Homogenization of materials with defects

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Crystals are like people, it is the defects in them which tend to make them interesting.


Let’s have a look at materials (media) with defects...
Composite material for the aerospace industry

(Courtesy of M. Thomas & EADS) Fiber reinforced material.
Assembly of fuel rods (Nuclear Eng. PWR)
Figure 1. SEM micrograph showing the Zircaloy-4 microstructure.
At the mesoscale: Realistic microstructure for cement paste

Courtesy of Navier Institute In silico reconstruction.
At the microscale: edge dislocation in metals

Schematic: An extra half-plane of atoms, the "defects", is inserted in the periodic lattice.
In my view, the major new features of Materials Science in the past three decades are:

- **MULTI-SCALE**: inclusion of the microscale in macroscale simulations (and now more often concurrently than sequentially)

- **DISORDERED ORDER**:
  - random: inclusion of random features in an otherwise deterministic model, genuinely random models
  - and/or non-periodic: defects in structures, dislocations in lattices, etc.
Common denominator of the works presented:

- go beyond the idealistic setting of periodic materials
- when possible, avoid fully general random materials (fine theoretically, but prohibitively expensive to address practically);
- consider materials that are, in a sense to be made precise, perturbations of periodic materials;
- adapt the modelling and the computational approach to have a quick reply in a limited time window (2h CPU).

Work on the simplest possible equation

$$\nabla \cdot \left( a(\frac{1}{\varepsilon}) \nabla u^\varepsilon \right) = f$$
Homogenization 1.0.1: the periodic setting

\[-\text{div} \left[ A_{\text{per}} \left( \frac{x}{\varepsilon} \right) \nabla u^\varepsilon \right] = f \quad \text{in} \quad \mathcal{D}, \quad u^\varepsilon = 0 \quad \text{on} \quad \partial \mathcal{D},\]

with $A_{\text{per}}$ symmetric and $\mathbb{Z}^d$-periodic: $A_{\text{per}}(x + k) = A_{\text{per}}(x)$ for any $k \in \mathbb{Z}^d$.

When $\varepsilon \to 0$, $u^\varepsilon$ converges to $u^*$ solution to

\[-\text{div} \left[ A^* \nabla u^* \right] = f \quad \text{in} \quad \mathcal{D}, \quad u^* = 0 \quad \text{on} \quad \partial \mathcal{D}.\]

The effective matrix $A^*$ is given by

$$[A^*]_{ij} = \int_Q (e_i + \nabla w_{e_i}(y))^T A_{\text{per}}(y) e_j \, dy,$$

with, for any $p \in \mathbb{R}^d$, $w_p$ solves the so-called \textbf{corrector} problem:

\[-\text{div} \left[ A_{\text{per}}(y) (p + \nabla w_p) \right] = 0 \quad \text{in} \quad \mathbb{R}^d, \quad w_p \text{ is } \mathbb{Z}^d\text{-periodic}.\]

$\rightarrow$ Solve $d$ PDEs (for $p = e_i$, $1 \leq i \leq d$) on the \textbf{bounded} domain $Q$: easy!

[Bensoussan/Lions/Papanicolaou, Jikov/Koslov/Oleinik, Tartar, Allaire, Avellaneda/Lin, Conca, Kenig/Shen, ...]
Homogenization 1.0.1: stationary ergodic setting

\[-\text{div} \left[ A \left( \frac{x}{\varepsilon}, \omega \right) \nabla u^\varepsilon \right] = f \quad \text{in} \quad \mathcal{D}, \quad u^\varepsilon = 0 \quad \text{on} \quad \partial \mathcal{D}.
\]

\(u^\varepsilon(\cdot, \omega)\) converges to \(u^*\) solution to

\[-\text{div} \left[ A^* \nabla u^* \right] = f \quad \text{in} \quad \mathcal{D}, \quad u^* = 0 \quad \text{on} \quad \partial \mathcal{D}, \quad \text{with}
\]

\([A^*]_{ij} = \mathbb{E} \left( \int_Q (e_i + \nabla w_e)(y, \cdot) A \left( y, \cdot \right) e_j \, dy \right),\]

where \(w_p\) solves

\[
\begin{cases}
-\text{div} \left[ A \left( y, \omega \right) (p + \nabla w_p(y, \omega)) \right] = 0 & \text{in} \quad \mathbb{R}^d, \quad p \in \mathbb{R}^d, \\
\nabla w_p \text{ stat.}, \quad \mathbb{E} \left( \int_Q \nabla w_p(y, \cdot) \, dy \right) = 0.
\end{cases}
\]

The corrector problem is set on \(\mathbb{R}^d\). Theoretically, the RVE is infinite.

[Papanicolaou/Varadhan, Koslov, Bourgeat/Piatnitski, Gloria/Otto, Armstrong/Smart, ... Caffarelli/Souganidis (nonlinear case)]
Numerical approximation

Since the corrector problem is set on $\mathbb{R}^d$:

\[
\begin{align*}
\mathcal{L}(w_p) &= 0 \quad \text{in} \quad \mathbb{R}^d, \\
\nabla w_p \text{ is stationary}
\end{align*}
\]

we need, in practice, to introduce truncation: introduce $Q_N = (-N, N)^d$ and approximate $w_p$ by $w_p^N$ with

\[
\begin{align*}
\mathcal{L}(w_p^N) &= 0 \quad \text{on} \quad Q_N, \\

w_p^N(\cdot, \omega) \text{ is } Q_N\text{-periodic}
\end{align*}
\]

and compute $A_N^*(\omega)$ from there: large domain ($N \gg 1$), random output, . . .

$\implies$ Often prohibitively expensive computationally!
A toolbox for modeling perturbations of a periodic structure
Random deformations

Φ(.,ω)

A ’real’ material ≡ a random deformation of a reference periodic material
Deformed structure

The periodic structure corresponds to identical inclusions centered on $\mathbb{Z}^2$. 
A variant of classical stochastic homogenization

Classical stochastic homogenization:

\[-\text{div} \left[ A \left( \frac{x}{\varepsilon}, \omega \right) \nabla u^\varepsilon(x, \omega) \right] = f(x) \text{ in } D, \quad u^\varepsilon = 0 \text{ on } \partial D\]

where the matrix $A$ is stationary.

We consider here a variant:

\[-\text{div} \left[ A_{\text{per}} \left( \Phi^{-1} \left( \frac{x}{\varepsilon}, \omega \right) \right) \nabla u^\varepsilon(x, \omega) \right] = f(x) \text{ in } D, \quad u^\varepsilon = 0 \text{ on } \partial D\]

for a periodic matrix $A_{\text{per}}$ and a random diffeomorphism $\Phi$, with $\nabla \Phi$ stationary.

In general, $A_{\text{per}} \circ \Phi^{-1}$ is NOT stationary.

(subsequently used in a variety of contexts: G. Roach et al. (2012), ... , W. Jing (2016), ... , T. Andrade et al. (2019), .... )
Random deformations

\[-\text{div} \left[ A_{\text{per}} \left( \Phi^{-1} \left( \frac{x}{\varepsilon}, \omega \right) \right) \nabla u^\varepsilon(x, \omega) \right] = f(x) \text{ in } \mathcal{D}, \quad u^\varepsilon = 0 \text{ on } \partial \mathcal{D}\]

\[u^\varepsilon(\cdot, \omega) \text{ converges (weakly in } H^1 \text{ and strongly in } L^2) \text{ to } u_* \text{ almost surely, with}\]

\[-\text{div} \left[ A^* \nabla u_*(x) \right] = f(x) \text{ in } \mathcal{D}, \quad u_* = 0 \text{ on } \partial \mathcal{D}\]

with the homogenized matrix

\[A^*_{ij} = \det \left[ \mathbb{E} \left[ \int_Q \nabla \Phi(y, \cdot) dy \right] \right]^{-1} \mathbb{E} \left[ \int_{\Phi(Q, \cdot)} (e_i + \nabla w_{e_i}(y, \cdot))^T A_{\text{per}} \left( \Phi^{-1}(y, \cdot) \right) e_j dy \right]\]

where, for all \( p \in \mathbb{R}^d \), \( w_p \) is the corrector defined by

\[
\begin{cases}
    -\text{div} \left[ A_{\text{per}} \left( \Phi^{-1}(x, \omega) \right) (p + \nabla w_p(x, \omega)) \right] = 0 \text{ in } \mathbb{R}^d, \\
    w_p(x, \omega) = \tilde{w}_p(\Phi^{-1}(x, \omega), \omega), \quad \nabla \tilde{w}_p \text{ is stationary,} \\
\end{cases}
\]

\[\mathbb{E} \left( \int_{\Phi(Q, \cdot)} \nabla w_p(y, \cdot) dy \right) = 0. \quad \text{... So what?}\]
Assume next that the diffeomorphism $\Phi$ is close to the identity:

$$\Phi(x, \omega) = x + \eta \Psi(x, \omega) + O(\eta^2),$$

for $\eta$ small. Then

$$w_p(x, \omega) = w_p^0(x) + \eta w_p^1(x, \omega) + O(\eta^2),$$

with

$$-\text{div} \left( A_{\text{per}} (p + \nabla w_p^0) \right) = 0, \quad w_p^0 \text{ is } \mathbb{Z}^d\text{-periodic},$$

and

$$\begin{cases}
-\text{div} \left[ A_{\text{per}} (\nabla w_p^1 - \nabla \Psi \nabla w_p^0) + (\nabla \Psi^T - (\text{div} \, \Psi)\text{Id}) A_{\text{per}} (p + \nabla w_p^0) \right] = 0, \\
\mathbb{E} \left( \int_Q \nabla w_p^1 \right) = \mathbb{E} \left( \int_Q (\nabla \Psi - (\text{div} \, \Psi)\text{Id}) \nabla w_p^0 \right), \quad \nabla w_p^1 \text{ stationary.}
\end{cases}$$
Random (small) deformations

Taking the expectation and setting \( \overline{w}_p^1 = \mathbb{E}(w_p^1) \),

\[
\begin{cases}
-\text{div} \left[ A_{\text{per}} \nabla \overline{w}_p^1 \right] = \text{RHS} \left( A_{\text{per}}, \mathbb{E}(\nabla \Psi), \nabla w_p^0 \right), \\
\int_Q \nabla \overline{w}_p^1 = \int_Q \left( \mathbb{E}(\nabla \Psi) - \mathbb{E}(\text{div} \, \Psi) \text{Id} \right) \nabla w_p^0, \quad \nabla \overline{w}_p^1 \text{ periodic}.
\end{cases}
\]

Eventually,

\[
A^* = A^0 + \eta A^1 + O(\eta^2),
\]

with

\[
A_{ij}^0 = \int_Q (e_i + \nabla w_{e_i}^0)^T A_{\text{per}} e_j,
\]

\[
A_{ij}^1 = \int_Q \text{fct} \left[ \mathbb{E}(\nabla \Psi), A^0, \nabla w^0, A_{\text{per}} \right] + \int_Q \left( \nabla \overline{w}_{e_i}^1 - \mathbb{E}(\nabla \Psi) \nabla w_{e_i}^0 \right)^T A_{\text{per}} e_j.
\]

Two periodic computations instead of an expensive stochastic one.
Define now a random “perturbation” in a different topology

A. Anantharaman/LB, SIAM MMS, 9, 2 (2011)
In the previous setting, we have considered \( a_{\text{per}}(\Phi^{-1}(x, \omega)) \) with

\[
\Phi_\eta(x, \omega) = x + \eta \Psi(x, \omega) + \ldots,
\]

and \( \eta \) a small scalar. We can alternately consider

\[
\Phi_\eta(x, \omega) = x + b_\eta(x, \omega) \Psi(x, \omega) + \ldots,
\]

with \( b_\eta \) small in some suitable (random) norm.

To keep things simple, let us assume

\[
a(x, \omega) = a_{\text{per}}(x) + b_\eta(x, \omega) c_{\text{per}}(x).
\]

The most interesting case is typically \( b_\eta(x, \omega) \) a Bernoulli random variable.
Randomly located defects

Remember the fibers in the composite, or the rods in the assembly...
Randomly located defects

Law of the material:

\[ \delta_a + \eta (\delta_c - \delta_a) \]

on each cell. Cells are independent from one another. Product. Expand at first order in \( \eta \):

\[
\prod_{k=1}^{N} \delta_a(\text{cell } k) + \eta N \left[ \delta_c(\text{cell } k = 1) \prod_{k=2}^{N} \delta_a(\text{cell } k) - \prod_{k=1}^{N} \delta_a(\text{cell } k) \right].
\]

Think of a jellium model in Physics, that is, a model for defects.

Next remark that in \(-\text{div}(A(x, \omega) (p + \nabla w(x, \omega)) = 0\), the only source of randomness is in \( A \). Put differently, \( w \) is a deterministic function of \( A \). Thus, we have the expansion

\[
A_{i,j}^* = \int \int (e_i + \nabla w e_i(A, y))^T A(y) e_j dy \rho(A) dA.
\]

\[
A^* = A_0 + \eta A_1 + \ldots
\]

Proof of the expansion at all orders: Mourrat (JMPA, 2015), Duerinckx et al. (ARMA, 2016)
Computation of the correctors associated to all possible geometries of one, two, etc, defects. That is, a collection of parameter-indexed elliptic PDEs.

Use of the Reduced Basis method to speed-up the computation (Y. Maday/A. Patera)

We shall soon return to such deterministic localized defects....
Fully random homogenization problems

Of course, if the weakly random model is deemed unfit, there is the option to address the fully random problem. Solve the corrector problem posed on a truncated large domain, and then embrace your enemy: the noise.

\[
A^* - A_N^*(\omega) = A^* - \mathbb{E}[A_N^*] + \mathbb{E}[A_N^*] - A_N^*(\omega)
\]

(small) systematic error  (large) statistical error

A selection of variance reduction approaches:

Blanc/Costaouec/LB/Legoll, MPRF, 2012. (Antithetic Variables)
Legoll/Minvielle, DCDS-S, Vol. 8 (1), 2015. (Control Variate)
LB/Legoll/Minvielle, MCMA, 22 (1), 2016. (Special Quasi-Random Structures, analysis by J. Fischer (ARMA, 2019))
Consider the HJB equation

\[ H(Du^\varepsilon, x/\varepsilon, \omega) = 0 \]

with (say) \( H = |p|^2 - V \) and \( V_\eta = V_{per} + \tilde{V}_\eta(., \omega) \) (Bernoulli of small parameter \( \eta \)). Then

\[
\lim_{\eta \to 0} \frac{H_\eta - H_{per}}{\eta}
\]

is zero for \( d \geq 2 \) (the optimal trajectories can avoid the bumps) and is \( \neq 0 \) for \( d = 1 \) (the trajectory necessarily hits the bump, however rare it is). It is (currently) unclear, for \( d \geq 2 \), what the first nontrivial term is...

Cardaliaguet/LB/Souganidis, viscous case, work in progress.
NONPERIODICITY BY DETERMINISTIC APPROACHES:
TOWARD A THEORY OF DEFECTS
"General" but "explicit" deterministic problems

What is the most general property that allows homogenization while keeping formulae explicit and staying deterministic?

Blanc/LB/Lions, 2002 → 2019 → ...
Non stochastic problems

Consider a set of points \( \{X_i\}_{i \in \mathbb{N}} \) s.t.

(H1) \( \sup_{x \in \mathbb{R}^3} \# \{ i \in \mathbb{N} \mid |x - X_i| < 1 \} < +\infty \),

(H2) \( \exists R_0 > 0, \inf_{x \in \mathbb{R}^3} \# \{ i \in \mathbb{N}, |x - X_i| < R_0 \} > 0 \),

(H3) the following limits exist:

\[
l^0 := \lim_{R \to \infty} \frac{1}{|B_R|} \# \{ i_0 \in \mathbb{N}, |X_{i_0}| \approx \leq R \}.
\]

\[
l^1(h_1) := \lim_{R \to \infty} \frac{1}{|B_R|} \# \{ (i_0, i_1) \in \mathbb{N}^2, |X_{i_0}| \approx \leq R, \ |X_{i_0} - X_{i_1}| \approx h_1 \}.
\]

etc.

Used for Thermodynamic limit problems for interacting particle systems (BLL, 2000’).

Next adapted to Homogenization Theory (BLL, 2010’).
With \( \{X_i\} \) now defined, we introduce the functions

\[
f(x) = \sum_{i \in \mathbb{N}} \varphi(x - X_i), \quad \varphi \in \mathcal{D}(\mathbb{R}^3).
\]

We consider the algebra generated by those functions and its closure for a certain functional norm.

Examples:

**Compactly perturbed periodic systems:** \( \{X_i\}_{i \in \mathbb{N}} = \mathbb{Z}^3 \setminus \{0\} \).

\[
\mathcal{A}^p(\{X_i\}) = L^p_{\text{per}}(\mathbb{Z}^3) + L^p_0(\mathbb{R}^3),
\]

where \( L^p_0(\mathbb{R}^3) = \{f \in L^p_{\text{loc}}(\mathbb{R}^3), \lim_{|x| \to \infty} \|f\|_{L^p(B+x)} = 0\} \).

**Two semi-crystals:**

\[
\mathcal{A}^p(\{X_i\}) = \left( L^p_{\text{per},1}(\mathbb{Z}^3-), L^p_{\text{per},2}(\mathbb{Z}^3+) \right) + L^p_0(\mathbb{R}^3).
\]
The question is homogenization for

$$-\text{div} \left( a\left(\frac{x}{\varepsilon}\right) \nabla u^\varepsilon \right) = f,$$

where $a$ is a function of the algebra, e.g.,

$$a(y) = 1 + \sum_{i \in \mathbb{N}} \varphi(y - X_i).$$

Homogenization does hold, but the issue we examine is the existence of an explicit expression for the limit.

Relation with works by G. N’Guetseng, J-L. Woukeng, et al.
Difficulty: show that the corrector problem is well posed in the algebra, that is, if \( a \in A \) then the corrector problem

\[ -\text{div} \left( a(y) \left( p + \nabla w_p \right) \right) = 0 \]

is uniquely solvable for \( \nabla w_p \in A \) and \( \langle \nabla w_p \rangle = 0 \).

The tools of elliptic problems posed on bounded domains are useless...

At present time, no general proof, valid for an abstract general algebra as defined above, is known.

A variety of particular cases are considered and solved.
Well-posedness of the corrector problem

Existence of correctors for nonperiodic homogenization problems

\[- \text{div} \left( a \left( p + \nabla w_p \right) \right) = 0 \quad \text{on } \mathbb{R}^d \]

Blanc/LB/Lions, Milan Journal of Maths (2012)
Blanc/LB/Lions, Comm. PDE, Vol. 43, 6 (2019)
Consider \( a = a^{\text{per}} + \tilde{a} \) where \( a^{\text{per}} \) denotes the (unperturbed) background, and \( \tilde{a} \) the perturbation.

We want to solve

\[
- \text{div} \left( (a^{\text{per}} + \tilde{a}) (p + \nabla w_p) \right) = 0
\]

in the suitable functional class, with \( w_p(x) = o(1 + |x|) \).

(a PDE problem)
Well-posedness of the corrector problem

Case considered: perturbation of a periodic background $a^{per}$, that is $a = a^{per} + \tilde{a}$. We would like to address the case

$$\tilde{a}(x) \xrightarrow{|x| \to \infty} 0,$$

but are only able to treat

$$\tilde{a} \in L^r(\mathbb{R}^d), \quad \text{for some} \quad 1 \leq r < +\infty.$$

Second case (not considered today): twin-boundaries, that is two different periodic structures separated by a flat interface.

$$a^{per}(x) = a_{per,1,2}(x) = \begin{cases} 
  a_{per,1}(x) & \text{when } x_1 \leq 0, \\
  a_{per,2}(x) & \text{when } x_1 > 0,
\end{cases}$$

(plus possibly a perturbation $\tilde{a}$ on top of that).
"Generic" Bi-crystal: "Twin boundaries"
A theoretical ingredient for MsFEM

- **Coarse mesh** with a P1 Finite Element basis functions $\phi_i^0$.

- **MsFEM basis**

$$
\begin{cases}
- \text{div}(A^\varepsilon(x) \nabla \phi_i^{\varepsilon,K}) = 0 & \text{in } K \\
\phi_i^{\varepsilon,K} = \phi_i^0|_K & \text{on } \partial K
\end{cases}
$$

and glue them together: $\phi_i^{\varepsilon}$ such that $\phi_i^{\varepsilon}|_K = \phi_i^{\varepsilon,K}$ for all $K$. The MsFEM functions are computed independently (in parallel) over each $K$.

- Solve the **macro problem** with MsFEM basis functions $\phi_i^{\varepsilon}$.

Efendiev, Hou, Allaire, Peterseim, ...
Relative errors using the periodic (left) and the adapted corrector (right).

\[
\frac{\| \nabla u^\varepsilon (\varepsilon \cdot) - \nabla u^\varepsilon_{\text{per}} (\varepsilon \cdot) \|_{L^2(\Omega)}}{\| \nabla u^\varepsilon (\varepsilon \cdot) \|_{L^2(\Omega)}} - \text{div} \left( (a_{\text{per}}(x/\varepsilon) + \tilde{a}(x/\varepsilon)) \, \nabla u^\varepsilon \right) \equiv f.
\]

Defect $\tilde{a} \in L^r(\mathbb{R}^d)$, $r \neq 2$

**Theorem** [Blanc/LB/Lions, Comm. PDE, 2015.]

(*$L^r$-perturbation of periodic*): Assume periodicity of the background and Hölder regularity. Then, the corrector problem has a unique solution $w_p$, up to the addition of a constant. Moreover, $w_p = w_{p,\text{per}} + \tilde{w}_p$, where $w_{p,\text{per}}$ is the periodic corrector and

- if $1 \leq r < d$, then, $\lim_{|x| \to +\infty} \tilde{w}_p(x) = 0$;
- if $2 \leq r$, then $\nabla \tilde{w}_p \in L^r$.

**Remarks**: Periodicity of $a^{\text{per}}$ and Hölder regularity of $a^{\text{per}}$ and $\tilde{a}$ are needed. The case $r = d$ is clearly critical.
Once the corrector equation is written under the form

\[- \text{div} \left( a \nabla \tilde{w}_p \right) = \text{div} \left( \tilde{a} \left( p + \nabla w_{p,\text{per}} \right) \right),\]

it is immediate to see that proving the existence/uniqueness of the corrector amounts to establishing the estimate

\[- \text{div} \left( a \nabla u \right) = \text{div} \left( f \right) \Rightarrow \| \nabla u \|_{L^q(\mathbb{R}^d)} \leq C_q \| f \|_{L^q(\mathbb{R}^d)}\]

for the coefficient \( a = a^{\text{per}} + \tilde{a} \) and \( \tilde{a} \in L^r(\mathbb{R}^d) \). (Apply to \( q = r \)).

We indeed show that such an estimate holds true, using concentration-compactness to reduce the problem to the periodic result of [Avellaneda-Lin]. And we do so in a variety of settings ...
Approximation theory for nonperiodic homogenization problems

"The corrector corrects"

\[ w_\varepsilon = w \left( \cdot / \varepsilon \right) \quad \Rightarrow \quad \text{rates of convergence} \]

Theorem: Assume $r \neq d$ and $b \in L^r(\mathbb{R}^d)$. Take $a = a_{per} + b$ with the usual properties of ellipticity and Hölder regularity. Consider a right-hand side $f \in L^p(\Omega)$ and the residual

$$R_\varepsilon = u_\varepsilon - u^* - \varepsilon \sum_{i=1}^{d} \partial_i u^*(\cdot) w_i(\cdot/\varepsilon).$$

Then

$$\| \nabla R_\varepsilon \|_{L^2(\Omega)} \leq C \varepsilon \min(1, d/r) \left( \| f \|_{L^2(\Omega)} + \| \nabla u^* \|_{L^\infty(\partial \Omega)} \right).$$

When in addition $f \in L^d(\Omega)$, we have

$$\| \nabla R_\varepsilon \|_{L^p(\Omega)} \leq C \varepsilon \min(1, d/r) \left( \| f \|_{L^p(\Omega)} + \| \nabla u^* \|_{L^\infty(\partial \Omega)} \right),$$

and ...
\[
\frac{1}{B(0, \varepsilon)} \int_{B(0, \varepsilon)} |\nabla R_\varepsilon|^2 \leq C \varepsilon^{\min(1, d/r) - d/p} \left( \|f\|_{L^p(\Omega)} + \|\nabla u^*\|_{L^\infty(\partial\Omega)} \right).
\]

If \( d \geq 3 \) and \( f \) is Hölder regular, then

\[
\|\nabla R_\varepsilon\|_{L^\infty(\Omega)} \leq C \varepsilon^{\min(1, d/r)} \left( 1 + |\ln \varepsilon^{-1}| \right) \|f\|_{C^{0, \beta}(\Omega)}.
\]

The point for the proof is \( w_\varepsilon = w(\cdot/\varepsilon) \).
The proof follows the same pattern as those by Avellaneda/Lin and Kenig/Lin/Shen in the periodic case. It concatenates

1. $L_\varepsilon$ converges to $L^*$ thus "what is true for the latter is true for the former when $\varepsilon$ is small"

2. estimate of the Green function $G_\varepsilon(x, y)$ by Grüter/Widman (only ellipticity)

3. estimate of its derivative $\partial_x G_\varepsilon(x, y)$ and $\partial_x \partial_y G_\varepsilon(x, y)$ (structure is needed)

4. estimate of the rate of convergence of $R_\varepsilon$ following for a regular right-hand side

5. argument by duality for the convergence of the Green functions $G_\varepsilon(x, y) - G^*(x, y)$
Extensions

- interface problems, M. Josien (CPDE, 2019)
- perforated domains, X. Blanc/S. Wolf (subm., 2019)
- defects "rare" at infinity, Blanc/Goudey/LB, work in progress
- ...
- nonlinear problems, ...
Not all equations behave like elliptic linear. An elliptic equation is indeed very forgiving...

Example (in 1D): $u^\varepsilon$ solution to

$$u^\varepsilon + |(u^\varepsilon)'| = b(x/\varepsilon)$$

for $b(0) = \inf_{\mathbb{R}} b < 0$, $b \in \mathcal{D}(\mathbb{R})$, converges uniformly to $\bar{u}$, solution to

$$\bar{u}(0) = b(0) \quad \text{and} \quad \bar{u}(x) + |(\bar{u})'(x)| = 0, \quad \forall x \neq 0$$

that is

$$\bar{u}(x) = b(0)e^{-|x|}$$

which is different from $u = 0$, the solution when $b \equiv 0$. The microscopic defect $b$ affects the equation macroscopically.
Coarse approximation of an oscillatory elliptic problem

"Homogenization with partial information"

LB/ Legoll/ Li, C. R. Acad. Sc., 351, (2013)
Gorynina/LB/Legoll, in preparation.
There exist many practical situations in

$$-\text{div} \left( A_\varepsilon \nabla u_\varepsilon \right) = f \text{ in } \Omega \subset \mathbb{R}^d,$$

for which

- $A_\varepsilon$ is not entirely known: one can only measure / observe the solution $u_\varepsilon$ for some loadings $f$ (think of mechanical experiments), so we have no access to the corrector equation.
- homogenization theory does not give explicit formulae for $A^*$
- even if explicit, $A^*$ is challenging to compute (or even as difficult as $A_\varepsilon$, like in the fractal case)

Can we nevertheless approximate $A_\varepsilon$ by a constant matrix, e.g. bypassing the computation of the correctors to compute $A^*$, or the computation of local problems in a dedicated Galerkin procedure?
Best constant matrix

Idea: approximate

\[-\text{div} \left( A_\varepsilon \nabla u_\varepsilon \right) = f\]

by

\[-\text{div} \left( \overline{A} \nabla \overline{u} \right) = f,\]

where \(\overline{A}\) is the best possible constant matrix so that \(\overline{u}\) is close to \(u_\varepsilon\).

- ideal choice for this matrix \(\overline{A}\)?
- when \(\varepsilon \rightarrow 0\), does this best matrix converge to the homogenized matrix \(A^*\) (in a setting when \(A^*\) is constant)?
- how to compute / approximate \(\overline{A}\)?

Related to Francfort/Garroni (ARMA, 2006), Blasselle/Maday (2011), and the whole area of inverse problems.
**Best constant matrix**

\[
I_\varepsilon = \inf_{\text{constant matrix } \bar{A} > 0} \sup_{f \in L^2(\Omega), \|f\|_{L^2(\Omega)} = 1} \|u_\varepsilon(f) - u(\bar{A}, f)\|^2_{L^2(\Omega)}
\]

Then

- \(\lim_{\varepsilon \to 0} I_\varepsilon = 0\).
- for any quasi-minimizing matrix \(\bar{A}_\varepsilon\) (i.e. \(I_\varepsilon \leq J_\varepsilon(\bar{A}_\varepsilon) \leq I_\varepsilon + \varepsilon\)), we have \(\lim_{\varepsilon \to 0} \bar{A}_\varepsilon = A^*\).

Ingredients of the proof:

- knowing \(R_{\bar{A}} = (-\text{div} \bar{A} \nabla)^{-1}\) amounts to knowing \(\bar{A}\) when \(\bar{A}\) is a constant matrix (in fact \(\|R_{\bar{A}} - R_B\| \approx \|\bar{A} - B\|\))
- the definition of \(I_\varepsilon\) guarantees the convergence of \(R_{\bar{A}_\varepsilon}\) to \(R_{A^*}\), thus that of \(\bar{A}_\varepsilon\) to \(A^*\).
Formally, we wish to consider

\[ I_\varepsilon = \inf_{\text{constant matrix } \overline{A} > 0} \sup_{f \in L^2(\Omega), \|f\|_{L^2(\Omega)} = 1} \left\| u_\varepsilon(f) - u(\overline{A}, f) \right\|^2_{L^2(\Omega)}. \]

Following an idea by Albert Cohen, we instead consider (compose by the 0-order operator \( \Delta^{-1} \text{div} \overline{A} \nabla \))

\[ I_\varepsilon = \inf_{\text{constant matrix } \overline{A} > 0} \sup_{f \in L^2(\Omega), \|f\|_{L^2(\Omega)} = 1} \left\| -\Delta^{-1} \left( -\text{div} \overline{A} \nabla u_\varepsilon(f) - f \right) \right\|^2_{L^2(\Omega)}. \]

Same theoretical result as above. Practically: much better because quadratic functional in \( \overline{A} \) and more robust!
Best constant matrix

- in practice, $\sup_f$ is replaced by $\max(f_1,\ldots,f_N)$ ⊕ strategy to choose the sample set of suitable r.h.s. $f_i$
- the corrector function is obtained by a post-process, using the two-scale expansion as a proxy
- the approach carries over to random homogenization
- an interesting variant introduced by R. Cottereau (IJNME, 2013): use the Arlequin coupling method (in order to avoid boundary effects) along with an optimization loop to identify the homogenized tensor (improved in Gorynina/LB/Legoll, work in progress).
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