Numerical Homogenization of PDE - inofficial lecture notes

April 26, 2016

Contents

Chapter 1

Introduction

1.1 Multiscale Problems

Applications include:

- Geophysical Flows in porous media
- Mechanical Simulation & Design of composite materials

For further information about Multiscale Problems in general see [**?**, Chapter 1].

1.2 Modeling of diffusion in heterogeneous media

Imagine a motionless medium (or fluid) filling a straight and very thin tube, and a substance diffusion through it. What we have given is the concentration of the substance $u(t)$ at some time $t = 0$, we are interested in the computation at later times. The amount of substance that passes the point x from left to right is called flux $q(x,t)$. We assume conservation of mass, i.e., for any control volume (x_0, x_1), the mass

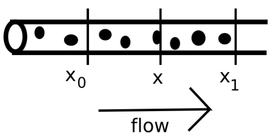

Figure 1.1: Multiscale setting of a thin tube; shows the flux at the point x

$$M = \int_{x_0}^{x_1} u(x,t)\,dx$$

changes in time only by *in-* or *outflow*, i.e. the change of mass

$$\frac{d}{dt}M = q(x_0, t) - q(x_1, t).$$

The above equation states that the mass changes due to inflow at x_0 and outflow at x_1 at time t (negative flow, i.e. outflow has negative sign).

We rewrite this as

$$\int_{x_0}^{x_1} \frac{d}{dt}u(x,t)\,dx = q(x_0, t) - q(x_1, t).$$

Differentiation w.r.t. x_1 and replacement of $x_1 \mapsto x$ leads (assuming the standard interval in space)

$$\frac{d}{dt}u = -\frac{d}{dx}q, \quad \text{in } Q = [0,1] \times [0,T].$$

This conservation law does not determine u and q. We need a second hypothesis that connects concentration and flux - a *diffusion law* (experimental / phenomenological law). The simplest diffusion law is **Fick's first law** and says that the flux depends linearly on u_x

$$q(x,t) = -A(x)\frac{d}{dx}u(x,t).$$

The diffusivity $A(x) > 0$ is a characteristic property of the medium (material) at point x. In homogeneous media, A may be treated as a global constant. In heterogeneous media, A varies with spatial location (e.g. A takes two different values in the fibers and in the background medium (*matrix*)). Finally, we model the process of diffusion by the linear PDE:

$$\frac{d}{dt}u = \frac{d}{dx}\left(A\frac{d}{dx}u\right) \quad \text{in } Q \tag{1.1}$$

along with the initial condition $u(x,0) = u_0(x)$, with u_0 denoting the given concentration at time $t = 0$. If we want to model that no substance can enter or escape the tube, then by *Fick's law* we have that

$$\frac{d}{dt}u(0,t) = \frac{d}{dx}u(1,t) = 0, \qquad 0 \le t \le T. \tag{1.2}$$

This is called *Neumann boundary condition.*

Eq. (1.1) also models heat diffusion in a thin wire.

The boundary condition in Eq. (1.2) then models perfect insulation at the end points. If instead a temperature is prescribed, we employ a *Dirichlet boundary condition*:

$$u(0,t) = g_1(t),\ u(1,t) = g_2(t), \quad 0 \le t \le T \tag{1.3}$$

for given functions g_1, g_2.

Often, we are interested in the steady-state solution of Eq. (1.1), i.e. the equilibrium concentration / temperature after long time if data remains unchange (i.e. $\frac{d}{dt}u = 0$). This leads to the stationary heat equation

$$\frac{d}{dx}\left(A(x)\frac{d}{dx}u(x)\right) = 0, \quad \text{in }]0,1[,$$

resp.

$$-\frac{d}{dx}\left(A(x)\frac{d}{dx}u(x)\right) = 0, \quad \text{in }]0,1[,$$

with Dirihlet boundary condition

$$u(0) = g_1, \quad u(1) = g_2,$$

for some $g_1, g_2 \in \mathbb{R}$. In the presence of further forces (gravity, external heat source) in a multi-dimensional setting, our model problem reads

$$\begin{aligned} -\operatorname{div}(A(x)\nabla u(x)) &= f(x), \quad x \in \Omega \subseteq \mathbb{R}^d \\ u(x) &= 0, \quad x \in \partial\Omega. \end{aligned}$$

In anisotropic materials, the diffusivity depends on the direction, and $A(x)$ is a positive definite matrix ($A \in \mathbb{R}^{d\times d}$).

1.3 Highly oscillatery diffusion in 1d

For the illustration of the critical scaling effects that motivate this lecture, we study the simple model problem

$$\left.\begin{aligned} -\operatorname{div}(A_\varepsilon(x)\nabla u_\varepsilon(x)) = {}& f(x), \quad x \in]0,1[\\ u_\varepsilon(0) = u_\varepsilon(1) = {}& 0 \end{aligned}\right\} \tag{1.4}$$

with some *forcing term* f and uniformly positive ε-periodic diffusion coefficient A_ε. ε reflects the period length.

The problem admits a unique solution $u_\varepsilon \in H_0^1(0,1)$, that is as well characterized by the variational problem

$$\int_0^1 A_\varepsilon(x)u_\varepsilon'(x)v'(x)\,dx = \int_0^1 f(x)v(x)\,dx, \quad \forall v \in H_0^1(0,1).$$

1.3.1 Naive Finite Element approximation

Consider the particular data $A_\varepsilon(x) = \frac{1}{2+\cos(2\pi\frac{x}{\varepsilon})}$, $f(x) = 1$ in Eq. (1.4). The problem we want to solve numerically is

$$\left.\begin{aligned} -(A(x)u'(x))' = {}& f(x), \quad \text{for } 0 \le x \le 1 \\ u(0) = u(1) = {}& 0 \end{aligned}\right\}$$

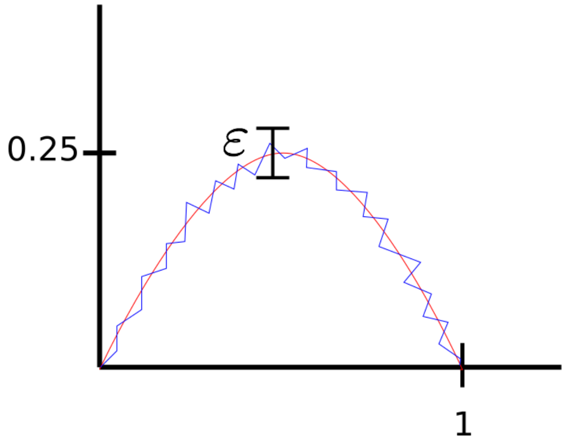

Figure 1.2: The true solution u_ε is a slightly perturbed version of $x - x^2$, perturbation is at most ε

In this case, an easy computation reads that

$$u_\varepsilon(x) = (x - x^2) + \varepsilon\left[\frac{1}{4\pi}\sin\left(2\pi\frac{x}{\varepsilon}\right) - \frac{1}{2\pi}x\sin\left(2\pi\frac{x}{\varepsilon}\right) - \frac{\varepsilon}{4\pi^2}\cos\left(2\pi\frac{x}{\varepsilon}\right) + \frac{\varepsilon}{4\pi^2}\right]$$

Numerical experiments with the standard FEM show that u_ε is just approximated if the meshsize h gets less or equal to ε.

1.3.2 Effective coefficient and periodic homogenization

Classical homogenization is a tool of mathematical modelling that seeks a simplified model (PDE) that is able to capture the macroscopic part of the (oscillatory) solution. For the example from Section 1.3.1, we had a solution of the form

$$u_\varepsilon(x) = \underbrace{x - x^2}_{=u_0(x)} + \varepsilon\left(u_1\left(\frac{x}{\varepsilon}\right)\right),$$

that is it consists of a **macroscopic part** $u_0 = x - x^2$ and some **microscopic part**

$$u_1 = u_\varepsilon - u_0 = -\varepsilon\left[\frac{1}{4\pi^2}\cos\left(\frac{2\pi}{\varepsilon}\right) - \frac{1}{2\varepsilon}x\sin\left(\frac{2\pi x}{\varepsilon}\right) - \frac{\varepsilon}{4\pi^2}\cos\left(\frac{2\pi}{\varepsilon}\right) + \frac{\varepsilon}{4\pi^2}\right]$$

that tends to 0 as $\varepsilon \to 0$ (strongly in $L^2(0,1)$). This means that

$$u_\varepsilon \xrightarrow{\varepsilon\to 0} u_0 \quad \text{strongly in } L^2(0,1).$$

Moreover, one observes that u_0 solves

$$\begin{cases} -\dfrac{d}{dx}A_0\dfrac{d}{dx}u_0 = & f, \quad 0 \le x \le 1 \\ u_0(0) = u_0(1) = & 0 \end{cases}$$

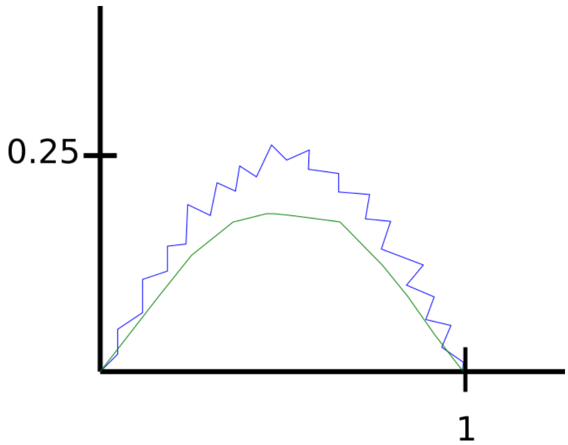

Figure 1.3: For $h > \varepsilon$ the sequence of FEM-solutions converges to some other function than the true solution of the problem

where $A_0 = \frac{1}{2} > 0$ is a global constant.

Question: Is this by coincidence or is there a general mechanismn behind?

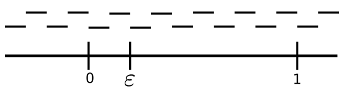

Figure 1.4: Example of a 1-periodic coefficient A_1 and it's scaling by ε

Assumption 1.1
Assume that $A \in L^\infty_{per}(0,1)$ is 1-periodic and define the ε-periodic coefficients A_ε (see also Fig. 1.4) by

$$A_\varepsilon(x) := A_1\left(\frac{x}{\varepsilon}\right).$$

Question (more precisely): Is there an effective (constant) coefficient $A_0 > 0$ such that the solution u_ε of our model problem converge to u_0, the solution of the problem from Section 1.3.1, uniformly w.r.t $f \in L^2(0,1)$.
If the answer is yes, then A_0 (resp. the problem) is called **homogenized/effective coefficient** (resp. solution, problem,...). There is the equally important question of computability of A_0!

In the simple 1d model, we will be able to answer both questions in a stroke!
Assume for the time being that $A_0 > 0$ exists. (We restrict ourselves to the case $\varepsilon^{-1} \in \mathbb{N}$).
We shall look at the L^2-error

$$u_\varepsilon - u_0 \in H^1_0(0,1) \subset L^2(0,1).$$

There exists a unique $z \in H_0^1(0,1)$ such that

$$\int_0^1 A_0 z' w' \, dx = \int_0^1 (u_\varepsilon - u_0) w \, dx, \quad \forall w \in H_0^1(0,1).$$

The choice $w = u_\varepsilon - u_0$ yields

$$\|u_\varepsilon - u_0\|_{L^2(0,1)}^2 = \int_0^1 A^0 z' (u_\varepsilon - u_0)' \, dx$$

(see the **Aubin-Nitsche duality trick**)
The solutions U_0 and u_ε are linked by the equality of the fluxes

$$(A_0 u_0')' = -f = (A_\varepsilon u_\varepsilon)'$$

so they coincide up to a constant, i.e.

$$A_0 u_0' = A_\varepsilon u_\varepsilon' \quad \text{in } H^{-1}(0,1) = [H_0^1(0,1)]^*.$$

Thus we have

$$\int_0^1 (A_0 u_0') w' \, dx = -\int_0^1 f w \, dx = \int_0^1 (A_\varepsilon u_\varepsilon') w' \, dx, \quad \forall w \in H_0^1.$$

This yields

$$\begin{aligned}
\|u_\varepsilon - u_0\|_{L^2(0,1)}^2 &= \int_0^1 z' (A_0 - A_\varepsilon) u_\varepsilon' \, dx \\
&= \sum_{j=1}^{\overbrace{\varepsilon^{-1}}^{=:N}} \int_{(j-1)\varepsilon}^{j\varepsilon} z' (A_0 - A_\varepsilon) u_\varepsilon' \, dx \\
&\overset{(*)}{=} \sum_{j=1}^{N} \int_{(j-1)\varepsilon}^{j\varepsilon} \left(z' - \varepsilon^{-1} \int_{(j-1)\varepsilon}^{j\varepsilon} z'(s) \, dS \right) (A_0 - A_\varepsilon) u_\varepsilon' \, dx \\
&\quad + \sum_{j=1}^{N} \left(\varepsilon^{-1} \int_{(j-1)\varepsilon}^{j\varepsilon} z'(s) \, dS \right) \int_{(j-1)\varepsilon}^{j\varepsilon} (A_0 - A_\varepsilon) \left(u_\varepsilon' - \varepsilon^{-1} \int_{(j-1)\varepsilon}^{j\varepsilon} u_\varepsilon'(s) \, dS \right) dx \\
&\quad + \sum_{j=1}^{N} \varepsilon^{-2} \int_{(j-1)\varepsilon}^{j\varepsilon} z'(s) \, dS \int_{(j-1)\varepsilon}^{j\varepsilon} u_\varepsilon'(s) \, dS \int_{(j-1)\varepsilon}^{j\varepsilon} (A_0 - A_\varepsilon) \, dx
\end{aligned}$$

Note that in $(*)$ we have added a zero, namely the mean value of z'. We have that z is the solution of a Poisson problem with a constant RHS, so it is in H^2. Thus it's derivative is still in H^1. Unfortunately for u_ε we just know that it is in L^2, so we have no regularity for u_ε'. Thus we make a further modification:

$$
\begin{aligned}
\|u_\varepsilon - u_0\|^2_{L^2(0,1)} &= \int_0^1 z'(A_0 - A_\varepsilon)u_\varepsilon'\,dx \\
&= \sum_{j=1}^{\overbrace{\varepsilon^{-1}}^{=:N}} \int_{(j-1)\varepsilon}^{j\varepsilon} z'(A_0 - A_\varepsilon)u_\varepsilon'\,dx \\
&\overset{(*)}{=} \sum_{j=1}^{N} \int_{(j-1)\varepsilon}^{j\varepsilon} \left(z' - \varepsilon^{-1}\int_{(j-1)\varepsilon}^{j\varepsilon} z'(s)\,dS\right) \frac{(A_0 - A_\varepsilon)}{A_\varepsilon} A_\varepsilon u_\varepsilon'\,dx \\
&\quad + \sum_{j=1}^{N} \left(\varepsilon^{-1}\int_{(j-1)\varepsilon}^{j\varepsilon} z'(s)\,dS\right) \int_{(j-1)\varepsilon}^{j\varepsilon} \frac{(A_0 - A_\varepsilon)}{A_\varepsilon} \left(A_\varepsilon u_\varepsilon' - \varepsilon^{-1}\int_{(j-1)\varepsilon}^{j\varepsilon} A_\varepsilon u_\varepsilon'\,dS\right) dx \\
&\quad + \sum_{j=1}^{N} \varepsilon^{-2} \int_{(j-1)\varepsilon}^{j\varepsilon} z'(s)\,dS \int_{(j-1)\varepsilon}^{j\varepsilon} A_\varepsilon u_\varepsilon'(s)\,dS \int_{(j-1)\varepsilon}^{j\varepsilon} \frac{(A_0 - A_\varepsilon)}{A_\varepsilon}\,dx.
\end{aligned}
$$

The third term on the right-hand side tends to 0 (as $\varepsilon \to 0$) if and only if it is actually 0, i.e.

$$
A_0 = \not\varepsilon \left(\varepsilon^{-1}\int_{(j-1)\varepsilon}^{j\varepsilon} A_\varepsilon^{-1}\,dx\right)^{-1}
$$

is chosen as the harmonic mean of A_ε. With this choice of A_0 and *Cauchy-Schwarz* we get

$$
\begin{aligned}
\|u_\varepsilon - u_0\|^2_{L^2(0,1)} &\le \sum_{j=1}^{N} \left\|\frac{A_0 - A_\varepsilon}{A_\varepsilon}\right\|_{L^\infty(0,1)} \\
&\quad \cdot \Big\{ \|z' - \overline{z'}\|_{L^2((j-1)\varepsilon,j\varepsilon)} \|A_\varepsilon u_\varepsilon'\|_{L^2((j-1)\varepsilon,j\varepsilon)} \\
&\quad + \|\overline{z'}\|_{L^2((j-1)\varepsilon,j\varepsilon)} \|A_\varepsilon u_\varepsilon' - \overline{A_\varepsilon u_\varepsilon'}\|_{L^2((j-1)\varepsilon,j\varepsilon)} \Big\} \\
&\le \frac{\varepsilon}{\pi} \left\|\frac{A_0 - A_\varepsilon}{A_\varepsilon}\right\|_{L^\infty(0,1)} \sum_{j=1}^{N} \Big(\|z''\|_{L^2((j-1)\varepsilon,j\varepsilon)} \|A_\varepsilon u_\varepsilon'\|_{L^2((j-1)\varepsilon,j\varepsilon)} \\
&\quad + \|z'\|_{L^2((j-1)\varepsilon,j\varepsilon)} \|(A_\varepsilon u_\varepsilon')'\|_{L^2((j-1)\varepsilon,j\varepsilon)} \Big).
\end{aligned}
$$

Define now constants α, β and assume that $\alpha \le A_\varepsilon \le \beta$. Then we have (continuing the previous estimate and using discrete Cauchy-Schwarz):

$$
\le \frac{\varepsilon}{\pi}\left(\frac{\beta}{\alpha} + 1\right)\left(\|z''\|_{L^2(0,1)}\|A_\varepsilon u_\varepsilon'\|_{L^2(0,1)} + \|z'\|_{L^2(0,1)}\|(A_\varepsilon u_\varepsilon')'\|_{L^2(0,1)}\right)
$$

where α, β are chosen as

$$
\begin{aligned}
\alpha &\coloneqq \inf_{0 \le x \le 1} A_1(x) \\
\beta &\coloneqq \sup_{0 \le x \le 1} A_1(x).
\end{aligned}
$$

Continuing we get

$$\leq \frac{\varepsilon}{\pi}\left(\frac{\beta}{\alpha}+1\right)\|u_\varepsilon - u_0\|_{L^2(0,1)}\sqrt{\frac{\beta}{\alpha}}\|f\|_{L^2(0,1)} + \frac{\|u_\varepsilon - u_0\|_{L^2(0,1)}}{\sqrt{A_0}}\|f\|_{L^2(0,1)}$$
$$\leq \frac{\varepsilon}{\pi}\left(\frac{\beta}{\alpha}+1\right)\left(\sqrt{\frac{\beta}{\alpha}}+\frac{1}{A_0}\right)\|f\|_{L^2(0,1)}\|u_\varepsilon - u_0\|_{L^2(0,1)}.$$

This shows that

$$\|u_\varepsilon - u_0\|_{L^2(0,1)} \leq C\varepsilon\|f\|_{L^2(0,1)}$$

with constant

$$C := \frac{1}{\pi}\left(1+\frac{\beta}{\alpha}\right)\left(\frac{\sqrt{\beta}+1}{\sqrt{\alpha}}+1\right).$$

Hence, for the choice

$$A_0 := \left(\fint_0^1 A_1^{-1}(x)\,dx\right)^{-1},$$

we have $u_\varepsilon \overset{\varepsilon\to 0}{\longrightarrow} u_0$ strongly in $L^2(0,1)$.

To summarize, we considered the problem:

$$\left.\begin{aligned} -(A_\varepsilon u_\varepsilon')' = &\quad f, \quad \text{in } [0,1] \\ u(0) = u(1) = &\quad\quad\quad\quad\quad 0 \end{aligned}\right\} \tag{P_ε}$$

and the corresponding for the macroscopic part:

$$\left.\begin{aligned} -(A_0 u_0')' = &\quad f, \quad \text{in } [0,1] \\ u(0) = u(1) = &\quad\quad\quad\quad\quad 0 \end{aligned}\right\} \tag{P_0}$$

The strategy for numerical approximation of the macroscopic part u_0 of u_ε is now pretty clear:

- Compute / approximate A_0 (high accuracy, as this is quite cheap)
- Approximately solve Problem P_0 by your favorite FEM-scheme, e.g. P1-FEM on a uniform grid of width $H > 0$, where H is chosen according to the desired accuracy

Remark 1.2. $H > 0$ is the **Discretization Parameter** and needs to be chosen according to level of accuracy needed.

1.3.3 Numerical homogenization of general L^∞-coefficients

The aim of this section is to revitisite the derivation of the preious section in order to understand the role of periodicity and to see how to generalize the concept. Let therefore $A \in L^\infty(0,1)$ and assume $\exists 0 < \alpha \leq \beta < \infty : \alpha \leq A(x) \leq \beta$. Moreover $f \in L^2(0,1)$ is assumed. Note that there is no ε occuring anymore, i.e. no periodicity is assumed from now on for the coefficient A!

Consider the model problem

$$\left.\begin{aligned} -(A(x)u'(x))' = &\quad f(x), \quad 0 \le x \le 1 \\ u(0) = u(1) = &\qquad\qquad\qquad\quad 0 \end{aligned}\right\} \tag{P}$$

The weak formulation reads: Find $u \in H_0^1(0,1)$ s.t.

$$\int_0^1 A(x)u'(x)v(x)\,dx = \int_0^1 f(x)v(x), \quad \forall v \in H_0^1(0,1)$$

Let $H > 0$ denote the mesh-size of some regular quasi-uniform subdivision $\mathcal{T}_H$ of $(0,1)$ into subintervals.

Our goal is to find $A_H \in P^0()$ s.t. for any $f \in L^2(0,1)$ it holds that

$$\|u_{A,f} - u_{A_H,f}\|_{L^2(0,1)} \le C_{\alpha,\beta} H \|f\|_{L^2(0,1)},$$

where $u_{A_H,f}$ solves

$$\int_0^1 A_H(x)u'_{A_h,f}(x)v'(x)\,dx = \int_0^1 f(x)v(x)\,dx, \quad \forall v \in H_0^1(0,1),$$

and $C_{\alpha,\beta}$ should be a universal constant independent of H, f and variations of A (it just depends on α, β).

Following the arguments of the previous section (Aubin-Nitsche-Argument, standard inequalities) we are able to show that

$$\begin{aligned} \|u_{A,f} - u_{A_H,f}\|_{L^2(0,1)} \le \sum_{T \in \mathcal{T}_H} \Bigg(& \pi^{-1} \|(A_H z')'\|_{L^2(T)} \left\| \frac{A_H - A}{A} \right\|_{L^\infty(T)} \|Au'\|_{L^2(T)} \\ & + \pi^{-1} H \|A_H z'\|_{L^2(T)} \left\| \frac{A_H - A}{A} \right\|_{L^\infty(T)} \| \underbrace{(Au')'}_{=f} \|_{L^2(T)} \\ & + \left| \fint_T A_H z'\,dx \fint_T Au'\,dx \fint_T \frac{A_H - A}{A}\,dx \right| \Bigg) \end{aligned}$$

where we assumed that A_H exists and is positive and where z solves

$$\int_0^1 A_H z' v'\,dx = \int_0^1 (U_{A,f} - u_{A_H,f}) v\,dx, \quad \forall v \in H_0^1(0,1).$$

Choose $A_{H|T}$ such that

$$\fint_T \frac{A_H - A}{A}\,dx = 0.$$

This leads to

$$A_{H|T} := \left(\fint_T A^{-1}\,dx \right)^{-1}.$$

Wit hthis choice, we get the desired results:

- $\alpha \leq A_H \leq \beta$
- $\exists! u_{A_H,f} \in H_0^1$ that solves

$$\int_0^1 A_H u'_{A_H,f} v' \, dx = \int_0^1 f v \, dx, \quad \forall v \in H_0^1(0,1)$$

- $$\|u_{A,f} - u_{A_H,f}\|_{L^2(0,1)} \leq C_{\alpha,\beta} H \|f\|_{L^2(0,1)}$$

In particular, A admits homogenization in the classical sense, if there is a mesh $\mathcal{T}_H$ such that

$$\fint_T A^{-1} \, dx = \fint_K A^{-1} \, dx, \quad \forall T, K \in \mathcal{T}_H.$$