

*Stochastic homogenization*¹

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¹Course material: S. Armstrong & T. Kuusi & J.-C. Mourrat : Quantitative stochastic homogenization and large-scale regularity, arXiv:1705.05300

Scope

The goal is to introduce basic concepts in stochastic homogenization for linear, uniformly elliptic equations of the form

$$-\nabla \cdot (\mathbf{a}^\varepsilon(x) \nabla u^\varepsilon(x)) = 0 \quad \text{in } U \subseteq \mathbb{R}^d, \quad \varepsilon > 0, \quad d \geq 2,$$

where $\mathbf{a}^\varepsilon(x) := \mathbf{a}(\frac{x}{\varepsilon})$ and the diffusion matrix $\mathbf{a}(\cdot)$ satisfies

$$|\xi|^2 \leq \mathbf{a}(x) \xi \cdot \xi \leq \Lambda |\xi|^2$$

for some $\Lambda \geq 1$ and for all $\xi \in \mathbb{R}^d$ and for almost every $x \in \mathbb{R}^d$.

If you are not familiar with the following concepts, please go through Appendixes from the course book. You should recall

- Basic knowledge about Sobolev spaces
- Knowledge about basic a priori estimates for elliptic equations is useful, but I will also discuss them during the course

Homogenization: Paradigm

Homogenization means that, in an appropriate way, the original equation

$$-\nabla \cdot (\mathbf{a}^\varepsilon(x) \nabla u^\varepsilon(x)) = 0 \quad \text{in } U \subseteq \mathbb{R}^d, \quad \varepsilon > 0, \quad d \geq 2,$$

homogenizes to an *effective* equation

$$-\nabla \cdot (\bar{\mathbf{a}} \nabla \bar{u}) = 0$$

with constant coefficients $\bar{\mathbf{a}}$ such that “ u^ε is close to \bar{u} ”

Two basic questions are:

- When can one expect homogenization? (Qualitative theory)
- How fast is homogenization happening? (Quantitative theory)

When can one expect homogenization?

Model assumptions for coefficients are that \mathbf{a} is

- periodic
- quasi-periodic
- almost periodic
- stationary random fields.

Let us first take a look of the easiest case, namely the periodic setting.
We assume that

$$\mathbf{a}(x + z) = \mathbf{a}(x) \quad \text{for every } x \in \mathbb{Z}^d \text{ and a.e. } x \in \mathbb{R}^d.$$

Periodic 1D

Let $\varepsilon = \frac{1}{k}$, $k \in \mathbb{N}$, and solve an ODE

$$\begin{cases} -(\mathbf{a}^\varepsilon(x)(u^\varepsilon)'(x))' = 0 \\ u^\varepsilon(0) = 0, \quad u^\varepsilon(1) = 1. \end{cases}$$

The unique solution is

$$u(x) = \left(\int_0^1 \frac{1}{\mathbf{a}^\varepsilon(t)} dt \right)^{-1} \int_0^x \frac{1}{\mathbf{a}^\varepsilon(t)} dt,$$

which can equivalently be written as

$$u^\varepsilon(x) = x + \left(\int_0^1 \frac{1}{\mathbf{a}(t)} dt \right)^{-1} \varepsilon \int_0^{x/\varepsilon - \lfloor x/\varepsilon \rfloor} \left(\frac{1}{\mathbf{a}(t)} - \int_0^1 \frac{1}{\mathbf{a}(t)} dt \right) dt$$

Periodic 1D

Set now, for $x \in \mathbb{R}$,

$$\phi(x) := \left(\int_0^1 \frac{1}{\mathbf{a}(t)} dt \right)^{-1} \int_0^{x - [x]} \left(\frac{1}{\mathbf{a}(t)} - \int_0^1 \frac{1}{\mathbf{a}(t)} dt \right) dt$$

The solution u^ε can be written by means of ϕ as

$$u(x) = x + \varepsilon \phi\left(\frac{x}{\varepsilon}\right).$$

Observe that u has two parts. Homogeneous solution $\bar{u}(x) = x$ and the small wiggles $\varepsilon \phi\left(\frac{\cdot}{\varepsilon}\right)$ coming from the anisotropic nature of the problem

Correctors

Following the analogue suggested by 1D-example, we define in the periodic first-order corrector. Denote the the periodic Sobolev space as

$$H_{\text{per}}^1([0,1]^d) := \{u \in H_{\text{loc}}^1(\mathbb{R}^d) : u(x+z) = u(x) \text{ for } z \in \mathbb{Z}^d \text{ and a.e } x \in \mathbb{R}^d\}.$$

One can identify this space as the completion of smooth \mathbb{Z}^d -periodic functions w.r.t. to the norm of $H^1([0,1]^d)$. This space is actually a Hilbert space.

First-order corrector $\phi_e \in H_{\text{per}}^1([0,1]^d)$, $e \in \partial B_1$, is the unique weak solution satisfying $\int_{[0,1]^d} \phi_e(x) dx = 0$ to the equation

$$-\nabla \cdot (\mathbf{a}(x) (e + \nabla \phi_e(x))) = 0 \quad \text{in } [0,1]^d.$$

Notice that since $\mathbf{a}(\cdot)$ is assumed to be \mathbb{Z}^d -periodic, the above equation is actually satisfied in the whole space.

Exercise. Prove that there exists a unique solution $\phi_e \in H_{\text{per}}^1([0,1]^d)$ modulo a constant satisfying the above equation.

Hint: One way is to find a suitable version of Lax-Millgram Lemma from the literature, state it, prove it, and apply it to obtain the existence.

Two-scale expansion

Let $\phi_j \in H_{\text{per}}^1([0,1]^d)$, $j \in \{1, \dots, d\}$, be the solution of

$$-\nabla \cdot (\mathbf{a}(\nabla \phi_j + \mathbf{e}_j)) = 0 \quad \text{in } [0,1]^d, \quad \int_{[0,1]^d} \phi_j(x) dx = 0,$$

where \mathbf{e}_j is the unit vector parallel to x_j -axis, and choose the constant so that ϕ_j has zero mean.

Denote by ϕ^ε and $\nabla \phi^\varepsilon$ the vector and the matrix, respectively, having the components, for $i, j \in \{1, \dots, d\}$,

$$(\phi^\varepsilon(x))_j := \phi_j\left(\frac{x}{\varepsilon}\right) \quad \text{and} \quad (\nabla \phi^\varepsilon(x))_{ij} := \partial_{x_i} \phi_j\left(\frac{x}{\varepsilon}\right).$$

We can test the equation of ϕ_j by itself, using the periodicity, and obtain by the Poincaré inequality that

$$\|\phi_j\|_{L^2([0,1]^d)} \leq C \|\nabla \phi_j\|_{L^2([0,1]^d)} \leq C.$$

Two-scale expansion

Suppose that we have the heterogeneous solution $u_\varepsilon \in H^1(U)$ and homogenized solution $u \in W^{2,\infty}(U)$ solving

$$\begin{cases} -\nabla \cdot (\mathbf{a}(\frac{x}{\varepsilon}) \nabla u^\varepsilon) = f & \text{in } U, \\ u^\varepsilon = g & \text{on } \partial U, \end{cases} \quad \begin{cases} -\nabla \cdot (\bar{\mathbf{a}} \nabla u) = f & \text{in } U, \\ u = g & \text{on } \partial U. \end{cases}$$

The very basic **two-scale expansion** around u is defined as

$$\tilde{w}_\varepsilon(x) := u(x) + \varepsilon \phi^\varepsilon(x) \cdot \nabla u(x)$$

We will show that using this it is possible to deduce estimates how close u^ε and u are in L^2 , and u^ε and w^ε in H^1

Two-scale expansion: The basic computation

We still want to tinker the definition of the two-scale expansion. Namely, we choose a smooth cut-off function $\eta^\varepsilon \in C_0^\infty(U)$ so that $\eta^\varepsilon = 1$ in ε away from ∂U and $\|\nabla \eta^\varepsilon\|_{L^\infty(U)} \leq C\varepsilon^{-1}$. Then w^ε and u have the same boundary values. Set

$$w^\varepsilon(x) := u(x) + \varepsilon \eta^\varepsilon(x) \phi^\varepsilon(x) \cdot \nabla u(x) = u(x) + \varepsilon \eta^\varepsilon(x) \sum_{k=1}^d \phi_k^\varepsilon\left(\frac{x}{\varepsilon}\right) \partial_{x_k} u(x)$$

Our goal is to show that

$$\|\nabla \cdot (\mathbf{a}^\varepsilon(\nabla w^\varepsilon - \nabla u^\varepsilon))\|_{H^{-1}(U)} \leq C\varepsilon \|u\|_{W^{2,\infty}(U)}.$$

Since $u^\varepsilon - w^\varepsilon \in H_0^1(U)$, this, in turn, implies

$$\|u^\varepsilon - u\|_{H^1(U)} + \|\nabla u^\varepsilon - \nabla w^\varepsilon\|_{H^1(U)} \leq C\varepsilon \|u\|_{W^{2,\infty}(U)}.$$

Two-scale expansion: The basic computation

Having

$$w^\varepsilon := u + \varepsilon \eta^\varepsilon \phi^\varepsilon \cdot \nabla u = u + \varepsilon \eta^\varepsilon(x) \sum_{k=1}^d \phi_k^\varepsilon \partial_{x_k} u,$$

compute

$$\nabla w^\varepsilon = \sum_{k=1}^d (\mathbf{e}_k + \nabla \phi_k^\varepsilon) \partial_{x_k} u + \mathbf{G}^\varepsilon,$$

where

$$\mathbf{G}^\varepsilon := (\eta^\varepsilon - 1) \sum_{k=1}^d \nabla \phi_k^\varepsilon \partial_{x_k} u + \varepsilon \sum_{k=1}^d \phi_k^\varepsilon \nabla (\eta^\varepsilon \partial_{x_k} u)$$

and then, using the equation of ϕ_k ,

$$\begin{aligned} \nabla \cdot (\mathbf{a}^\varepsilon \nabla w^\varepsilon) &= \sum_{k=1}^d \partial_{x_k} u \overbrace{\nabla \cdot (\mathbf{a}^\varepsilon (\mathbf{e}_k + \nabla \phi_k^\varepsilon))}^{=0} \\ &\quad + \sum_{k=1}^d \mathbf{a}^\varepsilon (\mathbf{e}_k + \nabla \phi_k^\varepsilon) \cdot \nabla \partial_{x_k} u + \nabla \cdot (\mathbf{a}^\varepsilon \mathbf{G}^\varepsilon). \end{aligned}$$

Two-scale expansion: The basic computation

We have thus found the following formula:

$$\nabla \cdot (\mathbf{a}^\varepsilon \nabla w^\varepsilon) = \sum_{k=1}^d \mathbf{a}^\varepsilon (\mathbf{e}_k + \nabla \phi_k^\varepsilon) \cdot \nabla \partial_{x_k} u + \nabla \cdot (\mathbf{a}^\varepsilon \mathbf{G}^\varepsilon).$$

and

$$\|\mathbf{a}^\varepsilon \mathbf{G}^\varepsilon\|_{L^2(U)} \leq C\varepsilon \|u\|_{W^{2,\infty}(U)}$$

This suggests to define the effective matrix as

$$\bar{\mathbf{a}} := \int_{[0,1]^d} \mathbf{a}(x) (\mathbf{I}_d + \nabla \phi(x)) \, dx$$

so that the above formula can be rewritten as

$$\nabla \cdot (\mathbf{a}^\varepsilon \nabla w^\varepsilon - \bar{\mathbf{a}} \nabla u) = \sum_{k=1}^d (\mathbf{a}^\varepsilon (\mathbf{e}_k + \nabla \phi_k^\varepsilon) - \bar{\mathbf{a}} \mathbf{e}_k) \cdot \nabla \partial_{x_k} u + \nabla \cdot (\mathbf{a}^\varepsilon \mathbf{G}^\varepsilon).$$

Notice, indeed, that since $\bar{\mathbf{a}}$ is a constant matrix,

$\nabla \cdot \bar{\mathbf{a}} \nabla u(x) = \bar{\mathbf{a}} : \nabla^2 u(x)$. Recall that

$$\mathbf{G}^\varepsilon := (\eta^\varepsilon - 1) \nabla \phi^\varepsilon \nabla u + \varepsilon \nabla (\eta^\varepsilon \nabla u) \phi^\varepsilon.$$

Two-scale expansion: The basic computation

The formula

$$\nabla \cdot (\mathbf{a}^\varepsilon \nabla w^\varepsilon - \bar{\mathbf{a}} \nabla u) = (\mathbf{a}^\varepsilon (\mathbf{I}_d + \nabla \phi^\varepsilon) - \bar{\mathbf{a}}) : \nabla^2 u + \nabla \cdot (\mathbf{a}^\varepsilon \mathbf{G}^\varepsilon),$$

tells now two sources of errors. Since $\|\mathbf{a}^\varepsilon \mathbf{G}^\varepsilon\|_{L^2(U)} \leq C\varepsilon \|u\|_{W^{2,\infty}(U)}$, we have that

$$\|\nabla \cdot (\mathbf{a}^\varepsilon \mathbf{G}^\varepsilon)\|_{H^{-1}(U)} \leq C\varepsilon \|u\|_{W^{2,\infty}(U)}.$$

We are thus left to establish

$$\|(\mathbf{a}^\varepsilon (\mathbf{I}_d + \nabla \phi^\varepsilon) - \bar{\mathbf{a}}) : \nabla^2 u\|_{H^{-1}(U)} \leq C\varepsilon \|u\|_{W^{2,\infty}(U)}.$$

Two-scale expansion: The basic computation

Set now

$$\mathbf{F}_e(x) := \mathbf{a}(x) (e + \nabla \phi_e(x)) - \bar{\mathbf{a}} e$$

By the equation of ϕ_e , \mathbf{F}_e is solenoidal (that is, $\nabla \cdot \mathbf{F}_e = 0$), \mathbb{Z}^d -periodic, and it has a zero mean. Therefore, one finds the following Helmholtz projection for \mathbf{F}_e :

$$\mathbf{F}_e(x) = \nabla \cdot \mathbf{S}_e,$$

and the matrix \mathbf{S}_e is \mathbb{Z}^d -periodic, zero mean, and skew-symmetric: $\mathbf{S}_{e,ij} = -\mathbf{S}_{e,ji}$. Moreover, by Poincaré's inequality,

$$\|\mathbf{S}_e\|_{L^2([0,1]^d)} \leq C \|\nabla \mathbf{S}_e\|_{L^2([0,1]^d)} \leq C.$$

Two-scale expansion: The basic computation

Using this computation, notice that

$$\begin{aligned}(\mathbf{a}^\varepsilon (\mathbf{I}_d + \nabla \phi^\varepsilon) - \bar{\mathbf{a}}) : \nabla^2 u &= \sum_{k=1}^d \mathbf{F}_{\mathbf{e}_k}^\varepsilon \cdot \nabla \partial_{x_k} u \\ &= \sum_{k=1}^d \varepsilon \nabla \cdot \mathbf{S}_{\mathbf{e}_k}^\varepsilon \cdot \nabla \partial_{x_k} u = \varepsilon \sum_{k=1}^d \nabla \cdot (\mathbf{S}_{\mathbf{e}_k}^\varepsilon \nabla \partial_{x_k} u)\end{aligned}$$

Here we used the following consequence of the skew-symmetry of $\mathbf{S}_{\mathbf{e}}$:

$$\begin{aligned}\nabla \cdot \mathbf{S}_{\mathbf{e}_k}^\varepsilon \cdot \nabla \partial_{x_k} u &= \sum_{i,j} \partial_{x_i} (\mathbf{S}_{\mathbf{e}_k}^\varepsilon)_{ij} \partial_{x_j x_k} u = \sum_{i,j} \partial_{x_i} \left((\mathbf{S}_{\mathbf{e}_k}^\varepsilon)_{ij} \partial_{x_j x_k} u \right) - \underbrace{\sum_{i,j} (\mathbf{S}_{\mathbf{e}_k}^\varepsilon)_{ij} \partial_{x_i x_j x_k} u}_{=0}\end{aligned}$$

Example: Periodic setting

We have now found the formula

$$\nabla \cdot (\mathbf{a}^\varepsilon \nabla w^\varepsilon - \bar{\mathbf{a}} \nabla u) = \nabla \cdot \left(\varepsilon \sum_{k=1}^d \mathbf{S}_{\mathbf{e}_k}^\varepsilon \nabla \partial_{x_k} u + \mathbf{a}^\varepsilon \mathbf{G}^\varepsilon \right),$$

and

$$\left\| \varepsilon \sum_{k=1}^d \mathbf{S}_{\mathbf{e}_k}^\varepsilon \nabla \partial_{x_k} u + \mathbf{a}^\varepsilon \mathbf{G}^\varepsilon \right\|_{L^2(U)} \leq C\varepsilon \|u\|_{W^{2,\infty}(U)}.$$

Since

$$\nabla \cdot (\bar{\mathbf{a}} \nabla u) = \nabla \cdot (\mathbf{a}^\varepsilon \nabla u^\varepsilon),$$

this yields

$$\|\nabla \cdot (\mathbf{a}^\varepsilon (\nabla w^\varepsilon - \nabla u^\varepsilon))\|_{H^{-1}(U)} \leq C\varepsilon \|u\|_{W^{2,\infty}(U)},$$

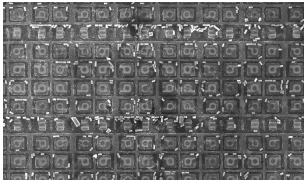
as desired.

Scope: Towards stochastic homogenization

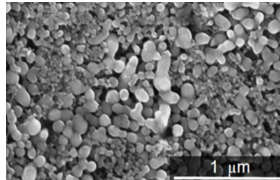
Before we were taking a look of periodic setting. However,

Real applications are more accurately modelled by random models

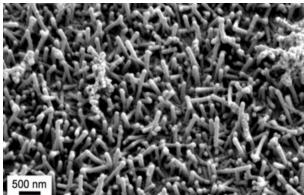
Scope: Towards stochastic homogenization



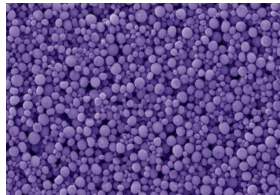
Microprocessor (scale 180nm)



Battery structure



Virus surface



Solar cell structure

Assumptions on coefficients

Reasonable assumptions for coefficients are as follows.

- $\Omega := \{\mathbf{a} : \mathbf{a} \text{ symmetric matrix } \mathbb{R}^{d \times d}, \lambda(\mathbf{a}) \subseteq [1, \Lambda]\}, \Lambda \geq 1.$
- For $U \subseteq \mathbb{R}^d$, \mathcal{F}_U denotes the σ -algebra generated by $\mathbf{a} \mapsto \int_U \mathbf{a}(x) \phi(x) dx$, $\phi \in C_c^\infty(U)$. Write $\mathcal{F} = \mathcal{F}(\mathbb{R}^d)$.
- \mathbb{P} is a probability measure on $(\Omega, \mathcal{F}_{\mathbb{R}^d})$
- Assumptions on \mathbb{P} .

(P1) Stationarity

$\mathbb{P} \circ T_z = \mathbb{P}$ for $z \in \mathbb{Z}^d$, where T_z is a translation $T_z f(x) = f(x + z)$

(P2) Unit range dependency

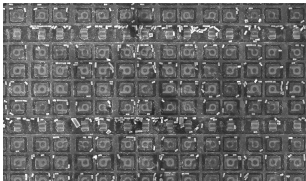
If $\text{dist}(U, V) \geq 1$, then \mathcal{F}_U and \mathcal{F}_V are \mathbb{P} -independent

We denote the expectation with respect to \mathbb{P} by \mathbb{E} . That is, if $X : \Omega \rightarrow \mathbb{R}$ is an \mathcal{F} -measurable random variable, we write

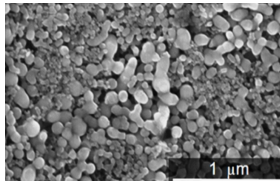
$$\mathbb{E}[X] := \int_{\Omega} X(\mathbf{a}) d\mathbb{P}(\mathbf{a})$$

In practice

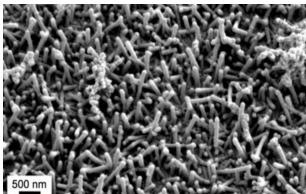
The probability distribution can be obtained by analyzing the material.



Microprocessor (scale 180nm)



Battery structure

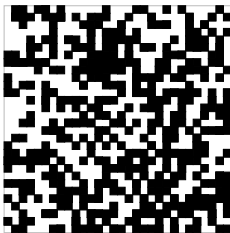


Virus surface



Solar cell structure

Another concrete example



A piece of the “random checkerboard”. The conductivity matrix equals identity matrix I in the white region, and $4I$ in the black region. Probability measure \mathbb{P} is a product measure so that at each cube a fair coin is tossed to decide the value I or $4I$.

- It can be shown by so-called *Dykhne formula* that $\bar{\mathbf{a}} = 2I$.
- Notice that $\mathbb{P}[\mathbf{a} \equiv 4I \text{ in macroscopic cube}] = 2^{-\#(\text{small cubes})}$.

Correctors

It turns out that so-called correctors play a central role in the theory. First-order corrector $\phi_e \in H_{\text{loc}}^1(\mathbb{R}^d)$, $e \in \mathbb{R}^d$, is the unique weak solution, modulo an additive constant, to the equation

$$-\nabla \cdot (\mathbf{a}(x) (e + \nabla \phi_e(x, \mathbf{a}(\cdot)))) = 0 \quad \text{in } \mathbb{R}^d.$$

Observe that ϕ_e depends on coefficients in the whole space.

Now, whenever we are referring to a solution, it is actually a function of both x and \mathbf{a} . This is to say that in reality the solution lives possibly in an **infinite** dimensional space. However, it is usually convenient to suppress \mathbf{a} from the notation for u since the PDE is cast in the physical space.

Following the reasoning from the periodic setting, one can show that the effective (homogenized) elliptic, symmetric and deterministic matrix $\bar{\mathbf{a}}$ is defined via

$$\bar{\mathbf{a}}e = \mathbb{E} \left[\int_{[0,1]^d} \mathbf{a}(x) (e + \nabla \phi_e(x)) \, dx \right] \quad \forall e \in \mathbb{R}^d.$$

Two-scale expansion

Suppose that we have the heterogeneous solution u_ε and homogenized solution \bar{u}

$$\begin{cases} -\nabla \cdot \left(\mathbf{a} \left(\frac{x}{\varepsilon} \right) \nabla u_\varepsilon \right) = f & \text{in } U, \\ u_\varepsilon = g & \text{on } \partial U, \end{cases} \quad \begin{cases} -\nabla \cdot (\bar{\mathbf{a}} \nabla \bar{u}) = f & \text{in } U, \\ \bar{u} = g & \text{on } \partial U. \end{cases}$$

Then, defining so-called two-scale expansion

$$w_\varepsilon(x) := \bar{u}(x) + \varepsilon \phi^\varepsilon(x) \cdot \nabla \bar{u}(x),$$

one of the main goals is to prove that

$$\begin{cases} \|u_\varepsilon - u\|_{L^2(U)} \leq \mathcal{X}\varepsilon, \\ \|\nabla u_\varepsilon - \nabla w_\varepsilon\|_{L^2(U)} \leq \mathcal{X}\varepsilon^{\frac{1}{2}} \end{cases}$$

with a **stochastic constant** \mathcal{X} .

Back to the checkerboard example

As noticed before, $\mathbb{P}[\mathbf{a} \equiv 4I \text{ in macroscopic cube}] = 2^{-\#(\text{small cubes})}$ and $\bar{\mathbf{a}} = 2I$. Consider thus the problem from before in this very unlikely event that $\mathbf{a} \equiv 4I$ in B_1 . We have

$$\begin{cases} -4\Delta u^\varepsilon = 1 & \text{in } B_1, \\ u_\varepsilon = 0 & \text{on } \partial B_1, \end{cases} \quad \begin{cases} -2\Delta u = 1 & \text{in } B_1, \\ u = 0 & \text{on } \partial B_1. \end{cases}$$

We can find an explicit solutions $2u^\varepsilon(x) = u(x) = \frac{1}{2d}(1 - |x|^2)$ and thus we have that

$$\|u_\varepsilon - u\|_{L^2(B_1)} = \frac{1}{4d} \|u\|_{L^2(B_1)} = c(d) \gg C(d)\varepsilon.$$

This shows that the stochastic constant \mathcal{X} in the error estimate is necessary, and the task is then to show that it is integrable in probability space stemming to $\mathbb{P}[\mathbf{a} \equiv 4I \text{ in macroscopic cube}] = 2^{-\#(\text{small cubes})}$.

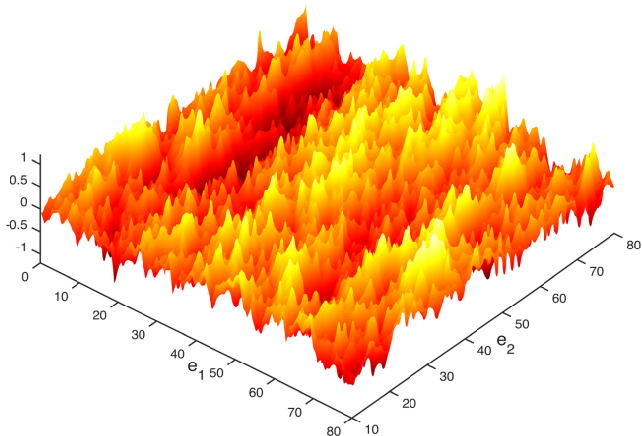
Correctors

Let us now go back to correctors, which satisfy the equation

$$-\nabla \cdot (\mathbf{a}(x) (e + \nabla \phi_e)) = 0 \quad \text{in } \mathbb{R}^d.$$

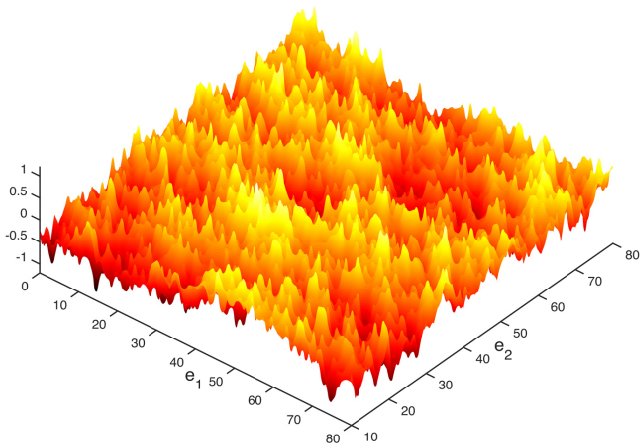
How do the correctors look like, for example, in the case of checkerboard?

Corrector



Approximation of the graph of ϕ_{e_1} solving $-\operatorname{div}(\mathbf{a}(x)(e_1 + \nabla \phi_{e_1}(x))) = 0$ in \mathbb{R}^2

Corrector



Approximation of the graph of ϕ_{e_2} solving $-\operatorname{div}(\mathbf{a}(x)(e_2 + \nabla \phi_{e_2}(x))) = 0$ in \mathbb{R}^2