname{var}(\int g \cdot \nabla u)$ Corrector φ_i corrects affine x_i such that $-\nabla \cdot a(e_i + \nabla \varphi_i) = 0$

for coordinate direction $i = 1, \dots, d$

Solution \overline{u} of homogenized equation $\nabla \cdot (\overline{a} \nabla \overline{u} + f) = 0$

Compare u to "two-scale expansion" $(1 + \varphi_i \partial_i) \overline{u}$ Einstein's summation rule



Naively expect $\operatorname{var}(\int g \cdot \nabla u) = \operatorname{var}(\int \nabla \cdot g u) \approx \operatorname{var}(\int \nabla \cdot g (1 + \varphi_i \partial_i) \overline{u})$ Hence study asymptotic covariance $\langle \varphi_i(x - y) \varphi_j(0) \rangle$

The subtle role of the two-scale expansion

Mourrat&O.'14: $\lim_{L\uparrow\infty} L^{d-2} \langle \varphi_i(L(\hat{x}-\hat{y}))\varphi_j(0) \rangle$ exists, but \neq a Green function $\bar{G}(\hat{x}-\hat{y})$ (Gaussian free field) Helffer-Sjöstrand, annealed Green's function bounds \rightsquigarrow 4-tensor \bar{Q}

Gu&Mourrat'15:
$$\lim_{L\uparrow\infty} L^d \operatorname{var}(\int g \cdot \nabla u)$$
 exists,
but $\neq \lim_{L\uparrow\infty} L^d \operatorname{var}(\int \nabla \cdot g (1 + \varphi_i \partial_i) \overline{u})$
Helffer-Sjöstrand \rightsquigarrow same 4-tensor \overline{Q} , Gaussianity, heuristics
i. e. two-scale expansion cannot be applied naively

Duerinckx&Gloria&O.'16: Two-scale expansion $\nabla u \approx \partial_i \bar{u}(e_i + \nabla \varphi_i)$ ok on level of "commutator" $\underline{a} \nabla u - \bar{a} \nabla u \approx \partial_i \bar{u} (\underline{a(e_i + \nabla \varphi_i) - \bar{a}(e_i + \nabla \varphi_i)})$ flux field $=: \equiv_i$

Leading-order fluctuation of macro observables ... $\Xi e_i = a(e_i + \nabla \varphi_i) - \overline{a}(e_i + \nabla \varphi_i)$ stationary tensor field I) $a\nabla u - \bar{a}\nabla u \approx \equiv \nabla \bar{u}$ holds in quantitative sense of L^{d} var $(\int g \cdot (a \nabla u - \overline{a} \nabla u - \Xi \nabla \overline{u})) = O(L^{-2})$, which implies L^{d} var $\left(\int g \cdot \nabla u - \int \nabla \overline{v} \cdot \Xi \nabla \overline{u}\right) = O(L^{-2}),$ where \overline{v} solves dual equation $\nabla \cdot (\overline{a}^* \nabla \overline{v} + g) = 0$ II) \equiv is local, ie $\equiv (a, x)$ depends little on a(y) for $|y - x| \gg 1$, $\Xi \approx$ tensorial white noise on large scales thus more precisely, $L^d | var(\int g \cdot \Xi f) - \int f \otimes g : \overline{Q} f \otimes g | = O(L^{-2})$ for four-tensor \overline{Q} from Mourrat&O. I)&II) $L^d |var(\int g \cdot \nabla u) - \int \nabla \overline{v} \otimes \nabla \overline{u} : \overline{Q} \nabla \overline{v} \otimes \nabla \overline{u} | = O(L^{-2})$... characterized via homogenization commutator

How to extract \bar{Q} from $\langle \cdot \rangle$?

Homogenization commutator $\equiv e_i = a(e_i + \nabla \varphi_i) - \bar{a}(e_i + \nabla \varphi_i)$

$$L^{d} \operatorname{var} \left(\int g \cdot \nabla u - \int \nabla \overline{v} \cdot \Xi \nabla \overline{u} \right) = O(L^{-2}), \quad \nabla \cdot (\overline{a}^{*} \nabla \overline{v} + g) = 0$$
$$L^{d} \left| \operatorname{var} \left(\int g \cdot \Xi f \right) - \int f \otimes g : \overline{Q} f \otimes g \right| = O(L^{-2})$$

Duerinckx&Gloria&O.'17: $|L^{d} \operatorname{var}_{\langle \cdot \rangle_{L}}(\bar{a}_{L}) - \bar{Q}| \leq C(d, \lambda) L^{-d} \ln^{d} L ,$

recall: $\langle \cdot \rangle_L$ ensemble of *a*'s with period *L*, solve $\nabla \cdot a(e_i + \nabla \varphi_i) = 0$ for φ_i of period *L*, Set $\bar{a}_L e_i = \oint_{[0,L)^d} a(e_i + \nabla \varphi_i)$.



In practise: Extract \bar{Q} from RVE ...

Recall periodized ensemble $\langle \cdot \rangle_L$ $\bar{a}_L e_i = \int_{[0,L)^d} a(e_i + \nabla \varphi_i)$ Previous result: $|\langle \bar{a}_L \rangle_L - \bar{a}|^2 \lesssim L^{-2d} \ln^d L$ Duerinckx&Gloria&O.'17: $|L^d \operatorname{var}_{\langle \cdot \rangle_L}(\bar{a}_L) - \bar{Q}|^2 \lesssim L^{-d} \ln^d L$ Hence get \bar{a} and \bar{Q} by same procedure: $N \sim L^{\frac{d}{2}}$ independent samples $\{a^{(n)}\}_{n=1,\dots,N}$ from $\langle \cdot \rangle_L$

$$ig\langle ig| rac{1}{N} \sum_{n=1}^{N} ar{a}_{L}^{(n)} - ar{a} ig|^{2} ig
angle_{L} \lesssim L^{-2d} \ln^{d} L, \ ig\langle ig| rac{L^{d}}{N-1} \sum_{m=1}^{N} ig(ar{a}_{L}^{(m)} - rac{1}{N} \sum_{n=1}^{N} ar{a}_{L}^{(n)} ig)^{\otimes 2} - ar{Q} ig|^{2} ig
angle_{L} \lesssim L^{-d} \ln^{d} L$$

... at no further cost than \bar{a}

Back to numerical example

$$N \sim L^{\frac{d}{2}} \text{ independent samples } \{a^{(n)}\}_{n=1,\cdots,N} \text{ from } \langle \cdot \rangle_L,$$
$$\Big\langle \Big| \frac{L^d}{N-1} \sum_{m=1}^N (\bar{a}_L^{(m)} - \frac{1}{N} \sum_{n=1}^N \bar{a}_L^{(n)})^{\otimes 2} - \bar{Q} \Big|^2 \Big\rangle_L \lesssim L^{-d} \ln^d L$$



L=20, N=500

$$\bar{Q} = 10^{-2} \times \begin{pmatrix} 1.00 & 0.00 & 0.00 & 0.23 \\ 0.00 & 0.56 & 0.23 & 0.00 \\ 0.00 & 0.23 & 0.56 & 0.00 \\ 0.23 & 0.00 & 0.00 & 1.01 \end{pmatrix}$$

Higher order comes naturally, i. e. 2nd order

2nd-order two-scale expansion: $u \approx (1+\phi_i\partial_i+\phi'_{ij}\partial_{ij})\bar{u}'$, where $\bar{u}' := \bar{u} + \tilde{u}'$ with $\nabla \cdot (a\nabla \tilde{u}' + \bar{a}'_i\nabla \partial_i \bar{u}) = 0$ and tensor \bar{a}'_i is 2nd-order homogenized coefficient.

k-the component of 2nd-order commutator: $\Xi'_{k}[u] := e_{k} \cdot (a - \bar{a}) \nabla u + \bar{a}_{k}^{*'} e_{l} \cdot \nabla \partial_{l} u,$ characterized by $\Xi_{k}[u] = \nabla^{2}$: something for *a*-harmonic *u*

Inject: $\equiv 0'[\bar{u}](x) := \equiv [(1+\phi_i\partial_i+\phi'_{ij}\partial_{ij})T'_x\bar{u}'](x),$ where $T'_x\bar{u}'$ is 2nd-order *Taylor polynomial* of \bar{u}' at x

A relative error of $O(L^{-\frac{d}{2}})$

Recipe: Inject two-scale expansion $(1+\phi_i\partial_i+\phi'_{ij}\partial_{ij})\bar{u}'$ into commutator $\Xi'_k[u] := e_k \cdot (a-\bar{a})\nabla u + \bar{a}_k^{*'}e_l \cdot \nabla \partial_l u$, in sense of $\Xi^{0'}[\bar{u}](x) := \Xi'[(1+\phi_i\partial_i+\phi'_{ij}\partial_{ij})T'_x\bar{u}'](x)$

Duerinckx&O.'18
$$(d = 3)$$
:
 $L^{d} \operatorname{var}(\int g \cdot \nabla u - \int \nabla \overline{v}' \cdot \Xi'[u])$
 $+ L^{d} \operatorname{var}(\int g \cdot \Xi'[u] - \int g \cdot \Xi^{0'}[\overline{u}]) \leq C(d, \lambda) L^{-d}$
where $\overline{v}' = \overline{v} + \widetilde{v}'$ with $\nabla \cdot (\overline{a}^* \nabla \widetilde{v}' + a_k^* \nabla \partial_k \overline{v}) = 0$

Relies on stochastic estimates of ϕ'_{ii} (Gu, Bella&Fehrman&Fischer&O)

Helpful tool: Flux correctors ...

1st-order:
$$ae_i = \bar{a}e_i - a\nabla\phi_i + \nabla\sigma_i$$
, σ_i skew,
2nd-order: $(\phi_i a - \sigma_i)e_j = \bar{a}'_i e_j - a\nabla\phi'_{ij} + \nabla \cdot \sigma'_{ij}$

2nd-order two-scale expansion; for \bar{a} -harmonic \bar{u} : $\nabla \cdot a \nabla (1 + \phi_i \partial_i + \phi'_{ij} \partial_{ij}) \bar{u}' = \nabla \cdot ((\phi'_{ij} a - \sigma'_{ij}) \nabla \partial_{ij} \bar{u}' + \bar{a}'_i \nabla \partial_i \tilde{u}'),$

2nd-order commutator; for a^* -harmonic u: $e_k \cdot (a - \bar{a}) \nabla u + a_k^{*'} e_l \cdot \nabla \partial_l u = \partial_l \nabla \cdot \left((\phi_{kl}^{*'} a + \sigma_{kl}^{*'}) \nabla u \right)$

stochastic estimates: σ_i, σ'_{ij} like ϕ_i, ϕ_{ij} (Gloria&Neukamm&O.'13)

... bring residue in divergence-form

Helpful tool: Malliavin calculus and spectral gap

Spectral gap: $\operatorname{var}(F) \leq \langle \int |\frac{\partial F}{\partial a}|^2 dx \rangle$ random variable F = functional of a, Malliavin-derivative = functional derivative

For 1st-order
$$F := \int g \cdot (a - \overline{a}) (\nabla u - \partial_i \overline{u} (e_i + \nabla \phi_i))$$

Crucial formula:
$$\delta a$$
 infinitesimal perturbation of a

$$\delta \Big(e_j \cdot (a - \bar{a}) \Big(\nabla u - \partial_i \bar{u} (e_i + \nabla \phi_i) \Big) \Big)$$

$$= \underbrace{(e_j + \nabla \phi_j^*)}_{O(1)} \cdot \delta a \Big(\underbrace{\nabla u - \partial_i \bar{u} (e_i + \nabla \phi_i)}_{O(L^{-1} \nabla \bar{u})} \Big)$$

$$- \underbrace{\nabla \cdot \Big((\phi_j^* a + \sigma_j^*) \underbrace{\nabla \delta u}_{O(1)} \Big) + \partial_i \bar{u} \nabla \cdot \Big((\phi_j^* a + \sigma_j^*) \underbrace{\nabla \delta \phi_i}_{O(\delta a)} \Big)$$

$$- \nabla \cdot \Big(\phi_j^* \delta a \nabla u \Big) + \partial_i \bar{u} \nabla \cdot \Big(\phi_j^* \delta a (e_i + \nabla \phi_i) \Big)$$

Credits

Gaussianity of various errors: Nolen'14 based on Stein/Chatterjee, Biskup&Salvi&Wolf'14, Rossignol'14, ...

Quartic tensor Q via Helffer-Sjöstrand and Mahrarens& O.'13: Mourrat&O'14, Gu&Mourrat'15

Heuristics of a path-wise approach $w/o \equiv$: Gu&Mourrat'15, based on variational approach by Armstrong&Smart '13

 $\nabla \varphi = \bar{a}$ -Helmholtz-projection of white noise: Armstrong&Mourrat&Kuusi'16, Gloria&O.'16 based on finite range rather than Spectral Gap

Summary

1) Error in Representative Volume Element (RVE) Method, Scaling of random $var(\bar{a}_L)$ and systematic contribution $\langle \bar{a}_L \rangle - \bar{a}$ in terms of RVE-size L

2) Fluctuations of macroscopic observables $\int g \cdot \nabla u$, leading-order pathwise characterization via two-scale expansion used on level of commutator Ξ in terms of fourth-order tensor \overline{Q} extract from RVE at no additional cost Natural higher-order versions