Construction of coarse approximations for a Schrödinger problem with highly oscillating potential

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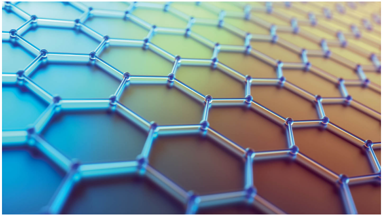
Outline

Inverse Problem : A new paradigm

Let Ω be a bounded open of $\mathbb{R}^d$.
Direct problem : For a given operator $\mathcal{L}$ and RHS f, find u that satisfies

$$\begin{cases} \mathcal{L}u = \Big(\sum_{i,j} a_{ij}(\cdot)\partial_{i,j} + \sum_i b_i(\cdot)\partial_i + c(\cdot) \Big) u = f \quad \text{in } \Omega, \\ u = 0 \quad \text{on } \partial\Omega. \end{cases} \tag{1}$$



Inverse Problem : A new paradigm

Let Ω be a bounded open of $\mathbb{R}^d$.

Direct problem : For a given operator $\mathcal{L}$ and RHS f, find u that satisfies (1).

Inverse problem : Assume the map $f \to u$ solution to (1) is known.

"Find" $\mathcal{L}$ such that (1) is satisfied.

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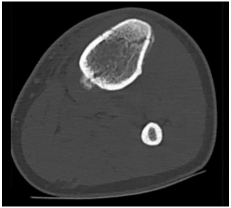


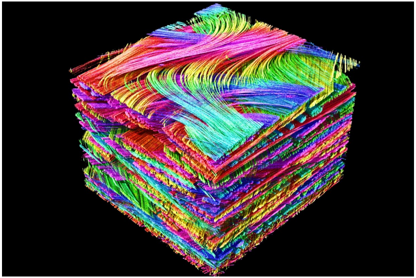
Inverse Problem : A new paradigm

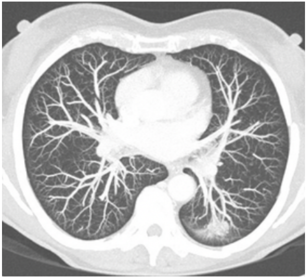
Inverse problems

- have been widely studied (Calderón problem, 1980)
- may involve more complexity (e.g. partial measurements available, finite number of available measurements, ...).
- are (very) HARD to solve ! (existence/uniqueness/stability issues...)

Multiscale Context

Our study focuses on multiscale systems (e.g. composite materials, lungs). Such systems naturally leads to ill-posed inverse problems (see [Lions05]).





Multiscale Context : ill-posed inverse problem

Consider the problem oscillating at the *small* length scall ε

$$\mathcal{L}_\varepsilon u_\varepsilon = (-\Delta + \varepsilon^{-1} V(\varepsilon^{-1} \cdot)) u_\varepsilon = f \text{ in } \Omega, \qquad u_\varepsilon = 0 \text{ on } \partial\Omega,$$

with potential **periodic** V such that $\langle V \rangle = 0$, and RHS $f \in L^2(\Omega)$.

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Homogenization theory[1] assesses the existence of a limit equation when $\varepsilon \to 0$.

$$\mathcal{L}_\star u_\star = (-\Delta + V_\star)u_\star = f \text{ in } \Omega, \qquad u_\star = 0 \text{ on } \partial\Omega.$$

which means $u_\varepsilon \to u_\star$ strongly in $L^2(\Omega)$ and weakly in $H^1(\Omega)$ when $\varepsilon \to 0$.

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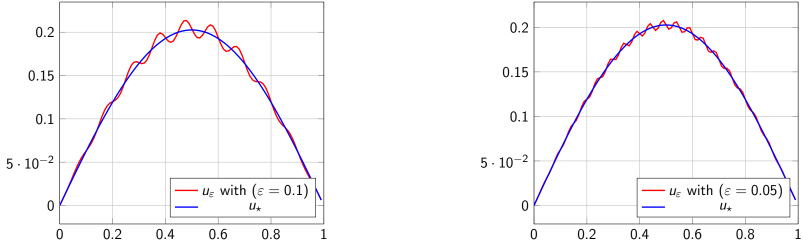

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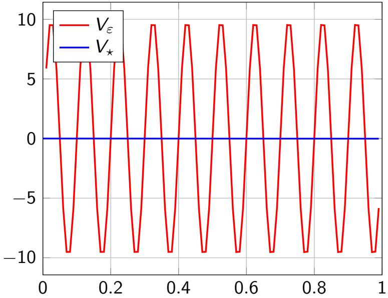
Multiscale Context : ill-posed inverse problem

Issue : in the limit $\varepsilon \to 0$, the quantity u_ε is very close to $u_\star$, whereas the operator we seek to reconstruct, $\mathcal{L}_\varepsilon$, is very different from $\mathcal{L}_\star$, its homogenized version.



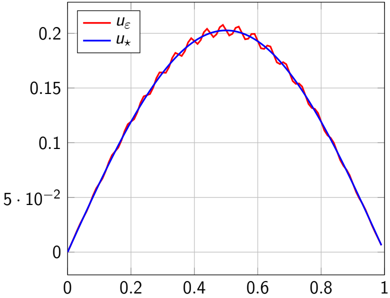


Figure: Two similar solutions associated to two very distinct potentials

An Inverse Multiscale Problem

How to tackle such problems ?

General approach :

- **Direct Inversion** (see [Uhlmann13]),
- **Perturbation** (see [Ammari08]),

Approach based on homogenization (see [Nolen12]):

- **Features Determination** (see [Engquist14]),
- **Regularization at order** 0, identifying effective quantity (see [Ammari16, Caiazzo20]),
- **Regularization at order** 1, beyond effective quantity : H^1 reconstruction (see [Garnier23, LeBris18]).
- **Inverse Homogenization** (see [Cherkaev01])

Our Approach

Consider the Schrödinger problem (2) involving a periodic potential V :

$$\mathcal{L}_\varepsilon u_\varepsilon = \left(-\Delta + \varepsilon^{-1} V\left(\varepsilon^{-1} \cdot\right)\right) u_\varepsilon = f \text{ in } \Omega, \qquad u_\varepsilon = 0 \text{ on } \partial\Omega. \tag{2}$$

From the knowledge of solutions u_ε for various rhs f, our aim is:

1. to propose a numerical methodology to build an effective operator $\overline{\mathcal{L}}$ approaching $\mathcal{L}_\varepsilon$ with satisfying L^2 error on the solutions,

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Our strategy

- is inspired by homogenization theory,
- does not rely on classical hypothesis for homogenization (such as periodicity) which may be too restrictive in practical situations,
- can be adapted to a wide range of other elliptic equations (see [LeBris18]),
- is valid outside the regime of homogenization (i.e. $\varepsilon \to 0$).

Recovering an effective potential

Let $\overline{V} \in \mathbb{R}$ be a *constant* potential, and $\overline{u} = u(\overline{V}, f)$ be the solution to (3) with RHS $f \in L^2(\Omega)$.

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The quality of the approximation of $\mathcal{L}_\varepsilon$ by $\overline{\mathcal{L}}$ can be quantified through the functional

$$\sup_{\|f\|_{L^2(\Omega)}=1} \left\| u_\varepsilon(f) - u(\overline{V}, f) \right\|_{L^2(\Omega)}^2$$

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$$\sup_{\|f\|_{L^2(\Omega)}=1} \left\| u_\varepsilon(f) - u(\overline{V}, f) \right\|^2_{L^2(\Omega)}$$

Hence we can minimize the worst case scenario with the optimization problem

$$\inf_{\overline{V}\in\mathbb{R}} \sup_{\|f\|_{L^2(\Omega)}=1} \| u_\varepsilon(f) - u(\overline{V}, f) \|^2_{L^2(\Omega)}$$

The choice of an $L^2(\Omega)$ norm is reminescent of the fact that $\| u_\varepsilon - u_\star \|_{L^2(\Omega)}$ tends to 0 with ε.

Recovering an effective potential

Practical considerations : To recover a **quadratic** optimization problem in $\overline{V}$, we consider the slightly different problem (4)

$$I_\varepsilon = \inf_{\overline{V}\in\mathbb{R}} \sup_{\|f\|_{L^2(\Omega)}=1} \left\|(-\Delta)^{-1}\left(-\Delta+\overline{V}\right)\left(u_\varepsilon(f)-\overline{u}(f)\right)\right\|^2_{L^2(\Omega)}. \quad (4)$$

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Theoretical considerations :

Proposition (Asymptotic consistency, periodic case)

Consider the problem (4)*. In the periodic setting, we have*

$$\lim_{\varepsilon\to 0} I_\varepsilon = 0. \qquad (5)$$

Furthermore, for $\varepsilon > 0$ fixed (sufficiently small), there exists a unique minimizer $\overline{V}^0_\varepsilon \in \mathbb{R}$. The following convergence holds :

$$\lim_{\varepsilon\to 0} \overline{V}^0_\varepsilon = V_\star. \qquad (6)$$

A consistency result

Let $\Phi_\varepsilon(\overline{V}) = \sup_{\|f\|_{L^2(\Omega)}=1} \left\| (-\Delta)^{-1} \left(-\Delta + \overline{V}\right) \left(u_\varepsilon(f) - \overline{u}(f)\right) \right\|^2_{L^2(\Omega)}.$

Lemma

In the periodic setting, we have

$$\lim_{\varepsilon \to 0} \Phi_\varepsilon(V_\star) = 0.$$

Lemma

For ε sufficiently small, the functional Φ_ε is continuous and convex.

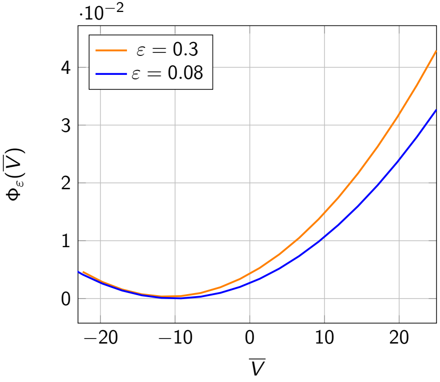

Figure: Convexity of Φ_ε.

Numerical results

We use an alternating direction algorithm in 2D ($\Omega = [0,1]^2$) using the potential

$$V(x,y) = \pi^2\sqrt{8}\,(\sin(2\pi x) + \sin(2\pi y))\,.$$

We approximate the supremum by a maximization over the first eigenmodes of $(-\Delta)$-operator. In practice, a *single* mode is sufficient in order to find the *single* coefficient $\overline{V}$.

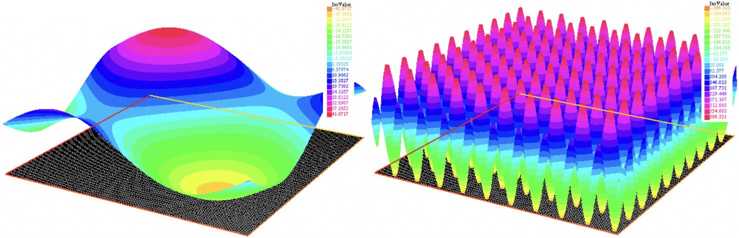

Figure: Potential V and Oscillating Potential $V_\varepsilon = \varepsilon^{-1}V(\varepsilon^{-1}\cdot)$.

Numerical results

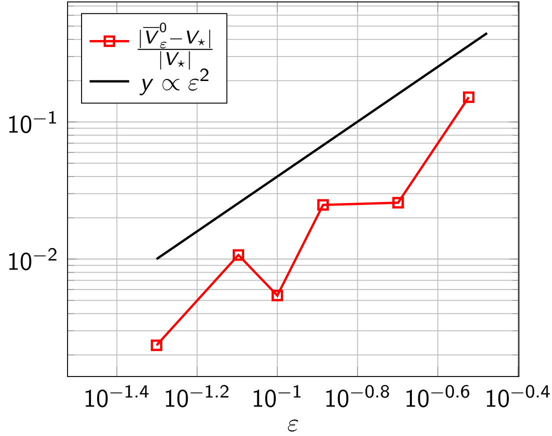

Figure: Error between the homogenized potential $V_\star$ and the effective potential $\overline{V}_\varepsilon^0$ as a function of ε.

Numerical results

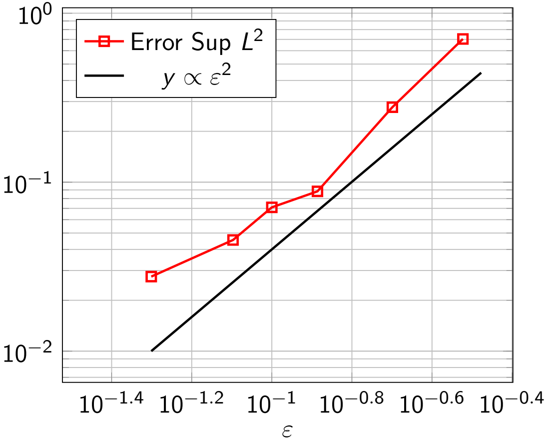

Figure: Error $\sup_{f \in \mathrm{Span}_{1 \leq p \leq 10}(f_p)} \left(\frac{\| u_\varepsilon(f) - u(\overline{V}^0_\varepsilon, f) \|_{L^2(\Omega)}}{\| u_\varepsilon(f) \|_{L^2(\Omega)}} \right)$ as a function of ε. ($\overline{V}^0_\varepsilon$ computed with $P = 3$)

Recovering an H^1-approximation

In the periodic setting, homogenization theory assesses that u_ε converges to $u_\star$ strongly in $L^2(\Omega)$, but only **weakly in** $H^1(\Omega)$. We wish to recover within our strategy a satisfying $H^1(\Omega)$ approximation. The strategy consisting in considering the problem (7) is a dead-end.

$$I_\varepsilon^{H^1} = \inf_{\overline{V}\in\mathbb{R}} \sup_{\|f\|_{L^2(\Omega)}=1} \|u_\varepsilon(f) - u(\overline{V}, f)\|_{H^1(\Omega)}. \tag{7}$$

How can we go further ?

Recovering an H^1-approximation

An essential tool in homogenization is the corrector. For our Schrödinger equation (2), it is the periodic solution to (8), denoted w.

$$\Delta w = V \tag{8}$$

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Homogenization theory assesses that $u_{\varepsilon,1} = u_\star(1 + \varepsilon w(\varepsilon^{-1}\cdot))$ is a good H^1 approximation of solution u_ε. Hence, we have :

$$\nabla u_\varepsilon(x) = \nabla u_\star(x) + u_\star(x)(\nabla w)\left(\frac{x}{\varepsilon}\right) + o_{L^2}(\varepsilon)$$

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Inspired by this statement, we define $\overline{C}_\varepsilon^0$, an approximation of $(\nabla w)(\varepsilon^{-1}\cdot)$, as the minimizer of (9).

$$I_\varepsilon^{corr} = \inf_{C \in \mathbb{P}^0} \sup_{\|f\|_{L^2}=1} \|\nabla u_\varepsilon(f) - \nabla u(\overline{V}_\varepsilon, f) - u(\overline{V}_\varepsilon, f) C\|_{L^2(\Omega)}^2. \tag{9}$$

where $u(\overline{V}_\varepsilon, f)$ is to be understood as an approximation of $u_\star(f)$ (which holds since $\overline{V}_\varepsilon \approx V_\star$).

Numerical results

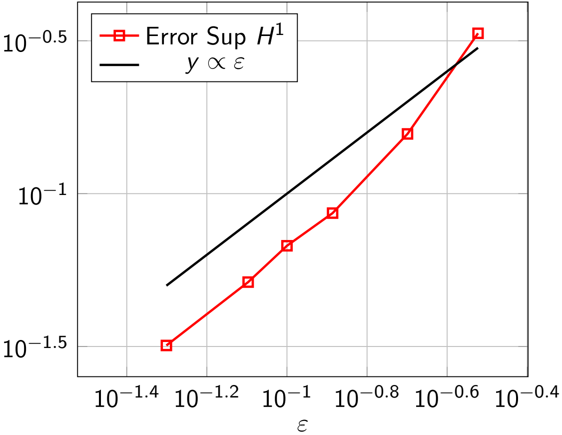

Figure: H^1 maximal error $\sup_{f \in \mathrm{Span}_{1 \leq p \leq 10}(f_p)} \left(\frac{\| \nabla u_\varepsilon(f) - \nabla u(\overline{V}_\varepsilon^0, f) - u(\overline{V}_\varepsilon^0, f) \overline{C}_\varepsilon^0 \|_{L^2(\Omega/\partial\Omega)}}{\| \nabla u_\varepsilon(f) \|_{L^2(\Omega/\partial\Omega)}} \right)$ as a function of ε. ($\overline{V}_\varepsilon^0$ and $\overline{C}_\varepsilon^0$ computed with $P = 3$)

Future Work

In progress :

- Robustness analysis : what happens if the data is blurred/perturbed/deteriorated/... ?
- Exploring other type of data : starting from the knowledge of macroscopic data $\left(\text{e.g. energy } \int_\Omega |\nabla u_\varepsilon|^2 + V_\varepsilon u_\varepsilon^2\right)$ instead of microscopic ones.

Thank you !

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Supremum or Maximum ?

For small ε, homogenization assesses $u_\varepsilon(f) \to u_\star(f)$ in $L^2(\Omega)$. Hence for all $f \in L^2(\Omega)$, we have

$$\left\|(-\Delta)^{-1}\left(-\Delta+\overline{V}\right)\left(u_\varepsilon(f)-\overline{u}(f)\right)\right\|^2_{L^2(\Omega)} \to \underbrace{\left\|(-\Delta)^{-1}\left(-\Delta+\overline{V}\right)\left(u_\star(f)-\overline{u}(f)\right)\right\|^2_{L^2(\Omega)}}_{=\int_\Omega \mathcal{H}_\star^{\overline{V}}(f)\, f}.$$

The study of $\mathcal{H}_\star^{\overline{V}}$ shows that it has the same eigenvalues (in the same order) as $-\Delta$.
Hence the supremum is well approximated by a maximization on the first eigenmodes :

$$\sup_{f\in L^2(\Omega)} \frac{\int_\Omega \mathcal{H}_\star^{\overline{V}}(f)\, f}{\|f\|^2_{L^2(\Omega)}} \approx \max_{f\in Span(\phi_p)_{p=1}^P} \frac{\int_\Omega \mathcal{H}_\star^{\overline{V}}(f)\, f}{\|f\|^2_{L^2(\Omega)}}$$