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[034] Homogenization Method and Multiscale Modeling

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Homogenization Method and Multiscale Modeling

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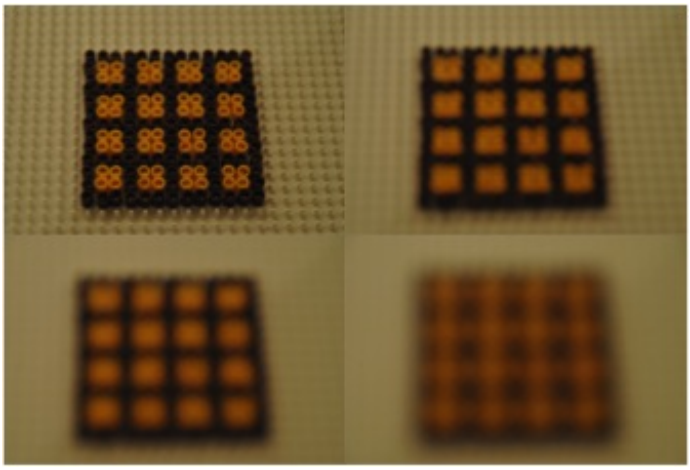

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Abstract. This mini-course addresses graduate students and young researchers in mathematics and engineering sciences interested in applying both formal and rigorous averaging methods to real-life problems described by means of partial differential equations (PDEs) posed in heterogeneous media. As a background application scenario we choose to look at the interplay between reaction, diffusion and flow in periodic porous materials, but broadly speaking, a similar procedure would apply for, e.g., acoustic and/or electromagnetic wave propagation phenomena in composite (periodic) media as well.

We start off with the study of oscillatory elliptic PDEs formulated firstly in fixed and, afterwards, in periodically-perforated domains. We remove the oscillations by means of a (formal) asymptotic homogenization method. The output of this procedure consists of a "guessed" averaged model equations and explicit rules (based on cell problems) for computing the effective coefficients.

As second step, we introduce the concept of two-scale convergence (and correspondingly, the two-scale compactness) in the sense of Allaire and Nguetseng and derive rigorously the averaged PDE models and coefficients obtained previously. This step uses the framework of Sobolev and Bochner spaces and relies on basic tools like weak convergence methods, compact embeddings as well as extension theorems in Sobolev spaces. We particularly emphasize the role the choice of microstructures (pores, perforations, subgrids, etc.) plays in performing the overall averaging procedure.

Finally, we focus our attention on a two-scale partly dissipative reaction-diffusion system with periodically distributed microstructure modeling chemical attack on concrete structures. We present a two-scale finite difference scheme able to approximate the unique weak solution to the two-scale system and prove its convergence. We illustrate numerically the typical micro-macro behavior of the active concentrations involved in the corrosion process and give details on how a two-scale FD scheme can be implemented in C.

The main objective of the course is to endow the audience with a rather flexible *mathematical homogenization* tool so that he/she can quickly start applying this averaging methodology to other PDEs scenarios describing physico-chemical processes in media with microstructures.

Per le nostre famiglie ...

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Thank you all for your patience and trust.

CHAPTER 1

Introduction

1.1. Aim of these notes. Choice of the teaching material

The objective of these lecture notes is to introduce quickly the reader[1] to the world of averaging techniques for partial differential equations. Deliberately, the presentation follows our favorite path—the applications-driven way. We mostly consider transport and reaction in porous media, but similar ideas apply to other related phenomena. Particularly, we refer to [**PPSW93**, **HH98**], or [**MV10**] for details on multiscale studies concerning scenarios arising in the mechanics of materials. For averaging techniques at the level of ODEs, the reader is referred to [**Hol95**] (standard matters) or [**Ver10**] (modern aspects, also touching upon geometric singular perturbations issues), [**PS08**] (useful for both deterministic and stochastic scenarios). Our standard reference book for (volume) averaging reaction, diffusion, and flow in heterogeneous porous media is [**Bea88**].

The choice of the material included here is rather personal. It is strongly influenced by our own work in the homogenization field, as well as by a series of mini-courses given by A. Muntean: "*Introduction to Homogenization*" given at the Department of Mathematics and Computer Science, Eindhoven University of Technology, The Netherlands during the period 2008–2011 (jointly with I. S. Pop), the Mastermath course "*Asymptotic Methods for Differential Equations*" during February–June 2011, University of Amsterdam, The Netherlands (jointly with A. Zagaris) as well as the mini-courses "*Homogenization: A Crash Course*" given firstly in February 2010 at the Department of Mathematics, University of Sussex (Falmer, UK), and then in March 2011 at the Institute of Mathematics for Industry, Kyushu University (Fukuoka, Japan).

The content and structure of the first five chapters owe very much to a few works from where we learned the techniques [**NR92**, **Hor97**, **All02**, **Hor93**]. See also [**PPSW93**] for complementary reading materials, organized very much in a textbook fashion. The last two chapters is the result of recent collaborations between V. Chalupecký and A. Muntean on multiscale computation issues strongly related to the topic of the PhD thesis by T. Fatima (TU Eindhoven, The Netherlands).

To get a decent overview on what happens today in the field of averaging techniques for PDEs, we kindly send the reader to dig into excellent monographs like [**Hor97**, **CD99**, **JKO94**, **PS08**, **CPS07**, **CS98**, **BLP78**, **MV10**], treating in an exhaustive way the case of periodically-distributed microstructures.

1.2. What means "homogenization" in this context?

In most fields of science and engineering the word *homogenization* typically refers to *mixing* (stirring). The same situation happens with the painter mixing colors, say black and white, to get a uniformly grayish nuance. Quite similarly, the role of statistical mechanics is to search for *ensembles* to get rid of microscopic fluctuations. In molecular dynamics simulations, much research interest is focussed on how to speed up calculations by *coarse graining*. At the continuum level, mixture theories [**M̈68**] combined eventually with volume averaging-type methods (e.g., [**Bea88**, **HW85**]) attempt to get an averaged perspective over the heterogeneities in both the distribution of matter and micro-geometry (microstructures). Such methods simply try to find simpler (easier to

[1] Most likely, the reader is a graduate student or young researcher in applied mathematics or in engineering sciences willing to apply a more fundamental averaging technique to his/her "baby problem".

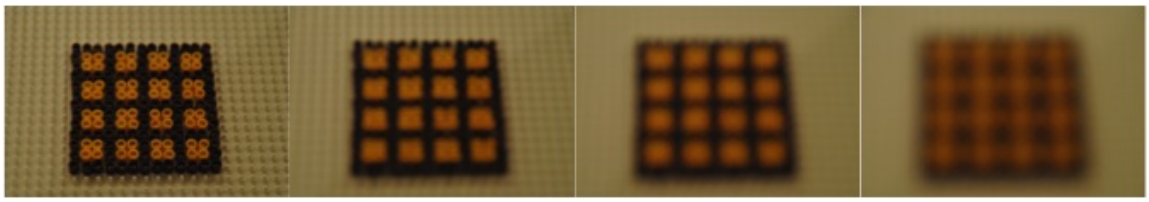

Figure 1.1 – The passing $\varepsilon \to \varepsilon_0$ $(0 \leq \varepsilon_0 \ll \varepsilon)$ can be imagined as the passing from high-contrast black-white regions to gray regions. Courtesy of S. A. Muntean (TU Eindhoven), who also produced the concept and photo of the cover.

compute) equations that smoothen out substructure variations, without loosing too much accuracy. In these equations, all material parameters and coefficients will possess, in most of the cases, a certain effective nature (i.e., we wish them to be independent of the microstructure shape). In the subsequent chapters, we focus on deterministic continuum-in-time events taking place at continuum in space levels, and hence, we stay away from scenarios involving random micro-geometries or discrete microstructures.

Well-understood oscillations occur inherently when periodic or almost periodic distributions of microstructures come into the game. The role of "mathematical homogenization"[2] is to efficiently use the special properties of periodic functions/structures in combination with the regularity of the weak solutions to the PDE models in questions in order to "remove" the oscillations (a visual hint for this is illustrated in Fig. 1.1), and finally, to derive averaged equations as well as constitutive laws for averaged (transport and reaction) coefficients (also called *effective* coefficients).

In this framework, we deal with averaging techniques tailored for media composed of a periodically-distributed substructure (that we refer to as *microstructure*). Note, however, that the techniques apply in a larger context including locally periodic microstructures or stationary distributions of pores assuming, among other things, precise ergodicity restrictions. Consequently, we are able to treat successfully geometries like the one pointed out in Fig. 1.2 and Fig 1.3 (i.e., "regular", uniformly periodic microstructures), and we will not attempt to treat non-uniform heterogeneities like those illustrated in Fig. 1.4 and Fig. 1.5.

1.3. Organization of the material

Chapter 2 describes the basic ideas of the asymptotic homogenization method by means of a relevant application posed in a media with periodically-distributed microstructures.

Chapter 3 briefly sketches the functional analysis prerequisites that the reader needs to understand in order to follow the subsequent chapters. This is the place where we introduce the central concept of two-scale convergence in the sense of Nguetseng and Allaire.

We use Chapter 4 to show how this two-scale concept of weak convergence works in the case of a linear elliptic problem posed in a fixed (non-oscillatory) domain, while in Chapter 5 we average (homogenize, scale-up) the same sort of equation as in Chapter 4, but now defined in a media with periodically-distributed microstructures. This part is mathematically a bit more involved, and it comes very close to current research questions in mathematical homogenization.

In Chapter 6 we study a reaction-diffusion scenario intimately connected to the corrosion of concrete with sulfates. The starting point here is a two-scale PDEs-ODE scenario (that can be obtained via the two-scale convergence technique detailed in Chapter 4 and Chapter 5). Our focus lies here on the construction and implementation of a convergent two-scale finite difference scheme to approximate the weak solution of the given two-scale problem.

[2] By "mathematical homogenization" we actually mean "two-scale convergence type techniques".

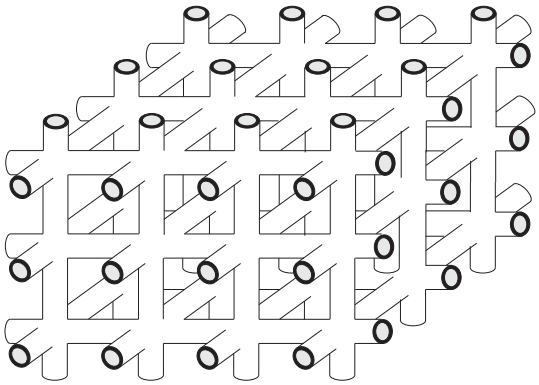

Figure 1.2 – Illustration of a periodically distributed array of microstructures approximating an unsaturated porous medium.

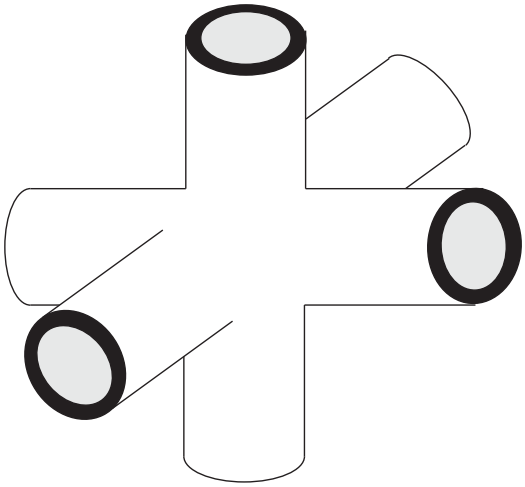

Figure 1.3 – Microstructure model in $\mathbb{R}^3$. The black part indicates the presence of a water film, while the interior of the tube is supposed to be subject to air diffusion. The solid part lies in the exterior of the tubes.

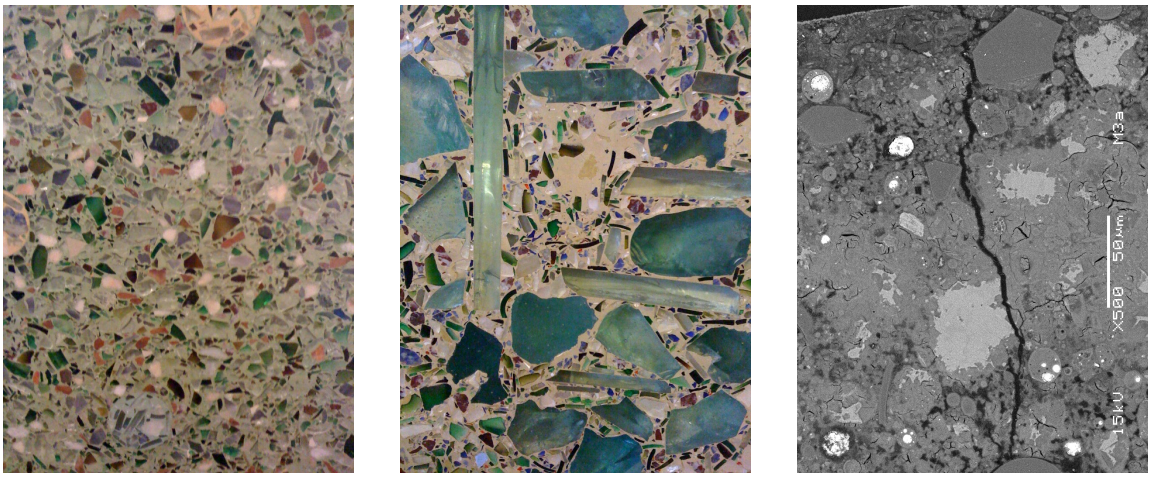

Figure 1.4 – Examples of heterogeneous media: Left and middle: Artistic composite wall with randomly placed inclusions; Right: Concrete microstructures attacked by sulfate ions. Courtesy of R. E. Beddoe and L. Urbonas (TU München).

Our computer implementation is the subject of Chapter 7. We describe the implementation at a sufficient level of detail such that even an unexperienced programmer can understand it easily in order to adapt it later to its own needs. The full source code is then listed in Appendix A.

1.4. Note

This material has a preliminary shape. The text is subject to continuous changes both in style as well as in content. If you spot errors, typos or have comments at the mathematical and/or

Figure 1.5 – Examples of heterogeneous media: Artistic representations with low regular inclusions.

teaching strategy level, then please get in contact with any of us. Your comments are welcome and very much appreciated.

Note that Chapter 2 and Chapter 5 can be offered as a crash course to PhD students and postdoctoral researchers in applied mathematics, having the background indicated in Chapter 3. Chapters 1–7 can be used as master course material structured in about 14 lessons and instructions, the target audience being then master students either in applied mathematics or in computational science and engineering.

CHAPTER 2

Formal asymptotic homogenization

In this chapter, we rely on formal two-spatial scale expansions to introduce the homogenization-type of thinking. This part plays a crucial role: if one believes the existence of such two-scale expansions, then these expansions simply "dislocate" the oscillations and successfully lead to upscaled model equations and effective coefficients, under the basic assumption of periodicity. This is only a formal way of working; analysis work is required to justify the validity of the two-scale expansion. The content of these notes follows partly [**NR92**, **Hor97**, **PS08**].

For a supplementary reading material, see [**PPSW93**].

2.1. Guessing the averaged model: A direct approach

This section presents a formal asymptotic technique (sometimes called *asymptotic homogenization*) that is able to derive, starting from microscopic models whose validity we trust, macroscopic models and constitutive laws for effective coefficients. We present the technique by means of a representative example—a model problem describing the interplay between stationary diffusion and chemical reactions in perforated media. It is worth noting that the applicability of this formal method covers wide classes of PDEs ranging, for instance, from Maxwell equations to free boundary problems modeling phase transitions in heterogeneous materials.

2.2. A model problem: Stationary diffusion and chemical reactions in perforated media

We consider the following linear elliptic equation

$$-\mathrm{div}(a_\varepsilon \nabla u_\varepsilon) = f_\varepsilon, \text{ in } \Omega_\varepsilon \subset \mathbb{R}^d, \tag{2.1}$$

together with the boundary conditions

$$u_\varepsilon = 0, \text{ on } \Gamma^{ext}, \tag{2.2}$$

$$-a_\varepsilon \nabla u\varepsilon \cdot n_\varepsilon = g_\varepsilon, \text{ on } \Gamma_\varepsilon, \tag{2.3}$$

where $\partial\Omega$ is a hypersurface in $\mathbb{R}^d$ and $\lambda^{d-1}(\Gamma_\varepsilon) \neq 0$, with λ^{d-1} being the $d-1$-dimensional Lebesgue measure. Furthermore, $\partial\Omega_\varepsilon = \Gamma^{ext} \cup \Gamma_\varepsilon$, where $\Gamma^{ext} \cap \Gamma_\varepsilon = \emptyset$. We take

$$f_\varepsilon\left(x, \frac{x}{\varepsilon}\right) := f_0(x) + \varepsilon f_1\left(x, \frac{x}{\varepsilon}\right)$$
$$g_\varepsilon\left(x, \frac{x}{\varepsilon}\right) := \varepsilon g_0\left(x, \frac{x}{\varepsilon}\right).$$

In this context, f_ε is a volume (bulk) chemical reaction, while g_ε is a surface chemical reaction. For the simplicity of the exposure, we keep the functions f_ε and g_ε dependent only on the x-variable. Minimal modifications are needed to adapt the following calculations for the case when f_ε and g_ε depend on t and on u_ε.

Let us assume for the moment that the parameters as well as the initial and boundary data are given such that our microscopic problem (P_ε) is well posed.

We refer to (2.1)–(2.2) as problem (P_ε); the limit problem (as $\varepsilon \to 0$) will be correspondingly denoted by (P_0). The task is now to remove (average out) the oscillatory behavior of the solution to (P_ε).

Let us briefly describe the geometry of our perforated domain Ω_ε. Let $Z \subset \mathbb{R}^d$ be a hypercube. Furthermore, let $k = (k_1, \dots, k_d) \in \mathbb{Z}^d$ be a vector of indices and $e = (e_1, \dots, e_d)$ be unit vectors in $\mathbb{R}^d$. For $X \subset Z$, we denote by X^k the shifted subset

$$X^k := X + \sum_{i=1}^{d} k_i e_i.$$

The pore matrix (or pore skeleton) is defined by

$$\Omega_0^\varepsilon := \bigcup_{k \in \mathbb{Z}^d} \{\varepsilon Y_0^k : Y_0^k \subset \Omega\},$$

while the total pore space is

$$\Omega^\varepsilon := \Omega - \Omega_0^\varepsilon.$$

εY_0^k is the ε-homotetic set of Y_0^k. The total (inner) surface of the skeleton is denoted by

$$\Gamma^\varepsilon := \partial\Omega_0^\varepsilon = \bigcup_{k \in \mathbb{Z}^d} \{\varepsilon \Gamma^k : \varepsilon \Gamma^k \subset \Omega\}.$$

Correspondingly, we introduce the unit normal vector n_ε to Γ^ε.

2.3. The asymptotics homogenization procedure or How to guess "macroscopic" models?

The key idea is to rely on the following ansatz (often called *homogenization ansatz*):

$$u_\varepsilon(x) := u_0(x, y) + \varepsilon u_1(x, y) + \varepsilon^2 u_2(x, y) + \mathcal{O}(\varepsilon^2)\big|_{\text{where } y := \frac{x}{\varepsilon}}. \tag{2.4}$$

If ψ is a sufficiently smooth function, then the following calculation rule applies:

$$\frac{\mathrm{d}}{\mathrm{d}x}\psi\left(x, \frac{x}{\varepsilon}\right) = \partial_x \psi\left(x, \frac{x}{\varepsilon}\right) + \frac{1}{\varepsilon}\partial_y \psi\left(x, \frac{x}{\varepsilon}\right)\Big|_{\text{where } y := \frac{x}{\varepsilon}}.$$

In order to simplify the writing, we will not carry with us the expression "where $y := \frac{x}{\varepsilon}$", but we implicitly mean it. Essentially, we imagine x and y to be independent variables.

Now, inserting the ansatz (2.4) into (P_ε), we get for (2.1) the following structure:

$$\left[\frac{1}{\varepsilon^2}T_{-2} + \frac{1}{\varepsilon}T_{-1} + \varepsilon^0 T_0\right](u_0, u_1, u_2, \dots) = [f_0 + \varepsilon f_1](u_0, u_1, u_2, \dots) \text{ in } \Omega_\varepsilon.$$

We obtain

$$\left(\nabla_x + \frac{1}{\varepsilon}\nabla_y\right) \cdot \left(A(y)\left(\nabla_x + \frac{1}{\varepsilon}\nabla_y\right)(u_0 + \varepsilon u_1 + \varepsilon^2 u_2 + \text{h.o.t.})\right) = f_0 + \varepsilon f_1 + \mathcal{O}(\varepsilon^2).$$

So,

$$\left(\nabla_x + \frac{1}{\varepsilon}\nabla_y\right) \cdot \Big(\frac{1}{\varepsilon}A(y)\nabla_y u_0 + \varepsilon^0\big(A(y)\nabla_x u_0 + A(y)\nabla_y u_1\big) + \varepsilon^1\big(A(y)\nabla_x u_1 + A(y)\nabla_y u_2\big) + \text{h.o.t}\Big) = f_0 + \text{h.o.t.}$$

Next, we group the terms by collecting those having the same powers of ε and get in $\Omega \times Y$ that

$$\begin{aligned}
&\frac{1}{\varepsilon^2} \quad \nabla_y \cdot \big(A(y)\nabla_y u_0\big) + \\
&\frac{1}{\varepsilon} \quad \Big(\nabla_y \cdot \big(A(y)\nabla_x u_0 + A(y)\nabla_y u_1\big) + \nabla_x \cdot \big(A(y)\nabla_y u_0\big)\Big) + \\
&\varepsilon^0 \quad \Big(\nabla_x \cdot \big(A(y)\nabla_x u_0 + A(y)\nabla_y u_1\big) + \nabla_y \cdot \big(A(y)\nabla_x u_1 + A(y)\nabla_y u_2\big)\Big) + \text{h.o.t} = f_0 + \text{h.o.t.}
\end{aligned}$$

We proceed in the same way with the boundary conditions and get

$$-A(y)\Big(\nabla_x + \frac{1}{\varepsilon}\nabla_y\Big)(u_0 + \varepsilon u_1 + \varepsilon^2 u_2) + \text{h.o.t.} = \varepsilon g_0 + \varepsilon^2 g_1$$

which leads to the relations at ∂Y_0, namely:

$$\begin{aligned}
\frac{1}{\varepsilon}: &\qquad -A(y)\nabla_y u_0 \cdot n(y) = 0,\\
\varepsilon^0: &\qquad -A(y)\nabla_x u_0 \cdot n(y) - A(y)\nabla_y u_1 \cdot n(y) = 0,\\
\varepsilon^1: &\qquad -\big(A(y)\nabla_x u_1 + A(y)\nabla_y u_2\big)n(y) = g_0(x,y).
\end{aligned}$$

Consequently, L'Hopital's rule indicates that as $\varepsilon \to 0$ we get in $\Omega \times Y$ the following auxiliary problems:

$$\begin{aligned}
T_{-2}(u_0) &= 0,\\
T_{-1}(u_0, u_1) &= 0,\\
T_0(u_0, u_1, u_2) &= F_0,
\end{aligned} \tag{2.5}$$

where Ω is the initial domain without the perforations, Y is the microstructure within the periodic cell Z, and F_0 is a zero order term in ε including f_0 and eventually some boundary terms. The precise structure of F_0 will be clear towards the end of this averaging procedure. Having a glance at (2.5), we expect already a certain structure for the macroscale equation, but what would be a good candidate for the solution of such a macroscopic equation?

Let's examine the first auxiliary problem, i.e., the one corresponding to T_{-2}:

Find $u_0 = u_0(x, y)$ solution of

$$\nabla_y \cdot \big(A(y)\nabla_y u_0(x,y)\big) = 0 \text{ in } Y, \tag{2.6}$$

$$-A(y)\nabla_y u_0(x,y) \cdot n(y) = 0 \text{ at } \partial Y_0, \tag{2.7}$$

$$u_0(x,\cdot) \text{ is } Y\text{-periodic for each given } x \in \Omega. \tag{2.8}$$

To ensure the uniqueness of solutions to (2.6)–(2.8), we impose

$$\int_Y u_0(x,y)\,\mathrm{d}y = c, \tag{2.9}$$

where $c \in \mathbb{R}$ is a constant. The structure of (2.6)–(2.8) indicates that u_0 is independent of the choice of y, and hence, we expect the function

$$u_0 = u_0(x)$$

to be the macroscopic solution we are looking for. Consequently, the constant c arising in (2.9) becomes a function of x and $c(x) := u_0(x)|Y|$.

Let us examine now the next auxiliary problem, i.e., the one corresponding to T_{-1}:

$$-\nabla_y \cdot \big(A(y)(\nabla u_0 + \nabla_y u_1)\big) = 0, \tag{2.10}$$

$$-A(y)\nabla_y u_1(x,y) \cdot n(y) = A(y)\nabla_x u_0(x) \cdot n(y), \text{ at } \partial Y_0, \tag{2.11}$$

$$u_1(x,\cdot) \text{ is } Y\text{-periodic for each given } x \in \Omega. \tag{2.12}$$

At this point, we need to recall a theoretical result ensuring the existence and uniqueness of periodic solutions to elliptic PDEs (see also [**PPSW93**, Lemma 2.1]).

LEMMA 2.1. *Let $F \in L^2(Y)$, and $g \in L^2(\partial Y)$. Consider the following boundary-value problem:*

$$-\nabla \cdot \big(A(y)\nabla\omega\big)\mathcal{A}\omega = F(y), \text{ in } Y, \tag{2.13}$$

$$-A(y)\nabla\omega \cdot n = g(y), \text{ at } \partial Y, \tag{2.14}$$

$$\omega \text{ is } Y-\text{periodic}. \tag{2.15}$$

Then following statements hold:

(i) *There exists a weak Y-periodic solution ω to (2.13) if and only if $\int F(y)\,\mathrm{d}y = \int g(y)\,\mathrm{d}\sigma_y$.*
(ii) *If (i) holds, then the uniqueness of weak solutions is ensured up to an additive constant.*

We apply now Lemma 2.1 to problem T_{-1}. Rearranging the terms in (2.10), we obtain after applying Gauß's theorem that

$$-\int_{\partial Y} A(y)\nabla_y u_1 \cdot n(y)\,\mathrm{d}\sigma_y = \int_{\partial Y_0} A(y)\nabla u_0 n(y)\,\mathrm{d}\sigma_y, \tag{2.16}$$

where $\mathrm{d}\sigma_y$ is the surface measure on ∂Y. Hence, Lemma 2.1 ensures the existence of a unique (weak) solution u_1 to T_{-1}.

For this problem, it is convenient to introduce the so-called *cell functions* and *cell problems*. Namely, we can rewrite u_1 as

$$u_1(x,y) = W(y)\cdot\nabla u_0(x) + \tilde{u}_1(x),$$

where the cell function(s)

$$W(y) = \big(W_1(y),\dots,W_d(y)\big)^t \in \mathbb{R}^d$$

satisfy the cell problems:

$$-\nabla_y \cdot \Big(A(y)\big(e_j + \nabla_y W_j(y)\big)\Big) = 0, \text{ in } Y, \tag{2.17}$$

$$A(y)\nabla_y W_j(y)\cdot n_j(y) = 0 \text{ at } \partial Y_0, \tag{2.18}$$

$$w_j \text{ is } Y\text{-periodic}, \quad \int_Y w\,\mathrm{d}y = 0. \tag{2.19}$$

Now, looking to the PDE for u_2, namely to the auxiliary problem T_0, we note that the following solvability condition has to be fulfilled:

$$\int_Y [\text{r. h. s.}]\,\mathrm{d}y = \int_{\partial Y} [\text{bdd. term}]\,\mathrm{d}\sigma_y. \tag{2.20}$$

A careful glance at equation (2.20) should recognize that this is actually a macroscopic (effective) equation in the sense that the microstructure variable y is averaged out from the equation.

2.4. Structure of the macroscopic equation. Effective coefficients

Now, it only remains to derive the precise structure of the macroscopic equation. The PDE for u_2, i.e., for the auxiliary problem T_0, is:

$$\begin{aligned} -\nabla_y\cdot\big(A(y)\nabla_y u_2\big) &= \nabla_x\cdot\big(A(y)\nabla_x u_0\big) + \nabla_x\cdot\big(A(y)\nabla_y u_1\big) + \nabla_y\cdot\big(A(y)\nabla_x u_1\big) + f_0, \text{ in } Y,\\ -A(y)\nabla_y u_2\cdot n(y) &= A(y)\nabla_x u_1\cdot n(y) + g_0, \text{ at } \partial Y_0,\\ u_2 &\text{ is } Y\text{-periodic}. \end{aligned}$$

Observe that (2.20) gives

$$I_1 + I_2 + I_3 = I_4 + I_5,$$

where the integral terms I_k ($k \in \{1,\dots,5\}$) are defined by

$$\begin{aligned} I_1 &:= \int_Y \nabla_x \cdot \big(A(y)\nabla_x u_0\big)\,\mathrm{d}y, \\ I_2 &:= \int_Y \nabla_x \cdot \big(A(y)\nabla_y u_1\big)\,\mathrm{d}y + \int_Y \nabla_y \cdot \big(A(y)\nabla_x u_1\big)\,\mathrm{d}y, \\ I_3 &:= \int_Y f_0\,\mathrm{d}y, \\ I_4 &:= \int_{\partial Y_0} A(y)\nabla_x u_1 \cdot n(y)\,\mathrm{d}\sigma_y, \\ I_5 &:= \int_{\partial Y_0} g_0\,\mathrm{d}\sigma_y. \end{aligned}$$

We have

$$I_1 = \int_Y \nabla_x \cdot \big(A(y)\nabla_x u_0\big)\,\mathrm{d}y = \nabla_x \cdot \left[\left(\int_Y A(y)\,\mathrm{d}y\right)\nabla_x u_0\right] = \left(\int_Y A(y)\,\mathrm{d}y\right) : \nabla_x\nabla_x u_0(x). \tag{2.21}$$

In (2.21), we have used the inner product between two matrices

$$A : B := \mathrm{tr}(A^t B) = \sum_{ij} a_{ij} b_{ij}.$$

This product[1], also called double dot product, is used to represent multiplying and summing across two indices. It is worth noting that the double dot product of two 2nd order tensors is a scalar. Some useful properties of the double dot product are listed, for instance, in [**PS08**, Section 2.2].

Furthermore, $I_2 = I_{21} + I_{22}$. Note that by periodicity and Gauß's theorem we obtain

$$I_{22} = I_4.$$

Let us now deal with the term I_{22}. We obtain that

$$\begin{aligned} I_{21} &= \int_Y \nabla_x \cdot \big(A(y)\nabla_y u_1\big)\,\mathrm{d}y = \int_Y A(y) : \nabla_x\nabla_y\big(W(y)\cdot\nabla_x u_0(x)\big)\,\mathrm{d}y \\ &= \int_Y \big(A(y)\nabla_y W(y)^t\big)\,\mathrm{d}y : \nabla_x\nabla_x u_0(x). \end{aligned}$$

Combining now the above results yields the following *macroscopic equation*:

$$-\frac{|Y|}{|Z|}\fint_Y \big(A(y) + A(y)\nabla_y W(y)^t\big)\,\mathrm{d}y : \nabla_x\nabla_x u_0(x) = \frac{|Y|}{|Z|} f_0(x) + \frac{|\partial Y_0|}{|Z|}\fint_{\partial Y_0} g_0(x,y)\,\mathrm{d}\sigma_y, \tag{2.22}$$

for a.e. $x \in \Omega$ with

$$u_0(x) = 0 \text{ for all } x \in \partial\Omega. \tag{2.23}$$

In (2.22), we denote by $\fint_{\mathcal{Y}} f(y)\,\mathrm{d}y$ the quantity $\frac{1}{|\mathcal{Y}|}\int_{\mathcal{Y}} f(y)\,\mathrm{d}y \in \mathbb{R}$ for any set $\mathcal{Y} \subset \mathbb{R}^\delta$ where $\delta \in \{1,\dots,d\}$. Note that the factor $\frac{|Y|}{|Z|}$ is the so-called *volumetric porosity*, while $\frac{|\partial Y_0|}{|Z|}$ is the *surface porosity*.

Remark 2.2. Equation (2.22) can also be obtained by integrating (2.20) with respect to y and then multiplying the result by $\frac{1}{|Z|}$; see [**Bea88**] for these and related concepts regarding modeling flow, diffusion and chemical reactions in porous media.

[1] Given vector fields a, v, we denote $a \cdot \nabla v := (\nabla v)a$. Similarly, if A is a 2nd order tensor, we denote $a \cdot \nabla A := (\nabla A)a$ and understand the notation component-wise. For any scalar function ψ, $\nabla\nabla\psi$ denotes the Hessian matrix. Note also that, since $\Delta\psi = \nabla\cdot\nabla\psi$ we can use the notation $\Delta\psi = \mathbb{I} : \nabla\nabla\psi$, where $\mathbb{I}$ is the identity matrix.

REMARK 2.3. We advise the reader to study from [**Hor97**, pp. 18–22], the (formal) derivation of a linear transmission problem for the stationary diffusion equations where the two diffusion coefficients, say D_1 and D_2, satisfy the very special scaling (in ϵ) $D_1 = \epsilon^2 D_2$. The resulting model is called in the literature a *double porosity* model or a *distributed microstructure* model.

2.5. Exercises

EXERCISE 2.1. Prove (2.16). Show also why Lemma 2.1 does actually apply in this context.

EXERCISE 2.2. (EFFECTIVE MODELS IN LAYERED MEDIA) Let ε be a small positive parameter. On the set $\Omega := (0,1)^2$ we define the ε-periodic function $a_\epsilon(x) := a(x_2/\epsilon)$ depending only on the second coordinate x_2, and satisfying

$$0 < m \leq a_\epsilon(x) \leq M < \infty$$

for some given (independent of ε) constants m, M. Let $\mathrm{q}^\varepsilon(x) := \mathrm{q}(x/\varepsilon)$ be a given ε-periodic velocity vector satisfying the divergence-free condition

$$\nabla \cdot \mathrm{q}^\varepsilon = 0.$$

For a given forcing term f, we consider the microscale equation

$$\nabla \cdot \left(\mathrm{q}^\varepsilon u^\varepsilon - a_\epsilon \nabla u^\epsilon\right) = f, \qquad \text{in } \Omega,$$

with homogeneous Dirichlet boundary conditions.

1. Apply the asymptotic expansion method to determine the effective (macro scale) equation.
2. Determine the effective diffusion tensor explicitly.

EXERCISE 2.3. Solve exercises 1c, 2 and 4 from [**Hol95**, pp. 231–233].

EXERCISE 2.4. Let's consider the context of Remark 2.3. Redo the calculations from [**Hor97**] (loc. cit.) for the case when $\frac{D_1}{D_2} = \mathcal{O}(1)$.

EXERCISE 2.5. (AN INVERSE HOMOGENIZATION PROBLEM) Consider the two-scale partially-dissipative coupled reaction-diffusion system discussed in Chapter 6. Propose a microstructure model that not only makes sense physically, but also gives as $\varepsilon \to 0$ the above mentioned two-scale system.

Hints

HINT FOR EXERCISE 2.3, PROBLEMS 1C AND 2. *Strategy 1 (recommended)*: Proceed as we worked in this chapter. You need to redo essentially the same calculations. Very few new terms will appear. Point them out!
Strategy 2 (not recommended): Holmes's working ideas described in pp. 224–228 can solve this, but they work only in 1D (due to the use of explicit solutions to the auxiliary problems). His approach can be "stretched" for other a bit more complex situations as well but it will generally not work when perforations are included. Try it for the fun, but make sure that you understand how strategy 1 works.

HINT FOR EXERCISE 2.3, PROBLEM 4. Use the mean-value theorem for integrals.

HINT FOR EXERCISE 2.4. Assume the context of Remark 2.3. Formulate the microscopic problem as a transmission problem by choosing $D_\epsilon(x) = D_{1,\epsilon}(x)$ if $x \in \Omega_\epsilon^1$ and $D_\epsilon(x) = D_{2,\epsilon}(x)$ if $x \in \Omega_\epsilon^2$, where Ω_1^ϵ and Ω_2^ϵ are the two periodic domains where the diffusion takes place.

HINT FOR EXERCISE 2.5. If you have really no clue, then adapt the setting from [**FAZM11**] to the current context.

CHAPTER 3

What should one know before thinking to applying homogenization?

In this chapter, we review the basic functional analytic notions[1] that the reader needs to be familiar with in order to be able to apply concepts like two-scale convergence to PDE models to derive in a rigorous manner upscaled model equations. Since the problems treated in this text are all linear, the key concept helping to pass to the limit $\varepsilon \to 0$ is connected to some kind of weak convergence. The role of this chapter is to elucidate these aspects.

3.1. Weak convergence

Let B be a real Banach space equipped with the norm $\|\cdot\|_B$. Correspondingly, B^* refers to the dual space of B, namely

$$B^* := \{\zeta : B \to \mathbb{R} \mid \zeta \text{ linear } \} =: \mathcal{L}(B, \mathbb{R}). \tag{3.1}$$

We endow the space B^* with the norm

$$\|\zeta\|_{B^*} := \sup_{x \in B - \{0\}} \frac{\langle \zeta, x \rangle_{B^*,B}}{\|x\|_B}, \tag{3.2}$$

for all $\zeta \in B^*$. In (3.2), for a $\zeta \in B^*$, the (dual) pairing $\langle \zeta, x \rangle_{B^*,B}$ represents the image $\zeta(x)$ of an element $x \in B$.

For what we are concerned, we are more interested in cases when

$$B \in \{L^p(\Omega), L^2(\Omega), H^1(\Omega), H^1_0(\Omega), H^1_{\#}(Y), L^2(\Omega, H^1_{\#}(Y))\},$$

where Ω and Y are open sets in $\mathbb{R}^d$ with Lipschitz boundary and where we take $d \in \{1, 2, 3\}$ and $p \in [1, \infty]$.

Note that $L^2(\Omega)$ or $H^1(\Omega)$ (or $H^1_0(\Omega)$ or $L^2(\Omega; H^1_{\#}(Y))$) are Hilbert spaces, say H. Then $\langle \zeta, x \rangle_{H^*,H} = (\zeta, x)$ and $H^{**} = H$, where (α, β) is the scalar product of the elements α and β from the Hilbert space H.

Let us introduce a generic sequence of positive numbers $(\epsilon_n) \subset \mathbb{R}_+$ such that $\lim_{n\to\infty} \epsilon_n = 0$. Let us abbreviate (ϵ_n) (together with all the convergent subsequences of (ϵ_n); see Remark 3.6) by calling it simply ϵ.

Definition 3.1. (Weak convergence) A sequence $(u_\epsilon) \subset B$ is said to converge weakly to $u \in B$ as $\epsilon \to 0$ if and only if

$$\text{for all } \zeta \in B^* \text{ we have } \langle \zeta, u_\epsilon \rangle_{B^*,B} \to \langle \zeta, u \rangle_{B^*,B} \text{ as } \varepsilon \to 0. \tag{3.3}$$

We denote the convergence (3.3) by $u^\epsilon \rightharpoonup u$.

Remark 3.2. Let $p \in]1, \infty[$. For the choice $B := L^p(\Omega)$, the expression $u_\varepsilon \rightharpoonup u$ in $L^p(\Omega)$ means that

$$\int_\Omega u_\varepsilon \varphi \, \mathrm{d}x \to \int_\Omega u\varphi \, \mathrm{d}x \tag{3.4}$$

[1] Ideally, the reader has previously followed a course related to introductory notions of functional analysis and a beginner course in partial differential equations.

for all $\varphi \in L^q(\Omega) = (L^p(\Omega))^*$, where $\frac{1}{p} + \frac{1}{q} = 1$.

PROPOSITION 3.3. (Strong convergence) Let $(u_\varepsilon) \in B$. We have $u_\varepsilon \to u$ (strongly) in B if and only if

(i) $u^\epsilon \rightharpoonup u$ in B;
(ii) $\|u^\epsilon\|_B \to \|u\|_B$.

REMARK 3.4. More on this subject can be found in [**CD99**] or in [**Eva98**].

3.2. Compactness

THEOREM 3.5. *(Eberlein-Smuljan) Let B be a reflexive Banach space and let (u_ε) be (uniformly) bounded in B. Then there exists a subsequence $(u_{\varepsilon_k}) \subset (u_\varepsilon)$ and a limit point $u \in B$ such that $u_{\varepsilon_k} \rightharpoonup u$ (weakly) in B as $k \to \infty$.*

REMARK 3.6. As a rule, we always denote the subsequence (u_{ε_k}) mentioned in Theorem 3.5 by (u_ε).

THEOREM 3.7. *(Rellich-Kondrachov) The space $W^{1,p}(\Omega)$ is compactly embedded in $L^q(\Omega)$ for any $q \in [1, p^*[$, where $p^* := \frac{dp}{d-p}$ is the so-called critical Sobolev exponent.*

For instance, if $d = 3$, Theorem 3.7 says that $H^1(\Omega)$ is compactly embedded in $L^6(\Omega)$.
We often use the fact that $H^1(\Omega)$ is compactly embedded in $L^2(\Omega)$.
The reader might find it useful to refresh their knowledge about the Fredholm alternative formulated for periodic elliptic PDEs (cf. e.g. [**PS08**, pp. 108–113]). We mention this mainly because we have seen in the previous chapter how important are Fredholm alternative-type results in handling the auxiliary problems arisen from the use of a two-scale (formal) expansion.

3.3. Two-scale convergence. Definition and properties

We start off this subsection by indicating a crucial property of periodic functions:

LEMMA 3.8 (First Oscillation Lemma). *Assume Ω to be a hypercube[2] in $\mathbb{R}^d$. For any $f \in C(\bar{\Omega}; C_\#(Y))$ it holds for $|Y| = 1$ that*

$$\lim_{\varepsilon \to 0} \int_\Omega f\left(x, \frac{x}{\varepsilon}\right) \mathrm{d}x = \int_\Omega \int_Y f(x, y) \, \mathrm{d}x \, \mathrm{d}y. \tag{3.5}$$

PROOF. This proof is taken from Maria Neuss-Radu's diploma thesis [**NR92**]. Let's denote $i := (i_1, \ldots, i_d) \in \mathbb{Z}^d$, $Y_i := i + Y$, and $J := \{i \in \mathbb{Z}^d : \varepsilon Y_i \subset \Omega\}$.
For each $\delta > 0$, we can find an $\epsilon_0 > 0$ such that

(1)
$$\int_{\Omega - \cup_{i \in J} \varepsilon Y_i} f\left(x, \frac{x}{\varepsilon}\right) < \delta$$

(2) $\|f(x, \cdot) - f(x', \cdot)\|_{C_\#(\bar{Y})} \leq \delta$ for all $|x - x'| < \varepsilon$ and for all $\varepsilon < \varepsilon_0$.

[2]This assumption on the geometry of Ω can be removed. We keep it here just for the sake of simplicity of the proofs.

We have that

$$\begin{aligned}\int_\Omega f\left(x,\frac{x}{\varepsilon}\right)\,\mathrm{d}x &= \sum_{\varepsilon Y_i\subset\Omega}\int_{\varepsilon Y_i} f\left(x,\frac{x}{\varepsilon}\right)\,\mathrm{d}x+\mathcal{O}(\delta)\\ &\overset{(2)}{=}\sum_{\varepsilon Y_i\subset\Omega}\int_{\varepsilon Y_i} f\left(x_i,\frac{x}{\varepsilon}\right)\,\mathrm{d}x+\mathcal{O}(\delta)\\ &=\sum_{\varepsilon Y_i\subset\Omega}\varepsilon^d\int_{Y_i} f\left(x_i,y\right)\,\mathrm{d}y+\mathcal{O}(\delta)\\ &=\int_\Omega\int_Y f(x,y)\,\mathrm{d}x\,\mathrm{d}y+\mathcal{O}(\delta).\end{aligned}$$

□

We introduce now the concept of two-scale convergence [**All92, Ngu89**].

REMARK 3.9. The key observation we make at this point is that we *expect* u_ε to behave like

$$u_0(x)+\varepsilon u_1\left(x,\frac{x}{\varepsilon}\right).$$

This idea complies with the formal asymptotic expansion we used earlier.

DEFINITION 3.10 (Two-scale convergence). Let (u^ϵ) be a sequence of functions in $L^2(\Omega)$. We say that (u^ϵ) converges two-scale to a unique function $u_0(x,y)\in L^2(\Omega\times Y)$ if and only if for any $\psi\in C_0^\infty(\Omega,C_\#^\infty(Y))$, we have

$$\lim_{\epsilon\to 0}\int_\Omega u^\epsilon\psi\Big(x,\frac{x}{\epsilon}\Big)\,\mathrm{d}x=\frac{1}{|Y|}\int_\Omega\int_Y u_0(t,x,y)\psi(x,y)\,\mathrm{d}x\,\mathrm{d}y. \tag{3.6}$$

We denote (3.6) by $u^\epsilon \overset{2}{\rightharpoonup} u_0$. Often, we will assume $|Y|=1$, but care needs to be paid whether this assumption makes sense physically and geometrically.[3]

REMARK 3.11. We mention at this point that, if convection dominates diffusion in periodic media, then the right convergence tool seems to be a variant of (3.6) called two-scale convergence with drift [**AMP10**]. A nice introduction to the study of (Taylor's) dispersion is [**vDMPR08**].

THEOREM 3.12 (Continuity theorem). *Let (u_ε) be a sequence in $L^2(\Omega)$ and let $u_0\in L^2(\Omega\times Y)$ such that $u_\varepsilon \overset{2}{\rightharpoonup} u_0\in L^2(\Omega\times Y)$. Then we have*

$$\liminf_{\varepsilon\to 0}\|u_\varepsilon\|_{L^2(\Omega)}\geq\|u_0\|_{L^2(\Omega\times Y)}. \tag{3.7}$$

For a proof, see [**NR92**].

The main result of this section is the following (two-scale) compactness result:

THEOREM 3.13 (Two-scale compactness). *The following statements hold:*

(i) *From each bounded sequence (u^ε) in $L^2(\Omega)$, one can extract a subsequence which two-scale converges to $u_0(x,y)\in L^2(\Omega\times Y)$.*

(ii) *Let (u^ϵ) be a bounded sequence in $H^1(\Omega)$, which converges weakly to a limit function $u_0(x,y)\in H^1(\Omega\times Y)$. Then there exists $u_1\in L^2(\Omega;H^1_\#(Y)/\mathbb{R})$ such that up to a subsequence (u^ϵ) two-scale converges to $u_0(x,y)$ and $\nabla u^\epsilon \overset{2}{\rightharpoonup}\nabla_x u_0+\nabla_y u_1$.*

(iii) *Let (u^ϵ) and $(\epsilon\nabla u^\epsilon)$ be bounded sequences in $L^2(\Omega)$. Then there exists $u_0\in L^2(\Omega;H^1_\#(Y))$ such that up to a subsequence u^ϵ and $\epsilon\nabla u^\epsilon$ two-scale converge to $u_0(x,y)$ and $\nabla_y u_0(x,y)$, respectively.*

[3] The use of $|Y|=1$ can be very misleading especially in the case when the periodic cell is denoted differently, say by Z, and periodically-placed microstructures are present (see next chapter for more in this direction). $Y\subset Z$ designates then the microstructure and, usually, we have $|Y|\neq 1$.

REMARK 3.14. You can now use the First Oscillation Lemma, part (i) of the two-scale compactness theorem in combination with the relation between two-scale convergence and weak convergence to prove rigorously Exercise 3.5 (iii).

As we will see later, we are particularly interested in treating the presence of a periodic array of inclusions (perforations, microstructures, ...). Consequently, a concept of two-scale convergence is needed to deal with the periodically arranged (hyper)surfaces (of the inclusions boundaries).

DEFINITION 3.15 (Two-scale convergence for ϵ-periodic surfaces; cf. [**NR96**]). A sequence of functions (u^ϵ) in $L^2(\Gamma_\epsilon)$ is said to two-scale converge to a limit $u_0 \in L^2(\Omega \times \Gamma)$ if and only if for any $\psi \in C_0^\infty(\Omega, C_\#^\infty(\Gamma))$ we have

$$\lim_{\epsilon\to 0} \epsilon \int_{\Gamma_\epsilon} u^\epsilon(x)\psi\Big(t, x, \frac{x}{\epsilon}\Big)\, \mathrm{d}\sigma_x = \int_\Omega \int_\Gamma u_0(x,y)\psi(x,y)\, \mathrm{d}\sigma_y\, \mathrm{d}x.$$

LEMMA 3.16 (Second Oscillation Lemma). *For all functions $f \in C^0(\bar\Omega; C_\#^0(\Gamma))$, it holds that*

$$\lim_{\varepsilon\to 0} \varepsilon \int_{\Gamma_\varepsilon} f\left(x, \frac{x}{\varepsilon}\right)\, \mathrm{d}\sigma_\varepsilon = \int_\Omega \int_\Gamma f(x,y)\, \mathrm{d}\sigma\, \mathrm{d}x. \tag{3.8}$$

THEOREM 3.17. *The following statements hold:*

(i) *From each bounded sequence $(u^\epsilon) \in L^2(\Gamma_\epsilon)$, one can extract a subsequence u^ϵ which two-scale converges to a function $u_0 \in L^2(\Omega \times \Gamma)$.*

(ii) *If a sequence of functions (u^ϵ) is bounded in $L^\infty(\Gamma_\epsilon)$, then u^ϵ two-scale converges to a function $u_0 \in L^\infty(\Omega \times \Gamma)$.*

PROOF. For the proof of (i), see [**NR96**]. The proof of (ii) is given for instance in [**MCP08**]. □

REMARK 3.18. In Chapter 6 we treat a real-world application—the corrosion of a concrete piece. Inherently, the underlying PDE model is of evolution type. The concepts introduced in this section are applicable to such evolution problems provided a few elementary modifications are made in order to to cope with the time variable; see e.g. [**Eva98**, **Lio63**].

REMARK 3.19. It is worth also noting that two-scale like convergence concepts have been adapted also to work with measures or to be applicable in the stochastic case; see for instance [**LW05**, **ZP06**].

3.4. Exercises

EXERCISE 3.1. Is the embedding $L^2(\Omega; H_\#^1(Y))$ into $L^2(\Omega; L_\#^2(Y))$ compact? Justify your answer.

EXERCISE 3.2. Show that $H_\#^1(Y)$ and $L^2(\Omega; H_\#^1(Y))$ are Hilbert spaces.

EXERCISE 3.3. Show that if $u_\epsilon \to u$ strongly in $L^2(\Omega)$, then following statements hold:

(i) $u_\epsilon \rightharpoonup u$ in $L^2(\Omega)$;

(ii) $u_\epsilon \overset{2}{\rightharpoonup} u_0(x,y)$ in $L^2(\Omega \times Y)$.

EXERCISE 3.4. Does the two-scale convergence in $L^2(\Omega \times Y)$ imply the weak convergence in $L^2(\Omega)$? Show your arguments.

EXERCISE 3.5. Let $u : \mathbb{R} \to [-1, 1]$ be defined by $u(y) := \cos 2\pi y$. Set $u_\epsilon(x) := u\left(\frac{x}{\epsilon}\right)$ for $x \in]a, b[$, where $a, b \in \mathbb{R}$ and $a < b$.

1. Show that $u_\epsilon \rightharpoonup 0$ in $L^2(a, b)$ as $\epsilon \to 0$.
2. Can one also have $u_\epsilon \to 0$ in $L^2(a, b)$? Justify your answer.

3. We expect that $u_\epsilon \overset{2}{\rightharpoonup} u_0$ in $L^2(\Omega \times Y)$. Can you guess what are the best candidates for u_0 and Y?

EXERCISE 3.6. Consider the domain $\Omega :=]-1, 1[$ and the function $u_\epsilon : \Omega \to \mathbb{R}$, where

$$u_\epsilon(x) := \begin{cases} \epsilon, & \text{if } x \in \left]0, \frac{1}{\epsilon}\right[, \\ 0, & \text{if } x \in \mathbb{R} \setminus \left]0, \frac{1}{\epsilon}\right[. \end{cases}$$

Show that the sequence (u_ϵ) is bounded in $L^1(\Omega)$ and calculate its weak limit.

EXERCISE 3.7. Derive (formally) the macroscopic equation and corresponding effective coefficients for the following microscopic problem, say (P_ϵ):

$$\begin{aligned} -\mathrm{div}(a_\epsilon(x)\nabla u_\epsilon) &= f(x), \quad \text{in } \Omega, \\ u_\epsilon(x) &= u_D(x), \quad \text{at } \partial\Omega, \end{aligned}$$

where $\Omega \subset \mathbb{R}^d$, the matrix $a_\epsilon(x) := A(\frac{x}{\epsilon})$ has periodic entries, the Dirichlet data u_D is smooth enough, and f is not oscillatory (i.e., f is uniform in ϵ). Assume that (P_ϵ) is a well-posed problem and pass to the formal homogenization limit $\epsilon \to 0$.

Hints

HINT FOR EXERCISE 3.3, (II). Use First Oscillation Lemma in combination with the Continuity Theorem.

HINT FOR EXERCISE 3.7. Make the transformation $v_\epsilon := u_\epsilon - u_D$ and impose the homogenization ansatz $v_\epsilon = v_0 + \epsilon v_1 + \mathcal{O}(\epsilon)$ to (P_ϵ) formulated in terms of v_ϵ. Note that your domain Ω is now not perforated, fact which will essentially simplify your arguments.

CHAPTER 4

Homogenization of a linear 2nd order elliptic equation. A two-scale approach

The plan here is to use the concept of two-scale convergence (as previously introduced in Definition 3.10) to perform the homogenization of a linear second order elliptic equation posed in a fixed (non-oscillatory) domain Ω. The structure of this chapter is inspired from lecture notes by G. Allaire [**All02**] and is meant to bring the concept of two scale convergence to "action".

4.1. Setting of the problem. Working hypotheses

Our objective now is to study the following model problem:
Find $u_\varepsilon \in H_0^1(\Omega)$ such that

$$-\operatorname{div}\big(a_\varepsilon(x)\nabla u_\varepsilon\big) = f, \text{ in } \Omega \subset \mathbb{R}^d, \tag{4.1}$$

$$u_\varepsilon = 0, \text{ on } \partial\Omega, \tag{4.2}$$

where $a_\varepsilon(x) := A\big(\frac{x}{\varepsilon}\big) \in \mathbb{R}^{d^2}$. We refer to (4.1)–(4.2) as problem (P_ε).

We consider the following assumptions (H1)–(H4) to be fulfilled:

(H1) The matrix A is Y-periodic and satisfies the coercivity condition:

$$\exists \alpha, \beta > 0, \alpha \leq \beta \text{ such that } \alpha|\zeta|^2 \leq \sum_{i,j=1}^{d} A_{ij}(y)\zeta_i\zeta_j \leq \beta|\zeta|^2 \forall \zeta \in \mathbb{R}^d; \tag{4.3}$$

(H2) $A_{ij} \in L^\infty(Y)$ for all $(i,j) \in \{1,\dots,d\}^2$, A symmetric;
(H3) $f \in L^2(\Omega)$;
(H4) Ω is a $\mathbb{R}^d$-parallelepiped, while Y is a hypercube of volume 1.

Remark 4.1. Assumptions (H1)–(H4) can be relaxed. However, in this chapter, we prefer to stick to them simply because they offer the simplest setting where the technique of two-scale convergence works.

4.1.1. Homogenization procedure. Assume (H1)–(H4). We split the application of the homogenization procedure into six steps as follows:

Step 1 (Well-posedness of (P_ε)). The first thing to do is to define a good concept of weak solution to problem (P_ε) (the microscopic problem). Then one needs to ensure the well-posedness of problem (P_ε). For our example, we have:

Definition 4.2 (Weak solution to (P_ε)). $u_\varepsilon \in H_0^1(\Omega)$ is a weak solution to (P_ε) if and only if for all $\varphi \in H_0^1(\Omega)$ the following identity holds

$$(a_\varepsilon \nabla u_\varepsilon, \nabla \varphi) = (f, \varphi). \tag{4.4}$$

A straightforward application of Lax-Milgram lemma (see, for instance, [**CD99**, Theorem 4.6]) gives the existence and uniqueness of $u_\varepsilon \in H_0^1(\Omega)$ solving (P_ε) in the sense of Definition 4.2. Showing the stability of u_ε with respect to the data of (P_ε) is an easy-to-do exercise; we leave this as homework.

Step 2 (ε-independent *a priori* estimates). Choosing in (4.4) as test function $\varphi = u_\varepsilon$ and using the coercivity condition (H1), we obtain

$$\alpha\|u_\varepsilon\|^2_{H^1_0(\Omega)} \leq (a_\varepsilon \nabla u_\varepsilon, \nabla u_\varepsilon) = (f, u_\varepsilon) \leq \|f\|_{L^2(\Omega)}\|u_\varepsilon\|_{L^2(\Omega)} \leq c_P\|f\|_{L^2(\Omega)}\|u_\varepsilon\|_{H^1_0(\Omega)},$$

where the constant $c_P > 0$ is the one entering Poincaré's inequality (note that $H^1_0(\Omega) \subset L^2(\Omega)$). Dividing in the latter expression by $\|u_\varepsilon\|_{H^1_0(\Omega)}$ we are led to the estimate

$$\|u_\varepsilon\|_{H^1_0(\Omega)} \leq \frac{c_P}{\alpha}\|f\|_{L^2(\Omega)}. \tag{4.5}$$

Note that the constant $\frac{c_P}{\alpha}$ entering the (energy) estimate (5.5) is independent of ε.

Step 3 (Compactness step). This is basically the true homogenization step. Now, we note that the hypotheses of the two-scale compactness theorem (i.e., of Theorem 3.13) are fulfilled, and hence, we can apply this theory to our setting.

Since (u_ε) is uniformly bounded in $H^1_0(\Omega)$, there exist

$$u_0 \in L^2(\Omega \times Y),$$
$$u_1 \in L^2(\Omega; H^1_\#(Y)/\mathbb{R}),$$

such that

$$u_\epsilon \overset{2}{\rightharpoonup} u_0,$$
$$\nabla u_\epsilon \overset{2}{\rightharpoonup} \nabla u_0 + \nabla_y u_1.$$

On the other hand, from the fact that the sequence (u_ε) is uniformly bounded in $H^1_0(\Omega)$ and from the compactness of the embedding $H^1_0(\Omega) \subset L^2(\Omega)$, we deduce that (up to subsequences) $u^\epsilon \rightharpoonup \hat{u}_0(x,y)$ (weakly), and respectively, $u_\varepsilon \to \bar{u}_0(x)$ (strongly). Consequently, by the uniqueness of the weak limit, we get

$$\bar{u}_0(x) = \hat{u}_0(x,y) = u_0(x), \text{ a.e. in } \Omega \times Y. \tag{4.6}$$

Essentially, this means that the limit function u_0 is independent of the microscopic variable y.

Step 4 (Weak formulation of the two-scale limit problem). Let $x \in \Omega$. Choosing in Definition 4.2 as test function

$$\varphi(x) = \phi(x) + \varepsilon\phi_1\left(x, \frac{x}{\varepsilon}\right), \tag{4.7}$$

where

$$(\phi, \phi_1) \in C^\infty_0(\Omega) \times C^\infty_0(\Omega; C^\infty_\#(Y)),$$

we obtain:

$$\int_\Omega A\Big(\frac{x}{\varepsilon}\Big)\nabla u_\varepsilon(x)\nabla\varphi(x) = \int_\Omega f(x)\varphi(x),$$

$$\int_\Omega A\Big(\frac{x}{\varepsilon}\Big)\nabla u_\varepsilon\Big(\nabla\phi(x) + \nabla_y\phi_1\Big(x, \frac{x}{\varepsilon}\Big) + \varepsilon\nabla_x\phi_1\Big(x, \frac{x}{\varepsilon}\Big)\Big) = \int_\Omega f(x)\Big(\phi(x) + \varepsilon\phi_1\Big(x, \frac{x}{\varepsilon}\Big)\Big).$$

Rearranging the terms, we have

$$\int_\Omega \nabla u_\varepsilon A^t\Big(\frac{x}{\varepsilon}\Big)\Big(\nabla\phi(x) + \nabla_y\phi_1\Big(x, \frac{x}{\varepsilon}\Big)\Big) + \varepsilon\int_\Omega \nabla u_\varepsilon A^t\Big(\frac{x}{\varepsilon}\Big)\nabla_x\phi_1\Big(x, \frac{x}{\varepsilon}\Big)$$
$$= \int_\Omega f(x)\phi(x) + \varepsilon\int_\Omega f(x)\phi_1\Big(x, \frac{x}{\varepsilon}\Big).$$

Passing now with $\varepsilon \to 0$, we get the weak form of the two-scale limit problem. Namely, we obtain

$$\int_\Omega\int_Y \big(\nabla u_0(x) + \nabla u_1(x,y)\big)A^t(y)\big(\nabla\phi(x) + \nabla_y\phi_1(x,y)\big) = \int_\Omega\int_Y f\phi,$$

and hence,

$$\int_\Omega \int_Y A(y)\big(\nabla u_0(x) + \nabla u_1(x,y)\big)\big(\nabla \phi(x) + \nabla_y \phi_1(x,y)\big) = \int_\Omega f\phi. \tag{4.8}$$

We consider (4.8) as the weak formulation of the limit two-scale problem, say (P_0).

Step 5 (Weak solvability of (P_0)). This step takes care of the existence and uniqueness of weak solutions to the two-scale limit problem (P_0).

The limiting process $\varepsilon \to 0$ guesses (by means of a subsequence) the existence[1] of a weak solution to (P_0). On the other hand, since the problem is linear, one can easily show, by standard arguments[2], the uniqueness of weak solutions to (P_0).

Step 6 (Strong formulation of the two-scale limit problem). Let us integrate by parts (P_0). We obtain

$$\int_\Omega \int_Y A(y)\nabla u_0(x)\nabla\phi(x) + \int_\Omega \int_Y A(y)\nabla_y u_1(x,y)\nabla\phi(x) + \int_\Omega \int_Y A(y)\nabla u_0(x)\nabla_y\phi_1(x,y) + \int_\Omega \int_Y A(y)\nabla_y u_1(x,y)\nabla_y\phi_1(x,y) = \int_\Omega f\phi.$$

This leads to

$$\int_\Omega -\mathrm{div}_x\left(\int_Y A(y)\big(\nabla u_0(x) + \nabla_y u_1(x,y)\big)\right)\phi(x) - \int_\Omega f\phi(x) = \int_{\Omega\times Y} \mathrm{div}_y\Big(A(y)\big(\nabla u_0(x) + \nabla_y u_1(x,y)\big)\Big)\phi_1(x,y)$$

for all $(\phi,\phi_1) \in C_0^\infty(\Omega)\times C_0^\infty(\Omega; C_\#^\infty(Y))$. Choosing firstly $\phi = 0$ and then $\phi_1 = 0$ (within the domains Ω and $\Omega\times Y$ and then at their boundaries), we obtain the strong formulation of the two-scale limit problem, viz.

$$-\mathrm{div}_y\Big(A(y)\big(\nabla u_0 + \nabla_y u_1\big)\Big) = 0, \text{ a.e. in } \Omega\times Y, \tag{4.9}$$

$$-\mathrm{div}\left(\int_Y A(y)\big(\nabla u_0(x) + \nabla_y u_1(x,y)\big)\right) = f, \text{ a.e. in } \Omega, \tag{4.10}$$

$$u = 0, \text{ on } \partial\Omega \text{ and } u_1 \text{ is } Y\text{-periodic}. \tag{4.11}$$

Note that (4.9) is precisely the ϵ^{-2} subproblem used to formulate the *cell problem* arising in the formal homogenization procedure. Their role was to eliminate the term u_1 in the expansion of u_ε. In the same spirit, we can use the PDE (4.9) to eliminate u_1 from the strong (and weak) formulation of the limit two-scale problem. As before, the solution of the cell problem admits the representation

$$u_1(x,y) = -\sum_{j=1}^d w_j(y)\partial_{x_j} u_0 + \tilde{u}_1(x), \tag{4.12}$$

---

[1] Alternatively, one can apply Lax-Milgram lemma this time for the Hilbert space

$$\mathcal{H} := H_0^1(\Omega)\times L^2(\Omega; H_\#^1(Y)/\mathbb{R})$$

endowed with the norm

$$\|(u_0,u_1)\|_{\mathcal{H}} := \|\nabla u_0\|_{L^2(\Omega)} + \|\nabla_y u_1\|_{L^2(\Omega\times Y)}.$$

[2] The uniqueness of weak solutions is obtained directly via a Lax-Milgram argument, or by testing conveniently with the difference of two distinct weak solutions to (P_ε).

where the cell functions w_j are solutions of the cell problems

$$-\mathrm{div}_y\big(A(y)\nabla_y w_j\big) = -\sum_{i=1}^{d} \partial_{y_i} A_{ij}(y), \text{ in } Y,$$
$$\int_Y w_j = 0 \text{ and } w_j \text{ is } Y\text{-periodic for all } j \in \{1,\dots,d\}.$$

Replacing now u_1 defined by (4.12) into (4.10), we obtain the desired (homogenized) macroscopic PDE

$$-\sum_{i,k=1}^{d} \left[\sum_{j=1}^{d} \int_Y \left(A_{ik} - A_{ij}\partial_{y_j} w_k\right) \mathrm{d}y\right] \partial^2_{x_i x_k} u_0 = |Y| f \text{ in } \Omega. \tag{4.13}$$

The coefficient $\bar{D}$, which is given by

$$\bar{D}_{ik} := \left[\sum_{j=1}^{d} \int_Y \left(A_{ik} - A_{ij}\partial_{y_j} w_k\right) \mathrm{d}y\right],$$

is the so called *effective* (macroscopic) diffusion coefficient.

4.2. A corrector estimate

4.2.1. How good is our averaging method? At this point, we have an averaged (homogenized) model with a computable effective transport coefficient. Inherently, the following unavoidable question arises: *How much information have we lost via averaging?* Looking to the structure of the asymptotic ansatz

$$u_\varepsilon = u_0 + \varepsilon u_1 + \mathcal{O}(\varepsilon) \tag{4.14}$$

makes us expect something like

$$\frac{u_\varepsilon - u_0}{\varepsilon} = u_1 + \mathcal{O}(\varepsilon).$$

In other words, we expect that showing that $u_\varepsilon \to u_0$ (strongly in $L^2(\Omega)$) is related to controlling the growth of u_1. With other words: the smaller ε is, the better the averaging.

Recall that the two-scale limit problem determines the unique pair $(u_0, u_1) \in H^1_0(\Omega) \times L^2(\Omega; H^1_\#(Y)/\mathbb{R})$. We claim that these u_0 and u_1 are precisely the same as those arising in (4.14). We have seen earlier that $\nabla u_\epsilon \overset{2}{\rightharpoonup} \nabla u_0 + \nabla_y u_1$ in $[L^2(\Omega; L^2(Y))]^d$. Can we turn this weak-type of convergence into a strong convergence result? The answer is yes, but *we need to extract some oscillations*[3] from the quantity $\nabla u_\varepsilon - \nabla u_0$ in order to get this behavior. But, how much oscillations should we then extract? Inspired by [**LNW02**, **CD99**], we give the precise answer in Theorem 4.3.

4.2.2. Main result—a corrector estimate. In this section, we prove the following strong convergence result:

THEOREM 4.3. *Let $1 \le s, t \le \infty$ such that $\frac{1}{s} + \frac{1}{t} = 1$. Assume that for all $(i,j) \in \{1,\dots,d\}^2$ we have*

$$\partial_{x_i} \in L^{2s}(\Omega), \quad \partial_{y_j} w_i \in L^2_\#(Y). \tag{4.15}$$

Then

$$\nabla u_\varepsilon - \nabla u_0 - \nabla_y u_1\Big(\cdot, \frac{\cdot}{\varepsilon}\Big) \to 0 \text{ in } [L^2(\Omega)]^d. \tag{4.16}$$

[3] *A priori* it is not quite clear how much oscillations can one actually extract. Intuitively, the more oscillations one can control the better the convergence is expected to be. Readers browsing attentively the literature will observe that the users of periodic unfolding techniques can use their unfolding ideas to derive better results. They don't get necessarily faster rates, just the class of microstructures that can be handled is larger. One requires then less regularity of the shapes of the microstructures.

PROOF. Using the coercivity condition on a_ε, we get

$$\begin{aligned}\alpha\int_\Omega |\nabla u_\varepsilon - \nabla u_0 - \nabla_y u_1|^2\,\mathrm{d}x &\le \int_\Omega A\Big(\frac{x}{\varepsilon}\Big)\left[\nabla u_\varepsilon - \nabla u_0 - \nabla_y u_1\right](\nabla u_\varepsilon - \nabla u_0 - \nabla_y u_1)\\ &= \int_\Omega A\Big(\frac{x}{\varepsilon}\Big)\nabla u_\varepsilon \nabla u_\varepsilon\,\mathrm{d}x - \int_\Omega \nabla u_\varepsilon\left(A + A^t\right)\Big(\frac{x}{\varepsilon}\Big)(\nabla u_0 + \nabla_y u_1)\,\mathrm{d}x\\ &\quad + \int_\Omega \Big[A\Big(\frac{x}{\varepsilon}\Big)(\nabla u_0 + \nabla_y u_1)\Big](\nabla u_0 + \nabla_y u_1)\,\mathrm{d}x\\ &= \sum_{k=1}^3 T_k,\end{aligned}$$

where the terms T_k ($k \in \{1,2,3\}$) are defined as follows:

$$\begin{aligned}T_1 &:= \int_\Omega A\Big(\frac{x}{\varepsilon}\Big)\nabla u_\varepsilon \nabla u_\varepsilon\,\mathrm{d}x,\\ T_2 &:= -\int_\Omega \nabla u_\varepsilon\left(A + A^t\right)\Big(\frac{x}{\varepsilon}\Big)(\nabla u_0 + \nabla_y u_1)\,\mathrm{d}x,\\ T_3 &:= \int_\Omega \Big[A\Big(\frac{x}{\varepsilon}\Big)(\nabla u_0 + \nabla_y u_1)\Big](\nabla u_0 + \nabla_y u_1)\,\mathrm{d}x.\end{aligned}$$

We proceed as follows: By the week formulation of (P_ε), we know that

$$\int_\Omega A\Big(\frac{x}{\varepsilon}\Big)\nabla u_\varepsilon \nabla u_\varepsilon\,\mathrm{d}x = \int_\Omega f u_\varepsilon\,\mathrm{d}x.$$

Passing in this inequality to the two-scale limit $\varepsilon \to 0$, we get that $T_1 \to \int_\Omega f u_0$. Now, using the symmetry of A, we can rewrite T_2 as

$$\begin{aligned}T_2 &= -2\int_\Omega \nabla u_\varepsilon A\Big(\frac{x}{\varepsilon}\Big)(\nabla u_0 + \nabla_y u_1)\,\mathrm{d}x\\ &\overset{\varepsilon\to 0}{\longrightarrow} -2\int_\Omega\int_Y A(y)[\nabla u_0(x) + \nabla_y u_1(x,y)](\nabla u_0(x) + \nabla_y u_1(x,y))\,\mathrm{d}x\,\mathrm{d}y.\end{aligned}$$

Similarly, T_3 goes to $\int_\Omega\int_Y A(y)[\nabla u_0(x) + \nabla_y u_1(x,y)](\nabla u_0(x) + \nabla_y u_1(x,y))$ as $\varepsilon \to 0$.

Combing the above relations, we get using the weak formulation of the two-scale limit problem (P_0) that

$$\begin{aligned}0 &\le \lim_{\varepsilon\to 0}\alpha\int_\Omega \Big|\nabla u_\varepsilon - \nabla u_0 - \nabla_y u_1\Big(x,\frac{x}{\varepsilon}\Big)\Big|^2\,\mathrm{d}x\\ &\le \int_\Omega f u_0\,\mathrm{d}x - \int_\Omega\int_Y A(y)\big[\nabla u_0 + \nabla_y u_1(x,y)\big]\big(\nabla u_0 + \nabla_y u_1(x,y)\big)\,\mathrm{d}x\,\mathrm{d}y = 0.\end{aligned}$$

□

REMARK 4.4. The French homogenization community typically call a result of type (4.15) a *corrector*. However, from the point of view of applications, more work is to be done to get *corrector estimates*, i.e. upper bound estimates on convergence rates inequalities expressing in terms of quantitative computable inequalities *how fast* one can approximate u_ε and ∇u_ε in terms of u_0 and $\nabla u_0 + \nabla_y u_1(\cdot, \frac{\cdot}{\varepsilon})$, respectively. We will briefly return to this issue at the end of the next chapter.

4.3. Exercises

EXERCISE 4.1. Show that $\varphi(x) := A^t\left(\frac{x}{\varepsilon}\right)\nabla_x\phi_1(x,\frac{x}{\varepsilon})$ is allowed as test function in the two-scale convergence.

EXERCISE 4.2. Establish the maximal regularity of the cell functions w_j, where $j \in \{1,\dots,d\}$.

EXERCISE 4.3. Formulate a variant of Lemma 2.34 [**PS08**, pp. 26–27] suitable for our setting.

EXERCISE 4.4. Why is the constant $\frac{c_P}{\alpha}$ entering (4.5) independent of the choice of ε?

EXERCISE 4.5. Prove (4.6).

EXERCISE 4.6. Derive (formally) the macroscopic equation and corresponding effective coefficients for the following microscopic problem, say (P_ϵ):

$$\begin{aligned} -\mathrm{div}\big(a_\epsilon(x)\nabla u_\epsilon\big) &= f(x), \text{ in } \Omega,\\ u_\epsilon(x) &= u_D(x), \text{ at } \partial\Omega, \end{aligned}$$

where $\Omega \subset \mathbb{R}^d$, the matrix $a_\epsilon(x) := A(\frac{x}{\epsilon})$ has periodic entries, the Dirichlet data u_D is smooth enough, and f is not oscillatory (i.e. f is uniform in ϵ). Assume that (P_ϵ) is a well-posed problem and do pass to the formal homogenization limit $\epsilon \to 0$.

EXERCISE 4.7. Consider the Exercise 4.6. Prove rigorously the asymptotic limit $\epsilon \to 0$.

Hints

HINT FOR EXERCISE 4.6. Make the transformation $v := u - u_D$ and work with the PDE in terms of v.

CHAPTER 5

Homogenization in periodically perforated media

The aim of this chapter is to use the concept of two-scale convergence to perform the homogenization of a linear second order elliptic equation posed in a domain with microstructures called Ω_ε. The mathematical community typically refers to Ω_ε as a perforated domain. Most of the steps mentioned in Chapter 4 will be redone now again, but the central question here is:

To which extent is the geometry of the perforation important for the averaging procedure and respective outcome?

5.1. Linear elliptic equation in periodically perforated domains

We are considering our model problem posed now in a perforated domain Ω_ε[1]:
Find $u_\varepsilon \in H_0^1(\Omega_\varepsilon)$ such that

$$-\mathrm{div}\big(a_\varepsilon(x)\nabla u_\varepsilon\big) = f, \text{ in } \Omega_\varepsilon \subset \mathbb{R}^d, \tag{5.1}$$

$$u_\varepsilon = 0, \text{ on } \partial\Omega_\varepsilon, \tag{5.2}$$

where $a_\varepsilon(x) := A\left(\frac{x}{\varepsilon}\right) \in \mathbb{R}^{d^2}$. We refer to (5.1)–(5.2) again as problem (P_ε).

As before[2], we consider the assumptions (H1)–(H4) to be fulfilled.

The relevant questions here are:

- What means Ω_ε?
- What are perforations? Microstructures?
- Can we repeat the same strategy as before (fixed domain case—Ω) to pass via two-scale convergence to the limit $\varepsilon \to 0$ in PDEs defined in perforated domains?

Let us define firstly the basic geometry of the perforations. This is the aim of the next section.

5.1.1. Geometry of perforations. Definition of Ω_ε. In this section, we rely on the following notation[3]: Let $Z \subset \mathbb{R}^d$ be a hypercube. Furthermore, let $k = (k_1, \ldots, k_d) \in \mathbb{Z}^d$ be a vector of indices and $e = (e_1, \ldots, e_d)$ be the unit vector in $\mathbb{R}^d$. For $X \subset Z$, we recall the notation X^k, which is the shifted subset

$$X^k := X + \sum_{i=1}^{d} k_i e_i.$$

[1] The perforated domain Ω_ε will be defined in Subsection 5.1.1.

[2] Similarly to the situation described in the previous chapter, we assume the following:
(H1) The matrix A is Y-periodic and satisfies the coercivity condition:

$$\exists \alpha, \beta > 0, \alpha \le \beta \text{ such that } \alpha|\zeta|^2 \le \sum_{i,j=1}^{d} A_{ij}(y)\zeta_i\zeta_j \le \beta|\zeta|^2 \forall \zeta \in \mathbb{R}^d; \tag{5.3}$$

The ellipticity constants α, β are taken to be independent of ε!
(H2) $A_{ij} \in L^\infty(Y)$ for all $(i,j) \in \{1, \ldots, d\}^2$; A symmetric
(H3) $f \in L^2(\Omega_\varepsilon)$
(H4) Ω_ε is the periodically perforated domain, Ω is a $\mathbb{R}^d$-parallelepiped, while Y is a hypercube of volume 1.

[3] This notation is inspired very much by the one used in [**HJ91**].

The pore matrix (or pore skeleton) is defined by

$$\Omega_0^\varepsilon := \bigcup_{k\in\mathbb{Z}^d} \{\varepsilon Y_0^k : Y_0^k \subset \Omega\},$$

while the total pore space is

$$\Omega^\varepsilon := \Omega - \Omega_0^\varepsilon.$$

εY_0^k is the ε-homotetic set of Y_0^k. The total (inner) surface of the skeleton is denoted by

$$\Gamma^\varepsilon := \partial\Omega_0^\varepsilon := \bigcup_{k\in\mathbb{Z}^d} \{\varepsilon\Gamma^k : \varepsilon\Gamma^k \subset \Omega\}.$$

Correspondingly, we introduce the unit normal vector n_ε to Γ^ε. Let $\mathrm{d}\sigma_\varepsilon$ be the corresponding (oscillating) measure defined on Γ_ε.

5.1.2. Homogenization procedure. Assume (H1)–(H4). We split the application of the homogenization procedure into seven steps as follows:

Step 1 (Well-posedness of (P_ε)).

Definition 5.1 (Weak solution to (P_ε)). $u_\varepsilon \in H_0^1(\Omega_\varepsilon)$ is a weak solution to (P_ε) if and only if for all $\varphi \in H_0^1(\Omega_\varepsilon)$ the following identity holds

$$(a_\varepsilon \nabla u_\varepsilon, \nabla\varphi) = (f, \varphi). \tag{5.4}$$

Lax-Milgram lemma ensures the existence and uniqueness of $u_\varepsilon \in H_0^1(\Omega_\varepsilon)$ solving (P_ε) in the sense of Definition 5.1.

Step 2 (ε-independent *a priori* estimates). Choosing in (5.4) as test function $\varphi = u_\varepsilon$ and using the coercivity condition (H1), we obtain

$$\alpha\|u_\varepsilon\|^2_{H_0^1(\Omega_\varepsilon)} \le (a_\varepsilon\nabla u_\varepsilon, \nabla u_\varepsilon) = (f, u_\varepsilon) \le \|f\|_{L^2(\Omega_\varepsilon)}\|u_\varepsilon\|_{L^2(\Omega_\varepsilon)} \le c_P\|f\|_{L^2(\Omega_\varepsilon)}\|u_\varepsilon\|_{H_0^1(\Omega_\varepsilon)},$$

where the constant $c_P > 0$ is the one entering Poincaré's inequality (note that $H_0^1(\Omega) \subset L^2(\Omega)$). Dividing the latter expression by $\|u_\varepsilon\|_{H_0^1(\Omega_\varepsilon)}$ we are led to the estimate

$$\|u_\varepsilon\|_{H_0^1(\Omega_\varepsilon)} \le \frac{c_P}{\alpha}\|f\|_{L^2(\Omega_\varepsilon)}. \tag{5.5}$$

Does the constant c_P depend on ε? In general the answer is yes, however, for some classes of (nice) microstructures one can prove that c_P is independent of ε. For the microstructure Y_0 chosen here, c_P does not depend on ε. Can we now find subsequences u_ε such that

$$u_\epsilon \overset{2}{\rightharpoonup} u_0, \tag{5.6}$$

$$\nabla u_\epsilon \overset{2}{\rightharpoonup} \nabla u_0 + \nabla_y u_1? \tag{5.7}$$

Not directly, one intermediate step needs to be made.

Step 3 (Extension to fixed domains). At this point, we need extension results for Sobolev spaces. Essentially, if we can show that the extension of u_ε is uniformly bounded in $H_0^1(\Omega)$, then we are done since we can simply use the two-scale convergence arguments as before.

(H5) Assume ∂Y_0 and $\partial\Omega_\varepsilon$ to be Lipschitz.

Lemma 5.2 (Extension lemma). *Assume (H5). The following statements hold:*

(i) *(Extension in the micro cell) If $u \in H^1(Y)$, then it exists $\tilde{u}$—extension into Y_0 (and thus on Z) of u—such that*

$$\|\tilde{u}\|_{H^1(Z)} \le c\|u\|_{H^1(Y)}.$$

(ii) *(Extension in the macro domain) If $u_\varepsilon \in H^1(\Omega^\varepsilon)$, it exists $\tilde{u}_\varepsilon$—extension to Ω of u_ε—such that*

$$\|\tilde{u}_\varepsilon\|_{H^1(\Omega)} \le c\|u_\varepsilon\|_{H^1(\Omega_\varepsilon)}.$$

PROOF. (i) See any good textbook on function spaces, e.g. [**AF03**].
(ii) As a basic rule, we consider that summation over k is such that $\varepsilon Y \subset \Omega$. We have

$$\begin{aligned}
\|\tilde{u}_\varepsilon\|^2_{H^1(\Omega)} &= \sum_{k\in\mathbb{Z}^d} \int_{\varepsilon Z^k} \left(|\tilde{u}_\varepsilon(x)|^2 + |\nabla \tilde{u}_\varepsilon(x)|^2\right) \mathrm{d}x \\
&\overset{y=\frac{x}{\varepsilon}}{=} \sum_{k\in\mathbb{Z}^d} \varepsilon^d \int_{Z^k} \left(|\tilde{u}_\varepsilon(\varepsilon y)|^2 + |\nabla \tilde{u}_\varepsilon(\varepsilon y)|^2\right) \mathrm{d}y \\
&\overset{extension}{\leq} c \sum_{k\in\mathbb{Z}^d} \varepsilon^d \int_{Y^k} \left(|\tilde{u}_\varepsilon(\varepsilon y)|^2 + |\nabla \tilde{u}_\varepsilon(\varepsilon y)|^2\right) \mathrm{d}y \\
&= c \sum_{k\in\mathbb{Z}^d} \int_{\varepsilon Y^k} \left(|\tilde{u}_\varepsilon(x)|^2 + |\nabla \tilde{u}_\varepsilon(x)|^2\right) \mathrm{d}x \\
&= c\|u_\varepsilon\|^2_{H^1(\Omega_\varepsilon)}.
\end{aligned}$$

□

REMARK 5.3. We just want to note in passing that the best extension result (applicable to homogenization problems) known until now is the one by Acerbi et al. [**ACPDMP92**]. The reader might take the challenge to sketch on paper what kind of microstructures fit to the setting from [**ACPDMP92**], and which one are pathological, in the sense that they cannot be treated due to the lack of extension results (and therefore no rigorous averaging statements can be made).

Using now the information from Step 2, we have just shown that the extension $\tilde{u}_\varepsilon$ is uniformly bounded in $H^1_0(\Omega)$. Consequently, the homogenization procedure takes the familiar road:
Step 4 (Compactness step).
Step 5 (Weak formulation of the limit two-scale problem).
Step 6 (Weak solvability of (P_0)).
Step 7 (Strong formulation of the two-scale limit problem).

5.2. Averaging boundary processes in perforated media

We focus our attention now on the following microscopic problem

$$-\mathrm{div}\left(a_\varepsilon(x)\nabla u_\varepsilon\right) = f_\varepsilon, \quad \text{in } \Omega_\varepsilon, \tag{5.8}$$

$$-a_\varepsilon(x)\nabla u_\varepsilon \cdot n_\varepsilon = \varepsilon g_\varepsilon, \quad \text{at } \Gamma_\varepsilon, \tag{5.9}$$

$$u_\varepsilon = 0, \quad \text{at } \partial\Omega. \tag{5.10}$$

Assume f_ε and g_ε to be uniformly bounded in $L^2(\Omega_\varepsilon)$ and $L^2(\Gamma_\varepsilon)$, respectively. Furthermore, assume (H1)–(H4) and (H5) to hold. Here we have in mind that $f_\varepsilon(x) := f\left(x, \frac{x}{\varepsilon}\right)$ and $g_\varepsilon(x) := g\left(x, \frac{x}{\varepsilon}\right)$. We refer to the problem (5.8)–(5.10) as $(\hat{P}_\varepsilon)$.

We introduce now the following Sobolev space:

$$H^1(\Omega_\varepsilon; \partial\Omega) := \{\varphi \in H^1(\Omega_\varepsilon) : \varphi = 0 \text{ at } \partial\Omega\}.$$

DEFINITION 5.4 (Weak solution to $(\hat{P}_\varepsilon)$). $u_\varepsilon \in H^1(\Omega_\varepsilon; \partial\Omega)$ is a weak solution to $(\hat{P}_\varepsilon)$ if and only if for all $\varphi \in H^1(\Omega_\varepsilon; \partial\Omega)$ the following identity holds

$$\int_{\Omega_\varepsilon} a_\varepsilon(x)\nabla u_\varepsilon(x)\nabla\varphi(x)\,\mathrm{d}x = \int_{\Omega_\varepsilon} f_\varepsilon(x)\varphi(x)\,\mathrm{d}x + \varepsilon\int_{\Gamma_\varepsilon} g_\varepsilon(x)\varphi(x)\,\mathrm{d}\sigma_\varepsilon. \tag{5.11}$$

Suitable application of the Lax-Milgram lemma ensures the existence and uniqueness of a $u_\varepsilon \in H^1(\Omega_\varepsilon; \partial\Omega)$ satisfying (5.11).

In order to perform the homogenization procedure in this case, a few crucial steps need to be made:

(i) $\|u_\varepsilon\|_{H^1(\Omega_\varepsilon;\partial\Omega)} \leq c$ uniformly in ε;

(ii) The concept of two-scale convergence of (hyper)surfaces is needed.

Main ingredients for (i) are suitable Poincaré and trace inequalities, while for (ii) we need a compactness theorem associated with this type of convergence on surfaces.

LEMMA 5.5 (A Poincaré-type inequality). *Let $Z, Y \subset \mathbb{R}^d$, Z connected, open set in $\mathbb{R}^d$, $Z \subseteq Y$ such that $0 < |Z| \leq |Y|$ with ∂Z and ∂Y of class C^1. Let also $p \in [1, \infty]$. Then there exists a constant c_P depending only on n, p, Z, and Y, such that*

$$\left\| \phi - \fint_Y \phi \, \mathrm{d}y \right\|_{L^p(Z)} \leq c_P \|\nabla \phi\|_{[L^p(Z)]^d} \tag{5.12}$$

for each $\phi \in W^{1,p}(Z)$.

PROOF. We follow the line of arguments of [**Eva98**, Theorem 1, pp. 275-276]. The proof goes by contradiction. Assuming (5.12) to be false, results in the fact there would exist, for all $k \in \mathbb{N}$, a function $\phi_k \in W^{1,p}(Z)$ satisfying

$$\left\| \phi_k - \fint_Y \phi \, \mathrm{d}y \right\|_{L^p(Z)} \geq k \|\nabla \phi_k\|_{[L^p(Z)]^d}. \tag{5.13}$$

For all $k \in \mathbb{N}$, we define the function

$$w_k(x) := \frac{\phi(x) - \fint_Y \phi \, \mathrm{d}y}{\|\phi - \fint_Y \phi \, \mathrm{d}y\|_{L^p(Z)}}. \tag{5.14}$$

It is easy to see that

$$\fint_Y w_k \, \mathrm{d}x = 0 \text{ and } \|w_k\|_{L^p(Z)} = 1. \tag{5.15}$$

Applying now (5.13) to w_k (a renormalized version of ϕ_k), we get

$$\|\nabla w_k\|_{[L^p(Z)]^n} < \frac{1}{k} \text{ for all } k \in \mathbb{N}. \tag{5.16}$$

Since w_k is bounded in $W^{1,p}(Z)$, and additionally, since the embedding $W^{1,p}(Z) \hookrightarrow L^p(Z)$ is compact (cf. Rellich-Kondrachov Theorem), we deduce that there exist at least a subsequence $(w_{k_j}) \subset (w_k)$ such that

$$w_{k_j} \to w \text{ strongly in } L^p(Z).$$

Using this strong convergence to pass to the limit $k \to \infty$ in (5.15), yields $\fint_Y w \, \mathrm{d}x = 0$ and

$$\|w\|_{L^p(Z)} = 1. \tag{5.17}$$

Furthermore, (5.16) also implies that, for all $i \in \{1, \ldots, d\}$ and all $\varphi \in C_c^\infty(Z)$, we have:

$$\int_Z w \frac{\partial \varphi}{\partial x_i} \, \mathrm{d}x = \lim_{k_j \to \infty} \int_Z w_{k_j} \frac{\partial \varphi_{k_j}}{\partial x_i} \, \mathrm{d}x = - \lim_{k_j \to \infty} \int_Z \frac{\partial w_{k_j}}{\partial x_i} \varphi \, \mathrm{d}x = 0.$$

So, $w \in W^{1,p}(Z)$ and $\nabla w = 0$ a.e. Thus w is constant, since Z is a connected set. But, on the other hand, $\fint_Y w \, \mathrm{d}y = 0$ implies that $w = 0$ a.e. in Y. From here, we deduce that $\|w\|_{L^p(Y)} = 0$, and hence, $\|w\|_{L^p(Z)} = 0$. This contradicts (5.17), and hence, the proof of the Lemma is completed. □

REMARK 5.6. If $Z = Y$, then the above Lemma reports on the standard Poincaré's inequality. A nice reference on Poincaré-type inequalities is [**SC02**].

LEMMA 5.7 (Poincaré's inequality for perforated media). *There exists a constant $c_P > 0$, independent of ε, such that*

$$\|u_\varepsilon\|_{L^2(\Omega_\varepsilon)} \leq c_P \|\nabla u_\varepsilon\|_{[L^2(\Omega_\varepsilon)]^d} \tag{5.18}$$

for all $u_\varepsilon \in H^1(\Omega_\varepsilon; \partial\Omega)$.

PROOF. We adapt the proof of [CS98, Lemma 2.1, pp. 14–15]). The extension lemma ensures the well-definiteness of a linear continuous extension operator

$$\mathcal{P} : H^1(\Omega_\varepsilon; \partial\Omega) \to H_0^1(\Omega)$$

such that $\mathcal{P}u_\varepsilon = u_\varepsilon$ a.e. on Ω_ε and

$$\|\nabla(\mathcal{P}u_\varepsilon)\|_{[L^2(\Omega)]^d} \leq c^* \|\nabla u_\varepsilon\|_{[L^2(\Omega)]^d}, \tag{5.19}$$

where c^* is the extension constant. Note that c^* is independent of the choice of ϵ. By the classical Poincaré's inequality, we have that

$$\|\mathcal{P}u_\varepsilon\|_{L^2(\Omega)} \leq \tilde{c}_P \|\nabla(\mathcal{P}u_\varepsilon)\|_{[L^2(\Omega)]^d}, \tag{5.20}$$

where, obviously, the positive constant $\tilde{c}_P$ does depend on Ω and d, but it is independent on ε. We conclude now the proof of this Lemma by noting that

$$\|u_\varepsilon\|_{L^2(\Omega_\varepsilon)} \overset{\text{extension in the interior}}{\leq} c_\star \|\mathcal{P}u_\varepsilon\|_{L^2(\Omega)} \overset{\text{Poincare's inequality}}{\leq} c_\star \tilde{c}_P \|\nabla(\mathcal{P}u_\varepsilon)\|_{[L^2(\Omega)]^d}$$
$$\overset{\text{extension in the exterior}}{\leq} c_\star \tilde{c}_P c^\star \|\nabla(\mathcal{P}u_\varepsilon)\|_{[L^2(\Omega_\varepsilon)]^d}.$$

Take now

$$c_P := c_\star \tilde{c}_P c^\star > 0 \tag{5.21}$$

and note that c_P is independent of ε. □

The following result is a trace inequality tailored for perforated media. This is a very useful inequality for those applications where (at least part of) the boundary is active. By "active boundary" we mean that boundary processes (and/or Cauchy fluxes; [Gur93]) are defined there. In mathematical terms, this is often described by the presence of a Robin-type boundary condition posed on a subset of Γ_ε.

LEMMA 5.8 (Trace inequality). *Let $\varphi \in H^1(\Omega_\varepsilon)$. Then there exists a constant $\hat{c} > 0$, independent of ε, such that the following inequality holds:*

$$\varepsilon \|\varphi\|^2_{L^2(\Gamma_\varepsilon)} \leq \hat{c} \|\varphi\|^2_{H^1(\Omega\varepsilon)}. \tag{5.22}$$

PROOF. Consider Fig. 5.1 as reference microstructure picture.

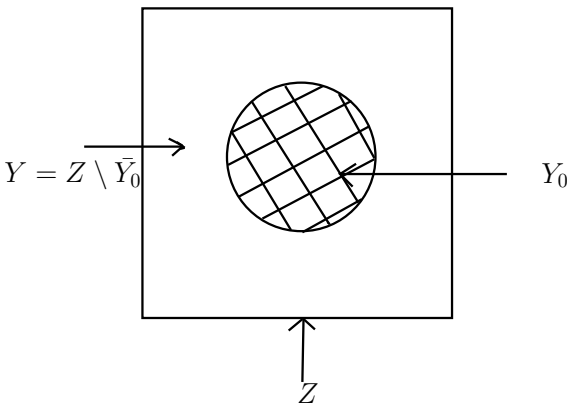

Figure 5.1 – Basic geometry of the microstructure.

To be more precise, we define

$$Y := Z - \bar{Y}_0 \text{ and } \Gamma := \partial Y_0,$$

and let n be the outer normal vector on Γ with $|n| = 1$, where $|\cdot|$ is here the Euclidean distance. We introduce the smooth extension $N := (N_1, \dots, N_d)$ of the normal unit vector n by

$$N_j(y) := n_j(y) \text{ on } \Gamma \tag{5.23}$$

for all $j \in \{1, \dots, d\}$ such that $\mathrm{supp} N_j$ is included in a closed "tubular" neighborhood of Γ.

Note that if $d = 2, 3$, then that tubular neighborhood of Γ is resembling the pillbox from Gurtin's Pillbox Lemma [**Gur93**].

Since Y_0 is a ball, the regularity C^∞ of Γ supports all following calculations[4]. We can therefore assume that we can choose $N_j \in C^1(\bar{Z})$. Due to periodicity and to the fact that $N \| n$ (and so $(N, n)_{\sigma_\varepsilon} = 1$), we have that

$$\begin{aligned}\int_{\Gamma_\varepsilon} \varphi^2 \, \mathrm{d}\sigma_\varepsilon &= \int_{\Gamma_\varepsilon} \varphi^2 \sum_{j=1}^{2} N_j\left(\frac{x}{\varepsilon}\right) n_j \, \mathrm{d}\sigma_\varepsilon = \int_{\Gamma_\varepsilon} \varphi^2(x) N\left(\frac{x}{\varepsilon}\right) n\left(\frac{x}{\varepsilon}\right) \, \mathrm{d}\sigma_\varepsilon \\ &= \int_{\Omega_\varepsilon} \mathrm{div}\left(\varphi^2(x)\right) N\left(\frac{x}{\varepsilon}\right) = \int_{\Omega_\varepsilon} \sum_{j=1}^{d} \frac{\partial}{\partial x_j}\left(\varphi^2(x)\right) N\left(\frac{x}{\varepsilon}\right) \, \mathrm{d}x \\ &= \sum_{j=1}^{d} \left[2 \int_{\Omega_\varepsilon} N_j\left(\frac{x}{\varepsilon}\right) \varphi(x) \frac{\partial \varphi}{\partial x_j}(x_j) + \frac{1}{\varepsilon} \int_{\Omega_\varepsilon} \int_{\Omega_\varepsilon} \frac{\partial N_j\left(\frac{x}{\varepsilon}\right)}{\partial x_j} \varphi^2(x) \, \mathrm{d}x \right].\end{aligned}$$

Consequently, we obtain

$$\begin{aligned}\|\varphi\|^2_{\Gamma_\varepsilon} &\le \sum_{j=1}^{d} \left[2 \max_{x \in \bar{\Omega}_\varepsilon} \left| N_j\left(\frac{x}{\varepsilon}\right) \right| \int_{\Omega_\varepsilon} \varphi(x) \frac{\partial \varphi}{\partial x_j}(x_j) + \frac{1}{\varepsilon} \max_{x \in \bar{\Omega}_\varepsilon} \left| \frac{\partial N_j\left(\frac{x}{\varepsilon}\right)}{\partial x_j} \right| \int_{\Omega_\varepsilon} \int_{\Omega_\varepsilon} \varphi^2(x) \, \mathrm{d}x \right] \\ &\le c_1 \|\varphi\|_{L^2(\Omega_\varepsilon)} \|\nabla \varphi\|_{[L^2(\Omega_\varepsilon)]^d} + \frac{1}{\varepsilon} c_2 \|\varphi\|^2_{L^2(\Omega_\varepsilon)}.\end{aligned}$$

We have taken here the constants $(c_1, c_2) := (\|N\|_\infty, \|\nabla N\|_\infty)$, where $N \in C^1(\bar{Z})$. We now have

$$\|\varphi\|^2_{L^2(\Gamma_\varepsilon)} \le c_1 \|\varphi\|_{L^2(\Omega_\varepsilon)} \|\nabla \varphi\|_{[L^2(\Omega_\varepsilon)]^d} + \frac{c_2}{\varepsilon} \|\varphi\|^2_{L^2(\Omega_\varepsilon)}.$$

Multiplying the last inequality by ε and then using the geometric-arithmetic mean leads to

$$\varepsilon \|\varphi\|^2_{L^2(\Gamma_\varepsilon)} \le \left(\frac{\varepsilon c_1^2}{2} + c_2 \right) \|\varphi\|^2_{L^2(\Omega_\varepsilon)} + \frac{1}{2} \|\nabla \varphi\|^2_{[L^2(\Omega_\varepsilon)]^2} \le \hat{c} \|\varphi\|^2_{H^1(\Omega_\varepsilon)}.$$

Note that $\hat{c} := \max\{c_1^2 + c_2, \frac{1}{2}\}$ is independent of the choice of ε. □

5.3. Exercises

EXERCISE 5.1. Why is the constant $\frac{c_P}{\alpha}$ entering (5.5) independent of the choice of ε? Justify your answer.

EXERCISE 5.2. Prove that the constant c_P entering (5.21) does not depend on ε.

EXERCISE 5.3. Let Ω be a bounded domain in $\mathbb{R}^2$ with Lipschitz $\partial\Omega$. Take the perforated domain $\Omega_\epsilon \subset \Omega$ to be connected such that the perforations do not touch each other, and additionally, that Γ_ϵ is Lipschitz. Consider the following problem, say (P_ϵ),

$$\begin{aligned} -\mathrm{div}\big(a_\epsilon(x) \nabla u_\epsilon\big) &= -\sqrt{\epsilon} u_\epsilon + f_\epsilon, && \text{in } \Omega_\epsilon, \\ -a_\epsilon(x) \nabla u_\epsilon \cdot n_\epsilon &= \epsilon u_\epsilon, && \text{at } \Gamma_\epsilon. \end{aligned}$$

Assume f_ϵ bounded (uniformly w.r.t ϵ) in $L^2(\Omega_\epsilon)$ and let a_ϵ satisfy the assumptions (H1)–(H4).

[4] We need at least $\Gamma \in C^2$.

1. Show the existence and uniqueness of a weak solution u_ϵ to (P_ϵ).
2. Prove that u_ϵ is uniformly bounded in $H^1(\Omega_\epsilon)$.
3. Show that u_ϵ is actually bounded in $H^1(\Omega)$.
4. Pass in (P_ϵ) via two-scale convergence to the limit $\epsilon \to 0$ and determine the weak form of the two-scale limit problem, say (P_0).
5. Prove the uniqueness of the weak solutions to (P_0).
6. Get the strong formulation of (P_0). Eliminate u_1.
7. Use the expansion $u_\epsilon(x) = u_0(x, \frac{x}{\epsilon}) + \epsilon u_1(x, \frac{x}{\epsilon}) + \mathcal{O}(\epsilon^2)$ and pass to the limit $\epsilon \to 0$ in (P_ϵ) via the formal asymptotic homogenization procedure. Compare your result with the answer to (vi).
8. *(Corrector estimate)* Which regularity we need to assume/show for the cell functions so that the following *corrector estimate* holds:

$$\nabla u_\epsilon - \nabla u_0 - \nabla_y u_1\Big(\cdot, \frac{\cdot}{\epsilon}\Big) \to 0 \text{ strongly in } L^2(\Omega)^2.$$

EXERCISE 5.4. Assume the hypothesis of Exercise 5.3, Question 8. Prove *the convergence rate*

$$\|u_\epsilon - u_0\|_{H^1(\Omega_\epsilon)} \leq c\epsilon^{\frac{1}{2}},$$

where the constant $c > 0$ is independent of ϵ.

EXERCISE 5.5. Let Ω be a bounded domain in $\mathbb{R}^2$ with Lipschitz $\partial\Omega$. Take the perforated domain $\Omega_\epsilon \subset \Omega$ to be connected such that the perforations do not touch each other, and that Γ_ϵ is Lipschitz. Additionally, take $\Gamma_\epsilon := \Gamma_\epsilon^D \cup \Gamma_\epsilon^N$, where $\Gamma_\epsilon^D \cap \Gamma_\epsilon^N = \emptyset$ and $meas(\Gamma_\varepsilon^D) \neq 0$. Γ_ε^D is the Dirichlet boundary, while Γ_ε^N is the corresponding Neumann boundary. Consider the following problem, say (P_ϵ),

$$\begin{aligned} -\mathrm{div}\big(a_\epsilon(x)\nabla u_\epsilon\big) &= -u_\epsilon + \epsilon|Y_0|, && \text{in } \Omega_\epsilon, \\ -a_\epsilon(x)\nabla u_\epsilon \cdot n_\epsilon &= \epsilon g_\epsilon, && \text{at } \Gamma_\epsilon^N, \\ u_\epsilon &= 0, && \text{at } \partial\Omega \cup \Gamma_\epsilon^D. \end{aligned}$$

Assume g_ϵ to be bounded (uniformly w.r.t ϵ) in $L^2(\Gamma_\epsilon)$. Additionally, let a_ϵ satisfy the assumptions (H1)–(H4). Note that here $|Y_0|$ denotes the volume of the set (void) $|Y_0|$.

1. Show the existence and uniqueness of a weak solution u_ϵ to (P_ϵ).
2. Prove that u_ϵ is uniformly bounded in $H_0^1(\Omega_\epsilon)$.
3. Show that u_ϵ is actually bounded in $H_0^1(\Omega)$.
4. Pass in (P_ϵ) via two-scale convergence to the limit $\epsilon \to 0$ and determine the weak form of the two-scale limit problem, say (P_0).
5. Prove the uniqueness of the weak solutions to (P_0).
6. Get the strong formulation of (P_0). Eliminate u_1.
7. *(Corrector estimate)* Assume sufficient regularity and prove that

$$\nabla u_\epsilon - \nabla u_0 - \nabla_y u_1\Big(\cdot, \frac{\cdot}{\epsilon}\Big) \to 0 \text{ strongly in } L^2(\Omega)^2.$$

EXERCISE 5.6. (DOUBLE POROSITY SCENARIO) Let Ω be a bounded domain in $\mathbb{R}^2$ with Lipschitz $\partial\Omega$. Take the perforated domain $\Omega_\epsilon \subset \Omega$ to be connected such that the perforations do not touch each other, and assume additionally that Γ_ϵ is Lipschitz. Consider the following problem,

say (P_ϵ),

$$\begin{aligned} -\mathrm{div}\big(a_\epsilon(x)\nabla u_\epsilon\big) + k_\epsilon(x)u_\epsilon &= v_\epsilon, && \text{in } \Omega_\epsilon,\\ -\mathrm{div}(\epsilon^2 b_\epsilon(x)\nabla v_\epsilon) &= u_\epsilon, && \text{in } \Omega_\epsilon,\\ -a_\epsilon(x)\nabla u_\epsilon \cdot n_\epsilon &= \epsilon b_\epsilon(x)\nabla v_\epsilon \cdot n_\epsilon, && \text{at } \Gamma_\epsilon,\\ u_\epsilon = v_\epsilon &= 0, && \text{at } \partial\Omega. \end{aligned}$$

Assume f_ϵ and g_ϵ to be bounded (uniformly w.r.t ϵ) in $L^2(\Omega_\epsilon)$ and, respectively, in $L^2(\Gamma_\epsilon)$. Additionally, let $k_\epsilon \in L^\infty_{\mathrm{per}}(Y)$ and a_ϵ, b_ϵ satisfy the assumptions (H1)–(H4).

1. Show the existence and uniqueness of a weak solution (u_ϵ, v_ϵ) to (P_ϵ).
2. Prove that u_ϵ is uniformly bounded in $H^1_0(\Omega_\epsilon)$. What happens with v_ϵ?
3. Show that u_ϵ is actually bounded in $H^1_0(\Omega)$. What happens with the extension of v_ϵ?
4. Pass in (P_ϵ) via two-scale convergence to the limit $\epsilon \to 0$ and determine the weak form of the two-scale limit problem, say (P_0).
5. Prove the uniqueness of the weak solutions to (P_0).
6. Get the strong formulation of (P_0). Eliminate u_1.

Hints

Hint for Exercise 5.4. Get inspiration from Cioranescu and St. Jean Paulin's book [CS98].

CHAPTER 6

Multiscale approximation

In this chapter, we present a numerical multiscale methodology applied to a real-world problem—the corrosion of concrete with sulfate ions. We motivate the need of using a multiscale approach, state the mathematical problem, and quickly get to the main issue—the numerical solution of a two-scale PDEs-ODE system by a two-scale finite difference method. The contents of this part extends the framework of our paper [**CM11**].

6.1. Multiscale concrete corrosion

Biogenic sulfide corrosion of concrete is a bacterially mediated process of forming hydrogen sulfide gas and the subsequent conversion to sulfuric acid that attacks concrete and steel within wastewater environments. The hydrogen sulfide gas is oxidized in the presence of moisture to form sulfuric acid that attacks the matrix of concrete. The effect of sulfuric acid on concrete and steel surfaces exposed to severe wastewater environments (like sewer pipes) is devastating, and is always associated with high maintenance costs.

The process can be briefly described as follows: Fresh domestic sewage entering a wastewater collection system contains large amounts of sulfates that, in the absence of dissolved oxygen and nitrates, are reduced by bacteria. Such bacteria identified primarily from the anaerobic species Desulfovibrio lead to the fast formation of hydrogen sulfide (H_2S) via a complex pathway of biochemical reactions. Once the gaseous H_2S diffuses into the headspace environment above the wastewater, a sulfur oxidizing bacteria—primarily Thiobacillus aerobic bacteria—metabolizes the H_2S gas and oxidize it to sulphuric acid. It is worth noting that Thiobacillus colonizes on pipe crowns above the waterline inside the sewage system. This oxidizing process prefers to take place where there is sufficiently high local temperature, enough productions of hydrogen sulfide gas, high relative humidity, and atmospheric oxygen; see Section 6.2.2 for more details on the involved chemistry and transport mechanisms. Good overviews of the civil engineering literature on the chemical aggression with acids of cement-based materials (focusing on sulfate ingress) can be found in [**BD05**, **JDM+01**, **MBH09**, **TMA03**].

If we decouple the mechanical corrosion part (leading to cracking and respective spalling of the concrete matrix) from the reaction-diffusion-flow part, and look only to the later one, the mathematical problem reduces to solving a partly dissipative reaction-diffusion system posed in heterogeneous domains. Now, assuming further that the concrete sample is perfectly covered by a locally-periodic repeated regular microstructure, averaged and two-scale reaction-diffusion systems modeling this corrosion processes can be derived; that is precisely what we have done in [**FAZM11**] (formal asymptotics for the locally-periodic case) and [**FM10**] (rigorous asymptotics via two-scale convergence for the periodic case).

Here, our attention focuses on the two-scale corrosion model. Besides performing the averaging procedure and ensuring the well-posedness of the resulting model(s), we are interested in simulating numerically the influence of the microstructural effects on observable (macroscopic) quantities. We refer the reader to [**CFM10**], where we performed numerical simulations of such a two-scale model.

6.2. Background and statement of the mathematical problem

6.2.1. Two-scale geometry. We consider the evolution of a chemical corrosion process (sulfate attack) taking place in one-dimensional macroscopic region $\Omega := (0, L)$, $L > 0$, that represents a concrete sample along a line perpendicular to the pipe surface with $x = 0$ being a point at the inner surface in contact with sewer atmosphere and $x = L$ being a point inside the concrete wall. Since we do not take into account bulging of the inner surface due to the growth of soft gypsum structures, the shape of the domain Ω does not change w.r.t. the time variable t.

We denote the typical microstructure (or standard cell [**Hor97**]) by $Y := (0, \ell)$, $\ell > 0$. Usually cells in concrete contain a stationary water film, and air and solid fractions in different ratios depending on the local porosity. Generally, we expect that, due to the randomness of the pores distribution in concrete, the choice of the microstructure essentially depends on the macroscopic position $x \in \Omega$, i.e., we would then have Y_x; see [**vNM11**] for averaging issues of double porosity media involving locally periodic ways of distributing microstructures, and [**FAZM11**] for more comments directly related to the sulfatation problem where pores are distributed in a locally periodic fashion. In this chapter, we restrict to the case when the medium Ω is made of the *same* microstructure Y periodically repeated to pave perfectly the region. Furthermore, since at the microscopic level the involved reaction and diffusion processes take place in the pore water, we choose to denote by Y only the wet part of the pore. Efficient direct computations (with controlled accuracy and known convergence rates) of scenarios involving Y_x as well as the corresponding error analysis are generally open problems in the field of multiscale numerical simulation.

6.2.2. Chemistry. Sewage is rich in sulphur-containing materials and normally it is without any action on concrete. Under suitable conditions like increased temperature or lower flow velocity oxygen in sewage can become depleted. Aerobic, purifying bacteria become inactive while anaerobic bacteria that live in slime layers at the bottom of the sewer pipe proliferate. They obtain needed oxygen by reducing sulfur compounds. Sulfur reacts with hydrogen and forms hydrogen sulfide (H_2S), which then diffuses in sewage and enters sewer atmosphere. It moves in the air space of the pipe and goes up towards the pipe wall. Gaseous H_2S (further denoted as $H_2S(g)$) enters into the concrete pores (microstructures) via both air and water parts. $H_2S(g)$ diffuses quickly through the air-filled part of the porous structure over macroscopic distances, while it dissolves in the thin, stationary water film of much smaller, microscopic thickness that clings on the surface of the fabric.

There are many chemical reactions taking place in the porous microstructure of sewer pipes which degrade the performance of the pipe structure depending on the intensity of the interaction between the chemical reactions and the local environment. Here we focus our attention on the following few relevant chemical reactions:

$$\mathrm{H_2S(aq)} + 2\mathrm{O_2} \to 2\mathrm{H^+} + \mathrm{SO_4^{2-}} \tag{6.1a}$$

$$10\mathrm{H^+} + \mathrm{SO_4^{-2}} + \text{organic matter} \to \mathrm{H_2S(aq)} + \ 4\mathrm{H_2O}\ + \text{oxidized matter} \tag{6.1b}$$

$$\mathrm{H_2S(aq)} \rightleftharpoons \mathrm{H_2S(g)} \tag{6.1c}$$

$$2\mathrm{H_2O} + \mathrm{H^+} + \mathrm{SO_4^{2-}} + \mathrm{CaCO_3} \to \mathrm{HCO_{3^-}} + \mathrm{CaSO_4 \cdot 2H_2O}. \tag{6.1d}$$

Dissolved hydrogen sulfide (further denoted as $H_2S(aq)$) undergoes oxidation by aerobic bacteria living in these films and sulfuric acid H_2SO_4 is produced (reaction (6.1a)). This aggressive acid reacts with calcium carbonate (i.e., with our concrete sample) and a soft gypsum layer ($CaSO_4 \cdot 2H_2O$) consisting of solid particles (unreacted cement, aggregate), pore air and moisture is formed (reaction (6.1d)).

The model considered in this chapter pays special attention to the following aspects:

(i) exchange of H_2S from water to the air phase and vice versa (reaction (6.1c);
(ii) production of gypsum at micro solid-water interfaces (reaction (6.1d)).

The transfer of H_2S is modeled by means of (deviations from) the Henry's law, while the production of gypsum is incorporated in a non-standard non-linear reaction rate, here denoted as η; see (6.7) for a precise choice. Equation (6.5) indicates the linearity of the Henry's law structure we have in

mind. The standard reference for modeling gas-liquid reactions at stationary interfaces (including a derivation via first principles of the Henry's law) is [**Dan70**].

6.2.3. Setting of the equations. Let $S := (0,T)$ (with $T \in (0,\infty)$) be the time interval during which we consider the process and let Ω and Y as described in Section 6.2.1. We look for the unknown functions (mass concentrations of active chemical species)

$$\begin{aligned}
&u_1 : \Omega \times S \to \mathbb{R} && \text{—concentration of } H_2S(g),\\
&u_2 : \Omega \times Y \times S \to \mathbb{R} && \text{—concentration of } H_2S(aq),\\
&u_3 : \Omega \times Y \times S \to \mathbb{R} && \text{—concentration of } H_2SO_4,\\
&u_4 : \Omega \times S \to \mathbb{R} && \text{—concentration of gypsum,}
\end{aligned}$$

that satisfy the following two-scale system composed of three weakly coupled PDEs and one ODE

$$\left\{\begin{aligned}
\partial_t u_1 - d_1 \partial_{xx} u_1 &= d_2 \partial_y u_2|_{y=0}, && \text{in } \Omega,\\
\partial_t u_2 - d_2 \partial_{yy} u_2 &= -\zeta(u_2, u_3), && \text{in } \Omega \times Y,\\
\partial_t u_3 - d_3 \partial_{yy} u_3 &= \zeta(u_2, u_3), && \text{in } \Omega \times Y,\\
\partial_t u_4 &= \eta(u_3|_{y=\ell}, u_4), && \text{in } \Omega,
\end{aligned}\right. \tag{6.2}$$

together with boundary conditions

$$\begin{aligned}
u_1 &= u_1^D, && \text{on } \{x=0\} \times S,\\
d_1 \partial_x u_1 &= 0, && \text{on } \{x=L\} \times S,\\
-d_2 \partial_y u_2 &= Bi^M (H u_1 - u_2), && \text{on } \Omega \times \{y=0\} \times S,\\
d_2 \partial_y u_2 &= 0, && \text{on } \Omega \times \{y=\ell\} \times S,\\
-d_3 \partial_y u_3 &= 0, && \text{on } \Omega \times \{y=0\} \times S,\\
d_3 \partial_y u_3 &= -\eta(u_3, u_4), && \text{on } \Omega \times \{y=\ell\} \times S,
\end{aligned} \tag{6.3}$$

and initial conditions

$$\begin{aligned}
u_1 &= u_1^0, && \text{on } \Omega \times \{t=0\},\\
u_2 &= u_2^0, && \text{on } \Omega \times Y \times \{t=0\},\\
u_3 &= u_3^0, && \text{on } \Omega \times Y \times \{t=0\},\\
u_4 &= u_4^0, && \text{on } \Omega \times \{t=0\}.
\end{aligned} \tag{6.4}$$

Here, d_k, $k \in \{1,2,3\}$, are the diffusion coefficients, Bi^M is a dimensionless Biot number, H is the Henry's constant, α, β are air-water mass transfer functions, and $\eta(\cdot)$ is a surface chemical reaction. Note that u_i $(i = 1, \dots, 4)$ are mass concentrations. Furthermore, all unknown functions, data and parameters carry dimensions.

Terms like

$$Bi^M \big(H u_1(x,t) - u_2(x, y=0, t)\big), \tag{6.5}$$

which appears on the right-hand side of (6.2), are usually referred to in the mathematical literature as production terms by Henry's or Raoult's law; see [**BJDR98**]. The special feature of the scenario studied in this chapter is that the term (6.5) *bridges* two distinct spatial scales: one macro with $x \in \Omega$ and one micro with $y \in Y$. We call this *micro-macro transmission condition*.

The initial and boundary data, the parameters as well as the involved chemical reaction rate are assumed to satisfy the following requirements:

(A1) $d_k > 0$, $k \in \{1,2,3\}$, $Bi^M > 0$, $H > 0$, $u_1^D > 0$ are constants.

(A2) The function ζ represents the biological oxidation volume reaction between the hydrogen sulfide and sulfuric acid and is defined by

$$\zeta : \mathbb{R}^2 \to \mathbb{R}, \quad \zeta(r,s) := \alpha r - \beta s, \tag{6.6}$$

where $\alpha, \beta \in L^\infty_+(Y)$.

(A3) We assume the reaction rate $\eta : \mathbb{R}^2 \to \mathbb{R}_+$ takes the form

$$\eta(r,s) = \begin{cases} kR(r)Q(s), & \text{for all } r \geq 0, s \geq 0, \\ 0, & \text{otherwise,} \end{cases} \tag{6.7}$$

where $k > 0$ is the corresponding reaction constant. We assume η to be (globally) Lipschitz in both arguments. Furthermore, R is taken to be sublinear (i.e., $R(r) \leq r$ for all $r \in \mathbb{R}$, in the spirit of [**Ber75**]), while Q is bounded from above by a threshold $\bar{c} > 0$. Furthermore, let $R \in W^{1,\infty}(0, M_3)$ and $Q \in W^{1,\infty}(0, M_4)$ be monotone functions (with R strictly increasing), where the constants M_3 and M_4 are the L^∞ bounds on u_3 and, respectively, on u_4. Note that [**CFM10**, Lemma 2] gives the constants M_3, M_4 explicitly.

(A4) $u_1^0 \in H^2(\Omega) \cap L^\infty_+(\Omega)$, $(u_2^0, u_3^0) \in \left[L^2(\Omega; H^1(Y))\right]^2 \times \left[L^\infty_+(\Omega \times Y)\right]^2$, $u_4^0 \in H^1(\Omega) \cap L^\infty_+(\Omega)$.

Furthermore, it is important to note that in the subsequent analysis we can replace (6.5) by a more general nonlinear relationship $\mathcal{B}(u_1, u_2)$. In that case assumption (A2) needs to be replaced, for instance, by

(A2')

$$\mathcal{B} \in C^1([0, M_1] \times [0, M_2]; \mathbb{R}), \quad \mathcal{B} \text{ is globally Lipschitz in both arguments,} \tag{6.8}$$

where M_1 and M_2 are sufficiently large positive constants[1].

Note that a derivation of the precise structure of $\mathcal{B}$ by taking into account (eventually by averaging of) the underlying microstructure information is still an open problem.

6.2.4. Weak formulation. As a next step, we first reformulate our problem (6.2), (6.3), (6.4) in an equivalent formulation that is more suitable for numerical treatment. We introduce the substitution $\tilde{u}_1 := u_1 - u_1^D$ to obtain

$$\begin{aligned} \partial_t \tilde{u}_1 - d_1 \partial_{xx} \tilde{u}_1 &= d_2 \partial_y u_2|_{y=0}, && \text{in } \Omega, \\ \partial_t u_2 - d_2 \partial_{yy} u_2 &= -\zeta(u_2, u_3), && \text{in } \Omega \times Y, \\ \partial_t u_3 - d_3 \partial_{yy} u_3 &= \zeta(u_2, u_3), && \text{in } \Omega \times Y, \\ \partial_t u_4 &= \eta(u_3|_{y=\ell}, u_4), && \text{in } \Omega, \end{aligned} \tag{6.9}$$

together with boundary conditions

$$\begin{aligned} \tilde{u}_1 &= 0, && \text{on } \{x = 0\} \times S, \\ d_1 \partial_x \tilde{u}_1 &= 0, && \text{on } \{x = L\} \times S, \\ -d_2 \partial_y u_2 &= Bi^M \big(H(\tilde{u}_1 + u_1^D) - u_2\big), && \text{on } \Omega \times \{y = 0\} \times S, \\ d_2 \partial_y u_2 &= 0, && \text{on } \Omega \times \{y = \ell\} \times S, \\ -d_3 \partial_y u_3 &= 0, && \text{on } \Omega \times \{y = 0\} \times S, \\ d_3 \partial_y u_3 &= -\eta(u_3, u_4), && \text{on } \Omega \times \{y = \ell\} \times S, \end{aligned} \tag{6.10}$$

[1] Typical choices for M_1, M_2 are the L^∞-estimates on u_1 and u_2; cf. [**CFM10**] (Lemma 2) such M_1, M_2 do exist.

and initial conditions

$$
\begin{aligned}
&\tilde{u}_1 = u_1^0 - u_1^D =: \tilde{u}_1^0, && \text{on } \Omega \times \{t = 0\},\\
&u_2 = u_2^0, && \text{on } \Omega \times Y \times \{t = 0\},\\
&u_3 = u_3^0, && \text{on } \Omega \times Y \times \{t = 0\},\\
&u_4 = u_4^0, && \text{on } \Omega \times \{t = 0\}.
\end{aligned} \tag{6.11}
$$

We refer to the system (6.9), (6.10), (6.11) as problem (P). Also, for the ease of notation, we denote $\tilde{u}_1$ again as u_1 and $\tilde{u}_1^0$ as u_1^0.

Now, we can introduce our concept of weak solution.

Definition 1 (Concept of weak solution). The vector of functions (u_1, u_2, u_3, u_4) with

$$u_1 \in L^2(S, H_0^1(\Omega)), \tag{6.12}$$

$$\partial_t u_1 \in L^2(S \times \Omega), \tag{6.13}$$

$$u_i \in L^2(S, L^2(\Omega, H^1(Y))), \qquad i \in \{2, 3\}, \tag{6.14}$$

$$\partial_t u_i \in L^2(S \times \Omega \times Y), \qquad i \in \{2, 3\}, \tag{6.15}$$

$$u_4(\cdot, x, y) \in H^1(S), \qquad \text{for a.e. } (x, y) \in \Omega \times Y, \tag{6.16}$$

is called *a weak solution* to problem (P) if the identities

$$
\begin{aligned}
\int_\Omega \partial_t u_1 \varphi_1 + d_1 \int_\Omega \partial_x u_1 \partial_x \varphi_1 &= \int_\Omega \partial_y u_2|_{y=0} \varphi_1,\\
\int_\Omega \int_Y \partial_t u_2 \varphi_2 + d_2 \int_\Omega \int_Y \partial_y u_2 \partial_y \varphi_2 &= -\int_\Omega \int_Y \zeta(u_2, u_3)\varphi_2 - \int_\Omega \partial_y u_2|_{y=0} \varphi_2,\\
\int_\Omega \int_Y \partial_t u_3 \varphi_3 + d_3 \int_\Omega \int_Y \partial_y u_3 \partial_y \varphi_3 &= \int_\Omega \int_Y \zeta(u_2, u_3)\varphi_3 - \int_\Omega \eta(u_3|_{y=\ell}, u_4)\varphi_3,
\end{aligned}
$$

and

$$\partial_t u_4 = \eta(u_3|_{y=\ell}, u_4),$$

hold for a.e. $t \in S$ and for all $\varphi := (\varphi_1, \varphi_2, \varphi_3) \in H_0^1(\Omega) \times \left[L^2(\Omega; H^1(Y))\right]^2$.

We refer the reader to [**CFM10**, Theorem 3] for statements regarding the global existence and uniqueness of such weak solutions to problem (P); see also [**MNR10**] for the analysis on a closely related problem.

6.3. Numerical scheme

In order to solve numerically our multiscale system (6.2)–(6.4), we use a semi-discrete approach leaving the time variable continuous and discretizing both space variables x and y by finite differences on rectangular grids. In the following paragraphs we introduce the necessary notation, the scheme and discrete scalar products and norms.

6.3.1. Grids and grid functions. For spatial discretization, we subdivide the domain Ω into N_x equidistant subintervals, the domain Y into N_y equidistant subintervals and we denote by $h_x := L/N_x$, $h_y := \ell/N_y$, the corresponding spatial step sizes. We denote by h the vector (h_x, h_y) with length $|h|$.

Let

$$\begin{aligned}
\Omega_h &:= \{x_i := ih_x \mid i = 0, \dots, N_x\},\\
\Omega_h^o &:= \{x_i \mid i = 1, \dots, N_x\},\\
Y_h &:= \{y_j := jh_y \mid i = 0, \dots, N_y\},\\
\Omega_h^e &:= \{x_{i+1/2} := (i+1/2)h_x \mid i = 0, \dots, N_x - 1\},\\
Y_h^e &:= \{y_{j+1/2} := (j+1/2)h_y \mid i = 0, \dots, N_y - 1\},
\end{aligned}$$

be, respectively, grid of all nodes in Ω, grid of nodes in Ω without the node at $x = 0$ (where Dirichlet boundary condition is imposed), grid of all nodes in Y, grid of nodes located in the middle of subintervals of Ω_h, and grid of nodes located in the middle of subintervals of Y_h. Finally, we define grids $\omega_h := \Omega_h \times Y_h$ and $\omega_h^e := \Omega_h \times Y_h^e$.

Next, we introduce grid functions defined on the grids just described. Let $\mathcal{G}_h := \{u_h \mid u_h : \Omega_h \to \mathbb{R}\}$, $\mathcal{G}_h^o := \{u_h \mid u_h : \Omega_h^o \to \mathbb{R}\}$ and $\mathcal{E}_h := \{\mathrm{v}_h | \mathrm{v}_h : \Omega_h^e \to \mathbb{R}\}$ be sets of grid functions approximating macro variables on Ω. Let $\mathcal{F}_h := \{u_h \mid u_h : \omega_h \to \mathbb{R}\}$ and $\mathcal{H}_h := \{\mathrm{v}_h \mid \mathrm{v}_h : \omega_h^e \to \mathbb{R}\}$ be sets of grid functions approximating micro variables on $\Omega \times Y$. These grid functions can be identified with vectors in $\mathbb{R}^N$, whose elements are the values of the grid function at the nodes of the respective grid. Hence, addition of functions and multiplication of a function by a scalar are defined as for vectors.

For $u_h \in \mathcal{G}_h$ we denote $u_i := u_h(x_i)$, and for $u_h \in \mathcal{F}_h$ we denote $u_{ij} := u_h(x_i, y_j)$. For $\mathrm{v}_h \in \mathcal{E}_h$ we denote $\mathrm{v}_{i+1/2} := \mathrm{v}_h(x_{i+1/2})$, and for $\mathrm{v}_h \in \mathcal{H}_h$ we denote $\mathrm{v}_{i,j+1/2} := \mathrm{v}_h(x_i, y_{j+1/2})$.

We frequently use functions from $\mathcal{F}_h$ restricted to the sets $\Omega_h \times \{y = 0\}$ or $\Omega_h \times \{y = \ell\}$. For $u_h \in \mathcal{F}_h$, we denote these restrictions as $u_h|_{y=0}$ and $u_h|_{y=\ell}$, and we interpret them as functions from $\mathcal{G}_h$, i.e., $u_h|_{y=0} \in \mathcal{G}_h$ and $u_h|_{y=\ell} \in \mathcal{G}_h$.

6.3.2. Discrete operators. In this section, we define difference operators defined on linear spaces of grid functions in such a way they mimic properties of the corresponding differential operators and, together with the scalar products defined in Section 6.3.4, fulfill similar integral identities.

The discrete gradient operators ∇_h and ∇_{yh} are defined as

$$\begin{aligned}
\nabla_h &: \mathcal{G}_h \to \mathcal{E}_h, & (\nabla_h u_h)_{i+\frac{1}{2}} &:= \frac{u_{i+1} - u_i}{h_x}, \quad u_h \in \mathcal{G}_h,\\
\nabla_{yh} &: \mathcal{F}_h \to \mathcal{H}_h, & (\nabla_{yh} u_h)_{i,j+\frac{1}{2}} &:= \frac{u_{i,j+1} - u_{ij}}{h_y}, \quad u_h \in \mathcal{F}_h,
\end{aligned}$$

while the discrete divergence operators div_h and div_{yh} is

$$\begin{aligned}
\mathrm{div}_h &: \mathcal{E}_h \to \mathcal{G}_h^o, & (\mathrm{div}_h\, \mathrm{v}_h)_i &:= \frac{\mathrm{v}_{i+\frac{1}{2}} - \mathrm{v}_{i-\frac{1}{2}}}{h_x}, \quad \mathrm{v}_h \in \mathcal{E}_h,\\
\mathrm{div}_{yh} &: \mathcal{H}_h \to \mathcal{F}_h, & (\mathrm{div}_{yh}\, \mathrm{v}_h)_{ij} &:= \frac{\mathrm{v}_{i,j+\frac{1}{2}} - \mathrm{v}_{i,j-\frac{1}{2}}}{h_y}, \quad \mathrm{v}_h \in \mathcal{H}_h.
\end{aligned}$$

The discrete Laplacian operators Δ_h and Δ_{yh} are defined as $\Delta_h := \mathrm{div}_h \nabla_h : \mathcal{G}_h \to \mathcal{G}_h^o$ and $\Delta_{yh} := \mathrm{div}_{yh} \nabla_{yh} : \mathcal{F}_h \to \mathcal{F}_h$, i.e., the following standard 3-point stencils are obtained:

$$\begin{aligned}
(\Delta_h u_h)_i &= \frac{u_{i-1} - 2u_i + u_{i+1}}{h_x^2}, \qquad u_h \in \mathcal{G}_h,\\
(\Delta_{yh} u_h)_{ij} &= \frac{u_{i,j-1} - 2u_{ij} + u_{i,j+1}}{h_y^2}, \qquad u_h \in \mathcal{F}_h.
\end{aligned}$$

To complete the definition of the discrete divergence and Laplacian operators, we need to specify values of grid functions on auxiliary nodes that fall outside their corresponding grid. At a later point, we obtain these values from the discretization of boundary conditions by centered differences.

6.3.3. Semi-discrete scheme. We can now construct a semi-discrete scheme for problem (6.2). Note that we omit the explicit dependence on t and we interchangeably use the notation $\frac{\mathrm{d}u_h}{\mathrm{d}t}$ and $\dot{u}_h$ for denoting the derivative of u_h with respect to t.

DEFINITION 2. A quadruple $\{u_h^1, u_h^2, u_h^3, u_h^4\}$ with

$$u_h^1, u_h^4 \in C^1([0,T]; \mathcal{G}_h) \text{ and } u_h^2, u_h^3 \in C^1([0,T]; \mathcal{F}_h)$$

is called semi-discrete solution of (6.2), if it satisfies the following system of ordinary differential equations

$$\frac{\mathrm{d}u_h^1}{\mathrm{d}t} = d_1 \Delta_h u_h^1 - Bi^M \big(H(u_h^1 + u_1^D) - u_h^2|_{y=0}\big), \qquad \text{on } \Omega_h^o, \tag{6.17a}$$

$$\frac{\mathrm{d}u_h^2}{\mathrm{d}t} = d_2 \Delta_{yh} u_h^2 - \zeta(u_h^2, u_h^3), \qquad \text{on } \omega_h, \tag{6.17b}$$

$$\frac{\mathrm{d}u_h^3}{\mathrm{d}t} = d_3 \Delta_{yh} u_h^3 + \zeta(u_h^2, u_h^3), \qquad \text{on } \omega_h, \tag{6.17c}$$

$$\frac{\mathrm{d}u_h^4}{\mathrm{d}t} = \eta(u_h^3|_{y=\ell}, u_h^4), \qquad \text{on } \Omega_h, \tag{6.17d}$$

together with the discrete boundary conditions ($i = 0, \dots, N_x$)

$$u_0^1 = 0, \tag{6.18a}$$

$$d_1 \frac{1}{2}\Big((\nabla_h u_h^1)_{N_x+\frac{1}{2}} + (\nabla_h u_h^1)_{N_x-\frac{1}{2}}\Big) = 0, \tag{6.18b}$$

$$-d_2 \frac{1}{2}\Big((\nabla_{yh} u_h^2)_{i,-\frac{1}{2}} + (\nabla_{yh} u_h^2)_{i,\frac{1}{2}}\Big) = Bi^M \big(H(u_i^1 + u_1^D) - u_{i,0}^2\big), \tag{6.18c}$$

$$d_2 \frac{1}{2}\Big((\nabla_{yh} u_h^2)_{i,N_y+\frac{1}{2}} + (\nabla_{yh} u_h^2)_{i,N_y-\frac{1}{2}}\Big) = 0, \tag{6.18d}$$

$$-d_3 \frac{1}{2}\Big((\nabla_{yh} u_h^3)_{i,-\frac{1}{2}} + (\nabla_{yh} u_h^3)_{i,\frac{1}{2}}\Big) = 0, \tag{6.18e}$$

$$d_3 \frac{1}{2}\Big((\nabla_{yh} u_h^3)_{i,N_y+\frac{1}{2}} + (\nabla_{yh} u_h^3)_{i,N_y-\frac{1}{2}}\Big) = -\eta(u_{i,N_y}^3, u_i^4), \tag{6.18f}$$

and the initial conditions

$$\begin{aligned} u_h^1(0) &= \mathcal{P}_h^1 u_1^0, \quad u_h^2(0) = \mathcal{P}_h^2 u_2^0, \\ u_h^3(0) &= \mathcal{P}_h^2 u_3^0, \quad u_h^4(0) = \mathcal{P}_h^1 u_4^0, \end{aligned} \tag{6.19}$$

where $\mathcal{P}_h^1$ and $\mathcal{P}_h^2$ are suitable projection operators from Ω to Ω_h and from $\Omega \times Y$ to ω_h, respectively.

PROPOSITION 3. *Assume (A1)–(A4) to be fulfilled. Then there exists a unique semi-discrete solution*

$$\{u_h^1, u_h^2, u_h^3, u_h^4\} \in C^1([0,T]; \mathcal{G}_h) \times C^1([0,T]; \mathcal{F}_h) \times C^1([0,T]; \mathcal{G}_h) \times C^1([0,T]; \mathcal{F}_h)$$

in the sense of Definition 2.

PROOF. The proof, based on the standard ode argument, follows in a straightforward manner. □

6.3.4. Discrete scalar products and norms. Next, we introduce scalar products and norms on the spaces of grid functions $\mathcal{G}_h$, $\mathcal{E}_h$, $\mathcal{F}_h$, $\mathcal{G}_h$ and we show some basic integral identities for the difference operators.

Let $(\gamma_i^1)_{i=0}^{N_x}$ and $(\gamma_j^2)_{j=0}^{N_y}$ be such that

$$\gamma_i^1 := \begin{cases} 1 & 1 \le i \le N_x - 1, \\ \frac{1}{2} & i \in \{0, N_x\}, \end{cases}, \qquad \gamma_j^2 := \begin{cases} 1 & 1 \le j \le N_y - 1, \\ \frac{1}{2} & j \in \{0, N_y\}, \end{cases} \tag{6.20}$$

and define the following discrete L^2 scalar products and the corresponding discrete L^2 norms

$$(u_h, v_h)_{\mathcal{G}_h} := h_x \sum_{x_i \in \Omega_h} \gamma_i^1 u_i v_i, \qquad u_h, v_h \in \mathcal{G}_h, \tag{6.21}$$

$$\|u_h\|_{\mathcal{G}_h} := \sqrt{(u_h, u_h)_{\mathcal{G}_h}}, \qquad u_h \in \mathcal{G}_h, \tag{6.22}$$

$$(u_h, v_h)_{\mathcal{G}_h^o} := h_x \sum_{x_i \in \Omega_h^o} \gamma_i^1 u_i v_i, \qquad u_h, v_h \in \mathcal{G}_h^o, \tag{6.23}$$

$$\|u_h\|_{\mathcal{G}_h^o} := \sqrt{(u_h, u_h)_{\mathcal{G}_h^o}}, \qquad u_h \in \mathcal{G}_h^o, \tag{6.24}$$

$$(u_h, v_h)_{\mathcal{F}_h} := h_x h_y \sum_{x_{ij} \in \omega_h} \gamma_i^1 \gamma_j^2 u_{ij} v_{ij}, \qquad u_h, v_h \in \mathcal{F}_h, \tag{6.25}$$

$$\|u_h\|_{\mathcal{F}_h} := \sqrt{(u_h, u_h)_{\mathcal{F}_h}}, \qquad u_h \in \mathcal{F}_h, \tag{6.26}$$

$$(\mathrm{u}_h, \mathrm{v}_h)_{\mathcal{E}_h} := h_x \sum_{x_{i+1/2} \in \Omega_h^e} \mathrm{u}_{i+1/2} \mathrm{v}_{i+1/2}, \qquad \mathrm{u}_h, \mathrm{v}_h \in \mathcal{E}_h, \tag{6.27}$$

$$\|\mathrm{u}_h\|_{\mathcal{E}_h} := \sqrt{(\mathrm{u}_h, \mathrm{u}_h)_{\mathcal{E}_h}}, \qquad \mathrm{u}_h \in \mathcal{E}_h, \tag{6.28}$$

$$(\mathrm{u}_h, \mathrm{v}_h)_{\mathcal{H}_h} := h_x h_y \sum_{x_{i,j+1/2} \in \omega_h^e} \gamma_i^1 \mathrm{u}_{i,j+1/2} \mathrm{v}_{i,j+1/2}, \qquad \mathrm{u}_h, \mathrm{v}_h \in \mathcal{H}_h, \tag{6.29}$$

$$\|\mathrm{u}_h\|_{\mathcal{H}_h} := \sqrt{(\mathrm{u}_h, \mathrm{u}_h)_{\mathcal{H}_h}}, \qquad \mathrm{u}_h \in \mathcal{H}_h. \tag{6.30}$$

It can be shown that a discrete equivalent of Green's formula holds for these scalar products as well as other identities as is stated in the following lemmas.

LEMMA 4 (Discrete macro Green-like formula). *Let $u_h \in \mathcal{G}_h$ and $\mathrm{v}_h \in \mathcal{E}_h$ such that*

$$u_0 = 0, \quad u_{N_x+1} = u_{N_x-1}, \tag{6.31}$$

$$\mathrm{v}_{N_x+1/2} = -\mathrm{v}_{N_x-1/2}. \tag{6.32}$$

Then the following identity holds:

$$(u_h, \operatorname{div}_h \mathrm{v}_h)_{\mathcal{G}_h^o} = -(\nabla_h u_h, \mathrm{v}_h)_{\mathcal{E}_h}. \tag{6.33}$$

PROOF. Let us define $\varphi_h^k \in \mathcal{G}_h$ as $\varphi_h^k(x_i) = 1$ for $k = i$, and $\varphi_h^k(x_i) = 0$ otherwise. Then, for $u_h \in \mathcal{G}_h$, $u_h = \sum_{x_i \in \Omega_h} u_i \varphi_h^i$. Note that for $i = 0, \ldots, N_x - 1$,

$$(\nabla_h \varphi_h^k)_{i+1/2} = \begin{cases} h_x^{-1}, & i = k-1, \\ -h_x^{-1}, & i = k, \\ 0, & \text{otherwise.} \end{cases}$$

Then, using the assumptions on u_h and v_h, for $k = 1, \ldots, N_x - 1$ we have

$$(\nabla_h \varphi_h^k, \mathrm{v}_h)_{\mathcal{E}_h} = h_x \left(\frac{\mathrm{v}_{k-1/2}}{h_x} - \frac{\mathrm{v}_{k+1/2}}{h_x} \right) = -h_x \frac{\mathrm{v}_{k+1/2} - \mathrm{v}_{k-1/2}}{h_x} = \\ - h_x (\operatorname{div}_h \mathrm{v}_h)_k = -h_x \gamma_k^1 \varphi_h^k(x_k) (\operatorname{div}_h \mathrm{v}_h)_k = -(\varphi_h^k, \operatorname{div}_h \mathrm{v}_h)_{\mathcal{G}_h},$$

for $k = 0$ we have

$$(\nabla_h \varphi_h^0, \mathrm{v}_h)_{\mathcal{E}_h} = -\mathrm{v}_{1/2},$$

and for $k = N_x$ we have

$$(\nabla_h \varphi_h^{N_x}, \mathrm{v}_h)_{\mathcal{E}_h} = h_x \frac{\mathrm{v}_{N_x-1/2}}{h_x} = \frac{h_x}{2}\frac{\mathrm{v}_{N_x-1/2}+\mathrm{v}_{N_x-1/2}}{h_x} =$$
$$-\frac{h_x}{2}\frac{\mathrm{v}_{N_x+1/2}-\mathrm{v}_{N_x-1/2}}{h_x} = -\frac{h_x}{2}(\mathrm{div}_h\,\mathrm{v}_h)_{N_x} = -h_x\gamma^1_{N_x}\varphi_h^{N_x}(x_{N_x})(\mathrm{div}_h\,\mathrm{v}_h)_{N_x} =$$
$$-(\varphi_h^{N_x}, \mathrm{div}_h\,\mathrm{v}_h)_{\mathcal{G}_h}.$$

Hence we obtain

$$(\nabla_h u_h, \mathrm{v}_h)_{\mathcal{E}_h} = \sum_{x_k\in\Omega_h} u_k(\nabla_h\varphi_h^k, \mathrm{v}_h)_{\mathcal{E}_h} = u_0(\nabla_h\varphi_h^0, \mathrm{v}_h)_{\mathcal{E}_h} + \sum_{k=1}^{N_x-1} u_k(\nabla_h\varphi_h^k, \mathrm{v}_h)_{\mathcal{E}_h}$$
$$+ u_{N_x}(\nabla_h\varphi_h^{N_x}, \mathrm{v}_h)_{\mathcal{E}_h} = -\sum_{k=0}^{N_x} u_k(\varphi_h^k, \mathrm{div}_h\,\mathrm{v}_h)_{\mathcal{G}_h} = -(u_h, \mathrm{div}_h\,\mathrm{v}_h)_{\mathcal{G}_h},$$

which proves (6.33). □

LEMMA 5 (Discrete micro-macro Green-like formula). *Let $u_h \in \mathcal{F}_h$ and $\mathrm{v}_h \in \mathcal{H}_h$ such that*

$$-\frac{1}{2}\left(\mathrm{v}_{k,-1/2}+\mathrm{v}_{k,1/2}\right) = \delta^1_k, \quad \frac{1}{2}\left(\mathrm{v}_{k,N_y-1/2}+\mathrm{v}_{k,N_y+1/2}\right) = \delta^2_k, \tag{6.34}$$

$$u_{k,-1} = u_{k,1} + 2h_y\delta^1_k, \qquad u_{k,N_y+1} = u_{k,N_y-1} + 2h_y\delta^2_k, \tag{6.35}$$

for $i = 0,\dots,N_x$, and $\delta^1_h, \delta^2_h \in \mathcal{G}_h$. Then the following identity holds:

$$(u_h, \mathrm{div}_{yh}\,\mathrm{v}_h)_{\mathcal{F}_h} = -(\nabla_{yh}u_h, \mathrm{v}_h)_{\mathcal{H}_h} + (u_h|_{y=0}, \delta^1_h)_{\mathcal{G}_h} + (u_h|_{y=N_y}, \delta^2_h)_{\mathcal{G}_h}. \tag{6.36}$$

PROOF. Similarly to the proof of the previous Lemma, let us define $\varphi_h^{kl} \in \mathcal{F}_h$ as $\varphi_h^{kl}(x_{ij}) = 1$ if $(k,l) = (i,j)$, and $\varphi_h^{kl}(x_{ij}) = 0$ otherwise. Then, for $u_h \in \mathcal{F}_h$, $u_h = \sum_{x_{ij}\in\omega_h} u_{ij}\varphi_h^{ij}$. Note that for $i = 0,\dots,N_x$, $j = 0,\dots,N_y-1$,

$$(\nabla_{yh}\varphi_h^{kl})_{i,j+1/2} = \begin{cases} h_y^{-1}, & j = l-1,\\ -h_y^{-1}, & j = l,\\ 0, & \text{otherwise.}\end{cases}$$

Using the assumptions on v_h, for $k = 0,\dots,N_x$, $l = 1,\dots,N_y-1$, we then have

$$(\nabla_{yh}\varphi_h^{kl}, \mathrm{v}_h)_{\mathcal{H}_h} = h_xh_y\gamma^1_k\left(\frac{\mathrm{v}_{k,l-1/2}}{h_y} - \frac{\mathrm{v}_{k,l+1/2}}{h_y}\right) = -h_xh_y\gamma^1_k\frac{\mathrm{v}_{k,l+1/2}-\mathrm{v}_{k,l-1/2}}{h_y} =$$
$$-h_xh_y\gamma^1_k(\mathrm{div}_{yh}\,\mathrm{v}_h)_{kl} = -h_xh_y\gamma^1_k\gamma^2_l\varphi_h^{kl}(x_{kl})(\mathrm{div}_{yh}\,\mathrm{v}_h)_{kl} = -(\varphi_h^{kl}, \mathrm{div}_{yh}\,\mathrm{v}_h)_{Fh};$$

for $l = 0$ we have

$$(\nabla_{yh}\varphi_h^{k,0}, \mathrm{v}_h)_{\mathcal{H}_h} = -h_xh_y\gamma^1_k\frac{\mathrm{v}_{k,1/2}}{h_y} = -h_xh_y\gamma^1_k\frac{1}{2}\frac{\mathrm{v}_{k,1/2}+\mathrm{v}_{k,1/2}}{h_y} =$$
$$= -h_xh_y\gamma^1_k\frac{1}{2}\frac{\mathrm{v}_{k,1/2}-\mathrm{v}_{k,-1/2}-2\delta^1_k}{h_y} = -h_xh_y\gamma^1_k\frac{1}{2}\frac{\mathrm{v}_{k,1/2}-\mathrm{v}_{k,-1/2}}{h_y} + h_x\gamma^1_k\delta^1_k =$$
$$-h_xh_y\gamma^1_k\gamma^2_l\varphi_h^{k,0}(x_{k,0})(\mathrm{div}_{yh}\,\mathrm{v}_h)_{k,0} + h_x\gamma^1_k\varphi_h^{k,0}(x_{k,0})\delta^1_k =$$
$$-(\varphi_h^{k,0}, \mathrm{div}_{yh}\,\mathrm{v}_h)_{\mathcal{F}_h} + (\varphi_h^{k,0}|_{y=0}, \delta^1_h)_{\mathcal{G}_h}.$$

Similarly, we can show that for $l = N_y$

$$(\nabla_{yh}\varphi_h^{k,N_y}, \mathrm{v}_h)_{\mathcal{H}_h} = -(\varphi_h^{k,N_y}, \mathrm{div}_{yh}\,\mathrm{v}_h)_{\mathcal{F}_h} + (\varphi_h^{k,N_y}|_{y=\ell}, \delta^2_h)_{\mathcal{G}_h}.$$

Hence we obtain

$$(\nabla_{yh}u_h, \mathrm{v}_h)_{\mathcal{H}_h} = \sum_{x_{kl}\in\omega_h} u_k(\nabla_{yh}\varphi_h^{kl}, \mathrm{v}_h)_{\mathcal{H}_h} = \sum_{k=0}^{N_x} u_{k,0}(\nabla_{yh}\varphi_h^{k,0}, \mathrm{v}_h)_{\mathcal{H}_h}$$
$$+ \sum_{k=0}^{N_x}\sum_{l=1}^{N_y-1} u_{kl}(\nabla_{yh}\varphi_h^{kl}, \mathrm{v}_h)_{\mathcal{H}_h} + \sum_{k=0}^{N_x} u_{k,N_y}(\nabla_{yh}\varphi_h^{k,N_y}, \mathrm{v}_h)_{\mathcal{H}_h} =$$
$$- \sum_{x_{kl}\in\omega_h} u_{kl}(\varphi_h^{kl}, \mathrm{div}_{yh}\,\mathrm{v}_h)_{\mathcal{F}_h} + \sum_{k=0}^{N_x} u_{k,0}(\varphi_h^{k,0}|_{y=0}, \delta_h^1)_{\mathcal{G}_h} + \sum_{k=0}^{N_x} u_{k,N_y}(\varphi_h^{k,N_y}|_{y=\ell}, \delta_h^2)_{\mathcal{G}_h} =$$
$$- (u_h, \mathrm{div}_{yh}\,\mathrm{v}_h)_{\mathcal{F}_h} + (u_h|_{y=0}, \delta_h^1)_{\mathcal{G}_h} + (u_h|_{y=\ell}, \delta_h^2)_{\mathcal{G}_h},$$

which proves (6.36). □

We also frequently make use of the following discrete trace inequality:

LEMMA 6 (Discrete trace inequality). *For $u_h \in \mathcal{F}_h$ there exists a positive constant C depending only on Ω such that*

$$\|u_h|_{y=\ell}\|_{\mathcal{G}_h} \le C(\|u_h\|_{\mathcal{F}_h} + \|\nabla_{yh}u_h\|_{\mathcal{H}_h}). \tag{6.37}$$

PROOF. Our proof follows the line of thought of [**GHV00**]. We have that for $u_h \in \mathcal{F}_h$

$$|u_{i,N_y}| \le \sum_{j=0}^{N_y-1} |u_{i,j+1} - u_{ij}| + \sum_{j=0}^{N_y} \gamma_j^2 h_y |u_{ij}|.$$

Squaring both sides of the inequality, we get

$$(u_{i,N_y})^2 \le A_i + B_i, \tag{6.38}$$

where

$$A_i := 2\left(\sum_{j=0}^{N_y-1} |u_{i,j+1} - u_{ij}|\right)^2 \quad \text{and } B_i := 2\left(\sum_{j=0}^{N_y} \gamma_j^2 h_y |u_{ij}|\right)^2.$$

Applying the Cauchy-Schwarz inequality to A_i, we obtain

$$A_i \le 2\sum_{j=0}^{N_y-1} h_y \left(\frac{u_{i,j+1} - u_{ij}}{h_y}\right)^2 \sum_{j=0}^{N_y-1} h_y = 2\ell \sum_{j=0}^{N_y-1} h_y \left(\frac{u_{i,j+1} - u_{ij}}{h_y}\right)^2.$$

Similarly, using the Cauchy-Schwarz inequality we get for B_i

$$B_i \le 2\sum_{j=0}^{N_y} \gamma_j^2 h_y (u_{ij})^2 \sum_{j=0}^{N_y} \gamma_j^2 h_y = 2\ell \sum_{j=0}^{N_y} \gamma_j^2 h_y (u_{ij})^2.$$

Multiplying (6.38) by $\gamma_i^1 h_x$, summing over $i \in \{0, \dots, N_x\}$ and then using the bounds on A_i and B_i, it yields that:

$$\sum_{i=0}^{N_x} \gamma_i^1 h_x (u_{i,N_y})^2 \le 2\ell\left(\sum_{i=0}^{N_x}\sum_{j=0}^{N_y-1} \gamma_i^1 h_x h_y \left((\nabla_{yh}u_h)_{i,j+\frac{1}{2}}\right)^2 + \sum_{x_{ij}\in\omega_h} \gamma_i^1\gamma_j^2 h_x h_y (u_{ij})^2\right),$$

that is

$$\|u_h|_{y=\ell}\|_{\mathcal{G}_h}^2 \le C\left(\|\nabla_{yh}u_h\|_{\mathcal{H}_h}^2 + \|u_h\|_{\mathcal{F}_h}^2\right),$$

from which the claim of the Lemma follows directly. □

6.4. Approximation estimates

The aim of this section is to derive *a priori* estimates on the semi-discrete solution. Based on weak convergence-type arguments, the estimates ensure, at least up to subsequences, a (weakly) convergent way to reconstruct the weak solution to problem (P).

6.4.1. A priori estimates. This is the place where we use the tools developed in Section 6.3. In subsequent paragraphs, we refer to the following relations: From scalar product of (6.17a) with $\varphi_h^1 \in \mathcal{G}_h$, (6.17b) and (6.17c) with $\varphi_h^2 \in \mathcal{F}_h$ and φ_h^3, respectively, and (6.17d) with $\varphi_h^4 \in \mathcal{G}_h$ to obtain

$$(\dot{u}_h^1, \varphi_h^1)_{\mathcal{G}_h^o} = d_1(\Delta_h u_h^1, \varphi_h^1)_{\mathcal{G}_h^o} - Bi^M\big(Hu_h^1 - u_h^2|_{y=0}, \varphi_h^1\big)_{\mathcal{G}_h^o}, \tag{6.39}$$

$$(\dot{u}_h^2, \varphi_h^2)_{\mathcal{F}_h} = d_2(\Delta_{yh} u_h^2, \varphi_h^2)_{\mathcal{F}_h} - \alpha(u_h^2, \varphi_h^2)_{\mathcal{F}_h} + \beta(u_h^3, \varphi_h^2)_{\mathcal{F}_h}, \tag{6.40}$$

$$(\dot{u}_h^3, \varphi_h^3)_{\mathcal{F}_h} = d_3(\Delta_{yh} u_h^3, \varphi_h^3)_{\mathcal{F}_h} + \alpha(u_h^2, \varphi_h^3)_{\mathcal{F}_h} - \beta(u_h^3, \varphi_h^3)_{\mathcal{F}_h}, \tag{6.41}$$

$$(\dot{u}_h^4, \varphi_h^4)_{\mathcal{G}_h} = \big(\eta(u_h^3|_{y=\ell}, u_h^4), \varphi_h^4\big)_{\mathcal{G}_h}. \tag{6.42}$$

Note that u_h^1 and $\nabla_h \varphi_h^1$ satisfy the assumptions of Lemma 4, u_h^2 and $\nabla_{yh}\varphi_h^2$ satisfy the assumptions of Lemma 5 with $\delta_k^1 = \frac{Bi^M}{d_2}(Hu_k^1 - u_{k,0}^2)$ and $\delta_k^2 = 0$, and u_h^3 and $\nabla_{yh}\varphi_h^3$ with $\delta_k^1 = 0$ and $\delta_k^2 = -\frac{1}{d_3}\eta(u_{k,N_y}^3, u_k^4)$. Thus, using Lemmas 4, 5 and properties of the discrete scalar products we get

$$(\dot{u}_h^1, \varphi_h^1)_{\mathcal{G}_h} + d_1(\nabla_h u_h^1, \nabla_h \varphi_h^1)_{\mathcal{E}_h} = -Bi^M\big(Hu_h^1 - u_h^2|_{y=0}, \varphi_h^1\big)_{\mathcal{G}_h}, \tag{6.43}$$

$$\begin{aligned}(\dot{u}_h^2, \varphi_h^2)_{\mathcal{F}_h} + d_2(\nabla_{yh} u_h^2, \nabla_{yh}\varphi_h^2)_{\mathcal{H}_h} &= Bi^M(Hu_h^1 - u_h^2|_{y=0}, \varphi_h^2|_{y=0})_{\mathcal{G}_h} \\ &\quad - \alpha(u_h^2, \varphi_h^2)_{\mathcal{F}_h} + \beta(u_h^3, \varphi_h^2)_{\mathcal{F}_h},\end{aligned} \tag{6.44}$$

$$\begin{aligned}(\dot{u}_h^3, \varphi_h^3)_{\mathcal{F}_h} + d_3(\nabla_{yh} u_h^3, \nabla_{yh}\varphi_h^3)_{\mathcal{H}_h} &= -\big(\eta(u_h^3|_{y=\ell}, u_h^4), \varphi_h^3|_{y=\ell}\big)_{\mathcal{G}_h} \\ &\quad + \alpha(u_h^2, \varphi_h^3)_{\mathcal{F}_h} - \beta(u_h^3, \varphi_h^3)_{\mathcal{F}_h},\end{aligned} \tag{6.45}$$

$$(\dot{u}_h^4, \varphi_h^4)_{\mathcal{G}_h} = \big(\eta(u_h^3|_{y=\ell}, u_h^4), \varphi_h^4\big)_{\mathcal{G}_h}. \tag{6.46}$$

Lemma 7 (Discrete energy estimates). *Let $\{u_h^1, u_h^2, u_h^3, u_h^4\}$ be a semi-discrete solution of (6.2) for some $T > 0$. Then it holds that*

$$\max_{t\in S}\Big(\|u_h^1(t)\|_{\mathcal{G}_h}^2 + \|u_h^2(t)\|_{\mathcal{F}_h}^2 + \|u_h^3(t)\|_{\mathcal{F}_h}^2 + \|u_h^4(t)\|_{\mathcal{G}_h}^2\Big) \le C, \tag{6.47}$$

$$\int_0^T \Big(\|\nabla_h u_h^1\|_{\mathcal{E}_h}^2 + \|\nabla_{yh} u_h^2\|_{\mathcal{H}_h}^2 + \|\nabla_{yh} u_h^3\|_{\mathcal{H}_h}^2\Big)\mathrm{d}t \le C, \tag{6.48}$$

where $C := \bar{C}\Big(\|u_h^1(0)\|_{\mathcal{G}_h}^2 + \|u_h^2(0)\|_{\mathcal{F}_h}^2 + \|u_h^3(0)\|_{\mathcal{F}_h}^2 + \|u_h^4(0)\|_{\mathcal{G}_h}^2\Big)$, with $\bar{C}$ being a positive constant independent of h_x, h_y.

Proof. In (6.43)–(6.46), taking $(\varphi_h^1, \varphi_h^2, \varphi_h^3, \varphi_h^4) = (u_h^1, u_h^2, u_h^3, u_h^4)$, summing the equalities, applying Young's inequality on terms with $(u_h^2, u_h^3)_{\mathcal{F}_h}$, dropping the negative terms on the right-hand side, and multiplying the resulting inequality by 2 give

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\Big(\|u_h^1\|_{\mathcal{G}_h}^2 + \|u_h^2\|_{\mathcal{F}_h}^2 + \|u_h^3\|_{\mathcal{F}_h}^2 + \|u_h^4\|_{\mathcal{G}_h}^2\Big) + 2d_1\|\nabla_h u_h^1\|_{\mathcal{E}_h}^2 + 2d_2\|\nabla_{yh} u_h^2\|_{\mathcal{H}_h}^2 + 2d_3\|\nabla_{yh} u_h^3\|_{\mathcal{H}_h}^2 \\ \le -2Bi^M(Hu_h^1 - u_h^2|_{y=0}, u_h^1)_{\mathcal{G}_h} + 2Bi^M(Hu_h^1 - u_h^2|_{y=0}, u_h^2|_{y=0})_{\mathcal{G}_h} \\ + C_1\|u_h^2\|_{\mathcal{F}_h}^2 + C_1\|u_h^3\|_{\mathcal{F}_h}^2 + 2\big(\eta(u_h^3|_{y=\ell}, u_h^4), u_h^4 - u_h^3|_{y=\ell}\big)_{\mathcal{G}_h},\end{aligned}$$

where $C_1 := \alpha + \beta > 0$. Expanding the first two terms on the right-hand side we get

$$\begin{aligned}-2(Hu_h^1 - u_h^2|_{y=0}, u_h^1)_{\mathcal{G}_h} + 2(Hu_h^1 - u_h^2|_{y=0}, u_h^2|_{y=0})_{\mathcal{G}_h} &= -2H\|u_h^1\|_{\mathcal{G}_h}^2 \\ + 2(1+H)(u_h^1, u_h^2|_{y=0})_{\mathcal{G}_h} - 2\|u_h^2|_{y=0}\|_{\mathcal{G}_h}^2 &\le \frac{1+H}{\varepsilon}\|u_h^1\|_{\mathcal{G}_h}^2 + \big((1+H)\varepsilon - 2\big)\|u_h^2|_{y=0}\|_{\mathcal{G}_h}^2,\end{aligned}$$

where we used Young's inequality with $\varepsilon > 0$. Choosing ε sufficiently small, the coefficient in front of the last term is negative, so we have that

$$-2(Hu_h^1 - u_h^2|_{y=0}, u_h^1)_{\mathcal{G}_h} + 2(Hu_h^1 - u_h^2|_{y=0}, u_h^2|_{y=0})_{\mathcal{G}_h} \le C_2\|u_h^1\|_{\mathcal{G}_h}^2,$$

where $C_2 := \frac{1+H}{\varepsilon} > 0$, and thus

(6.49)
$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\Big(\|u_h^1\|_{\mathcal{G}_h}^2 + \|u_h^2\|_{\mathcal{F}_h}^2 + \|u_h^3\|_{\mathcal{F}_h}^2 + \|u_h^4\|_{\mathcal{G}_h}^2\Big) + 2d_1\|\nabla_h u_h^1\|_{\mathcal{E}_h}^2 + 2d_2\|\nabla_{yh} u_h^2\|_{\mathcal{H}_h}^2 + 2d_3\|\nabla_{yh} u_h^3\|_{\mathcal{H}_h}^2 \\ \le C_2\|u_h^1\|_{\mathcal{G}_h}^2 + C_1\|u_h^2\|_{\mathcal{F}_h}^2 + C_1\|u_h^3\|_{\mathcal{F}_h}^2 + 2\big(\eta(u_h^3|_{y=\ell}, u_h^4), u_h^4 - u_h^3|_{y=\ell}\big)_{\mathcal{G}_h}.\end{aligned}$$

For the last term on the right-hand side of the previous inequality we have

$$\begin{aligned}2\big(\eta(u_h^3|_{y=\ell}, u_h^4), u_h^4 - u_h^3|_{y=\ell}\big)_{\mathcal{G}_h} &= 2k\big(R(u_h^3|_{y=\ell})Q(u_h^4), u_h^4\big)_{\mathcal{G}_h} \underbrace{-2k\big(R(u_h^3|_{y=\ell})Q(u_h^4), u_h^3|_{y=\ell}\big)_{\mathcal{G}_h}}_{\le 0} \\ \le 2k\bar{c}^q\big(R(u_h^3|_{y=\ell}), u_h^4\big)_{\mathcal{G}_h} &\le k\bar{c}^q\Big(\varepsilon\|R(u_h^3|_{y=\ell})\|_{\mathcal{G}_h}^2 + \frac{1}{\varepsilon}\|u_h^4\|_{\mathcal{G}_h}^2\Big) \le k\bar{c}^q\Big(\varepsilon\|u_h^3|_{y=\ell}\|_{\mathcal{G}_h}^2 + \frac{1}{\varepsilon}\|u_h^4\|_{\mathcal{G}_h}^2\Big) \\ &\le k\bar{c}^q\Big(C_3\varepsilon\|u_h^3\|_{\mathcal{F}_h}^2 + C_3\varepsilon\|\nabla_{yh} u_h^3\|_{\mathcal{H}_h}^2 + \frac{1}{\varepsilon}\|u_h^4\|_{\mathcal{G}_h}^2\Big),\end{aligned}$$

where we used the assumption (A_1), Young's inequality with $\varepsilon > 0$ and the discrete trace inequality (6.37) with the constant $C_3 > 0$. Using the result in (6.49) we obtain

(6.50)
$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\Big(\|u_h^1\|_{\mathcal{G}_h}^2 + \|u_h^2\|_{\mathcal{F}_h}^2 + \|u_h^3\|_{\mathcal{F}_h}^2 + \|u_h^4\|_{\mathcal{G}_h}^2\Big) + d_1\|\nabla_h u_h^1\|_{\mathcal{E}_h}^2 + d_2\|\nabla_{yh} u_h^2\|_{\mathcal{H}_h}^2 + C_4\|\nabla_{yh} u_h^3\|_{\mathcal{H}_h}^2 \\ \le C_2\|u_h^1\|_{\mathcal{G}_h}^2 + C_1\|u_h^2\|_{\mathcal{F}_h}^2 + C_5\|u_h^3\|_{\mathcal{F}_h}^2 + C_6\|u_h^4\|_{\mathcal{G}_h}^2,\end{aligned}$$

where $C_4 := d_3 - k\bar{c}^q C_3\varepsilon$ can be made positive for ε sufficiently small, $C_5 := C_1 + k\bar{c}^q C_3\varepsilon$, and $C_6 := k\bar{c}^q\frac{1}{\varepsilon}$.

Discarding the terms with discrete gradient, we get

$$\frac{\mathrm{d}}{\mathrm{d}t}\Big(\|u_h^1\|_{\mathcal{G}_h}^2 + \|u_h^2\|_{\mathcal{F}_h}^2 + \|u_h^3\|_{\mathcal{F}_h}^2 + \|u_h^4\|_{\mathcal{G}_h}^2\Big) \le C_7\Big(\|u_h^1\|_{\mathcal{G}_h}^2 + \|u_h^2\|_{\mathcal{F}_h}^2 + \|u_h^3\|_{\mathcal{F}_h}^2 + \|u_h^4\|_{\mathcal{G}_h}^2\Big),$$

where $C_7 := \max\{C_1, C_2, C_5, C_6\}$. Applying the Gronwall's lemma to the previous inequality we obtain

(6.51)
$$\begin{aligned}\max_{t\in S}\Big(\|u_h^1(t)\|_{\mathcal{G}_h}^2 + \|u_h^2(t)\|_{\mathcal{F}_h}^2 + \|u_h^3(t)\|_{\mathcal{F}_h}^2 + \|u_h^4(t)\|_{\mathcal{G}_h}^2\Big) \\ \le \Big(\|u_h^1(0)\|_{\mathcal{G}_h}^2 + \|u_h^2(0)\|_{\mathcal{F}_h}^2 + \|u_h^3(0)\|_{\mathcal{F}_h}^2 + \|u_h^4(0)\|_{\mathcal{G}_h}^2\Big)e^{C_7 T}.\end{aligned}$$

Finally, integrating (6.50) over $[0, T]$ and using (6.51) gives

(6.52)
$$\begin{aligned}\int_0^T \Big(\|\nabla_h u_h^1\|_{\mathcal{E}_h}^2 + \|\nabla_{yh} u_h^2\|_{\mathcal{H}_h}^2 + \|\nabla_{yh} u_h^3\|_{\mathcal{H}_h}^2\Big)\mathrm{d}t \\ \le \frac{1 + C_7 T e^{C_7 T}}{C_8}\Big(\|u_h^1(0)\|_{\mathcal{G}_h}^2 + \|u_h^2(0)\|_{\mathcal{F}_h}^2 + \|u_h^3(0)\|_{\mathcal{F}_h}^2 + \|u_h^4(0)\|_{\mathcal{G}_h}^2\Big),\end{aligned}$$

where $C_8 := \min\{d_1, d_2, C_4\}$. The claim of the lemma directly follows. □

LEMMA 8. *Let $\{u_h^1, u_h^2, u_h^3, u_h^4\}$ be a semi-discrete solution of (6.2) for some $T > 0$. Then it holds that*

$$\max_{t\in S}\Big(\|\dot{u}_h^1(t)\|_{\mathcal{G}_h}^2 + \|\dot{u}_h^2(t)\|_{\mathcal{F}_h}^2 + \|\dot{u}_h^3(t)\|_{\mathcal{F}_h}^2\Big) \le C, \tag{6.53}$$

$$\int_0^T \Big(\|\nabla_h \dot{u}_h^1\|_{\mathcal{E}_h}^2 + \|\nabla_{yh}\dot{u}_h^2\|_{\mathcal{H}_h}^2 + \|\nabla_{yh}\dot{u}_h^3\|_{\mathcal{H}_h}^2\Big)\mathrm{d}t \le C, \tag{6.54}$$

where C is a positive constant independent of h_x, h_y.

PROOF. We follow the steps of [**MNR10**, Theorem 4]. Differentiate (6.43)–(6.45) with respect to time, take $\varphi_h^i = \dot{u}_h^i, i = 1, \dots, 3$, discard the negative terms on the right-hand side and sum the inequalities to obtain

$$\begin{aligned}\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\Big(\|\dot{u}_h^1\|_{\mathcal{G}_h}^2 + \|\dot{u}_h^2\|_{\mathcal{F}_h}^2 + \|\dot{u}_h^3\|_{\mathcal{F}_h}^2\Big) + d_1\|\nabla_h\dot{u}_h^1\|_{\mathcal{E}_h}^2 + d_2\|\nabla_{yh}\dot{u}_h^2\|_{\mathcal{H}_h}^2 + d_3\|\nabla_{yh}\dot{u}_h^3\|_{\mathcal{H}_h}^2 \\ \le Bi^M(1+H)\big(\dot{u}_h^1, \dot{u}_h^2|_{y=0}\big)_{\mathcal{G}_h} - Bi^M\|\dot{u}_h^2|_{y=0}\|_{\mathcal{G}_h}^2 + (\alpha+\beta)\big(\dot{u}_h^2, \dot{u}_h^3\big)_{\mathcal{F}_h} \\ - \big(\partial_r\eta(u_h^3|_{y=\ell}, u_h^4)\dot{u}_h^3|_{y=\ell} + \partial_s\eta(u_h^3|_{y=\ell}, u_h^4)\dot{u}_h^4, \dot{u}_h^3|_{y=\ell}\big)_{\mathcal{G}_h}.\end{aligned}$$

As in the proof of Lemma 7, for the first two terms on the right-hand side we have that

$$Bi^M(1+H)\big(\dot{u}_h^1, \dot{u}_h^2|_{y=0}\big)_{\mathcal{G}_h} - Bi^M\|\dot{u}_h^2|_{y=0}\|_{\mathcal{G}_h}^2 \le C_1\|\dot{u}_h^1\|_{\mathcal{G}_h}^2,$$

and for the third term

$$(\alpha+\beta)\big(\dot{u}_h^2, \dot{u}_h^3\big)_{\mathcal{F}_h} \le C_2\big(\|\dot{u}_h^2\|_{\mathcal{F}_h}^2 + \|\dot{u}_h^3\|_{\mathcal{F}_h}^2\big).$$

Using the Lipschitz property of η, together with Schwarz's and Young's inequalities, and assuming the structural restriction $\partial_r\eta > 0$, we obtain for the last term on the right-hand side that

$$\begin{aligned}-\big(\partial_r\eta\dot{u}_h^3|_{y=\ell} + \partial_s\eta\dot{u}_h^4, \dot{u}_h^3|_{y=\ell}\big)_{\mathcal{G}_h} &= -\big(\partial_r\eta\dot{u}_h^3|_{y=\ell}, \dot{u}_h^3|_{y=\ell}\big)_{\mathcal{G}_h} - \big(\partial_s\eta\dot{u}_h^4, \dot{u}_h^3|_{y=\ell}\big)_{\mathcal{G}_h} \\ &\le \underbrace{-\big(\partial_r\eta\dot{u}_h^3|_{y=\ell}, \dot{u}_h^3|_{y=\ell}\big)_{\mathcal{G}_h}}_{\le 0} + C\left(\frac{1}{2\varepsilon}\big\|\dot{u}_h^4\big\|_{\mathcal{G}_h}^2 + \frac{\varepsilon}{2}\|\dot{u}_h^3|_{y=\ell}\big\|_{\mathcal{G}_h}^2\right).\end{aligned}$$

Choosing ε sufficiently small, we get that

$$-\big(\partial_r\eta(u_h^3|_{y=\ell}, u_h^4)\dot{u}_h^3|_{y=\ell} + \partial_s\eta(u_h^3|_{y=\ell}, u_h^4)\dot{u}_h^4, \dot{u}_h^3|_{y=\ell}\big)_{\mathcal{G}_h} \le C_3\big\|\dot{u}_h^4\big\|_{\mathcal{G}_h}^2.$$

Putting the obtained results together we finally obtain that

$$\begin{aligned}\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\Big(\|\dot{u}_h^1\|_{\mathcal{G}_h}^2 + \|\dot{u}_h^2\|_{\mathcal{F}_h}^2 + \|\dot{u}_h^3\|_{\mathcal{F}_h}^2\Big) + d_1\|\nabla_h\dot{u}_h^1\|_{\mathcal{E}_h}^2 + d_2\|\nabla_{yh}\dot{u}_h^2\|_{\mathcal{H}_h}^2 + d_3\|\nabla_{yh}\dot{u}_h^3\|_{\mathcal{H}_h}^2 \\ \le C_1\|\dot{u}_h^1\|_{\mathcal{G}_h}^2 + C_2\big(\|\dot{u}_h^2\|_{\mathcal{F}_h}^2 + \|\dot{u}_h^3\|_{\mathcal{F}_h}^2\big) + C_3\|\dot{u}_h^4\|_{\mathcal{G}_h}^2.\end{aligned} \tag{6.55}$$

Grönwall's inequality gives that

$$\max_{t\in S}\Big(\|\dot{u}_h^1\|_{\mathcal{G}_h}^2 + \|\dot{u}_h^2\|_{\mathcal{F}_h}^2 + \|\dot{u}_h^3\|_{\mathcal{F}_h}^2\Big) \le C_4\Big(\|\dot{u}_h^1(0)\|_{\mathcal{G}_h}^2 + \|\dot{u}_h^2(0)\|_{\mathcal{F}_h}^2 + \|\dot{u}_h^3(0)\|_{\mathcal{F}_h}^2\Big). \tag{6.56}$$

In order to estimate the right-hand side in the previous inequality, we evaluate (6.39)–(6.41) at $t = 0$ and test with $\big(\dot{u}_h^1(0), \dot{u}_h^2(0), \dot{u}_h^3(0)\big)$ to get

$$\begin{aligned}\|\dot{u}_h^1(0)\|_{\mathcal{G}_h}^2 + \|\dot{u}_h^2(0)\|_{\mathcal{F}_h}^2 + \|\dot{u}_h^3(0)\|_{\mathcal{F}_h}^2 = d_1(\Delta_h u_h^1(0), \dot{u}_h^1(0))_{\mathcal{G}_h^o} + d_2(\Delta_{yh}u_h^2(0), \dot{u}_h^2(0))_{\mathcal{F}_h} \\ + d_3(\Delta_{yh}u_h^3(0), \dot{u}_h^3(0))_{\mathcal{F}_h} - Bi^M\big(Hu_h^1(0) - u_h^2(0)|_{y=0}, \dot{u}_h^1(0)\big)_{\mathcal{G}_h} \\ + (\alpha u_h^2(0) - \beta u_h^3(0), \dot{u}_h^3(0) - \dot{u}_h^2(0))_{\mathcal{F}_h}.\end{aligned}$$

Schwarz's inequality and Young's inequality (with $\varepsilon > 0$ chosen sufficiently small) together with the regularity of the initial data yield the estimate

$$\|\dot{u}_h^1(0)\|_{\mathcal{G}_h}^2 + \|\dot{u}_h^2(0)\|_{\mathcal{F}_h}^2 + \|\dot{u}_h^3(0)\|_{\mathcal{F}_h}^2 \le C,$$

where C does not depend on the spatial step sizes. Returning back to (6.55), integrating it with respect to t and using (6.56) gives the claim of the lemma. □

In the following lemma we derive additional *a priori* estimates that will finally allow us to pass in the limit in the non-linear terms. In order to avoid introducing new grids, grid functions and associated scalar products for finite differences in x variable, we resort to sum notation in this proof. To this end, for $u_h \in \mathcal{F}_h$, let $\delta_x^+ u_{ij}$, $\delta_x^- u_{ij}$, $\delta_y^+ u_{ij}$, $\delta_y^- u_{ij}$ denote the forward and backward difference quotients at x_{ij} in x- and y-direction, i.e.,

$$(\delta_x^+ u_h)_{ij} := \frac{u_{i+1,j} - u_{ij}}{h_x}, \quad (\delta_x^- u_h)_{ij} := \frac{u_{ij} - u_{i-1,j}}{h_x},$$
$$(\delta_y^+ u_h)_{ij} := \frac{u_{i,j+1} - u_{ij}}{h_y}, \quad (\delta_y^- u_h)_{ij} := \frac{u_{ij} - u_{i,j-1}}{h_y}.$$

LEMMA 9 (Improved *a priori* estimates). *Let $\{u_h^1, u_h^2, u_h^3, u_h^4\}$ be a semi-discrete solution of (6.2) for some $T > 0$. Then it holds that*

$$\max_{t\in S} \left(h_x h_y \sum_{i=0}^{N_x-1} \sum_{j=0}^{N_y} (\delta_x^+ u_{ij}^2)^2 + h_x h_y \sum_{i=0}^{N_x-1} \sum_{j=0}^{N_y} (\delta_x^+ u_{ij}^3)^2 \right) \le C, \tag{6.57}$$

$$\int_0^T h_x h_y \sum_{i=0}^{N_x-1} \sum_{j=0}^{N_y-1} (\delta_x^+ \delta_y^+ u_{ij}^2)^2 \,\mathrm{d}t + \int_0^T h_x h_y \sum_{i=0}^{N_x-1} \sum_{j=0}^{N_y-1} (\delta_x^+ \delta_y^+ u_{ij}^3)^2 \,\mathrm{d}t \le C, \tag{6.58}$$

where C is a positive constant independent of h_x, h_y.

PROOF. Following the steps of [MNR10, Theorem 5], introduce a function $\vartheta \in C_0^\infty(\Omega)$ such that $0 \le \vartheta \le 1$ and let $\vartheta_h := \vartheta|_{\Omega_h} \in \mathcal{G}_h$. Test (6.17b) with $-\delta_x^-(\vartheta_i^2 \delta_x^+ u_h^2)_{ij}$, (6.17c) with $-\delta_x^-(\vartheta_i^2 \delta_x^+ u_h^3)_{ij}$, and sum over ω_h to form relations analogous to (6.44), (6.45). We get

$$\begin{aligned} &- h_y \sum_{i=1}^{N_x} \sum_{j=0}^{N_y} \gamma_i^1 \gamma_j^2 \dot{u}_{ij}^2 \delta_x^-(\vartheta_h^2 \delta_x^+ u_h^2)_{ij} - d_2 h_y \sum_{i=1}^{N_x} \sum_{j=0}^{N_y-1} \gamma_i^1 \gamma_j^2 \delta_y^+ u_{ij}^2 \delta_y^+ (\delta_x^-(\vartheta_h^2 \delta_x^+ u_h^2))_{ij} \\ &\quad = -Bi^m \sum_{i=1}^{N_x} \gamma_i^1 (H u_i^1 - u_{i,0}^2) \delta_x^-(\vartheta_i^2 \delta_x^+ u_h^2)_{i,0} + \alpha h_y \sum_{i=1}^{N_x} \sum_{j=0}^{N_y} \gamma_i^1 \gamma_j^2 u_{ij}^2 \delta_x^-(\vartheta_i^2 \delta_x^+ u_h^2)_{ij} \\ &\qquad - \beta h_y \sum_{i=1}^{N_x} \sum_{j=0}^{N_y} \gamma_i^1 \gamma_j^2 u_{ij}^3 \delta_x^-(\vartheta_i^2 \delta_x^+ u_h^2)_{ij}, \end{aligned}$$

$$\begin{aligned} &- h_y \sum_{i=1}^{N_x} \sum_{j=0}^{N_y} \gamma_i^1 \gamma_j^2 \dot{u}_{ij}^3 \delta_x^-(\vartheta_h^2 \delta_x^+ u_h^3)_{ij} - d_3 h_y \sum_{i=1}^{N_x} \sum_{j=0}^{N_y-1} \gamma_i^1 \gamma_j^2 \delta_y^+ u_{ij}^3 \delta_y^+ (\delta_x^-(\vartheta_h^2 \delta_x^+ u_h^3))_{ij} \\ &\quad = \sum_{i=1}^{N_x} \gamma_i^1 \eta(u_{i,N_y}^3, u_i^4) \delta_x^-(\vartheta_i^2 \delta_x^+ u_h^3)_{i,N_y} - \alpha h_y \sum_{i=1}^{N_x} \sum_{j=0}^{N_y} \gamma_i^1 \gamma_j^2 u_{ij}^2 \delta_x^-(\vartheta_i^2 \delta_x^+ u_h^3)_{ij} \\ &\qquad + \beta h_y \sum_{i=1}^{N_x} \sum_{j=0}^{N_y} \gamma_i^1 \gamma_j^2 u_{ij}^3 \delta_x^-(\vartheta_i^2 \delta_x^+ u_h^3)_{ij}. \end{aligned}$$

Summing the previous two equalities and using the discrete Green's theorem analogous to (6.33), Schwarz's inequality and Young's inequality we obtain

$$\begin{aligned}(6.59)\quad &\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\Big(h_y\sum_{i=0}^{N_x-1}\sum_{j=0}^{N_y}|\vartheta_i\delta_x^+u_{ij}^2|^2+h_y\sum_{i=0}^{N_x-1}\sum_{j=0}^{N_y}|\vartheta_i\delta_x^+u_{ij}^3|^2\Big)+d_2h_y\sum_{i=0}^{N_x-1}\sum_{j=0}^{N_y-1}|\vartheta_i\delta_x^+\delta_y^+u_{ij}^2|^2\\ &+d_3h_y\sum_{i=0}^{N_x-1}\sum_{j=0}^{N_y-1}|\vartheta_i\delta_x^+\delta_y^+u_{ij}^3|^2\le Bi^mHC_1\sum_{i=0}^{N_x-1}|\vartheta_i\delta_x^+u_i^1|^2+C_2h_y\sum_{i=0}^{N_x-1}\sum_{j=0}^{N_y}(\vartheta_i\delta_x^+u_{ij}^2)^2\\ &+C_3h_y\sum_{i=0}^{N_x-1}\sum_{j=0}^{N_y}(\vartheta_i\delta_x^+u_{ij}^3)^2-\sum_{i=0}^{N_x-1}(\delta_x^+\eta(u_{i,N_y}^3,u_i^4))(\vartheta_i^2\delta_x^+u_{i,N_y}^3).\end{aligned}$$

We rewrite the last term on the right-hand side as

$$\begin{aligned}&-k\sum_{i=0}^{N_x-1}(\delta_x^+(R(u_{i,N_y}^3)Q(u_i^4)))(\vartheta_i^2\delta_x^+u_{i,N_y}^3)\\ &\qquad=-k\sum_{i=0}^{N_x-1}\Big(Q(u_i^4)\delta_x^+R(u_{i,N_y}^3)+R(u_{i+1,N_y}^3)\delta_x^+Q(u_i^4)\Big)(\vartheta_i^2\delta_x^+u_{i,N_y}^3)\\ &\qquad=\underbrace{-k\sum_{i=0}^{N_x-1}\vartheta_i^2Q(u_i^4)\delta_x^+R(u_{i,N_y}^3)\delta_x^+u_{i,N_y}^3}_{\le0}-k\sum_{i=0}^{N_x-1}R(u_{i+1,N_y}^3)\delta_x^+Q(u_i^4)(\vartheta_i^2\delta_x^+u_{i,N_y}^3),\end{aligned}$$

where we used the monotonicity of R and boundedness of Q. To estimate the last term we exploit the Lipschitz continuity and boundedness of Q and use the discrete trace theorem so that

$$\begin{aligned}&-k\sum_{i=0}^{N_x-1}R(u_{i+1,N_y}^3)\delta_x^+Q(u_i^4)(\vartheta_i^2\delta_x^+u_{i,N_y}^3)\le C_4\sum_{i=0}^{N_x-1}\vartheta_i^2|\delta_x^+u_{i,N_y}^3\delta_x^+u_i^4|\\ &\qquad\le\frac{C_4\varepsilon}{2}\sum_{i=0}^{N_x-1}(\vartheta_i\delta_x^+u_{i,N_y}^3)^2+\frac{C_4}{2\varepsilon}\sum_{i=0}^{N_x-1}(\vartheta_i\delta_x^+u_i^4)^2\le C_5\varepsilon h_y\sum_{i=0}^{N_x-1}\sum_{j=0}^{N_y}(\vartheta_i\delta_x^+u_{ij}^3)^2\\ &\qquad\quad+C_5\varepsilon h_y\sum_{i=0}^{N_x-1}\sum_{j=0}^{N_y-1}(\vartheta_i\delta_x^+\delta_y^+u_{ij}^3)^2+\frac{C_4}{2\varepsilon}\sum_{i=0}^{N_x-1}(\vartheta_i\delta_x^+u_i^4)^2.\end{aligned}$$

Using the latter result in (6.59), we arrive at

$$\begin{aligned}(6.60)\quad &\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\Big(h_y\sum_{i=0}^{N_x-1}\sum_{j=0}^{N_y}(\vartheta_i\delta_x^+u_{ij}^2)^2+h_y\sum_{i=0}^{N_x-1}\sum_{j=0}^{N_y}(\vartheta_i\delta_x^+u_{ij}^3)^2\Big)+d_2h_y\sum_{i=0}^{N_x-1}\sum_{j=0}^{N_y-1}(\vartheta_i\delta_x^+\delta_y^+u_{ij}^2)^2\\ &+(d_3-C_5\varepsilon)h_y\sum_{i=0}^{N_x-1}\sum_{j=0}^{N_y-1}(\vartheta_i\delta_x^+\delta_y^+u_{ij}^3)^2\le Bi^mHC_1\sum_{i=0}^{N_x-1}|\vartheta_i\delta_x^+u_i^1|^2+C_2h_y\sum_{i=0}^{N_x-1}\sum_{j=0}^{N_y}(\vartheta_i\delta_x^+u_{ij}^2)^2\\ &+(C_3+C_5\varepsilon)h_y\sum_{i=0}^{N_x-1}\sum_{j=0}^{N_y}(\vartheta_i\delta_x^+u_{ij}^3)^2+\frac{C_4}{2\varepsilon}\sum_{i=0}^{N_x-1}(\vartheta_i\delta_x^+u_i^4)^2.\end{aligned}$$

Applying Gronwall's inequality and integrating with respect to time we obtain the claim of the lemma. □

6.5. Interpolation and compactness

In this section, we derive sufficient results that enable us to show the convergence of semi-discrete solutions of (6.2). To this end, we firstly introduce extensions of grid functions so that they are defined almost everywhere in Ω and ω and can be studied by the usual techniques of Lebesgue/Sobolev/Bochner spaces. Finally, we use the *a priori* estimates proved in Section 6.4 to show the necessary compactness for the sequences of extended grid functions.

6.5.1. Interpolation. In this subsection we introduce extensions of grid functions so that they are defined almost everywhere in Ω and ω.

Definition 10 (Dual and simplicial grids on Ω). Let Ω_h be a grid on Ω as defined in Section 6.3.1. Define the dual grid $\Omega_h^{\boxdot}$ as

$$\Omega_h^{\boxdot} := \{\mathcal{K}_i^{\boxdot} \subset \bar{\Omega} \mid \mathcal{K}_i^{\boxdot} := [x_i - h_x/2, x_i + h_x/2] \cap \bar{\Omega},\ x_i \in \Omega_h\},$$

and the simplicial grid $\Omega_h^{\boxbslash}$ as

$$\Omega_h^{\boxbslash} := \{\mathcal{K}_i^{\boxbslash} \subset \bar{\Omega} \mid \mathcal{K}_i^{\boxbslash} := [x_i, x_{i+1}] \cap \bar{\Omega},\ x_i \in \Omega_h\}.$$

Definition 11 (Dual and simplicial grids on $\Omega \times Y$). Let ω_h be a grid on $\Omega \times Y$ as defined in Section 6.3.1. Define the dual grid $\omega_h^{\boxdot}$ as

$$\begin{aligned}\omega_h^{\boxdot} := \{\mathcal{L}_{ij}^{\boxdot} \subset \bar{\Omega} \times \bar{Y} \mid \mathcal{L}_{ij}^{\boxdot} := [x_i - h_x/2, x_i + h_x/2] \\ \times [y_j - h_y/2, y_j + h_y/2] \cap \bar{\Omega} \times \bar{Y},\ x_i \in \Omega_h, y_j \in Y_h\},\end{aligned}$$

and the simplicial grid $\omega_h^{\boxbslash}$ as $\omega_h^{\boxbslash} := \omega_h^{\triangleleft} \cup \omega_h^{\triangleright}$, where

$$\begin{aligned}\omega_h^{\triangleleft} := \big\{\mathcal{L}_{ij}^{\triangleleft} \mid \mathcal{L}_{ij}^{\triangleleft} := \big[(x_i, y_j), (x_{i+1}, y_j), (x_i, y_{j+1})\big]_{\varkappa} \cap \bar{\Omega} \times \bar{Y}, \\ i = 0, \dots, N_x - 1, j = 0, \dots, N_y - 1\big\}, \\ \omega_h^{\triangleright} := \big\{\mathcal{L}_{ij}^{\triangleright} \mid \mathcal{L}_{ij}^{\triangleright} := \big[(x_{i+1}, y_{j+1}), (x_{i+1}, y_j), (x_i, y_{j+1})\big]_{\varkappa} \cap \bar{\Omega} \times \bar{Y}, \\ i = 0, \dots, N_x - 1, j = 0, \dots, N_y - 1\big\},\end{aligned}$$

where $[\mathrm{x}, \mathrm{y}, \mathrm{z}]_{\varkappa}$ denotes convex hull of points $\mathrm{x}, \mathrm{y}, \mathrm{z} \in \mathbb{R}^2$.

Definition 12 (Piecewise constant extension). For a grid function u_h we define its piecewise constant extension $\bar{u}_h$ as

$$\bar{u}_h(x) = \begin{cases} u_i, & x \in \mathcal{K}_i^{\boxdot},\ u_h \in \mathcal{G}_h, \\ u_{ij}, & x \in \mathcal{L}_{ij}^{\boxdot},\ u_h \in \mathcal{F}_h. \end{cases} \tag{6.61}$$

Definition 13 (Piecewise linear extension). For a grid function $u_h \in \mathcal{G}_h$ we define its piecewise linear extension $\hat{u}_h$ as

$$\hat{u}_h(x) = u_i + (\nabla_h u_h)_{i+1/2}(x - x_i), \quad x \in \mathcal{K}_i^{\boxbslash},\ u_h \in \mathcal{G}_h, \tag{6.62}$$

while for $u_h \in \mathcal{F}_h$ we define it as

$$\hat{u}_h(x) = \begin{cases} u_{ij} + \delta_x^+ u_{ij}(x - x_i) + (\nabla_{yh} u_h)_{i,j+1/2}(y - y_j), & x \in \mathcal{L}_{ij}^{\triangleleft}, \\ u_{i+1,j+1} + \delta_x^+ u_{i,j+1}(x_{i+1} - x) + (\nabla_{yh} u_h)_{i+1,j+1/2}(y_j - y), & x \in \mathcal{L}_{ij}^{\triangleright}. \end{cases} \tag{6.63}$$

The following lemma shows the relation between discrete scalar products of grid functions and scalar products of interpolated grid functions in $L^2(\Omega)$ and $L^2(\Omega \times Y)$ and follows by a direct calculation.

LEMMA 14. *It holds that*

$$
\begin{aligned}
(\bar{u}_h, \bar{v}_h)_{L^2(\Omega)} &= (u_h, u_h)_{\mathcal{G}_h}, && u_h, v_h \in \mathcal{G}_h,\\
(\nabla \hat{u}_h, \nabla \hat{v}_h)_{L^2(\Omega)} &= (\nabla_h u_h, \nabla_h v_h)_{\mathcal{E}_h}, && u_h, v_h \in \mathcal{G}_h,\\
(\bar{u}_h, \bar{v}_h)_{L^2(\Omega\times Y)} &= (u_h, v_h)_{\mathcal{F}_h}, && u_h, v_h \in \mathcal{F}_h,\\
(\nabla_y \hat{u}_h, \nabla_y \hat{v}_h)_{L^2(\Omega\times Y)} &= (\nabla_{yh} u_h, \nabla_{yh} v_h)_{\mathcal{H}_h}, && u_h, v_h \in \mathcal{F}_h.
\end{aligned}
$$

6.5.2. Compactness. In this subsection we prove our main result. To do this we essentially use the preliminary results shown in the previous paragraphs and the results of [**Lad85**]. Basically, we show the convergence of semi-discrete solutions to a weak solution of problem (P). This result is stated in the following theorem.

THEOREM 15. *Assume (A1)–(A4) to be fulfilled. Then the semi-discrete solution* $\{u_h^1, u_h^2, u_h^3, u_h^4\}$ *of* (6.2) *exists on* $[0,T]$ *for any* $T>0$ *and its interpolate* $\{\hat{u}_h^1, \hat{u}_h^2, \hat{u}_h^3, \hat{u}_h^4\}$ *converge in* $L^2(\Omega)$, $L^2(\Omega\times Y)$, $L^2(\Omega\times S)$, $L^2(\Omega)$, *respectively, as* $|h|\to 0$ *to a weak solution* (u_1, u_2, u_3, u_4) *to problem (P) in the sense of Definition 1.*

PROOF. We start off with recovering the initial data. The definition of interpolation of grid functions leads, as $|h|\to 0$, to

$$
\begin{aligned}
&\hat{u}_h^1(0) \to u_1^0 \text{ weakly in } H^1(\Omega),\\
&\hat{u}_h^2(0) \to u_2^0 \text{ weakly in } L^2(\Omega; H^1(Y)),\\
&\hat{u}_h^3(0) \to u_3^0 \text{ weakly in } L^2(\Omega; H^1(Y)),\\
&\hat{u}_h^4(0) \to u_4^0 \text{ weakly in } L^2(\Omega).
\end{aligned}
$$

Let h_n be a sequence of spatial space sizes such that $|h|\to 0$ as $n\to\infty$. Consequently, we obtain a sequence of solutions $\{u_{h_n}^1, u_{h_n}^2, u_{h_n}^3, u_{h_n}^4\}$ of (6.17) defined on the whole time interval S.

Let us pass to the limit $|h|\to 0$ in the ODE. Note that $\eta(\bar{u}_{h_n}^3|_{y=\ell}, \bar{u}_{h_n}^4) \rightharpoonup q$ weakly in $L^2(S; L^2(\Omega))$, and q still needs to be identified. The way we pass to the limit in the ODE is based on the following monotonicity-type argument (see [**FM10**]): using the monotonicity of η w.r.t. both variables, we can show that $\bar{u}_{h_n}^4$ is a Cauchy sequence, and therefore, it is strongly convergent to u^4.

Now, it only remains to pass to the limit in the PDEs. Note that the weak formulation contains a nonlinear boundary term involving $\eta(\cdot,\cdot)$. Exploiting the properties of the interpolations of grid functions (Lemma 14) we deduce that the same *a priori* estimates hold also for the interpolated solution (see also [**Lad85**]). On this way, we obtain

$$
\begin{aligned}
&\{\hat{u}_{h_n}^1\} \text{ is bounded in } L^\infty(0,T; L^2(\Omega)),\\
&\{\hat{u}_{h_n}^1\} \text{ is bounded in } L^2(0,T; H^1(\Omega)),\\
&\{\hat{u}_{h_n}^2\} \text{ is bounded in } L^\infty(0,T; L^2(\Omega)),\\
&\{\hat{u}_{h_n}^3\} \text{ is bounded in } L^\infty(0,T; L^2(\Omega)),\\
&\{\hat{u}_{h_n}^4\} \text{ is bounded in } L^\infty(0,T; L^2(\Omega)).
\end{aligned}
$$

Hence, there exists a subsequence of h_n (denoted again by h_n), such that

$$
\begin{aligned}
&\hat{u}_{h_n}^1 \rightharpoonup u^1 \text{ weakly in } L^2(S; H^1(\Omega)),\\
&\hat{u}_{h_n}^2 \rightharpoonup u^2 \text{ weakly in } L^2(S; L^2(\Omega)),\\
&\hat{u}_{h_n}^3 \rightharpoonup u^3 \text{ weakly in } L^2(S; L^2(\Omega)),\\
&\hat{u}_{h_n}^4 \rightharpoonup u^4 \text{ weakly in } L^2(S; L^2(\Omega)).
\end{aligned}
$$

Since

$$
\|\hat{u}_{h_n}^1\|_{L^2(S,H^1(\Omega))} + \|\partial_t \hat{u}_{h_n}^1\|_{L^2(S,L^2(\Omega))} \le C,
$$

Lions-Aubin's compactness theorem, see [**Lio63**, Theorem 1], implies that there exists a subset (again denoted by $\hat{u}^1_{h_n}$) such that

$$\hat{u}^1_{h_n} \longrightarrow u^1 \quad \text{strongly in} \quad L^2(S\times\Omega).$$

To get the desired strong convergence for the cell solutions $\hat{u}^2_{h_n}, \hat{u}^3_{h_n}$, we need the higher regularity with respect to the variable x, proved in Lemma 9. We remark that the two-scale regularity estimates imply that

$$\|\hat{u}^2_{h_n}\|_{L^2(S;H^1(\Omega,H^1(Y)))} + \|\hat{u}^3_{h_n}\|_{L^2(S;H^1(\Omega,H^1(Y)))} \leq C.$$

Moreover, from Lemma 8, we have that

$$\|\partial_t\hat{u}^2_{h_n}\|_{L^2(S\times\Omega\times Y)} + \|\partial_t\hat{u}^3_{h_n}\|_{L^2(S\times\Omega\times Y)} \leq C.$$

Since the embedding

$$H^1(\Omega,H^1(Y)) \hookrightarrow L^2(\Omega,H^\beta(Y))$$

is compact for all $\frac{1}{2} < \beta < 1$, it follows again from Lions-Aubin's compactness theorem that there exist subsequences (again denoted $\hat{u}^2_{h_n}, \hat{u}^3_{h_n}$), such that

$$(\hat{u}^2_{h_n}, \hat{u}^3_{h_n}) \longrightarrow (u^2, u^3) \quad \text{strongly in} \quad L^2(S\times L^2(\Omega,H^\beta(Y))), \tag{6.64}$$

for all $\frac{1}{2} < \beta < 1$. Now, (6.64) together with the continuity of the trace operator

$$H^\beta(Y) \hookrightarrow L^2(\partial Y), \quad \text{for} \quad \frac{1}{2} < \beta < 1,$$

yield the strong convergence of $\hat{u}^2_{h_n}$, $\hat{u}^3_{h_n}$ until the boundary $y = 0$. □

6.6. Numerical illustration of the two-scale FD scheme

We close this chapter by illustrating the behavior of the main chemical species driving the whole corrosion process, namely of $H_2S(g)$, and also the one of the corrosion product—the gypsum. To do these computations we use the reference parameters reported in [**CFM10**].

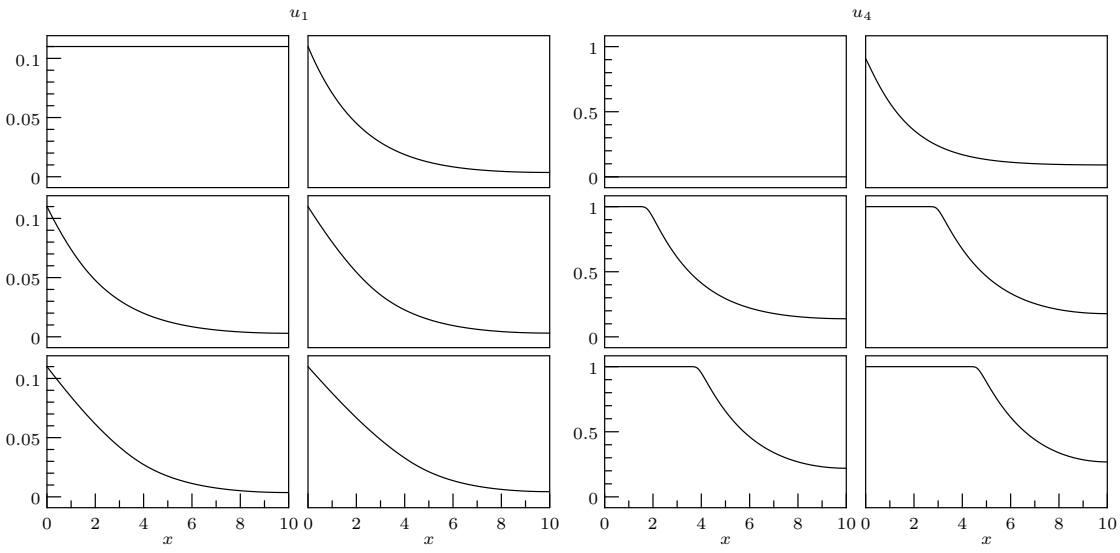

Figure 6.1 – Illustration of concentration profiles for the macroscopic concentration of gaseous H_2S (left) and of gypsum (right). Graphs plotted at times $t \in \{0, 80, 160, 240, 320, 400\}$ in a left-to-right and top-to-bottom order.

Fig. 6.1 shows the evolution of $u_1(x,t)$ and $u_4(x,t)$ as time elapses. Interestingly, although the behavior of u_1 is as expected (i.e., purely diffusive), we notice that a *macroscopic* gypsum layer (region where u_4 is produced) is formed (after a transient time $t^* > 80$) and grows in time. The figure clearly indicates that there are two distinct regions separated by a slowly moving intermediate layer: the left region, where the gypsum production reached saturation (a threshold), and the right region, the place of the ongoing sulfatation reaction (6.1d) (the gypsum production has not yet reached here the natural threshold). The precise position of the separating layer is *a priori unknown*. To capture it simultaneously with the computation of the concentration profile would require a moving-boundary formulation similar to the one reported in [**BJDR98**].

6.7. Exercises

EXERCISE 6.1. Before reading Chapter 7, implement in your favorite programming language the numerical scheme (6.17), (6.18), (6.19).

EXERCISE 6.2. Let us have a standard periodicity cell Y consisting of an aggregate $B \subset Y$ with smooth boundary Γ and of the remainder $F := Y \setminus B$. Outer normal vector to Γ is denoted by n. We consider a diffusion process in the whole Y, i.e., flow is allowed to take place within both B and F with largely disparate diffusivities. In this setting, the following two-scale model can be obtained by homogenization [**Hor97**, Chapter 1, Proposition 5.1]:

$$
\left\{
\begin{aligned}
|F|\partial_t u(t,x) + q(t,x) &= \nabla\cdot(A\nabla u(t,x)), && (t,x)\in(0,T)\times\Omega,\\
q(t,x) &= \int_\Gamma a_B(y)\nabla_y U(t,x,y)\cdot n\,\mathrm{d}\Gamma(y), && (t,x)\in(0,T)\times\Omega,\\
\partial_t U &= \nabla_y\cdot\left(a_B(y)\nabla_y U(t,x,y)\right), && (t,x,y)\in(0,T)\times\Omega\times B,\\
d(y)a_B(y)\nabla_y U(t,x,y)\cdot n &= c_F(y)u(t,x) - c_B(y)U(t,x,y), && (t,x,y)\in(0,T)\times\Omega\times\Gamma,\\
u(t,x) &= u_D(t,x), && (t,x)\in(0,T)\times\partial\Omega,\\
u(0,x) &= u_I(x), && x\in\Omega,\\
U(0,x,y) &= U_I(x,y), && (x,y)\in\Omega\times B.
\end{aligned}
\right. \tag{6.65}
$$

1. Propose a (semi-)discrete scheme for numerical solution of (6.65) assuming that $Y := (0,\ell)$ and $\Omega := (0,L)$.
2. Derive the needed *a priori* estimates and show the convergence of the numerical approximates to the weak solution to the original two-scale problem.
3. See what needs to be changed if we take $Y := (0,\ell)^2$.

CHAPTER 7

Computer implementation in C

Out goal in this chapter is to describe in a detailed way a possible computer implementation of the numerical scheme (6.17), (6.18), (6.19). Our presentation is truly didactic in order to help even novices in scientific programming to overcome the initial barrier so that they can start writing their own programs quickly. Also, there is nothing specific in our approach to multiscale problems and the program can be easily adapted to other scenarios as well. The complete source code is listed in Appendix A.

7.1. Introduction

Before we start description of the program, we give a general overview of our approach and what tools we use in the implementation. The particular program we describe here is written in portable ANSI C for its widespread use in scientific computing and for the sake of speed. However, other languages like for instance Python with its NumPy package are a viable alternative and thanks to its hiding of low-level implementation details might be more accessible to a novice scientific programmer. The reader is encouraged to write its own program in the language of his choice. It is out of the scope of this chapter to describe how to set up the development and visualization environment—the variety of operating systems, compilers and IDEs is simply too wide. We just assume that the reader has access to a text editor, a C compiler and the plotting tool Gnuplot. The authors developed and tested the program using gcc compiler version 4.2.1. and it should compile without any errors and warnings with this or any other modern compiler.

The program we present is a straightforward, single-purpose implementation of the numerical scheme, not a general, industrial-level approach. We wanted to keep things simple and short, and therefore we neglect many error-checking tests. Parsing of parameters and program options from disk or command line is another important feature of any serious scientific program that is nevertheless difficult to implement correctly from scratch unless an external library is used. Since we wanted to avoid as many external dependencies as possible, we solve it by hard-coding the problem parameters in the program as pre-processor macros. This approach is very primitive and the program needs to be recompiled every time we change a parameter, but it is sufficient for our purpose and is not an issue in our single source file. We do use an external library CVODE [**CH96**] for the time integration of the ODE system (6.17), but the use of this excellent, robust library simplifies the presentation and avoids the need to implement our own solver (which is also difficult to do in a robust way, see also Exercise 7.5). We recommend the reader to get acquainted with this library, its philosophy, interface, algorithms and data structures.

7.2. Review of the numerical scheme

In the program we try to follow closely the notation introduced in Chapter 6, so it is useful to rewrite the scheme and the boundary conditions again in index notation for the sake of clarity.

Thus, we are looking for the solution $(u_h^1, u_h^2, u_h^3, u_h^4)$ of the following system of ODEs:

$$\frac{\mathrm{d}u_i^1}{\mathrm{d}t} = d_1 \frac{u_{i-1}^1 - 2u_i^1 + u_{i+1}^1}{h_x^2} - Bi\big(Hu_i^1 - u_{i,0}^2\big), \qquad i = 1, \dots, N_x \tag{7.1}$$

$$\frac{\mathrm{d}u_{ij}^2}{\mathrm{d}t} = d_2 \frac{u_{i,j-1}^2 - 2u_{ij}^2 + u_{i,j+1}^2}{h_y^2} - k_2 u_{ij}^2 + k_3 u_{ij}^3, \qquad i = 0, \dots, N_x,\ j = 0, \dots, N_y, \tag{7.2}$$

$$\frac{\mathrm{d}u_{ij}^3}{\mathrm{d}t} = d_3 \frac{u_{i,j-1}^3 - 2u_{ij}^3 + u_{i,j+1}^3}{h_y^2} + k_2 u_{ij}^2 - k_3 u_{ij}^3, \qquad i = 0, \dots, N_x,\ j = 0, \dots, N_y, \tag{7.3}$$

$$\frac{\mathrm{d}u_i^4}{\mathrm{d}t} = \eta(u_{i,N_y}^3, u_i^4), \qquad i = 0, \dots, N_x, \tag{7.4}$$

with the boundary conditions

$$\begin{aligned} u_0^1 &= u_1^D, & u_{N_x+1}^1 &= u_{N_x-1}^1, \\ u_{i,-1}^2 &= u_{i,1}^2 + \frac{2h_y}{d_2} Bi\big(Hu_i^1 - u_{i,0}^2\big), & u_{i,N_y+1}^2 &= u_{i,N_y-1}^2, \\ u_{i,-1}^3 &= u_{i,1}^3, & u_{i,N_y+1}^3 &= u_{i,N_y-1}^3 - \frac{2h_y}{d_3}\eta(u_{i,N_y}^3, u_i^4). \end{aligned}$$

After choosing a suitable ordering of the unknowns, this system can be written as

$$\frac{\mathrm{d}\mathbf{u}}{\mathrm{d}t} = \mathbf{f}(\mathbf{u}), \tag{7.5}$$

where $\mathbf{u} : [0, T] \to \mathbb{R}^M$ is the vector of unknowns and $\mathbf{f} : \mathbb{R}^M \to \mathbb{R}^M$ is the right-hand side and $M := 2N_x + 1 + 2(N_x + 1)(N_y + 1)$. The number of unknowns is given by the fact that we look for two macroscopic quantities on a grid with $N_x + 1$ nodes (but we exclude from the computation the value of u_0^1, because it is given by the Dirichlet boundary condition) and two microscopic quantities on a grid with $(N_x + 1)(N_y + 1)$ nodes.

We are now ready to start writing the program.

7.3. Implementation

Include files

We first include standard C library header files together with mathematical library functions:

```
#include <stdlib.h>  /* standard library functions */
#include <stdio.h>   /* standard input/output functions */
#include <math.h>
```

We will use the following functions when saving the results to a file:

```
#include <time.h>
#include <sys/types.h>
#include <sys/stat.h>
```

Finally, we include header files for the CVODE library and its accompanying data structures:

```
#include <cvode/cvode.h>
#include <cvode/cvode_spgmr.h>
#include <nvector/nvector_serial.h>
#include <sundials/sundials_math.h>
```

Macro definitions and constants

As we stated in the introduction, we use a simple approach to specifying problem parameters in order to avoid reading a configuration file from disk and parsing its contents—we define them in the source code as symbolic constants using preprocessor directives. Thus, the Biot number Bi, Henry's constant H, maximum concentration of gypsum $\bar{c}$ and the reaction orders p and q are defined as

```
#define BIOT_NUMBER       864.0
#define H                 2.5
#define C_BAR             1.0
#define PARTIAL_ORDER_P   1.0
#define PARTIAL_ORDER_Q   1.0
```

the diffusion coefficients d_i, $i \in \{1, 2, 3\}$ as

```
#define D_1          864.0
#define D_2          0.0864
#define D_3          0.0864
```

and the reaction rates constants α, β and k as

```
#define ALPHA        7.2
#define BETA         0.84
#define K            1.0
```

The Dirichlet boundary condition for u_h^1 at $x = 0$ is given as

```
#define U1_D         0.1
```

and the initial conditions (constant functions) as

```
#define U1_INIT      U1_D
#define U2_INIT      0.0
#define U3_INIT      0.00001
#define U4_INIT      0.0
```

The two-scale geometry of the problem is given by L, ℓ, N_x, N_y, h_x and h_y as

```
#define L_X          500.0
#define L_Y          10.0
#define N_X          256
#define N_Y          32
#define DX           (L_X/N_X)
#define DY           (L_Y/N_Y)
```

For convenience we also define constants denoting the number of nodes in the x and y direction and the total number of unknowns in our ODE system (i.e., the length M of vector $\mathbf{u}$):

```
#define NEQ_X        (N_X+1)
#define NEQ_Y        (N_Y+1)
#define NEQ          (2*NEQ_X+2*NEQ_X*NEQ_Y-1)
```

Finally, the following constants define the time interval $(0, T)$, relative and absolute tolerances for the CVODE solver, number of output intervals and the time elapsed between two outputs:

```
#define T            1000.0
#define ABS_TOL      1.0e-9
#define REL_TOL      1.0e-9
#define N_OUT        100
#define DT           (T/N_OUT)
```

Ordering of unknowns

To obtain a system of ODEs in the form (7.5), we have to choose how to order the variables u_h^k in the vector $\mathbf{u}$. This ordering can be essentially arbitrary as long as we use it consistently throughout the program. However, it can have important impact on performance because, among other effects, it determines the memory access pattern and thus cache hit success rate. Furthermore, in CVODE there is a possibility to use a banded approximation to the Jacobian of $\mathbf{f}$ as a preconditioner in the Krylov linear solver and we would like to keep the bandwidth as small as possible.

The simplest ordering is to store the unknowns belonging to u_h^1 first, then u_h^2, u_h^3 and finally u_h^4 (of course, first we have to decide how to order u_h^2 and u_h^3, since they are indexed by two indeces i and j). However, this ordering is far from the best one. Consider evaluating the right-hand side of (7.2), where the values u_{ij}^2 and u_{ij}^3 are needed—these two values are $(N_x+1)(N_y+1)$ positions away from each other in the vector $\mathbf{u}$, which is against our goal of memory locality and small bandwidth of the Jacobian. This ordering is illustrated in Fig. 7.1.

u_1^1	u_2^1	$u_{0,0}^2$	$u_{0,1}^2$	$u_{1,0}^2$	$u_{1,1}^2$	$u_{2,0}^2$	$u_{2,1}^2$	$u_{0,0}^3$	$u_{0,1}^3$	$u_{1,0}^3$	$u_{1,1}^3$	$u_{2,0}^3$	$u_{2,1}^3$	u_0^4	u_1^4	u_2^4

Figure 7.1 – Example of a simple ordering of unknows in the vector $\mathbf{u}$ for $N_x = 2$ and $N_y = 1$.

A much better way and probably the best we can do is to "interlace" the unknowns in the following way: for each i, we store u_i^1, then $u_{i,0}^2$, $u_{i,0}^3$, $u_{i,1}^2$, $u_{i,1}^3$, …, u_{i,N_y}^2, u_{i,N_y}^3 and then u_i^4. Finally we increase i and repeat. This ordering is illustrated in Fig. 7.2.

$u_{0,0}^2$	$u_{0,0}^3$	$u_{0,1}^2$	$u_{0,1}^3$	u_0^4	u_1^1	$u_{1,0}^2$	$u_{1,0}^3$	$u_{1,1}^2$	$u_{1,1}^3$	u_1^4	u_2^1	$u_{2,0}^2$	$u_{2,0}^3$	$u_{2,1}^2$	$u_{2,1}^3$	u_2^4

Figure 7.2 – Example of a good ordering of unknows in the vector $\mathbf{u}$ for $N_x = 2$ and $N_y = 1$. Note that the unknown u_0^1 is omitted.

In the source code, we implement this ordering using preprocessor macros in the following way:

```
#define U1(u,xi)      u[(xi)*(2*NEQ_Y+2)-1]
#define U2(u,xi,yi)   u[(xi)*(2*NEQ_Y+2)+2*(yi)]
#define U3(u,xi,yi)   u[(xi)*(2*NEQ_Y+2)+2*(yi)+1]
#define U4(u,xi)      u[(xi)*(2*NEQ_Y+2)+2*NEQ_Y]
```

Here, `u` is expected to be a pointer to the solution vector, i.e., of type `double*`. Note the parenthesis around `xi` and `yi`—they are important to avoid problems with macro substitution and operator preference when invoking the macro with arguments like `U1(u,i-1)`. Another important observation is that we may not try to retrieve the value u_0^1, because it is given by the boundary condition and is not stored in the solution vector $\mathbf{u}$ (thus, nor in `u`). Invoking `U1(u,0)` leads to accessing memory at `u[-1]`, which is illegal and can lead to segmentation fault (or other unpredictable results).

Function declarations

Next, we declare the functions that we use in the program. We define them later. We have a function for printing parameters used in the computation

```
void   print_summary();
```

for initializing the solution vector with initial condition

```
void   set_initial_profiles(N_Vector u_vec);
```

and for setting up the CVODE solver

```
void* initialize_cvode(N_Vector u_0_vec, CVRhsFn rhs_fn);
```

Next, we declare the core function of the program—the implementation of the right-hand side function **f**

```
int    two_scale_corrosion_rhs(double t, N_Vector u_vec,
           N_Vector udot_vec, void* user_data);
```

Since this function is called by CVODE routines, its interface (the number and types of its arguments and the return type) must conform to what CVODE expects. Next, we declare the non-linear reaction rate function η

```
double eta(double a, double b);
```

a function for saving the solution to a file

```
void   save_output(N_Vector u_vec);
```

and for printing some final statistics for the CVODE solver

```
void   print_final_cvode_stats(void* cvode_mem);
```

The implementation of `print_summary`, `save_output` and `print_final_cvode_stats` is not described in this chapter, but it can be found in Appendix A.

Main function

Next, we define the main function, which is the entry point of the program

```
int main(void) {
```

followed by variable declarations. We declare the pointer to the CVODE solver memory block

```
    void*         cvode_mem;
```

the solution vector `u_vec` as a type `N_Vector` that CVODE can work with

```
    N_Vector      u_vec;
```

and finally variables for storing the reached time and the time step

```
    double        t, tout;
    int           iout;
```

We allocate the solution vector `u_vec` of `NEQ` elements, check for an error in memory allocation, immediately initialize its values and save the initial condition to a file

```
    u_vec = N_VNew_Serial((long)NEQ);
    if (u_vec == NULL) {
        exit(EXIT_FAILURE);
    }
    set_initial_profiles(u_vec);
    save_output(u_vec);
```

Then, we allocate and initialize the CVODE solver by calling our helper function giving it as arguments the solution vector and pointer to the function that implements the system's right-hand side

```
    cvode_mem = initialize_cvode(u_vec, two_scale_corrosion_rhs);
```

and we print the summary of used paramaters

```
    print_summary();
```

Next, we enter the main computational loop of the program: we iterate with `iout` over the number of output times given by `N_OUT`

```
    for (iout = 1; iout <= N_OUT; ++iout) {
```

In the body of the loop, we calculate the next output time and store it in `tout`, call the main routine of CVODE solver `CVode` and check for success, save the solution and print indication of progress to the screen

```
        tout = iout*DT;
        if (CVode(cvode_mem, tout, u_vec, &t, CV_NORMAL) != 0) {
            exit(EXIT_FAILURE);
        }
        save_output(u_vec);
        printf("Step␣%5u␣/␣%5u\r", iout, N_OUT);
        fflush(stdout);
    }
```

When the computation is finished, we print some statistics about the CVODE solver, free allocated memory and exit the program

```
    print_final_cvode_stats(cvode_mem);
    N_VDestroy_Serial(u_vec);
    CVodeFree(&cvode_mem);
    return EXIT_SUCCESS;
}
```

Initial condition

We initialize the values in `u_vec` from the initial condition, i.e., from the constants `U*_INIT` defined above. We do this in a helper function `set_initial_profiles` which also serves us here as an example of how to use the macros to access values of the functions u_h^k, $k \in \{1, 2, 3, 4\}$. We first extract the pointer to the actual data from the `N_Vector` structure using the macro `NV_DATA_S`. Then, in the outer loop we iterate over the x-direction, while in the inner loop we iterate over the y-direction. Note how the access pattern visits all the elements in `u_vec` sequentially and how we avoid accessing `U1(u,0)`.

```
void set_initial_profiles(N_Vector u_vec) {
    double* u = NV_DATA_S(u_vec);
    int xi, yi;

    for (xi = 0; xi <= N_X; ++xi) {
        if (xi != 0) {
            U1(u,xi) = U1_INIT;
        }
        for (yi = 0; yi <= N_Y; ++yi) {
            U2(u,xi,yi) = U2_INIT;
            U3(u,xi,yi) = U3_INIT;
        }
        U4(u,xi) = U4_INIT;
    }
}
```

Setting up the CVODE solver

We set up and initialize the CVODE solver in another helper function, `initialize_cvode`, which takes the vector with initial condition and the right-hand side function as parameters and returns a pointer to the allocated CVODE solver memory structure

```
void* initialize_cvode(N_Vector u_0_vec, CVRhsFn rhs_fn) {
    int flag;
```

Then, we call `CVodeCreate` to instantiate a solver object and specify Backward Differentiation Formula as the linear multistep method and the use of a Newton iteration for solving the non-linear system

```
    void* cvode_mem = CVodeCreate(CV_BDF, CV_NEWTON);
    if (cvode_mem == NULL) { exit(EXIT_FAILURE); }
```

Next, we call `CVodeInit` to allocate internal object memory and to initialize the solver giving it the right-hand side function, the initial time 0 and the initial dependent variable vector `u_0_vec`

```
    flag = CVodeInit(cvode_mem, rhs_fn, 0.0, u_0_vec);
    if (flag != 0 ) { exit(EXIT_FAILURE); }
```

As the next step, we set the scalar relative and absolute tolerances `REL_TOL` and `ABS_TOL` and we increase the internal maximum number of steps CVODE can take

```
    flag = CVodeSStolerances(cvode_mem, REL_TOL, ABS_TOL);
    if (flag != 0 ) { exit(EXIT_FAILURE); }
    flag = CVodeSetMaxNumSteps(cvode_mem, 1000000L);
    if (flag != 0 ) { exit(EXIT_FAILURE); }
```

Finally, we call `CVSpgmr` to specify the linear solver GMRES with no preconditioning (see also Exercise 7.4) and return the pointer to CVODE memory

```
    flag = CVSpgmr(cvode_mem, PREC_NONE, 30);
    if (flag != 0 ) { exit(EXIT_FAILURE); }
    return cvode_mem;
}
```

For additional details, we refer the reader to the CVODE User's Manual.

Right-hand side function

In this section we describe the core function of the program, `two_scale_corrosion_rhs`, that implements the right-hand side $\mathbf{f}$ of our system (7.5)

```
int two_scale_corrosion_rhs(double t, N_Vector u_vec,
        N_Vector udot_vec, void *user_data)
{
```

The arguments represent the current time `t` (not used in the function, because the right-hand side does not depend explicitly on time), the vector with dependent variable `u_vec` (should not and is not changed in the function), the output vector containing $\mathbf{f}(\mathbf{u})$ and a pointer to user data, which is not used in this function because all the parameters are available as global macro constants. Should our program grow in size and be split into several files, it would be advisable and convenient gather the parameters into a structure and pass a pointer to this structure when initializing CVode solver memory. That pointer then would be available here as `user_data`.

Next, we extract pointers to the actual data from `u_vec` and `udot_vec`

```
    double* u = NV_DATA_S(u_vec);
    double* udot = NV_DATA_S(udot_vec);
```

and we declare some variables that we need below

```
    double  u1, u2, u3;
    double  BHu1u2, etau3u4;
    double  u1_left, u1_right;
    double  u2_left, u2_right;
```

```
double  u3_left, u3_right;
int     xi, yi;
```

Now, we employ the familiar nested loop iterating over the nodes of our two-scale grids and start evaluating the right-hand side

```
for (xi = 0; xi <= N_X; ++xi) {
```

First, we deal with the equation (7.1) by evaluating the two-scale sink/source coupling term $Bi(Hu_i^1 - u_{i,0}^2)$, which we store in a local variable for later use when computing the boundary condition for u_h^2

```
    if (xi != 0) {
        u1 = U1(u,xi);
    } else {
        u1 = U1_D;
    }
    BHu1u2 = BIOT_NUMBER*(H*u1 - U2(u,xi,0));
```

For the evaluation of discrete Laplacian we need neighboring values at nodes $i-1$ and $i+1$, but we have to take into account the Dirichlet boundary condition at $x = 0$ and zero Neumann condition at $x = L$

```
    if (xi != 0) {
        if (xi != 1) {
            u1_left = U1(u,xi-1);
        } else {
            u1_left = U1_D;
        }
        u1_right = (xi != N_X) ? U1(u,xi+1) : u1_left;
```

Finally, we evaluate the right-hand side of (7.1) and store the value in the `udot_vec` vector

```
        U1(udot,xi) = D_1*(u1_left - 2.0*u1 + u1_right)/(DX*DX)
          - BHu1u2;
    }
```

Next, we evaluate the right-hand side of (7.2) and (7.3). We iterate in a loop over nodes of the grid covering the micro-cell Y

```
    for (yi = 0; yi <= N_Y; ++yi) {
```

and extract the values of u_h^2 and u_h^3 at nodes $i-1$, i and $i+1$ taking into account the boundary conditions. Note that we store the value of $\eta(u_{i,N_y}^3, u_i^4)$ for later reuse to avoid recomputing this (possibly expensive) function

```
        if (yi != 0) {
            u2_left = U2(u,xi,yi-1);
            u3_left = U3(u,xi,yi-1);
        } else {
            u2_left = U2(u,xi,1) + 2.0*DY/D_2*BHu1u2;
            u3_left = U3(u,xi,1);
        }
        u2 = U2(u,xi,yi);
        u3 = U3(u,xi,yi);
        if (yi != N_Y) {
            u2_right = U2(u,xi,yi+1);
            u3_right = U3(u,xi,yi+1);
        } else {
```

```
            etau3u4 = eta(u3, U4(u,xi));
            u2_right = u2_left;
            u3_right = u3_left - 2.0*DY/D_3*etau3u4;
        }
```

Now, all that remains is to evaluate the right-hand side of (7.2)

```
        U2(udot,xi,yi) = D_2*(u2_left - 2.0*u2 + u2_right)/(DY*DY)
          - ALPHA*u2 + BETA*u3;
```

of (7.3)

```
        U3(udot,xi,yi) = D_3*(u3_left - 2.0*u3 + u3_right)/(DY*DY)
          + ALPHA*u2 - BETA*u3;
    }
```

of (7.4)

```
    U4(udot,xi) = etau3u4;
}
```

and exit the function return 0 to indicate success to the caller

```
    return 0;
}
```

We conclude the description of the program by listing the function `eta`, whose implementation is straightforward

```
double eta(double a, double b) {
    if (a > 0.0 && b < C_BAR) {
        return K*pow(a, PARTIAL_ORDER_P)*pow(C_BAR - b, PARTIAL_ORDER_Q);
    } else {
        return 0.0;
    }
}
```

7.4. Exercises

EXERCISE 7.1. Even if the program described in this chapter consists of only single file, it depends on an external library, whose header and library files can be located in different places depending on the operating system and compiler. As the source code and number of files grows, there arise internal dependencies between individual components. In order to facilitate portability and ease of compilation under different environments, various tools have been developed over years. As you extend the program and write your own, knowledge of such a tool can come very handy. CMake[1] is one such popular, modern tool that enables portable compilation under Windows as well as UNIX-based systems (e.g., Linux or Mac OS X). Write a CMake script for compiling our simple program and try to compile it under different operating systems and compilers.

EXERCISE 7.2. Learn how to use Gnuplot[2] and write a script for visualization of the numerical data from our program.

EXERCISE 7.3. Implement the simple ordering described in the text of this chapter and see if and how it affects the performance compared to our good ordering. Determine the bandwidth of the Jacobian of $\mathbf{f}$ in both cases.

[1] http://www.cmake.org/
[2] http://www.gnuplot.info/

EXERCISE 7.4. CVODE library offers various dense and Krylov iterative linear solvers (with or without preconditioning) that are used in the non-linear Newton solver.

1. Learn how to set up CVODE to use these solvers and modify the code accordingly.
2. Experiment with different solvers and see if and how they affect the performance of the program.
3. Modify the source code to use the built-in preconditioner CVBANDPRE and experiment, how the simple and good ordering affect the performance.

EXERCISE 7.5. Remove the dependence on the external CVODE library by implementing your own time integration solver. For instance, try to implement an explicit Runge-Kutta method with embedded higher-order estimate so that you can change the time step size adaptively, and compare the performance of both solvers. As a simpler alternative, try to use a Runge-Kutta solver as implemented, e.g., in GSL[3].

EXERCISE 7.6. Taking inspiration from the program presented in this chapter implement the numerical scheme from Exercise 6.2. Start with Ω and Y being one-dimensional as in this chapter. To make the simulation more interesting, try to take the relevant problem parameters (like $d(y)$, $c_F(y)$ and $c_B(y)$) non-constant depending on y. Try to extend the program for Y being two-dimensional.

[3] http://www.gnu.org/s/gsl/

APPENDIX A

Source code

```
#include <stdlib.h>  /* standard library functions */
#include <stdio.h>   /* standard input/output functions */
#include <math.h>
#include <time.h>
#include <sys/types.h>
#include <sys/stat.h>

/* CVODE header files */
#include <cvode/cvode.h>
#include <cvode/cvode_spgmr.h>
#include <nvector/nvector_serial.h>
#include <sundials/sundials_math.h>

/* parameters */
#define BIOT_NUMBER       864.0
#define H                 2.5
#define C_BAR             1.0
#define PARTIAL_ORDER_P   1.0
#define PARTIAL_ORDER_Q   1.0

/* diffusivities */
#define D_1         864.0
#define D_2         0.0864
#define D_3         0.0864

/* rate constants */
#define ALPHA       7.2
#define BETA        0.84
#define K           1.0

/* boundary and initial conditions */
#define U1_D        0.1
#define U1_INIT     U1_D
#define U2_INIT     0.0
#define U3_INIT     0.00001
#define U4_INIT     0.0

/* geometry */
#define L_X         500.0
#define L_Y         10.0
#define N_X         256
```

```
#define N_Y          32
#define DX           (L_X/N_X)
#define DY           (L_Y/N_Y)
#define NEQ_X        (N_X+1)
#define NEQ_Y        (N_Y+1)
#define NEQ          (2*NEQ_X+2*NEQ_X*NEQ_Y-1)

/* time integration and output*/
#define T            1000.0
#define ABS_TOL      1.0e-9
#define REL_TOL      1.0e-9
#define N_OUT        100
#define DT           (T/N_OUT)

/* macros to access solution vector */
#define U1(u,xi)     u[(xi)*(2*NEQ_Y+2)-1]
#define U2(u,xi,yi)  u[(xi)*(2*NEQ_Y+2)+2*(yi)]
#define U3(u,xi,yi)  u[(xi)*(2*NEQ_Y+2)+2*(yi)+1]
#define U4(u,xi)     u[(xi)*(2*NEQ_Y+2)+2*NEQ_Y]

void   print_summary();
void   set_initial_profiles(N_Vector u_vec);
void*  initialize_cvode(N_Vector u_0_vec, CVRhsFn rhs_fn);
int    two_scale_corrosion_rhs(double t, N_Vector u_vec,
           N_Vector udot_vec, void* user_data);
double eta(double a, double b);
void   save_output(N_Vector u_vec);
void   print_final_cvode_stats(void* cvode_mem);

int main(void) {
    void*        cvode_mem;
    N_Vector     u_vec;
    double       t, tout;
    int          iout;

    u_vec = N_VNew_Serial((long)NEQ);
    if (u_vec == NULL) {
        exit(EXIT_FAILURE);
    }
    set_initial_profiles(u_vec);
    save_output(u_vec);

    cvode_mem = initialize_cvode(u_vec, two_scale_corrosion_rhs);

    print_summary();

    for (iout = 1; iout <= N_OUT; ++iout) {
        tout = iout*DT;
        if (CVode(cvode_mem, tout, u_vec, &t, CV_NORMAL) != 0) {
            exit(EXIT_FAILURE);
```

```
        }
        save_output(u_vec);
        printf("Step␣%5u␣/␣%5u\r", iout, N_OUT);
        fflush(stdout);
    }
    print_final_cvode_stats(cvode_mem);
    N_VDestroy_Serial(u_vec);
    CVodeFree(&cvode_mem);
    return EXIT_SUCCESS;
}

void set_initial_profiles(N_Vector u_vec) {
    double* u = NV_DATA_S(u_vec);
    int xi, yi;

    for (xi = 0; xi <= N_X; ++xi) {
        if (xi != 0) {
            U1(u,xi) = U1_INIT;
        }
        for (yi = 0; yi <= N_Y; ++yi) {
            U2(u,xi,yi) = U2_INIT;
            U3(u,xi,yi) = U3_INIT;
        }
        U4(u,xi) = U4_INIT;
    }
}

void* initialize_cvode(N_Vector u_0_vec, CVRhsFn rhs_fn) {
    int flag;

    void* cvode_mem = CVodeCreate(CV_BDF, CV_NEWTON);
    if (cvode_mem == NULL) { exit(EXIT_FAILURE); }
    flag = CVodeInit(cvode_mem, rhs_fn, 0.0, u_0_vec);
    if (flag != 0 ) { exit(EXIT_FAILURE); }
    flag = CVodeSStolerances(cvode_mem, REL_TOL, ABS_TOL);
    if (flag != 0 ) { exit(EXIT_FAILURE); }
    flag = CVodeSetMaxNumSteps(cvode_mem, 1000000L);
    if (flag != 0 ) { exit(EXIT_FAILURE); }
    flag = CVSpgmr(cvode_mem, PREC_NONE, 30);
    if (flag != 0 ) { exit(EXIT_FAILURE); }
    return cvode_mem;
}

int two_scale_corrosion_rhs(double t, N_Vector u_vec,
        N_Vector udot_vec, void *user_data)
{
    double* u = NV_DATA_S(u_vec);
    double* udot = NV_DATA_S(udot_vec);
    double  u1, u2, u3;
    double  BHu1u2, etau3u4;
```

```
    double  u1_left, u1_right;
    double  u2_left, u2_right;
    double  u3_left, u3_right;
    int     xi, yi;

    for (xi = 0; xi <= N_X; ++xi) {
        if (xi != 0) {
            u1 = U1(u,xi);
        } else {
            u1 = U1_D;
        }
        BHu1u2 = BIOT_NUMBER*(H*u1 - U2(u,xi,0));
        if (xi != 0) {
            if (xi != 1) {
                u1_left = U1(u,xi-1);
            } else {
                u1_left = U1_D;
            }
            u1_right = (xi != N_X) ? U1(u,xi+1) : u1_left;
            U1(udot,xi) = D_1*(u1_left - 2.0*u1 + u1_right)/(DX*DX)
              - BHu1u2;
        }
        for (yi = 0; yi <= N_Y; ++yi) {
            if (yi != 0) {
                u2_left = U2(u,xi,yi-1);
                u3_left = U3(u,xi,yi-1);
            } else {
                u2_left = U2(u,xi,1) + 2.0*DY/D_2*BHu1u2;
                u3_left = U3(u,xi,1);
            }
            u2 = U2(u,xi,yi);
            u3 = U3(u,xi,yi);
            if (yi != N_Y) {
                u2_right = U2(u,xi,yi+1);
                u3_right = U3(u,xi,yi+1);
            } else {
                etau3u4 = eta(u3, U4(u,xi));
                u2_right = u2_left;
                u3_right = u3_left - 2.0*DY/D_3*etau3u4;
            }
            U2(udot,xi,yi) = D_2*(u2_left - 2.0*u2 + u2_right)/(DY*DY)
              - ALPHA*u2 + BETA*u3;
            U3(udot,xi,yi) = D_3*(u3_left - 2.0*u3 + u3_right)/(DY*DY)
              + ALPHA*u2 - BETA*u3;
        }
        U4(udot,xi) = etau3u4;
    }

    return 0;
}
```

```
double eta(double a, double b) {
    if (a > 0.0 && b < C_BAR) {
        return K*pow(a, PARTIAL_ORDER_P)*pow(C_BAR - b, PARTIAL_ORDER_Q);
    } else {
        return 0.0;
    }
}

void print_summary() {
    printf("Omega = (0,%f)\n", L_X);
    printf("Y = (0,%f)\n", L_Y);
    printf("grid size = %u x %u\n", NEQ_X, NEQ_Y);
    printf("step sizes: h_x = %f, h_y = %f\n", DX, DY);
    printf("d_1 = %f, d_2 = %f, d_3 = %f\n", D_1, D_2, D_3);
    printf("alpha = %f, beta = %f, k = %f\n", ALPHA, BETA, K);
    printf("Biot = %f, c_bar = %f, H = %f, p = %f, q = %f\n",
        BIOT_NUMBER, C_BAR, H, PARTIAL_ORDER_P, PARTIAL_ORDER_Q);
    printf("u1_D = %f\n", U1_D);
    printf("u1_0 = %f, u2_0 = %f, u3_0 = %f, u4_0 = %f\n",
        U1_INIT, U2_INIT, U3_INIT, U4_INIT);
    printf("time interval = (0,%f)\n", T);
    printf("relative tolerance = %g\nabsolute tolerance = %g\n\n",
        REL_TOL, ABS_TOL);
}

void save_output(N_Vector u_vec) {
    static int  count = 0;
    static char output_dir[256];
    char        filename[512];
    int         xi, yi;
    FILE*       fout;
    double*     u = NV_DATA_S(u_vec);

    if (count == 0) {
        time_t     rawtime;
        struct tm* timeinfo;
        time(&rawtime);
        timeinfo = localtime(&rawtime);
        strftime(output_dir, (size_t)255, "result_%Y%m%d_%H%m%S", timeinfo);
        if (0 != mkdir(output_dir, 0755)) {
            perror("Failed to create output directory");
            exit(EXIT_FAILURE);
        } else {
            printf("Writing results to directory: %s\n", output_dir);
        }
    }

    sprintf(filename, "%s/u1_%05u.dat", output_dir, count);
    fout = fopen(filename, "wt");
```

```
    if (fout == NULL) {
        perror("Failed␣to␣create␣output␣file␣for␣u1");
        exit(EXIT_FAILURE);
    }
    fprintf(fout, "%f␣%f\n", 0.0, U1_D);
    for (xi = 1; xi <= N_X; ++xi) {
        fprintf(fout, "%f␣%f\n", xi*DX, U1(u,xi));
    }
    fclose(fout);

    sprintf(filename, "%s/u2_%05u.dat", output_dir, count);
    fout = fopen(filename, "wt");
    if (fout == NULL) {
        perror("Failed␣to␣create␣output␣file␣for␣u2");
        exit(EXIT_FAILURE);
    }
    for (xi = 0; xi <= N_X; ++xi) {
        for (yi = 0; yi <= N_Y; ++yi) {
            fprintf(fout, "%f␣%f␣%f\n", xi*DX, yi*DY, U2(u,xi,yi));
        }
        fprintf(fout, "\n");
    }
    fclose(fout);

    sprintf(filename, "%s/u3_%05u.dat", output_dir, count);
    fout = fopen(filename, "wt");
    if (fout == NULL) {
        perror("Failed␣to␣create␣output␣file␣for␣u3");
        exit(EXIT_FAILURE);
    }
    for (xi = 0; xi <= N_X; ++xi) {
        for (yi = 0; yi <= N_Y; ++yi) {
            fprintf(fout, "%f␣%f␣%f\n", xi*DX, yi*DY, U3(u,xi,yi));
        }
        fprintf(fout, "\n");
    }
    fclose(fout);

    sprintf(filename, "%s/u4_%05u.dat", output_dir, count);
    fout = fopen(filename, "wt");
    if (fout == NULL) {
        perror("Failed␣to␣create␣output␣file␣for␣u4");
        exit(EXIT_FAILURE);
    }
    for (xi = 0; xi <= N_X; ++xi) {
        fprintf(fout, "%f␣%f\n", xi*DX, U4(u, xi));
    }
    fclose(fout);

    ++count;
```

```
}

void print_final_cvode_stats(void* cvode_mem) {
    long int lenrw, leniw ;
    long int lenrwLS, leniwLS;
    long int nst, nfe, nsetups, nni, ncfn, netf;
    long int nli, npe, nps, ncfl, nfeLS;

    /* CVODE solver stats */
    CVodeGetWorkSpace(cvode_mem, &lenrw, &leniw);
    CVodeGetNumSteps(cvode_mem, &nst);
    CVodeGetNumRhsEvals(cvode_mem, &nfe);
    CVodeGetNumLinSolvSetups(cvode_mem, &nsetups);
    CVodeGetNumErrTestFails(cvode_mem, &netf);
    CVodeGetNumNonlinSolvIters(cvode_mem, &nni);
    CVodeGetNumNonlinSolvConvFails(cvode_mem, &ncfn);

    /* Spils (linear solver) stats */
    CVSpilsGetWorkSpace(cvode_mem, &lenrwLS, &leniwLS);
    CVSpilsGetNumLinIters(cvode_mem, &nli);
    CVSpilsGetNumPrecEvals(cvode_mem, &npe);
    CVSpilsGetNumPrecSolves(cvode_mem, &nps);
    CVSpilsGetNumConvFails(cvode_mem, &ncfl);
    CVSpilsGetNumRhsEvals(cvode_mem, &nfeLS);

    printf("\n\nFinal␣CVODE␣statistics:\n\n");
    printf("Real␣workspace␣size␣=␣%5ld\n", lenrw);
    printf("Integer␣workspace␣size␣=␣%5ld\n", leniw);
    printf("Linear␣solver␣real␣workspace␣size␣=␣%5ld\n", lenrwLS);
    printf("Linear␣solver␣integer␣workspace␣size␣=␣%5ld\n", leniwLS);
    printf("Number␣of␣steps␣taken␣=␣%5ld\n", nst);
    printf("Number␣of␣RHS␣evaluations␣=␣%5ld\n", nfe);
    printf("Number␣of␣RHS␣evaluations␣in␣linear␣solver␣=␣%5ld\n", nfeLS);
    printf("Number␣of␣nonlinear␣solver␣iterations␣=␣%5ld\n", nni);
    printf("Number␣of␣linear␣solver␣iterations␣=␣%5ld\n", nli);
    printf("Number␣of␣linear␣solver␣setups␣=␣%5ld\n", nsetups);
    printf("Number␣of␣error␣test␣fails␣=␣%5ld\n", netf);
    printf("Number␣of␣preconditioner␣evaluations␣=␣%5ld\n", npe);
    printf("Number␣of␣preconditioner␣solves␣=␣%5ld\n", nps);
    printf("Number␣of␣nonlinear␣convergence␣fails␣=␣%5ld\n", ncfn);
    printf("Number␣of␣linear␣solver␣convergence␣fails␣=␣%5ld\n\n", ncfl);
}
```

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