Fluctuation in random homogenization: motivations, corrector theory, and algorithm test

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Outline

- Motivations
  - Uncertainty quantification
  - PDE-based Inverse problems
  - Test algorithms
- Corrector theory for elliptic equations with stochastic multiscale potential
  - Corrector theory for random diffusion, 1D only
  - Corrector theory for elliptic equations with random potential .
  - Important factor: short-range v.s. long-range correlations
  - Important factor: Singularity of Green's function
- Corrector test for multiscale algorithms
  - Well-known benchmark: capturing homogenization
  - A new benchmark: capturing fluctuation ?
  - Some results

Typical problems

- Homogenization

$$F(D^2u_\varepsilon, Du_\varepsilon, u_\varepsilon, x, \frac{x}{\varepsilon}, \omega) = 0 \Longrightarrow \overline{F}(D^2u_0, Du_0, u_0, x, \omega) = 0.$$

e.g., Dirichlet problem of stationary diffusion

$$-\nabla \cdot A\left(\frac{x}{\varepsilon}, \omega\right) \cdot \nabla u_\varepsilon(x, \omega) = f(x) \Longrightarrow -A^* : D^2u_0 = f(x).$$

- Randomness is parametrized by (y, ω). Here y set to be $\frac{x}{\varepsilon}$, multi-scale (two-scale).
- e.g., $A(y, \omega)$ a random field in $(\Omega, \mathcal{F}, \mathbb{P})$ valued in uniformly elliptic matrices.
- Just mild conditions: stationarity and ergodicity. The underlying mechanism is essentially Law of large numbers, Birkhoff's ergodic theorem.

Typical problems

- Corrector Theory: $u_\varepsilon - u_0$.
  - Convergence rate: $\mathbb{E}\|u_\varepsilon - u_0\|_{L^2}^2 \le \varepsilon^\gamma$.
  - Statistics of the corrector.

$$u_\varepsilon - u_0 = (\mathbb{E}u_\varepsilon - u_0) + (u_\varepsilon - \mathbb{E}u_\varepsilon).$$

    That is, a decomposition into deterministic and stochastic correctors.

  - Want to write

$$u_\varepsilon(x) - u_0(x) = \varepsilon^{\gamma_1}(\text{deterministic}) + \varepsilon^{\gamma_2}(\text{mean-zero random}).$$

  - Limit of the deterministic corrector
  - Limit distribution of the random corrector

$$\frac{u_\varepsilon - \mathbb{E}u_\varepsilon}{\varepsilon^{\gamma_2}} \xrightarrow[\varepsilon\to 0]{\text{distr.}} \text{certain statistics, e.g. Gaussian}$$

This requires more information regarding the random field.

Motivation I: Uncertainty quantification

Forward UQ: uncertainty of coefficient propagate to solutions, etc.

- PDE model is given: physics is known .
- Corrector theory provides information about the statistics of solution.
- Good estimate of measurable events, e.g.,

$$\mathbb{P}\{u_\varepsilon(x_0) > \alpha\} \approx ?$$

- In the setting we have, we will see that not much information of the randomness is propagated.
- The limiting distribution depends on u_0 , and integrated information of the randomness.

Motivation II: PDE-based inverse problems

$$
\begin{array}{ccc}
\text{input} : q & \xrightarrow[\text{physics}]{T} & \text{output} : T(q) \\
\Big\| & & \text{noise} \Big\downarrow \text{(observation)} \\
q & & Y = G(q) + E \\
\text{prior} \Big\uparrow & & \Big\uparrow \text{noise model} \\
\pi_{\text{prior}}(q) & & \pi_{\text{noise}}(e)
\end{array}
$$

Then the Bayesian formulation becomes:

$$\pi(q|Y) \propto \pi_{\text{pr}}(q)\pi(Y|q) = \pi_{\text{pr}}(q)\pi_{\text{noise}}(Y - G(q)).$$

Motivation II: PDE-based inverse problems

- Typically in an inverse problem, the high frequency part of q cannot be stably reconstructed.
- Model high frequency effect as noise.
- Corrector theory provides well-tailored noise model.

$$
\begin{array}{lccc}
\text{low frequency} & q & \xrightarrow[\text{physics}]{T} & u_0 \\
 & \text{uncertainty} \downarrow & & \downarrow \text{(observation)} \\
\text{random} & q + q_\varepsilon & \xrightarrow{\text{propagation}} & u_\varepsilon = u_0 + E
\end{array}
$$

Motivation III: Test algorithms

- Numerical schemes have been designed to approximate the homogenized solution without resolving the ε-scale, or calculating the effective coefficients.
- Fluctuation is important sometimes, but can we use these (given by the scheme)?
- To analyze, we want to know what to compare with, i.e., what the corrector is for the continuous equation.
- Multiscale scheme yields u_ε^h; standard scheme for homogenized equation yields u_0^h. Test:

$$\frac{u_\varepsilon^h - u_0^h}{\varepsilon^{\gamma_2}} \xrightarrow[?]{h,\varepsilon\to 0} \mu \xleftarrow{\varepsilon\to 0} \frac{u_\varepsilon - u_0}{\varepsilon^{\gamma_2}}$$

Part II: Corrector theory

- The divergence equation $-\nabla \cdot A\left(\frac{x}{\varepsilon}, \omega\right) \cdot \nabla u_\varepsilon = f$ in 1D
  - · mixing random field with short-range correlation.
  - · function of Gaussian random field with long-range correlation.
- Elliptic equation with multiscale random potential

$$(P(x, D) + q_0(x))u_\varepsilon + q\left(\frac{x}{\varepsilon}, \omega\right) u_\varepsilon = f,$$

with Dirichlet boundary condition.

  - · assume Green's function $\sim |x - y|^{d-\beta}$, the effect of β.

1D divergence equation

$$-\frac{d}{dx}a_\varepsilon(x,\omega)\frac{d}{dx}u_\varepsilon = f(x), x \in (0,1), \quad \text{with Dirichlet boundary.}$$

- Random field model for $a(x,\omega)$
  - Problem is well-posed for almost all realizations. Here, uniform ellipticity, i.e.,
    $$0 < \lambda \leq a(x,\omega) \leq \Lambda.$$
  - Stationarity and ergodicity.
  - Define the harmonic mean ,
    $$a^* := \left(\mathbb{E}\frac{1}{a(0,\omega)}\right)^{-1}, \qquad q(x,\omega) = \frac{1}{a(x,\omega)} - \frac{1}{a^*}.$$
- Then u_ε converges, e.g. in $H^1(0,1)$ for a.e. ω, to $u_0(x)$ which solves the equation with effective coefficient a^*.

Corrector for the 1D divergence equation: Short-range case

Corrector theory requires finer knowledge of q. A standard assumption is:
Strong mixing, ρ-mixing

Strong mixing coefficient $\rho(r)$ is a non-negative function s.t.

$$|\mathbb{E}(\xi\eta) - \mathbb{E}\xi\ \mathbb{E}\eta| \le \rho(r)(\mathrm{Var}\xi\ \mathrm{Var}\eta)^{\frac{1}{2}},$$

for any ξ and η that are $\mathcal{F}_{\le t}$ and $\mathcal{F}_{\ge t+r}$ measurable with finite variance.

- Assumption: $\rho(r) \le Cr^{-\alpha}$ for $\alpha > 1$. [$\alpha > d$ in d-dimension case.]
  In particular, this implies that the (auto)-correlation function

$$R(x) := \mathbb{E}\{q(0)q(x)\},$$

  is integrable. $q(x,\omega)$ is then said to have "short-range correlation".

Corrector for the 1D divergence equation: Short-range case

Theorem [Bourgeat and Piatnitski '99] For short-range correlated field, the convergence rate in $L^2(\Omega, L^2([0,1]))$ is $\sqrt{\varepsilon}$.

$$\mathbb{E}\|u_\varepsilon - u_0\|^2 \leq C\varepsilon\|f\|^2.$$

Further, with the mixing condition, the corrector satisfies

$$\frac{u_\varepsilon(x) - u_0(x)}{\varepsilon^{\frac{1}{2}}} \xrightarrow[\varepsilon\to 0]{\text{distribution}} -\sigma \int_0^1 L(x,t)dW_t.$$

Remark:

- The deterministic corrector is of order ε. The random corrector has variance of order $\sqrt{\varepsilon}$, giving the central limit scaling.
- $\sigma^2 = \int R(x)dx$; strength of correlation.
- W_t is the standard Brownian motion. The integral explicitly determines a Gaussian distribution on $C([0,1])$.
- The mixing condition is needed to apply central limit theorem.
- The kernel $L(x,t) = a^{*2}\partial_y G(x,t)u_0'(t)$.

Corrector for the 1D divergence equation: Long-range case

No CLT available. Consider special model:

· Let $g(x,\omega)$ be a centered unit-variance Gaussian field, with long-range correlation:

$$R_g(x) := \mathbb{E}\{g(y)g(y+x)\} \sim \frac{\kappa_g}{|x|^\alpha}, \alpha < d, \text{ for } |x| \text{ large} .$$

· Let $q(x,\omega) = \Phi(g(x))$ with $\Phi : \mathbb{R} \to \mathbb{R}$ being a nice function satisfying:

$$\mathbb{E}\Phi(g(0)) = 0, \quad \mathbb{E}\{g(0)\Phi(g(0))\} =: V_1 \neq 0 \quad (\text{define } \kappa = \kappa_g V_1^2).$$

The above can be written as:

$$\int_{\mathbb{R}} H_0(x)\Phi(x)d^g x = 0, \quad \int_{\mathbb{R}} H_1(x)\Phi(x)d^g x \neq 0, \quad \{H_n(x)\} \text{ Hermite polynomials.}$$

Define *Hermite rank* to be the index of the first non-zero coefficient in the expansion of Φ in Hermite polynomials. The above condition can be rephrased as: Φ has Hermite rank one .

Corrector for the 1D divergence equation: Long-range case

Theorem [Bal, Garnier, Motsch and Perrier '08] With the special model, the convergence rate in $L^2(\Omega, L^2([0,1]))$ is $\sqrt{\varepsilon^\alpha}$.

$$\mathbb{E}\|u_\varepsilon - u_0\|^2 \leq C\varepsilon^\alpha \|f\|^2.$$

Further, the corrector satisfies

$$\frac{u_\varepsilon(x) - u_0(x)}{\varepsilon^{\frac{\alpha}{2}}} \xrightarrow[\varepsilon\to 0]{\text{distribution}} -\sigma_H \int_0^1 L(x,t) dW_t^H.$$

Remark

- Deterministic corrector is of order ε^α; variance of the random corrector is of order ε^α.
- $H = 1 - \alpha/2$ is called the Hurst index. $\sigma_H^2 = \kappa/H(2H-1)$.
- W_t^H is the standard fractional Brownian motion with Hurst index H. The integral explicitly determines a Gaussian distribution over $C([0,1])$ that has strong correlation.
- This is not central limit *per se*.
- The previous results are convergence in distribution in the space of continuous functions.
- Non-Gaussian corrector if Φ has Hermite rank ≥ 2 .

Corrector for elliptic equation with random potential

Elliptic equation with multiscale stochastic potential

$$P(x,D)u_\varepsilon + (q_0(x) + q_\varepsilon(x,\omega))u_\varepsilon = f, \quad \text{with Dirichlet Boundary.}$$

- The Green's function $G(x,y)$ associated to $P + q_0$ satisfies

  $$|G(x,y)| \leq C|x-y|^{-d+\beta}.$$

  Smaller β corresponds to higher singularity near the origin.
- The random equation is well-posed under mild conditions e.g. $q_0 + q_\varepsilon \geq 0$.
- Solution operator of the random equation can be bounded uniformly in ε.
- Assume $q(x)$ satisfies the condition in item two, in addition to stationarity and ergodicity.

Examples of elliptic equations

For $\beta = 2$, we can consider

$$\begin{cases} (-\Delta + q_0(x))u_\varepsilon + q_\varepsilon(x)u_\varepsilon = f, & x \in X, \\ u = 0, & x \in \partial X. \end{cases}$$

For $\beta < 2$, we can consider

$$\begin{cases} (-(-(-\Delta)^{\frac{\beta}{2}}) + q_0(x))u_\varepsilon + q_\varepsilon(x)u_\varepsilon = f, & x \in X, \\ u = 0, & x \in X^c = \mathbb{R}^d \backslash X. \end{cases}$$

Random fields

- Short-range correlated field
  - ρ-mixing with $\rho(r) \le Cr^{-\alpha}$, $\alpha > d$.
  - Estimates for moments of sufficient order.
  - Superposition of Poisson bumps.
- Long-range correlated field
  - As before $q = \Phi(g)$, $R_g(x) \sim \kappa_g |x|^{-\alpha}$, $\alpha < d$.
  - Further conditions on Φ can lead to estimates of higher order moments, e.g., a control of

$$\mathbb{E}\prod_{i=1}^{4} q(x_i) - \mathbb{E}q(x_1)q(x_2)\mathbb{E}q(x_3)q(x_4) - \mathbb{E}q(x_1)q(x_3)\mathbb{E}q(x_2)q(x_4) \\ -\mathbb{E}q(x_1)q(x_4)\mathbb{E}q(x_2)q(x_3).$$

Corrector for elliptic equation: short-range potential

Theorem [Bal and J. CMS '11] With short-range correlated field, the convergence rate is

$$\mathbb{E}\|u_\varepsilon - u_0\|^2 \le C\|f\|^2 \begin{cases} \varepsilon^{2\beta}, & \text{if } 2\beta < d, \\ \varepsilon^d |\log \varepsilon|, & \text{if } 2\beta = d, \\ \varepsilon^d, & \text{if } 2\beta > d. \end{cases}$$

Further, the following holds in distribution in $L^2(X)$.

$$\frac{u_\varepsilon - \mathbb{E}u_\varepsilon}{\varepsilon^{d/2}} \xrightarrow[\varepsilon\to 0]{\text{distribution}} -\sigma \int_X G(x,y) u_0(y) dW_y.$$

Remark:

- Random corrector has variance of order ε^d, indicating the central limit scaling; deterministic corrector is larger if $\beta < d/2$ (Green's function singular enough).
- Deterministic corrector can be estimated as well. For $P = (-\Delta + \lambda^2)^{-\frac{1}{2}}$ on the whole space $\mathbb{R}^2$, we have $\lim \varepsilon^{-1}(\mathbb{E}u_\varepsilon - u_0) = \varepsilon \tilde{R} \mathcal{G} u_0$ and $\tilde{R} := \int R(y)/2\pi|y|dy$.

Corrector for elliptic equation: long-range potential

Theorem [Bal, Garnier, Gu and J.] With the long-range field and assume $2\beta < d$, the convergence rate (in homogenization) is

$$\mathbb{E}\|u_\varepsilon - u_0\|^2 \le C\|f\|^2 \begin{cases} \varepsilon^\alpha, & \text{if } \alpha < 2\beta, \\ \varepsilon^{2\beta}|\log \varepsilon|, & \text{if } \alpha = 2\beta, \\ \varepsilon^{2\beta}, & \text{if } \alpha > 2\beta. \end{cases}$$

Assume $\alpha < 4\beta$; the following holds in distribution in $L^2(X)$:

$$\frac{u_\varepsilon - \mathbb{E}\{u_\varepsilon\}}{\varepsilon^{\alpha/2}} \xrightarrow[\varepsilon\to 0]{\text{distribution}} -\int_X G(x,y)u_0(y)W^\alpha(dy).$$

Remark:

- The deterministic corrector is of order ε^α or ε^β, whichever is larger.
- Here, $W^\alpha(dy) := \dot{W}^\alpha(y)dy$, and $\dot{W}^\alpha(y)$ is a centered Gaussian field with covariance function $\kappa|x-y|^{-\alpha}$.

Part III: Corrector theory for multiscale algorithms

Given multiscale algorithm, test its ability to capture corrector.

$$\begin{array}{ccc} \dfrac{u_\varepsilon^h - u_0^h}{\varepsilon^{\frac{\alpha\wedge 1}{2}}}(x,\omega) & \xrightarrow[(i)]{h\to 0} & \dfrac{u_\varepsilon - u_0}{\varepsilon^{\frac{\alpha\wedge 1}{2}}}(x,\omega) \\ {\scriptstyle \varepsilon\to 0}\Big\downarrow{\scriptstyle (ii)} & & {\scriptstyle (iii)}\Big\downarrow{\scriptstyle \varepsilon\to 0} \\ \mathcal{U}^h_{\alpha\wedge 1}(x; W^{\alpha\wedge 1}) & \xrightarrow[(iv)]{h\to 0} & \mathcal{U}_{\alpha\wedge 1}(x; W^{\alpha\wedge 1}) \end{array}$$

- Testing on the 1D divergence equation.
- u_ε^h is yielded by a given algorithm; u_0^h is yielded by applying it to the homogenized equation.
- Clearly, (i) and (iii) hold. All convergence are in distribution in $C([0,1])$.

MsFEM: multi-scale finite element method

Weak formulation of the random ODE is $A_\varepsilon(u_\varepsilon, v) = F(v)$,

$$\int_0^1 a_\varepsilon(x) u_\varepsilon'(x) v'(x) = \int_0^1 f(x) v(x), \quad \forall v \in H_0^1.$$

- Finite element: approximate H_0^1; approximate A_ε.
- Standard FEM: $V_0^h \subset H_0^1$; hat base functions; h: discretization size
- MsFEM: multi-scale base function ϕ_ε^j; for each ϕ_0^j, construct

$$\begin{cases} \mathcal{L}_\varepsilon \phi_\varepsilon^j(x) = 0, & x \in I_1 \cup I_2 \cup \cdots \cup I_{N-1}, \\ \phi_\varepsilon^j = \phi_0^j, & x \in \{x_k\}_{k=0}^N. \end{cases}$$

- Linear system:

$$A_\varepsilon^h U^\varepsilon = F^\varepsilon.$$

- Reference: Hou, Wu and Cai ’99; Efendiev and Hou ’09

HMM: heterogeneous multi-scale method

HMM aims to approximate u_0. Given by minimizer of

$$I[u] := \frac{1}{2}A_0(u,u) - F(u) = \frac{1}{2}\int_0^1 a^* \left(\frac{du}{dx}\right)^2 \, dx - \int_0^1 fu \, dx.$$

Approximate bilinear form by

$$A_0(u,u) \approx \sum_{j=1}^N a^*(x^j)\left(\frac{du}{dx}(x^j)\right)^2 h$$

Without calculating a^*, approximate further by

$$A_\varepsilon^\delta(w,v) := \sum_{j=1}^N \frac{h}{\delta}\int_{I_j^\delta} a_\varepsilon \, \frac{d(\mathscr{L}w)}{dx}\frac{d(\mathscr{L}v)}{dx} \, dx.$$

Due to the homogenization result: $a_\varepsilon u_\varepsilon' \xrightarrow{L^2} a^* u_0'$.

HMM continued

The operator $\mathscr{L}$ is defined by

$$\begin{cases} \mathcal{L}_\varepsilon(\mathscr{L}w) = 0, & x \in I_1^\delta \cup \cdots \cup I_{N-1}^\delta, \\ \mathscr{L}w = w, & x \in \{\partial I_j^\delta\}_{j=1}^{N-1}. \end{cases}$$

- I_k^δ: a small patch of size δ inside I_k, $\varepsilon \ll \delta < h$
- HMM: minimization problem with A_ε^δ, in the space V_0^h (hat base functions).
- Equivalent with
$$A_\varepsilon^{h,\delta} U^{\varepsilon,\delta} = F^0.$$

Reference: E, Ming and Zhang '05

The diagram commutes for MsFEM

Theorem [Bal and J., submitted]
(i) In random medium with short range correlation,

$$\frac{u_\varepsilon^h(x) - u_0^h(x)}{\sqrt{\varepsilon}} \xrightarrow[\varepsilon\to 0]{\text{distribution}} \mathcal{U}^h(x;W) \xrightarrow[h\to 0]{\text{distribution}} \mathcal{U}(x;W).$$

$\mathcal{U}^h(x;W)$ is a stochastic integral with integrand $L^h(x,t)$ and Brownian motion integrator.
(ii) In random medium with long range correlation,

$$\frac{u_\varepsilon^h(x) - u_0^h(x)}{\varepsilon^{\frac{\alpha}{2}}} \xrightarrow[\varepsilon\to 0]{\text{distribution}} \mathcal{U}_H^h(x;W^H) \xrightarrow[h\to 0]{\text{distribution}} \mathcal{U}_H(x;W^H).$$

$\mathcal{U}_H^h(x;W^H)$ has fBm integrator. Here,

$$L^h(x,t) = \sum_{k=1}^{N} \mathbf{1}_{I_k}(t) a^{*2} \frac{D^- G_0^h(x,x_k)}{h} \frac{D^- U_k^0}{h} + \text{sth. else}$$

HMM: depends on correlation ranges

Theorem (i) In random medium with short range correlation,

$$\frac{u_\varepsilon^{h,\delta}(x) - u_0^h(x)}{\sqrt{\varepsilon}} \xrightarrow[\varepsilon\to 0]{\text{distribution}} \mathcal{U}^{h,\delta}(x;W) \xrightarrow[h\to 0]{\text{distribution}} \sqrt{\frac{h}{\delta}}\,\mathcal{U}(x;W).$$

$\mathcal{U}^{h,\delta}(x;W)$ is a stochastic integral with integrand $L^{h,\delta}(x,t)$ and Brownian motion integrator.

(ii) In random medium with long range correlation,

$$\frac{u_\varepsilon^{h,\delta}(x) - u_0^h(x)}{\varepsilon^{\frac{\alpha}{2}}} \xrightarrow[\varepsilon\to 0]{\text{distribution}} \mathcal{U}_H^{h,\delta}(x;W^H) \xrightarrow[h\to 0]{\text{distribution}} \mathcal{U}_H(x;W^H).$$

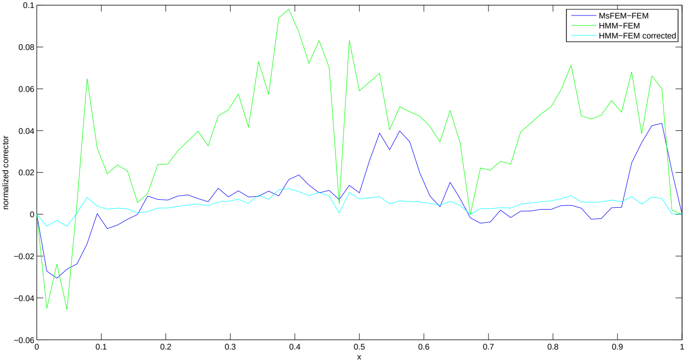
$\mathcal{U}_H^{h,\delta}(x;W^H)$ has fBm integrator. Here,

$$L^{h,\delta}(x,t) = \frac{h}{\delta}\sum_{k=1}^{N} \mathbf{1}_{I_k^\delta}(t)\,\frac{a^* D^- G_0^h(x,x_k)}{h}\,\frac{a^* D^- U_k^0}{h}.$$

Remarks

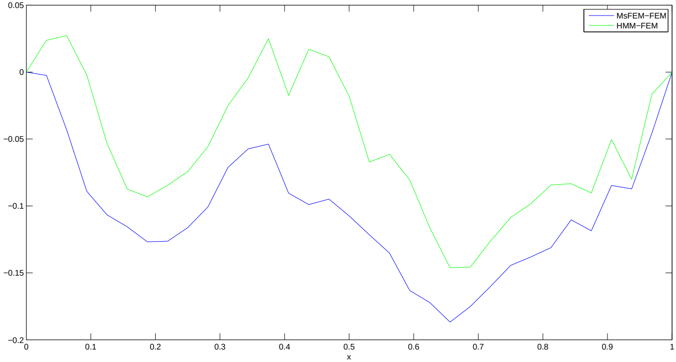
- Roughly, what is happening is: In each interval I_j, we have $X_1^j, \cdots, X_N^j$ be i.d with mean one and variance one; HMM approximate $S_j = \sum X_i^j$ by NX_1^j.
- When $X_1^j, \cdots, X_N^j$ are independent, the variance is amplified by N.
- For long-range media, the fluctuation lives at a macroscopic scale, and the scaling is correct.

- Other schemes; higher dimensional test.



- The equation: $-\frac{d}{dx}a(\frac{x}{\varepsilon},\omega)\frac{d}{dx}u_\varepsilon(x,\omega) = f(x)$, $x \in (0,1)$,
- $f = \cos(\pi x)$, $a^* = 1$, $q(x,\omega)$ is the sign function of a Orstein-Uhlenbeck process. $a(x,\omega) = 1/(q(x,\omega) + a^{*-1})$.
- $h = 2^{-6}$, $\delta = 2^{-9}$, $\varepsilon = 2^{-14}$.

Numerical implementation - II: long-range media



- The equation: $-\frac{d}{dx}a(\frac{x}{\varepsilon},\omega)\frac{d}{dx}u_\varepsilon(x,\omega) = f(x)$, $x \in (0,1)$,
- $f = \cos(\pi x)$, $a^* = 1$, $q(x,\omega)$ is the sign function of fBm increments. $a(x,\omega) = 1/(q(x,\omega) + {a^*}^{-1})$.
- $h = 2^{-5}$, $\delta = 2^{-8}$, $\varepsilon = 2^{-12}$.

Summary

- Corrector theory, i.e., fluctuations about the homogenized solution, has important applications in uncertainty quantification, PDE-based inverse problems, and setting tests for multiscale algorithms.

- For elliptic equations with random multiscale potential, we develop a systematic theory for the corrector. In particular, regularity of the Green's function and correlation range of the random field are important factors.

- We found that multiscale numerical methods that captures homogenization does not necessarily capture the right corrector. In particular, long-range correlations is more "robust" w.r.t. sampling.

THANKS!

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