Liblice 2013, MOdelling REvisited + MOdel REduction

A quantitative theory in stochastic homogenization

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Stochastic homogenization:

Early explicit approximate treatment,

recent numerical applications

Maxwell: Effective resistance of a composite

A TREATISE

ON

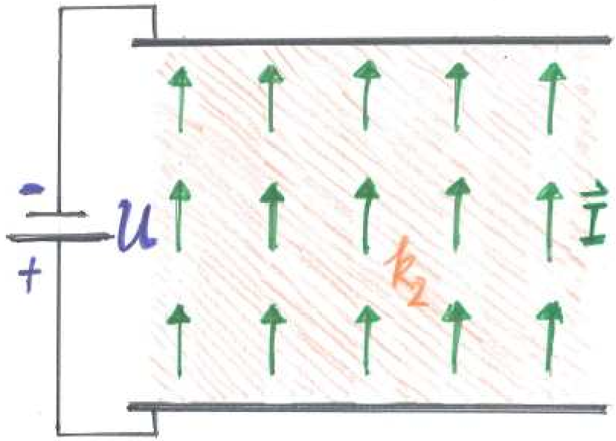
ELECTRICITY AND MAGNETISM

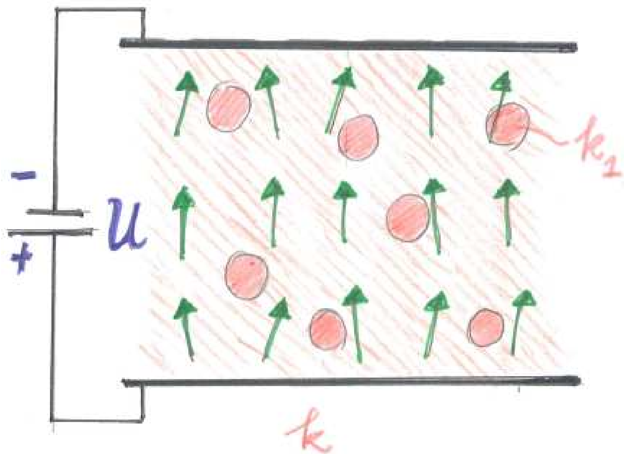
MAXWELL

That the one expression should be equivalent to the other,

$$K = \frac{2k_1 + k_2 + p(k_1 - k_2)}{2k_1 + k_2 - 2p(k_1 - k_2)} k_2. \qquad (17)$$

This, therefore, is the specific resistance of a compound medium consisting of a substance of specific resistance k_2, in which are disseminated small spheres of specific resistance k_1, the ratio of the volume of all the small spheres to that of the whole being p. In order that the action of these spheres may not produce effects depending on their interference, their radii must be small compared with their distances, and therefore p must be a small fraction.





Einstein: Effective viscosity of a suspension

EINE NEUE BESTIMMUNG
DER MOLEKÜLDIMENSIONEN

INAUGURAL-DISSERTATION
ZUR
ERLANGUNG DER PHILOSOPHISCHEN DOKTORWÜRDE
DER
HOHEN PHILOSOPISCHEN FAKULTÄT
(MATHEMATISCH-NATURWISSENSCHAFTLICHE SEKTION)
DER
UNIVERSITÄT ZÜRICH

VORGELEGT
VON
ALBERT EINSTEIN
AUS ZÜRICH

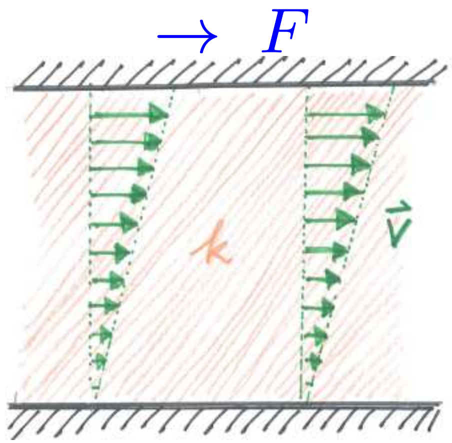
§ 2. Berechnung des Reibungskoeffizienten einer Flüssigkeit, in welcher sehr viele kleine Kugeln in regelloser Verteilung suspendiert sind.

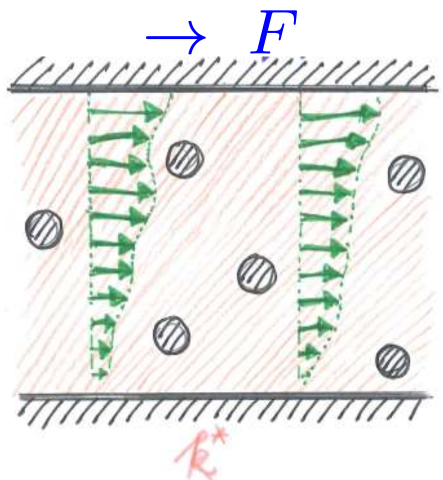
Aus den drei letzten Gleichungen erhält man unter Vernachlässigung von unendlich Kleinem höherer Ordnung:

$$k^* = k\,(1 + \varphi).$$

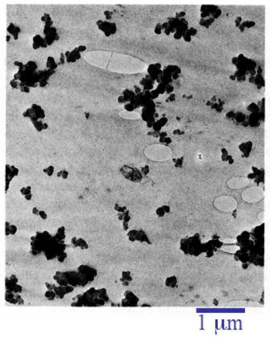
Wir erhalten also das Resultat:

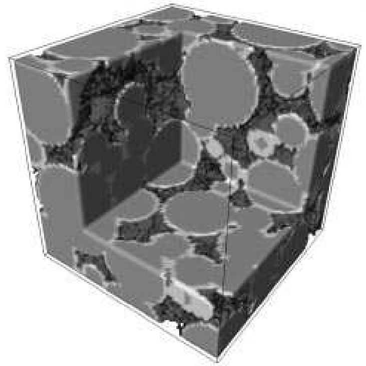
Werden in einer Flüssigkeit sehr kleine starre Kugeln suspendiert, so wächst dadurch der Koeffizient der inneren Reibung um einen Bruchteil, der gleich ist dem Gesamtvolumen der in der Volumeneinheit suspendierten Kugeln, vorausgesetzt, dass dieses Gesamtvolumen sehr klein ist.





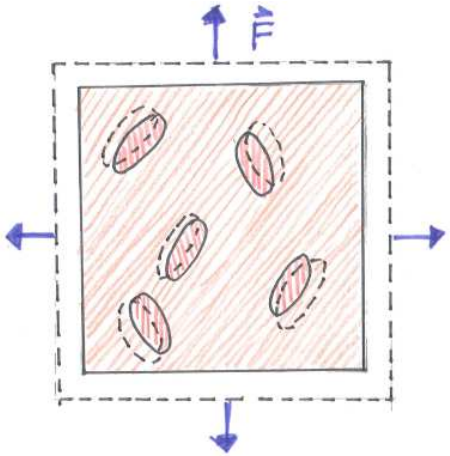
Recent: composite materials & porous media





Effective elasticity

Effective permeability



Effective behavior by simulation on

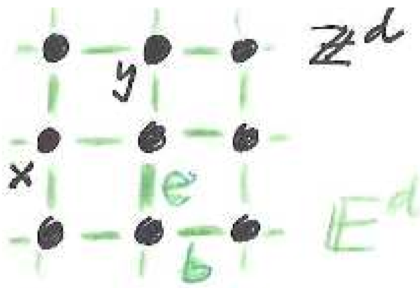
"Representative Volume Element"

Stochastic homogenization of elliptic equations:

a discrete, scalar toy model.

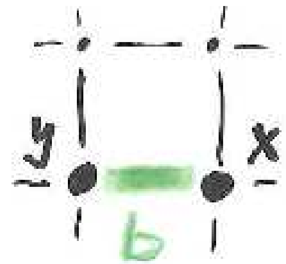
Setting and qualitative theory

Discrete calculus



Lattice,
sites x, $y \in \mathbb{Z}^d$
bonds b, $e \in \mathbb{E}^d$

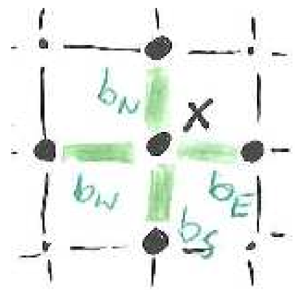
Gradient ∇.



Scalar field $\zeta\colon \mathbb{Z}^d \to \mathbb{R}$ $\rightsquigarrow$ vector field $\nabla\zeta\colon \mathbb{E}^d \to \mathbb{R}$

$\nabla\zeta(b) = \zeta(x) - \zeta(y)$

(negative) Divergence ∇^*. ℓ^2-adjoint.

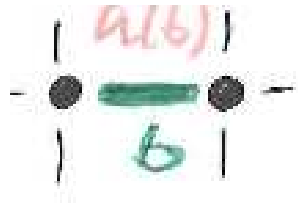


Vector field $g\colon \mathbb{E}^d \to \mathbb{R}$ $\rightsquigarrow$ scalar field $\nabla^* g\colon \mathbb{Z}^d \to \mathbb{R}$

$\nabla^* g(x) = g(b_E) + g(b_N) - g(b_W) - g(b_S)$

Discrete elliptic operator and its interpretation

Coefficients a.

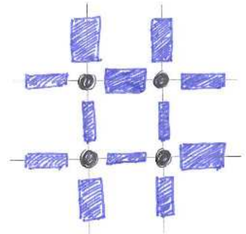


Tensor field $a\colon \mathbb{E}^d \to \mathbb{R}$,

Uniformly elliptic: $\exists\, \lambda > 0 \quad \forall b \in \mathbb{E}^d \quad \lambda \le a(b) \le 1$.

Elliptic operator: $\nabla^* a \nabla$ maps scalar fields on scalar fields

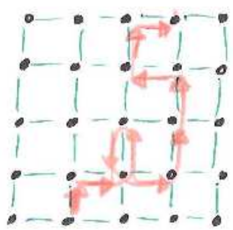
Network of resistors



a conductivity, a^{-1} resistance, u potential,

$j = a\nabla u$ current, stationary iff $\nabla^* j = 0$

Random walk in heterogen. environm.



generator given by $\nabla^* a \nabla$

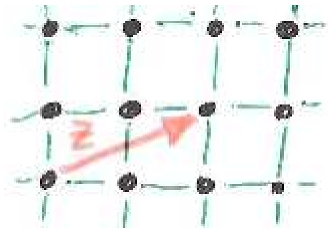
Random discrete elliptic operator

Field of coefficients a is random variable,

ensemble average $\langle\cdot\rangle$

Simplest setting: $\{a(b)\}_{b\in\mathbb{E}^d}$ are **i**ndependent and **i**dentically **d**istributed

Most general setting: $\mathbb{Z}^d$ acts on space of a's by translation



Stationarity: $\forall\, z\in\mathbb{Z}^d \quad a$ and $a(\cdot+z)$ have same distribution

Ergodicity: If $\forall\, z\in\mathbb{Z}^d\ \zeta(a(\cdot+z))=\zeta(a)$ then $\zeta=\langle\zeta\rangle$ a. s.

Qualitative homogenization

Kozlov ['79], Papanicolaou & Varadhan ['79].

Suppose $\langle\cdot\rangle$ is stationary and ergodic.

$\exists \ a_{hom} \in \mathbb{R}^{d\times d}$, symmetric, $\lambda \le a_{hom} \le 1$ such that:

Given $f_0(\hat{x})$ consider right hand side $f(x) = \frac{1}{L^2} f_0(\frac{x}{L})$

Solve discrete Dirichlet problem : for $u(a;x)$
$$\begin{cases} \nabla^* a \nabla u = f & \text{in } ((0,L)\cap\mathbb{Z})^d \\ u = 0 & \text{outside } ((0,L)\cap\mathbb{Z})^d \end{cases}$$

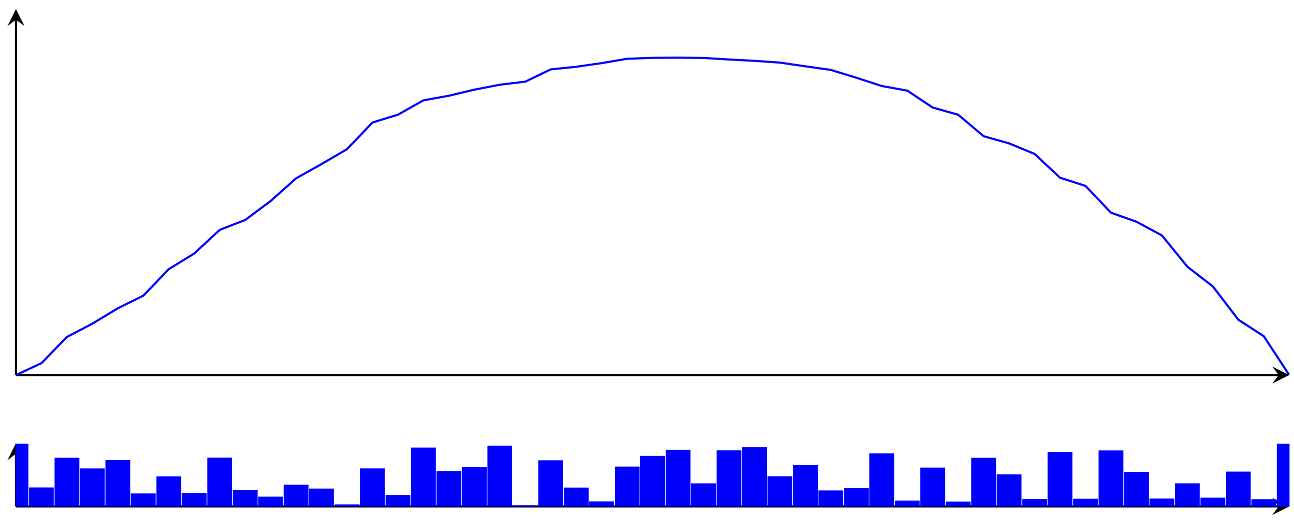
Solve continuum Dirichlet problem : for $u_0(\hat{x})$
$$\begin{cases} -\hat{\nabla}\cdot a_{hom}\hat{\nabla} u_0 = f_0 & \text{in } (0,1)^d \\ u_0 = 0 & \text{outside } (0,1)^d \end{cases}$$

Then $\lim_{L\uparrow\infty} u(a, L\hat{x}) = u_0(\hat{x})$ for $\langle\cdot\rangle$-a. e. a

$$\nabla^* a(x) \nabla u(x) \; = \; L^{-2}, \qquad x \in (0, L) \cap \mathbb{Z}, \qquad L \gg 1$$

$$u(0) = u(L) \; = \; 0$$

statistics of a **i**ndependent, **i**dentically, **d**istributed uniformly in $(0.2, 1)$



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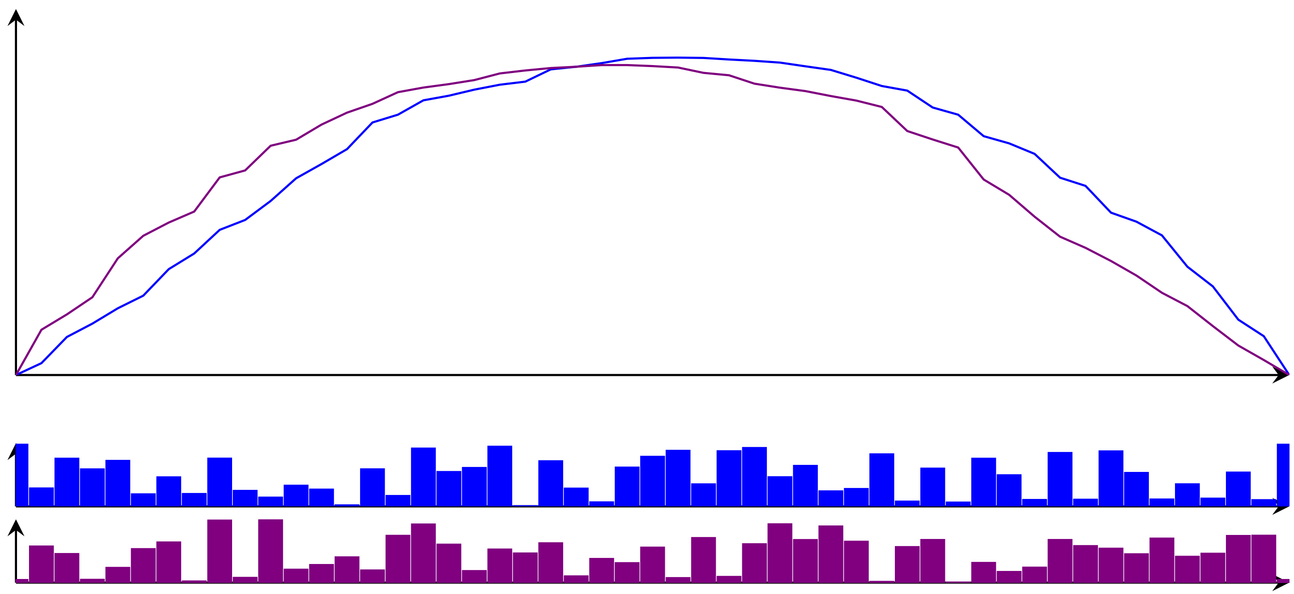

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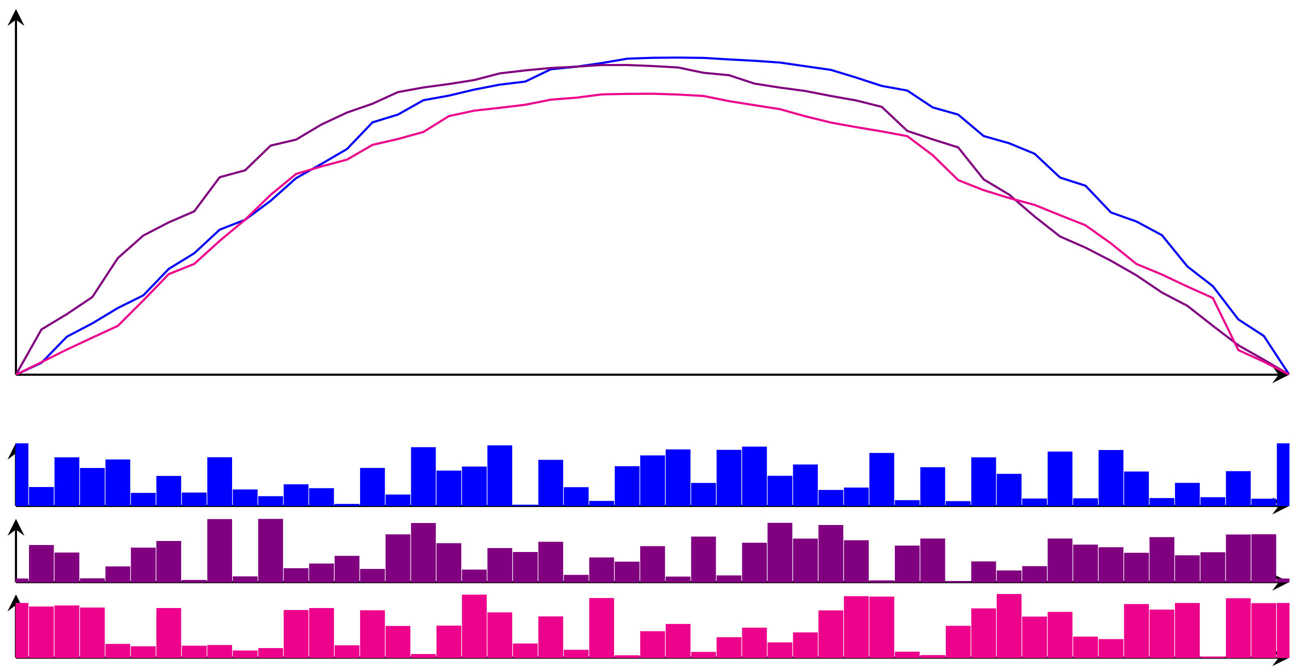
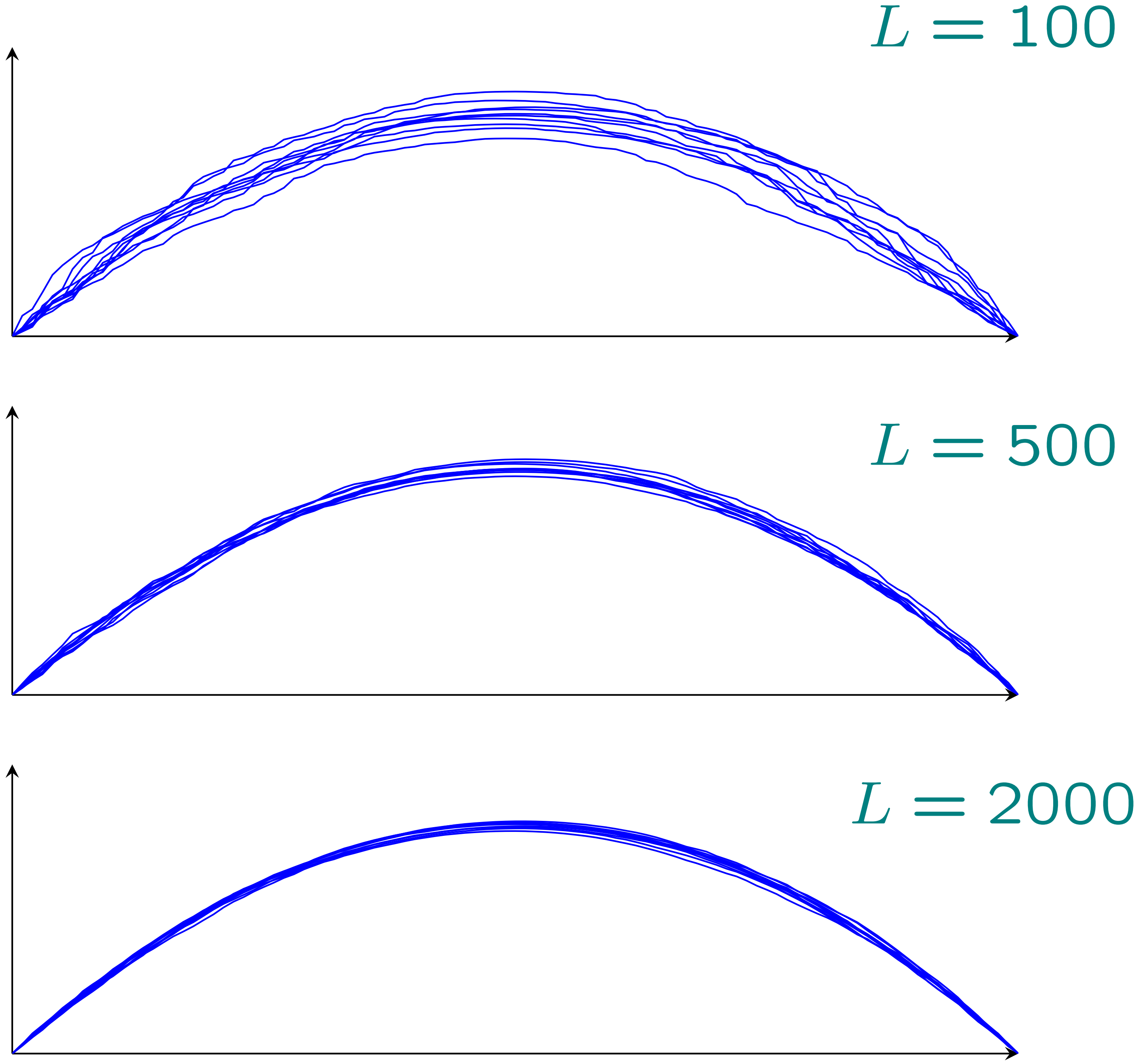
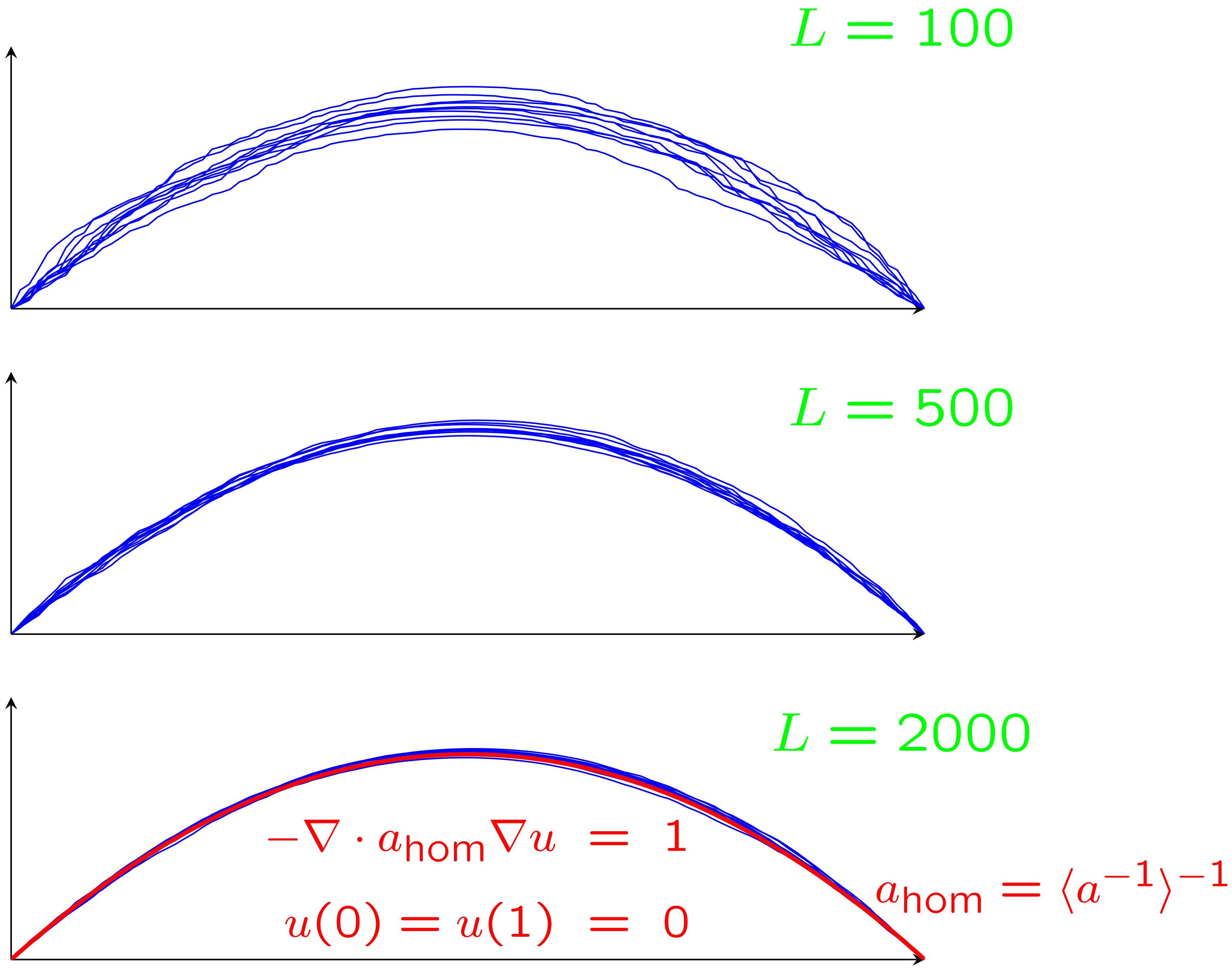



$L = 100$
$L = 500$
$L = 2000$



$L = 100$
$L = 500$
$L = 2000$
$-\nabla \cdot a_{\mathrm{hom}} \nabla u = 1$
$u(0) = u(1) = 0$
$a_{\mathrm{hom}} = \langle a^{-1} \rangle^{-1}$

Prediction of a_{hom} from statistics of $a(e)$?

Conductivity^{-1} = Resistance

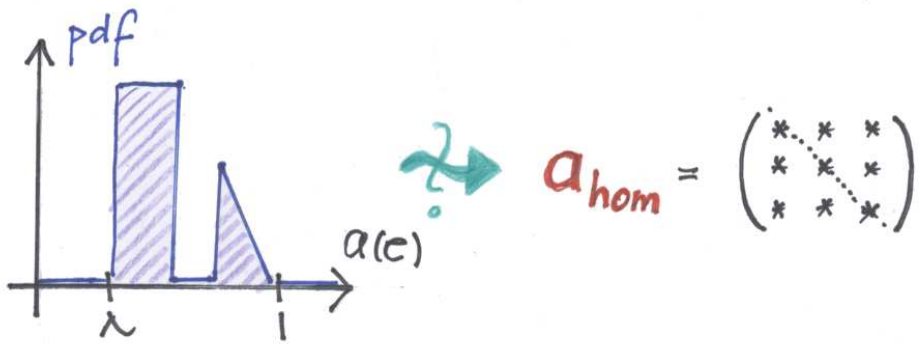
For d=1: $\langle a^{-1} \rangle^{-1} = a_{hom}$

For any d: $\langle a^{-1} \rangle^{-1} \leq a_{hom} \leq \langle a \rangle$

in series in parallel

No simple general formula for

(just expansions in $1 - \lambda \ll 1$)



A computable approximation of a_{hom},

i. e. "Representative Volume Element":

concept of corrector,

two errors and their scaling

Intuition of homogenized coefficient and corrector

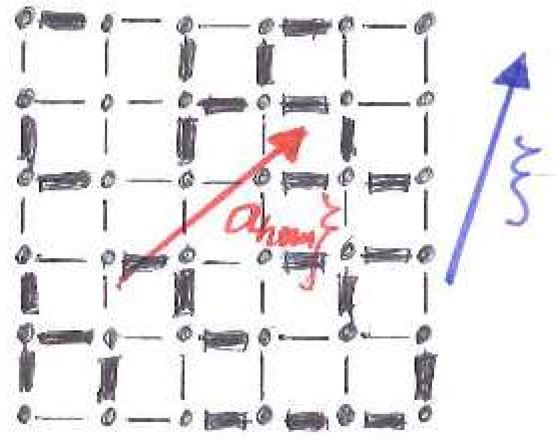
Physical: Consider $\nabla^* a \nabla u = 0$.

Average potential gradient

$$\xi = \lim_{L\uparrow\infty} \frac{1}{L^d} \sum_{b\in[0,L)^d} \nabla u$$

$\rightsquigarrow$ average current

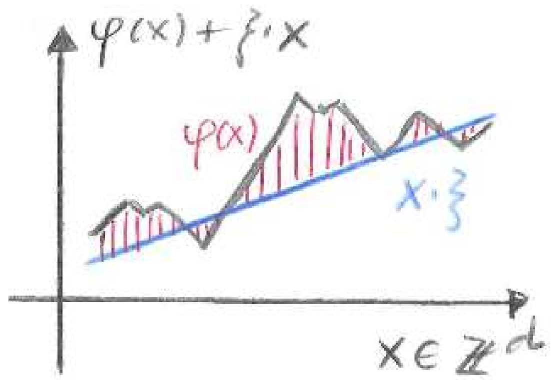
$$a_{hom}\xi = \lim_{L\uparrow\infty} \frac{1}{L^d} \sum_{b\in[0,L)^d} a\nabla u$$



Geometrical: Given affine function $x \cdot \xi$,

find φ s. t. $\varphi(x) + x \cdot \xi$ is a-harmonic:

$\nabla^* a(\nabla\varphi + \xi) = 0$.



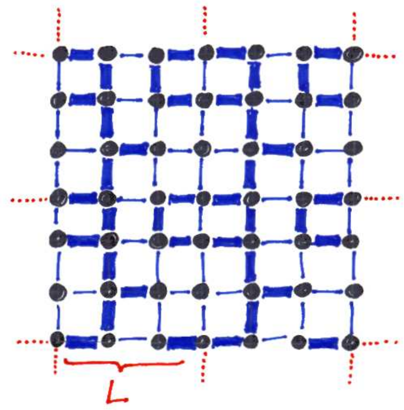
... boundary conditions for corrector φ?

Artificial boundary conditions, modified ensemble

Artificial periodic boundary cond.:

a has period L, i. e. $a(b + Le_i) = a(b)$

$\rightsquigarrow$ φ has period L



Modified, periodic ensemble:

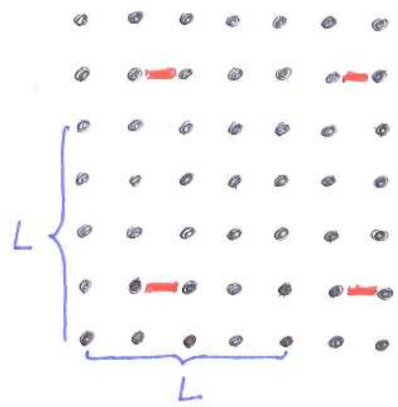
$\langle \cdot \rangle_L := \langle \cdot | a$ has period $L\rangle$

$\langle \cdot \rangle$ i. i. d. $\Longrightarrow$ $\langle \cdot \rangle_L$ i. i. d.

i. e. a has period L,

$\{a(b)\}_{b \in [0,L)^d}$ independent,

identically distributed



... artificial long-range correlations

Practical approximation of homogenized coefficient

Pick a according to $\langle\cdot\rangle_L$, **solve** for φ (period L),
compute spatial average $a_{hom,L}\xi := \frac{1}{L^d}\sum_{b\in[0,L)^d} a(\nabla\varphi+\xi)$

Take *random variable* $a_{hom,L}$ **as approximation to** a_{hom}

$\langle$**error**$^2\rangle_L$ = **random**^{2} + **systematic**^{2}:

$$\langle|a_{hom,L}-a_{hom}|^2\rangle_L = \mathrm{var}_{\langle\cdot\rangle_L}[a_{hom,L}] + |\langle a_{hom,L}\rangle_L - a_{hom}|^2$$

Qualitative theory yields:

$$\lim_{L\uparrow\infty}\mathrm{var}_{\langle\cdot\rangle_L}[a_{hom,L}] = 0, \qquad \lim_{L\uparrow\infty}\langle a_{hom,L}\rangle_L = a_{hom}$$

... why is scaling in L of interest?

Number of samples N vs. artificial period L

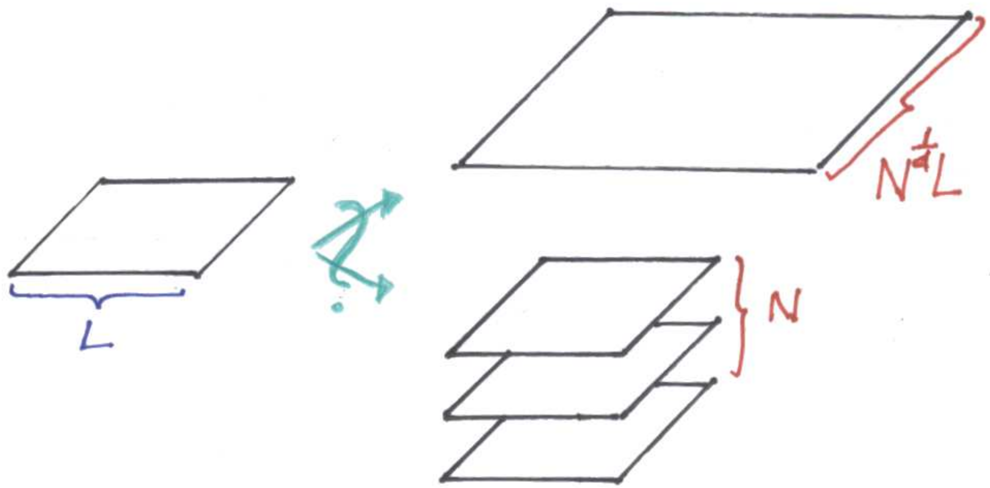
Take **N** samples, i. e. N independent picks $a_1, \cdots, a_N$ from $\langle\cdot\rangle_L$.

Compute empirical mean $\frac{1}{N}\sum_{n=1}^{N}\frac{1}{L^d}\sum_{b\in[0,L)^d} a_n(\nabla\varphi_n+\xi)$

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

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, where $\{a(b)\}_{b\in[0,L)^d}$ independent, identically distributed

For a with period L

solve $\nabla^* a(\nabla\varphi+\xi)=0$ for φ of period L.

Set $a_{hom,L}\xi=\frac{1}{L^d}\sum_{b\in[0,L)^d} a(\nabla\varphi+\xi)$.

Theorem [Gloria&Neukamm&O. '13]

Random error $=\mathrm{var}^{\frac{1}{2}}_{\langle\cdot\rangle_L}\left[a_{hom,L}\right]\ \le\ C(d,\lambda)L^{-\frac{d}{2}}$

Systematic error $=\left|\langle a_{hom,L}\rangle_L-a_{hom}\right|\ \le\ C(d,\lambda)L^{-d}\ln^{\frac{d}{2}}L$

Concepts in the proof:

horizontal vs. vertical derivatives

Spectral gap and semigroup decay

parabolic regularity

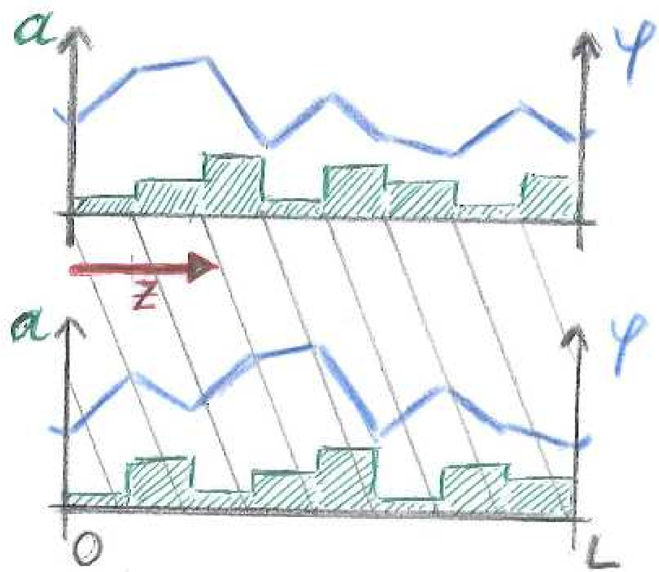
Stationarity of corrector φ

Recall $\nabla^*(a\nabla\varphi + \xi) = 0$

$\varphi(a;x)$ is "stationary"

i. e. for all shifts $z \in \mathbb{Z}^d$

$\varphi(a(\cdot + z);x) = \varphi(a;x+z)$

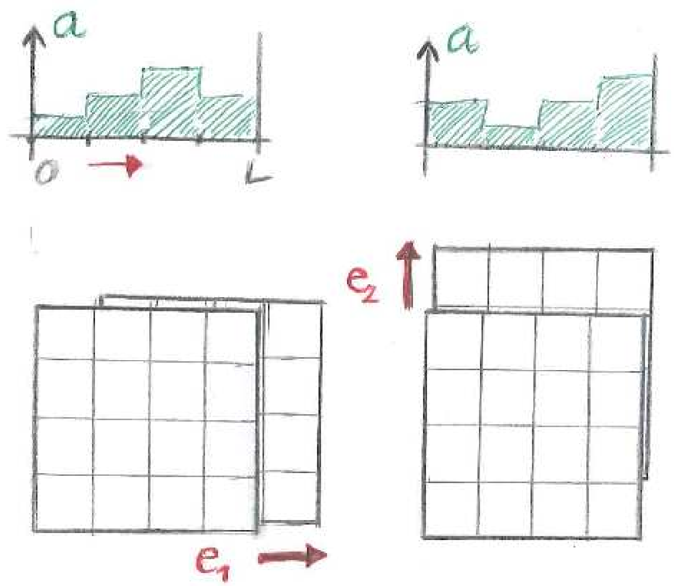


All information on φ contained in $\phi(a) := \varphi(a;0)$

Goal: Reformulate equation for $\varphi(a;x)$ in terms of $\phi(a)$

Horizontal derivatives

How sensitively does ϕ depend on shifting its argument a?



$$
\begin{aligned}
(D_i\phi)(a) &= \phi\big(a(\cdot + e_i)\big) - \phi\big(a\big), \\
(D_i^*\phi)(a) &= \phi\big(a(\cdot - e_i)\big) - \phi\big(a\big)
\end{aligned}
\qquad \text{for} \quad i = 1, \cdots, d
$$

Horizontal derivatives D_i, D_i^* allow to reformulate equation for φ in terms of ϕ

Reformulation of corrector equation

Recall $\left\{ \begin{array}{lcl} (D_i\phi)(a) & = & \phi\big(a(\cdot + e_i)\big) - \phi\big(a\big), \\ (D_i^*\phi)(a) & = & \phi\big(a(\cdot - e_i)\big) - \phi\big(a\big) \end{array} \right\}$ for $i = 1, \cdots, d$

In terms of $\varphi(a;x)$: $\nabla^* a(\nabla\varphi + \xi) = 0$

In terms of $\phi(a) = \varphi(a;0)$: $\sum_{i=1}^{d} D_i^* a(e_i)(D_i\phi + \xi\cdot e_i) = 0$

$\rightsquigarrow$ discrete elliptic PDE in **high dimensions**:
dL^d variables $\{a(b)\}_{b\in[0,L)^d}$

No Poincaré estimate for horizontal derivative

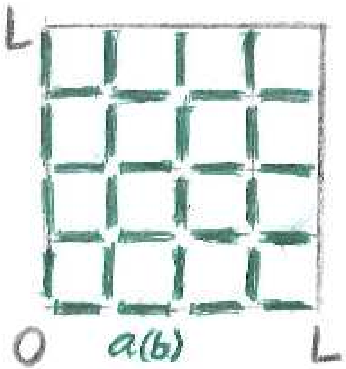
Recall elliptic problem $\sum_{i=1}^{d} D_i^* a(e_i)(D_i \phi + \xi \cdot e_i) = 0$

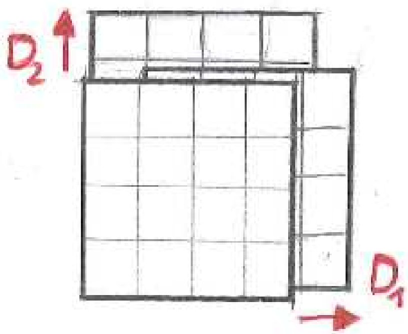
No Poincaré: $\left\langle (\phi - \langle \phi \rangle_L)^2 \right\rangle_L \not\leq C(d) \left\langle \sum_{i=1}^{d} (D_i \phi)^2 \right\rangle_L$

no surprise:

dL^d variables $\{a(b)\}_{b \in [0,L)^d}$

d derivatives $\{D_i\}_{i=1,\cdots,d}$



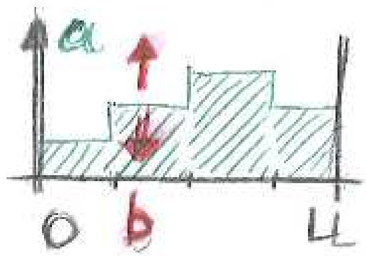


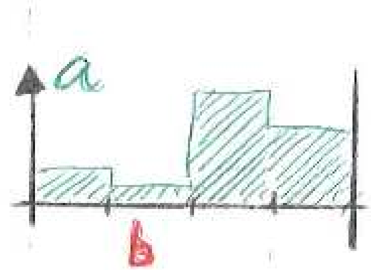
Elliptic operator $\sum_{i=1}^{d} D_i^* a(e_i) D_i$ is **highly degenerate**

Vertical derivative

Recall elliptic problem $$\left\{ \begin{array}{l} \sum_{i=1}^{d} D_i^* a(e_i)(D_i\phi + \xi \cdot e_i) = 0 \\ \nabla^* a(\nabla\varphi + \xi) = 0 \end{array} \right\}$$

How sensitively does $\phi = \varphi(0)$ depend on changing $a(b)$ for given edge b?





Vertical derivative: $$\frac{\partial \phi}{\partial b} = \phi - \langle \phi | \{a(e)\}_{e \neq b} \rangle_L \sim \frac{\partial \phi}{\partial a(b)}$$

Note $\frac{\partial}{\partial b}^* = \frac{\partial}{\partial b}$

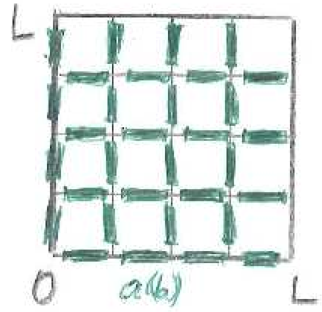
Poincaré estimate holds for vertical derivative

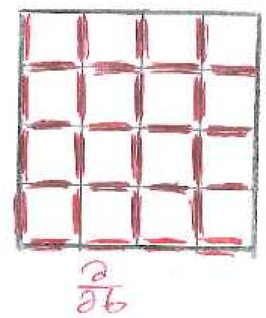
For $\langle\cdot\rangle$ **i. i. d.**: $$\Big\langle(\phi-\langle\phi\rangle_L)^2\Big\rangle_L \le \Big\langle \sum_{b\in[0,L)^d}\Big(\frac{\partial\phi}{\partial b}\Big)^2\Big\rangle_L$$

no surprise:

dL^d variables $\{a(b)\}_{b\in[0,L)^d}$

dL^d derivatives $\{\frac{\partial}{\partial b}\}_{b\in[0,L)^d}$





Elliptic operator $\displaystyle\sum_{b\in[0,L)^d}\frac{\partial}{\partial b}^*\frac{\partial}{\partial b}$ is non-degenerate

— but not directly related to $\displaystyle\sum_{i=1}^{d} D_i^* a(e_i) D_i$

Corrector expressed and estimated via semigroup

We have $\phi = \int_0^\infty U(t)dt$ where

$$\partial_t U + \sum_{i=1}^{d} D_i^* a(e_i) D_i U = 0 \text{ and } U(t=0) = -\sum_{i=1}^{d} D_i^* a(e_i)\xi\cdot e_i$$

Theorem[Gloria&Neukamm&O.].
Suppose $\langle\cdot\rangle$ is stationary
and has Spectral Gap $\rho > 0$ w. r. t. $\{\frac{\partial}{\partial b}\}_{b\in[0,L)^d}$.
Then for all $p < \infty$

$$\left\langle |U(t)|^p \right\rangle^{\frac{1}{p}} \leq C(d,\lambda,\rho,p)\, t^{-\frac{d}{4}-\frac{1}{2}}.$$

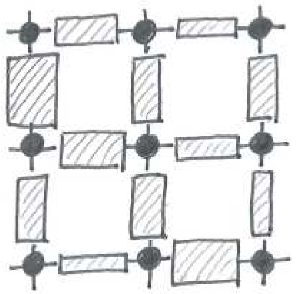
... error estimates are corollary

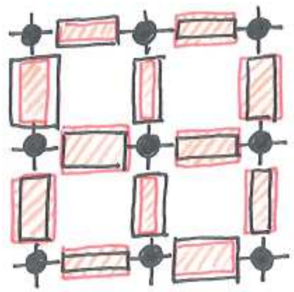
Two processes on space of coefficient fields

reversible w. r. t. ensemble $\langle\cdot\rangle$ of coefficient fields $a(b)$

heat-bath
Glauber dynamics

– unrelated to
homogenization

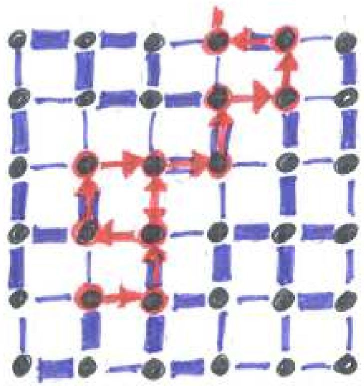


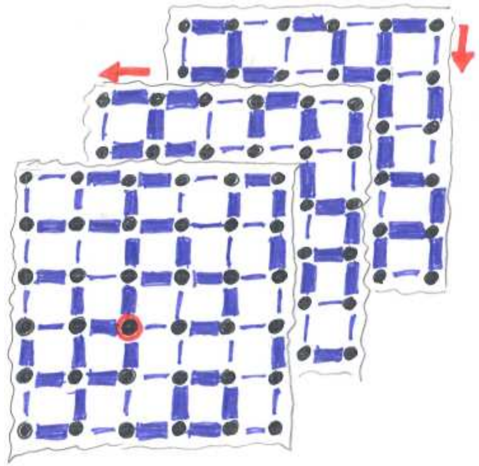


“Environment
as seen from
a random walker”

– related to
homogenization

[Sznitman&Sidoravicius 04 ...]





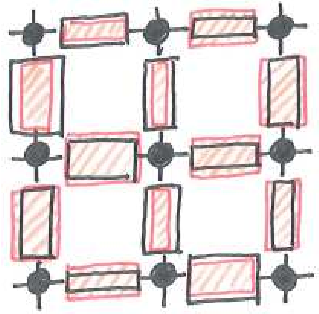
... seemingly unrelated

Spectral gap of generators

Glauber dynamics:

Generator $\sum_{\text{bonds } b} (\frac{\partial}{\partial b})^* \frac{\partial}{\partial b}$

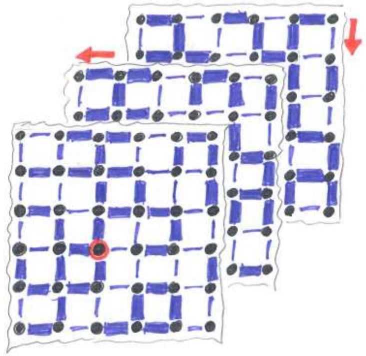
typically has spectral gap (in i. i. d. case)



Random walker dynamics:

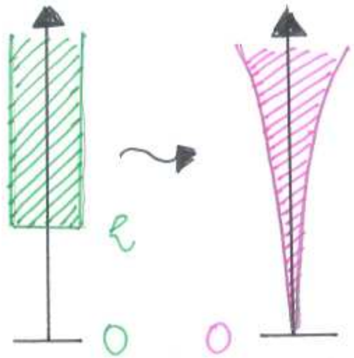
Generator $\sum_{i=1}^{d} D_i^* a(e_i) D_i$

does *not* have spectral gap,
but decay of semi-group (ergodicity)



Idea: spectral gap for $\sum_{\text{bonds } b} (\frac{\partial}{\partial b})^* \frac{\partial}{\partial b}$

$\rightsquigarrow$ quantified decay of $\exp(-t \sum_{i=1}^{d} D_i^* a(e_i) D_i)$



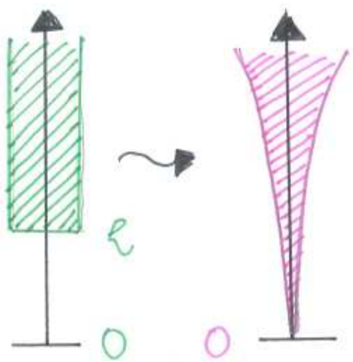
A more general view on our result

Theorem[Gloria&Neukamm&O.]. Suppose $\langle\cdot\rangle$ is stationary and that $\sum_{\text{bonds}\,b}(\frac{\partial}{\partial b})^*\frac{\partial}{\partial b}$ has spectral gap $\rho > 0$. Then for all $\zeta(a)$ and $1 \ll p < \infty$

$$\left\langle\left|\exp(-t\sum_{i=1}^{d} D_i^* a(e_i) D_i)\ D_1\zeta\right|^p\right\rangle^{\frac{1}{p}}$$

$$\leq\ C(d,\lambda,\rho,p)\ t^{-\frac{d}{4}-\frac{1}{2}} \sum_{\text{bonds}\,b}\left\langle\left(\frac{\partial\zeta}{\partial b}\right)^p\right\rangle^{\frac{1}{p}}.$$

Optimal semi-group decay for $\sum_{i=1}^{d} D_i^* a(e_i) D_i$



Proof: connecting horizontal to vertical derivative

From D to ∇: $u(a;x) = U(a(\cdot + x))$ satisfies

$$\partial_t u + \nabla^* a \nabla u = 0, \quad u(t=0) = -\nabla^* a \xi$$

From ∇ to ∂: $\partial u = \{\frac{\partial u}{\partial b}\}_b$ satisfies

$$\partial_t \frac{\partial u}{\partial b} + \nabla^* a \nabla \frac{\partial u}{\partial b} = -\nabla^* \delta(\cdot - b) \nabla u(b)$$

$$\frac{\partial u}{\partial b}(t=0) = -\nabla^* \delta(\cdot - b) \xi$$

Proof: Green's function and parabolic regularity

Representation via parabolic Green's function $G(a;t,0,x)$:

$$\frac{\partial u}{\partial b}(t,0) = -\int_0^t \nabla G(t-s,0,b)\nabla u(s,b)\,ds - \nabla G(t,0,b)\xi(b)$$

Parabolic regularity theory $\exists\, q(d,\lambda) > 1 \;\; \forall\, \alpha < \infty$

$$\sum_b \Big(\big(\tfrac{|b|^2}{t+1} + 1\big)^{\alpha}\big(\nabla G(a;t,0,b)\big)^2\Big)^q \le C(d,\lambda,\alpha)(t+1)^{\frac{d}{2}-2q(\frac{d}{2}+\frac{1}{2})}$$

Nash, Caccioppoli, Meyers (Naddaf& Spencer)

Ongoing and future projects

Random errors $\approx$ Gaussian:

[Biskup&Salvi&Wolff, Nolen, Rossignol]

Continuum medium: Finite correlation length ok

Systems:

Moment bounds on corrector ok

Other boundary conditions:

half-space ok

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