

Homogenization Techniques for Lower Dimensional Structures

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Dissertation

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Abstract

This thesis is concerned with extensions and applications of the theory of periodic unfolding in the field of (mathematical) homogenization.

The first part extends the applicability of homogenization in domains with evolving microstructure to the case of evolving hypersurfaces: We consider a diffusion-reaction equation inside a perforated domain, where also surface diffusion and reaction takes place. Upon a transformation to a referential geometry, we (formally) obtain a transformed set of equations. We show that homogenization techniques can be applied to this transformed formulation. Special emphasis is placed on possible nonlinear reaction rates on the surface, a fact which requires special results for estimation and convergence results. In the limit, we obtain a macroscopic system, where each point of the domain is coupled to a system posed in the reference (micro-)geometry. Additionally, this reference geometry is evolving.

In a second part, we are concerned with an extension of the notion of periodic unfolding to some Riemannian manifolds: We develop a notion of periodicity on nonflat structures in a local fashion with the help of a special atlas. If this atlas satisfies a compatibility condition, unfolding operators can be defined which operate on the manifold. We show that continuity and compactness theorems hold, generalizing the well-known results from the established theory. As an application of this newly developed results, we apply the unfolding operators to a strongly elliptic model problem. Again, we obtain a generalization of results well-known in homogenization. Moreover, we are also able to show some additional smoothness-properties of the solution of the cell problem, and we construct an equivalence relation for different atlases. With respect to this relation, the limit problem is independent of the parametrization of the manifold.

Zusammenfassung

Diese Dissertationsschrift befasst sich mit Erweiterungen und Anwendungen der Theorie des "Periodic Unfolding" auf dem Gebiet der Homogenisierung.

Im ersten Teil zeigen wir, dass Homogenisierung in Gebieten mit veränderlicher Mikrostruktur auch bei sich verändernden Hyperflächen angewandt werden kann: Wir betrachten eine Diffusions-Reaktionsgleichung in einem Gebiet mit periodisch verteilten Löchern, an deren Rändern ebenfalls Diffusion und Reaktion stattfindet. Nach Transformation der erhaltenen Gleichungen auf eine Referenzgeometrie erhalten wir (formal) ein transformiertes Gleichungssystem. Wir zeigen, dass Homogenisierungstechniken auf diese Formulierung des Problems angewendet werden können. Dabei betrachten wir insbesondere nichtlineare Oberflächenreaktionsraten – dies macht weitere Resultate nötig, um Konvergenzaussagen und Abschätzungen zu gewinnen. Im Grenzwert erhalten wir ein System in der makroskopischen Geometrie, welches an jedem Punkt mit einem System in der mikroskopischen Geometrie gekoppelt ist. Die Evolution der Struktur findet nur dort statt.

Im zweiten Teil erweitern wir die Theorie des "Periodic Unfolding" auf Riemannsche Mannigfaltigkeiten: Wir entwickeln den Begriff der Periodizität für solche Objekte lokal mit Hilfe eines ausgezeichneten Atlases. Falls dieser eine Kompatibilitätsbedingung erfüllt, können Entfaltungsooperatoren auf der Mannigfaltigkeit definiert werden. Wir zeigen, dass sich viele Resultate aus der bisher entwickelten Theorie übertragen lassen. Als Anwendung betrachten wir eine elliptische Modellgleichung. Im Grenzwert erhalten wir wiederum eine Verallgemeinerung bekannter Resultate. Zusätzlich zeigen wir Glattheitseigenschaften der Lösung des Zellproblems, und wir konstruieren eine Äquivalenzrelation für Atlanten. Bezüglich dieser Relation ist der Grenzwert des homogenisierten Problems unabhängig von der Parametrisierung.

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List of Symbols

Ω	Domain in \mathbb{R}^n , page 38
\mathbb{R}_u^n	Halfspace of \mathbb{R}^n , characterized by some vector $u \in \mathbb{R}^n$, page 92
Id	Identity map, page 39
$\det F$	Determinant of the linear map F , page 39
\longrightarrow	(Strong) convergence, page 36
\rightharpoonup	Weak convergence, page 36
$[\cdot, \cdot]$	Euclidean scalar product in \mathbb{R}^n or induced Euclidean scalar product on M , page 32
$(\cdot, \cdot)_H$	Scalar product on the Hilbert space H , page 50
$[\cdot, \cdot]$	Lie bracket for vector fields; also used for closed intervals in \mathbb{R} , page 93
δ_{ij}, δ_j^i	Kronecker delta, page 44
\mathcal{O}	Landau symbol, “big O” notation, page 111
e_i	i -th unit vector of \mathbb{R}^n , page 92
$\text{dist}(z, A)$	Distance of the point z to the set A , page 39
X^*	Dual space of the Banach space X , page 50
$\ \cdot\ _X$	Norm on the Banach space X , page 52
$L^p(G)$	Banach space of measurable functions on G whose p -th power is Lebesgue integrable, $p \in [1, \infty)$, page 50
$L^\infty(G)$	Banach space of measurable, essentially bounded functions on G , page 50
$\mathcal{C}^k(G)$	Space of k times continuously differentiable functions on G , page 50
$W^{k,p}(G)$	Sobolev space of k times weakly differentiable functions with derivatives in $L^p(G)$, page 154
$W^{r,p}E$	Sobolev space of sections of a vector bundle E (of differentiability r and integrability p), page 159

$L^p(0, T; X)$	L^p -Bochner space of functions on $[0, T]$ with values in the Banach space X , page 50
$H^1(G)$	Shorthand notation for $W^{1,2}(G)$, page 50
H	The space $L^2(\Omega^\varepsilon(0))$, page 50
H_Γ	The space $L^2(\Gamma^\varepsilon(0))$, page 50
V	The space $H^1(\Omega^\varepsilon(0))$, page 50
V_Γ	The space $H^1(\Gamma^\varepsilon(0))$, page 50
\mathcal{V}	The space $L^2(0, T; V)$, page 50
\mathcal{V}_Γ	The space $L^2(0, T; V_\Gamma)$, page 50
\mathcal{W}	The space $\{u \in \mathcal{V} : u' \in \mathcal{V}^*\}$, page 50
\mathcal{W}_Γ	The space $\{u \in \mathcal{V} : \Gamma : u' \in \mathcal{V}_\Gamma^*\}$, page 50
$\#$	Number of; when used as a subscript: periodicity with respect to the reference cell of functions in the corresponding function space, page 38
\mathcal{D}	Total derivative, page 134
∇	Gradient operator; a subscript indicates the variable with respect to which the derivative is taken, page 32
∇^Γ	Surface gradient operator; a subscript indicates the variable with respect to which the derivative is taken, page 42
∇_M	Gradient on M with respect to the metric g_M , page 105
$\nabla_Y^{(x,\varepsilon)}$	Gradient on Y with respect to the metric $\mathcal{T}_{\mathcal{A}}^\varepsilon(g_M)$, page 105
$\nabla_Y^{(x)}$	Gradient on Y with respect to the (fixed) metric coefficients $g_{ij}(x)$, page 105
div	Divergence operator; a subscript indicates the variable with respect to which the derivative is taken, page 32
div^Γ	Surface divergence operator; a subscript indicates the variable with respect to which the derivative is taken, page 42
div_M	Divergence on M with respect to the metric g_M , page 105
$\text{div}_Y^{(x,\varepsilon)}$	Divergence on Y with respect to the metric $\mathcal{T}_{\mathcal{A}}^\varepsilon(g_M)$, page 105
$\text{div}_Y^{(x)}$	Divergence on Y with respect to the (fixed) metric coefficients $g_{ij}(x)$, page 105

d	Exterior derivative; a subscript indicates the variable with respect to which the derivative is taken, page 32
$\frac{Dc}{Dt}$	Lagrangian derivative of the function c , page 31
κ	Mean curvature; in general used with superscript, page 41
V	Normal velocity; in general used with superscript, page 41
v_M	Tangential velocity; in general used with superscript, page 41
\mathcal{T}^ε	Domain unfolding operator, page 35
$\mathcal{T}_b^\varepsilon$	Boundary unfolding operator, page 35
$\mathcal{T}_\phi^\varepsilon$	Unfolding operator acting on the chart ϕ , page 93
$\mathcal{T}_{\mathcal{A}}^\varepsilon$	Global unfolding operator with respect to the atlas \mathcal{A} , page 101
$[z] + \{z\}$	Decomposition of $z \in \mathbb{R}^n$ used in Periodic Unfolding, page 34
\simeq	Relation for the unfolding of integral expressions, page 102
Y	Reference cell, in general the unit cube of dimension $n \in \mathbb{N}$, page 38
$Y^{(x,\varepsilon)}$	Reference cell Y , endowed with an equivalent metric, page 101
$Y^{(x)}$	Reference cell Y , endowed with another equivalent metric, page 130
$(\cdot)_Y, (\cdot)_M$	Transport operators for vector fields, page 107
M	Manifold in Euclidean space, page 30
∂M	Boundary of M , page 92
\mathcal{A}	Atlas of a manifold, page 91
TM	Tangent bundle of M , page 92
g_M	Riemannian metric on M , page 92
dvol_M	Volume form on M with respect to the metric g_M , page 101
$\mathfrak{X}(M)$	Set of vector fields over M , page 33
$\Gamma(E)$	Set of smooth sections of the vector bundle E , page 92
$\frac{\partial}{\partial x^i}$	Local basis tangent vectors for the chart $\phi = (x^1, \dots, x^n)$, page 93
dx^i	Local basis 1-form stemming from the chart $\phi = (x^1, \dots, x^n)$, page 94
ϕ^*	Pullback with ϕ , page 93
ϕ_*	Pushforward with ϕ , page 93

$T_z \psi$	Tangential map of the function ψ in z , page 30
\wedge	Exterior product, page 95
$\Omega_k(G)$	Set of k -forms over G , page 94
$\Omega_k^n(G, F)$	Set of n -times continuously differentiable differential forms over G of degree k with values in the Banach space F , page 162
q^l	Shifted function q , $q^l(t, x) := q(t, x + l\varepsilon)$, page 72
δq	Difference $\delta q := q^l - q$, page 72
q^+	Positive part of the function q , $q^+ = \max\{0, q\}$, page 86
q^-	Negative part of the function q , $q^- = -\min\{0, q\}$, page 86

1 Introduction

Homogenization emerged during the 1960-1970s with the advent of more and more complex materials, like fibre reinforced plastic, carbon fibre filaments and other composite materials (see e.g. Chung [Chu10] for an overview). They are characterized by

- the existence of at least two length scales: A macroscopic scale on the level of the whole object (ranging e.g. from km to cm), and a microscale defining the internal structure (on the range of e.g. mm to nm);
- an internal structure which is given approximately by a periodic repetition of a reference structure.

Since simulations of objects with a total size in the order of meters requiring a spatial resolution of mm are not feasible even with modern computers, periodic homogenization is a method to derive effective material properties by employing the periodic structure of the underlying medium. This facilitates numerical simulations (see also the corresponding chapter in this work).

Homogenization relies on a description of material properties in the form

$$\mathcal{L}^\varepsilon u^\varepsilon = f, \tag{1.1}$$

where \mathcal{L}^ε is a known differential operator, u^ε is an unknown function and f is a given right hand side. The variable ε refers to the scale of the microstructure. It is assumed that the global structure can be obtained by a periodic repetition of a ε -scaled version of a reference structure being defined on a so-called reference cell (commonly denoted in the field by Y). Therefore, we obtain a family of problems depending on the scale parameter $\varepsilon > 0$.

One is now interested in showing that there exists a function u^0 such that u^ε converges to u^0 in a suitable sense for $\varepsilon \rightarrow 0$, and that there exists a differential operator \mathcal{L}^0 such that u^0 fulfills

$$\mathcal{L}^0 u^0 = f.$$

This equation is then interpreted to represent an effective description of the material.

Several methods have been devised to obtain the effective material properties:

- The method of **asymptotic expansion** (see for example the book by Bensoussan, Lions, and Papanicolaou [BLP78]) stipulates the existence of a series expansion of the unknown function u^ε

$$u^\varepsilon(x) = u^0\left(x, \frac{x}{\varepsilon}\right) + \varepsilon u_1\left(x, \frac{x}{\varepsilon}\right) + \varepsilon^2 u_2\left(x, \frac{x}{\varepsilon}\right) + \dots,$$

with functions u^0 and u_i , $i = 1, 2, \dots$. They depend on two variables x and $y = \frac{x}{\varepsilon}$, the first in the actual domain and the latter in the reference cell, extended by

periodicity. By inserting this expansion into the problem (1.1) and comparing terms of different orders of ε , one can derive equations for the summands on the right hand side. Note, however, that this method is only a formal one, yielding no mathematical proof of convergence.

- A mathematical proof of convergence can be obtained by the method of **oscillating test functions** developed by Tartar (see again [BLP78] or Cioranescu and Donato [CD99]). Unfortunately, for complex problems this method becomes tedious to apply.
- Therefore, Nguetseng and Allaire [Ngu89], [All92] developed the notion of **two-scale convergence**, a special notion of convergence being suitable for the problems described above. One advantage is that no special auxiliary functions have to be constructed, but the method works on its own.
- The latest development in the field is the method of **Periodic Unfolding** (see Cioranescu [CDG02], [CDZ06] or Damlamian [Dam05]). It is equivalent to two-scale convergence, but instead of using a special notion of convergence, it relies on "established" types of convergence (like weak and strong convergence in Banach spaces). This method has also been proven to be useful in the treatment of nonlinear problems, see for instance Neuss-Radu [NRJ07].

Periodic homogenization has long been used in the mathematical community only – however, results obtained by this technique seem to appear in the engineering literature more often recently: In [BMSS11], Brandmeier, Müller et. al. investigate elastic properties of solder materials in microelectronic devices. They derive effective material properties by using several methods, including an asymptotic expansion of the above type. Similarly, Bonnet [Bon07] investigates elastic properties of media with a periodic structure of fibers with the help of (mathematical) well known asymptotic results.

This thesis deals with extensions of the method of periodic unfolding in mathematical homogenization. In this work, the focus lies on two techniques: Homogenization with evolving microstructure (developed by Alber [Alb00] and Peter [Pet07]) – allowing for an evolution of the structure to be included in a homogenization setting, and the newly developed homogenization on Riemannian manifolds – permitting to treat homogenization problems on nonflat objects. The organization is as follows:

- In Chapter 2 we give an overview of heterogeneous catalysis and marine aggregates. These chemical and biological processes represent real world applications with respect to which the mathematical tools are developed.
- Chapter 3 extends the method of homogenization with evolving microstructure to domains containing an evolving hypersurface.
- In Chapter 4 we extend the notion of Periodic Unfolding to some Riemannian manifolds.
- Finally, in Chapter 5 we present some numerical simulations to illustrate the effectiveness of the homogenization method.

The different chapters can be read independently of each other. However, the reader should be familiar with the following two subjects: The notion of Periodic Unfolding – we refer to the introductory works by Cioranescu and Damlamian [CDG08] and [Dam05] and to Section 3.1.4 on page 33; and the basic constructions of differential geometry as

they appear for example in Amann and Escher [AE01]. Especially Chapter 4 of this work relies heavily on the definition of pushforwards and pullbacks, the tangential mapping and local representations, local basis vectors etc.

2 Porous Materials in Biology and Chemistry

In this chapter we describe several real life phenomena stemming from the fields of biology and chemistry, namely marine aggregates and some aspects of heterogeneous catalysis. In both cases, accurate and effective models are needed for the treatment of important aspects, the estimation of material exchange and the enhancement of industrial and other processes. We are going to deal with structures which – at least as an approximation – possess a periodic structure. Thus, homogenization techniques should in principle be applicable. On the other hand, however, all the examples also exhibit some features which are not amenable to mathematical techniques and results known today. This will be the guideline for the new tools and theorems we are going to develop in subsequent chapters.

2.1 Heterogeneous Catalysis

Where no further references are given, this section is based on Thomas and Thomas [TT97] as well as Campbell [Cam88]. According to [TT97], a catalyst is

”[a] substance that increases the rate of attainment of chemical equilibrium without itself undergoing chemical change.”

At the end of the 1990’s, 90% of all industrial processes involving chemistry used at least one catalyst in one production stage. Areas where catalysts are needed include

- Fuel: Cracking of the heavy parts of crude oil; desulfurization of fuel to avoid the poisoning of catalytic converters.
- Medicine: Fabrication of drugs.
- Food: Hydrogenation of fats to produce margarine which is not so prone to becoming rancid; production of fertilizers for the food industry; production of high fructose corn syrup from glucose syrup; production of L-aspartic acid (an artificial sweetener known as Aspartame).
- Fabrics and building materials: Polymers like PVC or nylon, for example.

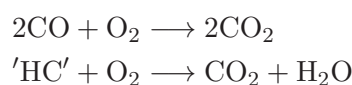
One has to distinguish between homogeneous and heterogeneous catalysis: The first refers to the fact that the catalyst is present in the same phase as the reactant, whereas the latter means that the phase of the catalysis is different from that of the reactants. This allows for an easy separation of the catalyst from the products stemming from the reaction. Due to that property, the majority of industrial relevant processes involve the heterogeneous flavour of catalysis. In the sequel, we only deal with heterogeneous catalysis.

2.1.1 Examples

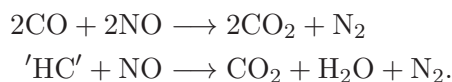
Automobile Exhaust Catalysts

The emergence of catalytic converters for automobiles started in the 1970s in California, due to a more restrictive legislation regarding exhaust gases.¹ Prior to the introduction of these "catcons", it contained larger amounts of carbon monoxide (CO), oxides of nitrogen (NO and NO₂, together named NO_x) and hydrocarbons (termed HC). These gases are toxic and are known to cause smog and acid rain. Furthermore, they also represent effective greenhouse gases, contributing to global warming.

Inside the catalytic converter, these substances react to the less harmful nitrogen (N₂), carbon dioxide (CO₂) and water H₂O according to the schematic reactions



as well as



These reactions are facilitated by the noble metals platinum (Pt), rhodium (Rh), and palladium (Pd). Due to their high price, there is a demand for an efficient converter design. Nowadays, a honeycomb ceramic structure is used, consisting of channels oriented in the direction of the flow of the exhaust gas. On the channel walls, highly porous aluminum oxide (Al₂O₃, also known as alumina) is attached such that the noble metals are embedded inside the porous matrix. In addition, stabilizing chemical compounds such as cerium oxide (Ce₂O) and barium oxide (BaO) are added.

The effectiveness of a catalytic converter depends on several factors, among them the distribution of the active components and the exhaust flow inside the converter. Since an effective catalytic reaction only takes place in a narrow temperature range and under sufficient feed of oxygen, these parameters have to be controlled as well. As one can see, the design and operation of catalytic converters is a complex task. Since the processes inside of it are not arbitrarily accessible, efficient simulations are very important in the developmental process. In the future, this will even play a more important role due to new legislation demanding an even further reduction of emissions.

Petroleum Processing

Crude oil harvested from drilling sites is of almost no direct use. First, it has to be distilled in columns leading to products like liquid petroleum gas, naphtha and gas oil. The latter two are treated further and finally yield fuel and petrol. Three important steps in this process are reforming, cracking, and desulfurization:

¹Comments on the history and development of automobile exhaust catalysts can be found in Ghandi, Graham and McCabe [GGM03] as well as [TT97], for example.

Reforming is the process of treating naphtha products such that one obtains gasoline with higher octane numbers (which is needed for modern high performance engines). This is obtained by catalytically restructuring hydrocarbons into more complex molecules. Traditionally, one uses Pt on a porous Al_2O_3 -support as a catalyst. The reaction takes place at around 500°C at a pressure between 5 and 40 bar. Modern bimetallic catalysts also contain iridium (Ir), rhenium (Re), or germanium (Ge).

The goal of **cracking** is to obtain a higher proportion of gasoline from crude oil. This is achieved by catalytically breaking down carbon-carbon bonds of larger molecules to get smaller ones while keeping the proportion of carcinogenic components low. This process is carried out at about 500°C and 70 bar with the help of zeolites charged with rare-earth metals. Zeolites are microporous minerals consisting of aluminum (Al), silicon (Si), and oxygen (O). Due to their complex structure, they are used to control the size of molecules which are "allowed" to undergo the catalytic reaction.

Desulfurization has to be carried out prior to the above processing steps. It designates the removal of unwanted elements (in this case sulfur) from crude oil. The reason for this is that sulfur (S) poisons the catalyst: It (more or less) permanently attaches to the active sites of it, thus reducing the catalytic effectiveness. Moreover, desulfurization improves the color and stability of the final gasoline product. A prototypical reaction is given by



The process is carried out with the help of supported cobalt/molybdenum oxides or nickel/tungsten oxides. Newer catalysts are based on molybdenum disulfide (MoS_2). Findings imply that the reactivity is different for edge and basal planes of the catalyst (see Skrabalak and Suslick [SS05]) – thus, the surface structure of the catalyst plays an important role. Hence, advanced manufacturing methods to obtain a high surface area have recently been investigated: Figure 2.1 shows catalysts used in methanol fuel cell electrodes manufactured by spray pyrolysis, see Bang, Han et. al. [BHS⁺07] for the results as well as Kodas and Hampden-Smith [KHS99] for an introduction to the process. Similar techniques are also used in the production of MoS_2 -catalysts for desulfurization in [SS05], yielding structures closely resembling those shown in the figure.

2.1.2 Aspects of Physics and Modeling

Chemisorption

A catalyst facilitates reactions by adsorbing² molecules to its surface (see again the references cited at the beginning of this chapter). There, bonds between the atoms are weakened, facilitating chemical reactions. Here, one has to distinguish between two types of adsorption: Physical adsorption and chemisorption. Whereas the former is characterized by van-der-Waals forces, the latter is established due to a rearrangement of electrons and a rupture of chemical bonds. In heterogeneous catalysis, first the physical adsorption keeps molecules in the vicinity of active sites, followed by chemisorption which

²Note that the term "adsorption" designates the adhesion of substances to the surface of the adsorbate, whereas "absorption" means the incorporation of a substance into another one.

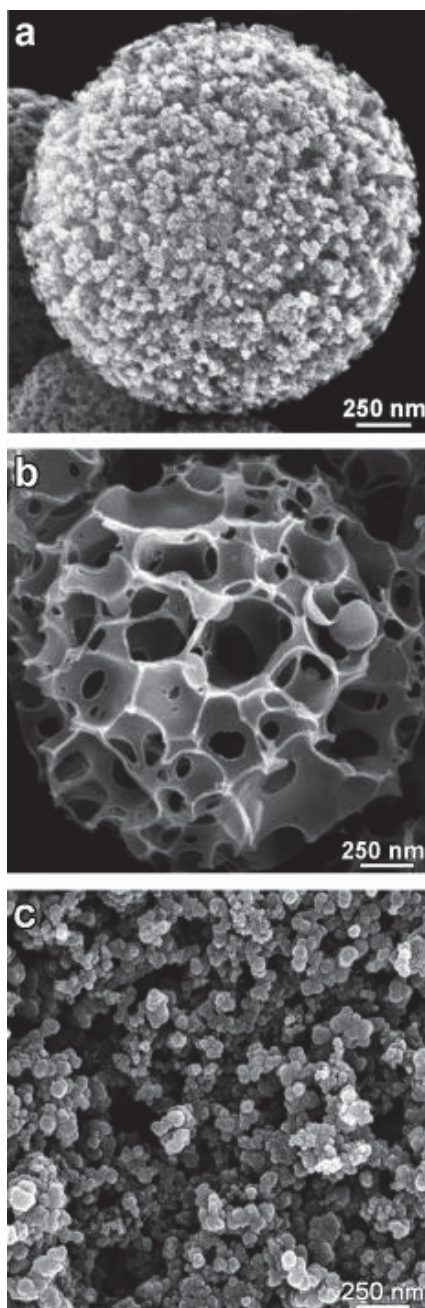


Figure 2.1: Microscopic images of porous catalysts used in methanol fuel cells produced by spray pyrolysis. Reprinted with permission from [BHS⁺07]. Copyright 2007 American Chemical Society.

bounds the molecules closer to the surface. After adsorption, the excess energy of the molecules is "transformed" into a surface diffusion of the chemical species.

Modeling of the adsorption process is usually based on the proportionality principle (see e.g. Böhm [Böh08]) and an exchange towards an equilibrium concentration: Denote by c the concentration of a species in a bulk phase and by c_Γ the corresponding concentration on the catalyst's surface, then a simple model would be to assume that desorption is a constant process being proportional to c_Γ , with adsorption being proportional to c . Denoting the proportionality constants by k_a (for adsorption) and k_d (for desorption), then the equilibrium between ad- and desorption is characterized by

$$k_a c = k_d c_\Gamma \quad \Longleftrightarrow \quad 0 = c - \frac{k_d}{k_a} c_\Gamma.$$

Setting $H := \frac{k_d}{k_a}$ as the Henry constant, exchange towards equilibrium would be characterized by the Henry-type law

$$f_{\text{exch}}(c, c_\Gamma) = (c - H c_\Gamma),$$

where f_{exch} denotes a function characterizing the exchange of c and c_Γ . Further details can be found in Section 3.3.1. Usually, the constants k_a and k_d depend on temperature, pressure, and the surface characteristics of the catalyst, among others.

Often, the number of active sites on the catalyst is limited. If this has to be taken into account, one assumes additionally that adsorption is proportional to $(c_{\Gamma, \text{max}} - c_\Gamma)$, where $c_{\Gamma, \text{max}}$ characterizes the amount of free sites on the catalyst's surface. In this case, the proportionality principle yields for the equilibrium concentrations

$$k_d c_\Gamma = k_a (c_{\Gamma, \text{max}} - c_\Gamma) c \quad \Longleftrightarrow \quad 0 = \frac{k c_{\Gamma, \text{max}} c}{k_d + k_a c} - c_\Gamma.$$

This yields $f_{\text{exch}}(c, c_\Gamma) = \left(\frac{k c_{\Gamma, \text{max}} c}{k_d + k_a c} - c_\Gamma \right)$, which is known as Langmuir adsorption kinetics (and usually based on the partial pressures of the species, see [TT97]). Variants of this formula can be obtained by assuming that adsorbed species occupy $m \in \mathbb{N}$ adsorption sites and that desorption can only occur if $l \in \mathbb{N}$ molecules detach simultaneously from the surface; in this case (where ' \sim ' denotes proportionality)

$$\text{adsorption} \sim (c_{\Gamma, \text{max}} - c_\Gamma)^m, \quad \text{adsorption} \sim c \quad \text{and} \quad \text{desorption} \sim c_\Gamma^l$$

gives the equilibrium equation

$$k_d c_\Gamma^l = k_a (c_{\Gamma, \text{max}} - c_\Gamma)^m c$$

as a starting point. More realistic models also involve hysteresis effects. Depending on the pore size, the pore distribution and the interconnectivity, different hysteresis curves have to be taken into account, see [TT97].

Since we are interested in developing new mathematical tools and not in an exact simulation of adsorption kinetics, we will use Henry's law throughout this work.

Diffusional and Surface Effects

Molecules reach the active sites of the catalyst mainly by diffusion. In heterogeneous catalysts, one distinguishes three types:

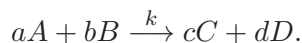
Bulk diffusion denotes the "standard" diffusion found in most liquids. It is characterized by the fact that collisions of molecules with each other are much more frequent than collisions with the walls of the catalyst.

Inside small pores, one can find **Knudsen diffusion**. Here, collisions of the molecules with the walls of the catalyst are much more frequent than collisions of molecules within the liquid. Experimental findings imply that the corresponding diffusion coefficient D_K is proportional to the reciprocal of the surface area. As a side note, we would like to point out that in applications of homogenization in \mathbb{R}^3 , this corresponds to the choice of the diffusion coefficient $D_K = \varepsilon^2 D$, where $\varepsilon > 0$ is the scale parameter and $D > 0$ the dimensionless diffusion coefficient. Since the inclusion of such a coefficient in PDE models leads to so called distributed microstructure models (see e.g. Hornung [Hor97] or Clark [Cla98], Showalter and Visarraga [SV04] for mathematical results), we suggest to investigate the applicability of such models in the field of catalysis.

Finally, **surface diffusion** denotes the diffusion of molecules on the surface of the catalyst after having been adsorbed to it.

Reaction Rates

As seen above, the surface and pore distribution of the catalyst has important effects on the catalytic reaction. Experiments suggest that its rate is proportional to the surface area to the power of $\gamma \in [\frac{1}{2}, 1]$, with $\gamma = 1$ for wider pores and $\gamma = \frac{1}{2}$ for narrow channels. Similarly, one has to distinguish between diffusion-controlled and reaction-controlled processes. We consider the example of a simple reaction



If the chemical reaction is rate determining (i.e. the supply of educts is high enough to allow the reaction to take place with the highest possible velocity), the reaction velocity η is given by the law of mass action. In this case, this yields $\eta = kc_A^a c_B^b$ with corresponding concentrations c_A of A and c_B of B . If the supply of one species, say A , is limited such that the reaction becomes diffusion-controlled, Thomas and Thomas [TT97] (based on the classical work of Thiele [Thi39]) argue that in this case the speed k has to be replaced by the effective constant $k^{\frac{1}{2}}$, and that the order of the reaction becomes $a_D = \frac{a+1}{2}$, yielding the reaction rate $\eta_D = k^{\frac{1}{2}} c_A^{a_D} c_B^b$. Special characteristics of adsorption sites can also lead to reaction rates of the form $\tilde{\eta} = kc_A^\gamma$, with $\gamma \in [0, \frac{1}{2}]$, see Campbell [Cam88].

2.1.3 Recent Trends

In this section, we will summarize recent trends in manufacturing and simulation of heterogeneous catalysts.

Concerning the catalysts used in industrial processes, more and more complex and structured surfaces are used nowadays. If one wants to employ different catalysts at the

same time, instead of simply "mixing" the active substances, one constructs catalysts with a well-designed distribution of the ingredients on a carrier substance. This leads to so-called bifunctional catalysts with enhanced reaction rate and throughput. See e.g. Blomsma, Martens and Jacobs [BMJ97] for the description of a bimetallic catalyst used for the cracking of heptane or the works of Guo, Dong and their coworkers [GLDW10] and [WGWD10] about the synthesis of bimetallic catalytic nanoparticles.

Moreover, one tries to integrate enzymes into catalytic settings. Enzymes are proteins, occurring naturally in living organisms. They trigger catalytic reactions, with a rate one to two orders of magnitude higher than that of man-made catalysts. However, enzymes usually are present in a liquid phase, making them inconvenient for industrial processes (see the beginning of Section 2.1). To overcome this drawback, one tries to attach enzymes to the surface of a carrier material and thus immobilizing the active proteins (see Sheldon [She07] for a description of corresponding methods). This has led to very efficient catalysts which can be used on an industrial scale, cf. for example Iso, Chen et. al. [ICE⁺01]. In this reference, immobilized lipase is used to produce biodiesel.

Nowadays, the design and development of new catalysts is not possible without the use of computers and efficient simulations. However, due to the number of complex processes happening at different scales, a complete and satisfactory model is not yet available. Even if all the processes could be modeled correctly, still the dimensional "bridge" connecting molecular interactions (size of 10^{-10} m) with the pores of the support material (size of 10^{-9} m to 10^{-8} m), the support itself (size of 10^{-3} m to 10^{-2} m) and finally the whole catalyst (size of 10^{-1} m to 10^0 m) makes exact simulations infeasible due to limitations in memory and computational power. Thus, only effective models focussing on a choice of aspects can be used.

To allow for more detailed models taking into account hardware restrictions, the chemical community became interested in multiscale-modeling recently: In [KNŠ⁺10], Kočí, Novák and their coworkers proposed a computational 3-scale model for the oxidation of CO in Al₂O₃-supported exhaust gas catalysts. Based on their model for the porous support material in [KŠKM07], they examined

1. Simple packed Al₂O₃-particles supporting Pt-particles as a catalyst.
2. The porous washcoat formed by stacking the catalytic entities.
3. A channel from an automobile exhaust catalyst, where the walls are occupied by the washcoat layer.

Progressing from one step to the other, the authors derived effective material properties needed in the computations of the n -th step from the $(n - 1)$ -th step, $n = \{2, 3\}$.

A similar approach was undertaken by Sundmacher, Pfafferoth and Heidebrecht to model a steam reforming unit of a carbonate fuel cell: In [HPS11], they simulated a small catalytic device (the "Detailed Model" in their terminology). Lead from the appearance of several reaction zones, they devised a meso-scale model (the "Zone Model") to explicitly model such a behavior. This was then used to build a macro-model of the whole reforming unit (the "Phase Model"). Detailed descriptions of the first two simulations together with a comprehensive list of material parameters can be found in [PHS⁺08]. For a description of the industrial application and the reactions taking place, see [PHS10].

2.2 Marine Aggregates

Marine aggregates are particles found in the pelagic zone of the oceans. They consist of detritus, dead material and living organisms like phytoplankton and microorganisms, and inorganic matter, for example clay minerals. Their size ranges from $500\mu\text{m}$ to some mm. Aggregates smaller than 0.5mm in diameter are called microaggregates, whereas those with size greater than 0.5mm are called marine snow (cf. Logan and Wilkinson [LW90]). The concentration of marine aggregates in the water ranges from 1 to 10 aggregates per litre in the surface water region, with numbers up to two orders of magnitude lower in the deeper regions, see Alldredge and Silver [AS88]. One should keep in mind, however, that the term "marine aggregate" or "marine snow" is applied to a whole family of particles, ranging from fragile to robust and from porous to gelatinous, with very different shapes and forms (like plates, shells, spheres etc.).

Due to the sinking of these aggregates to the seabed, a constant transportation process of chemical and biological material to the sea floor is maintained. According to Fowler and Knauer [FK86], this is the main process driving vertical fluxes in the ocean. Recently, there has been renewed interest in this flux in the field of climate modeling: Marine aggregates bury carbon in the seabed and thus can be an important factor when estimating global warming (see Kiørboe [Ki01]). However, Azam and Long [AL01] pointed out that these processes have never been included into a global climate study: Up to now, it is unknown whether the oceans are a source or a sink of carbon. Only after having obtained these information, it is possible to estimate the effectiveness of methods to artificially bury carbon in the sea, like putting iron in the sea water to enhance the production of algae.

The genesis of marine aggregates begins with the formation of microaggregates – from the remains of other organisms, mucus of plankton or fecal pellets. Due to Brownian motion and fluid shear in the water, microaggregates meet and coagulate to greater particles. They stuck together due to van-der-Waals forces, biological glue, or mechanical surface characteristics of the aggregates, see [Ki01] and [AS88].

The breakdown and loss of aggregates is caused by several mechanisms: Due to shear stress, the particle may be torn apart; or it may be consumed in part by plankton or as a whole by fish (an event that, however, leads to the transformation to fecal pellets, which constitute a source of aggregates). Moreover, bacterial colonies can lead to decomposition. Finally, settlement of the marine snow on the sea floor is the main process of removal from the water column (cf. the references cited above).

Inside the aggregate, microorganisms like algae and bacteria can be found in concentrations one to three orders of magnitude higher than in the surrounding water (cf. [AS88]). They stem from fecal pellets containing those organisms as well as organisms which were attracted by the aggregate.

Therefore, marine aggregates are places of elevated biological and chemical activity. Various biological and chemical reactions take place inside the aggregate, for instance the production of ammonium and carbon dioxide. This leaves a plume of higher concentration in the water. Additional substances exchanged with the surrounding water are oxygen, nitrate, sulfur, minerals, dissolved organic material and trace metals. This trail is attracting other microorganisms (see Kiørboe and Thygesen [KT01] for estimations via simulations).

In order to understand the transport and aggregation phenomena, one has to know the advective and diffusive exchange of the aggregate with the surrounding water. Due to [FK86], aggregates can be considered as a porous medium.

Flow around solid and porous particles has been studied by various authors: See for example von Wolfersdorf [vW88] for the derivation of a potential flow past a porous cylinder or the works of Jäger and Mikelić, [JM00] and [JM96] on the derivation of boundary conditions between a porous medium and a free flow. In this context, see also [DB10] for generalizations.

Simulations related to marine aggregates on the other hand are rare; they have been carried out by Kiørboe et. al. [KPT01] as well as [KT01] in the case of a 2-dimensional solid sphere. Here, the focus lies on the estimation of the plume behind the aggregate and the attraction of microorganisms. Another related work is Bhattacharyya, Dhinakaran, and Kahili [BDK06] on the simulation of a porous sphere by using a single-domain approach.

Nevertheless, in these simulations the reactive, diffusive and advective processes inside the marine aggregate have completely or partially been neglected.

2.3 Implications for Research

As it has become clear in the previous two sections, both industrial applications of heterogeneous catalysis and marine aggregates are multi-scale systems: Whereas for catalysts, one can at least distinguish between the catalytically active substance (e.g. Pt-atoms), its carrier substance (e.g. porous Al_2O_3) and the whole unit (for instance a catalytic converter to treat exhaust gases), marine snow can be considered on the level of its constituents (for example fecal pellets or mucus), as an agglomerate (i.e. the whole aggregate) and on the level of a large volume fraction of the sea, that is an ensemble of sinking aggregates.

Since in both situations (at least as an approximation) the structure is given by a periodic repetition of basic constituents, the methods and tools of periodic homogenization should in principle be applicable (see Cioranescu and Donato [CD99] for an introduction to the mathematical theory and Hornung [Hor97] for basic applications to porous media). However, for a reasonable study of the processes above, the following features must be taken into account:

Complex Multiscale Models

All situations discussed above possess at least three scales. While multiscale convergence is well-developed in the field of homogenization (see the classical work of Allaire and Briane [AB96] or the hints given at the end of the paper by Damlamian [Dam05]), all applications so far only treat the case that the whole domain has the same multi-scale structure. What is lacking is the possibility to create complex geometries on multiple scales, such that different parts of the domain can be equipped with different structures.

Processes on Evolving Surfaces

In the case of marine snow, the grazing of bacteria leads to a change of the surface of the aggregates. However, important exchange- and chemical processes are happening at these surfaces.

The concept of an evolution of the microstructure in homogenization has recently been introduced by Peter and Meier – see [Pet06], [Pet07] and [Mei08]. In these works, however, only reaction-diffusion processes in the bulk have been considered. The case of reaction and diffusion on the surface of an evolving structure has not been treated so far.

Structured and Non-Flat Surfaces

While surface diffusion and reaction have been considered in some cases in the homogenization literature (see e.g. Neuss-Radu [NR92] or Allaire, Damlamian, and Hornung [ADH95]), all the processes only happened on a boundary with no structure in itself. Although there are some works deriving surface equations with the help of two-scale convergence-like constructions in Neuss-Radu and Jäger [NRJ07], no structured surface or nonflat domain has been considered in the context of periodic homogenization to the knowledge of the author. However, especially for the modeling of the fine structure of catalysts (cf. Figure 2.1), such an approach seems appropriate.

In this work, we investigate the latter two situations (see also the introduction): The next chapter deals with diffusion-reaction processes on evolving surfaces inside a homogenization setting; and the subsequent chapter is concerned with the development of a homogenization calculus applicable to manifolds itself.

3 Homogenization of Evolving Hypersurfaces

In this chapter we carry out a homogenization procedure for chemical processes in a domain containing an array of embedded hypersurfaces. These surfaces are assumed to evolve with time, where the evolution is a-priori known and might depend on the position in the domain of interest.

Starting with the works of Alber [Alb00], Peter [Pet06], and Meier [Mei08], homogenization together with an evolution of the microstructure has become an accepted tool when deriving effective material properties. To the author's knowledge, however, all works so far concerned only an evolution of different subdomain structures. The evolution of an embedded hypersurface has not yet been considered. This is the aim of this chapter. There are two essential difficulties: First, the treatment of the evolution process of the hypersurface; and second, the treatment of the nonlinearities in the reaction rates.

The outline is as follows: Transport theorems for evolving hypersurfaces are hard to find in the literature. Thus for the convenience of the reader, we summarize the theorems which are needed to derive reasonable mass balance equations in the introductory Section 3.1, where we also give an overview of Periodic Unfolding. In Section 3.2 we present our method of describing the domain with embedded hypersurfaces. In the next Section 3.3 we use these transport theorems to derive mass balance equations for a model reaction taking place in the domain and on the hypersurface. After nondimensionalization, we arrive at the equations to be homogenized. Existence theorems together with a-priori estimates are derived in Sections 3.3.3 and 3.3.5. Finally, the rigorous homogenization procedure is carried out in Section 3.4. We conclude this chapter with some remarks concerning L^∞ -estimates for the solutions: In our approach, we tried to avoid the use of these estimates since they impose some restrictions on the situation considered; however when modeling real-life situations with some a-priori information at hand, they might be useful in the treatment of nonlinearities.

3.1 Coordinate Systems, Transport Theorems and Periodic Unfolding

3.1.1 Coordinate Transformations

In this section we recall some basic definitions and properties of coordinate transformations in continuum mechanics, see e.g. Marsden and Hughes [MH94] for an introduction or Meier [Mei08].

In this paragraph, let $S := [0, T)$ be a given time interval with $T > 0$ and let $\Omega_0 \subset \mathbb{R}^n$, $n \in \mathbb{N}$ be a given domain (which is assumed sufficiently regular). Assume that $\Sigma \subset \Omega_0$

is a compact \mathcal{C}^2 -hypersurface. Furthermore, let $M \subset \mathbb{R}^n$ be a smooth m -dimensional submanifold of \mathbb{R}^n with induced Riemannian metric. In the sequel, the reader should keep the choices $M = \Omega_0$ and $M = \Sigma$ in mind.

3.1.1 Definition.

A function $\psi : S \times M \rightarrow \mathbb{R}^n$ is called a regular \mathcal{C}^k -motion ($k \in \mathbb{N}_0$) if

1. $\psi \in \mathcal{C}^k(S \times M)$
2. For all $t \in S$ the function $\psi(t, \cdot) : M \rightarrow M(t) := \psi(t, M)$ is bijective, and the inverse function is of class $\mathcal{C}^k(M(t))$.
3. There exist constants $c, C > 0$ such that for the tangent map¹ $T_z \psi$ of $\psi(t, \cdot)$ it holds

$$c \leq \det T_z \psi \leq C$$

for all $(t, z) \in S \times M$.

We define the linear map $F(z) := T_z \psi$ for $z \in M$. Note that due to the implicit function theorem and condition 3 the function ψ^{-1} is continuously differentiable, which also gives the existence of F^{-1} as a continuous linear function. We will use the notation F^T to denote the adjoint of F with respect to the induced Euclidean scalar product on M , and F^{-T} to denote the inverse of F^T .

3.1.2 Transport Theorems

When deriving mass balance equations in a time-dependent set, one has to use transport theorems for the differentiation of time-dependent integrals. For the usual domain-case, these theorems are well-known in the mathematical and engineering literature (see e.g. the references cited below); however for the hypersurface-case, only few works are available. Here the reader is referred to the book by Slattery [Sla90] (from an engineering point of view) and the paper by Bothe, Prüss, and Simonett [BPS05].

We begin by reviewing the well-known transport theorem of Reynold. Let $\psi : S \times \bar{\Omega}_0 \rightarrow \mathbb{R}^n$ be a \mathcal{C}^1 -motion. The (Lagrangian) velocity of the transformation is given by $\tilde{v}(t, z) := \frac{\partial \psi}{\partial t}(t, z)$ for $(t, z) \in S \times \bar{\Omega}_0$. The corresponding Eulerian velocity is then given by

$$v(t, x) = \tilde{v}(t, \psi^{-1}(t, x)) \quad \text{for } t \in S, x \in \psi(t, \bar{\Omega}_0),$$

where the inverse is taken with respect to the spatial coordinates. With the notations and definitions above, the following results holds:

3.1.2 Proposition (Reynold's transport theorem).

Let $c \in \mathcal{C}^1(S \times \Omega(t))$, where $\Omega(t) = \psi(t, \Omega_0)$. It holds

$$\frac{d}{dt} \int_{\Omega(t)} c(t, y) \, dy = \int_{\Omega(t)} \partial_t c(t, y) \, dy + \int_{\Omega(t)} \operatorname{div}(cv)(t, y) \, dy.$$

¹As a reminder: For M, N manifolds and a smooth map $f : M \rightarrow N$ the tangent map $T_z f$ in $z \in M$ is a map $T_z f : T_z M \rightarrow T_z N$ defined as follows: Choose a $v \in T_z M$, then there exists a $\delta > 0$ and a smooth curve $\gamma : (-\delta, \delta) \rightarrow M$ with $\gamma(0) = z$, $\gamma'(0) = v$. Define $T_z f(v) = (f \circ \gamma)'(0)$. One can show that this definition is actually independent of the specific choice of the curve γ .

Proof. See e.g. [Mei08] or [EGK08]. ◆

For the case of a hypersurface, we have the following result:

3.1.3 Proposition (Transport theorem for hypersurfaces).

Let $\psi : S \times \bar{\Omega}_0 \rightarrow \mathbb{R}^n$ be a \mathcal{C}^2 -motion and let $\Sigma \subset \Omega_0$ be a compact \mathcal{C}^2 -hypersurface. Let $\Gamma(t) := \psi(t, \Sigma)$ be the transported material surface and let $c_\Gamma \in \mathcal{C}^1(S \times \Gamma(t))$. Then it holds

$$\begin{aligned} \frac{d}{dt} \int_{\Gamma(t)} c_\Gamma \, d\sigma_t &= \int_{\Gamma(t)} \left(\frac{Dc_\Gamma}{Dt} + c_\Gamma \operatorname{div}^\Gamma(v) \right) d\sigma_t \\ &= \int_{\Gamma(t)} \left(\frac{Dc_\Gamma}{Dt} + c_\Gamma \operatorname{div}^\Gamma(v_\Gamma) - c_\Gamma \kappa V \right) d\sigma_t. \end{aligned}$$

Here σ_t denotes the surface measure on $\Gamma(t)$, and $\kappa(t, x)$ is the mean curvature of $\Gamma(t)$ at x . $\operatorname{div}^\Gamma$ denotes the divergence-operator on $\Gamma(t)$, and v_Γ and V denote the tangential and normal component of the velocity v :

$$v_\Gamma := v - (v \cdot \nu)\nu, \quad V := v \cdot \nu.$$

Here ν denotes the outer unit normal vector. The term $\frac{Dc_\Gamma}{Dt}$ is the Lagrangian derivative of c_Γ given by

$$\frac{Dc_\Gamma}{Dt}(t, x) = \left. \frac{d}{ds} c_\Gamma(t + s, \psi(t + s, \psi^{-1}(t, x))) \right|_{s=0}.$$

The Lagrangian derivative appears due to the fact that one cannot consider the function $t \mapsto c_\Gamma(t, x)$ for fixed x , since x can only be chosen from a set depending on t itself.

Proof. This is a reformulation of the result presented in [BPS05]. In that paper, the Eulerian velocity v is given, and the transformation ψ is obtained as $\psi(t, z) = \phi(t; 0, z)$ via the solution $\phi(t; t_0, z_0)$ of the ODE

$$\phi'(t) = v(t, \phi(t)), \quad \phi(t_0) = z_0$$

(neglecting the expression " t_0, z_0 " in ϕ). This gives the assertion for $c_\Gamma \in \mathcal{C}^1(S \times \Gamma(t))$, where $\frac{Dc_\Gamma}{Dt}(t, x) := \left. \frac{d}{ds} c_\Gamma(t + s, \phi(t + s; t, x)) \right|_{s=0}$. Here $\phi(t + s; t, x) = \psi(t + s, \psi^{-1}(t, x))$. ◆

These transport theorems are frequently used in order to derive balance equations. However, one has to keep in mind that its use is only justified when the motion *transports* the quantity under consideration. In our case, we deal with a structural change of the domain which does not transport any substances itself. That is why we have to use another transport theorem:

3.1.4 Proposition (Transport theorem).

Let $c \in \mathcal{C}^1(S \times \Omega(t))$. Extend c by 0 outside $\Omega(t)$ in \mathbb{R}^n . Assume that $\Gamma(t)$ is a smooth

evolving hypersurface in the sense of Eck et. al. [EGK08]. Let $\Omega' \subset \mathbb{R}^n$ be an open control volume. Then it holds

$$\frac{d}{dt} \int_{\Omega'} c \, dx = \int_{\Omega' \cap \Omega(t)} \partial_t c \, dx + \int_{\Omega' \cap \Gamma(t)} c V \, d\sigma.$$

Here V denotes again the normal velocity of the surface as above.

Proof. This is a special case of the transport theorem 7.3 in [EGK08], where we set the function c to be 0 in one part of the domain. Note the direction of the normal vector, which in the case of the cited reference is an *inner* normal vector. \blacklozenge

When deriving mass balance equations, one has to assume the regularity of the involved functions – that is why we refrained from giving the most general results for weakly differentiable functions in this section, which may be found in the literature.

3.1.3 Transformation Formulas

3.1.5 Definition.

Let $c(t, x)$ be a scalar quantity and let $j(t, x)$ be a tangential vector field defined in $(t, x) \in S \times M(t)$. Assume that c and j are sufficiently smooth. We associate to these functions the so-called material representations \tilde{c} and \tilde{j} defined via

$$\tilde{c}(t, z) = c(t, \psi(t, z)) \quad \tilde{j}(t, z) = j(t, \psi(t, z)) \quad \text{with } (t, z) \in S \times \bar{\Omega}_0.$$

c and j are called quantities described in Eulerian coordinates, whereas \tilde{c} and \tilde{j} are described in Lagrangian coordinates (or material coordinates).

In order to be able to transform equations defined in $M(t)$ to M , we have to relate the differential operators on the different manifolds. The following lemma gives these results ($\llbracket \cdot, \cdot \rrbracket$ denotes the Euclidean scalar product in \mathbb{R}^n):

3.1.6 Lemma.

Let ∇_x be the gradient and let div_x be the divergence operator on $M(t)$ induced by the corresponding operators in Euclidean space. Analogously, let ∇_z and div_z be the corresponding operators on M . Then the following relations hold:

$$\begin{aligned} \nabla_x c &= F^{-T} \nabla_z \tilde{c} \\ \text{div}_x(j) &= \text{div}_z(F^{-1} \tilde{j}) \\ \partial_t c &= \partial_t \tilde{c} - \llbracket F^{-T} \nabla_z \tilde{c}, v \rrbracket, \end{aligned}$$

where $v(t, z) = \partial_t \psi(t, z)$.

Proof. By the chain rule, we have for the derivative in $z \in M$ that $T_z \tilde{c} = T_{\psi(t, z)} c \circ T_z \psi = T_x c \circ F$. By the definition of the gradient on a Riemannian manifold, we have for $v \in T_z M$

$$\begin{aligned} \llbracket \nabla_z \tilde{c}(t, z), v \rrbracket &= T_z \tilde{c}(v) = T_x c(Fv) \\ &= \llbracket \nabla_x c(t, x), Fv \rrbracket = \llbracket F^T \nabla_x c(t, x), v \rrbracket \end{aligned}$$

where $x = \psi(t, z)$. Thus we obtain $\nabla_z \tilde{c} = F^T \nabla_x c$, which by application of F^{-T} to both sides gives the first equality.

For the second equality, note that the divergence is the formal adjoint of the gradient operator. Carrying out an integration by parts, we obtain for a smooth vector field $\tilde{q} \in \mathfrak{X}(M)$ having compact support

$$\int_M \llbracket F^{-T} \nabla_z \tilde{c}, \tilde{q} \rrbracket \, \text{dvol}_M = - \int_M \tilde{c} \, \text{div}_z(F^{-1} \tilde{q}) \, \text{dvol}_M,$$

which shows that $\text{div}_z(F^{-1} \cdot)$ is the adjoint to $F^{-T} \nabla_z$; and thus the second equality follows. The third relation follows by an application of the chain rule and the transformation formula for the gradient. \blacklozenge

3.1.7 Lemma.

Denote by $\tilde{\nu}$ the outward unit normal at Σ . The corresponding unit normal at $\Gamma(t)$ is given by

$$\nu(t) = \frac{F^{-T} \tilde{\nu}}{|F^{-T} \tilde{\nu}|}.$$

Proof. See e.g. [Mei08]. \blacklozenge

For the Lagrangian derivative, we have the following transformation result:

3.1.8 Lemma.

We use the assumptions and definitions of Proposition 3.1.3. Define the function \tilde{c}_Γ in Lagrangian coordinates via

$$\tilde{c}_\Gamma(t, z) = c_\Gamma(t, \psi(t, z)).$$

Then it holds

$$\frac{\text{D}c_\Gamma}{\text{D}t} = \partial_t \tilde{c}_\Gamma.$$

Proof. By setting $x = \psi(t, z)$ we obtain by definition of the Lagrangian derivative

$$\begin{aligned} \frac{\text{D}c_\Gamma}{\text{D}t}(t, x) &= \left. \frac{\text{d}}{\text{d}s} c_\Gamma(t + s, \psi(t + s, \psi^{-1}(t, x))) \right|_{s=0} \\ &= \left. \frac{\text{d}}{\text{d}s} c_\Gamma(t + s, \psi(t + s, z)) \right|_{s=0} \\ &= \left. \frac{\text{d}}{\text{d}s} \tilde{c}_\Gamma(t + s, z) \right|_{s=0} = \partial_t \tilde{c}_\Gamma(t, z). \end{aligned} \quad \blacklozenge$$

3.1.4 Overview of Periodic Unfolding

To facilitate convergence proofs in the field of homogenization, Nguetseng and Allaire developed the notion of two-scale convergence, see [Ngu89] and [All92]. This notion has been proven to be extremely useful, and a lot of extensions and generalizations emerged: See for example the works of Neuss-Radu [NR96] and Allaire, Damlamian and Hornung [ADH95] for convergence on periodic surfaces (similar to our situation) or

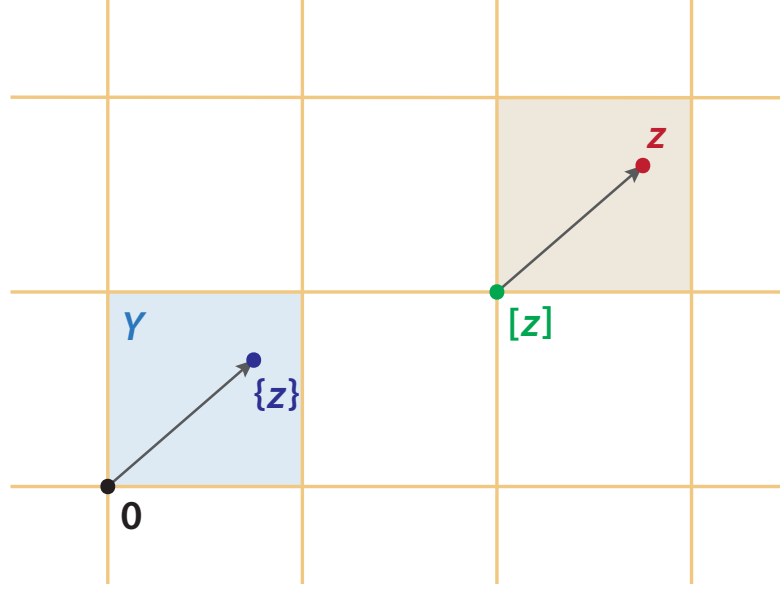


Figure 3.1: The construction of $[z]$ and $\{z\}$ for given $z \in \Omega$.

Bourgeat, Mikelić and Wright [BMW94] as well as Zhikov [Zhi00] for extensions to a stochastic microstructure and a more measure-theoretic approach. In this connection see also Lukkassen and Wall [LW05] for a similar approach for monotone operators. A characterization of admissible test functions may be found in Valadier [Val97]. For recent developments in order to extend the notion of two-scale convergence to other classes of functions (e.g. smooth functions or distributions) we refer the reader to the works of Visintin [Vis04], [Vis06] and [Vis07]. Finally, see Lukkassen, Nguetseng and Wall [LNW02] for a good summary of the method together with common caveats and errors.

Two-scale convergence uses special test functions and function spaces, whose characterization is difficult in some circumstances (see the references above). With the help of the notion of Periodic Unfolding, developed by Cioranescu, Damlamian, and Griso in [CDG02], one can use the usual weak convergence in L^p -spaces to treat homogenization problems. Good introductory papers are available with the works of Damlamian [Dam05] and Cioranescu, Donato and Zaki [CDZ06] (where specifically perforated domains are treated). A general formulation, unifying all concepts, can be found in Holmbom, Silfver et al. [HSSW06]. The reader is especially referred to the newer work [CDG08], where also a literature survey with applications of the method in various fields is contained.

In order to have the main results concerning two-scale convergence and Periodic Unfolding at hand, we give an overview of the most important definitions and results:

As for the notation in the field of Periodic Unfolding, we have: Let $z \in \mathbb{R}^N$. Define $[z]$ to be the unique linear combination $\sum_{j=1}^N k_j e_j$ with $k \in \mathbb{Z}^N$ and e_j the j -th unit vector, $j = 1, \dots, N$, such that $z - [z] \in Y$. Define $\{z\} = z - [z]$ (see also Figure 3.1). We denote the reference cell by Y ; in this work, we assume that $Y = [0, 1]^n$. For the definition of the boundary unfolding operator, we assume that Y can be decomposed in two disjoint parts $Y = Y_S \cup Y_R$, such that Y_S is strictly included in Y . Let $\Omega \subset \mathbb{R}^n$ be a given domain of interest and define $\Omega^\varepsilon = \bigcup_{k \in \mathbb{Z}^n} \varepsilon(k + Y_R) \cap \Omega$ as well as $\Gamma^\varepsilon = \bigcup_{k \in \mathbb{Z}^n} \varepsilon(k + \partial Y_S) \cap \Omega$.

3.1.9 Definition.

For a function ϕ with domain Ω , let $\hat{\phi}$ be the function extended by 0 outside of Ω . We define the following unfolding operators:

1. For $\phi : \Omega \rightarrow \mathbb{R}$ define the unfolding operator

$$\begin{aligned} \mathcal{T}^\varepsilon(\phi) : \mathbb{R}^N \times Y &\rightarrow \mathbb{R} \\ \mathcal{T}^\varepsilon(\phi)(x, y) &= \hat{\phi}\left(\varepsilon \begin{bmatrix} x \\ \varepsilon \end{bmatrix} + \varepsilon y\right). \end{aligned}$$

2. For $\phi_\Gamma : \Gamma^\varepsilon \rightarrow \mathbb{R}$ define the boundary unfolding operator

$$\begin{aligned} \mathcal{T}_b^\varepsilon(\phi_\Gamma) : \mathbb{R}^N \times \partial Y_S &\rightarrow \mathbb{R} \\ \mathcal{T}_b^\varepsilon(\phi_\Gamma)(x, y) &= \hat{\phi}_\Gamma\left(\varepsilon \begin{bmatrix} x \\ \varepsilon \end{bmatrix} + \varepsilon y\right). \end{aligned}$$

It is obvious that both operators are linear and that $\mathcal{T}^\varepsilon(f \cdot g) = \mathcal{T}^\varepsilon(f) \cdot \mathcal{T}^\varepsilon(g)$ for appropriate functions f and g (the same holds true for $\mathcal{T}_b^\varepsilon$). We present some standard results in the field of Periodic Unfolding, whose proofs can for example be found in [CDZ06]:

3.1.10 Proposition.

Let $p \in [1, \infty)$, let $\phi, \phi^1 \in L^p(\Omega)$ and $\phi_\Gamma, \phi_\Gamma^1 \in L^p(\Gamma^\varepsilon)$.

1. The following integral identities hold:

$$\begin{aligned} \int_{\Omega} \phi(x) \, dx &= \frac{1}{|Y|} \int_{\Omega \times Y} \mathcal{T}^\varepsilon(\phi)(x, y) \, dx \, dy, \\ \int_{\Gamma^\varepsilon} \phi_\Gamma(x) \, d\sigma_x &= \frac{1}{\varepsilon|Y|} \int_{\Omega \times \partial Y_S} \mathcal{T}_b^\varepsilon(\phi_\Gamma)(x, y) \, dx \, d\sigma_y. \end{aligned}$$

2. The operators $\mathcal{T}^\varepsilon : L^p(\Omega) \rightarrow L^p(\Omega \times Y)$ and $\mathcal{T}_b^\varepsilon : L^p(\Gamma^\varepsilon) \rightarrow L^p(\Omega \times \partial Y_S)$ are linear and continuous with norm estimate

$$\begin{aligned} \|\mathcal{T}^\varepsilon(\phi)\|_{L^p(\Omega \times Y)} &\leq \sqrt[p]{|Y|} \|\phi\|_{L^p(\Omega)}, \\ \|\mathcal{T}_b^\varepsilon(\phi_\Gamma)\|_{L^p(\Omega \times \partial Y_S)} &\leq \sqrt[p]{\varepsilon|Y|} \|\phi_\Gamma\|_{L^p(\Gamma^\varepsilon)}. \end{aligned}$$

3.1.11 Proposition.

Let $\phi \in W^{1,p}(\Omega)$. Then $\varepsilon \mathcal{T}^\varepsilon(\nabla \phi) = \nabla_y \mathcal{T}^\varepsilon(\phi)$ a.e. in $\Omega \times Y$. Similarly, for $\phi_\Gamma \in W^{1,p}(\Gamma^\varepsilon)$ one has $\varepsilon \mathcal{T}_b^\varepsilon(\nabla_\Gamma^\Gamma \phi_\Gamma) = \nabla_y^\Gamma \mathcal{T}_b^\varepsilon(\phi_\Gamma)$ a.e. in $\Omega \times \partial Y_S$.

Proof. For the gradient in the domain, the result is well-known in Periodic Unfolding (see above). For the surface gradient, denote by ν^ε the unit normal vector for $\Gamma^\varepsilon(0)$, and by ν^Γ the unit normal for $\Gamma(0) = \partial Y_S$. Due to the construction of the domain via summation and scaling, it is obvious that $\nu^\varepsilon(x) = \nu^\Gamma(\{\frac{x}{\varepsilon}\})$ and thus $\mathcal{T}^\varepsilon(\nu^\varepsilon)(x, y) = \nu^\Gamma(y)$. Now let $\phi_\Gamma : \Gamma^\varepsilon(0) \rightarrow \mathbb{R}$ be a smooth function. Extend ϕ_Γ to Ω in any smooth manner and denote the extension by ϕ . Since $\mathcal{T}_b^\varepsilon = \mathcal{T}^\varepsilon|_{\Omega \times \partial Y_S}$, we obtain due to the definition of the

surface gradient

$$\begin{aligned}\varepsilon \mathcal{T}_b^\varepsilon(\nabla^\Gamma \phi_\Gamma) &= \varepsilon \mathcal{T}^\varepsilon(\nabla \phi - \llbracket \nabla \phi, \nu^\varepsilon \rrbracket \nu^\varepsilon)|_{\Omega \times \partial Y_S} \\ &= \nabla_y \mathcal{T}^\varepsilon(\phi)|_{\Omega \times \partial Y_S} - \llbracket \nabla_y \mathcal{T}^\varepsilon(\phi)|_{\Omega \times \partial Y_S}, \nu^\Gamma \rrbracket \nu^\Gamma \\ &= \nabla_y^\Gamma \mathcal{T}_b^\varepsilon(\phi_\Gamma).\end{aligned}$$

In this connection, note that the surface gradients only depend on the values of ϕ_Γ and $\mathcal{T}_b^\varepsilon(\phi_\Gamma)$ on the respective surface, and thus the specific form of the extension ϕ plays no role. \blacklozenge

For the convergence proof we need an extension operator, which is recalled in the following lemma:

3.1.12 Lemma (Extension Operator).

Let $u \in W^{1,p}(Y_R)$. Then there exists an extension $\tilde{u} \in W^{1,p}(Y)$ into all of Y and a constant $C > 0$, independent of ε , such that $\|\tilde{u}\|_{W^{1,p}(Y)} \leq C \|u\|_{W^{1,p}(Y_R)}$. If $u \in L^p(Y_F)$, the extension satisfies $\|\tilde{u}\|_{L^p(Y)} \leq C \|u\|_{L^p(Y_R)}$.

Let $u^\varepsilon \in W^{1,p}(\Omega^\varepsilon)$. There exists an extension $\tilde{u}^\varepsilon \in W^{1,p}(\Omega)$ such that $\|\tilde{u}^\varepsilon\|_{W^{1,p}(\Omega)} \leq C \|u^\varepsilon\|_{W^{1,p}(\Omega^\varepsilon)}$. If $u \in L^p(\Omega^\varepsilon)$, the extension satisfies $\|\tilde{u}^\varepsilon\|_{L^p(\Omega)} \leq C \|u^\varepsilon\|_{L^p(\Omega^\varepsilon)}$. The constant C is the same as above.

Proof. The proof can be found in Hornung and Jäger [HJ91] or in Chiadò, Dal Maso et al. [ACMP92]. \blacklozenge

In the following theorem, the subscript $\#$ indicates periodicity of functions with respect to Y :

3.1.13 Theorem.

Let u^ε be a sequence in $L^2(\Omega)$ such that $u^\varepsilon \rightarrow u$ strongly in $L^2(\Omega)$. Then $\mathcal{T}^\varepsilon(u^\varepsilon) \rightarrow u$ strongly in $L^2(\Omega \times Y)$.

Let u^ε be a sequence in $H^1(\Omega^\varepsilon)$, let u_Γ^ε be a sequence in $H^1(\Gamma^\varepsilon)$.

1. If $\|u^\varepsilon\|_{L^2(\Omega^\varepsilon)} + \|\nabla u^\varepsilon\|_{L^2(\Omega^\varepsilon)}$ is bounded independently of ε , then there exists a $u_0 \in H^1(\Omega)$ and a $u_1 \in L^2(\Omega; H_{\#}^1(Y))$ such that along a subsequence the convergence

$$\begin{aligned}\mathcal{T}^\varepsilon(\tilde{u}^\varepsilon) &\rightharpoonup u_0 \quad \text{in } L^2(\Omega \times Y), \\ \mathcal{T}^\varepsilon(\nabla \tilde{u}^\varepsilon) &\rightharpoonup \nabla_x u_0 + \nabla_y u_1 \quad \text{in } L^2(\Omega \times Y)\end{aligned}$$

holds for the extended functions \tilde{u}^ε from the previous lemma. In that case also $\varepsilon \|u^\varepsilon\|_{L^2(\Gamma^\varepsilon(0))}^2$ is bounded independently of ε , and along a subsequence it holds

$$\mathcal{T}_b^\varepsilon(u^\varepsilon) \rightharpoonup u_0 \quad \text{in } L^2(\Omega \times \partial Y_S).$$

2. If $\|u^\varepsilon\|_{L^2(\Omega^\varepsilon)} + \varepsilon \|\nabla u^\varepsilon\|_{L^2(\Omega^\varepsilon)}$ is bounded independently of ε , then there exists a $u \in L^2(\Omega; H_{\#}^1(Y))$ such that along a subsequence the convergence

$$\begin{aligned}\mathcal{T}^\varepsilon(\tilde{u}^\varepsilon) &\rightharpoonup u \quad \text{in } L^2(\Omega \times Y), \\ \mathcal{T}^\varepsilon(\nabla \tilde{u}^\varepsilon) &\rightharpoonup \nabla_y u \quad \text{in } L^2(\Omega \times Y)\end{aligned}$$

holds for the extended functions \tilde{u}^ε .

3. If $\varepsilon \|u_\Gamma^\varepsilon\|_{L^2(\Gamma^\varepsilon)}^2 + \varepsilon^3 \|\nabla^\Gamma u_\Gamma^\varepsilon\|_{L^2(\Gamma^\varepsilon)}^2$ is bounded independent of ε , then there exists a $u_\Gamma \in L^2(\Omega; H^1(\partial Y_S))$ such that

$$\begin{aligned} \mathcal{T}_b^\varepsilon(u_\Gamma^\varepsilon) &\rightharpoonup u_\Gamma \quad \text{in } L^2(\Omega \times \partial Y_S), \\ \varepsilon \mathcal{T}_b^\varepsilon(\nabla^\Gamma u_\Gamma^\varepsilon) &\rightharpoonup \nabla_y^\Gamma u_\Gamma \quad \text{in } L^2(\Omega \times \partial Y_S). \end{aligned}$$

3.1.14 Remark.

The same results also hold if the functions depend on an additional parameter, like time. In this connection see e.g. Neuss-Radu [NR92] or the literature cited above. If the sequence u^ε is defined on the whole of Ω , variants of the results for $\mathcal{T}^\varepsilon(u^\varepsilon)$ from the previous theorem hold. The reader is again referred to the works mentioned above or to Section 4.2.7 in this work.

We finish this paragraph by presenting a generalized version of the usual trace inequality which takes into account the dependence of the constants on the scale-factor ε :

3.1.15 Lemma (General trace inequality).

Fix $k \in \mathbb{N}_0$ and let $u \in H^{k+1}(\Omega)$. Then it holds

$$\sqrt{\varepsilon} \left(\sum_{j=0}^k \varepsilon^j \left\| (\nabla^\Gamma)^{(j)} u \right\|_{L^2(\Gamma^\varepsilon(0))} \right) \leq C \left(\sum_{j=0}^{k+1} \varepsilon^j \left\| \nabla^{(j)} u \right\|_{L^2(\Omega^\varepsilon(0))} \right)$$

with a constant $C > 0$ independent of ε . Here $\|\nabla^{(j)} u\|_{L^2(\Omega^\varepsilon)}$ denotes the seminorm of the j -th derivatives of u in $H^{k+1}(\Omega^\varepsilon)$; analogously for the spaces over Γ^ε .

Proof. The continuous embedding $H^k(\partial Y_S) \hookrightarrow H^{k+1}(Y_R)$ yields the trace estimate

$$\sum_{j=0}^k \left\| (\nabla^\Gamma)^{(j)} w \right\|_{L^2(\partial Y_S)}^2 \leq K \sum_{j=0}^{k+1} \left\| \nabla^{(j)} w \right\|_{L^2(Y_R)}^2$$

for $w \in H^{k+1}(Y_R)$. Using the boundary unfolding operator $\mathcal{T}_b^\varepsilon$ (see Definition 3.1.9) together with the results for the unfolding of gradients in Proposition 3.1.11 and the inequality above, we obtain for u as above

$$\begin{aligned} \varepsilon \left(\int_{\Gamma^\varepsilon} \sum_{j=0}^k |\varepsilon^j (\nabla^\Gamma)^{(j)} u|^2 \, d\sigma \right) &\leq \frac{C}{|Y|} \int_{\Omega \times \partial Y_S} \sum_{j=0}^k |(\nabla_y^\Gamma)^{(j)} \mathcal{T}_b^\varepsilon(u)|^2 \, d\sigma_y \, dx \\ &\leq \frac{CK}{|Y|} \int_{\Omega \times Y_R} \sum_{j=0}^{k+1} \underbrace{|(\nabla_y)^{(j)} \mathcal{T}^\varepsilon(u)|^2}_{= \varepsilon^j |\nabla_x^{(j)} \mathcal{T}^\varepsilon(u)|^2} \, dy \, dx \\ &\leq CK \int_{\Omega^\varepsilon} \sum_{j=0}^{k+1} \varepsilon^{2j} |(\nabla)^{(j)} u|^2 \, dx. \end{aligned}$$

Taking the square root on both sides now gives the result. ◆

3.2 Construction of the Domain

3.2.1 The General Setting

We consider a fixed domain $\Omega \subset \mathbb{R}^n$ with piecewise smooth boundary. This domain is divided into two parts: A pore space part Ω_R (later called Ω^ε) and a solid part Ω_S . We assume that the following process happens in Ω : A substance A diffuses and reacts inside Ω_R . Other chemical species contributing to the reaction as well as its products are not considered at this place; they might however easily be incorporated into the model. The substance A is also present at the pore walls $\partial\Omega_S$, where it is denoted by A_Γ . A_Γ undergoes diffusion and reaction on the pore boundary. Furthermore, there is an exchange with the pore space.

The main feature of our model is the fact that the solid part changes with time – thus all the domains presented above depend on a time-parameter t . This change might be due to the chemical reaction (for example formation of crystals or precipitation/sedimentation of the chemical educts/products). In this work we assume that the evolution of Ω_S is a-priori known.

The same model can be applied to biological processes, see Chapter 2. However, note that there is an ongoing debate on whether to model such processes as a surface or as a bulk reaction.²

3.2.2 The Periodic Homogenization Setting

In order to be able to use techniques from formal asymptotic analysis, we assume that our domain is constructed in a locally periodic fashion (compare the works of Muntean et. al. [FAZM11] and [vNM10]).

Evolution via Reference Cells

Let $Y = [0, 1]^n$ be a reference cell, divided into two parts $Y_R =: Y_R(0)$ (the reaction part) and $Y_S =: Y_S(0)$ (the solid part), such that Y_S is strictly included in Y .

Since we assume the evolution of the domain to be a-priori known, we postulate the existence of a function $\psi : S \times \Omega \times Y \rightarrow Y$ such that

$$\psi(t, x, \cdot) : Y_R(0, x) \rightarrow Y_R(t, x) \quad \text{and} \quad \psi_\Gamma(t, x, \cdot) := \psi(t, x)|_{\partial Y_S} : \Gamma(0, x) \rightarrow \Gamma(t, x)$$

are orientation-preserving motions of \mathbb{R}^n for all $(t, x) \in S \times \Omega$. Here $Y_R(t, x) := \psi(t, x, Y_R(0))$ and $\Gamma(t, x) := \psi(t, x, \partial Y_S(0))$. We make the following assumptions:

3.2.1 Assumption.

For the regularity of the coordinate transformation, we assume:

- $\psi \in \mathcal{C}^2(S; \mathcal{C}^3(\Omega) \times \mathcal{C}_\#^3(Y))$.

²Private communication, MATCH-Workshop Analytical and Numerical Methods for Multiscale Systems, Heidelberg.

- Let $\nu(t, x, y)$ be the field of exterior normal vectors (with respect to $Y_R(t, x)$) on $\Gamma(t, x)$. We require $\nu(t, x, \cdot) \in \mathcal{C}^2(\Gamma(t, x))^n$ for all $(t, x) \in S \times \Omega$.

Note that these strong assumptions are only needed to treat the nonlinear reaction rates which we are going to use in our model. Concerning the structure of the motions, we require

- $\psi(0, x, \cdot) = \text{Id}$ for all $x \in \Omega$.
- There exist constants $c, C > 0$ such that

$$c \leq \det T_y \psi \leq C, \quad c \leq \det T_y \psi_\Gamma \leq C \quad (3.1)$$

in $S \times \Omega \times Y$.

- There exists a $\delta > 0$ such that for all $(t, x) \in S \times \Omega$ it holds:

$$\text{dist}(z, \partial Y) > \delta \quad \text{for all } z \in \Gamma(t, x)$$

as well as

$$\psi(t, x, \cdot) = \text{Id} \quad \text{on } \left\{ y \in Y : \text{dist}(y, \partial Y) < \frac{\delta}{2} \right\}.$$

Roughly speaking, this means that the surface in the reference cell never touches the boundary in the course of its evolution.

We now construct a periodic domain: Choose a scale-parameter $\varepsilon > 0$ and define

$$\Omega^\varepsilon(0) := \Omega \cap \left(\bigcup_{k \in \mathbb{Z}^n} \varepsilon(Y_R + k) \right), \quad \Gamma^\varepsilon(0) = \Omega \cap \left(\bigcup_{k \in \mathbb{Z}^n} \varepsilon(\partial Y_S + k) \right),$$

i.e. we pave Ω by scaled and translated copies of Y_R . In order to apply the motion defined above to each scaled and translated copy, we use the notation from periodic unfolding (see Section 3.1.4) and define

$$\psi^\varepsilon(t, x) := \psi\left(t, \varepsilon \begin{bmatrix} x \\ \varepsilon \end{bmatrix}, \left\{ \frac{x}{\varepsilon} \right\}\right).$$

Then we have

$$\begin{aligned} \Omega^\varepsilon(t) &= \left\{ \varepsilon \begin{bmatrix} x \\ \varepsilon \end{bmatrix} + \varepsilon \psi^\varepsilon(t, x); x \in \Omega^\varepsilon(0) \right\} \\ \Gamma^\varepsilon(t) &= \left\{ \varepsilon \begin{bmatrix} x \\ \varepsilon \end{bmatrix} + \varepsilon \psi^\varepsilon(t, x); x \in \Gamma^\varepsilon(0) \right\}. \end{aligned}$$

Thus the "global transformation" for fixed ε is given by $\phi^\varepsilon(t, x) := \varepsilon \begin{bmatrix} x \\ \varepsilon \end{bmatrix} + \varepsilon \psi^\varepsilon(t, x)$. Note that similar ideas also appear in Peter [Pet06]. In the sequel, we need the two linear maps $F(t, x) : \mathbb{R}^n \rightarrow \mathbb{R}^n$ as well as $F_\Gamma(t, x) : T_x \Gamma^\varepsilon(0) \rightarrow T_{\phi^\varepsilon(x)} \Gamma^\varepsilon(t)$ defined via the tangential maps

$$\begin{aligned} F(t, x) &:= T_x \phi^\varepsilon(t, x) \\ F_\Gamma(t, x) &:= T_x \phi_\Gamma^\varepsilon(t, x). \end{aligned}$$

Note that F and F_Γ also depend on ε , however we are not going to write down this dependence explicitly. With F^T and F_Γ^T we denote the Hilbert-space adjoint of F and F_Γ with respect to $[\cdot, \cdot]$ and $[\cdot, \cdot]_\Gamma$.

Since F is defined in \mathbb{R}^n , we can equivalently characterize this map as a matrix $F(t, x) = \nabla \phi^\varepsilon(t, x)$, with F^T being the usual transpose matrix.

3.2.2 Lemma.

For $\phi^\varepsilon(t) : \Omega^\varepsilon(0) \longrightarrow \Omega^\varepsilon(t)$ and $\phi_\Gamma^\varepsilon(t) : \Gamma^\varepsilon(0) \longrightarrow \Gamma^\varepsilon(t)$, $\phi_\Gamma^\varepsilon(t) := \phi^\varepsilon(t)|_{\Gamma^\varepsilon(0)}$ it holds

$$T_x \phi^\varepsilon(t, x) = T_y \psi(t, \varepsilon \left[\frac{x}{\varepsilon} \right], \left\{ \frac{x}{\varepsilon} \right\}), \quad T_x \phi_\Gamma^\varepsilon(t, x) = T_y \psi_\Gamma(t, \varepsilon \left[\frac{x}{\varepsilon} \right], \left\{ \frac{x}{\varepsilon} \right\}),$$

where we used the identification $T_x \Gamma^\varepsilon(0) \cong T_{\left\{ \frac{x}{\varepsilon} \right\}} \partial Y_S$. Thus especially $c \leq \det F \leq C$, $c \leq \det F_\Gamma \leq C$, and these bounds are independent of ε .

Proof. Since $\psi = \text{Id}$ for $\{y \in Y : \text{dist}(y, \partial Y) < \frac{\delta}{2}\}$, we have $\phi^\varepsilon(t, x) = \text{Id}(x)$ for $t \in [0, T]$, $x \in M := \{x \in \Omega : \text{dist}(x, \bigcup_{k \in \mathbb{Z}^n} \varepsilon(\partial Y + k)) < \varepsilon \frac{\delta}{2}\}$. Thus

$$\nabla \phi^\varepsilon = \text{Id} = \nabla_y \psi \quad \text{on } [0, T] \times M.$$

For $x \notin M$, we can find an open neighborhood of x with diameter less than $\varepsilon \frac{\delta}{2}$ that lies entirely in one translated and scaled reference cell $\varepsilon(Y + k')$, $k' \in \mathbb{Z}^n$. Therefore $x \mapsto \varepsilon \left[\frac{x}{\varepsilon} \right]$ is constant in that neighborhood and by the chain rule

$$\nabla \phi^\varepsilon(t, x) = \varepsilon \nabla \psi^\varepsilon(t, x) = \varepsilon \left(\frac{1}{\varepsilon} \nabla_y \psi(t, \varepsilon \left[\frac{x}{\varepsilon} \right], \left\{ \frac{x}{\varepsilon} \right\}) \right).$$

Thus by the identification of ∇ with T in \mathbb{R}^n we obtain the result.

For the second equality, let $v \in T_x \Gamma^\varepsilon(0)$ and let $\gamma : [-1, 1] \longrightarrow \Gamma^\varepsilon(0)$ be a smooth curve with $\gamma'(0) = v$. Then

$$\begin{aligned} T_x \phi_\Gamma^\varepsilon(t, x)(v) &= \frac{d}{ds} \varepsilon \psi^\varepsilon(t, \gamma(s)) \\ &= \frac{d}{ds} \varepsilon \psi(t, \varepsilon \left[\frac{\gamma(s)}{\varepsilon} \right], \left\{ \frac{\gamma(s)}{\varepsilon} \right\}) \\ &= \frac{d}{ds} \varepsilon \psi(t, \varepsilon \left[\frac{\gamma(s)}{\varepsilon} \right], \tilde{\gamma}(s)) \\ &= T_y \psi(t, \left[\frac{x}{\varepsilon} \right], \left\{ \frac{x}{\varepsilon} \right\})(v) \end{aligned}$$

where we used the fact that $\left[\frac{\gamma(s)}{\varepsilon} \right]$ is constant since γ is continuous, and that $\tilde{\gamma} = \varepsilon^{-1} \gamma$ is a smooth curve in ∂Y_S with $\varepsilon \tilde{\gamma}'(0) = v$. Property (3.1) now yields the estimates. \blacklozenge

We construct the induced velocity field of the transformation: Let

$$\tilde{v}^\varepsilon(t, x) := \partial_t \phi^\varepsilon(t, x) = \varepsilon \partial_t \psi(t, \varepsilon \left[\frac{x}{\varepsilon} \right], \left\{ \frac{x}{\varepsilon} \right\})$$

be the velocity at $(t, x) \in [0, T] \times \Omega^\varepsilon(0) \cup \Gamma^\varepsilon(0)$ in referential coordinates. Then the velocity in natural coordinates is given by $v^\varepsilon = \partial_t \phi^\varepsilon(t, ((\phi^\varepsilon)^{-1}(t, z))$ for $(t, z) \in [0, T] \times \Omega^\varepsilon(t) \cup \Gamma^\varepsilon(t)$.

Define

$$\begin{aligned} V^\varepsilon &:= v^\varepsilon \cdot \nu^\varepsilon && \text{the normal velocity,} \\ v_M^\varepsilon &:= v^\varepsilon - V^\varepsilon \nu^\varepsilon && \text{the tangential velocity,} \\ \kappa^\varepsilon &:= -\operatorname{div}^\Gamma(\nu^\varepsilon) && \text{the mean curvature.} \end{aligned}$$

Here $\nu^\varepsilon(t, x)$ is the outer unit normal vector at $(t, x) \in [0, T] \times \Gamma^\varepsilon(t)$.

By the Transformation Lemma 3.1.7 we obtain for the corresponding quantities in referential coordinates

$$\begin{aligned} \tilde{V}^\varepsilon(t, x) &= \varepsilon \partial_t \psi(t, \varepsilon \left[\frac{x}{\varepsilon} \right], \left\{ \frac{x}{\varepsilon} \right\}) \cdot \frac{F_\Gamma^{-T}(t, x) \tilde{\nu}^\varepsilon(x)}{|F_\Gamma^{-T}(t, x) \tilde{\nu}^\varepsilon(x)|}, \\ \tilde{v}_M^\varepsilon(t, x) &= \varepsilon \partial_t \psi(t, \varepsilon \left[\frac{x}{\varepsilon} \right], \left\{ \frac{x}{\varepsilon} \right\}) - \tilde{V}^\varepsilon(t, x) \frac{F_\Gamma^{-T}(t, x) \tilde{\nu}^\varepsilon(x)}{|F_\Gamma^{-T}(t, x) \tilde{\nu}^\varepsilon(x)|}, \\ \tilde{\kappa}^\varepsilon(t, x) &= -\operatorname{div}(F^{-1}(t, x) \frac{F_\Gamma^{-T}(t, x) \tilde{\nu}^\varepsilon(x)}{|F_\Gamma^{-T}(t, x) \tilde{\nu}^\varepsilon(x)|}), \end{aligned}$$

where $\tilde{\nu}^\varepsilon(x)$ is the unit normal at $x \in \Gamma^\varepsilon(0)$. Obviously $\tilde{\nu}^\varepsilon$ has a representation $\tilde{\nu}^\varepsilon(x) = \tilde{\nu}(\{\frac{x}{\varepsilon}\})$, where $\tilde{\nu}$ is the normal field on ∂Y_S .

In order to avoid technical difficulties, we assume that $\Gamma^\varepsilon(t) \cap \partial\Omega = \emptyset$ for all $t \in [0, T]$. This can for example be achieved if Ω is a rectangular domain of the form

$$\Omega = \varepsilon_0 \prod_{i=1}^n (a_i, b_i) \tag{3.2}$$

with $a_i, b_i \in \mathbb{Z}, a_i < b_i$ and an initial scaling factor ε_0 ; or if Ω can be represented by a scaled union of translated reference cells.

3.3 Derivation of the Equations

In this section we present the derivation and the full mathematical treatment of our "basic" equations.

We have the following situation in mind: We consider a chemical species which is present in the domain $\Omega^\varepsilon(t)$ and on the boundary of the pores $\Gamma^\varepsilon(t)$. The species is subject to diffusion and reaction both in the bulk and on the boundary, and an exchange between the domain and the pore boundary takes place. We are only considering one species at this place since our focus lies on the treatment of the evolving surfaces. However, all the assumptions and methods which follow will be chosen in a way that they can also be applied to systems with several species.

In order to simplify the derivations, we will drop the index ε for the moment.

3.3.1 Mass Balance

Denote by $c : S \times \Omega(t) \rightarrow \mathbb{R}$ the volume-concentration of the chemical species, and by $c_\Gamma : S \times \Gamma(t) \rightarrow \mathbb{R}$ its surface-concentration. Extend c by 0 outside $\Omega(t)$.

For simplicity, we assume that the mass densities of the species are constant (and w.l.o.g. have a value of 1). Let f and f_Γ be a volume- and surface source-term for the reaction. We denote by $f_{\text{exch}}(c, c_\Gamma)$ an exchange-term describing the exchange of the concentrations along the boundary $\Gamma(t)$. The diffusive flux in the domain and on the surface is assumed to be given by Fick's law, thus by $q := -D \nabla c$ as well as $q_\Gamma := -D_\Gamma \nabla^\Gamma c_\Gamma$. Here we use ∇^Γ to denote a surface gradient (in this case on $\Gamma(t)$). Later, we will also use ∇^Γ for surface gradient on ∂Y_S and other surfaces. Since it is always clear from the context on which surface the gradient has to be taken, we refrain from using a more specific notation. The corresponding adjoint operators are denoted by div^Γ .

Let $\Omega' \subset \mathbb{R}^n$ be a sufficiently regular open control set such that $\Omega' \cap \Gamma(t)$ does not have a nonzero $n - 2$ -dimensional surface measure.

We can now derive the following balance equations in the domain (for a detailed introduction into the idea of these considerations see Böhm [Böh08] or Eck, Garcke, and Knabner [EGK08]):

$$\begin{aligned} \frac{d}{dt} \int_{\Omega'} c \, dx &= - \int_{\partial\Omega'} q \cdot \nu \, d\sigma + \int_{\Omega'} f(c) \, dx - \int_{\Omega' \cap \Gamma(t)} f_{\text{exch}}(c, c_\Gamma) \, d\sigma \\ \Leftrightarrow \int_{\Omega'} \partial_t c + \text{div}(q) \, dx + \int_{\Omega' \cap \Gamma(t)} cV - q \cdot \nu \, d\sigma &= \int_{\Omega'} f(c) \, dx - \int_{\Omega' \cap \Gamma(t)} f_{\text{exch}}(c, c_\Gamma) \, d\sigma, \end{aligned} \quad (3.3)$$

where we used Proposition 3.1.4 and the fact that

$$\begin{aligned} \int_{\partial\Omega'} q \cdot \nu \, d\sigma &= \int_{(\partial\Omega' \cap \bar{\Omega}(t)) \cup (\Gamma(t) \cap \Omega')} q \cdot \nu \, d\sigma - \int_{\Gamma(t) \cap \Omega'} q \cdot \nu \, d\sigma \\ &= \int_{\Omega' \cap \Omega(t)} \text{div}(q) \, dx - \int_{\Omega' \cap \Gamma(t)} q \cdot \nu \, d\sigma \\ &= \int_{\Omega'} \text{div}(q) \, dx - \int_{\Omega' \cap \Gamma(t)} q \cdot \nu \, d\sigma, \end{aligned}$$

keeping in mind that $q = 0$ in $\Omega(t)^C$. Choosing Ω' such that $\bar{\Omega}' \subset \Omega(t)$ in (3.3), one obtains by the arbitrariness of the set

$$\partial_t c + \text{div}(q) = f(c) \quad \text{in } \Omega(t). \quad (3.4)$$

Arguing similarly for $\Omega' \cap \Gamma(t)$ leaves

$$q \cdot \nu - cV = f_{\text{exch}}(c, c_\Gamma) \quad \text{on } \Gamma(t). \quad (3.5)$$

In order to derive balance equations on the surface, let $\Gamma'_0 \subset \Gamma(0)$ and set $\Gamma'(t) = \psi(t, \Gamma'_0)$. The mass balance on the surface reads as follows, where τ denotes the $n - 2$ -dimensional

measure on $\partial\Gamma'(t)$:

$$\begin{aligned} \frac{d}{dt} \int_{\Gamma'(t)} c_\Gamma \, d\sigma &= - \int_{\partial\Gamma'(t)} q_\Gamma \cdot \nu_\Gamma \, d\tau + \int_{\Gamma'(t)} f_{\text{exch}}(c, c_\Gamma) + f_\Gamma(c_\Gamma) \, d\sigma \\ \Leftrightarrow \int_{\Gamma'(t)} \left(\frac{Dc_\Gamma}{Dt} + \text{div}^\Gamma(q_\Gamma) + c \text{div}^\Gamma(v_\Gamma) - c_\Gamma \kappa V \right) d\sigma &= \int_{\Gamma'(t)} f_\Gamma(c_\Gamma) + f_{\text{exch}}(c, c_\Gamma) \, d\sigma \end{aligned}$$

by the divergence theorem for div^Γ and Proposition 3.1.3. By the arbitrariness of $\Gamma'(t)$ we obtain

$$\frac{Dc_\Gamma}{Dt} + \text{div}^\Gamma(q_\Gamma) + c \text{div}^\Gamma(v_\Gamma) - c_\Gamma \kappa V = f_\Gamma(c_\Gamma) + f_{\text{exch}}(c, c_\Gamma) \quad \text{on } \Gamma(t). \quad (3.6)$$

We would like to point the reader to one important aspect of these derivations: We assumed that the motion of the domain $\Omega(t)$ does not have an effect on the bulk concentration itself. Such an effect could be caused by advective fluxes stemming from a carrier substance. As stated above, we chose to neglect such a substance. For these reasons we have to chose the Transport Theorem 3.1.4 when deriving the mass balance equations in the bulk.

The situation is different when we consider the surface concentration: Even with no exchange with the bulk part, no source term and zero flux (i.e. $q_\Gamma = 0$), a change of the solid surface would change the surface concentration of the substance. That is why we have to consider a moving reference surface-element $\Gamma'(t)$ when deriving the mass balance equations on the surface.

In order to obtain a closed system at $\Gamma(t)$, one condition has to be added. Among the possibilities are:

1. In the case of an instantaneous exchange, one keeps f_{exch} as a formal expression to equal the equations and adds an equilibrium condition in the form

$$c_\Gamma = \gamma(c)$$

with a known function γ . This is often used for free boundary problems (see e.g. [BPS05]). Cf. also the work of Ptashnyk and Roose [PR10] for a homogenization procedure involving such a boundary condition.

2. One specifies f_{exch} . If one assumes a slow exchange towards an equilibrium of concentrations of the form $c = Hc_\Gamma$ with a Henry constant H , one can choose

$$f_{\text{exch}}(c, c_\Gamma) = k(c - Hc_\Gamma)$$

(see also Section 2.1.2). Sometimes in the literature (see again [BPS05]) the term with the normal velocity is dropped in the exchange conditions (3.5). That is why we are also going to investigate

$$f_{\text{exch}}(c, c_\Gamma) = k(c - Hc_\Gamma) - cV.$$

Introducing initial conditions $c_0 : \Omega(0) \rightarrow \mathbb{R}$ as well as outer boundary conditions $c_{\text{ext}} : S \times \Omega(t) \rightarrow \mathbb{R}$ we obtain the following full system from (3.4), (3.5) and (3.6):

Bulk equations:

$$\partial_t c - \operatorname{div}(D \nabla c) = f(c) \quad \text{in } S \times \Omega(t) \quad (3.7a)$$

$$-D \nabla c \cdot \nu - cV = f_{\text{exch}}(c, c_\Gamma) \quad \text{on } S \times \Gamma(t) \quad (3.7b)$$

$$-D \nabla c \cdot \nu = c - c_{\text{ext}} \quad \text{on } S \times \partial\Omega(t) \quad (3.7c)$$

$$c(0, \cdot) = c_0(\cdot) \quad \text{in } \Omega(0) \quad (3.7d)$$

Surface equations:

$$\frac{Dc_\Gamma}{Dt} - \operatorname{div}^\Gamma(D_\Gamma \nabla^\Gamma c_\Gamma) + c_\Gamma \operatorname{div}^\Gamma v_M - c_\Gamma \kappa V \quad (3.8a)$$

$$-f_\Gamma(c_\Gamma) = f_{\text{exch}}(c, c_\Gamma) \quad \text{on } S \times \Gamma(t) \quad (3.8a)$$

$$c_\Gamma(0, \cdot) = c_{0,\Gamma}(\cdot) \quad \text{on } \Gamma(0) \quad (3.8b)$$

Here v_M is the tangential and V the normal velocity of Γ , and κ denotes the mean curvature. The expression $\frac{Dc_\Gamma}{Dt}$ is the time derivative along the moving interface. Fix the model case $i \in \{1, 2\}$, then we are going to investigate

$$f_{\text{exch}}(c, c_\Gamma) = -\delta_{i2}cV + k(x - Hc_\Gamma)$$

where δ_{ij} is the Kronecker delta. Keep in mind that the choice $i = 1$ is more reasonable from a modeling point of view.

3.3.2 Nondimensionalization

In order to have a reasonable scaling of our equations in the ε -periodic domain at hand, we carry out a nondimensionalization procedure. We introduce the following characteristic parameters:

- Characteristic time T
- Characteristic length of the domain L ; characteristic length of the boundary L_Γ
- Characteristic concentration in the domain C ; characteristic concentration on the surface C_Γ
- Characteristic tangential velocity V_T ; characteristic normal velocity V_N
- Characteristic mean curvature K

Later, we will impose assumptions on these quantities which make their relations clear.

In order to derive the nondimensionalized equations, define the new quantities

$$\begin{aligned} \bar{c}(t, x) &= \frac{1}{HC} c(tT, xL), & \bar{c}_\Gamma(t, x) &= \frac{1}{C_\Gamma} c_\Gamma(tT, xL) \\ \bar{v}_\Gamma(t, x) &= \frac{1}{V_T} v_\Gamma(tT, xL), & \bar{V}(t, x) &= \frac{1}{V_N} V(tT, xL), & \bar{\kappa}(t, x) &= \frac{1}{K} \kappa(tT, xL) \end{aligned}$$

and keep the following transformation rules in mind

$$\begin{aligned}\partial_t c &= (HC \frac{1}{T}) \partial_t \bar{c}, & \operatorname{div}(D \nabla c) &= (HC \frac{1}{L^2}) \operatorname{div}(D \nabla \bar{c}), \\ D \nabla c \cdot \nu &= (HC \frac{1}{L}) D \nabla \bar{c} \cdot \nu, & \operatorname{div}^\Gamma(D_\Gamma \nabla^\Gamma c_\Gamma) &= (C_\Gamma \frac{1}{L^2}) \operatorname{div}^\Gamma(D_\Gamma \nabla^\Gamma \bar{c}_\Gamma), \\ c_\Gamma \operatorname{div}^\Gamma(v_\Gamma) &= (C_\Gamma V_T \frac{1}{L}) \bar{c}_\Gamma \operatorname{div}^\Gamma(\bar{v}_\Gamma), & c_\Gamma \kappa V &= (C_\Gamma K V_N) \bar{v}_\Gamma \bar{\kappa} \bar{V}.\end{aligned}$$

For the transformation of the Lagrangian derivative, we have the following lemma:

3.3.1 Lemma.

It holds

$$\frac{D c_\Gamma}{D t} = (C_\Gamma \frac{1}{T}) \frac{D \bar{c}_\Gamma}{D t}.$$

Proof. We use the characterization of $\frac{D}{D t}$ as given in the proof of Proposition 3.1.3. Define the shorthand notation $\hat{c}_\Gamma(s; \tau, X) := c_\Gamma(s, \phi(s; \tau, X))$, where we consider \hat{c}_Γ as a function of s only. We obtain

$$\begin{aligned}\frac{D \bar{c}_\Gamma}{D t}(t, x) &= \left. \frac{d}{d s} \bar{c}_\Gamma(t + s, \phi(t + s; t, x)) \right|_{s=0} \\ &= \left. \frac{1}{C_\Gamma} \frac{d}{d s} c_\Gamma(T(t + s), \phi(T(t + s); tT, xL)) \right|_{s=0} \\ &= \left. \frac{1}{C_\Gamma} \frac{d}{d s} \hat{c}_\Gamma(T(t + s); Tt, xL) \right|_{s=0} \\ &= \left. \frac{T}{C_\Gamma} \frac{d}{d s} \hat{c}_\Gamma(tT + s; Tt, xL) \right|_{s=0} \\ &= \frac{T}{C_\Gamma} \frac{D c_\Gamma}{D t}(tT, xL),\end{aligned}$$

where we used the usual chain rule of differentiation in the fourth line. \blacklozenge

Inserting these formulas into equations (3.7) and (3.8), we obtain for the processes itself

$$\partial_t \bar{c} - \operatorname{div}(\bar{D} \nabla \bar{c}) = g(\bar{c})$$

with

$$\bar{D} = D \frac{T}{L^2}, \quad g(\bar{c}) = \frac{T}{HC} f(HC \bar{c})$$

as well as

$$\frac{D \bar{c}_\Gamma}{D t} - \operatorname{div}^\Gamma(\bar{D}_\Gamma^* \nabla^\Gamma \bar{c}_\Gamma) + \frac{V_T T}{L} \bar{c}_\Gamma \operatorname{div}^\Gamma(\bar{v}_\Gamma) - (K V_N T) \bar{c}_\Gamma \bar{\kappa} \bar{V} - g_\Gamma(\bar{c}_\Gamma) = g_{\text{exch}}(\bar{c}, \bar{c}_\Gamma)$$

with

$$\bar{D}_\Gamma^* = D_\Gamma \frac{T}{L^2}, \quad g_\Gamma(\bar{c}_\Gamma) = \frac{T}{C_\Gamma} f_\Gamma(C_\Gamma \bar{c}_\Gamma), \quad g_{\text{exch}}(\bar{c}, \bar{c}_\Gamma) = \frac{T}{C_\Gamma} f_{\text{exch}}(HC \bar{c}, C_\Gamma \bar{c}_\Gamma).$$

For the boundary conditions, we obtain on the inner parts

$$-\bar{D} \nabla \bar{c} \cdot \nu - \frac{TV_N}{L} \bar{c} \bar{V} = \frac{C_\Gamma}{HCL} g_{\text{exch}}(\bar{c}, \bar{c}_\Gamma)$$

as well as on the outer boundary

$$-\bar{D} \nabla \bar{c} \cdot \nu = \frac{T}{L} \left(\bar{c} - \frac{1}{HC} c_{\text{ext}} \right).$$

For our specific choice of f_{exch} , we obtain

$$\frac{C_\Gamma}{HCL} g_{\text{exch}}(\bar{c}, \bar{c}_\Gamma) = \frac{T}{HCL} f_{\text{exch}}(HC\bar{c}, C_\Gamma \bar{c}_\Gamma) = -\delta_{i2} \frac{L_\Gamma}{L} \bar{c} \bar{V} + k \frac{T}{L} \bar{c} - k \frac{TC_\Gamma}{LC} \bar{c}_\Gamma.$$

Looking at these results, one sees that \bar{D} , g , g_Γ and g_{exch} are already in dimensionless form, since these expressions relate quantities in the domain with scales of the domain and surface-quantities with its corresponding scales. In order to deal with the remaining terms, we make the following assumptions:

3.3.2 Assumption.

For the characteristic parameters we assume the following:

1. The ratio of length scales is of order ε , i.e. $\frac{L_\Gamma}{L} = \varepsilon$.
2. The ratio of the diffusivities is given by $\frac{D_\Gamma}{D} \approx \left(\frac{L_\Gamma}{L} \right)^2$.
3. For the velocities we have $V_N = V_T = \frac{L_\Gamma}{T}$.
4. For the mean curvature $K = \frac{1}{L}$.
5. The characteristic concentrations are related via the Henry equilibrium relation $C_\Gamma = HC$.
6. The exchange at the pore boundaries is controlled by a dimensionless factor $\tilde{k} = k \frac{T}{L_\Gamma}$ stemming from the surface-scale.

Now we obtain for the remaining terms

$$\bar{D}_\Gamma^* = D_\Gamma \frac{T}{L_\Gamma^2} \frac{L_\Gamma^2}{L^2} = \varepsilon^2 \bar{D}_\Gamma$$

with a constant \bar{D}_Γ of surface-order 1, as well as

$$\frac{V_N T}{L} = \frac{V_T T}{L} = \frac{L_\Gamma}{L} = \varepsilon, \quad KV_N T = \frac{L_\Gamma}{L} = \varepsilon, \quad k \frac{T}{L} = k \frac{T}{L_\Gamma} \frac{L_\Gamma}{L} = \varepsilon \tilde{k}.$$

Switching back to the old name of the terms, we arrive at the following nondimensionalized system of equations:

$$\partial_t c^\varepsilon - \text{div}(D \nabla c^\varepsilon) = f_{\text{reac}}(c^\varepsilon) \quad \text{in } S \times \Omega^\varepsilon(t) \quad (3.9a)$$

$$-D \nabla c^\varepsilon \cdot \nu = \varepsilon [\delta_{i1} c^\varepsilon V^\varepsilon + k(c^\varepsilon - H c_\Gamma^\varepsilon)] \quad \text{on } S \times \Gamma^\varepsilon(t) \quad (3.9b)$$

$$-D \nabla c^\varepsilon \cdot \nu = c^\varepsilon - c_{\text{ext}} \quad \text{on } S \times \partial\Omega(t) \quad (3.9c)$$

$$c^\varepsilon(0, \cdot) = c_0(\cdot) \quad \text{in } \Omega(0) \quad (3.9d)$$

as well as

$$\frac{Dc_{\Gamma}^{\varepsilon}}{Dt} - \varepsilon^2 \operatorname{div}^{\Gamma}(D_{\Gamma} \nabla^{\Gamma} c_{\Gamma}^{\varepsilon}) + \varepsilon c_{\Gamma}^{\varepsilon} \operatorname{div}^{\Gamma} v_M^{\varepsilon} - \varepsilon c_{\Gamma}^{\varepsilon} \kappa^{\varepsilon} V^{\varepsilon}$$

$$-f_{\Gamma}(c_{\Gamma}^{\varepsilon}) = -\delta_{i2} c^{\varepsilon} V^{\varepsilon} + k(c^{\varepsilon} - H c_{\Gamma}^{\varepsilon}) \quad \text{on } \Gamma^{\varepsilon}(t) \quad (3.10a)$$

$$c_{\Gamma}^{\varepsilon}(0, \cdot) = c_{0,\Gamma}(\cdot) \quad \text{on } \Gamma^{\varepsilon}(0) \quad (3.10b)$$

The choice $i \in \{1, 2\}$ corresponds to the form of f_{exch} discussed above.

Since our focus lies on the rigorous treatment of a homogenization process in a domain with an evolving hypersurface, we tried to keep our model rather simple. For more realistic models (capturing more features of *specific* processes), the reader is referred to the following references:

A detailed model of crystal formation is presented in the work of van Duijn and Pop, [vDP04]. An upscaling approach using the model (based on a free boundary problem) can be found in van Noorden, Pop et. al. [vNPEH10].

Furthermore, we did not include any carrier substance for the chemical reaction into our model. This would lead to an advective flux-term. If the underlying velocity is divergence-free, such a process might easily be incorporated into the homogenization setting (see e.g. the works of Hornung, Jäger and Mikelić [HJ91] and [HJM94]). If the divergence does not vanish, one can use more recent techniques like for instance the method of two-scale convergence with drift by Allaire, Mikelić and Piatnitski [AMP10].

3.3.3 Existence and Uniqueness of a Solution

Transformation to a Fixed Domain

The equations (3.9) and (3.10) represent one example of so-called equations in noncylindrical domains. Usually, they appear in the theory of the Navier-Stokes equations, see e.g. the works of Inoue, Wakimoto [IW77], Miyakawa, Teramoto [MT82] or Miranda and Ferrel [MF97]. The common approach to treat these types of equations is the transformation to a fixed domain. Several techniques can be used:

1. One transforms the equations formally by using the results given in Section 3.1.3. This is used in most works on problems in noncylindrical domains, for instance in the references cited above.
2. One writes down a weak formulation of the problem in natural coordinates and uses integral transformations to obtain a weak formulation in referential coordinates. This rigorous method is used for example in [Mei08], where a two-scale parabolic system is transformed. After the transformation, a degenerate parabolic system is obtained which is solved by using methods presented in Showalter [Sho97].

Under some regularity assumptions on the transformation, both approaches are equivalent.³ Since our focus lies mainly on the derivation of effective equations via homogenization, we use the first approach at this place.

³Meier and Peter, private communications.

Note that in order to use the second approach, it is recommended to employ weak formulations which do not rely on the existence of the time derivative $\partial_t c^\varepsilon$ and $\partial_t c_\Gamma^\varepsilon$. Such approaches can for example be found in [Sho97] or [Mei08].⁴

By using the transformation formulas in Section 3.1.3 we obtain for the transformed quantities \tilde{c}^ε and $\tilde{c}_\Gamma^\varepsilon$:

$$\partial_t \tilde{c}^\varepsilon - \nabla \tilde{c}^\varepsilon \cdot F^{-1} \tilde{v}^\varepsilon - \operatorname{div}(DF^{-1} F^{-T} \nabla \tilde{c}^\varepsilon) = \tilde{f}(\tilde{c}^\varepsilon) \quad \text{in } S \times \Omega(0) \quad (3.11a)$$

$$-DF^{-T} \nabla \tilde{c}^\varepsilon \cdot \tilde{\nu} = \delta_{i1} \tilde{c}^\varepsilon \tilde{V}^\varepsilon + \varepsilon \tilde{k}(\tilde{c}^\varepsilon - H \tilde{c}_\Gamma^\varepsilon) \quad \text{on } S \times \Gamma^\varepsilon(0) \quad (3.11b)$$

$$-DF^{-T} \nabla \tilde{c}^\varepsilon \cdot \tilde{\nu} = \tilde{c}^\varepsilon - \tilde{c}_{\text{ext}} \quad \text{on } S \times \partial\Omega \quad (3.11c)$$

$$\tilde{c}^\varepsilon(0, \cdot) = \tilde{c}_0 \quad \text{in } \Omega(0) \quad (3.11d)$$

$$\begin{aligned} \partial_t \tilde{c}_\Gamma^\varepsilon - \varepsilon^2 \operatorname{div}^\Gamma(D_\Gamma F_\Gamma^{-1} F_\Gamma^{-T} \nabla^\Gamma \tilde{c}_\Gamma^\varepsilon) + \tilde{c}_\Gamma^\varepsilon \operatorname{div}^\Gamma(F_\Gamma^{-1} \tilde{v}_M^\varepsilon) \\ - \tilde{c}_\Gamma^\varepsilon \tilde{\kappa} \tilde{V}^\varepsilon - \tilde{f}_\Gamma(\tilde{c}_\Gamma^\varepsilon) = -\delta_{i2} \frac{1}{\varepsilon} \tilde{c}^\varepsilon \tilde{V}^\varepsilon + \tilde{k}(\tilde{c}^\varepsilon - H \tilde{c}_\Gamma^\varepsilon) \quad \text{on } S \times \Gamma^\varepsilon(0) \end{aligned} \quad (3.12a)$$

$$\tilde{c}_\Gamma^\varepsilon(0, \cdot) = \tilde{c}_{0,\Gamma} \quad \text{on } \Gamma^\varepsilon(0) \quad (3.12b)$$

where

$$F = T_x \phi^\varepsilon \quad F_\Gamma = T_x \phi_\Gamma^\varepsilon,$$

cf. Section 3.2.2. Note that F and F_Γ depend on ε , however we do not write this dependence explicitly. The missing factors of ε as compared to equations (3.9) and (3.10) stem from the fact that the definition of \tilde{v}^ε from Section 3.2.2 already contains a factor of ε , the underlying "dimensionless" velocity there is given by $\partial_t \psi$, see page 40.

3.3.3 Assumption.

For the coefficients and the data of the problem, we assume the following:

- $D, D_\Gamma > 0$ (this assumption can easily be generalized to functions or matrices).
- $\tilde{k} \in \mathcal{C}^1(0, T; \mathcal{C}^2(\bar{\Omega}))$, $\tilde{k} \geq 0$
- $c_{\text{ext}} \in H^1(0, T; L^2(\partial\Omega))$, $c_{\text{ext}} \geq 0$
- $\tilde{c}_0 \in H^3(\Omega)$
- $\tilde{c}_{0,\Gamma} \in H^4(\Omega)$

⁴The deeper reason for this need is a missing characterization of the dual spaces of L^p -spaces in noncylindrical domains: $L^p(S; X(s))$ -spaces can only be defined for scales of Banach-spaces $X(s)$ ranging from $\mathcal{C}_0^\infty(\Omega(s))$ up to $X(s) = L^p(\Omega(s))$. A usual setting for parabolic problems would involve function spaces like $L^p(S; W^{-1,q}(\Omega(s)))$. Of course, such a space can formally be defined as the dual space of $L^{p^*}(S; W^{1,q^*}(\Omega(s)))$. However, one lacks an embedding of the form $L^p(S; W^{-1,q}(\Omega(s))) \subset L^p(S; Y)$:

The main difficulty is to find a Banach space Y which is reasonable and "big enough" to contain all $W^{-1,q}(\Omega(s))$. Due to passing to dual spaces, inclusions like $W_0^{1,p}(\Omega(s)) \subset W_0^{1,p}(\Omega)$ turn into $W^{-1,p'}(\Omega) \subset W^{-1,p'}(\Omega(s))$ – where the space to the right is not even contained in a space of measures. This illustrates the difficulties of finding a suitable space Y . (Since the set of distributions does not form a Banach space, it is not obvious how to construct a space like $L^p(S; \mathcal{D}'(\Omega(s)))$, which would be a good candidate). Since this part of the work [Mei08] received great attention, it is recommended to further investigate these types of function spaces.

- The Henry constant H fulfills $H > 0$
- $\tilde{f}, \tilde{f}_\Gamma : \Omega \times \mathbb{R} \rightarrow \mathbb{R}$ are continuous and Lipschitz-continuous in the second argument with constant $L > 0$ independent of the first argument.
- \tilde{f}_Γ is also Lipschitz-continuous in the first argument with constant $L_\Gamma > 0$ independent of the second argument

For the estimation of terms involving the reaction functions \tilde{f} and \tilde{f}_Γ , we need the following lemma.

3.3.4 Lemma.

With the assumptions above, there exists a constant $C > 0$ such that

$$|\tilde{f}(x, z)| \leq C(1 + |z|) \quad \text{and} \quad |\tilde{f}_\Gamma(x, z)| \leq C(1 + |z|).$$

Proof. We only prove the first result, the second follows completely analogously. It holds

$$\begin{aligned} |\tilde{f}(x, z)| &\leq |\tilde{f}(x, z) - \tilde{f}(x, 0)| + |\tilde{f}(x, 0)| \\ &\leq L|z - 0| + \|\tilde{f}(\cdot, 0)\|_{L^\infty(\bar{\Omega})} \leq C(1 + |z|) \end{aligned}$$

due to the Lipschitz-continuity of \tilde{f} in the second argument and the continuity in the first. \blacklozenge

In the sequel, we will keep the notations $\tilde{f}(\tilde{c}^\varepsilon)$ and $\tilde{f}_\Gamma(\tilde{c}_\Gamma^\varepsilon)$ etc. from equations (3.11a), (3.12a) to designate the functions $(t, x) \mapsto \tilde{f}(x, \tilde{c}^\varepsilon(t, x))$ and $(t, x) \mapsto \tilde{f}_\Gamma(x, \tilde{c}_\Gamma^\varepsilon(t, x))$.

3.3.5 Lemma.

For all $\varepsilon > 0$ and $(t, x, x') \in [0, T] \times \Omega \times \Gamma^\varepsilon(0)$, the linear operators $F^{-1}(t, x)F^{-T}(t, x)$ as well as $F_\Gamma^{-1}(t, x')F_\Gamma^{-T}(t, x')$ are symmetric, bounded and positive definite in the sense that there exist constants $d_0, K > 0$ (independent of ε, t, x and x') such that for all $\xi, \xi' \in \mathbb{R}^n$ and $\tilde{\xi}, \tilde{\xi}' \in T_{x'}\Gamma^\varepsilon(0)$

$$\begin{aligned} \|[F^{-1}(t, x)F^{-T}(t, x)\xi, \xi']\| &\leq K|\xi||\xi'| \quad \text{and} \quad d_0|\xi|^2 \leq \|[F^{-1}(t, x)F^{-T}(t, x)\xi, \xi]\| \\ \|[F_\Gamma^{-1}(t, x')F_\Gamma^{-T}(t, x')\tilde{\xi}, \tilde{\xi}']_\Gamma\| &\leq K|\tilde{\xi}|_\Gamma|\tilde{\xi}'|_\Gamma \quad \text{and} \quad d_0|\tilde{\xi}|_\Gamma^2 \leq \|[F_\Gamma^{-1}(t, x')F_\Gamma^{-T}(t, x')\tilde{\xi}, \tilde{\xi}]_\Gamma\|. \end{aligned}$$

Here $\llbracket \cdot, \cdot \rrbracket$ denotes the usual scalar product in \mathbb{R}^n , whereas $\llbracket \cdot, \cdot \rrbracket_\Gamma$ denotes the scalar product (i.e. the Riemannian metric) on $\Gamma^\varepsilon(0)$, which is given as the induced scalar product from \mathbb{R}^n . The corresponding norms are denoted by $|\cdot|$ and $|\cdot|_\Gamma$.

Proof. The symmetry of the linear operators is clear. Due to Lemma 3.2.2, we obtain estimates on the eigenvalues of the maps as well. A spectral decomposition now yields the estimates (see e.g. [Dob09], pages 31ff). \blacklozenge

Weak Formulation

In order to derive a solution theory for the coupled system, we use a weak formulation of the equations similar to Zeidler [Zei90]. We need the following spaces, where we fix the parameter $\varepsilon > 0$ for the rest of this section:

3.3.6 Definition.

In the sequel, we will use the following function spaces:

$$\begin{aligned} H &:= L^2(\Omega^\varepsilon(0)) & H_\Gamma &:= L^2(\Gamma^\varepsilon(0)) \\ V &:= H^1(\Omega^\varepsilon(0)) & V_\Gamma &:= H^1(\Gamma^\varepsilon(0)) \\ \mathcal{V} &:= L^2(0, T; V) & \mathcal{V}_\Gamma &:= L^2(0, T; V_\Gamma) \\ \mathcal{W} &:= \{u \in \mathcal{V} : u' \in \mathcal{V}^*\} & \mathcal{W}_\Gamma &:= \{u \in \mathcal{V} : \Gamma : u' \in \mathcal{V}_\Gamma^*\} \end{aligned}$$

Note that the sequences $V \subset H \subset V^*$ and $V_\Gamma \subset H_\Gamma \subset V_\Gamma^*$ form evolution triples.

3.3.7 Definition.

The weak formulation of Problem (3.11), (3.12) is given by: Find $(\tilde{c}^\varepsilon, \tilde{c}_\Gamma^\varepsilon) \in \mathcal{W} \times \mathcal{W}_\Gamma$ such that for all $(\phi, \phi_\Gamma) \in V \times V_\Gamma$ it holds

$$\begin{aligned} \frac{d}{dt}(\tilde{c}^\varepsilon(t), \phi)_H + a^1(\tilde{c}^\varepsilon(t), \phi; t) + a^2(\tilde{c}^\varepsilon(t), \phi; t) \\ + a^3(\tilde{c}^\varepsilon(t), \phi; t) = b(\phi; t, \tilde{c}^\varepsilon, \tilde{c}_\Gamma^\varepsilon) \quad a.e. [0, T] \end{aligned} \quad (3.13a)$$

$$\tilde{c}^\varepsilon(0) = \tilde{c}_0 \quad (3.13b)$$

as well as

$$\begin{aligned} \frac{d}{dt}(\tilde{c}_\Gamma^\varepsilon(t), \phi_\Gamma)_{H_\Gamma} + a_\Gamma^1(\tilde{c}_\Gamma^\varepsilon(t), \phi_\Gamma; t) + a_\Gamma^2(\tilde{c}_\Gamma^\varepsilon(t), \phi_\Gamma; t) \\ = b_\Gamma(\phi_\Gamma; t, \tilde{c}^\varepsilon, \tilde{c}_\Gamma^\varepsilon) \quad a.e. [0, T] \end{aligned} \quad (3.14a)$$

$$\tilde{c}_\Gamma^\varepsilon(0) = \tilde{c}_{0,\Gamma}. \quad (3.14b)$$

Here the following (bi-)linear forms are used:

$$\begin{aligned} a^1(c, \phi; t) &:= (DF^{-T}(t) \nabla c, F^{-T}(t) \nabla \phi)_H \\ a^2(c, \phi; t) &:= (\nabla c \cdot F^{-1}(t) \tilde{v}^\varepsilon(t), \phi)_H \\ a^3(c, \phi; t) &:= \varepsilon(\tilde{k}(t)c|_{\Gamma^\varepsilon(0)}, \phi|_{\Gamma^\varepsilon(0)})_{H_\Gamma} + (\delta_{i1} \tilde{V}^\varepsilon c|_{\Gamma^\varepsilon(0)}, \phi|_{\Gamma^\varepsilon(0)})_{H_\Gamma} + (c|_{\partial\Omega}, \phi|_{\partial\Omega})_{L^2(\partial\Omega)} \\ b(\phi; t, \tilde{c}^\varepsilon, \tilde{c}_\Gamma^\varepsilon) &:= (\tilde{f}(\tilde{c}^\varepsilon(t)), \phi)_H + \varepsilon(\tilde{k}(t)H\tilde{c}_\Gamma^\varepsilon(t), \phi|_{\Gamma^\varepsilon(0)})_{H_\Gamma} + (c_{\text{ext}}(t), \phi|_{\partial\Omega})_{L^2(\partial\Omega)} \end{aligned}$$

and

$$\begin{aligned} a_\Gamma^1(c_\Gamma, \phi_\Gamma; t) &:= \varepsilon^2(D_\Gamma F_\Gamma^{-T}(t) \nabla^\Gamma c_\Gamma, F_\Gamma^{-T}(t) \phi_\Gamma)_{H_\Gamma} \\ a_\Gamma^2(c_\Gamma, \phi_\Gamma; t) &:= ([\text{div}^\Gamma(F_\Gamma^{-1}(t) \tilde{v}_M^\varepsilon(t)) - \tilde{\kappa}(t) \tilde{V}^\varepsilon(t) + \tilde{k}(t)H]c_\Gamma, \phi_\Gamma)_{H_\Gamma} \\ b_\Gamma(\phi_\Gamma; t, \tilde{c}^\varepsilon, \tilde{c}_\Gamma^\varepsilon) &:= (\tilde{f}_\Gamma(\tilde{c}_\Gamma^\varepsilon(t)), \phi_\Gamma)_{H_\Gamma} + (\tilde{k}(t)\tilde{c}^\varepsilon(t), \phi_\Gamma)_{H_\Gamma} - \frac{\delta_{i2}}{\varepsilon}(\tilde{V}^\varepsilon(t)\tilde{c}^\varepsilon(t)|_{\Gamma^\varepsilon(0)}, \phi_\Gamma)_{H_\Gamma} \end{aligned}$$

Formally, the weak formulation is obtained by multiplying (3.11a) by ϕ and carrying out an integration by parts; analogously for (3.12a) by multiplying with ϕ_Γ .

3.3.8 Lemma.

Fix $t \in [0, T]$, $\tilde{c}^\varepsilon \in L^2(0, T; V)$ as well as $\tilde{c}_\Gamma^\varepsilon \in L^2(0, T; H_\Gamma)$. The following maps are

linear and continuous between the indicated spaces:

$$\begin{aligned} a^j(\cdot, \cdot; t) : V \times V &\longrightarrow \mathbb{R}, & j \in \{1, 2, 3\} & & a_\Gamma^j(\cdot, \cdot; t) : V_\Gamma \times V_\Gamma &\longrightarrow \mathbb{R}, & j \in \{1, 2\} \\ b(\cdot; t, \tilde{c}^\varepsilon, \tilde{c}_\Gamma^\varepsilon) : V &\longrightarrow \mathbb{R} & & & b_\Gamma(\cdot; t, \tilde{c}^\varepsilon, \tilde{c}_\Gamma^\varepsilon) : V_\Gamma &\longrightarrow \mathbb{R} \end{aligned}$$

Moreover, a^2, a^3, a_Γ^2 are compact.

Proof. These results are standard in the theory of parabolic equations, see e.g. Zeidler [Zei90]. See also the assumed regularity for the data and Corollary 3.3.11. \blacklozenge

We are going to prove the following theorem:

3.3.9 Theorem.

There exists a unique weak solution $(\tilde{c}^\varepsilon, \tilde{c}_\Gamma^\varepsilon) \in \mathcal{W} \times \mathcal{W}_\Gamma$ in the sense of Definition 3.3.7.

This theorem will be proven in the next section. Basically, the result is obtained by carrying out the following steps:

1. We consider the decoupled and linearized system: We solve the weak formulation with right hand sides $b(\phi; t, \bar{c}, \bar{c}_\Gamma)$ and $b_\Gamma(\phi_\Gamma; t, \bar{c}, \bar{c}_\Gamma)$, where \bar{c} and \bar{c}_Γ are given functions. We can use the linear theory of parabolic equations to obtain the existence result in this case.
2. Next, we still consider the decoupled problem, but with nonlinear right hand sides given by $b(\phi; t, \tilde{c}^\varepsilon, \bar{c}_\Gamma)$ and $b_\Gamma(\phi_\Gamma; t, \bar{c}, \tilde{c}_\Gamma^\varepsilon)$. We obtain existence in this case by using the Leray-Schauder principle based on appropriate a-priori estimates.
3. Finally, we consider the full system. By using the solution operators from the previous step, we prove the existence of a fixed point for the surface equations via the Leray-Schauder principle. This gives the existence of a solution of the full system.
4. By estimating the difference of two possible solutions, one shows the uniqueness of the solution of the system.

We are also going to use the following regularity result, which is by no means optimal:

3.3.10 Proposition.

The solution $(\tilde{c}^\varepsilon, \tilde{c}_\Gamma^\varepsilon)$ is contained in the space

$$H^1(0, T; V) \times H^1(0, T; V_\Gamma).$$

Proof. Since the right hand sides of the problem are functionals in $H^{\frac{3}{4}}(\Omega^\varepsilon(0))$ and H_Γ as well, well-known parabolic regularity results apply, see for instance [Wlo92] or [LSU88]. By using a bootstrapping argument, one can gain arbitrary regularity provided the data of the problem are sufficiently smooth. \blacklozenge

We conclude this paragraph with an estimate that we are going to use frequently:

3.3.11 Corollary.

For $\phi \in V$, $\phi_\Gamma \in V_\Gamma$ it holds

$$a^1(\phi, \phi; t) \geq d_0 \|\nabla \phi\|_H^2 \quad \text{as well as} \quad a_\Gamma^1(\phi_\Gamma, \phi_\Gamma; t) \geq d_0 \|\nabla^\Gamma \phi_\Gamma\|_{H_\Gamma}^2;$$

and for $u \in \mathcal{V}$, $u_\Gamma \in \mathcal{V}_\Gamma$ we obtain

$$\int_0^T a^1(u(t), u(t); t) dt \geq d_0 \|\nabla u\|_{L^2(0, T; H)}^2$$

$$\int_0^T a_\Gamma^1(u_\Gamma(t), u_\Gamma(t); t) dt \geq d_0 \|\nabla^\Gamma u_\Gamma\|_{L^2(0, T; H_\Gamma)}^2$$

Proof. Integration over the pointwise estimates on the right hand side of Lemma 3.3.5 yields the result. \blacklozenge

3.3.4 Proof of the Existence- and Uniqueness-Theorem

Note that in this section, we do not consider the dependence of constants on ε explicitly, i.e. all the appearing constants might depend on the scale factor.

The following well-known lemma is used frequently:

3.3.12 Lemma (Ehrling's inequality).

Let X, Y, Z be Banach-spaces with compact embedding $X \hookrightarrow Y$ and continuous embedding $Y \hookrightarrow Z$. Then for each $\delta > 0$ there exists a constant $C(\delta) > 0$ such that

$$\|u\|_Y \leq \delta \|u\|_X + C(\delta) \|u\|_Z$$

for all $u \in X$.

Proof. Assume that the asserted inequality is not true. Then there exists a $\delta > 0$ and a sequence $(u_n) \in X^\mathbb{N}$ with

$$\|u_n\|_Y > \delta \|u_n\|_X + n \|u_n\|_Z. \quad (3.15)$$

for all $n \in \mathbb{N}$. Dividing by $\|u_n\|_X$, we may assume that $\|u_n\|_X = 1$. Due to the compact embedding, there exists a $u \in Y$ such that along a subsequence $u_n \rightarrow u$ in Y . Due to the second embedding we thus also have $u_n \rightarrow u$ in Z . Neglecting the right term on the right hand side in (3.15) we obtain $\|u\|_Y > \delta$, thus $u \neq 0$. Neglecting the left term on the right hand side of the same equation, we get after division by n the relation $\|u\|_Z = 0$, thus $u = 0$ – which is a contradiction. \blacklozenge

3.3.13 Corollary.

We will often use the preceding lemma in the following variants:

- With the sequence $H^1(\Omega) \hookrightarrow H^{\frac{3}{4}}(\Omega) \hookrightarrow L^2(\Omega)$ we obtain

$$\begin{aligned} \|u\|_{L^2(\partial\Omega)} &\leq \|u\|_{H^{\frac{1}{4}}(\partial\Omega)} \leq \|u\|_{H^{\frac{3}{4}}(\Omega)} \leq \delta \|u\|_{H^1(\Omega)} + C(\delta) \|u\|_{L^2(\Omega)} \\ &\leq C\delta \|\nabla u\|_{L^2(\Omega)} + C(\delta) \|u\|_{L^2(\Omega)} \quad \text{for } u \in H^1(\Omega). \end{aligned}$$

- Squaring both sides of the previous estimate gives $\|u\|_{L^2(\partial\Omega)}^2 \leq C\delta \|\nabla u\|_{L^2(\Omega)}^2 + C(\delta) \|u\|_{L^2(\Omega)}^2$. Integrating over $[0, T]$ for a $u \in L^2(0, T; H^1(\Omega))$ thus gives the analogous estimate for Bochner-spaces:

$$\|u\|_{L^2(0, T; L^2(\partial\Omega))}^2 \leq C\delta \|\nabla u\|_{L^2(0, T; L^2(\Omega))}^2 + C(\delta) \|u\|_{L^2(0, T; L^2(\Omega))}^2$$

This estimate is used for various boundary terms in the sequel as well as for spaces over $\Omega^\varepsilon(0)$.

Decoupled, Linearized Equations

3.3.14 Lemma.

The forms $a^1 + a^2 + a^3$ and $a_\Gamma^1 + a_\Gamma^2$ are regular Gårding forms, i.e. the embeddings $H \hookrightarrow V$ and $H_\Gamma \hookrightarrow V_\Gamma$ are compact and there exist constants $C, C_\Gamma > 0$ and $K, K_\Gamma \in \mathbb{R}$ such that

$$\begin{aligned} a^1(\phi, \phi; t) + a^2(\phi, \phi; t) + a^3(\phi, \phi; t) &\geq C \|\phi\|_V^2 - K \|\phi\|_H^2 \text{ and} \\ a_\Gamma^1(\phi_\Gamma, \phi_\Gamma; t) + a_\Gamma^2(\phi_\Gamma, \phi_\Gamma; t) &\geq C_\Gamma \|\phi_\Gamma\|_{V_\Gamma}^2 - K_\Gamma \|\phi_\Gamma\|_{H_\Gamma}^2. \end{aligned}$$

Proof. We start by estimating the different terms separately: Due to Corollary 3.3.11 we have

$$a^1(\phi, \phi; t) \geq d_0 \|\nabla \phi\|_{L^2(\Omega^\varepsilon(0))}^2 = d_0 \|\phi\|_V^2 - d_0 \|\phi\|_H^2.$$

Next we have

$$\begin{aligned} |a^2(\phi, \phi; t)| &\leq \|F^{-1}(t)v(t)\|_{L^\infty([0, T] \times \Omega^\varepsilon(0))} \|\nabla \phi\|_{L^2(\Omega^\varepsilon(0))} \|\phi\|_{L^2(\Omega^\varepsilon(0))} \\ &\leq C\delta \|\phi\|_V^2 + C(\delta) \|\phi\|_H^2 \end{aligned}$$

by the scaled Young's inequality, thus

$$a^2(\phi, \phi; t) \geq -C\delta \|\phi\|_V^2 - C(\delta) \|\phi\|_H^2.$$

For the estimation of a^3 note that

$$\begin{aligned} |a^3(\phi, \phi; t)| &\leq (\varepsilon \|\tilde{k}\|_{L^\infty([0, T] \times \Gamma^\varepsilon(0))} + \|\delta_{i1} \tilde{V}^\varepsilon\|_{L^\infty([0, T] \times \Gamma^\varepsilon(0))}) \|\phi\|_{L^2(\Gamma^\varepsilon(0))}^2 + \|\phi\|_{L^2(\partial\Omega)}^2 \\ &\leq C \|\phi\|_{L^2(\Gamma^\varepsilon(0) \cup \partial\Omega)}^2 \leq C \|\phi\|_{H^{\frac{3}{4}}(\Omega^\varepsilon(0))}^2. \end{aligned}$$

By using Ehrling's inequality for $L^2(\Omega^\varepsilon(0)) \subset H^{\frac{3}{4}}(\Omega^\varepsilon(0)) \subset H^1(\Omega^\varepsilon(0))$ and arguing similarly as for a^2 , we obtain

$$a^3(\phi, \phi; t) \geq -C\delta \|\phi\|_V^2 - C(\delta) \|\phi\|_H^2.$$

By summing up, one sees that

$$(a^1 + a^2 + a^3)(\phi, \phi; t) \geq (d_0 - 2C\delta) \|\phi\|_V^2 - (d_0 + 2C(\delta)) \|\phi\|_H^2,$$

thus choosing δ small enough gives the first estimate.

The estimation of the boundary terms a_Γ^1 and a_Γ^2 follows along the same lines and is left to the reader. \blacklozenge

3.3.15 Proposition.

Let $\bar{c} \in L^2(0, T; H)$, $\hat{c} \in \mathcal{V}$ and $\bar{c}_\Gamma \in L^2(0, T; H_\Gamma)$ be given. Then there exist $(\tilde{c}^\varepsilon, \tilde{c}_\Gamma^\varepsilon) \in \mathcal{W} \times \mathcal{W}_\Gamma$ such that

$$\begin{aligned} \frac{d}{dt}(\tilde{c}^\varepsilon(t), \phi)_H + a^1(\tilde{c}^\varepsilon(t), \phi; t) + a^2(\tilde{c}^\varepsilon(t), \phi; t) \\ + a^3(\tilde{c}^\varepsilon(t), \phi; t) = b(\phi; t, \bar{c}, \bar{c}_\Gamma) \quad a.e. [0, T] \end{aligned} \quad (3.16a)$$

$$\tilde{c}^\varepsilon(0) = \tilde{c}_0 \quad (3.16b)$$

holds for all $\phi \in V$ and

$$\begin{aligned} \frac{d}{dt}(\tilde{c}_\Gamma^\varepsilon(t), \phi_\Gamma)_{H_\Gamma} + a_\Gamma^1(\tilde{c}_\Gamma^\varepsilon(t), \phi_\Gamma; t) + a_\Gamma^2(\tilde{c}_\Gamma^\varepsilon(t), \phi; t) = b_\Gamma(\phi; t, \hat{c}, \bar{c}_\Gamma) \quad a.e. [0, T] \\ \tilde{c}_\Gamma^\varepsilon(0) = \tilde{c}_{0,\Gamma} \end{aligned}$$

holds for all $\phi_\Gamma \in V_\Gamma$. Moreover, the estimates

$$\|\tilde{c}^\varepsilon\|_{\mathcal{W}} \leq C(\|b(\cdot; \cdot, \bar{c}, \bar{c}_\Gamma)\|_{L^2(0, T; V^*)} + \|\tilde{c}_0\|_H) \quad (3.17)$$

$$\|\tilde{c}_\Gamma^\varepsilon\|_{\mathcal{W}_\Gamma} \leq C(\|b_\Gamma(\cdot; \cdot, \bar{c}, \bar{c}_\Gamma)\|_{L^2(0, T; V_\Gamma^*)} + \|\tilde{c}_{0,ext}\|_{H_\Gamma}) \quad (3.18)$$

are valid with some constant $C > 0$.

Proof. Due to the estimates in Lemma 3.3.14, we can use Theorem 23.A in [Zei90] to obtain the assertions. In connection with this also note Remark 23.25 in this reference. \blacklozenge

For the moment we neglect the dependence of b on \bar{c}_Γ and that of b_Γ on \bar{c} . Thus the proposition above gives us solution operators

$$\begin{aligned} S : L^2(0, T; H) \longrightarrow \mathcal{W} \quad \text{and} \quad S_\Gamma : L^2(0, T; H_\Gamma) \longrightarrow \mathcal{W}_\Gamma \\ S(\bar{c}) = \tilde{c}^\varepsilon \quad \quad \quad S_\Gamma(\bar{c}_\Gamma) = \tilde{c}_\Gamma^\varepsilon \end{aligned}$$

Decoupled, Nonlinear Equations

We begin by showing some properties of the operators S and S_Γ :

3.3.16 Lemma.

The operators S and S_Γ as defined above are Lipschitz-continuous.

Proof. Let \bar{c}_1 and \bar{c}_2 be two functions in $L^2(0, T; H)$. Then the difference $S(\bar{c}_1) - S(\bar{c}_2)$ solves the problem (3.16) with initial value zero and right hand side $b(\phi; t, \bar{c}_1, \bar{c}_\Gamma) -$

$b(\phi; t, \bar{c}_2, \bar{c}_\Gamma)$. Thus the estimate (3.17) gives

$$\|\tilde{c}^\varepsilon\|_{\mathcal{W}} \leq C \|b(\cdot; \cdot, \bar{c}_1, \bar{c}_\Gamma) - b(\cdot; \cdot, \bar{c}_2, \bar{c}_\Gamma)\|_{L^2(0, T; V^*)}.$$

Now

$$\begin{aligned} |b(\phi; t, \bar{c}_1, \bar{c}_\Gamma) - b(\phi; t, \bar{c}_2, \bar{c}_\Gamma)| &= |(\tilde{f}(\bar{c}_1(t)), \phi)_H - (\tilde{f}(\bar{c}_2(t)), \phi)_H| \\ &\leq \left\| (\tilde{f}(\bar{c}_1(t)) - \tilde{f}(\bar{c}_2(t))) \right\|_H \|\phi(t)\|_H \\ &\leq L \|\bar{c}_1(t) - \bar{c}_2(t)\|_H \|\phi(t)\|_V \end{aligned}$$

due to the Lipschitz-continuity of \tilde{f} . Now integration in time gives

$$\|b(\cdot; \cdot, \bar{c}_1, \bar{c}_\Gamma) - b(\cdot; \cdot, \bar{c}_2, \bar{c}_\Gamma)\|_{L^2(0, T; V^*)} \leq L \|\bar{c}_1 - \bar{c}_2\|_{L^2(0, T; H)},$$

and the result for S follows. A similar argument applies to S_Γ as well. \blacklozenge

Now we can give an existence proof for the decoupled nonlinear system:

3.3.17 Proposition.

Consider the operators S and S_Γ as self-maps $S : L^2(0, T; H) \rightarrow L^2(0, T; H)$ and $S_\Gamma : L^2(0, T; H_\Gamma) \rightarrow L^2(0, T; H_\Gamma)$. Then these operators possess a fixed point in their domains of definition, that is a solution of the problems: Find $(\tilde{c}^\varepsilon, \tilde{c}_\Gamma^\varepsilon) \in \mathcal{W} \times \mathcal{W}_\Gamma$ with

$$\begin{aligned} \frac{d}{dt}(\tilde{c}^\varepsilon(t), \phi)_H + a^1(\tilde{c}^\varepsilon(t), \phi; t) + a^2(\tilde{c}^\varepsilon(t), \phi; t) \\ + a^3(\tilde{c}^\varepsilon(t), \phi; t) = b(\phi; t, \tilde{c}^\varepsilon, \bar{c}_\Gamma) \quad a.e. [0, T] \end{aligned} \quad (3.19a)$$

$$\tilde{c}^\varepsilon(0) = \tilde{c}_0 \quad (3.19b)$$

for all $\phi \in V$, and

$$\frac{d}{dt}(\tilde{c}_\Gamma^\varepsilon(t), \phi_\Gamma)_{H_\Gamma} + a_\Gamma^1(\tilde{c}_\Gamma^\varepsilon(t), \phi_\Gamma; t) + a_\Gamma^2(\tilde{c}_\Gamma^\varepsilon(t), \phi; t) = b_\Gamma(\phi; t, \hat{c}, \tilde{c}_\Gamma^\varepsilon) \quad a.e. [0, T] \quad (3.20a)$$

$$\tilde{c}_\Gamma^\varepsilon(0) = \tilde{c}_{0, \Gamma} \quad (3.20b)$$

for all $\phi_\Gamma \in V_\Gamma$, with given functions $\hat{c} \in \mathcal{V}$ and $\bar{c}_\Gamma \in L^2(0, T; H_\Gamma)$.

Proof. Since the embeddings $\mathcal{W} \hookrightarrow L^2(0, T; H)$ and $\mathcal{W} : \Gamma \hookrightarrow L^2(0, T; H_\Gamma)$ are compact and continuous, the operators S and S_Γ as given in the proposition are compact and continuous as well.

We want to apply the Leray-Schauder principle to show the existence of a fixed point. Therefore we have to derive estimates for a solution of the scaled equations

$$\tilde{c}^\varepsilon = \lambda S(\tilde{c}^\varepsilon) \quad \text{and} \quad \tilde{c}_\Gamma^\varepsilon = \lambda S_\Gamma(\tilde{c}_\Gamma^\varepsilon), \quad \lambda \in (0, 1].$$

These equations correspond to the Problems (3.19) and (3.20), with right hand sides replaced by λb and λb_Γ and initial values $\lambda \tilde{c}_0$ and $\lambda \tilde{c}_{0, \Gamma}$, resp.

We begin with the bulk equation, considered on a smaller time-intervall $[0, s]$, $s > 0$. Due to the continuous embedding $\{u \in L^2(0, s; V), \partial_t u \in L^2(0, s; V^*)\} \subset \mathcal{C}([0, s]; H)$, estimate

(3.17) yields

$$\|\tilde{c}^\varepsilon(s)\|_H \leq C(\lambda \|b(\cdot; \cdot, \tilde{c}^\varepsilon, \bar{c}_\Gamma)\|_{L^2(0, s; V^*)} + \lambda \|\tilde{c}_0\|_H).$$

Similarly to the proof of the previous lemma, we obtain

$$\begin{aligned} |b(\phi; t, \tilde{c}^\varepsilon, \bar{c}_\Gamma)| &\leq \|\tilde{f}(\tilde{c}^\varepsilon(t))\|_H \|\phi\|_H + \|\varepsilon k(t)H\bar{c}_\Gamma(t)\|_{L^2(\Gamma^\varepsilon(0))} \|\phi\|_{L^2(\Gamma^\varepsilon(0))} + \|c_{\text{ext}}\|_{L^2(\partial\Omega)} \|\phi\|_{L^2(\partial\Omega)} \\ &\leq (L \|\tilde{c}^\varepsilon(t)\|_H + C) \|\phi\|_V, \end{aligned}$$

where we used the Lipschitz-continuity of \tilde{f} and $\tilde{f}(0) = 0$. Integration over $[0, s]$ and insertion in the right hand side of the above estimate gives

$$\|\tilde{c}^\varepsilon(s)\|_H^2 \leq \lambda(CL \int_0^s \|\tilde{c}^\varepsilon(s)\|_H^2 ds + K) \leq CL \int_0^s \|\tilde{c}^\varepsilon(s)\|_H^2 ds + TK \quad \forall s \in [0, T],$$

thus Gronwall's lemma implies a bound on $\|\tilde{c}^\varepsilon\|_{L^\infty(0, T; H)}$ independent of λ , thus also on $\|\tilde{c}^\varepsilon\|_{L^2(0, T; H)}$. The same argument also applies to the surface equations. Therefore we can employ the Leray-Schauder principle to obtain the existence of a fixed point of the operators S and S_Γ . \blacklozenge

Thus for given $\hat{c} \in \mathcal{V}$ and $\bar{c}_\Gamma \in L^2(0, T; H_\Gamma)$, we obtain solutions of the decoupled nonlinear problems. This gives us two solution operators

$$\begin{aligned} T : L^2(0, T; H_\Gamma) &\longrightarrow \mathcal{W} & \text{and} & & T_\Gamma : L^2(0, T; V) &\longrightarrow \mathcal{W}_\Gamma \\ T(\bar{c}_\Gamma) &= \tilde{c}^\varepsilon & & & T_\Gamma(\bar{c}) &= \tilde{c}_\Gamma^\varepsilon. \end{aligned}$$

Full System

A solution of the full system is clearly given by fixed point of the map

$$\begin{pmatrix} \bar{c}_\Gamma \\ \bar{c} \end{pmatrix} \mapsto \begin{pmatrix} T_\Gamma(\bar{c}) \\ T(\bar{c}_\Gamma) \end{pmatrix}. \quad (3.21)$$

In a lot of situations, one can show that this map is contracting on $\mathcal{C}([0, T]; L^2(\Omega \times \Gamma^\varepsilon(0)))$, which then gives a fixed point due to Banach's theorem. However, this approach does not work at this place, since the regularity $\tilde{c}^\varepsilon \in \mathcal{C}([0, T]; L^2(\Omega))$ is not enough to ensure the existence of the trace $\tilde{c}^\varepsilon|_{\Gamma^\varepsilon(0)}$, which is needed in the solution of (3.20).

Therefore we use the following approach: Assume that we have a fixed point of the map $T_\Gamma \circ T : L^2(0, T; H_\Gamma) \longrightarrow L^2(0, T; H_\Gamma)$ given by $\bar{c}_\Gamma = T_\Gamma(T(\bar{c}_\Gamma))$. Define $\bar{c} := T(\bar{c}_\Gamma)$. Then obviously $\bar{c}_\Gamma = T_\Gamma(\bar{c})$, and $(\bar{c}_\Gamma, \bar{c})$ is a fixed point of the map given in (3.21). This means that $(\bar{c}_\Gamma, \bar{c})$ is a solution of the full system!

3.3.18 Lemma.

The operators T and T_Γ as defined above are Lipschitz continuous.

Proof. The result follows along the same lines as Lemma 3.3.16. \blacklozenge

3.3.19 Proposition.

Consider the operator $T_\Gamma \circ T : L^2(0, T; H_\Gamma) \longrightarrow L^2(0, T; H_\Gamma)$. Then there exists a fixed point of $T_\Gamma \circ T$.

Proof. Since the embedding $\mathcal{W}_\Gamma \hookrightarrow L^2(0, T; H_\Gamma)$ is compact and continuous, the operator $T_\Gamma \circ T$ is compact and continuous (see also the previous lemma). Thus we can again use the Leray-Schauder principle to obtain the result. Thus we have to consider the equation

$$\bar{c}_\Gamma = \lambda T_\Gamma(T(\bar{c}_\Gamma)), \quad \lambda \in (0, 1],$$

i.e. the system

$$\begin{aligned} \frac{d}{dt}(\bar{c}_\Gamma(t), \phi_\Gamma)_{H_\Gamma} + a_\Gamma^1(\bar{c}_\Gamma(t), \phi_\Gamma; t) + a_\Gamma^2(\bar{c}_\Gamma(t), \phi; t) &= \lambda b_\Gamma(\phi; t, T(\bar{c}_\Gamma), \bar{c}_\Gamma) \quad \text{a.e. } [0, T] \\ \bar{c}_\Gamma(0) &= \lambda \tilde{c}_{0, \Gamma} \quad \forall \phi_\Gamma \in V_\Gamma, \end{aligned}$$

where $T(\bar{c}_\Gamma) =: \bar{c}$ satisfies

$$\begin{aligned} \frac{d}{dt}(\bar{c}(t), \phi)_H + a^1(\bar{c}(t), \phi; t) + a^2(\bar{c}(t), \phi; t) + a^3(\bar{c}(t), \phi; t) &= b(\phi; t, \bar{c}, \bar{c}_\Gamma) \quad \text{a.e. } [0, T] \\ \bar{c}^\varepsilon(0) &= \tilde{c}_0 \quad \forall \phi \in V \end{aligned}$$

We will first derive estimates for $\|\bar{c}\|_{L^2(0, T; V)}$. Subsequently, these estimates are used in the estimation of $\|\bar{c}_\Gamma\|_{L^2(0, T; H_\Gamma)}$ independent of λ .

Since

$$\|b(\cdot; \cdot, \bar{c}, \bar{c}_\Gamma)\|_{L^2(0, s; V^*)}^2 \leq L \|\bar{c}\|_{L^2(0, s; H)}^2 + C \|\bar{c}_\Gamma\|_{L^2(0, s; H_\Gamma)}^2 + C, \quad (3.24)$$

equation (3.17) adapted to the interval $[0, s]$ together with the embedding into $\mathcal{C}([0, s]; H)$ yield as in the proof of Proposition 3.3.17

$$\begin{aligned} \|\bar{c}(s)\|_H^2 &\leq \|\bar{c}\|_{\{u \in L^2(0, s; V); \partial_t u \in L^2(0, s; V^*)\}}^2 \\ &\leq L \|\bar{c}\|_{L^2(0, s; H)}^2 + C' \|\bar{c}_\Gamma\|_{L^2(0, s; H_\Gamma)}^2 + C. \end{aligned}$$

Gronwall's lemma implies that

$$\|\bar{c}\|_{L^2(0, T; H)} \leq TC + TC' \|\bar{c}_\Gamma\|_{L^2(0, T; H_\Gamma)}^2.$$

Going back to estimate (3.17) together with the result (3.24), we see that

$$\|\bar{c}\|_{L^2(0, T; V)} \leq \|\bar{c}\|_{\mathcal{W}} \leq C + C' \|\bar{c}_\Gamma\|_{L^2(0, T; H_\Gamma)}. \quad (3.25)$$

Now we return to the estimation of \bar{c}_Γ as given by the formulation above: Similar to the above derivation, it holds

$$\begin{aligned} \|b_\Gamma(\cdot; \cdot, \bar{c}, \bar{c}_\Gamma)\|_{L^2(0, s; V_\Gamma^*)}^2 &\leq L \|\bar{c}_\Gamma\|_{L^2(0, s; H_\Gamma)}^2 + C \|\bar{c}\|_{L^2(0, s; H_\Gamma)}^2 \\ &\leq L \|\bar{c}_\Gamma\|_{L^2(0, s; H_\Gamma)}^2 + C \|\bar{c}\|_{L^2(0, s; V)}, \end{aligned}$$

thus inequality (3.18) on $[0, s]$ yields together with the continuous embedding $\{u \in L^2(0, s; V_\Gamma); \partial_t u \in L^2(0, s; V_\Gamma^*)\} \hookrightarrow \mathcal{C}(0, s; H_\Gamma)$

$$\begin{aligned} \|\bar{c}_\Gamma(s)\|_{H_\Gamma}^2 &\leq \lambda(C + C' \|\bar{c}_\Gamma\|_{L^2(0, s; H_\Gamma)}^2) \\ &\leq C + C' \|\bar{c}_\Gamma\|_{L^2(0, s; H_\Gamma)}^2. \end{aligned}$$

Now Gronwall's lemma implies that $\|\bar{c}_\Gamma\|_{L^2(0, T; H_\Gamma)}$ is bounded independent of λ . Thus the Leray-Schauder principle applies. \blacklozenge

3.3.20 Proposition.

The solution of the full nonlinear system (3.13), (3.14) is unique.

Proof. Let $(\bar{c}^1, \bar{c}_\Gamma^1)$ and $(\bar{c}^2, \bar{c}_\Gamma^2)$ be two solutions of the full system. Then the difference $(c, c_\Gamma) := (\bar{c}^1, \bar{c}_\Gamma^1) - (\bar{c}^2, \bar{c}_\Gamma^2)$ fulfills the equations (3.13) and (3.14) with right hand sides $b(\phi; t, \bar{c}^1, \bar{c}_\Gamma^1) - b(\phi; t, \bar{c}^2, \bar{c}_\Gamma^2)$ as well as $b_\Gamma(\phi_\Gamma; t, \bar{c}^1, \bar{c}_\Gamma^1) - b_\Gamma(\phi_\Gamma; t, \bar{c}^2, \bar{c}_\Gamma^2)$ and initial value 0. The proof is now based on testing the weak formulations with (c, c_Γ) and estimating the terms appropriately. Finally, one arrives at

$$\|c(s)\|_H^2 + \|c_\Gamma(s)\|_{H_\Gamma}^2 \leq C \|c\|_{L^2(0, s; H)}^2 + C \|c_\Gamma\|_{L^2(0, s; H_\Gamma)}^2,$$

such that Gronwall's lemma implies that $\|c(s)\|_H^2 + \|c_\Gamma(s)\|_{H_\Gamma}^2 \leq 0$ a.e., which gives the result. Since we carry out similar calculations in Sections 3.3.5 and 3.5.1, we do not give the full details at this place. \blacklozenge

Proof of Theorem 3.3.9. Existence is obtained by Proposition 3.3.19, whereas the uniqueness-result is contained in Proposition 3.3.20. \blacklozenge

3.3.5 A-priori Estimates

In this section we prove a-priori estimates for the solution of the Problems (3.11) and (3.12). Since we need to treat the dependence on the scale-factor ε explicitly, we are not using the abstract approach from Section 3.3.3. Instead, we choose specific test functions for the weak formulation and estimate the terms obtained by this procedure.

We are going to prove the following result:

3.3.21 Theorem (A-priori estimates).

There exists a constant $C > 0$, independent of ε , such that for the solutions \tilde{c}^ε and $\tilde{c}_\Gamma^\varepsilon$ of the Problems (3.11) and (3.12) the following estimates hold:

- *The functions $\tilde{c}^\varepsilon, \tilde{c}_\Gamma^\varepsilon$ fulfill the bounds*

$$\begin{aligned} & \|\tilde{c}^\varepsilon\|_{L^\infty(0, T; L^2(\Omega^\varepsilon(0)))} + \|\nabla \tilde{c}^\varepsilon\|_{L^2(0, T; L^2(\Omega^\varepsilon(0)))} \leq C \\ & \varepsilon^{\frac{1}{2}} \|\tilde{c}_\Gamma^\varepsilon\|_{L^\infty(0, T; L^2(\Gamma^\varepsilon(0)))} + \varepsilon^{\frac{3}{2}} \|\nabla^\Gamma \tilde{c}_\Gamma^\varepsilon\|_{L^2(0, T; L^2(\Gamma^\varepsilon(0)))} \leq C. \end{aligned}$$

- *For the corresponding time derivatives, we have the estimates*

$$\begin{aligned} & \|\partial_t \tilde{c}^\varepsilon\|_{L^\infty(0, T; L^2(\Omega^\varepsilon(0)))} + \|\nabla \partial_t \tilde{c}^\varepsilon\|_{L^2(0, T; L^2(\Omega^\varepsilon(0)))} \leq C \\ & \varepsilon^{\frac{1}{2}} \|\partial_t \tilde{c}_\Gamma^\varepsilon\|_{L^\infty(0, T; L^2(\Gamma^\varepsilon(0)))} + \varepsilon^{\frac{3}{2}} \|\nabla^\Gamma \partial_t \tilde{c}_\Gamma^\varepsilon\|_{L^2(0, T; L^2(\Gamma^\varepsilon(0)))} \leq C. \end{aligned}$$

Before presenting the proofs, we give some estimates for the data:

3.3.22 Lemma.

The following estimates hold:

- $\|\tilde{V}^\varepsilon\|_{L^\infty([0, T] \times \Omega)} \leq C\varepsilon$
- $\|\operatorname{div}^\Gamma(F_\Gamma^{-1}\tilde{v}_M^\varepsilon)\|_{L^\infty([0, T] \times \Omega)} \leq C$
- $\|\varepsilon\tilde{\kappa}^\varepsilon\|_{L^\infty([0, T] \times \Omega)} \leq C$, thus especially $\|\tilde{\kappa}^\varepsilon\tilde{V}^\varepsilon\|_{L^\infty([0, T] \times \Omega)} \leq C$
- $\|\tilde{v}^\varepsilon\|_{L^\infty([0, T] \times \Omega)} \leq C\varepsilon$
- $\|\tilde{k}\|_{L^\infty([0, T] \times \Omega)} \leq C$
- $\|\partial_t\tilde{V}^\varepsilon\|_{L^\infty([0, T] \times \Omega)} \leq C\varepsilon$
- $\|\operatorname{div}^\Gamma(\partial_t(F_\Gamma^{-1}\tilde{v}_M^\varepsilon))\|_{L^\infty([0, T] \times \Omega)} \leq C$
- $\|\varepsilon\partial_t\tilde{\kappa}^\varepsilon\|_{L^\infty([0, T] \times \Omega)} \leq C$, thus especially $\|\partial_t(\tilde{\kappa}^\varepsilon\tilde{V}^\varepsilon)\|_{L^\infty([0, T] \times \Omega)} \leq C$
- $\|\partial_t\tilde{v}^\varepsilon\|_{L^\infty([0, T] \times \Omega)} \leq C\varepsilon$
- $\|\partial_t\tilde{k}\|_{L^\infty([0, T] \times \Omega)} \leq C$
- $\|\partial_t(F^{-1}F^{-T})\|_{L^\infty([0, T] \times \Omega)} \leq C$
- $\|\partial_t(F_\Gamma^{-1}F_\Gamma^{-T})\|_{L^\infty([0, T] \times \Omega)} \leq C$

Proof. All the estimates follow by using the regularity of the auxiliary functions. We elaborate on some of the terms: We have

$$\tilde{v}^\varepsilon(t, x) = \partial_t\phi^\varepsilon(t, x) = \varepsilon\partial_t\psi(t, \varepsilon\left[\frac{x}{\varepsilon}\right], \left\{\frac{x}{\varepsilon}\right\}),$$

where ψ is bounded in $L^\infty([0, T] \times \Omega \times Y)$. Since the transformed normal vector

$$\frac{F_\Gamma^{-T}\tilde{\nu}^\varepsilon}{|F_\Gamma^{-T}\tilde{\nu}^\varepsilon|} = \frac{(\nabla_y\psi^{-1}(t, \left[\frac{x}{\varepsilon}\right], \left\{\frac{x}{\varepsilon}\right\}))^T\tilde{\nu}(\left\{\frac{x}{\varepsilon}\right\})}{|(\nabla_y\psi^{-1}(t, \left[\frac{x}{\varepsilon}\right], \left\{\frac{x}{\varepsilon}\right\}))^T\tilde{\nu}(\left\{\frac{x}{\varepsilon}\right\})|}$$

is bounded independent of ε , we obtain an estimate for \tilde{V}^ε as well. Next we get

$$\begin{aligned} \operatorname{div}^\Gamma(F_\Gamma^{-1}\tilde{v}_M^\varepsilon)(t, x) &= \frac{1}{\varepsilon}\operatorname{div}_y^\Gamma\left(\nabla_y^\Gamma\psi_\Gamma(t, \left[\frac{x}{\varepsilon}\right], \left\{\frac{x}{\varepsilon}\right\}) \cdot \varepsilon\partial_t\psi_\Gamma(t, \left[\frac{x}{\varepsilon}\right], \left\{\frac{x}{\varepsilon}\right\})\right) \\ &= \operatorname{div}_y^\Gamma\left(\nabla_y^\Gamma\psi_\Gamma(t, \left[\frac{x}{\varepsilon}\right], \left\{\frac{x}{\varepsilon}\right\}) \cdot \partial_t\psi_\Gamma(t, \left[\frac{x}{\varepsilon}\right], \left\{\frac{x}{\varepsilon}\right\})\right), \end{aligned}$$

the right hand side being bounded independently of ε by the regularity assumptions on ψ . Moreover

$$\begin{aligned} \varepsilon\tilde{\kappa}^\varepsilon(t, x) &= -\varepsilon\operatorname{div}\left(F^{-1}\frac{F_\Gamma^{-T}\tilde{\nu}^\varepsilon}{|F_\Gamma^{-T}\tilde{\nu}^\varepsilon|}\right)(t, x) \\ &= -\operatorname{div}_y\left(\nabla_y\psi^{-1}(t, \left[\frac{x}{\varepsilon}\right], \left\{\frac{x}{\varepsilon}\right\}) \frac{(\nabla_y\psi^{-1}(t, \left[\frac{x}{\varepsilon}\right], \left\{\frac{x}{\varepsilon}\right\}))^T\tilde{\nu}(\left\{\frac{x}{\varepsilon}\right\})}{|(\nabla_y\psi^{-1}(t, \left[\frac{x}{\varepsilon}\right], \left\{\frac{x}{\varepsilon}\right\}))^T\tilde{\nu}(\left\{\frac{x}{\varepsilon}\right\})|}\right), \end{aligned}$$

again with a bounded right hand side due to the regularity assumptions on ψ and $\tilde{\nu}$. The estimation of the remaining terms follows along the same lines. \blacklozenge

Bounds for the Functions

We begin with the following estimates:

3.3.23 Proposition.

There exists a constant $C \geq 0$ independent of ε such that

$$\begin{aligned} & \|\tilde{c}^\varepsilon\|_{L^\infty(0,T;L^2(\Omega^\varepsilon(0)))} + \|\nabla \tilde{c}^\varepsilon\|_{L^2(0,T;L^2(\Omega^\varepsilon(0)))} \leq C, \\ & \varepsilon \|\tilde{c}_\Gamma^\varepsilon\|_{L^\infty(0,T;L^2(\Gamma^\varepsilon(0)))} + \varepsilon^{\frac{3}{2}} \|\nabla^\Gamma \tilde{c}_\Gamma^\varepsilon\|_{L^2(0,T;L^2(\Gamma^\varepsilon(0)))} \leq C. \end{aligned}$$

Proof. Choose $\phi = \tilde{c}^\varepsilon(t)$ in (3.13a), $\phi_\Gamma(t) = \varepsilon \tilde{c}_\Gamma^\varepsilon(t)$ in (3.14a) and integrate from 0 to t . We estimate the terms in each equation separately: For the bulk equation we obtain

$$\begin{aligned} & \int_0^t \int_{\Omega^\varepsilon(0)} \frac{d}{dt} |\tilde{c}^\varepsilon|^2 \, dx \, dt = \frac{1}{2} \|\tilde{c}^\varepsilon(t)\|_H^2 - \frac{1}{2} \|\tilde{c}_0\|_H^2; \\ & d_0 \|\nabla \tilde{c}^\varepsilon\|_{L^2(0,t;H)}^2 \leq \int_0^t (DF^{-T} \nabla \tilde{c}^\varepsilon, F^{-T} \nabla \tilde{c}^\varepsilon)_H \, dt; \\ & \int_0^t |(\nabla \tilde{c}^\varepsilon \cdot F^{-1} v^\varepsilon, \tilde{c}^\varepsilon)_H| \, dt \leq \|F^{-1} v^\varepsilon\|_{L^\infty([0,T] \times \Omega^\varepsilon(0))} \left(\int_0^t \|\nabla \tilde{c}^\varepsilon\|_H \|\tilde{c}^\varepsilon\|_H \, dt \right) \\ & \leq C \varepsilon \delta \|\nabla \tilde{c}^\varepsilon\|_{L^2(0,t;H)}^2 + C(\delta) \varepsilon \|\tilde{c}^\varepsilon\|_{L^2(0,t;H)}^2; \\ & \int_0^t |\varepsilon(\tilde{k} \tilde{c}^\varepsilon + \delta_{i1} \tilde{V}^\varepsilon \tilde{c}^\varepsilon, \tilde{c}^\varepsilon)_{H_\Gamma}| \, dt \leq (\|\tilde{k}\|_{L^\infty([0,T] \times \Omega^\varepsilon(0))} + \|\tilde{V}^\varepsilon\|_{L^\infty([0,T] \times \Omega^\varepsilon(0))}) \int_0^t \varepsilon \|\tilde{c}^\varepsilon\|_{H_\Gamma}^2 \, dt \\ & \leq C(\|\tilde{c}^\varepsilon\|_{L^2(0,t;H)}^2 + \varepsilon^2 \|\nabla \tilde{c}^\varepsilon\|_{L^2(0,t;H)}^2) \end{aligned}$$

(see also Lemma 3.1.15 with $k = 0$), together with

$$\int_0^t |(\tilde{c}^\varepsilon, \tilde{c}^\varepsilon)_{L^2(\partial\Omega)}| \, dt \leq \|\tilde{c}^\varepsilon\|_{L^2(0,t;H^{\frac{1}{4}}(\partial\Omega))}^2 \leq C \delta \|\nabla \tilde{c}^\varepsilon\|_{L^2(0,t;H)}^2 + C(\delta) \|\tilde{c}^\varepsilon\|_{L^2(0,t;H)}^2$$

by Corollary 3.3.13. Moreover

$$\begin{aligned} & \int_0^t |(\tilde{f}(\tilde{c}^\varepsilon), \tilde{c}^\varepsilon)_H| \, dt \leq C(1 + \|\tilde{c}^\varepsilon\|_{L^2(0,t;H)}) \|\tilde{c}^\varepsilon\|_{L^2(0,t;H)} \leq C + C \|\tilde{c}^\varepsilon\|_{L^2(0,t;H)}^2; \\ & \int_0^t \varepsilon(\tilde{k}(t) H \tilde{c}_\Gamma^\varepsilon(t), \tilde{c}^\varepsilon(t))_{H_\Gamma} \, dt \leq \|H \tilde{k}\|_{L^\infty(\Omega^\varepsilon(0))} (\|\tilde{c}_\Gamma^\varepsilon\|_{L^2(0,t;H_\Gamma)} \|\tilde{c}^\varepsilon\|_{L^2(0,t;H_\Gamma)}) \\ & \leq C \varepsilon \|\tilde{c}_\Gamma^\varepsilon\|_{L^2(0,t;H_\Gamma)}^2 + C \varepsilon \|\tilde{c}^\varepsilon\|_{L^2(0,t;H_\Gamma)}^2 \\ & \leq C \varepsilon \|\tilde{c}_\Gamma^\varepsilon\|_{L^2(0,t;H_\Gamma)}^2 + C(\|\tilde{c}^\varepsilon\|_{L^2(0,t;H)}^2 + \varepsilon^2 \|\nabla \tilde{c}^\varepsilon\|_{L^2(0,t;H)}^2); \end{aligned}$$

$$\begin{aligned} \int_0^t (c_{\text{ext}}(t), \tilde{c}^\varepsilon)_{L^2(\partial\Omega)} dt &\leq C \|\tilde{c}^\varepsilon\|_{L^2(0,t;L^2(\partial\Omega))} \leq C + C \|\tilde{c}^\varepsilon\|_{L^2(0,t;L^2(\partial\Omega))}^2 \\ &\leq C + C\delta \|\nabla \tilde{c}^\varepsilon\|_{L^2(0,t;H)}^2 + C(\delta) \|\tilde{c}^\varepsilon\|_{L^2(0,t;H)}^2. \end{aligned}$$

For the surface equation we get

$$\begin{aligned} \int_0^t \int_{\Gamma^\varepsilon(0)} \frac{d}{dt} \varepsilon |\tilde{c}_\Gamma^\varepsilon|^2 dx dt &= \frac{\varepsilon}{2} \|\tilde{c}_\Gamma^\varepsilon(t)\|_{H_\Gamma}^2 - \frac{\varepsilon}{2} \|\tilde{c}_{0,\Gamma}\|_{H_\Gamma}^2; \\ d_0 \varepsilon^3 \|\nabla \tilde{c}_\Gamma^\varepsilon\|_{L^2(0,t;H_\Gamma)}^2 &\leq \int_0^t \varepsilon^3 (D_\Gamma F_\Gamma^{-T}(t) \nabla^\Gamma \tilde{c}_\Gamma^\varepsilon(t), F_\Gamma^{-T}(t) \nabla^\Gamma \tilde{c}_\Gamma^\varepsilon(t))_{H_\Gamma} dt; \\ \int_0^t \varepsilon ([\text{div}^\Gamma(F_\Gamma^{-1}(t) \tilde{v}_M^\varepsilon(t)) - \tilde{\kappa}(t) \tilde{V}^\varepsilon(t) + \tilde{k}(t)H] \tilde{c}_\Gamma^\varepsilon(t), \tilde{c}_\Gamma^\varepsilon(t))_{H_\Gamma} dt \\ &\leq \varepsilon \left(\left\| |\text{div}^\Gamma(F_\Gamma^{-1} \tilde{v}_M^\varepsilon)| + |\tilde{\kappa} \tilde{V}^\varepsilon| + |\tilde{k}H| \right\|_{L^\infty([0,T] \times \Omega)} \right) \|\tilde{c}_\Gamma^\varepsilon\|_{L^2(0,t;H_\Gamma)}^2 \\ &\leq C\varepsilon \|\tilde{c}_\Gamma^\varepsilon\|_{L^2(0,t;H_\Gamma)}^2; \\ \int_0^t \varepsilon (\tilde{f}_\Gamma(\tilde{c}_\Gamma^\varepsilon(t)), \tilde{c}_\Gamma^\varepsilon(t))_{H_\Gamma} dt &\leq C\varepsilon(1 + \|\tilde{c}_\Gamma^\varepsilon\|_{L^2(0,t;H_\Gamma)}) \|\tilde{c}_\Gamma^\varepsilon\|_{L^2(0,t;H_\Gamma)} \leq C\varepsilon + C\varepsilon \|\tilde{c}_\Gamma^\varepsilon\|_{L^2(0,t;H_\Gamma)}^2 \end{aligned}$$

and finally

$$\begin{aligned} \int_0^t \varepsilon \left(\tilde{k}(t) + \frac{\delta_{i2}}{\varepsilon} \tilde{V}^\varepsilon \right) \tilde{c}^\varepsilon(t), \tilde{c}_\Gamma^\varepsilon(t) \Big)_{H_\Gamma} &\leq \varepsilon \left\| |\tilde{k}| + \left| \frac{1}{\varepsilon} \tilde{V}^\varepsilon \right| \right\|_{L^\infty([0,T] \times \Omega)} \|\tilde{c}^\varepsilon\|_{L^2(0,t;H_\Gamma)} \|\tilde{c}_\Gamma^\varepsilon\|_{L^2(0,t;H_\Gamma)} \\ &\leq C\varepsilon \|\tilde{c}_\Gamma^\varepsilon\|_{L^2(0,t;H_\Gamma)}^2 + C(\|\tilde{c}^\varepsilon\|_{L^2(0,t;H)}^2 + \varepsilon^2 \|\nabla \tilde{c}^\varepsilon\|_{L^2(0,t;H)}^2). \end{aligned}$$

Now we put everything together; note that the first two estimates for each equation are used on the left hand side of the following relation, whereas all the remaining terms are put on the right hand side: Adding up (3.13a) with $\phi = \tilde{c}^\varepsilon(t)$, and (3.14a) with $\phi_\Gamma(t) = \varepsilon \tilde{c}_\Gamma^\varepsilon(t)$ (both integrated from 0 to t) gives with the help of the estimates above

$$\begin{aligned} \|\tilde{c}^\varepsilon(t)\|_H^2 + (d_0 - C\varepsilon^2 - C\varepsilon\delta) \|\nabla \tilde{c}^\varepsilon\|_{L^2(0,t;H)}^2 + \varepsilon \|\tilde{c}_\Gamma^\varepsilon(t)\|_{H_\Gamma}^2 + C\varepsilon^3 \|\nabla^\Gamma \tilde{c}_\Gamma^\varepsilon\|_{L^2(0,t;H_\Gamma)}^2 \\ \leq C + C(\delta) \|\tilde{c}^\varepsilon\|_{L^2(0,t;H)}^2 + C\varepsilon \|\tilde{c}_\Gamma^\varepsilon\|_{L^2(0,t;H_\Gamma)}^2. \end{aligned}$$

Choose δ and ε small enough such that $(d_0 - C\varepsilon^2 - C\varepsilon\delta) > 0$, then neglecting the terms containing a gradient gives with the help of Gronwall's inequality

$$\begin{aligned} \|\tilde{c}^\varepsilon(t)\|_H^2 &\leq C \quad \text{for almost all } t \in [0, T] \\ \varepsilon \|\tilde{c}_\Gamma^\varepsilon(t)\|_{H_\Gamma}^2 &\leq C \quad \text{for almost all } t \in [0, T], \end{aligned}$$

which gives the bounds in $L^\infty(0, T; H)$. Due to the continuous embedding $L^\infty([0, T]) \hookrightarrow L^2([0, T])$, we get the same bounds in $L^2(0, T; H)$ and $L^2(0, T; H_\Gamma)$, resp. Inserting these bounds in the right hand side of the last estimate for $t = T$ gives the remaining estimate on the gradients. \blacklozenge

Bounds for the Time-Derivatives

For the estimation of the nonlinear reaction rates, we need the following lemma:

3.3.24 Lemma.

Let $c \in H^1(0, T; L^2(\Omega^\varepsilon(0)))$ and $c_\Gamma \in H^1(0, T; L^2(\Gamma^\varepsilon(0)))$. Then it holds

$$\begin{aligned} \|\partial_t \tilde{f}(\cdot, c)\|_{L^2(0, T; L^2(\Omega^\varepsilon(0)))} &\leq L \|\partial_t c\|_{L^2(0, T; L^2(\Omega^\varepsilon(0)))}, \\ \|\partial_t \tilde{f}_\Gamma(\cdot, c_\Gamma)\|_{L^2(0, T; L^2(\Gamma^\varepsilon(0)))} &\leq L \|\partial_t c_\Gamma\|_{L^2(0, T; L^2(\Gamma^\varepsilon(0)))}. \end{aligned}$$

Proof. The proof is carried out in several steps: First we show the estimate for smooth c : Choose a $c \in \mathcal{C}^1([0, T] \times \Omega^\varepsilon(0))$. Fix a $\delta > 0$ and let $0 < h < \delta$. Due to the Lipschitz-continuity of \tilde{f} , we obtain the estimate

$$\left| \frac{\tilde{f}(x, c(t+h, x)) - \tilde{f}(x, c(t, x))}{h} \right|^2 \leq \frac{L^2}{h^2} |c(t+h, x) - c(t, x)|^2. \quad (3.26)$$

Now the left hand side converges to $|\partial_t \tilde{f}(x, c(t, x))|^2$ for $h \rightarrow 0$, whereas the right hand side goes to $L^2 |\partial_t c(t, x)|^2$. Integration over $[0, T - \delta] \times \Omega^\varepsilon(0)$ yields

$$\int_0^{T-\delta} \int_{\Omega^\varepsilon(0)} |\partial_t \tilde{f}(x, c(t, x))|^2 dx dt \leq \int_0^{T-\delta} \int_{\Omega^\varepsilon(0)} L^2 |\partial_t c(t, x)|^2 dx dt.$$

Since δ is arbitrary, the first assertion holds for smooth c .

In a second step, we show the existence of $\partial_t \tilde{f}(c)$ for $c \in H^1(0, T; L^2(\Omega^\varepsilon(0)))$: Assume that c has the latter regularity. Due to Lemma 3.3.4, \tilde{f} is a map $L^2(0, T; L^2(\Omega^\varepsilon(0))) \rightarrow L^2(0, T; L^2(\Omega^\varepsilon(0)))$, thus $\frac{\tilde{f}(\cdot, c(\cdot+h, \cdot)) - \tilde{f}(\cdot, c(\cdot, \cdot))}{h} \in L^2(0, T - \delta; L^2(\Omega^\varepsilon(0)))$. Integrating the estimate (3.26), one obtains

$$\begin{aligned} \int_0^{T-\delta} \int_{\Omega^\varepsilon(0)} \left| \frac{\tilde{f}(x, c(t+h, x)) - \tilde{f}(x, c(t, x))}{h} \right|^2 dx dt &\leq \int_0^{T-\delta} \int_{\Omega^\varepsilon(0)} \frac{L^2}{h^2} |c(t+h, x) - c(t, x)|^2 dx dt \\ &\rightarrow \int_0^{T-\delta} \int_{\Omega^\varepsilon(0)} L^2 |\partial_t c(t, x)|^2 dx dt, \end{aligned}$$

which shows that $\frac{\tilde{f}(\cdot, c(\cdot+h, \cdot)) - \tilde{f}(\cdot, c(\cdot, \cdot))}{h}$ is bounded in $L^2(0, T - \delta; L^2(\Omega^\varepsilon(0)))$ independent of h . By the theorem of Eberlein-Shmulyian, there exists a $g_\delta \in L^2(0, T - \delta; L^2(\Omega^\varepsilon(0)))$

such that along some sequence $h_n \rightarrow 0$

$$\frac{\tilde{f}(\cdot, c(\cdot + h_n, \cdot)) - \tilde{f}(\cdot, c(\cdot, \cdot))}{h_n} \rightharpoonup g_\delta \quad \text{in } L^2(0, T - \delta; L^2(\Omega^\varepsilon(0))).$$

Now choose a $\phi \in C_0^\infty(0, T)$ with $\text{supp}(\phi) \subset (\delta, T - \delta)$ and fix a $v \in L^2(0, T; L^2(\Omega^\varepsilon(0)))$. By the integration by parts-formula for difference quotients (see e.g. [Mei08], Lemma B.2.3), we obtain

$$\begin{aligned} & \int_{\delta}^T \int_{\Omega^\varepsilon(0)} \frac{\phi(t) - \phi(t-h)}{h} \tilde{f}(x, c(t, x)) v(x) \, dx \, dt \\ &= - \int_0^{T-\delta} \int_{\Omega^\varepsilon(0)} \frac{\tilde{f}(x, c(t+h, x)) - \tilde{f}(x, c(t, x))}{h} \phi(t) v(x) \, dx \, dt \\ & \quad + \underbrace{\frac{1}{h} \int_t^{t+h} \int_{\Omega^\varepsilon(0)} \phi(\tau) \tilde{f}(x, c(\tau, x)) v(x) \, dx \, d\tau}_{=0} \Bigg|_{t=0}^{t=T-\delta}. \end{aligned}$$

For $h = h_n \rightarrow 0$ the left hand side converges to $\int_{\delta}^T \int_{\Omega^\varepsilon(0)} \phi'(t) \tilde{f}(x, c(t, x)) v(x) \, dx \, dt$, and the right hand side to $-\int_0^{T-\delta} \int_{\Omega^\varepsilon(0)} g_\delta(t, x) \phi(t) v(x) \, dx \, dt$ and thus

$$\int_0^T \int_{\Omega^\varepsilon(0)} \phi'(t) \tilde{f}(x, c(t, x)) v(x) \, dx \, dt = - \int_0^T \int_{\Omega^\varepsilon(0)} g_\delta(t, x) \phi(t) v(x) \, dx \, dt$$

for some extension of g_δ . By the definition of weak time-derivatives (see e.g. Zeidler [Zei90]), this means that $g_\delta(t, x) = \partial_t \tilde{f}(x, c(t, x))$ on $[\delta, T_\delta]$. Since the derivative is unique, we can construct such functions on an increasing sequence of sets to obtain the function $\partial_t \tilde{f}(x, c(t, x)) \in L^2(0, T; L^2(\Omega^\varepsilon(0)))$. In this connection note that the estimate for this time derivative can actually be chosen independent of δ .

Finally, by density of $C^1([0, T] \times \Omega^\varepsilon(0))$ in $H^1(0, T; L^2(\Omega^\varepsilon(0)))$ the first estimate follows. The proof of the remaining estimate follows along the same lines. \blacklozenge

3.3.25 Proposition.

There exists a constant $C \geq 0$ independent of ε such that

$$\begin{aligned} & \|\partial_t \tilde{c}^\varepsilon\|_{L^\infty(0, T; L^2(\Omega^\varepsilon(0)))} + \|\nabla \partial_t \tilde{c}^\varepsilon\|_{L^2(0, T; L^2(\Omega^\varepsilon(0)))} \leq C, \\ & \varepsilon^{\frac{1}{2}} \|\partial_t \tilde{c}_\Gamma^\varepsilon\|_{L^\infty(0, T; L^2(\Gamma^\varepsilon(0)))} + \varepsilon^{\frac{3}{2}} \|\nabla^\Gamma \partial_t \tilde{c}_\Gamma^\varepsilon\|_{L^2(0, T; L^2(\Gamma^\varepsilon(0)))} \leq C. \end{aligned}$$

Proof. We carry out the proof by differentiating the defining equations for \tilde{c}^ε and $\tilde{c}_\Gamma^\varepsilon$, (3.11) and (3.12) with respect to time in order to derive the defining equations for $\partial_t \tilde{c}^\varepsilon$ and $\partial_t \tilde{c}_\Gamma^\varepsilon$. Using a test function approach similar to 3.3.23, we obtain the estimates. For a justification of this technique, see Wloka [Wlo92], Section 27.

We obtain the following equations:

$$\begin{aligned}
& \partial_{tt}\tilde{c}^\varepsilon - \nabla \partial_t \tilde{c}^\varepsilon \cdot F^{-1} \tilde{v}^\varepsilon - \nabla \tilde{c}^\varepsilon \cdot \partial_t(F^{-1} \tilde{v}^\varepsilon) - \operatorname{div}(DF^{-1}F^{-T} \nabla \partial_t \tilde{c}^\varepsilon) \\
& \quad - \operatorname{div}(D\partial_t(F^{-1}F^{-T}) \nabla \tilde{c}^\varepsilon) = \partial_t \tilde{f}(\tilde{c}^\varepsilon) \quad \text{in } \Omega(0) \\
& (-DF^{-T} \nabla \partial_t \tilde{c}^\varepsilon - D\partial_t F^{-T} \nabla \tilde{c}^\varepsilon) \cdot \tilde{v} = \delta_{i1} \partial_t \tilde{c}^\varepsilon \tilde{V}^\varepsilon + \delta_{i1} \tilde{c}^\varepsilon \partial_t \tilde{V}^\varepsilon \\
& \quad + \varepsilon \tilde{k}(\partial_t \tilde{c}^\varepsilon - H \partial_t \tilde{c}_\Gamma^\varepsilon) + \varepsilon \partial_t \tilde{k}(\tilde{c}^\varepsilon - H \tilde{c}_\Gamma^\varepsilon) \quad \text{on } \Gamma^\varepsilon(0) \\
& (-DF^{-T} \nabla \partial_t \tilde{c}^\varepsilon - D\partial_t F^{-T} \nabla \tilde{c}^\varepsilon) \cdot \tilde{v} = \partial_t \tilde{c}^\varepsilon - \partial_t \tilde{c}_{\text{ext}} \quad \text{on } \partial\Omega \\
& \partial_t \tilde{c}^\varepsilon(0, \cdot) = \tilde{c}_1 \quad \text{in } \Omega(0).
\end{aligned}$$

Here the initial condition is given by

$$\tilde{c}_1 = \tilde{f}(0, \tilde{c}_0) - \operatorname{div}(DF^{-1}(0)F^{-T}(0) \nabla \tilde{c}_0),$$

see [Wlo92]. We obtain

$$\begin{aligned}
\|\tilde{c}_1\|_V & \leq \|f(0, \tilde{c}_0)\|_H + \|\nabla f(0, \tilde{c}_0)\|_H + C \|\tilde{c}_0\|_{H^2(\Omega^\varepsilon(0))} + C \|\nabla \tilde{c}_0\|_{H^2(\Omega^\varepsilon(0))} \\
& \leq C + C \|\tilde{c}_0\|_H + L \|\nabla \tilde{c}_0\|_H + C \|\tilde{c}_0\|_{H^3(\Omega^\varepsilon(0))} \\
& \leq C \|\tilde{c}_0\|_{H^3(\Omega^\varepsilon(0))} \leq C
\end{aligned}$$

with bounds independent of ε . Here we used Rademacher's theorem for $\nabla f(0, \tilde{c}_0)$, the Lipschitz-continuity of \tilde{f} , and the regularity and boundedness of F . Similarly we get

$$\begin{aligned}
& \partial_{tt}\tilde{c}_\Gamma^\varepsilon - \varepsilon^2 \operatorname{div}^\Gamma(D_\Gamma F_\Gamma^{-1} F_\Gamma^{-T} \nabla^\Gamma \partial_t \tilde{c}_\Gamma^\varepsilon) - \varepsilon^2 \operatorname{div}^\Gamma(D_\Gamma \partial_t(F_\Gamma^{-1} F_\Gamma^{-T}) \nabla^\Gamma \tilde{c}_\Gamma^\varepsilon) \\
& + \partial_t \tilde{c}_\Gamma^\varepsilon \operatorname{div}^\Gamma(F_\Gamma^{-1} \tilde{v}_M^\varepsilon) + \tilde{c}_\Gamma^\varepsilon \operatorname{div}^\Gamma(\partial_t(F_\Gamma^{-1} \tilde{v}_M^\varepsilon)) - \partial_t \tilde{c}_\Gamma^\varepsilon \tilde{\kappa}^\varepsilon \tilde{V}^\varepsilon - \tilde{c}_\Gamma^\varepsilon \partial_t(\tilde{\kappa}^\varepsilon \tilde{V}^\varepsilon) - \partial_t \tilde{f}(\tilde{c}_\Gamma^\varepsilon) \\
& = -\frac{\delta_{i2}}{\varepsilon} \partial_t \tilde{c}^\varepsilon \tilde{V}^\varepsilon - \frac{\delta_{i2}}{\varepsilon} \tilde{c}^\varepsilon \partial_t \tilde{V}^\varepsilon + \tilde{k}(\partial_t \tilde{c}^\varepsilon - H \partial_t \tilde{c}_\Gamma^\varepsilon) + \partial_t \tilde{k}(\tilde{c}^\varepsilon - H \tilde{c}_\Gamma^\varepsilon) \quad \text{on } \Gamma^\varepsilon(0) \\
& \partial_t \tilde{c}_\Gamma^\varepsilon(0, \cdot) = \tilde{c}_{1,\Gamma} \quad \text{on } \Gamma^\varepsilon(0)
\end{aligned}$$

with an initial condition

$$\tilde{c}_{1,\Gamma} = \tilde{f}_\Gamma(0, \tilde{c}_{0,\Gamma}) - \varepsilon^2 \operatorname{div}^\Gamma(F_\Gamma^{-1} F_\Gamma^{-T} \nabla \tilde{c}_{0,\Gamma}).$$

Using the same arguments as above, we obtain that $\tilde{c}_{1,\Gamma} \in V_\Gamma$ (which is needed for the regularity result of [Wlo92]); however we do *not* get reasonable bounds in the space V_Γ . Since we only need estimates in H_Γ in the estimation of the time derivatives, the following inequality is sufficient: Due to the general trace inequality 3.1.15 we have

$$\begin{aligned}
\sqrt{\varepsilon} \|\tilde{c}_{1,\Gamma}\|_{H_\Gamma} & \leq \sqrt{\varepsilon} \left\| \tilde{f}_\Gamma(0, \tilde{c}_{0,\Gamma}) \right\|_{H_\Gamma} + \varepsilon^{\frac{5}{2}} \left\| \operatorname{div}^\Gamma(F_\Gamma^{-1} F_\Gamma^{-T} \nabla \tilde{c}_{0,\Gamma}) \right\|_{H_\Gamma} \\
& \leq C\sqrt{\varepsilon} + C\sqrt{\varepsilon} \|\tilde{c}_{0,\Gamma}\|_{H_\Gamma} + C\varepsilon^{\frac{5}{2}} \|\tilde{c}_{0,\Gamma}\|_{H^2(\Gamma^\varepsilon(0))} \\
& \leq C + C\sqrt{\varepsilon} \|\tilde{c}_{0,\Gamma}\|_{H_\Gamma} + C\varepsilon^{\frac{3}{2}} \|\nabla^\Gamma \tilde{c}_{0,\Gamma}\|_{H_\Gamma} + C\varepsilon^{\frac{5}{2}} \|\nabla^\Gamma \nabla^\Gamma \tilde{c}_{0,\Gamma}\|_{H_\Gamma} \\
& \leq C + C \|\tilde{c}_{0,\Gamma}\|_H + C\varepsilon \|\nabla \tilde{c}_{0,\Gamma}\|_H + C\varepsilon^2 \|\nabla \nabla \tilde{c}_{0,\Gamma}\|_H + C\varepsilon^3 \|\nabla \nabla \nabla \tilde{c}_{0,\Gamma}\|_H \\
& \leq C + C \|\tilde{c}_{0,\Gamma}\|_{H^3(\Omega)} \leq C
\end{aligned}$$

independent of ε .

The weak formulation of the problems above reads: Find $(\partial_t \tilde{c}^\varepsilon, \partial_t \tilde{c}_\Gamma^\varepsilon) \in \mathcal{W} \times \mathcal{W}_\Gamma$ such that for all $(\phi, \phi_\Gamma) \in V \times V_\Gamma$ it holds

$$\begin{aligned} & \frac{d}{dt} (\partial_t \tilde{c}^\varepsilon, \phi)_H + (DF^{-T} \nabla \partial_t \tilde{c}^\varepsilon, F^{-T} \nabla \phi)_H + (D \partial_t (F^{-1} F^{-T}) \nabla \tilde{c}^\varepsilon, \nabla \phi)_H \\ & - (\nabla \partial_t \tilde{c}^\varepsilon \cdot F^{-1} \tilde{v}^\varepsilon, \phi)_H - (\nabla \tilde{c}^\varepsilon \cdot \partial_t (F^{-1} \tilde{v}^\varepsilon), \phi)_H + (\delta_{i1} \partial_t \tilde{c}^\varepsilon \tilde{V}^\varepsilon, \phi)_{H_\Gamma} + (\delta_{i1} \tilde{c}^\varepsilon \partial_t \tilde{V}^\varepsilon, \phi)_{H_\Gamma} \\ & + \varepsilon (\tilde{k} (\partial_t \tilde{c}^\varepsilon - H \partial_t \tilde{c}_\Gamma^\varepsilon), \phi)_{H_\Gamma} + \varepsilon (\partial_t \tilde{k} (\tilde{c}^\varepsilon - H \tilde{c}_\Gamma^\varepsilon), \phi)_{H_\Gamma} - (\partial_t \tilde{c}^\varepsilon - \partial_t \tilde{c}_{\text{ext}}, \phi)_{L^2(\partial\Omega)} \\ & = (\partial_t \tilde{f}(\tilde{c}^\varepsilon), \phi)_H \quad (3.27) \end{aligned}$$

and

$$\begin{aligned} & \frac{d}{dt} (\partial_t \tilde{c}_\Gamma^\varepsilon, \phi_\Gamma)_{H_\Gamma} + \varepsilon^2 (D_\Gamma F_\Gamma^{-T} \nabla^\Gamma \partial_t \tilde{c}_\Gamma^\varepsilon F_\Gamma^{-T} \nabla^\Gamma \phi_\Gamma)_{H_\Gamma} + \varepsilon^2 (D_\Gamma \partial_t (F_\Gamma^{-1} F_\Gamma^{-T}) \nabla^\Gamma \tilde{c}_\Gamma^\varepsilon, \nabla^\Gamma \phi_\Gamma)_{H_\Gamma} \\ & + (\partial_t \tilde{c}_\Gamma^\varepsilon \operatorname{div}^\Gamma (F_\Gamma^{-1} \tilde{v}_M^\varepsilon), \phi_\Gamma)_{H_\Gamma} + (\tilde{c}_\Gamma^\varepsilon \operatorname{div}^\Gamma (\partial_t (F_\Gamma^{-1} \tilde{v}_M^\varepsilon)), \phi_\Gamma)_{H_\Gamma} - (\partial_t \tilde{c}_\Gamma^\varepsilon \tilde{\kappa}^\varepsilon \tilde{V}^\varepsilon, \phi_\Gamma)_{H_\Gamma} \\ & - (\tilde{c}_\Gamma^\varepsilon \partial_t (\tilde{\kappa}^\varepsilon \tilde{V}^\varepsilon), \phi_\Gamma)_{H_\Gamma} - (\partial_t \tilde{f}_\Gamma(\tilde{c}_\Gamma^\varepsilon), \phi_\Gamma)_{H_\Gamma} \\ & = -\frac{\delta_{i2}}{\varepsilon} (\partial_t \tilde{c}^\varepsilon \tilde{V}^\varepsilon, \phi_\Gamma)_{H_\Gamma} - \frac{\delta_{i2}}{\varepsilon} (\tilde{c}^\varepsilon \partial_t \tilde{V}^\varepsilon, \phi_\Gamma)_{H_\Gamma} + (\tilde{k} (\partial_t \tilde{c}^\varepsilon - H \partial_t \tilde{c}_\Gamma^\varepsilon), \phi_\Gamma)_{H_\Gamma} \\ & + (\partial_t \tilde{k} (\tilde{c}^\varepsilon - H \tilde{c}_\Gamma^\varepsilon), \phi_\Gamma)_{H_\Gamma}, \quad (3.28) \end{aligned}$$

both supplemented with the corresponding initial conditions.

We now use $(\partial_t \tilde{c}^\varepsilon(t), \varepsilon \partial_t \tilde{c}_\Gamma^\varepsilon(t))$ as a test function and integrate from 0 to t . Again we start by estimating each term separately: For the bulk equation we obtain:

$$\begin{aligned} & \int_0^t \int_{\Omega^\varepsilon(0)} \frac{d}{dt} |\partial_t \tilde{c}^\varepsilon|^2 \, dx \, dt = \frac{1}{2} \|\partial_t \tilde{c}^\varepsilon(t)\|_H^2 - \frac{1}{2} \|\tilde{c}_1\|_H^2; \\ & d_0 \|\nabla \partial_t \tilde{c}^\varepsilon\|_{L^2(0,t;H)}^2 \leq \int_0^t (DF^{-T} \nabla \partial_t \tilde{c}^\varepsilon, F^{-T} \nabla \partial_t \tilde{c}^\varepsilon)_H \, dt; \\ & \int_0^t |(\nabla \partial_t \tilde{c}^\varepsilon \cdot F^{-1} \tilde{v}^\varepsilon, \partial_t \tilde{c}^\varepsilon)_H| \, dt \leq \|F^{-1} \tilde{v}^\varepsilon\|_{L^\infty([0,T] \times \Omega^\varepsilon(0))} \left(\int_0^t \|\nabla \partial_t \tilde{c}^\varepsilon\|_H \|\partial_t \tilde{c}^\varepsilon\|_H \, dt \right) \\ & \leq C \varepsilon \delta \|\nabla \partial_t \tilde{c}^\varepsilon\|_{L^2(0,t;H)}^2 + C(\delta) \varepsilon \|\partial_t \tilde{c}^\varepsilon\|_{L^2(0,t;H)}^2; \\ & \int_0^t |\varepsilon (\tilde{k} \partial_t \tilde{c}^\varepsilon + \delta_{i1} \tilde{V}^\varepsilon \partial_t \tilde{c}^\varepsilon, \partial_t \tilde{c}^\varepsilon)_{H_\Gamma}| \, dt \leq (\|\tilde{k}\|_{L^\infty([0,T] \times \Omega^\varepsilon(0))} + \|\tilde{V}^\varepsilon\|_{L^\infty([0,T] \times \Omega^\varepsilon(0))}) \int_0^t \varepsilon \|\partial_t \tilde{c}^\varepsilon\|_{H_\Gamma}^2 \, dt \\ & \leq C (\|\partial_t \tilde{c}^\varepsilon\|_{L^2(0,t;H)}^2 + \varepsilon^2 \|\nabla \partial_t \tilde{c}^\varepsilon\|_{L^2(0,t;H)}^2) \end{aligned}$$

(see also Lemma 3.1.15 with $k = 0$), as well as

$$\int_0^t |(\partial_t \tilde{c}^\varepsilon, \partial_t \tilde{c}^\varepsilon)_{L^2(\partial\Omega)}| \, dt \leq \|\partial_t \tilde{c}^\varepsilon\|_{L^2(0,t;H^{\frac{1}{4}}(\partial\Omega))}^2 \leq C \delta \|\nabla \partial_t \tilde{c}^\varepsilon\|_{L^2(0,t;H)}^2 + C(\delta) \|\partial_t \tilde{c}^\varepsilon\|_{L^2(0,t;H)}^2$$

by Corollary 3.3.13. Similarly

$$\begin{aligned}
& \int_0^t |(\partial_t \tilde{f}(\tilde{c}^\varepsilon), \partial_t \tilde{c}^\varepsilon)_H| \, dt \leq CL \|\partial_t \tilde{c}^\varepsilon\|_{L^2(0,t;H)}^2; \\
& \int_0^t \varepsilon(\tilde{k}(t)H\partial_t \tilde{c}_\Gamma^\varepsilon(t), \partial_t \tilde{c}^\varepsilon(t))_{H_\Gamma} \, dt \leq \varepsilon \|H\tilde{k}\|_{L^\infty(\Omega^\varepsilon(0))} (\|\partial_t \tilde{c}_\Gamma^\varepsilon\|_{L^2(0,t;H_\Gamma)} \|\partial_t \tilde{c}^\varepsilon\|_{L^2(0,t;H_\Gamma)}) \\
& \leq C\varepsilon \|\partial_t \tilde{c}_\Gamma^\varepsilon\|_{L^2(0,t;H_\Gamma)}^2 + C\varepsilon \|\partial_t \tilde{c}^\varepsilon\|_{L^2(0,t;H_\Gamma)}^2 \\
& \leq C\varepsilon \|\partial_t \tilde{c}_\Gamma^\varepsilon\|_{L^2(0,t;H_\Gamma)}^2 + C(\|\partial_t \tilde{c}^\varepsilon\|_{L^2(0,t;H)}^2 + \varepsilon^2 \|\nabla \partial_t \tilde{c}^\varepsilon\|_{L^2(0,t;H)}^2); \\
& \int_0^t (\partial_t c_{\text{ext}}(t), \partial_t \tilde{c}^\varepsilon)_{L^2(\partial\Omega)} \, dt \leq C \|\partial_t \tilde{c}^\varepsilon\|_{L^2(0,t;L^2(\partial\Omega))} \leq C + C \|\partial_t \tilde{c}^\varepsilon\|_{L^2(0,t;L^2(\partial\Omega))}^2 \\
& \leq C + C\delta \|\nabla \partial_t \tilde{c}^\varepsilon\|_{L^2(0,t;H)}^2 + C(\delta) \|\partial_t \tilde{c}^\varepsilon\|_{L^2(0,t;H)}^2.
\end{aligned}$$

Moreover, we have

$$\begin{aligned}
& \int_0^t |(D\partial_t(F^{-1}F^{-T})\nabla \tilde{c}^\varepsilon, \nabla \partial_t \tilde{c}^\varepsilon)_H| \, dt \leq D \|\partial_t(F^{-1}F^{-T})\|_{L^\infty([0,T] \times \Omega)} \|\nabla \tilde{c}^\varepsilon\|_{L^2(0,T;H)} \|\nabla \partial_t \tilde{c}^\varepsilon\|_{L^2(0,t;H)} \\
& \leq C(\delta) \|\nabla \tilde{c}^\varepsilon\|_{L^2(0,T;H)}^2 + C\delta \|\nabla \partial_t \tilde{c}^\varepsilon\|_{L^2(0,t;H)}^2 \leq C(\delta) + C\delta \|\nabla \partial_t \tilde{c}^\varepsilon\|_{L^2(0,t;H)}^2; \\
& \int_0^t |(\nabla \tilde{c}^\varepsilon \partial_t(F^{-1}\tilde{v}^\varepsilon), \partial_t \tilde{c}^\varepsilon)_H| \, dt \leq \|\partial_t(F^{-1}\tilde{v}^\varepsilon)\|_{L^\infty([0,T] \times \Omega)} \|\nabla \tilde{c}^\varepsilon\|_{L^2(0,T;H)} \|\partial_t \tilde{c}^\varepsilon\|_{L^2(0,t;H)} \\
& \leq C + C \|\partial_t \tilde{c}^\varepsilon\|_{L^2(0,t;H)}^2; \\
& \int_0^t |(\delta_{i1}\tilde{c}^\varepsilon \partial_t \tilde{V}^\varepsilon, \partial_t \tilde{c}^\varepsilon)_{H_\Gamma}| \, dt \leq \|\partial_t \tilde{V}^\varepsilon\|_{L^\infty([0,T] \times \Omega)} \|\tilde{c}^\varepsilon\|_{L^2(0,T;H_\Gamma)} \|\partial_t \tilde{c}^\varepsilon\|_{L^2(0,t;H_\Gamma)} \\
& \leq C\varepsilon \|\tilde{c}^\varepsilon\|_{L^2(0,T;H_\Gamma)} \|\partial_t \tilde{c}^\varepsilon\|_{L^2(0,t;H_\Gamma)} \leq C\varepsilon \|\tilde{c}^\varepsilon\|_{L^2(0,T;H_\Gamma)}^2 + C\varepsilon \|\partial_t \tilde{c}^\varepsilon\|_{L^2(0,t;H_\Gamma)}^2 \\
& \leq C(\|\tilde{c}^\varepsilon\|_{L^2(0,T;H)}^2 + \varepsilon^2 \|\nabla \tilde{c}^\varepsilon\|_{L^2(0,T;H)}^2) + C(\|\partial_t \tilde{c}^\varepsilon\|_{L^2(0,t;H)}^2 + \varepsilon^2 \|\nabla \partial_t \tilde{c}^\varepsilon\|_{L^2(0,t;H)}^2) \\
& \leq C + C(\|\partial_t \tilde{c}^\varepsilon\|_{L^2(0,t;H)}^2 + \varepsilon^2 \|\nabla \partial_t \tilde{c}^\varepsilon\|_{L^2(0,t;H)}^2); \\
& \int_0^t \varepsilon |(\partial_t \tilde{k}(\tilde{c}^\varepsilon - H\tilde{c}_\Gamma^\varepsilon), \partial_t \tilde{c}^\varepsilon)_{H_\Gamma}| \, dt \leq \|(1+H)\partial_t \tilde{k}\|_{L^\infty([0,T] \times \Omega)} (\varepsilon \|\tilde{c}^\varepsilon\|_{L^2(0,T;H_\Gamma)}^2 + \varepsilon \|\tilde{c}_\Gamma^\varepsilon\|_{L^2(0,T;H_\Gamma)}^2 \\
& \quad + 2\varepsilon \|\partial_t \tilde{c}^\varepsilon\|_{L^2(0,t;H_\Gamma)}^2) \\
& \leq C(\|\tilde{c}^\varepsilon\|_{L^2(0,T;H)}^2 + \varepsilon^2 \|\nabla \tilde{c}^\varepsilon\|_{L^2(0,T;H)}^2) + C + C(\|\partial_t \tilde{c}^\varepsilon\|_{L^2(0,t;H)}^2 + \varepsilon^2 \|\nabla \partial_t \tilde{c}^\varepsilon\|_{L^2(0,t;H)}^2) \\
& \leq C + C(\|\partial_t \tilde{c}^\varepsilon\|_{L^2(0,t;H)}^2 + \varepsilon^2 \|\nabla \partial_t \tilde{c}^\varepsilon\|_{L^2(0,t;H)}^2).
\end{aligned}$$

For the surface equations we obtain analogously

$$\begin{aligned}
& \int_0^t \int_{\Gamma^\varepsilon(0)} \frac{d}{dt} \varepsilon |\partial_t \tilde{c}_\Gamma^\varepsilon|^2 \, dx \, dt = \frac{\varepsilon}{2} \|\partial_t \tilde{c}_\Gamma^\varepsilon(t)\|_{H_\Gamma}^2 - \frac{\varepsilon}{2} \|\tilde{c}_{1,\Gamma}\|_{H_\Gamma}^2; \\
& d_0 \varepsilon^3 \|\nabla \partial_t \tilde{c}_\Gamma^\varepsilon\|_{L^2(0,t;H_\Gamma)}^2 \leq \int_0^t \varepsilon^3 (D_\Gamma F_\Gamma^{-T} \nabla^\Gamma \partial_t \tilde{c}_\Gamma^\varepsilon, F_\Gamma^{-T}(t) \nabla^\Gamma \partial_t \tilde{c}_\Gamma^\varepsilon)_{H_\Gamma} \, dt; \\
& \int_0^t \varepsilon ([\operatorname{div}^\Gamma (F_\Gamma^{-1} \tilde{v}_M^\varepsilon) - \tilde{\kappa} \tilde{V}^\varepsilon + \tilde{k} H] \partial_t \tilde{c}_\Gamma^\varepsilon, \partial_t \tilde{c}_\Gamma^\varepsilon)_{H_\Gamma} \, dt \\
& \leq \varepsilon \left(\left\| \operatorname{div}^\Gamma (F_\Gamma^{-1} \tilde{v}_M^\varepsilon) + |\tilde{\kappa} \tilde{V}^\varepsilon| + |\tilde{k} H| \right\|_{L^\infty([0,T] \times \Omega)} \right) \|\partial_t \tilde{c}_\Gamma^\varepsilon\|_{L^2(0,t;H_\Gamma)}^2 \\
& \leq C \varepsilon \|\partial_t \tilde{c}_\Gamma^\varepsilon\|_{L^2(0,t;H_\Gamma)}^2; \\
& \int_0^t \varepsilon (\partial_t \tilde{f}_\Gamma(\tilde{c}_\Gamma^\varepsilon), \partial_t \tilde{c}_\Gamma^\varepsilon(t))_{H_\Gamma} \, dt \leq +CL\varepsilon \|\partial_t \tilde{c}_\Gamma^\varepsilon\|_{L^2(0,t;H_\Gamma)}^2; \\
& \int_0^t \varepsilon \left(\left(\tilde{k} + \frac{\delta_{i2} \tilde{V}^\varepsilon}{\varepsilon} \right) \partial_t \tilde{c}^\varepsilon, \partial_t \tilde{c}_\Gamma^\varepsilon \right)_{H_\Gamma} \leq \varepsilon \left\| \tilde{k} + \left| \frac{1}{\varepsilon} \tilde{V}^\varepsilon \right| \right\|_{L^\infty([0,T] \times \Omega)} \|\partial_t \tilde{c}^\varepsilon\|_{L^2(0,t;H)} \|\partial_t \tilde{c}_\Gamma^\varepsilon\|_{L^2(0,t;H_\Gamma)} \\
& \leq C \varepsilon \|\partial_t \tilde{c}_\Gamma^\varepsilon\|_{L^2(0,t;H_\Gamma)}^2 + C (\|\partial_t \tilde{c}^\varepsilon\|_{L^2(0,t;H)}^2 + \varepsilon^2 \|\nabla \partial_t \tilde{c}^\varepsilon\|_{L^2(0,t;H)}^2)
\end{aligned}$$

as well as

$$\begin{aligned}
& \int_0^t \varepsilon^3 |(D_\Gamma \partial_t (F_\Gamma^{-1} F_\Gamma^{-T}) \nabla^\Gamma \tilde{c}_\Gamma^\varepsilon, \nabla^\Gamma \partial_t \tilde{c}_\Gamma^\varepsilon)_{H_\Gamma}| \, dt \leq \varepsilon^3 D_\Gamma \|\partial_t (F_\Gamma^{-1} F_\Gamma^{-T})\|_{L^\infty([0,T] \times \Omega)} \\
& \quad \cdot \|\nabla^\Gamma \tilde{c}_\Gamma^\varepsilon\|_{L^2(0,T;H_\Gamma)} \|\nabla^\Gamma \partial_t \tilde{c}_\Gamma^\varepsilon\|_{L^2(0,t;H_\Gamma)} \\
& \leq \varepsilon^3 (C(\delta) \|\nabla^\Gamma \tilde{c}_\Gamma^\varepsilon\|_{L^2(0,T;H_\Gamma)}^2 + C\delta \|\nabla^\Gamma \partial_t \tilde{c}_\Gamma^\varepsilon\|_{L^2(0,t;H_\Gamma)}^2) \leq C(\delta) + C\varepsilon^3 \delta \|\nabla^\Gamma \partial_t \tilde{c}_\Gamma^\varepsilon\|_{L^2(0,t;H_\Gamma)}^2; \\
& \int_0^t \varepsilon ([\operatorname{div}^\Gamma (\partial_t (F_\Gamma^{-1} \tilde{v}_M^\varepsilon)) - \partial_t (\tilde{\kappa} \tilde{V}^\varepsilon)] \tilde{c}_\Gamma^\varepsilon, \partial_t \tilde{c}_\Gamma^\varepsilon)_{H_\Gamma} \, dt \\
& \leq \varepsilon \left\| \operatorname{div}^\Gamma (\partial_t (F_\Gamma^{-1} \tilde{v}_M^\varepsilon)) + |\partial_t (\tilde{\kappa} \tilde{V}^\varepsilon)| \right\|_{L^\infty([0,T] \times \Omega)} \|\tilde{c}_\Gamma^\varepsilon\|_{L^2(0,T;H_\Gamma)} \|\partial_t \tilde{c}_\Gamma^\varepsilon\|_{L^2(0,t;H_\Gamma)} \\
& \leq C \varepsilon \|\tilde{c}_\Gamma^\varepsilon\|_{L^2(0,T;H_\Gamma)}^2 + C \varepsilon \|\partial_t \tilde{c}_\Gamma^\varepsilon\|_{L^2(0,t;H_\Gamma)}^2 \leq C + C \varepsilon \|\partial_t \tilde{c}_\Gamma^\varepsilon\|_{L^2(0,t;H_\Gamma)}^2; \\
& \int_0^t \varepsilon |(\partial_t \tilde{k}(\tilde{c}^\varepsilon - H \tilde{c}_\Gamma^\varepsilon) + \frac{\delta_{i2}}{\varepsilon} \partial_t \tilde{V}^\varepsilon \tilde{c}^\varepsilon, \partial_t \tilde{c}_\Gamma^\varepsilon)_{H_\Gamma}| \, dt \leq C \left\| (1+H) \partial_t \tilde{k} + \left| \frac{1}{\varepsilon} \partial_t \tilde{V}^\varepsilon \right| \right\|_{L^\infty([0,T] \times \Omega)} \\
& \quad \cdot (\varepsilon \|\tilde{c}^\varepsilon\|_{L^2(0,T;H_\Gamma)}^2 + \varepsilon \|\tilde{c}_\Gamma^\varepsilon\|_{L^2(0,T;H_\Gamma)}^2 + 2\varepsilon \|\partial_t \tilde{c}_\Gamma^\varepsilon\|_{L^2(0,t;H_\Gamma)}^2) \\
& \leq C (\|\tilde{c}^\varepsilon\|_{L^2(0,T;H)}^2 + \varepsilon^2 \|\nabla \tilde{c}^\varepsilon\|_{L^2(0,T;H)}^2) + C + C \varepsilon \|\partial_t \tilde{c}_\Gamma^\varepsilon\|_{L^2(0,T;H_\Gamma)}^2 \\
& \leq C + C \varepsilon \|\partial_t \tilde{c}_\Gamma^\varepsilon\|_{L^2(0,T;H_\Gamma)}^2.
\end{aligned}$$

We now use the first two estimates for each equation on the left hand side of the following relation; all the remaining terms are put on the right hand side: Adding up (3.27) with $\phi = \partial_t \tilde{c}^\varepsilon(t)$, and (3.28) with $\phi_\Gamma(t) = \varepsilon \partial_t \tilde{c}_\Gamma^\varepsilon(t)$ and integrating from 0 to t gives due to the estimates above

$$\begin{aligned} & \|\partial_t \tilde{c}^\varepsilon(t)\|_H^2 + (d_0 - C\varepsilon^2 - C\varepsilon\delta) \|\nabla \partial_t \tilde{c}^\varepsilon\|_{L^2(0,t;H)}^2 + \varepsilon \|\partial_t \tilde{c}_\Gamma^\varepsilon(t)\|_{H_\Gamma}^2 \\ & \quad + (C - C'\delta)\varepsilon^3 \|\nabla^\Gamma \partial_t \tilde{c}_\Gamma^\varepsilon\|_{L^2(0,t;H_\Gamma)}^2 \\ & \leq C(\delta) + C(\delta) \|\partial_t \tilde{c}^\varepsilon\|_{L^2(0,t;H)} + C\varepsilon \|\partial_t \tilde{c}_\Gamma^\varepsilon\|_{L^2(0,t;H_\Gamma)}. \end{aligned}$$

Choose δ and ε small enough such that $(d_0 - C\varepsilon^2 - C\varepsilon\delta) > 0$ as well as $(C - C'\delta) > 0$. Neglecting the terms containing a gradient for a moment gives with the help of Gronwall's inequality

$$\begin{aligned} \|\partial_t \tilde{c}^\varepsilon(t)\|_H^2 & \leq C \quad \text{for almost all } t \in [0, T] \\ \varepsilon \|\partial_t \tilde{c}_\Gamma^\varepsilon(t)\|_{H_\Gamma}^2 & \leq C \quad \text{for almost all } t \in [0, T], \end{aligned}$$

which gives the bounds in $L^\infty(0, T; H)$. Again, due to the continuous embedding $L^\infty([0, T]) \hookrightarrow L^2([0, T])$, we get the same bounds in $L^2(0, T; H)$ and $L^2(0, T; H_\Gamma)$, resp. Inserting these bounds in the right hand side of the last estimate for $t = T$ gives the remaining estimate on the gradients. \blacklozenge

3.4 Homogenization of the Evolving-Surface Model

3.4.1 Convergence Results

Due to the estimates from Theorem 3.3.21, we obtain the following proposition:

3.4.1 Proposition.

There exists a function $c^0 \in L^2(0, T; H^1(\Omega))$ with $\partial_t c^0 \in L^2(0, T; L^2(\Omega))$ and functions $c^1 \in L^2(0, T; L^2(\Omega; H_{\#}^1(Y)))$ as well as $c_\Gamma^0 \in L^2(0, T; L^2(\Omega; H^1(\partial Y_S)))$ such that along a subsequence of ε the following convergence statements hold:

$$\tilde{c}^\varepsilon \rightharpoonup c^0 \quad \text{in } L^2(0, T; H^1(\Omega)) \quad (3.29)$$

$$\partial_t \tilde{c}^\varepsilon \rightharpoonup \partial_t c^0 \quad \text{in } L^2(0, T; L^2(\Omega)) \quad (3.30)$$

$$\tilde{c}^\varepsilon \rightarrow c^0 \quad \text{in } L^2(0, T; L^2(\Omega)) \quad (3.31)$$

for the extension of \tilde{c}^ε according to Lemma 3.1.12, as well as

$$\mathcal{T}^\varepsilon(\tilde{c}^\varepsilon) \rightarrow c^0 \quad \text{in } L^2(0, T; L^2(\Omega)) \quad (3.32)$$

$$\mathcal{T}^\varepsilon(\nabla \tilde{c}^\varepsilon) \rightarrow \nabla_x c^0 + \nabla_y c^1 \quad \text{in } L^2(0, T; L^2(\Omega \times Y)) \quad (3.33)$$

$$\mathcal{T}^\varepsilon(\partial_t \tilde{c}^\varepsilon) \rightarrow \partial_t c^0 \quad \text{in } L^2(0, T; L^2(\Omega)) \quad (3.34)$$

$$\mathcal{T}_b^\varepsilon(\tilde{c}^\varepsilon) \rightarrow c^0 \quad \text{in } L^2(0, T; L^2(\Omega \times \partial Y_S)) \quad (3.35)$$

and

$$\mathcal{T}_b^\varepsilon(\tilde{c}_\Gamma^\varepsilon) \rightharpoonup c_\Gamma^0 \quad \text{in } L^2(0, T; L^2(\Omega \times \partial Y_S)) \quad (3.36)$$

$$\varepsilon \mathcal{T}_b^\varepsilon(\nabla^\Gamma \tilde{c}_\Gamma^\varepsilon) \rightharpoonup \nabla_y^\Gamma c_\Gamma^0 \quad \text{in } L^2(0, T; L^2(\Omega \times \partial Y_S)) \quad (3.37)$$

$$\mathcal{T}_b^\varepsilon(\partial_t \tilde{c}_\Gamma^\varepsilon) \rightharpoonup \partial_t c_\Gamma^0 \quad \text{in } L^2(0, T; L^2(\Omega \times \partial Y_S)) \quad (3.38)$$

Proof. For the extended function \tilde{c}^ε we have the estimate $\|\tilde{c}^\varepsilon\|_{L^2(0, T; H^1(\Omega))} \leq C$, which gives (3.29) due to weak compactness. Analogously, since $\|\partial_t \tilde{c}^\varepsilon\|_{L^2(0, T; L^2(\Omega))} \leq C$ there exists a $g \in L^2(0, T; L^2(\Omega))$ such that $\partial_t \tilde{c}^\varepsilon \rightharpoonup g$ in that space. By standard results, this forces $g = \partial_t c^0$ in weak sense (see e.g. Zeidler [Zei90], Proposition 23.19). Now the compact embedding $\{u \in L^2(0, T; H^1(\Omega)); \partial_t u \in L^2(0, T; L^2(\Omega))\} \hookrightarrow L^2(0, T; L^2(\Omega))$ yields (3.31).

This last strong convergence statement together with the first result in Theorem 3.1.13 gives the strong convergence (3.32). Similarly, the same theorem leads to (3.33) and (3.35).

In order to obtain the result for the time derivative, first note that $\mathcal{T}^\varepsilon(\partial_t \tilde{c}^\varepsilon)$ is bounded in $L^2(0, T; L^2(\Omega \times Y_R))$, thus there exists a g' in that space such that along a subsequence $\mathcal{T}^\varepsilon(\partial_t \tilde{c}^\varepsilon) \rightharpoonup g'$. Now choose a $\phi \in C_0^\infty([0, T] \times \Omega \times Y_R)$ and unfold the integral identity $\int_0^T \int_\Omega \partial_t \tilde{c}^\varepsilon(t, x) \phi(t, x, \frac{x}{\varepsilon}) \, dx \, dt = - \int_0^T \int_\Omega \tilde{c}^\varepsilon(t, x) \partial_t \phi(t, x, \frac{x}{\varepsilon}) \, dx \, dt$. Since $\mathcal{T}^\varepsilon(\phi(t, x, \frac{x}{\varepsilon})) \rightarrow \phi(t, x, y)$ as well as $\mathcal{T}^\varepsilon(\partial_t \tilde{c}^\varepsilon) \rightarrow \partial_t \phi(t, x, y)$ strongly, we get

$$\begin{aligned} \int_0^T \int_{\Omega \times Y} \mathcal{T}^\varepsilon(\partial_t \tilde{c}^\varepsilon) \mathcal{T}^\varepsilon(\phi(t, x, \frac{x}{\varepsilon})) \, dy \, dx \, dt &= - \int_0^T \int_{\Omega \times Y} \mathcal{T}^\varepsilon(\tilde{c}^\varepsilon) \mathcal{T}^\varepsilon(\partial_t \phi(t, x, \frac{x}{\varepsilon})) \, dy \, dx \, dt \\ &\quad \downarrow \qquad \qquad \qquad \downarrow \\ \int_0^T \int_{\Omega \times Y} g'(t, x, y) \phi(t, x, y) \, dy \, dx \, dt &= - \int_0^T \int_{\Omega \times Y} c^0(t, x) \partial_t \phi(t, x, y) \, dy \, dx \, dt \end{aligned}$$

for $\varepsilon \rightarrow 0$. Thus by using the same argument as above $g' = \partial_t c^0$, which is (3.34).

Due to the boundedness properties $\varepsilon \|\tilde{c}_\Gamma^\varepsilon\|_{L^2(0, T; H_\Gamma)}^2 + \varepsilon^3 \|\tilde{c}_\Gamma^\varepsilon\|_{L^2(0, T; H_\Gamma)}^2 \leq C$, Theorem 3.1.13 gives the convergences (3.36) and (3.37). Finally, the convergence for the time derivative follows as in the bulk-case. \blacklozenge

3.4.2 Treatment of the Nonlinear Reaction Rates

The weak convergence (3.36) is not enough to pass to the limit in the nonlinear reaction rate \tilde{f}_Γ . However, since the set on which $\tilde{c}_\Gamma^\varepsilon$ is defined varies with ε , we cannot expect any convergence in a $H^1(\Gamma^\varepsilon)$ -space. Thus we have no compact embedding at hand. The best result which can be obtained is the strong convergence of the unfolded sequence $\mathcal{T}_b^\varepsilon(\tilde{c}_\Gamma^\varepsilon)$. As we will see below, this result is sufficient to pass to the limit.

In order to prove this result, we follow the approach suggested by Neuss-Radu and Jäger in [NRJ07]. It is based on the Kolmogoroff compactness criterion, which is recalled next for the convenience of the reader:

3.4.2 Theorem (Kolmogoroff compactness criterion).

Let $1 \leq p < \infty$. Let $G \subset \mathbb{R}^N$ be a bounded open set. A bounded set $S \subset L^p(G)$ is compact if and only if it is p -mean equicontinuous, i.e. for all $\eta > 0$ there exists a $\delta > 0$ such that for all $h \in \mathbb{R}$ with $|h| < \delta$ it holds

$$\sup_{u \in S} \int_G |u(x+h) - u(x)|^p dx \leq \eta.$$

Proof. See e.g. Hanche-Olsen and Holden [HOH10] for a modern proof or Rafeiro [Raf09] for extensions. \blacklozenge

We are going to show the following theorem:

3.4.3 Theorem.

The set $\{\mathcal{T}_b^\varepsilon(\tilde{c}_\Gamma^\varepsilon)\}_{\varepsilon>0}$ is compact in $L^2([0, T] \times \Omega \times \partial Y_S)$, thus along a subsequence we have the strong convergence

$$\mathcal{T}_b^\varepsilon(\tilde{c}_\Gamma^\varepsilon) \longrightarrow c_\Gamma^0 \quad \text{in } L^2([0, T] \times \Omega \times \partial Y_S). \quad (3.39)$$

The proof is carried out in several steps: First, we show that $\{\mathcal{T}_b^\varepsilon(\tilde{c}_\Gamma^\varepsilon)\}$ fulfills the Kolmogoroff compactness criterion in t and y . The difficult part is to show the criterion in x . As it will turn out, a Taylor expansion of $\tilde{k}, F^{-1}, \tilde{V}^\varepsilon$ etc. will allow us to gain a useful power of h in the estimates. Together with the strong convergence of \tilde{c}^ε , this forces the criterion to hold.

Proof. Step 1: Compactness criterion in t and y .

Let e be one of the unit vectors e_1, \dots, e_n of \mathbb{R}^n and let $h > 0$. A Taylor expansion gives

$$\|\mathcal{T}_b^\varepsilon(\tilde{c}_\Gamma^\varepsilon)(t, x, y + he) - \mathcal{T}_b^\varepsilon(\tilde{c}_\Gamma^\varepsilon)(t, x, y)\|_{L^2([0, T] \times \Omega \times \partial Y_S)} \leq Ch \|\nabla_y \mathcal{T}_b^\varepsilon(\tilde{c}_\Gamma^\varepsilon)\|_{L^2([0, T] \times \Omega \times \partial Y_S)}.$$

Since $\|\nabla_y \mathcal{T}_b^\varepsilon(\tilde{c}_\Gamma^\varepsilon)\|_{L^2([0, T] \times \Omega \times \partial Y_S)}$ is bounded independent of ε (see Proposition 3.1.10), the criterion can be satisfied in y . A similar argument with $\|\partial_t \mathcal{T}_b^\varepsilon(\tilde{c}_\Gamma^\varepsilon)\|_{L^2([0, T] \times \Omega \times \partial Y_S)}$ gives the same result in the variable t .

Step 2: Reduction to a simpler estimate.

In the sequel we will assume that Ω can always be represented by a union of scaled and translated reference cells, see also the remarks accompanying equation (3.2) in Section 3.2. Fix $\varepsilon > 0$ and let $I \subset \mathbb{Z}^n$ be an index set such that

$$\Omega = \bigcup_{i \in I} \varepsilon(Y + i) =: \bigcup_{i \in I} \varepsilon Y_i.$$

Note that $x \in \varepsilon Y_i \Leftrightarrow \left\lceil \frac{x}{\varepsilon} \right\rceil = i$. Fix $i \in I$. For given $\xi \in \mathbb{R}^n$ subdivide εY_i as follows: For $k \in \{0, 1\}^n$ define

$$\varepsilon Y_i^k := \left\{ x \in \varepsilon Y_i : \varepsilon \left\lceil \frac{x + \left\{ \frac{\xi}{\varepsilon} \right\} \varepsilon}{\varepsilon} \right\rceil = \varepsilon(i + k) \right\}$$

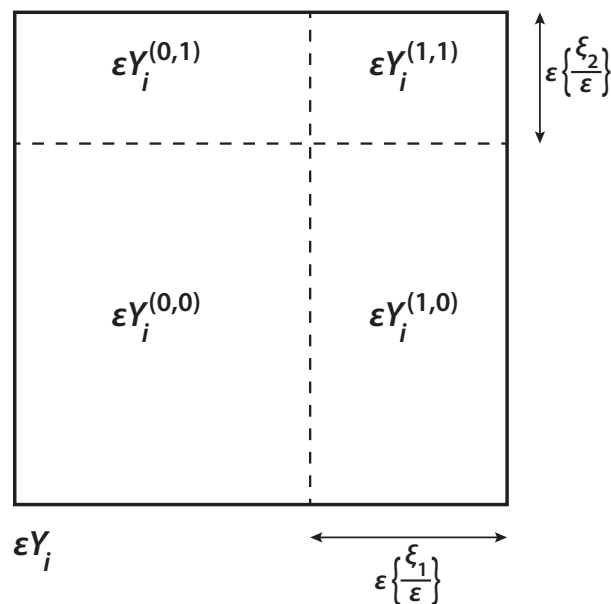


Figure 3.2: Illustration of the sets εY_i^k in the two-dimensional case for $\xi = \begin{pmatrix} \xi_1 \\ \xi_2 \end{pmatrix}$.

(see also Figure 3.2 for the two-dimensional case). It holds $\varepsilon Y_i = \bigcup_{k \in \{0,1\}^n} \varepsilon Y_i^k$. Now

$$\begin{aligned}
& \left\| \mathcal{T}_b^\varepsilon(\tilde{c}_\Gamma^\varepsilon)(t, x + \xi, y) - \mathcal{T}_b^\varepsilon(\tilde{c}_\Gamma^\varepsilon)(t, x, y) \right\|_{L^2([0, T] \times \Omega \times \partial Y_S)}^2 \\
&= \sum_{i \in I} \int_0^T \int_{\varepsilon Y_i} \int_{\partial Y_S} \left| \tilde{c}_\Gamma^\varepsilon(t, \varepsilon \left[\frac{x + \xi}{\varepsilon} \right] + \varepsilon y) - \tilde{c}_\Gamma^\varepsilon(t, \varepsilon \left[\frac{x}{\varepsilon} \right] + \varepsilon y) \right|^2 d\sigma_y dx dt \\
&= \sum_{i \in I} \sum_{k \in \{0,1\}^n} \int_0^T \int_{\varepsilon Y_i^k} \int_{\partial Y_S} \left| \tilde{c}_\Gamma^\varepsilon(t, \varepsilon(i + k + \left[\frac{\xi}{\varepsilon} \right]) + \varepsilon y) - \tilde{c}_\Gamma^\varepsilon(t, \varepsilon i + \varepsilon y) \right|^2 d\sigma_y dx dt \\
&\leq \sum_{i \in I} \sum_{k \in \{0,1\}^n} \int_0^T \int_{\varepsilon Y_i} \int_{\partial Y_S} \left| \tilde{c}_\Gamma^\varepsilon(t, \varepsilon(i + k + \left[\frac{\xi}{\varepsilon} \right]) + \varepsilon y) - \tilde{c}_\Gamma^\varepsilon(t, \varepsilon i + \varepsilon y) \right|^2 d\sigma_y dx dt,
\end{aligned}$$

which by undoing the unfolding operation and remarking that $i = \left[\frac{x}{\varepsilon} \right]$ is equal to

$$\sum_{k \in \{0,1\}^n} \varepsilon \int_0^T \int_{\Gamma^\varepsilon(0)} \left| \tilde{c}_\Gamma^\varepsilon(t, x + \varepsilon \left(\left[\frac{\xi}{\varepsilon} \right] + k \right)) - \tilde{c}_\Gamma^\varepsilon(t, x) \right|^2 d\sigma dt.$$

For given small $h > 0$, we can choose an ε small enough such that $|\varepsilon \left[\frac{\xi}{\varepsilon} \right] + \varepsilon k| < h$.

This amounts to saying that in order to obtain the compactness criterion in x for $\mathcal{T}_b^\varepsilon(\tilde{c}_\Gamma^\varepsilon)$, it is sufficient to obtain estimates for given $l \in \mathbb{Z}^n$, $|l\varepsilon| < h$ of

$$\boxed{\varepsilon \left\| \tilde{c}_\Gamma^\varepsilon(t, x + l\varepsilon) - \tilde{c}_\Gamma^\varepsilon(t, x) \right\|_{L^2([0, T] \times \Gamma^\varepsilon(0))}^2} \cdot \quad (3.40)$$

Step 3: Estimation of the Difference-PDE.

In order to estimate the norm (3.40), we introduce the following assumptions and definitions: We assume that Ω is of rectangular shape. We extend $\tilde{c}_\Gamma^\varepsilon$ to the whole \mathbb{R}^n by successively reflecting $\tilde{c}_\Gamma^\varepsilon$ with respect to the planes $\{(x_1, \dots, x_n) : x_i = 0\}$ for $i = 1, \dots, n$, followed by an extension by periodicity (see [NRJ07] for the details). For a function q defined on $[0, T] \times \mathbb{R}^n$ set

$$\begin{aligned} q^l(t, x) &:= q(t, x + l\varepsilon) \\ \delta q &:= q^l - q \end{aligned}$$

and note that for a similar function ρ we have

$$q^l \rho^l - q\rho = q^l(\delta\rho) + (\delta q)\rho = \rho^l(\delta q) + (\delta\rho)q. \quad (3.41)$$

Define $\tilde{g} = \operatorname{div}^\Gamma(F_\Gamma^{-1}\tilde{v}_M^\varepsilon) - \tilde{\kappa}^\varepsilon\tilde{V}^\varepsilon$ and consider the difference $\delta\tilde{c}_\Gamma^\varepsilon = (\tilde{c}_\Gamma^\varepsilon)^l - \tilde{c}_\Gamma^\varepsilon$. By subtracting the weak formulations of $(\tilde{c}_\Gamma^\varepsilon)^l$ and $\tilde{c}_\Gamma^\varepsilon$, we obtain

$$\begin{aligned} \frac{d}{dt}((\tilde{c}_\Gamma^\varepsilon)^l - \tilde{c}_\Gamma^\varepsilon, \eta)_{H_\Gamma} + \varepsilon^2(D_\Gamma(F_\Gamma^{-1}F_\Gamma^{-T})^l \nabla(\tilde{c}_\Gamma^\varepsilon)^l - D_\Gamma F_\Gamma^{-1}F_\Gamma^{-T} \nabla \tilde{c}_\Gamma^\varepsilon, \nabla \eta)_{H_\Gamma} \\ + (\tilde{g}^l(\tilde{c}_\Gamma^\varepsilon)^l - \tilde{g}\tilde{c}_\Gamma^\varepsilon, \eta)_{H_\Gamma} = (\tilde{f}_\Gamma^l((\tilde{c}_\Gamma^\varepsilon)^l) - \tilde{f}_\Gamma(\tilde{c}_\Gamma^\varepsilon), \eta)_{H_\Gamma} \\ + (\tilde{k}^l(\tilde{c}_\Gamma^\varepsilon)^l - \tilde{k}\tilde{c}_\Gamma^\varepsilon, \eta)_{H_\Gamma} - (H\tilde{k}^l(\tilde{c}_\Gamma^\varepsilon)^l - H\tilde{k}\tilde{c}_\Gamma^\varepsilon, \eta)_{H_\Gamma} \end{aligned}$$

for $\eta \in H_\Gamma$. We use $\eta = \varepsilon\delta\tilde{c}_\Gamma^\varepsilon$ as a test function, integrate from 0 to t and estimate the terms with the help of (3.41): We obtain

$$\int_0^t \frac{d}{dt} \varepsilon((\tilde{c}_\Gamma^\varepsilon)^l - \tilde{c}_\Gamma^\varepsilon, \delta\tilde{c}_\Gamma^\varepsilon)_{H_\Gamma} dt = \varepsilon \|\delta\tilde{c}_\Gamma^\varepsilon(t)\|_{H_\Gamma}^2 - \varepsilon \|\delta\tilde{c}_{0,\Gamma}\|_{H_\Gamma}^2$$

and

$$\begin{aligned} &\int_0^t \varepsilon^3(D_\Gamma(F_\Gamma^{-1}F_\Gamma^{-T})^l \nabla(\tilde{c}_\Gamma^\varepsilon)^l - D_\Gamma F_\Gamma^{-1}F_\Gamma^{-T} \nabla \tilde{c}_\Gamma^\varepsilon, \nabla \delta\tilde{c}_\Gamma^\varepsilon)_{H_\Gamma} dt \\ &= \int_0^t \varepsilon^3(D_\Gamma \delta(F_\Gamma^{-1}F_\Gamma^{-T}) \nabla(\tilde{c}_\Gamma^\varepsilon)^l, \nabla \delta\tilde{c}_\Gamma^\varepsilon)_{H_\Gamma} dt + \int_0^t \varepsilon^3(D_\Gamma F_\Gamma^{-1}F_\Gamma^{-T} \nabla \delta\tilde{c}_\Gamma^\varepsilon, \nabla \delta\tilde{c}_\Gamma^\varepsilon)_{H_\Gamma} dt \\ &=: I_1 + I_2 \end{aligned}$$

with the estimates

$$\begin{aligned} I_2 &\geq \varepsilon^3 d_0 \|\nabla \delta\tilde{c}_\Gamma^\varepsilon\|_{L^2(0, t; H_\Gamma)}^2 \\ |I_1| &\leq \varepsilon^3 D_\Gamma \underbrace{\left\| \delta(F_\Gamma^{-1}F_\Gamma^{-T}) \right\|_{L^\infty([0, T] \times \Omega)}}_{\leq C\varepsilon} \cdot 2 \underbrace{\|\nabla \tilde{c}_\Gamma^\varepsilon\|_{L^2(0, t; H_\Gamma)}^2}_{\leq C\varepsilon^{-3}} \leq C\varepsilon, \end{aligned}$$

since $\|\nabla \delta \tilde{c}_\Gamma^\varepsilon\|_{H_\Gamma} \leq 2 \|\nabla \tilde{c}_\Gamma^\varepsilon\|_{H_\Gamma}$ and by Taylor expansion of $F_\Gamma^{-1} F_\Gamma^{-T}$. Next

$$\begin{aligned} & \int_0^t \varepsilon |(\tilde{g}^l(\tilde{c}_\Gamma^\varepsilon)^l - \tilde{g}_\Gamma^\varepsilon, \eta)_{H_\Gamma}| dt = \int_0^t \varepsilon |(\tilde{g}^l \delta \tilde{c}_\Gamma^\varepsilon, \delta \tilde{c}_\Gamma^\varepsilon)_{H_\Gamma}| dt + \int_0^t \varepsilon |(\delta \tilde{g} \tilde{c}_\Gamma^\varepsilon, \delta \tilde{c}_\Gamma^\varepsilon)_{H_\Gamma}| dt \\ & \leq \varepsilon \|\tilde{g}\|_{L^\infty([0, T] \times \Omega)} \|\delta \tilde{c}_\Gamma^\varepsilon\|_{L^2(0, t; H_\Gamma)}^2 + C\varepsilon \underbrace{\|\delta \tilde{g}\|_{L^\infty([0, T] \times \Omega)}}_{\leq C\varepsilon} \underbrace{(\|\tilde{c}_\Gamma^\varepsilon\|_{L^2(0, T; H_\Gamma)}^2)}_{\leq C\varepsilon^{-1}} + \|\delta \tilde{c}_\Gamma^\varepsilon\|_{L^2(0, t; H_\Gamma)}^2 \\ & \leq C\varepsilon + C\varepsilon \|\delta \tilde{c}_\Gamma^\varepsilon\|_{L^2(0, t; H_\Gamma)}^2 \end{aligned}$$

and

$$\begin{aligned} & \int_0^t \varepsilon |(\tilde{f}_\Gamma^l((\tilde{c}_\Gamma^\varepsilon)^l) - \tilde{f}_\Gamma(\tilde{c}_\Gamma^\varepsilon), \delta \tilde{c}_\Gamma^\varepsilon)_{H_\Gamma}| dt \leq \int_0^t \varepsilon |(\tilde{f}_\Gamma^l((\tilde{c}_\Gamma^\varepsilon)^l) - \tilde{f}_\Gamma((\tilde{c}_\Gamma^\varepsilon)^l), \delta \tilde{c}_\Gamma^\varepsilon)_{H_\Gamma}| dt \\ & + \int_0^t \varepsilon |(\tilde{f}_\Gamma((\tilde{c}_\Gamma^\varepsilon)^l) - \tilde{f}_\Gamma(\tilde{c}_\Gamma^\varepsilon), \delta \tilde{c}_\Gamma^\varepsilon)_{H_\Gamma}| dt \leq \varepsilon L_\Gamma \|\delta \tilde{c}_\Gamma^\varepsilon\|_{L^2(0, t; H_\Gamma)}^2 + \varepsilon L \|\delta \tilde{c}_\Gamma^\varepsilon\|_{L^2(0, t; H_\Gamma)}^2 \\ & \leq C\varepsilon + C\varepsilon \|\delta \tilde{c}_\Gamma^\varepsilon\|_{L^2(0, t; H_\Gamma)}^2 \end{aligned}$$

due to the Lipschitz-continuity of \tilde{f}_Γ in both arguments. Since

$$\varepsilon \|\tilde{c}^\varepsilon\|_{L^2(0, T; H_\Gamma)}^2 \leq C \|\tilde{c}^\varepsilon\|_{L^2(0, T; H)}^2 + C\varepsilon^2 \|\nabla \tilde{c}^\varepsilon\|_{L^2(0, T; H)}^2 \leq C$$

as well as

$$\begin{aligned} \varepsilon \|\delta \tilde{c}^\varepsilon\|_{L^2(0, T; H_\Gamma)}^2 & \leq C \|\delta \tilde{c}^\varepsilon\|_{L^2(0, T; H)}^2 + C\varepsilon^2 \|\nabla \delta \tilde{c}^\varepsilon\|_{L^2(0, T; H)}^2 \\ & \leq C \|\delta \tilde{c}^\varepsilon\|_{L^2(0, T; H)}^2 + 2C\varepsilon^2 \|\nabla \tilde{c}^\varepsilon\|_{L^2(0, T; H)}^2 \\ & \leq C \|\delta \tilde{c}^\varepsilon\|_{L^2(0, T; H)}^2 + C\varepsilon, \end{aligned} \tag{3.42}$$

we obtain the estimate

$$\begin{aligned} & \int_0^t \varepsilon |(\tilde{k}^l(\tilde{c}^\varepsilon)^l - \tilde{k} \tilde{c}^\varepsilon, \delta \tilde{c}_\Gamma^\varepsilon)_{H_\Gamma}| dt \leq \int_0^t \varepsilon |((\delta \tilde{k}) \tilde{c}^\varepsilon, \delta \tilde{c}_\Gamma^\varepsilon)_{H_\Gamma}| dt + \int_0^t \varepsilon |(\tilde{k} \delta \tilde{c}^\varepsilon, \delta \tilde{c}_\Gamma^\varepsilon)_{H_\Gamma}| dt \\ & \leq C \underbrace{\|\delta \tilde{k}\|_{L^\infty([0, T] \times \Omega)}}_{\leq C\varepsilon} (\varepsilon \|\tilde{c}^\varepsilon\|_{L^2(0, T; H_\Gamma)}^2 + \varepsilon \|\delta \tilde{c}_\Gamma^\varepsilon\|_{L^2(0, t; H_\Gamma)}^2) \\ & + C \underbrace{\|\tilde{k}\|_{L^\infty([0, T] \times \Omega)}}_{\leq C\varepsilon} (\varepsilon \|\delta \tilde{c}^\varepsilon\|_{L^2(0, T; H_\Gamma)}^2 + \varepsilon \|\delta \tilde{c}_\Gamma^\varepsilon\|_{L^2(0, t; H_\Gamma)}^2) \\ & \leq C\varepsilon + C\varepsilon \|\delta \tilde{c}_\Gamma^\varepsilon\|_{L^2(0, t; H_\Gamma)}^2 + C \|\delta \tilde{c}^\varepsilon\|_{L^2(0, T; H)}^2. \end{aligned}$$

For the last term we get

$$\begin{aligned}
& \int_0^t \varepsilon |(H\tilde{k}^l(\tilde{c}_\Gamma^\varepsilon)^l - H\tilde{k}\tilde{c}_\Gamma^\varepsilon, \delta\tilde{c}_\Gamma^\varepsilon)_{H_\Gamma}| dt \leq \int_0^t \varepsilon |(H(\delta\tilde{k})(\tilde{c}_\Gamma^\varepsilon)^l, \delta\tilde{c}_\Gamma^\varepsilon)_{H_\Gamma}| dt \\
& \quad + \int_0^t \varepsilon |(H\tilde{k}\delta\tilde{c}_\Gamma^\varepsilon, \delta\tilde{c}_\Gamma^\varepsilon)_{H_\Gamma}| dt \\
& \leq CH \underbrace{\|\delta\tilde{k}\|_{L^\infty([0,t] \times \Omega)}}_{\leq C\varepsilon} \underbrace{(\varepsilon \|\tilde{c}_\Gamma^\varepsilon\|_{L^2(0,T;H_\Gamma)}^2 + \varepsilon \|\delta\tilde{c}_\Gamma^\varepsilon\|_{L^2(0,t;H_\Gamma)}^2)}_{\leq C} + \varepsilon H \|\tilde{k}\|_{L^\infty([0,T] \times \Omega)} \|\delta\tilde{c}_\Gamma^\varepsilon\|_{L^2(0,t;H_\Gamma)}^2 \\
& \leq C\varepsilon + C\varepsilon \|\delta\tilde{c}_\Gamma^\varepsilon\|_{L^2(0,t;H_\Gamma)}^2.
\end{aligned}$$

Putting everything together and neglecting the terms containing a gradient on the left hand side, we obtain the estimate

$$\varepsilon \|\delta\tilde{c}_\Gamma^\varepsilon(t)\|_{H_\Gamma}^2 \leq C\varepsilon \|\delta\tilde{c}_\Gamma^\varepsilon\|_{L^2(0,t;H_\Gamma)}^2 + C\varepsilon \|\delta\tilde{c}_{0,\Gamma}\|_{H_\Gamma}^2 + C\varepsilon + C \|\delta\tilde{c}^\varepsilon\|_{L^2(0,T;H)}^2$$

which gives due to Gronwall's inequality

$$\varepsilon \|\delta\tilde{c}_\Gamma^\varepsilon\|_{L^2(0,T;H_\Gamma)}^2 \leq C\varepsilon \|\delta\tilde{c}_{0,\Gamma}\|_{H_\Gamma}^2 + C\varepsilon + C \|\delta\tilde{c}^\varepsilon\|_{L^2(0,T;H)}^2.$$

Inserting the estimate

$$\begin{aligned}
\varepsilon \|\delta\tilde{c}_{0,\Gamma}\|_{H_\Gamma}^2 & \leq C \|\delta\tilde{c}_{0,\Gamma}\|_H^2 + C\varepsilon^2 \|\nabla \delta\tilde{c}_{0,\Gamma}\|_H^2 \\
& \leq C \|\delta\tilde{c}_{0,\Gamma}\|_H^2 + 2C\varepsilon^2 \|\nabla \tilde{c}_{0,\Gamma}\|_H^2 \\
& \leq C \|\delta\tilde{c}_{0,\Gamma}\|_H^2 + C\varepsilon,
\end{aligned}$$

we finally arrive at

$$\boxed{\varepsilon \|\delta\tilde{c}_\Gamma^\varepsilon\|_{L^2(0,T;H_\Gamma)}^2 \leq C \|\delta\tilde{c}_{0,\Gamma}\|_{L^2(\Omega)}^2 + C\varepsilon + C \|\delta\tilde{c}^\varepsilon\|_{L^2(0,T;L^2(\Omega))}^2.} \quad (3.43)$$

Note that $\|\delta\tilde{c}_{0,\Gamma}\|_{H^1(\Omega)} \leq 2\|\tilde{c}_{0,\Gamma}\|_{H^1(\Omega)} \leq C$ independent of ε . By an analogous argument, we see that $\delta\tilde{c}^\varepsilon$ is bounded in $\{u \in L^2(0,T;H^1(\Omega)); \partial_t u \in L^2(0,T;H^{-1}(\Omega))\}$. These spaces are compactly embedded in $L^2(\Omega)$ and $L^2(0,T;L^2(\Omega))$, resp.; thus $\|\delta\tilde{c}_{0,\Gamma}\|_H^2$ and $\|\delta\tilde{c}^\varepsilon\|_{L^2(0,T;L^2(\Omega))}^2$ satisfy the Kolmogoroff compactness criterion!

Therefore, for all $\mu > 0$ there exists a $h > 0$ such that for all l with $|\varepsilon| < h$ we have

$$\|\delta\tilde{c}_{0,\Gamma}\|_{L^2(\Omega)}^2 \leq \frac{\mu}{3C}, \quad \|\delta\tilde{c}^\varepsilon\|_{L^2(0,T;L^2(\Omega))}^2 \leq \frac{\mu}{3C}, \quad \text{and} \quad \varepsilon \leq \frac{\mu}{3C}.$$

Upon insertion into (3.43) we get

$$\varepsilon \|\delta\tilde{c}_\Gamma^\varepsilon\|_{L^2(0,T;H_\Gamma)}^2 \leq \eta,$$

which proves in conjunction with (3.40) that $\mathcal{T}_b^\varepsilon(\tilde{c}_\Gamma^\varepsilon)$ satisfies the Kolmogoroff compactness criterion in the variable x . \blacklozenge

3.4.4 Remark.

If one takes a look at estimate (3.42) and the considerations that follow, one sees that it is essentially the strong convergence of \tilde{c}^ε on the boundary which forces the unfolded boundary concentrations to converge strongly.

3.4.5 Remark.

As stated before, we did not want to rely on estimates in L^∞ for the concentrations at this place. If, however, such estimates are available, one can reduce the regularity assumptions on the data in the estimates above. In this case, it is sufficient to require only regularity of the type $\tilde{g} \in H^1(\Omega)$, $\tilde{k} \in H^1(\Omega)$.

3.4.3 The Limit Problem

In order to give the limit problem, we need some auxiliary functions which are defined in the following lemma:

3.4.6 Lemma.

We have the following convergences:

1. $\mathcal{T}^\varepsilon(F^{-1})(t, x, y) \longrightarrow \nabla_y \psi^{-1}(t, x, y) =: F_y^{-1}(t, x, y)$ in $\mathcal{C}([0, T] \times \Omega \times Y_R)$
2. $\mathcal{T}_b^\varepsilon(F_\Gamma^{-1})(t, x, y) \longrightarrow \nabla_y^\Gamma \psi^{-1}(t, x, y) =: F_{\Gamma, y}^{-1}(t, x, y)$ in $\mathcal{C}([0, T] \times \Omega \times \partial Y_S)$
3. $\mathcal{T}_b^\varepsilon(\tilde{\nu}^\varepsilon)(t, x, y) \longrightarrow \frac{F_y^{-T}(t, x, y)\tilde{\nu}(y)}{|F_y^{-T}(t, x, y)\tilde{\nu}(y)|} =: \nu_y(t, x, y)$ in $\mathcal{C}([0, T] \times \Omega \times \partial Y_S)$
4. $\frac{1}{\varepsilon}\mathcal{T}_b^\varepsilon(\tilde{\nu}^\varepsilon)(t, x, y) \longrightarrow \partial_t \psi(t, x, y) =: \tilde{\nu}(t, x, y)$ in $\mathcal{C}([0, T] \times \Omega \times \partial Y_S)$
5. $\frac{1}{\varepsilon}\mathcal{T}_b^\varepsilon(\tilde{V}^\varepsilon)(t, x, y) \longrightarrow \partial_t \psi(t, x, y) \cdot \nu_y(t, x, y) =: \tilde{V}(t, x, y)$ in $\mathcal{C}([0, T] \times \Omega \times \partial Y_S)$
6. $\frac{1}{\varepsilon}\mathcal{T}_b^\varepsilon(\tilde{\nu}_M^\varepsilon)(t, x, y) \longrightarrow \tilde{\nu}(t, x, y) - (\tilde{\nu}(t, x, y) \cdot \nu_y(t, x, y))\nu_y(t, x, y) =: \tilde{\nu}_M(t, x, y)$ in $\mathcal{C}([0, T] \times \Omega \times \partial Y_S)$
7. $\varepsilon\mathcal{T}_b^\varepsilon(\tilde{\kappa}^\varepsilon)(t, x, y) \longrightarrow \operatorname{div}_y(F_{\Gamma, y}^{-1}(t, x, y)\nu_y(t, x, y)) =: \tilde{\kappa}_y(t, x, y)$ in $\mathcal{C}([0, T] \times \Omega \times \partial Y_S)$

Note that the convergence statements also hold in the corresponding L^2 -spaces.

Proof. We have (cf. the definitions in Section 3.2.2)

$$\begin{aligned} \mathcal{T}^\varepsilon(F^{-1})(t, x, y) &= \mathcal{T}^\varepsilon((\nabla \phi^\varepsilon)^{-1})(t, x, y) = \mathcal{T}^\varepsilon((\nabla_y \psi^\varepsilon)^{-1})(t, x, y) \\ &= \nabla_y \psi^{-1}\left(t, \varepsilon \left[\frac{\varepsilon \left[\frac{x}{\varepsilon} \right] + \varepsilon y}{\varepsilon} \right], \left\{ \frac{\varepsilon \left[\frac{x}{\varepsilon} \right] + \varepsilon y}{\varepsilon} \right\}\right) \\ &= \nabla_y \psi^{-1}\left(t, \varepsilon \left[\frac{x}{\varepsilon} \right], y\right) \\ &\longrightarrow \nabla_y \psi^{-1}(t, x, y), \end{aligned}$$

due to $\varepsilon \left[\frac{x}{\varepsilon} \right] \rightarrow x$ and the continuity of ψ^{-1} . See also Lemma 3.2.2. The second assertion follows analogously. For the third property use the fact that $\mathcal{T}_b^\varepsilon(fg) = \mathcal{T}_b^\varepsilon(f)\mathcal{T}_b^\varepsilon(g)$ and

$\mathcal{T}_b^\varepsilon(|f|) = |\mathcal{T}_b^\varepsilon(f)|$ together with the usual rules for products and quotients of limits. Next

$$\begin{aligned} \frac{1}{\varepsilon} \mathcal{T}_b^\varepsilon(\tilde{v}^\varepsilon)(t, x, y) &= \frac{1}{\varepsilon} \mathcal{T}^\varepsilon(\partial_t \phi^\varepsilon)(t, x, y) = \mathcal{T}^\varepsilon(\partial_t \psi^\varepsilon)(t, x, y) \\ &= \partial_t \psi(t, \varepsilon \left[\frac{\frac{x}{\varepsilon}}{\varepsilon} + \varepsilon y \right], \left\{ \frac{\varepsilon \left[\frac{x}{\varepsilon} \right] + \varepsilon y}{\varepsilon} \right\}) \\ &= \partial_t \psi(t, \varepsilon \left[\frac{x}{\varepsilon} \right], y) \\ &\longrightarrow \partial_t \psi(t, x, y). \end{aligned}$$

For the fifth and sixth assertion use the same arguments as above. Similarly

$$\begin{aligned} \varepsilon \mathcal{T}_b^\varepsilon(\tilde{\kappa}^\varepsilon)(t, x, y) &= \varepsilon \mathcal{T}_b^\varepsilon(\operatorname{div}(F^{-1} \tilde{v}^\varepsilon))(t, x, y) = \operatorname{div}_y(\mathcal{T}_b^\varepsilon(F^{-1}) \mathcal{T}_b^\varepsilon(\tilde{v}^\varepsilon))(t, x, y) \\ &\longrightarrow \operatorname{div}_y(F_{\Gamma, y}^{-1}(t, x, y) \nu_y(t, x, y)). \end{aligned} \quad \blacklozenge$$

3.4.7 Theorem (Homogenized System).

The limit functions from Proposition 3.4.1 satisfy the equations

$$\begin{aligned} |Y_R(0)| \partial_t c^0 - \operatorname{div}(D^* \nabla c^0) + \delta_{i1} c^0 \int_{\partial Y_S} \tilde{V} \, d\sigma_y &= |Y_R(0)| \tilde{f}(c^0) \\ &\quad - \int_{\partial Y_S} \tilde{k}(c^0 - H c_\Gamma^0) \, d\sigma_y \quad \text{in } [0, T] \times \Omega \\ -D^* \nabla c^0 \cdot \nu &= |Y|(c^0 - c_{\text{ext}}) \quad \text{on } [0, T] \times \partial\Omega \\ c^0(0) &= \tilde{c}_0 \quad \text{in } \Omega \end{aligned}$$

and

$$\begin{aligned} \partial_t c_\Gamma^0 - \operatorname{div}_y^\Gamma(D_\Gamma F_{\Gamma, y}^{-1} F_{\Gamma, y}^{-T} \nabla_y^\Gamma c_\Gamma^0) + c_\Gamma^0 \operatorname{div}_y^\Gamma(F_{\Gamma, y}^{-1} \tilde{v}_M) - c_\Gamma^0 \tilde{\kappa}_y \tilde{V} \\ = \tilde{f}_\Gamma(c_\Gamma^0) + \tilde{k}(c^0 - H c_\Gamma^0) - \delta_{i2} c^0 \tilde{V} \quad \text{in } [0, T] \times \Omega \times \partial Y_S \\ c_\Gamma^0(0, x, y) = \tilde{c}_{0, \Gamma}(x) \quad \text{in } \Omega \times \partial Y_S, \end{aligned}$$

where the effective diffusivity matrix D^* is given by

$$D^*(t, x) = \int_{Y_R(0)} D F_y^{-1}(t, x, y) F^{-T}(t, x, y) ([\delta_{ij}]_{i, j=1}^n + [\frac{\partial w_j}{\partial y_i}(t, x, y)]_{i, j=1}^n) \, dy.$$

D^* is symmetric and positive definite. Here w_j for $j = 1, \dots, n$ is a parameter-dependent solution of the cell problem

$$\begin{aligned} -\operatorname{div}_y(D(F^{-1} F^{-T})(t, x, y) \nabla_y w_j(t, x, y)) &= \operatorname{div}_y(D(F^{-1} F^{-T})(t, x, y) e_j) \quad \text{in } Y_R(0) \\ -D(F^{-1} F^{-T})(t, x, y) \nabla_y w_j(t, x, y) \cdot \nu(y) &= D(F^{-1} F^{-T})(t, x, y) e_j \cdot \nu(y) \quad \text{on } \partial Y_S \\ w_j(t, x, \cdot) &\text{ is } Y\text{-periodic} \end{aligned}$$

The surface equation and the cell problem correspond to a problem with an evolving structure in the reference cell Y , the evolution given by the motion $(t, y) \mapsto \psi(t, x, y)$ for fixed $x \in \Omega$. We are going to prove this theorem in several steps:

3.4.8 Proposition.

In the bulk part, the limit functions satisfy the following weak two-scale system: For all test functions $\phi_0 \in \mathcal{C}^\infty([0, T]; \mathcal{C}^\infty(\bar{\Omega}))$ with $\phi_0(0) = \phi_0(T) = 0$ and $\phi_1 \in \mathcal{C}^\infty([0, T] \times \bar{\Omega} \times Y)$, periodic in y with $\phi_1(0) = \phi_1(T) = 0$ it holds $c^0(0) = \tilde{c}_0$ and

$$\begin{aligned}
|Y_R(0)| \int_0^T \int_{\Omega} \partial_t c^0 \phi_1 \, dx \, dt + \int_0^T \int_{\Omega} \int_{Y_R(0)} DF_y^{-1} F_y^{-T} (\nabla_x c^0 + \nabla_y c^1) (\nabla_x \phi_0 + \nabla_y \phi_1) \, dy \, dx \, dt \\
+ \int_0^T \int_{\Omega} \int_{\partial Y_S} \tilde{k} (c^0 - Hc_{\Gamma}^0) \phi_0 + \delta_{i1} c^0 \tilde{V} \phi_0 \, d\sigma_y \, dx \, dt + |Y| \int_0^T \int_{\partial \Omega} (c^0 - c_{\text{ext}}) \phi_0 \, d\sigma_x \, dt \\
= |Y_R(0)| \int_0^T \int_{\Omega} \tilde{f}(c^0) \phi_0 \, dx \, dt \tag{3.44}
\end{aligned}$$

Proof. We are going to use $\phi_0(t, x) + \varepsilon \phi_1(t, x, \{\frac{x}{\varepsilon}\}) =: \phi_0(t, x) + \varepsilon \phi_1^\varepsilon(t, x) =: \phi^\varepsilon(t, x)$ as a test function in the weak formulation (3.13). We first consider the term $\int_0^T \int_{\Omega^\varepsilon(0)} \frac{d}{dt} \tilde{c}_\Gamma^\varepsilon(t) \phi^\varepsilon \, dx \, dt$. Since $\frac{d}{dt} (\tilde{c}^\varepsilon(t), \phi^\varepsilon)_H = \langle \partial_t \tilde{c}^\varepsilon, \phi^\varepsilon \rangle_V$, we get upon unfolding

$$\begin{aligned}
& \int_0^T \int_{\Omega^\varepsilon(0)} \partial_t(t, x) \tilde{c}_\Gamma^\varepsilon(\phi_0(t, x) + \varepsilon \phi_1(t, x, \{\frac{x}{\varepsilon}\})) \, dx \, dt \\
&= \int_0^T \int_{\Omega} \partial_t \tilde{c}_\Gamma^\varepsilon(t, x) \chi_{Y_R(0)}(\{\frac{x}{\varepsilon}\}) (\phi_0(t, x) + \varepsilon \phi_1(t, x, \{\frac{x}{\varepsilon}\})) \, dx \, dt \\
&= \frac{1}{|Y|} \int_0^T \int_{\Omega} \int_Y \mathcal{T}^\varepsilon(\partial_t \tilde{c}_\Gamma^\varepsilon)(t, x, x) \chi_{Y_R(0)}(y) (\mathcal{T}^\varepsilon(\phi_0) + \varepsilon \mathcal{T}^\varepsilon(\phi_1^\varepsilon))(t, x, y) \, dy \, dx \, dt \\
&= \frac{1}{|Y|} \int_0^T \int_{\Omega} \int_{Y_R(0)} \mathcal{T}^\varepsilon(\partial_t \tilde{c}_\Gamma^\varepsilon)(t, x, y) (\mathcal{T}^\varepsilon(\phi_0) + \varepsilon \mathcal{T}^\varepsilon(\phi_1^\varepsilon))(t, x, y) \, dy \, dx \, dt \\
&\longrightarrow \frac{1}{|Y|} \int_0^T \int_{\Omega} \int_{Y_R(0)} \partial_t c^0(t, x) \phi_0(t, x) \, dy \, dx \, dt
\end{aligned}$$

due to convergence (3.34) and $\mathcal{T}^\varepsilon(\phi_0) \rightarrow \phi_0$ as well as $\varepsilon\mathcal{T}^\varepsilon(\phi_1^\varepsilon) \rightarrow 0$. Next

$$\begin{aligned} & \int_0^T \int_{\Omega^\varepsilon(0)} D(F^{-1}F^{-T} \nabla \tilde{c}_\Gamma^\varepsilon \cdot \nabla(\phi_0 + \varepsilon\phi_1^\varepsilon)) \, dx \, dt \\ &= \frac{1}{|Y|} \int_0^T \int_{\Omega} \int_{Y_R(0)} D\mathcal{T}^\varepsilon(F^{-1})\mathcal{T}^\varepsilon(F^{-T})\mathcal{T}^\varepsilon(\nabla \tilde{c}_\Gamma^\varepsilon)(\mathcal{T}^\varepsilon(\nabla_x \phi_0) + \nabla_y \mathcal{T}^\varepsilon(\phi_1^\varepsilon)) \, dy \, dx \, dt \\ &\rightarrow \frac{1}{|Y|} \int_0^T \int D F_y^{-1} F_y^{-T} (\nabla_x c^0 + \nabla_y c^1) \cdot (\nabla_x \phi_0 + \nabla_y \phi_1) \, dy \, dx \, dt, \end{aligned}$$

where we used (3.33), Lemma 3.4.6 as well as $\mathcal{T}^\varepsilon(\nabla \phi_0) \rightarrow \nabla \phi_0$ and $\mathcal{T}^\varepsilon(\varepsilon \nabla \phi_1^\varepsilon) = \nabla_y \mathcal{T}^\varepsilon(\phi_1^\varepsilon) \rightarrow \nabla_y \phi_1$. Moreover

$$\int_0^T \int_{\Omega^\varepsilon(0)} \nabla \tilde{c}_\Gamma^\varepsilon \cdot F^{-1} \tilde{v}^\varepsilon(\phi_0 + \varepsilon\phi_1^\varepsilon) \, dx \, dt \rightarrow 0$$

since $\|\tilde{v}^\varepsilon\|_{L^\infty} \leq C\varepsilon$ and the other terms are bounded. For the boundary terms we obtain

$$\begin{aligned} & \varepsilon \int_0^T \int_{\Gamma^\varepsilon(0)} \frac{\delta_{i1}}{\varepsilon} \tilde{c}^\varepsilon \tilde{V}^\varepsilon(\phi_0 + \varepsilon\phi_1^\varepsilon) + \tilde{k} \tilde{c}^\varepsilon(\phi_0 + \varepsilon\phi_1^\varepsilon) - H \tilde{k} \tilde{c}_\Gamma^\varepsilon(\phi_0 + \varepsilon\phi_1^\varepsilon) \, d\sigma_x \, dt \\ &= \frac{1}{|Y|} \int_0^T \int_{\Omega} \int_{\partial Y_S} \delta_{i1} \frac{1}{\varepsilon} \mathcal{T}_b^\varepsilon(\tilde{V}^\varepsilon) \mathcal{T}_b^\varepsilon(\tilde{c}^\varepsilon)(\mathcal{T}_b^\varepsilon(\phi_0) + \varepsilon \mathcal{T}_b^\varepsilon(\phi_1^\varepsilon)) \\ &\quad + \mathcal{T}_b^\varepsilon(\tilde{k}) \mathcal{T}_b^\varepsilon(\tilde{c}^\varepsilon)(\mathcal{T}_b^\varepsilon(\phi_0) + \varepsilon \mathcal{T}_b^\varepsilon(\phi_1^\varepsilon)) - H \mathcal{T}_b^\varepsilon(\tilde{k}) \mathcal{T}_b^\varepsilon(\tilde{c}_\Gamma^\varepsilon)(\mathcal{T}_b^\varepsilon(\phi_0) \\ &\quad \quad \quad + \varepsilon \mathcal{T}_b^\varepsilon(\phi_1^\varepsilon)) \, d\sigma_y \, dx \, dt \\ &\rightarrow \frac{1}{|Y|} \int_0^T \int_{\Omega} \int_{\partial Y_S} \delta_{i1} \tilde{V} c^0 \phi_0 + \tilde{k}(c^0 - H c_\Gamma^0) \, d\sigma_y \, dx \, dt \end{aligned}$$

due to (3.35), (3.36) as well as Lemma 3.4.6 and $\mathcal{T}_b^\varepsilon(\phi_0) \rightarrow \phi_0$, $\varepsilon \mathcal{T}_b^\varepsilon(\phi_1^\varepsilon) \rightarrow 0$.

Since the first embedding in the chain $\{u \in L^2(0, T; H^1(\Omega)); \partial_t u \in L^2(0, T; H^{-1}(\Omega))\} \hookrightarrow L^2(0, T; H^{\frac{3}{4}}(\Omega)) \hookrightarrow L^2(0, T; L^2(\partial\Omega))$ is compact, (3.29) implies that $\tilde{c}^\varepsilon \rightarrow c^0$ strongly in $L^2(0, T; L^2(\partial\Omega))$, thus

$$\int_0^T \int_{\partial\Omega} (\tilde{c}_\Gamma^\varepsilon - c_{\text{ext}})(\phi_0 + \varepsilon\phi_1^\varepsilon) \, dx \, dt \rightarrow \int_0^T \int_{\partial\Omega} (\tilde{c}_\Gamma^\varepsilon - c_{\text{ext}})\phi_0 \, dx \, dt.$$

Finally, due to the strong convergence (3.32), we have almost everywhere convergence along a subsequence of $\mathcal{T}^\varepsilon(\tilde{c}^\varepsilon)$ towards c^0 . Since \tilde{f} is continuous, we obtain along that

subsequence

$$\mathcal{T}^\varepsilon(\tilde{f}(\tilde{c}_\Gamma^\varepsilon))(t, x, y) = \tilde{f}\left(\varepsilon \left\lfloor \frac{x}{\varepsilon} \right\rfloor + \varepsilon y, \mathcal{T}^\varepsilon(\tilde{c}_\Gamma^\varepsilon)(t, x, y)\right) \longrightarrow \tilde{f}(x, c^0(t, x, y)) \quad \text{a.e.}$$

Since \tilde{c}^ε converges strongly in $L^2(0, T; L^2(\Omega))$, there exists a subsequence (still denoted by ε) and a majorizing function $v \in L^2(0, T; L^2(\Omega))$ such that $|\tilde{c}^\varepsilon(t, x)| \leq v(t, x)$ for all ε and almost all $(t, x) \in [0, T] \times \Omega$. Thus, due to Lemma 3.3.4, we obtain the bound $|\mathcal{T}^\varepsilon(\tilde{f}(\tilde{c}^\varepsilon))(\phi_0 + \varepsilon\phi_1^\varepsilon)| \leq C(1 + |\tilde{c}^\varepsilon|) \leq C(1 + v)$. Since the right hand side is square integrable, with integral bounded independent of ε , Lebesgues dominated convergence theorem yields that

$$\begin{aligned} \int_0^T \int_{\Omega^\varepsilon(0)} \tilde{f}(\tilde{c}^\varepsilon)((\phi_0 + \varepsilon\phi_1^\varepsilon)) \, dx \, dt &= \frac{1}{|Y|} \int_0^T \int_{\Omega} \int_{Y_R(0)} \mathcal{T}^\varepsilon(\tilde{f}(\tilde{c}^\varepsilon))(\mathcal{T}^\varepsilon(\phi_0) + \varepsilon\mathcal{T}^\varepsilon(\phi_1^\varepsilon)) \, dy \, dx \, dt \\ &\longrightarrow \frac{1}{|Y|} \int_0^T \int_{\Omega} \int_{Y_R(0)} \tilde{f}(c^0)\phi_0 \, dy \, dx \, dt = \frac{|Y_R(0)|}{|Y|} \int_0^T \int_{\Omega} \tilde{f}(c^0)\phi_0 \, dx \, dt. \end{aligned}$$

Putting everything together, we obtain the integral identity of the proposition.

In order to recover the initial condition, choose a $\phi_0 \in \mathcal{C}^\infty(0, T; \mathcal{C}^\infty(\bar{\Omega}))$ with $\phi_0(T) = 0$. We have $\int_0^T \int_{\Omega} \partial_t \tilde{c}^\varepsilon \phi_0 \, dx \, dt = - \int_0^T \int_{\Omega} \tilde{c}^\varepsilon \partial_t \phi_0 \, dx \, dt - \int_{\Omega} \tilde{c}_0 \phi_0(0) \, dx$. Passing to the limit on both sides gives

$$\int_0^T \int_{\Omega} \partial_t c^0 \phi_0 \, dx \, dt = - \int_0^T \int_{\Omega} c^0 \partial_t \phi_0 \, dx \, dt - \int_{\Omega} \tilde{c}_0 \phi_0(0) \, dx,$$

thus $c^0(0) = \tilde{c}_0$. ◆

3.4.9 Proposition.

Concerning the surface part of the equations, the limit functions satisfy the following weak two-scale system: For all test functions $\phi_\Gamma \in \mathcal{C}^\infty([0, T] \times \bar{\Omega} \times \partial Y_S)$, periodic in y with $\phi_\Gamma(0) = \phi_\Gamma(T) = 0$ it holds $c_\Gamma^0(0, x, y) = \tilde{c}_{0,\Gamma}(x)$ and

$$\begin{aligned} &\int_0^T \int_{\Omega} \int_{\partial Y_S} \partial_t c_\Gamma^0 \phi_\Gamma \, d\sigma_y \, dx \, dt + \int_0^T \int_{\Omega} \int_{\partial Y_S} D_\Gamma F_{\Gamma,y}^{-1} F_{\Gamma,y}^{-T} \nabla_y^\Gamma c_\Gamma^0 \cdot \nabla_y^\Gamma \phi_\Gamma \, d\sigma_y \, dx \, dt \\ &+ \int_0^T \int_{\Omega} \int_{\partial Y_S} c_\Gamma^0 \operatorname{div}_y^\Gamma (F_{\Gamma,y}^{-1} \tilde{v}_M) \phi_\Gamma \, d\sigma_y \, dx \, dt - \int_0^T \int_{\Omega} \int_{\partial Y_S} c_\Gamma^0 \tilde{\kappa}_y \tilde{V} \phi_\Gamma \, d\sigma_y \, dx \, dt \\ &= \int_0^T \int_{\Omega} \int_{\partial Y_S} \tilde{f}_\Gamma(c_\Gamma^0) \phi_\Gamma \, d\sigma_y \, dx \, dt + \int_0^T \int_{\Omega} \int_{\partial Y_S} \tilde{k}(c^0 - H c_\Gamma^0) \phi_\Gamma \, d\sigma_y \, dx \, dt \\ &\quad - \int_0^T \int_{\Omega} \int_{\partial Y_S} \delta_{i2} c^0 \tilde{V} \phi_\Gamma \, d\sigma_y \, dx \, dt. \end{aligned}$$

Proof. We use $\varepsilon\phi_\Gamma(t, x, \{\frac{x}{\varepsilon}\}) =: \varepsilon\phi_\Gamma^\varepsilon(t, x)$ as a test function in the weak formulation (3.14). We get for the different terms via boundary unfolding

$$\begin{aligned} \varepsilon \int_0^T \int_{\Gamma^\varepsilon(0)} \partial_t \tilde{c}_\Gamma^\varepsilon \phi_\Gamma^\varepsilon \, d\sigma_x \, dt &= \frac{1}{|Y|} \int_0^T \int_\Omega \int_{\partial Y_S} \mathcal{T}_b^\varepsilon(\partial_t \tilde{c}_\Gamma^\varepsilon) \mathcal{T}_b^\varepsilon(\phi_\Gamma^\varepsilon) \, d\sigma_y \, dx \, dt \\ &\longrightarrow \int_0^T \int_\Omega \int_{\partial Y_S} \partial_t c_\Gamma^0 \phi_\Gamma \, d\sigma_y \, dx \, dt \end{aligned}$$

due to (3.38) and $\mathcal{T}_b^\varepsilon(\phi_\Gamma^\varepsilon) \rightarrow \phi_\Gamma$. Moreover (note (3.37) and Lemma 3.4.6)

$$\begin{aligned} \varepsilon \int_0^T \int_{\Gamma^\varepsilon(0)} \varepsilon^2 D_\Gamma F_\Gamma^{-1} F_\Gamma^{-T} \nabla^\Gamma \tilde{c}_\Gamma^\varepsilon \cdot \nabla^\Gamma \phi_\Gamma^\varepsilon \, d\sigma_x \, dt \\ &= \frac{1}{|Y|} \int_0^T \int_\Omega \int_{\partial Y_S} D_\Gamma \mathcal{T}_b^\varepsilon(F_\Gamma^{-1}) \mathcal{T}_b^\varepsilon(F_\Gamma^{-T}) \varepsilon \mathcal{T}_b^\varepsilon(\nabla \tilde{c}_\Gamma^\varepsilon) \cdot \varepsilon \mathcal{T}_b^\varepsilon(\nabla \phi_\Gamma^\varepsilon) \, d\sigma_y \, dx \, dt \\ &= \frac{1}{|Y|} \int_0^T \int_\Omega \int_{\partial Y_S} D_\Gamma \mathcal{T}_b^\varepsilon(F_\Gamma^{-1}) \mathcal{T}_b^\varepsilon(F_\Gamma^{-T}) \varepsilon \mathcal{T}_b^\varepsilon(\nabla \tilde{c}_\Gamma^\varepsilon) \cdot \nabla_y^\Gamma \mathcal{T}_b^\varepsilon(\phi_\Gamma^\varepsilon) \, d\sigma_y \, dx \, dt \\ &\longrightarrow \frac{1}{|Y|} \int_0^T \int_\Omega \int_{\partial Y_S} D_\Gamma F_{\Gamma,y}^{-1} F_{\Gamma,y}^{-T} \nabla_y^\Gamma c_\Gamma^0 \cdot \nabla_y^\Gamma \phi_\Gamma \, d\sigma_y \, dx \, dt. \end{aligned}$$

With (3.36) and the unfolding result for the tangential part of the velocity we obtain

$$\begin{aligned} \varepsilon \int_0^T \int_{\Gamma^\varepsilon(0)} \tilde{c}_\Gamma^\varepsilon \operatorname{div}^\Gamma(F_\Gamma^{-1} \tilde{v}_M^\varepsilon) \phi_\Gamma^\varepsilon \, d\sigma_x \, dt \\ &= \frac{1}{|Y|} \int_0^T \int_\Omega \int_{\partial Y_S} \mathcal{T}_b^\varepsilon(\tilde{c}_\Gamma^\varepsilon) \varepsilon \mathcal{T}_b^\varepsilon(\operatorname{div}^\Gamma(F_\Gamma^{-1} \frac{1}{\varepsilon} \tilde{v}_M^\varepsilon)) \mathcal{T}_b^\varepsilon(\phi_\Gamma^\varepsilon) \, d\sigma_y \, dx \, dt \\ &= \frac{1}{|Y|} \int_0^T \int_\Omega \int_{\partial Y_S} \mathcal{T}_b^\varepsilon(\tilde{c}_\Gamma^\varepsilon) \operatorname{div}_y^\Gamma(\mathcal{T}_b^\varepsilon(F_\Gamma^{-1}) \frac{1}{\varepsilon} \mathcal{T}_b^\varepsilon(\tilde{v}_M^\varepsilon)) \mathcal{T}_b^\varepsilon(\phi_\Gamma^\varepsilon) \, d\sigma_y \, dx \, dt \\ &\longrightarrow \frac{1}{|Y|} \int_0^T \int_\Omega \int_{\partial Y_S} c_\Gamma^0 \operatorname{div}_y^\Gamma(F_{\Gamma,y}^{-1} \tilde{v}_M) \phi_\Gamma \, d\sigma_y \, dx \, dt. \end{aligned}$$

Analogously

$$\begin{aligned} \varepsilon \int_0^T \int_{\Gamma^\varepsilon(0)} \tilde{c}_\Gamma^\varepsilon \tilde{\kappa}^\varepsilon \tilde{V}^\varepsilon \phi_\Gamma^\varepsilon \, d\sigma_x \, dt &= \frac{1}{|Y|} \int_0^T \int_\Omega \int_{\partial Y_S} \mathcal{T}_b^\varepsilon(\tilde{c}_\Gamma^\varepsilon) \varepsilon \mathcal{T}_b^\varepsilon(\tilde{\kappa}^\varepsilon) \frac{1}{\varepsilon} \mathcal{T}_b^\varepsilon(\tilde{V}^\varepsilon) \mathcal{T}_b^\varepsilon(\phi_\Gamma^\varepsilon) \, d\sigma_y \, dx \, dt \\ &\rightarrow \frac{1}{|Y|} \int_0^T \int_\Omega \int_{\partial Y_S} c_\Gamma^0 \tilde{\kappa}_y \tilde{V} \phi_\Gamma \, d\sigma_y \, dx \, dt. \end{aligned}$$

The limit for the remaining terms can be obtained by the same way as for the corresponding terms in the proof of the last proposition. Putting everything together, we obtain the result for the integral identity.

In order to obtain the initial condition, choose a $\phi_\Gamma \in \mathcal{C}^\infty([0, T] \times \bar{\Omega} \times \partial Y_S)$, periodic in y with $\phi_\Gamma(T) = 0$ and set $\phi_\Gamma^\varepsilon = \phi_\Gamma(t, x, \{\frac{x}{\varepsilon}\})$ as above. We have

$$\varepsilon \int_0^T \int_{\Gamma^\varepsilon(0)} \partial_t \tilde{c}_\Gamma^\varepsilon \phi_\Gamma^\varepsilon \, d\sigma_x \, dt = -\varepsilon \int_0^T \int_{\Gamma^\varepsilon(0)} \tilde{c}_\Gamma^\varepsilon \partial_t \phi_\Gamma^\varepsilon \, d\sigma_x \, dt - \varepsilon \int_{\Gamma^\varepsilon(0)} \tilde{c}_{0,\Gamma} \phi_\Gamma^\varepsilon(0) \, d\sigma_x.$$

Upon unfolding we obtain

$$\begin{aligned} \frac{1}{|Y|} \int_0^T \int_\Omega \int_{\partial Y_S} \mathcal{T}_b^\varepsilon(\partial_t \tilde{c}_\Gamma^\varepsilon) \mathcal{T}_b^\varepsilon(\phi_\Gamma^\varepsilon) \, d\sigma_y \, dx \, dt &= \frac{1}{|Y|} \int_0^T \int_\Omega \int_{\partial Y_S} \mathcal{T}_b^\varepsilon(\tilde{c}_\Gamma^\varepsilon) \mathcal{T}_b^\varepsilon(\partial_t \phi_\Gamma^\varepsilon) \, d\sigma_y \, dx \, dt \\ &\quad - \int_\Omega \int_{\partial Y_S} \mathcal{T}_b^\varepsilon \tilde{c}_{0,\Gamma} \mathcal{T}_b^\varepsilon(\phi_\Gamma^\varepsilon(0)) \, d\sigma_y \, dx. \end{aligned}$$

Since $\mathcal{T}_b^\varepsilon \tilde{c}_{0,\Gamma} \rightarrow \tilde{c}_{0,\Gamma}$ in $L^2(\Omega \times \partial Y_S)$ we get in the limit

$$\frac{1}{|Y|} \int_0^T \int_\Omega \int_{\partial Y_S} \partial_t c_\Gamma^0 \phi_\Gamma \, d\sigma_y \, dx \, dt = \frac{1}{|Y|} \int_0^T \int_\Omega \int_{\partial Y_S} c_\Gamma^0 \partial_t \phi_\Gamma \, d\sigma_y \, dx \, dt - \int_\Omega \int_{\partial Y_S} \tilde{c}_{0,\Gamma} \phi_\Gamma(0) \, d\sigma_y \, dx,$$

which shows that also the asserted initial condition is valid. \blacklozenge

We now come back to equation (3.44) and show how this formulation can be split into a bulk equation and a cell problem: Define the functions $w_j(t, x, \cdot)$ for $j = 1, \dots, n$ and given $(t, x) \in [0, T] \times \Omega$ via

$$\begin{aligned} -\operatorname{div}_y(DF^{-1}(t, x, y)F^{-T}(t, x, y) \nabla_y w_j(t, x, y)) \\ = \operatorname{div}_y(DF^{-1}(t, x, y)F^{-T}(t, x, y)e_j) &\quad \text{in } Y_R(0) \\ -DF^{-1}(t, x, y)F^{-T}(t, x, y) \nabla_y w_j(t, x, y) \cdot \nu = DF^{-1}(t, x, y)F^{-T}(t, x, y)e_j \cdot \nu &\quad \text{on } \partial Y_S \\ w_j(t, x, \cdot) \text{ is } Y\text{-periodic in } y. \end{aligned}$$

3.4.10 Lemma.

Fix $(t, x) \in [0, T] \times \Omega$ and write $w_j(\cdot) = w_j(t, x, \cdot)$. Then there exists a solution to the above problem in $H_{\#}^1(Y_R(0))$ which is unique up to constants.

Proof. Multiplying the first equation with a test function $\phi \in H_{\#}^1(Y_R(0))$ and integrating both sides by parts yields

$$\int_{Y_R(0)} DF_y^{-1}(t, x) F_y^{-T}(t, x) \nabla_y w_j \cdot \nabla_y \phi \, dy = - \int_{Y_R(0)} DF_y^{-1}(t, x) F_y^{-T}(t, x) e_j \cdot \nabla_y \phi \, dy \quad (3.45)$$

for all $\phi \in H_{\#}^1(Y_R(0))/\mathbb{R}$. This is a well defined weak formulation in $H_{\#}^1(Y_R(0))/\mathbb{R}$, thus the Lax-Milgram lemma gives the existence of a w_j in that function space. \blacklozenge

3.4.11 Remark.

Results concerning the smoothness of w_j in direction of t and x can be obtained by using the implicit function theorem for Banach-spaces, see [Dob09]. In short, the differentiability properties of the matrix F carry over to the solution w_j .

Proof of Theorem 3.4.7. Choosing $\phi_0 = 0$ in (3.44), one obtains the equation

$$\int_0^T \int_{\Omega} \int_{Y_R(0)} DF_y^{-1} F_y^{-T} (\nabla_x c^0 + \nabla_y c^1) (\nabla_y \phi_1) \, dy \, dx \, dt = 0,$$

which upon an integration by parts gives the strong formulation

$$\begin{aligned} -\operatorname{div}_y (DF_y^{-1} F_y^{-T} (\nabla_x c^0 + \nabla_y c^1)) &= 0 \quad \text{in } Y_R(0) \\ -DF_y^{-1} F_y^{-T} (\nabla_x c^0 + \nabla_y c^1) \cdot \nu &= 0 \quad \text{on } \partial Y_S \\ c^1 &\text{ is } y\text{-periodic in } Y_R(0). \end{aligned}$$

Here we are looking for a function $c^1 \in H^1(Y_R(0))/\mathbb{R}$. Making the ansatz

$$c^1 = \sum_{j=1}^n \frac{\partial c^0}{\partial x_j} w_j,$$

a short calculation using the definition of w_j shows that c^1 solves the problem above. Next, we choose $\phi_1 = 0$ in (3.44) and consider the term $I := \int_0^T \int_{\Omega} \int_{Y_R(0)} DF_y^{-1} F_y^{-T} (\nabla_x c^0 + \nabla_y c^1) \nabla_x \phi_0 \, dy \, dx \, dt$. Carrying out an integration by parts, we get

$$\begin{aligned} I &= - \int_0^T \int_{\Omega} \int_{Y_R(0)} \operatorname{div}_x (DF_y^{-1} F_y^{-T} (\nabla_x c^0 + \nabla_y c^1)) \phi_0 \, dy \, dx \, dt \\ &\quad + \int_0^T \int_{\partial \Omega} \int_{Y_R(0)} DF_y^{-1} F_y^{-T} (\nabla_x c^0 + \nabla_y c^1) \phi_0 \cdot \nu \, dy \, d\sigma_x \, dt \end{aligned}$$

$$\begin{aligned}
&= - \int_0^T \int_{\Omega} \operatorname{div}_x \left(\int_{Y_R(0)} F_y^{-1} F_y^{-T} (\nabla_x c^0 + \nabla_y c^1) \, dy \right) \phi_0 \, dx \, dt \\
&\quad + \int_0^T \int_{\partial\Omega} \left(\int_{Y_R(0)} DF_y^{-1} F_y^{-T} (\nabla_x c^0 + \nabla_y c^1) \cdot \nu \, dy \right) \phi_0 \, d\sigma_x \, dt.
\end{aligned}$$

By the form of c^1 , we now obtain that

$$\begin{aligned}
\int_{Y_R(0)} DF_y^{-1} F_y^{-T} (\nabla_x c^0 + \nabla_y c^1) \, dy &= \int_{Y_R(0)} DF_y^{-1} F_y^{-T} (\nabla_x c^0 + \sum_{j=1}^n \frac{\partial c^0}{\partial x_j} \nabla_y w_j) \, dy \\
&= \int_{Y_R(0)} DF_y^{-1} F_y^{-T} ([\delta_{ij}]_{i,j=1}^n + [\frac{\partial w_j}{\partial y_i}]_{i,j=1}^n) \nabla_x c^0 \, dy \\
&= D^* \nabla_x c^0,
\end{aligned}$$

where D^* is defined in the assertion of the theorem. Inserting this term in the above integrals and arguing with the fundamental lemma of variational calculus, we obtain the strong form of the bulk equations from the result of Proposition 3.4.8. Similarly, since

$$\begin{aligned}
&\int_0^T \int_{\Omega} \int_{\partial Y_S} D_{\Gamma} F_{\Gamma,y}^{-1} F_{\Gamma,y}^{-T} \nabla_y^{\Gamma} c_{\Gamma}^0 \cdot \nabla_y^{\Gamma} \phi_{\Gamma} \, d\sigma_y \, dx \, dt \\
&= - \int_0^T \int_{\Omega} \int_{\partial Y_S} \operatorname{div}_y^{\Gamma} (D_{\Gamma} F_{\Gamma,y}^{-1} F_{\Gamma,y}^{-T} \nabla_y^{\Gamma} c_{\Gamma}^0) \phi_{\Gamma} \, d\sigma_y \, dx \, dt
\end{aligned}$$

we can apply the same argument to the result of Proposition 3.4.9 to deduce the strong form of the surface equations.

It remains to show that D^* is positive definite: To begin with, fix $i, j \in \{1, \dots, n\}$. All gradients that appear in the sequel are always considered with respect to the variable y . Now we choose $\phi = w_i$ in (3.45) to obtain

$$\begin{aligned}
\int_{Y_R(0)} DF_y^{-1}(t, x) F_y^{-T}(t, x) \nabla w_j \cdot \nabla w_i \, dy &= - \int_{Y_R(0)} DF_y^{-1}(t, x) F_y^{-T}(t, x) e_j \cdot \nabla w_i \, dy \\
&= \int_{Y_R(0)} DF_y^{-1}(t, x) F_y^{-T}(t, x) \nabla y_j \cdot \nabla w_i \, dy,
\end{aligned}$$

where – by abuse of notation – we used y_j to denote the function $y_j : \mathbb{R}^n \rightarrow \mathbb{R}$, $\begin{pmatrix} y_1 \\ \vdots \\ y_n \end{pmatrix} \mapsto y_j$. This gives

$$\int_{Y_R(0)} DF_y^{-1}(t, x) F_y^{-T}(t, x) (\nabla y_j - \nabla w_j) \cdot \nabla w_i \, dy = 0. \quad (3.46)$$

Since the j -th column of D^* is given by

$$\int_{Y_R(0)} DF_y^{-1}(t, x) F_y^{-T}(t, x) (e_j - \nabla w_j) \, dy = \int_{Y_R(0)} DF_y^{-1}(t, x) F_y^{-T}(t, x) (\nabla y_j - \nabla w_j) \, dy,$$

we get

$$\begin{aligned} (D^*)_{ij} &= \int_{Y_R(0)} DF_y^{-1}(t, x) F_y^{-T}(t, x) (\nabla y_j - \nabla w_j) \cdot e_i \, dy \\ &= \int_{Y_R(0)} DF_y^{-T}(t, x) (\nabla y_j - \nabla w_j) \cdot F_y^{-T}(t, x) \nabla y_i \, dy \\ &= \int_{Y_R(0)} DF_y^{-T}(t, x) (\nabla y_j - \nabla w_j) \cdot F_y^{-T}(t, x) (\nabla y_i - \nabla w_i) \, dy \end{aligned}$$

by (3.46). This last equation clearly shows that D^* is symmetric. Next, let $\xi \in \mathbb{R}^n$ be a vector and define $\zeta = \sum_{j=1}^n (y_j - w_j) \xi_j$, then by the last identity

$$\begin{aligned} \xi^T D^* \xi &= \sum_{i,j=1}^n \int_{Y_R(0)} DF_y^{-T}(t, x) (\nabla y_j - \nabla w_j) \xi_j \cdot F_y^{-T}(t, x) (\nabla y_i - \nabla w_i) \xi_i \, dy \\ &= \int_{Y_R(0)} DF_y^{-T}(t, x) \sum_{j=1}^n [(\nabla y_j - \nabla w_j) \xi_j] \cdot F_y^{-T}(t, x) \sum_{i=1}^n [(\nabla y_i - \nabla w_i) \xi_i] \, dy \\ &= \int_{Y_R(0)} DF_y^{-T}(t, x) \nabla \zeta \cdot F_y^{-T}(t, x) \nabla \zeta \, dy \geq d_0 \int_{Y_R(0)} |\nabla \zeta|^2 \, dy \geq 0. \end{aligned}$$

This proves that D^* is positive. Assume that there exists a $\xi \in \mathbb{R}^n$ such that $\xi^T D^* \xi = 0$. In that case, by the last result we obtain $\nabla \zeta = 0$, i.e. $\zeta = \text{const.}$ or

$$\sum_{i=1}^n \xi_i y_i = \sum_{i=1}^n \xi_i w_i(t, x, y) + \text{const.}$$

for $(t, x) \in [0, T] \times \Omega$ and $y \in Y_R(0)$. Whereas the right hand side is periodic in y , the left hand side is periodic in y only for $\xi = 0$. This shows the definiteness of D^* and finishes the proof of Theorem 3.4.7. \blacklozenge

3.4.12 Proposition.

The solution (c^0, c_Γ^0) of the limit problem from Theorem 3.4.7 is unique.

Proof. This result can be proven as in Proposition 3.3.20 by choosing adequate test functions. \blacklozenge

Due to this last proposition, we do not only get convergence along a subsequence, but convergence of the whole sequence $(\tilde{c}^\varepsilon, \tilde{c}_\Gamma^\varepsilon)$.

3.5 Appendix: L^∞ -estimates for the solutions

In this section we present one possible approach which can be used to estimate the solution $(\tilde{c}^\varepsilon, \tilde{c}_\Gamma^\varepsilon)$ of the evolving hypersurface-problem in the space $L^\infty([0, T] \times \Omega)$. One can use the standard regularity theory for parabolic problems (see e.g. Ladyzhenskaya, Solonnikov, and Uralt'ceva [LSU88]) to obtain such estimates for fixed ε ; however, to use them in the homogenization process, one has to have an explicit control on the estimates in terms of ε .

In the sequel, we prove an abstract comparison principle which is independent of the scale parameter. One then has to construct special upper and lower solutions to obtain estimates on the solution. For further information about this way of obtaining estimates, see e.g. Knabner [Kna91], Friedmann [FK92], Meier [Mei08] for works on similar situations as ours or Pao [Pao92] for the general theory.

The advantage of this approach is that it allows the reader to exploit additional information when applying our results to real life problems. We illustrate this with the example of a hypersurface which is only growing (or shrinking), i.e. the normal velocity is negative (or positive) everywhere and with additional assumptions on the reaction rates \tilde{f} and \tilde{f}_Γ .

3.5.1 Abstract Comparison Principle

We start by defining weak upper and lower solutions:

3.5.1 Definition (Weak Upper and Lower Solutions).

We say that

1. $(\bar{c}^\varepsilon, \bar{c}_\Gamma^\varepsilon) \in \mathcal{W} \times \mathcal{W}_\Gamma$ is a weak upper solution of Problem (3.13) and (3.14) if for all $(\phi, \phi_\Gamma) \in V \times V_\Gamma$ with $\phi, \phi_\Gamma \geq 0$ it holds

$$\begin{aligned} \frac{d}{dt}(\bar{c}^\varepsilon(t), \phi)_H + a^1(\bar{c}^\varepsilon(t), \phi; t) + a^2(\bar{c}^\varepsilon(t), \phi; t) + a^3(\bar{c}^\varepsilon(t), \phi; t) \\ \geq b(\phi; t, \bar{c}^\varepsilon, \bar{c}_\Gamma^\varepsilon, c_{\text{ext}}) \quad a.e. [0, T] \end{aligned} \quad (3.47a)$$

$$\bar{c}^\varepsilon(0) \geq \tilde{c}_0 \quad (3.47b)$$

and

$$\begin{aligned} \frac{d}{dt}(\bar{c}_\Gamma^\varepsilon(t), \phi_\Gamma)_{H_\Gamma} + a_\Gamma^1(\bar{c}_\Gamma^\varepsilon(t), \phi_\Gamma; t) + a_\Gamma^2(\bar{c}_\Gamma^\varepsilon(t), \phi_\Gamma; t) \\ \geq b_\Gamma(\phi; t, \bar{c}^\varepsilon, \bar{c}_\Gamma^\varepsilon) \quad a.e. [0, T] \end{aligned} \quad (3.48a)$$

$$\bar{c}_\Gamma^\varepsilon(0) \geq \tilde{c}_{0,\Gamma}. \quad (3.48b)$$

2. $(\underline{c}^\varepsilon, \underline{c}_\Gamma^\varepsilon) \in \mathcal{W} \times \mathcal{W}_\Gamma$ is a weak lower solution of problem (3.13) and (3.14) if for all $(\phi, \phi_\Gamma) \in V \times V_\Gamma$ with $\phi, \phi_\Gamma \geq 0$ it holds

$$\begin{aligned} \frac{d}{dt}(\underline{c}^\varepsilon(t), \phi)_H + a^1(\underline{c}^\varepsilon(t), \phi; t) + a^2(\underline{c}^\varepsilon(t), \phi; t) + a^3(\underline{c}^\varepsilon(t), \phi; t) \\ \leq b(\phi; t, \underline{c}^\varepsilon, \underline{c}_\Gamma^\varepsilon, c_{\text{ext}}) \quad a.e. [0, T] \end{aligned} \quad (3.49a)$$

$$\underline{c}^\varepsilon(0) \leq \tilde{c}_0 \quad (3.49b)$$

and

$$\begin{aligned} \frac{d}{dt}(\underline{c}_\Gamma^\varepsilon(t), \phi_\Gamma)_{H_\Gamma} + a_\Gamma^1(\underline{c}_\Gamma^\varepsilon(t), \phi_\Gamma; t) + a_\Gamma^2(\underline{c}_\Gamma^\varepsilon(t), \phi; t) \\ \leq b_\Gamma(\phi; t, \underline{c}^\varepsilon, \underline{c}_\Gamma^\varepsilon) \quad \text{a.e. } [0, T] \end{aligned} \quad (3.50a)$$

$$\underline{c}_\Gamma^\varepsilon(0) \leq \tilde{c}_{0,\Gamma}. \quad (3.50b)$$

Here b is given by $b(\phi; t, \tilde{c}^\varepsilon, \tilde{c}_\Gamma^\varepsilon, c_{\text{ext}}) = (\tilde{f}(\tilde{c}^\varepsilon(t)), \phi)_H + \varepsilon(\tilde{k}(t)H\tilde{c}_\Gamma^\varepsilon(t), \phi|_{\Gamma^\varepsilon(0)})_{H_\Gamma} + (c_{\text{ext}}(t), \phi|_{\partial\Omega})_{L^2(\partial\Omega)}$. The form of the other terms can be found in Definition 3.3.7.

3.5.2 Theorem (Comparison Principle).

Let $(\bar{c}^\varepsilon, \bar{c}_\Gamma^\varepsilon)$ be a weak upper solution with initial conditions \bar{c}_0 and $\bar{c}_{0,\Gamma}$ and boundary condition \bar{c}_{ext} . Let $(\underline{c}^\varepsilon, \underline{c}_\Gamma^\varepsilon)$ be a weak upper solution with initial conditions \underline{c}_0 and $\underline{c}_{0,\Gamma}$ and boundary condition $\underline{c}_{\text{ext}}$. In the case $i = 2$, assume that $\text{sign}(\tilde{V}^\varepsilon) \leq 0$.

If $\underline{c}_0 \leq \bar{c}_0$ a.e., $\underline{c}_{0,\Gamma} \leq \bar{c}_{0,\Gamma}$ a.e. and $\underline{c}_{\text{ext}} \leq \bar{c}_{\text{ext}}$ a.e., then the inequalities

$$\begin{aligned} \underline{c}^\varepsilon &\leq \bar{c}^\varepsilon \\ \underline{c}_\Gamma^\varepsilon &\leq \bar{c}_\Gamma^\varepsilon \end{aligned}$$

hold almost everywhere in $[0, T] \times \Omega^\varepsilon(0)$ and $[0, T] \times \Gamma^\varepsilon(0)$, resp.

The restriction on $\text{sign}(\tilde{V}^\varepsilon)$ means that in the model case $i = 2$ the solid part is only allowed to grow.

Proof. Define $c := \underline{c}^\varepsilon - \bar{c}^\varepsilon$ as well as $c_\Gamma := \underline{c}_\Gamma^\varepsilon - \bar{c}_\Gamma^\varepsilon$. Subtract equation (3.47a) from (3.49a) and subtract equation (3.48a) from (3.50a). This gives

$$\begin{aligned} \frac{d}{dt}(c(t), \phi)_H + a^1(c(t), \phi; t) + a^2(c(t), \phi; t) + a^3(c(t), \phi; t) \\ \leq b(\phi; t, \underline{c}^\varepsilon, \underline{c}_\Gamma^\varepsilon, \underline{c}_{\text{ext}}) - b(\phi; t, \bar{c}^\varepsilon, \bar{c}_\Gamma^\varepsilon, \bar{c}_{\text{ext}}) \quad \text{a.e. } [0, T] \\ c(0) \leq 0 \end{aligned}$$

as well as

$$\begin{aligned} \frac{d}{dt}(c_\Gamma(t), \phi_\Gamma)_{H_\Gamma} + a_\Gamma^1(c_\Gamma(t), \phi_\Gamma; t) + a_\Gamma^2(c_\Gamma(t), \phi; t) \\ \leq b_\Gamma(\phi; t, \underline{c}^\varepsilon, \underline{c}_\Gamma^\varepsilon) - b_\Gamma(\phi; t, \bar{c}^\varepsilon, \bar{c}_\Gamma^\varepsilon) \quad \text{a.e. } [0, T] \\ c_\Gamma(0) \leq 0. \end{aligned}$$

We choose $\phi = c^+$ as a test function in the first equation and $\phi_\Gamma = \varepsilon c_\Gamma^+$ in the second and integrate from 0 to t . Since the sign and the position of each individual term is important in the following estimate, we use the symbolic notation $A (\leq) B$ to underline that the term A appears on the left hand side of the inequality, whereas B appears on the right. We start by estimating the terms in the bulk equation separately:

$$\int_0^t \frac{d}{dt}(c, c^+)_{H} dt = \int_0^t \frac{d}{dt}(c^+, c^+)_{H} dt = \frac{1}{2} \|c^+(t)\|_H^2 - \frac{1}{2} \|c^+(0)\|_H^2;$$

since $c^+(0) = 0$, this gives $\|c^+(t)\|_H (\leq)$. Next

$$d_0 \|\nabla c^+\|_{L^2(0,t;H)}^2 \leq \int_0^t (DF^{-T} \nabla c^+, F^{-T} \nabla c^+)_H dt = \int_0^t (DF^{-T} \nabla c, F^{-T} \nabla c^+)_H dt$$

and thus $d_0 \|\nabla c^+\|_{L^2(0,t;H)}^2 (\leq)$. We use

$$\begin{aligned} (\leq) \int_0^t |(\nabla c \cdot F^{-1} \tilde{v}^\varepsilon, c^+)_H| dt &= \int_0^t |(\nabla c^+ \cdot F^{-1} \tilde{v}^\varepsilon, c^+)_H| dt \\ &\leq C(\delta) \|c^+\|_{L^2(0,t;H)}^2 + C\varepsilon\delta \|\nabla c^+\|_{L^2(0,t;H)}^2, \end{aligned}$$

see also the proof of Proposition 3.3.23. This yields the estimate $-C\varepsilon\delta \|\nabla c^+\|_{L^2(0,t;H)}^2 (\leq) C(\delta) \|c^+\|_{L^2(0,t;H)}^2$. Moreover

$$\begin{aligned} (\leq) - \int_0^t \varepsilon(\tilde{k}c, c^+)_{H_\Gamma} dt &= - \int_0^t \varepsilon(\tilde{k}c^+, c^+)_{H_\Gamma} dt \leq 0; \\ (\leq) \int_0^t |(\delta_{i1} \tilde{V}^\varepsilon c, c^+)_{H_\Gamma}| dt &= \int_0^t |(\delta_{i1} \tilde{V}^\varepsilon c^+, c^+)_{H_\Gamma}| dt \leq C\varepsilon \|c^+\|_{L^2(0,t;H_\Gamma)}^2 \\ &\leq C \|c^+\|_{L^2(0,t;H)}^2 + C\varepsilon^2 \|\nabla c^+\|_{L^2(0,t;H)}^2, \end{aligned}$$

which gives $-C\varepsilon^2 \|\nabla c^+\|_{L^2(0,t;H)}^2 (\leq) C \|c^+\|_{L^2(0,t;H)}^2$. Next

$$(\leq) \int_0^t |(c, c^+)_{L^2(\partial\Omega)}| dt = \int_0^t |(c^+, c^+)_{L^2(\partial\Omega)}| dt \leq C(\delta) \|c^+\|_{L^2(0,t;H)}^2 + C\delta \|\nabla c^+\|_{L^2(0,t;H)}^2$$

and thus $-C\delta \|\nabla c^+\|_{L^2(0,t;H)}^2 (\leq) C(\delta) \|c^+\|_{L^2(0,t;H)}^2$. For the terms stemming from the right hand side of the bulk equations we obtain

$$\begin{aligned} (\leq) \int_0^t (\tilde{f}(\underline{c}^\varepsilon) - \tilde{f}(\bar{c}^\varepsilon), c^+)_H dt &\leq L \int_0^t (\underline{c}^\varepsilon - \bar{c}^\varepsilon, c^+)_H dt = L \int_0^t (c, c^+)_H dt \\ &= L \int_0^t (c^+, c^+)_H dt = L \|c^+\|_{L^2(0,t;H)}^2 \end{aligned}$$

and

$$(\leq) \int_0^t \underbrace{(c_{\text{ext}} - \bar{c}_{\text{ext}})}_{\leq 0}, c^+)_H dt \leq 0$$

as well as

$$\begin{aligned}
(\leq) & \int_0^t \varepsilon(\tilde{k}H c_\Gamma, c^+)_{H_\Gamma} dt = \int_0^t \varepsilon(\tilde{k}H c_\Gamma^+, c^+)_{H_\Gamma} \underbrace{-\varepsilon(\tilde{k}H c_\Gamma^-, c^+)_{H_\Gamma}}_{\leq 0} dt \\
& \leq \int_0^t \varepsilon(\tilde{k}H c_\Gamma^+, c^+)_{H_\Gamma} dt \leq C\varepsilon \|c_\Gamma^+\|_{L^2(0,t;H_\Gamma)}^2 + C\varepsilon \|c^+\|_{L^2(0,t;H_\Gamma)}^2 \\
& \leq C\varepsilon \|c_\Gamma^+\|_{L^2(0,t;H_\Gamma)}^2 + C \|c^+\|_{L^2(0,t;H)}^2 + C\varepsilon^2 \|\nabla c^+\|_{L^2(0,t;H)}^2.
\end{aligned}$$

This gives $-C\varepsilon^2 \|\nabla c^+\|_{L^2(0,t;H)}^2 (\leq) C\varepsilon \|c_\Gamma^+\|_{L^2(0,t;H_\Gamma)}^2 + C \|c^+\|_{L^2(0,t;H)}^2$.

Now we come to the surface equation:

$$\int_0^t \frac{d}{dt} \varepsilon(c_\Gamma, c_\Gamma^+)_{H_\Gamma} dt = \int_0^t \frac{d}{dt} \varepsilon(c_\Gamma^+, c_\Gamma^+)_{H_\Gamma} dt = \frac{1}{2} \varepsilon \|c_\Gamma^+(t)\|_{H_\Gamma}^2 - \frac{1}{2} \varepsilon \|c_\Gamma^+(0)\|_{H_\Gamma}^2$$

Due to $c_\Gamma^+(0) = 0$ we obtain $\varepsilon \|c_\Gamma^+(t)\|_{H_\Gamma}^2 (\leq) 0$. Next

$$\begin{aligned}
d_0 \varepsilon^3 \|\nabla^\Gamma c_\Gamma^+\|_{L^2(0,t;H_\Gamma)}^2 & \leq \int_0^t \varepsilon^3 (DF_\Gamma^{-T} \nabla^\Gamma c_\Gamma^+, F_\Gamma^{-T} \nabla^\Gamma c_\Gamma^+)_{H_\Gamma} dt \\
& = \int_0^t \varepsilon^3 (DF_\Gamma^{-T} \nabla^\Gamma c, F_\Gamma^{-T} \nabla^\Gamma c_\Gamma^+)_{H_\Gamma} dt
\end{aligned}$$

and thus $d_0 \varepsilon^3 \|\nabla^\Gamma c_\Gamma^+\|_{L^2(0,t;H_\Gamma)}^2 (\leq) 0$. Now

$$\begin{aligned}
(\leq) & \int_0^t \varepsilon |(\operatorname{div}^\Gamma(F_\Gamma^{-1} \tilde{v}_M^\varepsilon) - \tilde{\kappa} \tilde{V}^\varepsilon + \tilde{k}H) c_\Gamma, c_\Gamma^+|_{H_\Gamma} dt \\
& = \int_0^t \varepsilon |(\operatorname{div}^\Gamma(F_\Gamma^{-1} \tilde{v}_M^\varepsilon - \tilde{\kappa} \tilde{V}^\varepsilon + \tilde{k}H) c_\Gamma^+, c_\Gamma^+)|_{H_\Gamma} dt \\
& \leq C\varepsilon \|c_\Gamma^+\|_{L^2(0,t;H_\Gamma)}^2.
\end{aligned}$$

Finally

$$\begin{aligned}
(\leq) & \int_0^t \varepsilon(\tilde{f}_\Gamma(\underline{c}_\Gamma^\varepsilon) - \tilde{f}_\Gamma(\bar{c}_\Gamma^\varepsilon), c_\Gamma^+)_{H_\Gamma} dt \leq L \int_0^t \varepsilon(\underline{c}_\Gamma^\varepsilon - \bar{c}_\Gamma^\varepsilon, c_\Gamma^+)_{H_\Gamma} dt \\
& = L \int_0^t \varepsilon(c_\Gamma, c_\Gamma^+)_{H_\Gamma} dt = L \int_0^t \varepsilon(c_\Gamma^+, c_\Gamma^+)_{H_\Gamma} dt = L \|c_\Gamma^+\|_{L^2(0,t;H_\Gamma)}^2
\end{aligned}$$

as well as

$$\begin{aligned}
& (\leq) \int_0^t \varepsilon(\tilde{k}c, c_\Gamma^+)_{H_\Gamma} - \delta_{i2}(\tilde{V}^\varepsilon c, c_\Gamma^+)_{H_\Gamma} dt \\
& = \int_0^t \varepsilon(\tilde{k}c^+, c_\Gamma^+)_{H_\Gamma} \underbrace{-\varepsilon(\tilde{k}c^-, c_\Gamma^+)_{H_\Gamma}}_{\leq 0} - \delta_{i2}(\tilde{V}^\varepsilon c^+, c_\Gamma^+)_{H_\Gamma} \underbrace{+\delta_{i2}(\tilde{V}^\varepsilon c^-, c_\Gamma^+)_{H_\Gamma}}_{\leq 0} dt \\
& \leq C\varepsilon \|c_\Gamma^+\|_{L^2(0,t;H_\Gamma)} \|c^+\|_{L^2(0,t;H_\Gamma)} \\
& \leq C\varepsilon \|c_\Gamma^+\|_{L^2(0,t;H_\Gamma)}^2 + C \|c^+\|_{L^2(0,t;H)}^2 + C\varepsilon^2 \|\nabla c^+\|_{L^2(0,t;H)}^2
\end{aligned}$$

by the assumption on $\text{sign}(\tilde{V}^\varepsilon)$. Adding up the estimates for the bulk and for the surface equation, we obtain

$$\begin{aligned}
& \|c^+(t)\|_H^2 + \varepsilon \|c_\Gamma^+(t)\|_{H_\Gamma}^2 + (d_0 - C\varepsilon\delta - C\varepsilon^2) \|\nabla c^+\|_{L^2(0,t;H)}^2 + d_0\varepsilon^3 \|\nabla^\Gamma c_\Gamma^+\|_{L^2(0,t;H_\Gamma)}^2 \\
& \leq C \|c^+\|_{L^2(0,t;H)}^2 + C\varepsilon \|c_\Gamma^+\|_{L^2(0,t;H_\Gamma)}^2.
\end{aligned}$$

Choosing δ small enough, we can neglect the terms on the left hand side containing gradients. Then Gronwall's inequality shows that

$$\|c^+(t)\|_H^2 + \varepsilon \|c_\Gamma^+(t)\|_{H_\Gamma}^2 \leq 0,$$

which means that $c^+ = 0$ as well as $c_\Gamma^+ = 0$. This implies $c = \underline{c}^\varepsilon - \bar{c}^\varepsilon \leq 0$, $c_\Gamma = \underline{c}_\Gamma^\varepsilon - \bar{c}_\Gamma^\varepsilon \leq 0$, which is the asserted inequality. \blacklozenge

3.5.2 Positivity of the Solutions

With the help of the comparison principle of Theorem 3.5.2 we can show that – under mild assumptions – the solutions of the evolving surface problem are positive (which is reasonable for concentrations):

3.5.3 Proposition.

Assume that $\tilde{f}(x,0) \geq 0$, $\tilde{f}_\Gamma(x,0) \geq 0$ for all $x \in \Omega$ as well as $\tilde{c}_0 \geq 0$, $\tilde{c}_{0,\Gamma} \geq 0$ and $c_{\text{ext}} \geq 0$. In the model case $i = 2$, assume further that $\text{sign}(\tilde{V}^\varepsilon) \leq 0$. Then the solutions of problems (3.13) and (3.14) are non-negative, i.e.

$$\tilde{c}_\Gamma^\varepsilon \geq 0 \quad \text{as well as} \quad \bar{c}_\Gamma^\varepsilon \geq 0.$$

Proof. By the assumption on the reaction rates, the zero function $(0,0)$ is a weak lower solution for initial values and exterior boundary values zero. The comparison principle now yields the result. \blacklozenge

3.5.3 Boundedness of the Solution

If we are in the model case $i = 1$ and assume that the solid domain is shrinking at all points, we can show that the concentrations are bounded by a constant:

3.5.4 Proposition.

Assume that $i = 1$ and $\text{sign}(\tilde{V}^\varepsilon) \geq 0$. Let there exists a constant $M > 0$ such that $c_{\text{ext}}, \tilde{c}_0, \tilde{c}_{0,\Gamma} \leq M$. Moreover, assume that the reaction rates satisfy the estimate $\tilde{f}(x, u) \leq Au$, $\tilde{f}_\Gamma(x, u) \leq Au$ for a constant $A > 0$ and all $u \geq M$, $x \in \Omega$. Then there exists a constant $M_\infty > 0$ independent of ε such that

$$\tilde{c}^\varepsilon \leq M_\infty \quad \text{as well as} \quad \tilde{c}_\Gamma^\varepsilon \leq M_\infty.$$

Proof. We make the following ansatz for an upper weak solution: Set

$$\bar{c}(t, x) = Me^{\lambda t} \quad \text{and} \quad \bar{c}_\Gamma(t, x) = \frac{1}{H}\bar{c}(t, x).$$

The parameter λ will be determined later. We will insert these functions into the equation (3.47a) and consider the scalar products in the bulk and on the surface separately. Since $\frac{d}{dt}(\bar{c}, \phi)_H = \lambda(\bar{c}, \phi)_H$, $\nabla \bar{c} = 0$ and $-(\tilde{f}(\bar{c}), \phi)_H \geq -(A\bar{c}, \phi)_H$ for positive $\phi \in V$, we obtain from the bulk scalar products the condition

$$\lambda(\bar{c}, \phi)_H - (\tilde{f}(\bar{c}), \phi)_H \geq \lambda(\bar{c}, \phi)_H - (A\bar{c}, \phi)_H \stackrel{!}{\geq} 0 \quad \forall \phi \geq 0$$

which leads to the condition

$$\boxed{\lambda - A \geq 0.} \tag{3.51}$$

Since $\bar{c} - c_{\text{ext}} \geq 0$ we can neglect the contribution from the term $(\bar{c} - c_{\text{ext}}, \phi)_{L^2(\partial\Omega)}$. It remains

$$\varepsilon(\tilde{k}(\bar{c} - H\bar{c}_\Gamma))_{H_\Gamma} + (\delta_{i1}\tilde{V}^\varepsilon\bar{c}, \phi)_{H_\Gamma} = (\delta_{i1}\tilde{V}^\varepsilon\bar{c}, \phi)_{H_\Gamma} \stackrel{!}{\geq} 0 \quad \forall \phi \geq 0.$$

Due to the assumption on $\text{sign}(\tilde{V}^\varepsilon)$ in case $i = 1$, this condition is always satisfied.

We now consider equation (3.48a). We use $\frac{d}{dt}(\bar{c}_\Gamma, \phi_\Gamma)_{H_\Gamma} = \lambda(\bar{c}_\Gamma, \phi_\Gamma)_{H_\Gamma}$, $\nabla^\Gamma \bar{c}_\Gamma = 0$, $\bar{c} - H\bar{c}_\Gamma = 0$ and $-(\tilde{f}_\Gamma(\bar{c}), \phi_\Gamma)_{H_\Gamma} \geq -(A\bar{c}_\Gamma, \phi_\Gamma)_{H_\Gamma}$ to obtain

$$\lambda(\bar{c}_\Gamma, \phi_\Gamma)_{H_\Gamma} + ([\text{div}^\Gamma(F_\Gamma^{-1}\tilde{v}_M^\varepsilon) - \tilde{\kappa}\tilde{V}^\varepsilon]\bar{c}_\Gamma, \phi_\Gamma)_{H_\Gamma} - (A\bar{c}_\Gamma, \phi_\Gamma)_{H_\Gamma} \stackrel{!}{\geq} 0 \quad \forall \phi_\Gamma \geq 0$$

which leads to the condition

$$\boxed{\lambda + \text{div}^\Gamma(F_\Gamma^{-1}\tilde{v}_M^\varepsilon) - \tilde{\kappa}\tilde{V}^\varepsilon - A \geq 0.} \tag{3.52}$$

Choosing λ large enough, one can always satisfy conditions (3.51) and (3.52) independently of the scale parameter. Then $\bar{c} \leq Me^{\lambda T}$ and the comparison principle implies the bound on the solutions. \blacklozenge

4 Periodic Unfolding on Compact Riemannian Manifolds

4.1 Introduction

In this chapter we present an unfolding approach for compact Riemannian manifolds in \mathbb{R}^m . The main idea is to stipulate the existence of a designated atlas \mathcal{A} such that locally the image of a chart is ε -periodic in the usual (\mathbb{R}^n -)sense. By requiring a compatibility condition for the charts, we are able to transfer most of the basic results from the theory of Periodic Unfolding to Riemannian manifolds.

This chapter is organized as follows: In Section 4.2 we introduce the notion of periodicity with respect to a given atlas and present the local unfolding operators. Afterwards we prove results which are well-known for the usual Periodic Unfolding in the context of manifolds. In the next Section 4.3 we show that a spherical zone, i.e. the part of the sphere lying between two parallel planes, fulfills the assumptions on the charts when considering spherical coordinates. Finally, we present the homogenization procedure for an elliptic model problem on a Riemannian manifold. One can think of this as an example of a simple stationary reaction-diffusion or heat equation. This is done in Section 4.4. To show that the new notion of unfolding is compatible with the established one, we consider two multiscale problems in Section 4.5. For the convenience of the reader, we finally collect some results about function spaces on manifolds in Section 4.6, having the character of an appendix.

In applications, we have to restrict ourselves to compact manifolds since we can only define unfolding operators locally, acting on charts. We will then use a partition of unity to "patch" the local results together. Since this partition of unity is finite, no problems arise with the exchange of limit processes. In order to generalize this concept to arbitrary Riemannian manifolds, one would have to introduce and prove some decay-properties of the functions and operators involved.

The reader should have some familiarity with the notion of Periodic Unfolding as it appears in the literature. We refer to Section 3.1.4 and the papers by Cioranescu, Damlamian et. al. [CDG08] as well as [Dam05]. Moreover, basic knowledge of differential geometry is required (for instance to the extend of Amann and Escher [AE01]).

4.2 Unfolding Operators on Riemannian Manifolds

In this section, let $M \subset \mathbb{R}^m$ be a n -dimensional Riemannian manifold (with or without boundary in the sense of Schwarz [Sch95]): We denote an atlas by

$$\mathcal{A} = \{(U_\alpha, \phi_\alpha); \alpha \in I\}$$

with some index set I and the charts $\phi_\alpha : U_\alpha \rightarrow V_\alpha$. Here for $\alpha \in I$, V_α is an open subset (with respect to the relative topology) of $\mathbb{R}_{u_\alpha}^n$, where $\mathbb{R}_{u_\alpha}^n := \{x \in \mathbb{R}^n; \llbracket u_\alpha, x \rrbracket \geq 0\}$ is a halfspace characterized by some vector $u_\alpha \neq 0$, and $\llbracket \cdot, \cdot \rrbracket$ denotes the Euclidean scalar product. The boundary ∂M of M is then given by $\partial M = \{z \in M; \exists \alpha \in I : \llbracket \phi_\alpha(z), u_\alpha \rrbracket = 0\}$. On M , let there be given a smooth Riemannian metric $g_M \in \Gamma(TM^* \otimes TM^*)$ with local representation $\sum_{i,j=1}^n g_{ij} dx^i \otimes dx^j$. Finally, denote by $Y := [0, 1]^n$ (or any other rectangular connected subset of \mathbb{R}^n) the reference cell in \mathbb{R}^n , endowed with the topology of the torus. We consider a fixed sequence $\varepsilon_i \rightarrow 0$ with $\varepsilon_i > 0$, $i \in \mathbb{N}$. As usual in the theory of homogenization, we denote this sequence and its elements by ε . Moreover, we will also use the same letter ε to denote subsequences.

To be able to prove our main results, we require the manifold M and the metric g_M to be at least of class \mathcal{C}^1 . However for a concrete application, the reader should keep in mind that more regularity might be required to be able to define suitable Sobolev-spaces, see Section 4.6.

4.2.1 Periodicity with Respect to Charts

We start with a more or less philosophical definition of periodicity on a manifold. Note that similar ideas appear in the article by Neuss, Neuss-Radu, and Mikić [NNRM06] and the current work of Maria Neuss-Radu.¹

4.2.1 Definition.

We say that an object is $\varepsilon_{\mathcal{A}}$ -periodic, if it is Y -periodic in \mathbb{R}^n after transformation with a chart ϕ from a designated atlas \mathcal{A} .

For example, if we take a smooth εY -periodic function $f : Y \rightarrow \mathbb{R}$ and a $\phi_\alpha \in \mathcal{A}$, then $\tilde{f} := f \circ \phi_\alpha = \phi_\alpha^* f$ is $\varepsilon_{\mathcal{A}}$ -periodic on U_α . One can also think of M itself being $\varepsilon_{\mathcal{A}}$ -periodic, if we image M to represent a material body whose properties (for example heat conductivity etc.) vary in an $\varepsilon_{\mathcal{A}}$ -periodic way. We need the following compatibility condition:

4.2.2 Definition (UC-criterion).

The atlas \mathcal{A} is said to be compatible with unfolding (UC) if for all $\alpha, \beta \in I$ with $U_\alpha \cap U_\beta \neq \emptyset$ and for all ε there exists a $k(\varepsilon) \in \mathbb{Z}^n$ such that

$$\phi_\alpha = \phi_\beta + \varepsilon \sum_{i=1}^n k_i(\varepsilon) e_i \quad \text{in } U_\alpha \cap U_\beta, \quad (4.1)$$

where e_i denotes the i -th unit vector in \mathbb{R}^n .

This definition immediately yields the following lemma by definition of $\{\cdot\}$ (see page 34):

4.2.3 Lemma.

Let ϕ_α and ϕ_β be two charts of an UC-atlas \mathcal{A} with $U_\alpha \cap U_\beta \neq \emptyset$. For all admissible ε and $x \in U_\alpha \cap U_\beta$ it holds

$$\left\{ \begin{array}{c} \phi_\alpha(x) \\ \varepsilon \end{array} \right\} = \left\{ \begin{array}{c} \phi_\beta(x) \\ \varepsilon \end{array} \right\}.$$

¹Private communication, Workshop "Scale transitions in chemistry and biology", Edinburgh 2012.

4.2.4 Lemma.

Let $\phi_\alpha = (x^1, \dots, x^n)$ and $\phi_\beta = (\tilde{x}^1, \dots, \tilde{x}^n)$ be two charts of an UC-atlas \mathcal{A} with $U_\alpha \cap U_\beta \neq \emptyset$. For the tangent vectors, the identity

$$\frac{\partial}{\partial x^i} = \frac{\partial}{\partial \tilde{x}^i}, \quad i = 1, \dots, n$$

holds in $U_\alpha \cap U_\beta$.

Proof. Fix $\varepsilon > 0$. Then there is a $k(\varepsilon) \in \mathbb{Z}^n$ such that $\phi_\alpha = \phi_\beta + K$, where $K = \varepsilon \sum_{i=1}^n k_i(\varepsilon) e_i$. This identity also yields $\phi_\alpha^{-1}(z) = \phi_\beta^{-1}(z - K)$ for $z \in V_\alpha$. Now by the definition of $\frac{\partial}{\partial x^i}$ and the chain rule we obtain for $z = \phi_\alpha(x)$, $x \in U_\alpha \cap U_\beta$ with the help of the tangent map (see page 30)

$$\begin{aligned} \frac{\partial}{\partial x^i}(x) &= T_{\phi_\alpha(x)}(\phi_\alpha^{-1})(e_i) \\ &= T_z(\phi_\alpha^{-1})(e_i) = T_{z-K}(\phi_\beta^{-1})(e_i) \\ &= T_{\phi_\beta(x)}(\phi_\beta^{-1})_{\phi_\beta(x)}(e_i) = \frac{\partial}{\partial \tilde{x}^i}(x), \end{aligned}$$

since $z - K = \phi_\beta(x)$. ◆

If M satisfies the UC-criterion, then by Lemma 4.2.4 there exist n smooth vector fields $X_i = \frac{\partial}{\partial x^i}$, $i = 1, \dots, n$ such that $(X_1(x), \dots, X_n(x))$ constitutes a basis for $T_x M$ for all $x \in M$. This means that the manifold M is necessarily parallelizable. Moreover, if we denote by $[\cdot, \cdot]$ the Lie bracket then we obtain $[X_i, X_j] = 0$ for all $i, j \in \{1, \dots, n\}$ (since the coefficients of the X_i 's are constant). It is an open question whether these conditions are also sufficient.²

4.2.2 Unfolding on Charts

We can now define local unfolding operators for functions, vector fields and forms. Note that the usual unfolding operator \mathcal{T}^ε on \mathbb{R}^n maps objects defined on a set Ω to objects defined on $\Omega \times Y$. Translated to the language of manifolds, an object defined on M should be mapped to an object defined on the product manifold $M \times Y$ (which is indeed a manifold with boundary since Y has empty boundary, see e.g. Amann, Escher [AE01]).

4.2.5 Definition.

Choose a chart $\phi \in \mathcal{A}$ with corresponding domain $U \subset M$.

1. For a function $f : U \rightarrow \mathbb{R}$ we define

$$\mathcal{T}_\phi^\varepsilon(f) = (\phi \times \text{Id})^* \mathcal{T}^\varepsilon(\phi_* f), \quad (4.2)$$

where \mathcal{T}^ε denotes the usual unfolding operator in \mathbb{R}^n . Obviously $\mathcal{T}_{\text{Id}}^\varepsilon = \mathcal{T}^\varepsilon$.

²In this case, at least locally the existence of a chart, having the given vector fields as local basis vectors is ensured, see e.g. Michor [Mic08], Theorem 3.17.

2. For a vector field $F \in \mathfrak{X}(U)$ define analogously

$$\mathcal{T}_\phi^\varepsilon(F) = (\phi \times \text{Id})^* \mathcal{T}^\varepsilon(\phi_* F). \quad (4.3)$$

3. For a k -form $\eta \in \Omega_k(U)$ with $\eta = \sum_{(j)} a_{(j)} dx^{(j)}$ set

$$\mathcal{T}_\phi^\varepsilon(\eta) = \sum_{(j)} \mathcal{T}_\phi^\varepsilon(a_{(j)}) dy^{(j)}, \quad (4.4)$$

where the forms $dy^{(j)}$ stem from the trivial chart Id for Y .

Here $\mathfrak{X}(U)$ denotes the set of smooth vector fields on U , and for η we use the representation

$$\eta = \sum_{(j)} a_{(j)} dx^{(j)} := \sum_{(j) \in \mathbb{J}_k} a_{(j)} dx^{(j)},$$

where $\mathbb{J}_k = \{(j) = (j_1, \dots, j_k) \in \mathbb{N}^k; 1 \leq j_1 < \dots < j_k \leq n\}$ as well as $dx^{(j)} = dx^{j_1} \wedge \dots \wedge dx^{j_k}$. The $a_{(j)}$'s are the scalar coefficients of the k -forms $dx^{(j)}$ constituting a basis of $\Omega^k(U)$. (See also Section 4.6.6.)

4.2.6 Remark.

Note that we have the following implications (see also the next lemma):

1. $f : U \rightarrow \mathbb{R} \implies \mathcal{T}_\phi^\varepsilon(f) : U \times Y \rightarrow \mathbb{R}$
2. $F \in \mathfrak{X}(U) \implies \mathcal{T}_\phi^\varepsilon(F) \in \mathfrak{X}(Y)^U$
3. $\eta \in \Omega_k(U) \implies \mathcal{T}_\phi^\varepsilon(\eta) \in \Omega_k(Y)^U$

4.2.7 Remark.

For a scalar function $f : U \rightarrow \mathbb{R}$ we obtain the following explicit form for $\mathcal{T}_\phi^\varepsilon(f)$:

$$\mathcal{T}_\phi^\varepsilon(f)(x, y) = f\left(\phi^{-1}\left(\varepsilon \left[\frac{\phi(x)}{\varepsilon} \right] + \varepsilon y\right)\right).$$

The following lemma shows that the definition of $\mathcal{T}_\phi^\varepsilon(F)$ and $\mathcal{T}_\phi^\varepsilon(\eta)$ is compatible:

4.2.8 Lemma.

Let $F = \sum_{i=1}^n F^i \frac{\partial}{\partial x^i} \in \mathfrak{X}(U)$ be a vector field with coefficients $F^i : U \rightarrow \mathbb{R}$, $i = 1, \dots, n$. Then

$$\mathcal{T}_\phi^\varepsilon(F) = \sum_{i=1}^n \mathcal{T}_\phi^\varepsilon(F^i) \frac{\partial}{\partial y^i},$$

where $\frac{\partial}{\partial y^i}$ is the tangent vector with respect to the trivial chart Id of Y .

Proof. The pushforward $\phi_* \frac{\partial}{\partial x^i}$ of $\frac{\partial}{\partial x^i}$ is equal to e_i . Thus

$$\begin{aligned} \mathcal{T}_\phi^\varepsilon(F) &= (\phi \times \text{Id})^* \mathcal{T}^\varepsilon(\phi_* F) \\ &= (\phi \times \text{Id})^* \mathcal{T}^\varepsilon\left(\sum_{i=1}^n (F^i \circ \phi^{-1}) \cdot e_i\right) \end{aligned}$$

$$\begin{aligned}
&= \sum_{i=1}^n (\phi \times \text{Id})^* \mathcal{T}^\varepsilon(\phi_* F^i) \frac{\partial}{\partial y^i} \\
&= \sum_{i=1}^n \mathcal{T}_\phi^\varepsilon(F^i) \frac{\partial}{\partial y^i},
\end{aligned}$$

since $e_i = \text{Id}_*(\frac{\partial}{\partial y^i})$. ◆

4.2.3 Properties of the Unfolding Operator

4.2.9 Lemma.

Choose a chart $\phi \in \mathcal{A}$ with corresponding domain $U \subset M$. Let $f, g : U \rightarrow \mathbb{R}$ be two functions. The unfolding operator $\mathcal{T}_\phi^\varepsilon$ respects summation and multiplication, i.e. it holds

$$\mathcal{T}_\phi^\varepsilon(f + g) = \mathcal{T}_\phi^\varepsilon(f) + \mathcal{T}_\phi^\varepsilon(g) \quad \text{and} \quad \mathcal{T}_\phi^\varepsilon(f \cdot g) = \mathcal{T}_\phi^\varepsilon(f) \cdot \mathcal{T}_\phi^\varepsilon(g)$$

We give a proof which is slightly too general, in order to facilitate generalizations:

Proof. For the sum, note that pushforwards, pullbacks and \mathcal{T}^ε are linear operators. The multiplication of two scalar functions can be expressed by the wedge product due to $f \cdot g = f \wedge g$. Since pullbacks and pushforwards commute with \wedge , we obtain

$$\begin{aligned}
\mathcal{T}_\phi^\varepsilon(f \cdot g) &= (\phi \times \text{Id})^* \mathcal{T}^\varepsilon(\phi_*(f \wedge g)) \\
&= (\phi \times \text{Id})^* \mathcal{T}^\varepsilon(\phi_* f \wedge \phi_* g) = (\phi \times \text{Id})^* \mathcal{T}^\varepsilon(\phi_* f \cdot \phi_* g) \\
&= (\phi \times \text{Id})^* [\mathcal{T}^\varepsilon(\phi_* f) \wedge \mathcal{T}^\varepsilon(\phi_* g)] \\
&= (\phi \times \text{Id})^* \mathcal{T}^\varepsilon(\phi_* f) \wedge (\phi \times \text{Id})^* \mathcal{T}^\varepsilon(\phi_* g) \\
&= \mathcal{T}_\phi^\varepsilon(f) \cdot \mathcal{T}_\phi^\varepsilon(g)
\end{aligned}$$
◆

4.2.10 Corollary.

For a scalar function $f : U \rightarrow \mathbb{R}$ and a matrix-valued function $A : U \rightarrow \mathbb{R}^{n \times n}$ with $A = (a_{ij})$, we obtain for $k, p \in \mathbb{N}$

1. $\mathcal{T}_\phi^\varepsilon(f^{\frac{k}{p}}) = \mathcal{T}_\phi^\varepsilon(f)^{\frac{k}{p}}$
2. $\mathcal{T}_\phi^\varepsilon(\sqrt{f}) = \sqrt{\mathcal{T}_\phi^\varepsilon(f)}$
3. $\mathcal{T}_\phi^\varepsilon(\det A) = \det \mathcal{T}_\phi^\varepsilon(A)$, where $\mathcal{T}_\phi^\varepsilon$ is applied to the entries of A .
4. $\mathcal{T}_\phi^\varepsilon(|f|) = |\mathcal{T}_\phi^\varepsilon(f)|$

Proof. For the first identity, note that by the preceding lemma we have

$$\mathcal{T}_\phi^\varepsilon(f^{\frac{k}{p}})^p = \mathcal{T}_\phi^\varepsilon(f^k) = \mathcal{T}_\phi^\varepsilon(f)^k.$$

Now taking the p -th root on both sides gives the result. For the second result choose $k = 1, p = 2$, whereas for the third note that the determinant is a polynomial in the entries of A , thus Lemma 4.2.9 applies as well. For the last statement use the identity $|f| = \sqrt{f^2}$ and the second assertion of this corollary. ◆

The following lemma shows that some sort of "calculation" with the charts is possible.

4.2.11 Lemma.

Let $\phi_1, \phi_2 : U \rightarrow \mathbb{R}^n$ be two charts defined on a common open set $U \subset M$ and fix $\varepsilon > 0$. Then the equivalence

$$\mathcal{T}_{\phi_1}^\varepsilon = \mathcal{T}_{\phi_2}^\varepsilon \iff \mathcal{T}_{\phi_2 \circ \phi_1^{-1}}^\varepsilon = \mathcal{T}_{\text{Id}}^\varepsilon$$

holds for the scalar unfolding operators.

Note that in this assertion we do not give exact function spaces on which an identity like $\mathcal{T}_{\phi_1}^\varepsilon = \mathcal{T}_{\phi_2}^\varepsilon$ is supposed to hold. In the proof we are going to use arbitrarily smooth functions, such that by using density results, if necessary, the asserted equalities hold on a wide range of function spaces like $\mathcal{C}^\infty(M)$, $\mathcal{C}(M)$ or $L^2(M)$.

Proof. Choose a $f : U \rightarrow \mathbb{R}$ (and note the remarks at the beginning of this paragraph). We have that

$$\begin{aligned} \mathcal{T}_{\phi_1}^\varepsilon(f) = \mathcal{T}_{\phi_2}^\varepsilon(f) &\Leftrightarrow \mathcal{T}^\varepsilon((\phi_1)_*f) \circ (\phi_1 \times \text{Id}) = \mathcal{T}^\varepsilon((\phi_2)_*f) \circ (\phi_2 \times \text{Id}) \\ &\Leftrightarrow \mathcal{T}^\varepsilon((\phi_1)_*f) = \mathcal{T}^\varepsilon((\phi_2)_*f) \circ (\phi_2 \circ \phi_1^{-1} \times \text{Id}) \\ &\Leftrightarrow (\phi_2 \circ \phi_1^{-1} \times \text{Id})^* \mathcal{T}^\varepsilon((\phi_2)_*f) = \mathcal{T}^\varepsilon((\phi_1)_*f) \end{aligned}$$

which upon choosing a function g via $f = g \circ \phi_1$ yields

$$\begin{aligned} &\Leftrightarrow (\phi_2 \circ \phi_1^{-1} \times \text{Id})^* \mathcal{T}^\varepsilon(\underbrace{g \circ \phi_1 \circ \phi_2^{-1}}_{=g \circ (\phi_2 \circ \phi_1^{-1})^{-1}}) = \mathcal{T}^\varepsilon(g) \\ &\Leftrightarrow (\phi_2 \circ \phi_1^{-1} \times \text{Id})^* \mathcal{T}^\varepsilon((\phi_2 \circ \phi_1^{-1})_*g) = \mathcal{T}^\varepsilon(g) \\ &\Leftrightarrow \mathcal{T}_{\phi_2 \circ \phi_1^{-1}}^\varepsilon(g) = \mathcal{T}_{\text{Id}}^\varepsilon(g). \end{aligned}$$

Since f and g are arbitrary, the result follows. ◆

We conclude this section with a result which shows that the unfolding operators are well defined on sets where two charts overlap. Later, we will use this result to define a global unfolding operator on the whole manifold M .

4.2.12 Proposition.

Let ϕ_α and ϕ_β be two charts of an UC-atlas \mathcal{A} with $U_\alpha \cap U_\beta \neq \emptyset$. Then

$$\mathcal{T}_{\phi_\alpha}^\varepsilon = \mathcal{T}_{\phi_\beta}^\varepsilon \quad \text{on } U_\alpha \cap U_\beta$$

Proof. We first show the result for the scalar unfolding operator. Thus let $f : U_\alpha \cap U_\beta \rightarrow \mathbb{R}$ be a scalar function. Since \mathcal{A} is a UC-atlas, we have (compare Lemma 4.2.4) $\phi_\alpha = \phi_\beta + \varepsilon K(\varepsilon)$, where $K(\varepsilon) = \sum_{i=1}^n k_i(\varepsilon) e_i$ with $k(\varepsilon) \in \mathbb{Z}^n$. Then $\phi_\alpha^{-1}(z) = \phi_\beta^{-1}(z - \varepsilon K(\varepsilon))$ and

$$\begin{aligned} \mathcal{T}_{\phi_\alpha}^\varepsilon(f)(x, y) &= f(\phi_\alpha^{-1}(\varepsilon \left[\frac{\phi_\alpha(x)}{\varepsilon} \right] + \varepsilon y)) \\ &= f(\phi_\beta^{-1}(\varepsilon \left[\frac{\phi_\alpha(x)}{\varepsilon} \right] + \varepsilon y - \varepsilon K(\varepsilon))) \end{aligned}$$

$$\begin{aligned}
&= f(\phi_\beta^{-1}(\varepsilon \underbrace{\left[\frac{\phi_\beta(x) + \varepsilon K(\varepsilon)}{\varepsilon} \right]}_{= \left[\frac{\phi_\beta(x)}{\varepsilon} \right] + K(\varepsilon)} + \varepsilon y - \varepsilon K(\varepsilon))) \\
&= f(\phi_\beta^{-1}(\varepsilon \left[\frac{\phi_\beta(x)}{\varepsilon} \right] + \varepsilon y)) = \mathcal{T}_{\phi_\beta}^\varepsilon(f)(x, y).
\end{aligned}$$

This shows the result for the first operator from Definition 4.2.5. Since the correspondence $\frac{\partial}{\partial x^i} \sim \frac{\partial}{\partial y^i}$ and $dx^i \sim dy^i$ is unique due to Lemma 4.2.4, the result follows for the other operators as well (cf. also Lemma 4.2.8). \blacklozenge

4.2.4 Unfolding and Derivatives

Exterior Derivatives of Forms

Let d be the exterior derivative on M and let d_y be the exterior derivative in Y . Similar to the equality $\varepsilon \mathcal{T}^\varepsilon(\nabla f) = \nabla_y \mathcal{T}^\varepsilon(f)$ for the unfolding of functions $f : \mathbb{R}^n \rightarrow \mathbb{R}$ we obtain:³

4.2.13 Proposition.

Let $\phi : U \rightarrow \mathbb{R}^n$ be a chart, let $\eta \in \Omega_k(U)$. Then

$$\varepsilon \mathcal{T}_\phi^\varepsilon(d\eta) = d_y \mathcal{T}_\phi^\varepsilon(\eta). \quad (4.5)$$

Proof. Let $f \in \Omega_0(U)$ be a scalar function. Then $df = \sum_{i=1}^n \frac{\partial f}{\partial x^i} dx^i$. Due to the construction of $\varepsilon \mathcal{T}_\phi^\varepsilon(df)$, we have to consider the term $\varepsilon \mathcal{T}_\phi^\varepsilon(\frac{\partial f}{\partial x^i})$ first. Since for the unfolding operator on \mathbb{R}^n we have $\varepsilon \mathcal{T}^\varepsilon(\frac{\partial}{\partial x^i} \cdot) = \frac{\partial \mathcal{T}^\varepsilon(\cdot)}{\partial y^i}$, we obtain

$$\varepsilon \mathcal{T}_\phi^\varepsilon(\frac{\partial f}{\partial x^i}) = \varepsilon(\phi \times \text{Id})^* \mathcal{T}^\varepsilon(\phi_* \frac{\partial f}{\partial x^i}) \quad (4.6a)$$

$$= \varepsilon(\phi \times \text{Id})^* \mathcal{T}^\varepsilon(\frac{\partial(\phi_* f)}{\partial x^i}) \quad (4.6b)$$

$$= (\phi \times \text{Id})^* \frac{\partial(\mathcal{T}^\varepsilon(\phi_* f))}{\partial y^i} \quad (4.6c)$$

$$= \frac{\partial \mathcal{T}_\phi^\varepsilon(f)}{\partial y^i}. \quad (4.6d)$$

Thus

$$\varepsilon \mathcal{T}_\phi^\varepsilon(df) = \varepsilon \sum_{i=1}^n \mathcal{T}_\phi^\varepsilon(\frac{\partial f}{\partial x^i}) dy^i = \sum_{i=1}^n \frac{\partial \mathcal{T}_\phi^\varepsilon(f)}{\partial y^i} dy^i = d_y \mathcal{T}_\phi^\varepsilon(f).$$

³Note that the exterior derivative is the "natural" notion of derivation on a manifold. This can also be seen by comparing the identity (4.5) with (4.7): While the former can be obtained directly, the latter involves more objects and auxiliary constructions for its proof.

Now let $\eta \in \Omega_k(U)$. The form η has a representation

$$\eta = \sum_{(j)} a_{(j)} dx^{(j)}$$

with scalar functions $a_{(j)}$, see page 94. Now by the preceding part of the proof

$$\begin{aligned} \varepsilon \mathcal{T}_\phi^\varepsilon(d\eta) &= \varepsilon \sum_{(j)} \mathcal{T}_\phi^\varepsilon(da_{(j)}) \wedge dy^{(j)} \\ &= \sum_{(j)} d_y \mathcal{T}_\phi^\varepsilon(a_{(j)}) \wedge dy^{(j)} = d_y \mathcal{T}_\phi^\varepsilon(\eta). \end{aligned} \quad \blacklozenge$$

Gradients

We now investigate the unfolding of gradients. For this, we have to take care of the Riemannian metric $g_M \in \Gamma(TM^* \otimes TM^*)$ in the following way:

4.2.14 Definition.

Let $\phi : U \rightarrow \mathbb{R}^n$ be a chart, $U \subset M$. For fixed $x \in U$, $\varepsilon > 0$ associate to the Riemannian metric g_M on U a (x, ε) -dependent metric $g_Y^{(x, \varepsilon)}$ on Y via $g_Y^{(x, \varepsilon)}(x, \cdot) = \mathcal{T}_\phi^\varepsilon(g_M)(x, \cdot)$ in the sense that

$$\mathcal{T}_\phi^\varepsilon(g_M) = \mathcal{T}_\phi^\varepsilon\left(\sum_{i,j} g_{ij} dx^i \otimes dx^j\right) = \sum_{i,j} \mathcal{T}_\phi^\varepsilon(g_{ij}) dy^i \otimes dy^j.$$

$\mathcal{T}_\phi^\varepsilon(g_M)$ is indeed a Riemannian metric: For $x \in U$, the matrix $G(x) = [g_{ij}(x)]_{i,j=1,\dots,n}$ consisting of the metric coefficients g_{ij} at x is symmetric, invertible and positive definite. Since this is a pointwise property, the same holds true for the matrix $\mathcal{T}_\phi^\varepsilon(G)(x, y)$ containing the unfolded metric coefficients $\mathcal{T}_\phi^\varepsilon(g_{ij})(x, y)$, where $x \in M$ and $y \in Y$. Thus the expression $\sum_{i,j} \mathcal{T}_\phi^\varepsilon(g_{ij})(x, \cdot) dy^i \otimes dy^j$ defines (at least locally) a Riemannian metric on Y . Since the atlas for Y consists only of the trivial chart Id , this metric is well-defined on the whole reference cell.

Finally, by taking into account the exact form of the unfolded coefficients $\mathcal{T}_\phi^\varepsilon(g_{ij})(x, y) = g_{ij}(\phi^{-1}(\varepsilon \left[\frac{\phi(x)}{\varepsilon} \right] + \varepsilon y))$, one sees that for x and ε treated as parameters the metric $g_Y^{(x, \varepsilon)}(y)$ is smooth in y .

The following proposition shows that the unfolding operator is compatible with respect to the metrics defined above:

4.2.15 Proposition.

Let $\phi : U \rightarrow \mathbb{R}^n$ be a chart, and let $F, G \in \mathfrak{X}(U)$. Then

$$\mathcal{T}_\phi^\varepsilon(g_M(F, G))(x, y) = g_Y^{(x, \varepsilon)}(\mathcal{T}_\phi^\varepsilon(F)(x, y), \mathcal{T}_\phi^\varepsilon(G)(x, y)).$$

This result generalizes the relation $\mathcal{T}^\varepsilon(\llbracket F, G \rrbracket) = \llbracket \mathcal{T}^\varepsilon(F), \mathcal{T}^\varepsilon(G) \rrbracket$, where F and G are vector fields in \mathbb{R}^n , and $\llbracket \cdot, \cdot \rrbracket$ is the usual Euclidean scalar product.

Proof. We prove the assertion in local coordinates: Let $F = \sum_i F^i \frac{\partial}{\partial x^i}$ and $G = \sum_i G^i \frac{\partial}{\partial x^i}$ be two vector fields. Then $g_M(F, G) = \sum_{i,j} g_{ij} F^i G^j$ and thus by the properties of $\mathcal{T}_\phi^\varepsilon$ we obtain

$$\mathcal{T}_\phi^\varepsilon(g_M(F, G)) = \sum_{i,j} \mathcal{T}_\phi^\varepsilon(g_{ij}) \mathcal{T}_\phi^\varepsilon(F^i) \mathcal{T}_\phi^\varepsilon(G^j) = g_Y^{(x,\varepsilon)}(\mathcal{T}_\phi^\varepsilon(F), \mathcal{T}_\phi^\varepsilon(G))$$

since $\mathcal{T}_\phi^\varepsilon(F) = \sum_i \mathcal{T}_\phi^\varepsilon(F^i) \frac{\partial}{\partial y^i}$. ◆

Note that since smooth functions are dense in L^2TU and the unfolding operator is continuous acting on vector fields in L^2 (see Corollary 4.2.25 below), the same result also holds true for L^2 -vector fields.

In the sequel, we denote the gradient on M with respect to g_M by ∇_M , and the gradient on Y with respect to $g_Y^{(x,\varepsilon)}$ by $\nabla_Y^{(x,\varepsilon)}$. We obtain the following result for the unfolding of gradients:

4.2.16 Proposition.

Let $\phi : U \rightarrow \mathbb{R}^n$ be a chart, and let $f : U \rightarrow \mathbb{R}^n$ be a differentiable function. Then the identity

$$\varepsilon \mathcal{T}_\phi^\varepsilon(\nabla_M f)(x, y) = \nabla_Y^{(x,\varepsilon)} \mathcal{T}_\phi^\varepsilon(f)(x, y) \quad (4.7)$$

holds.

Proof. Again, we use local coordinates: We have that $\nabla_M f = \sum_{i,j} g^{ij} \frac{\partial f}{\partial x^i} \frac{\partial}{\partial x^j}$, where $G^{-1} := [g^{ij}]_{i,j=1,\dots,n}$ is the inverse of $G := [g_{ij}]_{i,j=1,\dots,n}$. Keeping in mind the construction of g^{ij} via the matrix of cofactors, $g^{ij} = \det(G)^{-1} \cdot (-1)^{i+j} \det G'_{ji}$ (where $\det G'_{ji}$ denotes the (j, i) -th minor of G), one can apply the rules from Corollary 4.2.10 to obtain $\mathcal{T}_\phi^\varepsilon([g^{ij}]) = \mathcal{T}_\phi^\varepsilon([g_{ij}]^{-1}) = \mathcal{T}_\phi^\varepsilon([g_{ij}])^{-1}$. Now we obtain

$$\begin{aligned} \varepsilon \mathcal{T}_\phi^\varepsilon(\nabla_M f)(x, y) &= \varepsilon [(\phi \times \text{Id})^* \mathcal{T}^\varepsilon(\sum_{i,j} g^{ij} \circ \phi^{-1} \frac{\partial(f \circ \phi^{-1})}{\partial x^i} e_j)](x, y) \\ &= [(\phi \times \text{Id})^* \sum_{i,j} \mathcal{T}^\varepsilon(g^{ij} \circ \phi^{-1}) \frac{\partial \mathcal{T}^\varepsilon(f \circ \phi^{-1})}{\partial y^i} e_j](x, y) \\ &= \sum_{i,j} \mathcal{T}_\phi^\varepsilon(g^{ij})(x, y) \frac{\partial \mathcal{T}_\phi^\varepsilon(f)}{\partial y^i}(x, y) \frac{\partial}{\partial y^j} = \nabla_Y^{(x,\varepsilon)} \mathcal{T}_\phi^\varepsilon(f), \end{aligned}$$

where we used the considerations for $\mathcal{T}_\phi^\varepsilon(G^{-1})$ in the last equality. ◆

Again, the same results hold for weakly differentiable vector fields due to density. In the same manner one obtains:

4.2.17 Lemma.

Let $\phi : U \rightarrow \mathbb{R}^n$ be a chart, and let $F \in \mathfrak{X}(U)$ be a vector field. Then

$$\varepsilon \mathcal{T}_\phi^\varepsilon(\text{div}_M F)(x, y) = \text{div}_Y^{(x,\varepsilon)} \mathcal{T}_\phi^\varepsilon(F)(x, y).$$

Proof. In local coordinates, we have for $F = \sum_i F^i \frac{\partial}{\partial x^i}$

$$\begin{aligned} \varepsilon \mathcal{T}_\phi^\varepsilon(\operatorname{div}_M F)(x, y) &= \varepsilon \mathcal{T}_\phi^\varepsilon \left[\frac{1}{\sqrt{|G|}} \sum_i \frac{\partial(\sqrt{|G|} F^i)}{\partial x^i} \right] \\ &= \frac{1}{\sqrt{|\mathcal{T}_\phi^\varepsilon(G)|}} \sum_i \frac{\partial(\sqrt{|\mathcal{T}_\phi^\varepsilon(G)|} \mathcal{T}_\phi^\varepsilon(F^i))}{\partial y^i} \\ &= \operatorname{div}_Y^{(x, \varepsilon)} \mathcal{T}_\phi^\varepsilon(F) \end{aligned}$$

due to the identity (4.6). ◆

We conclude this section by showing that the Riesz isomorphisms are compatible with unfolding as well:

4.2.18 Proposition.

Let $\phi : U \rightarrow \mathbb{R}^n$ be a chart. We consider the Riesz isomorphisms

$$\begin{aligned} \Theta_M : \mathfrak{X}(U) &\longrightarrow \Omega^1(U) \quad \text{and} \\ \Theta_Y^{(x, \varepsilon)} : \mathfrak{X}(Y) &\longrightarrow \Omega^1(Y) \end{aligned}$$

belonging to g_M and $g_Y^{(x, \varepsilon)}$, where x and ε are treated as parameters. For the unfolding operators acting on vector fields and on forms, the identity

$$\mathcal{T}_\phi^\varepsilon \circ \Theta_M(\cdot)(x, y) = \Theta_Y^{(x, \varepsilon)} \circ \mathcal{T}_\phi^\varepsilon(\cdot)(x, y)$$

holds.

Proof. Let $F \in \mathfrak{X}(U)$ with local representation $F = \sum_i F^i \frac{\partial}{\partial x^i}$. Then $\Theta_M F = \sum_{i,j} g_{ij} F^i dx^j$ and thus

$$\begin{aligned} \mathcal{T}_\phi^\varepsilon(\Theta_M F)(x, y) &= \left[\sum_{i,j} \mathcal{T}_\phi^\varepsilon(g_{ij}) \mathcal{T}_\phi^\varepsilon(F^i) dy^j \right](x, y) \\ &= \Theta_Y^{(x, \varepsilon)} \circ \mathcal{T}_\phi^\varepsilon(F)(x, y). \end{aligned} \quad \blacklozenge$$

4.2.19 Corollary.

Similarly we obtain

$$\mathcal{T}_\phi^\varepsilon \circ \Theta_M^{-1}(\cdot)(x, y) = (\Theta_Y^{(x, \varepsilon)})^{-1} \circ \mathcal{T}_\phi^\varepsilon(\cdot)(x, y).$$

Proof. Let $\eta \in \Omega_1(U)$, then

$$\mathcal{T}_\phi^\varepsilon(\eta)(x, y) = \mathcal{T}_\phi^\varepsilon(\Theta_M(\Theta_M^{-1}\eta))(x, y) = \Theta_Y^{(x, \varepsilon)} \mathcal{T}_\phi^\varepsilon(\Theta_M^{-1}\eta).$$

Now apply $(\Theta_Y^{(x, \varepsilon)})^{-1}$ on both sides. ◆

4.2.5 Integral Identities

We now consider a n -dimensional compact Riemannian manifold $M \subset \mathbb{R}^m$ with Riemannian metric g_M and UC-compatible atlas $\mathcal{A} = \{(U_\alpha, \phi_\alpha); \alpha \in I\}$. Since the manifold is compact, the index set I can be chosen as finite. Moreover, we denote by $\{\pi_\alpha; \alpha \in I\}$ a smooth (finite) partition of unity subordinate to the covering $\{U_\alpha\}$. All the other prerequisites of the previous section remain valid.

We start by defining a global unfolding operator:

4.2.20 Definition.

The global unfolding operator $\mathcal{T}_{\mathcal{A}}^\varepsilon$ with respect to the atlas \mathcal{A} is defined as

$$\mathcal{T}_{\mathcal{A}}^\varepsilon(\cdot)(x, y) = \mathcal{T}_{\phi_\alpha}^\varepsilon(\cdot)(x, y) \quad \text{for } x \in U_\alpha.$$

Due to the compatibility result in Proposition 4.2.12, an equivalent definition is given by

$$\mathcal{T}_{\mathcal{A}}^\varepsilon(\cdot) = \sum_{\alpha \in I} \pi_\alpha \mathcal{T}_{\phi_\alpha}^\varepsilon(\cdot|_{U_\alpha}).$$

4.2.21 Lemma.

Let $f \in \mathcal{C}(\bar{M})$, then

$$\mathcal{T}_{\phi_\alpha}^\varepsilon(f|_{U_\alpha}) \longrightarrow f|_{U_\alpha} \quad \text{in } L^\infty(U_\alpha \times Y).$$

Proof. An analogous result holds true for the usual unfolding operator \mathcal{T}^ε (see e.g. the works cited in Section 3.1.4). Due to the continuity of the charts and of the function f , we obtain

$$\mathcal{T}^\varepsilon((\phi_\alpha)_* f|_{U_\alpha}) \longrightarrow (\phi_\alpha)_* f|_{U_\alpha} \quad \text{in } L^\infty(V_\alpha \times Y).$$

By application of the continuous function $(\phi_\alpha \times \text{Id})^*$ on both sides we obtain the result. \blacklozenge

Since $\text{supp } \pi_\alpha \subset\subset U_\alpha$ holds for the partition of unity and I is finite, there exists a $\delta^* > 0$, where $\delta^* := \min_{\alpha \in I} \text{dist}[\text{supp}((\phi_\alpha)_* \pi_\alpha), \partial V_\alpha]$. In the sequel we will always assume $\varepsilon < \delta^*$. In integral and norm expressions we will additionally use the two manifolds $M \times Y$ and $M \times Y^{(x, \varepsilon)}$; here $M \times Y$ is endowed with the volume form $\text{dvol}_M \, dy = \sqrt{|G|} \, dx \, dy$, whereas for $M \times Y^{(x, \varepsilon)}$ we use the volume form $\mathcal{T}_{\mathcal{A}}^\varepsilon(\sqrt{|G|}) \, dx \, dy$. Note that since we are dealing with compact manifolds, all volume-forms generate norms which are mutually equivalent! Similar to Lemma 4.4.7 one can show that the constant of equivalence can be chosen independent of the parameters x and ε .

In order to motivate the next definition, we start with the following observation: Assume $f \in L^1(M)$. The next proposition shows that the estimate $\|\mathcal{T}_{\mathcal{A}}^\varepsilon(f)\|_{L^1(M \times Y)} < \infty$ holds. Due to $\varepsilon < \delta^*$, we have that $\text{supp}(\mathcal{T}_{\phi_\alpha}^\varepsilon(\pi_\alpha)) \subset \phi_\alpha(U_\alpha) \times Y$ and thus

$$\int_M f \, \text{dvol}_M = \sum_{\alpha \in I} \int_{\phi_\alpha(U_\alpha)} (\phi_\alpha)_*(\pi_\alpha) (\phi_\alpha)_* f (\phi_\alpha)_* \sqrt{|G|} \, dx \quad (4.8a)$$

$$= \sum_{\alpha \in I} \frac{1}{|Y|} \int_{\phi_\alpha(U_\alpha) \times Y} \mathcal{T}^\varepsilon((\phi_\alpha)_*(\pi_\alpha)) \mathcal{T}^\varepsilon((\phi_\alpha)_* f) \mathcal{T}^\varepsilon((\phi_\alpha)_* \sqrt{|G|}) \, dy \, dx \quad (4.8b)$$

$$= \sum_{\alpha \in I} \int_{U_\alpha \times Y} \mathcal{T}_{\phi_\alpha}^\varepsilon(\pi_\alpha) \mathcal{T}_{\phi_\alpha}^\varepsilon(f) \overline{\mathcal{T}_{\phi_\alpha}^\varepsilon(\sqrt{|G|})} \, dy \, dx. \quad (4.8c)$$

We obtain the estimate

$$\begin{aligned} & \left| \int_M f \, d\text{vol}_M - \frac{1}{|Y|} \int_{M \times Y} \mathcal{T}_{\mathcal{A}}^\varepsilon(f) \mathcal{T}_{\mathcal{A}}^\varepsilon(\sqrt{|G|}) \, dy \, dx \right| \\ &= \left| \int_M f \, d\text{vol}_M - \frac{1}{|Y|} \sum_{\alpha \in I} \int_{U_\alpha \times Y} \pi_\alpha \mathcal{T}_{\phi_\alpha}^\varepsilon(F) \mathcal{T}_{\phi_\alpha}^\varepsilon(\sqrt{|G|}) \, dy \, dx \right| \\ &\leq \sum_{\alpha \in I} \frac{1}{|Y|} \int_{U_\alpha \times Y} |\pi_\alpha - \mathcal{T}_{\phi_\alpha}^\varepsilon(\pi_\alpha)| \cdot |\mathcal{T}_{\phi_\alpha}^\varepsilon(f)| \mathcal{T}_{\phi_\alpha}^\varepsilon(\sqrt{|G|}) \, dy \, dx \\ &\leq Cr(\varepsilon) \|\mathcal{T}_{\mathcal{A}}^\varepsilon(f)\|_{L^1(M \times Y)}, \end{aligned}$$

where we used the fact that $|\pi_\alpha - \mathcal{T}_{\phi_\alpha}^\varepsilon(\pi_\alpha)| \leq r(\varepsilon)$ for some function $r : \mathbb{R}^+ \rightarrow \mathbb{R}$ with $r(\varepsilon) \rightarrow 0$ as $\varepsilon \rightarrow 0$ and the norm equivalence $\|\cdot\|_{L^1(M \times Y^{(x,\varepsilon)})}$ with $\|\cdot\|_{L^1(M \times Y)}$. Therefore we define

4.2.22 Definition.

A sequence $\{f^\varepsilon\}$ in $L^1(M)$ is said to fulfill the unfolding criterion on manifolds (UCM) if there exists a function $r : \mathbb{R}^+ \rightarrow \mathbb{R}$ such that $r(\varepsilon) \rightarrow 0$ as $\varepsilon \rightarrow 0$ and

$$\int_M f^\varepsilon \, d\text{vol}_M = \frac{1}{|Y|} \int_{M \times Y} \mathcal{T}_{\mathcal{A}}^\varepsilon(f^\varepsilon) \mathcal{T}_{\mathcal{A}}^\varepsilon(\sqrt{|G|}) \, dy \, dx + r(\varepsilon).$$

We write in this case

$$\int_M f^\varepsilon \, d\text{vol}_M \simeq \frac{1}{|Y|} \int_{M \times Y} \mathcal{T}_{\mathcal{A}}^\varepsilon(f^\varepsilon) \mathcal{T}_{\mathcal{A}}^\varepsilon(\sqrt{|G|}) \, dy \, dx.$$

4.2.23 Example.

Keeping the next proposition in mind, the following (sequences of) functions fulfill the (UCM)-criterion:

- $f \in L^1(M)$.
- $\{f^\varepsilon\} \subset L^1(M)$ such that $\|f^\varepsilon\|_{L^1(M)}$ is bounded independently of ε .
- Since the functions are defined on a compact manifold, the same is true if we replace $L^1(M)$ with $L^p(M)$ with $1 \leq p \leq \infty$.

4.2.24 Proposition.

The operators

$$\mathcal{T}_{\mathcal{A}}^\varepsilon : L^p(M) \rightarrow L^p(M \times Y^{(x,\varepsilon)})$$

are linear and continuous with operator norm less than $((1 + \text{card}(I)\delta)|Y|)^{\frac{1}{p}}$, where $\delta > 0$ is arbitrary and $\varepsilon \leq \varepsilon_0(\delta)$.

Proof. Step 1: $p = 1$

Choose a small $\delta > 0$. Since $\mathcal{T}_{\phi_\alpha}^\varepsilon(\pi_\alpha) \rightarrow \pi_\alpha$ in $\mathcal{C}(\bar{U}_\alpha \times Y)$, there exists an $\varepsilon_0(\delta) > 0$ such

that for all $\varepsilon \leq \varepsilon_0(\delta)$

$$\mathcal{T}_{\phi_\alpha}^\varepsilon(\pi_\alpha) \geq \pi_\alpha - \delta.$$

By making ε_0 smaller, if necessary, this can be obtained uniformly for all $\alpha \in I$. Now let $f \in L^1(M)$, then

$$\begin{aligned} \int_M \pi_\alpha |f| \, d\text{vol}_M &\geq \frac{1}{|Y|} \int_{U_\alpha \times Y} \mathcal{T}_{\phi_\alpha}^\varepsilon(\pi_\alpha) |\mathcal{T}_{\phi_\alpha}^\varepsilon(f)| \mathcal{T}_{\phi_\alpha}^\varepsilon(\sqrt{|G|}) \, dy \, dy \\ &\geq \frac{1}{|Y|} \int_{U_\alpha \times Y} (\pi_\alpha - \delta) |\mathcal{T}_{\phi_\alpha}^\varepsilon(f)| \mathcal{T}_{\phi_\alpha}^\varepsilon(\sqrt{|G|}) \, dy \, dx. \end{aligned}$$

Thus

$$\frac{1}{|Y|} \int_{U_\alpha \times Y} \pi_\alpha |\mathcal{T}_{\phi_\alpha}^\varepsilon(f)| \mathcal{T}_{\phi_\alpha}^\varepsilon(\sqrt{|G|}) \, dy \, dy \leq \frac{1}{|Y|} \int_{U_\alpha \times Y} (\delta + \mathcal{T}_{\phi_\alpha}^\varepsilon(\pi_\alpha)) |\mathcal{T}_{\phi_\alpha}^\varepsilon(f)| \mathcal{T}_{\phi_\alpha}^\varepsilon(\sqrt{|G|}) \, dy \, dx.$$

By using the same derivations as in (4.8), one gets

$$\frac{1}{|Y|} \int_{U_\alpha \times Y} \delta |\mathcal{T}_{\phi_\alpha}^\varepsilon(f)| \mathcal{T}_{\phi_\alpha}^\varepsilon(\sqrt{|G|}) \, dy \, dx = \delta \int_{U_\alpha} |f| \, d\text{vol}_M \leq \delta \int_M |f| \, d\text{vol}_M$$

as well as

$$\frac{1}{|Y|} \int_{U_\alpha \times Y} \mathcal{T}_{\phi_\alpha}^\varepsilon(\pi_\alpha) |\mathcal{T}_{\phi_\alpha}^\varepsilon(f)| \mathcal{T}_{\phi_\alpha}^\varepsilon(\sqrt{|G|}) \, dy \, d = \int_{U_\alpha} \pi_\alpha |f| \, d\text{vol}_M.$$

Now summation over $\alpha \in I$ yields

$$\frac{1}{|Y|} \int_{M \times Y} \pi_\alpha |\mathcal{T}_{\phi_\alpha}^\varepsilon(f)| \mathcal{T}_{\phi_\alpha}^\varepsilon(\sqrt{|G|}) \, dy \, dy \leq (1 + \text{card}(I)\delta) \int_M |f| \, d\text{vol}_M$$

which is the result for $p = 1$.

Step 2: $1 < p < \infty$

Using the product rule from Corollary 4.2.10, we obtain for $f \in L^p(M)$

$$\begin{aligned} \|\mathcal{T}_{\mathcal{A}}^\varepsilon(f)\|_{L^p(M \times Y^{(x,\varepsilon)})}^p &= \|\mathcal{T}_{\mathcal{A}}^\varepsilon(f^p)\|_{L^1(M \times Y^{(x,\varepsilon)})} \leq (1 + \text{card}(I)\delta) |Y| \|f^p\|_{L^1(M)} \\ &= (1 + \text{card}(I)\delta) |Y| \|f\|_{L^p(M)}^p. \end{aligned}$$

Now taking the p -th root on both sides yields the result. ◆

4.2.25 Corollary.

Take a vector field $F \in \mathfrak{X}(M)$ and set $f := g_M(F, F)$. Then

$$\begin{aligned} \|\mathcal{T}_{\mathcal{A}}^\varepsilon(F)\|_{L^2(M \times Y^{(x,\varepsilon)})}^2 &= \left\| g_Y^{(x,\varepsilon)}(\mathcal{T}_{\mathcal{A}}^\varepsilon(F), \mathcal{T}_{\mathcal{A}}^\varepsilon(F)) \right\|_{L^1(M \times Y^{(x,\varepsilon)})} = \|\mathcal{T}_{\mathcal{A}}^\varepsilon(f)\|_{L^1(M \times Y^{(x,\varepsilon)})} \\ &\leq (1 + \text{card}(I)\delta) |Y| \|f\|_{L^1(M)} \\ &= (1 + \text{card}(I)\delta) |Y| \|F\|_{L^2(M)}^2, \end{aligned}$$

and we see that $\mathcal{T}_{\mathcal{A}}^\varepsilon$ is also a continuous map for L^2 -vector fields with the same operator norm as in the scalar case.

4.2.6 Convergence Statements

4.2.26 Lemma.

Let $w \in L^p(M)$ with $p \in [1, \infty)$. Then

$$\mathcal{T}_{\mathcal{A}}^\varepsilon(w) \longrightarrow w \quad \text{in } L^p(M \times Y).$$

An analogous result holds for $w \in \mathcal{C}^k(M)$, $k \in \mathbb{N}_0$.

Proof. Let $w \in \mathcal{C}^1(M)$. Then

$$\begin{aligned} \|\mathcal{T}_{\mathcal{A}}^\varepsilon(w) - w\|_{L^p(M \times Y)}^p &= \int_{M \times Y} |\mathcal{T}_{\mathcal{A}}^\varepsilon(w) - w|^p \sqrt{|G|} \, dy \, dx \\ &\leq C \max_{(x,y) \in M \times Y} |\mathcal{T}_{\mathcal{A}}^\varepsilon(w)(x,y) - w(x)| \longrightarrow 0, \end{aligned}$$

since $\mathcal{T}_{\mathcal{A}}^\varepsilon(w) \rightarrow w$ pointwise in $L^\infty(M \times Y)$ due to Lemma 4.2.21. By density, the result follows for L^p . Looking at the estimate above, the other assertion is obvious. \blacklozenge

4.2.27 Lemma.

Let $\{w^\varepsilon\} \subset L^p(M)$, $p \in [1, \infty)$ be a sequence such that $w^\varepsilon \rightarrow w$ in $L^p(M)$ for some $w \in L^p(M)$. Then

$$\mathcal{T}_{\mathcal{A}}^\varepsilon(w^\varepsilon) \longrightarrow w \quad \text{in } L^p(M \times Y).$$

Proof. We have

$$\begin{aligned} \|\mathcal{T}_{\mathcal{A}}^\varepsilon(w^\varepsilon) - w\|_{L^p(M \times Y)} &= \|\mathcal{T}_{\mathcal{A}}^\varepsilon(w^\varepsilon) - \mathcal{T}_{\mathcal{A}}^\varepsilon(w) + \mathcal{T}_{\mathcal{A}}^\varepsilon(w) - w\|_{L^p(M \times Y)} \\ &\leq \|\mathcal{T}_{\mathcal{A}}^\varepsilon(w^\varepsilon - w)\|_{L^p(M \times Y)} + \|\mathcal{T}_{\mathcal{A}}^\varepsilon(w) - w\|_{L^p(M \times Y)} \\ &\leq C \|\mathcal{T}_{\mathcal{A}}^\varepsilon(w^\varepsilon - w)\|_{L^p(M \times Y^{(x,\varepsilon)})} + \|\mathcal{T}_{\mathcal{A}}^\varepsilon(w) - w\|_{L^p(M \times Y)} \\ &\leq C \|w^\varepsilon - w\|_{L^p(M)} + \|\mathcal{T}_{\mathcal{A}}^\varepsilon(w) - w\|_{L^p(M \times Y)} \longrightarrow 0, \end{aligned}$$

where we used (starting from the second line) the norm equivalence $\|\cdot\|_{L^p(M \times Y)}$ with $\|\cdot\|_{L^p(M \times Y^{(x,\varepsilon)})}$, the continuity of $\mathcal{T}_{\mathcal{A}}^\varepsilon$, see Proposition 4.2.24, as well as the previous lemma. \blacklozenge

4.2.28 Proposition.

Let $\{w^\varepsilon\} \subset L^p(M)$, $p \in [1, \infty)$ be a sequence such that $\mathcal{T}_{\mathcal{A}}^\varepsilon w^\varepsilon \rightarrow \hat{w}$ in $L^p(M \times Y)$, where $\hat{w} \in L^p(M \times Y)$. Then w^ε converges weakly to w in $L^p(M)$, where

$$w := \int_Y \hat{w} \, dy.$$

Proof. Choose a $\psi \in L^{p'}(M)$. Since weakly convergent sequences are bounded, the product $w^\varepsilon \psi$ is a bounded sequence in $L^1(M)$ and thus fulfills the UCM-criterion. Thus

we obtain

$$\int_M w^\varepsilon \psi \, \text{dvol}_M \simeq \int_{M \times Y} \mathcal{T}_{\mathcal{A}}^\varepsilon(w^\varepsilon) \mathcal{T}_{\mathcal{A}}^\varepsilon(\psi) \mathcal{T}_{\mathcal{A}}^\varepsilon(\sqrt{|G|}) \, \text{d}y \, \text{d}x.$$

Since $\mathcal{T}_{\mathcal{A}}^\varepsilon(w^\varepsilon) \rightarrow \hat{w}$, $\mathcal{T}_{\mathcal{A}}^\varepsilon(\psi) \rightarrow \psi$ and $\mathcal{T}_{\mathcal{A}}^\varepsilon(\sqrt{|G|}) \rightarrow \sqrt{|G|}$ (see Lemma 4.2.26) we obtain in the limit for $\varepsilon \rightarrow 0$

$$\int_{M \times Y} \hat{w} \psi \sqrt{|G|} \, \text{d}y \, \text{d}x = \int_M \left(\int_Y \hat{w} \, \text{d}y \right) \psi \, \text{dvol}_M$$

which proves the assertion. \blacklozenge

4.2.7 Unfolding of Gradients in the Hilbert-Space Setting

In this section we consider sequences w^ε in $H^1(M)$. We analyze two different situations: In the first one, we assume that we have a bound on the gradient of the form $\varepsilon \|\nabla_M w^\varepsilon\|_{L^2} \leq C$ with a constant C independent of ε . We call this a situation with "weak gradient estimates". Secondly, we assume that we have the stronger bound $\|\nabla_M w^\varepsilon\|_{L^2} \leq C$ without the factor of ε .

The main difficulty is that the usual results like $\mathcal{T}^\varepsilon(\nabla u^\varepsilon) \rightarrow \nabla_x u_0 + \nabla_y u_1$ relate two objects which cannot be coupled on general manifolds: Whereas $\nabla_x u_0$ corresponds to $\nabla_M u_0$ and is thus a vector field on M , the term $\nabla_y u_1$ represents a vector field in Y ! This is why, in the general case, a transport operator $(\cdot)_Y$ appears, which maps vector fields on M to vector fields in Y .

In the sequel, we need three different gradient operators, which we denote by ∇_M , $\nabla_Y^{(x,\varepsilon)}$ and $\nabla_Y^{(x)}$:

- ∇_M denotes the gradient on M with respect to the metric g_M .
- For fixed $x \in M$ and $\varepsilon > 0$, $\nabla_Y^{(x,\varepsilon)}$ denotes the gradient on Y with respect to the parameter-dependent metric $g_Y^{(x,\varepsilon)}$.
- Finally, for fixed $x \in M$ the operator $\nabla_Y^{(x)}$ is defined to be the gradient on Y with respect to the parameter-dependent metric $g_Y^{(x)} := \lim_{\varepsilon \rightarrow 0} \mathcal{T}_{\mathcal{A}}^\varepsilon(g_M)(x, \cdot)$, i.e. with respect to the metric on Y with metric coefficients $g_Y^{(x)}(\frac{\partial}{\partial y^i}, \frac{\partial}{\partial y^j}) = g_{ij}(x)$.

We will use the same index notation for divergence operators, which are defined as the (formal) negative L^2 -adjoint of the corresponding gradient operators.

Using Weak Gradient Estimates

4.2.29 Theorem.

Let $\{w^\varepsilon\} \subset W^{1,2}(M)$ be a sequence such that

$$\begin{aligned} \|w^\varepsilon\|_{L^2(M)} &\leq C \\ \varepsilon \|\nabla_M w^\varepsilon\|_{L^2 TM} &\leq C, \end{aligned}$$

with a constant $C > 0$ independent of ε . Then there exists a $w \in L^2(M; W_{\#}^{1,2}(Y))$ such that along a subsequence

$$\begin{aligned} \mathcal{T}_{\mathcal{A}}^{\varepsilon}(w^{\varepsilon}) &\rightharpoonup w && \text{in } L^2(M \times Y) \\ \varepsilon \mathcal{T}_{\mathcal{A}}^{\varepsilon}(\nabla_M w^{\varepsilon}) &\rightharpoonup \nabla_Y^{(x)} w && \text{in } L^2(M; L^2TY), \end{aligned}$$

where by abuse of notation we use $\nabla_Y^{(x)} w$ to denote a function $(x, y) \mapsto \nabla_Y^{(x)} w(x, y)$.

Proof. Due to Proposition 4.2.16 we have $\varepsilon \mathcal{T}_{\mathcal{A}}^{\varepsilon}(\nabla_M w^{\varepsilon}) = \nabla_Y^{(x,\varepsilon)} \mathcal{T}_{\mathcal{A}}^{\varepsilon}(w^{\varepsilon})$ and thus the norm estimate shows that $\|\mathcal{T}_{\mathcal{A}}^{\varepsilon}(w^{\varepsilon})\|_{L^2(M \times Y)}$ as well as $\|\nabla_Y^{(x,\varepsilon)} \mathcal{T}_{\mathcal{A}}^{\varepsilon}(w^{\varepsilon})\|_{L^2(M \times Y)}$ are bounded independent of ε . Thus there exist limits $w \in L^2(M \times Y)$ and $\xi \in L^2(M; L^2TY)$ such that along a subsequence

$$\begin{aligned} \mathcal{T}_{\mathcal{A}}^{\varepsilon}(w^{\varepsilon}) &\rightharpoonup w && \text{in } L^2(M \times Y) \\ \nabla_Y^{(x,\varepsilon)} \mathcal{T}_{\mathcal{A}}^{\varepsilon}(w^{\varepsilon}) &\rightharpoonup \xi && \text{in } L^2(M; L^2TY). \end{aligned}$$

It remains to show that $\xi = \nabla_Y^{(x)} w$. To this end, choose a test function $\psi \in \mathcal{C}_0^{\infty}(M; \mathcal{C}_{\#}^{\infty}(Y))^n$ and consider the term $\int_{M \times Y} g_Y^{(x,\varepsilon)}(\nabla_Y^{(x,\varepsilon)} \mathcal{T}_{\mathcal{A}}^{\varepsilon}(w^{\varepsilon}), \psi) \mathcal{T}_{\mathcal{A}}^{\varepsilon}(\sqrt{|G|}) \, dy \, dx$. Upon an integration by parts with respect to the metric $g_Y^{(x,\varepsilon)}$ we obtain

$$\int_{M \times Y} g_Y^{(x,\varepsilon)}(\nabla_Y^{(x,\varepsilon)} \mathcal{T}_{\mathcal{A}}^{\varepsilon}(w^{\varepsilon}), \psi) \mathcal{T}_{\mathcal{A}}^{\varepsilon}(\sqrt{|G|}) \, dy \, dx = - \int_{M \times Y} \mathcal{T}_{\mathcal{A}}^{\varepsilon}(w^{\varepsilon}) \operatorname{div}_Y^{(x,\varepsilon)} \psi \mathcal{T}_{\mathcal{A}}^{\varepsilon}(\sqrt{|G|}) \, dy \, dx.$$

Since the metric coefficients g_{ij} are smooth, we obtain that $\mathcal{T}_{\mathcal{A}}^{\varepsilon}(g_{ij}) \rightarrow g_{ij}$. This implies that $\operatorname{div}_Y^{(x,\varepsilon)} \psi \rightarrow \operatorname{div}_Y^{(x)} \psi$ and $g_Y^{(x,\varepsilon)} \rightarrow g_Y^{(x)}$ in the sense that if $\chi^{\varepsilon} \rightarrow \chi$ in L^2TY and $\eta^{\varepsilon} \rightarrow \eta$ in L^2TY , then $g_Y^{(x,\varepsilon)}(\chi^{\varepsilon}, \eta^{\varepsilon}) \rightarrow g_Y^{(x)}(\chi, \eta)$. Thus passing to the limit $\varepsilon \rightarrow 0$ in the previous expression yields

$$\int_{M \times Y} g_Y^{(x)}(\xi, \psi) \, dy \, \operatorname{dvol}_M = - \int_{M \times Y} w \operatorname{div}_Y^{(x)} \psi \, dy \, \operatorname{dvol}_M.$$

Choosing a test function ψ such that $\operatorname{div}_Y^{(x)} \psi = 0$, we see that ξ is orthogonal to divergence-free functions in the variable y . We can thus use Hodge-theory (see for example Agricola and Friedrich [AF02]) to obtain that ξ can be represented as a gradient with

$$\xi = \nabla_Y^{(x)} \zeta, \quad \zeta \in L^2(M; W_{\#}^{1,2}(Y)).$$

Inserting this form for ξ in the last integral identity and carrying out another integration by parts, we see that

$$\int_{M \times Y} (w - \zeta) \operatorname{div}_y^{(x)} \psi \, dy \, \operatorname{dvol}_M = 0$$

for all ψ . Since the set of all functions $\{\operatorname{div}_y^{(x)} \psi; \psi \in \mathcal{C}_0^{\infty}(M; \mathcal{C}_{\#}^{\infty}(Y))^n\}$ is dense in the set $L^2(M; L_0^2(Y)) = L_0^2(M \times Y)$ of functions with mean value 0, we obtain that

$(w - \zeta) \perp L_0^2(M \times Y)$, i.e. $w = \zeta + K$ with some constant K . Thus

$$\nabla_Y^{(x)} w = \nabla_Y^{(x)} \zeta = \xi,$$

which finishes the proof. \blacklozenge

Transport Operators

In order to be able to give the convergence result when we have stronger estimates on the gradient, we need some preparatory constructions and results:

4.2.30 Definition.

For a vector field $F \in \mathfrak{X}(M)$ we define a transport operator $(\cdot)_Y$ with

$$\begin{aligned} (\cdot)_Y : \mathfrak{X}(M) &\longrightarrow \mathfrak{X}(Y)^M \\ F &\longmapsto F_Y, \end{aligned}$$

where for $F = \sum_i F^i \frac{\partial}{\partial x^i}$ the field F_Y is defined via

$$F_Y(x, y) = \sum_i F^i(x) \frac{\partial}{\partial y^i}.$$

Analogously, we construct a transport operator which maps vector fields on Y to vector fields on M :

4.2.31 Definition.

For a vector field $G \in \mathfrak{X}(Y)$ we define a transport operator $(\cdot)_M$ with

$$\begin{aligned} (\cdot)_M : \mathfrak{X}(Y) &\longrightarrow \mathfrak{X}(M)^Y \\ G &\longmapsto G_M, \end{aligned}$$

where for $G = \sum_i G^i \frac{\partial}{\partial y^i}$ the field G_M is defined via

$$G_M(x, y) = \sum_i G^i(y) \frac{\partial}{\partial x^i}.$$

4.2.32 Remark.

Note that Lemma 4.2.4 allows a one-to-one correspondence between $\frac{\partial}{\partial x^i}$ and $\frac{\partial}{\partial y^i}$ even across different charts, thus the transport operators are well defined.

We will use the same operators on parameter-dependent vector fields; e.g. for $\tilde{F} \in \mathfrak{X}(M)^Y$, $F(x, y) = \sum_i F^i(x, y) \frac{\partial}{\partial x^i}$ we set $\tilde{F}_Y(x, y) = \sum_i F^i(x, y) \frac{\partial}{\partial y^i}$ (analogously for a $\tilde{G} \in \mathfrak{X}(Y)^M$ and $(\cdot)_M$). We obtain the following results:

4.2.33 Lemma.

Let $V_i \in \mathfrak{X}(M)^Y$, $W_i \in \mathfrak{X}(Y)^M$ for $i = 1, 2$. Then

$$\bullet \left((V_1)_Y \right)_M = V_1, \quad \left((W_1)_M \right)_Y = W_1,$$

- $g_Y^{(x)}(W_1, W_2) = g_M\left((W_1)_M, (W_2)_M\right)$,
- $g_M(V_1, V_2) = g_Y^{(x)}\left((V_1)_Y, (V_2)_Y\right)$.

Proof. For the first assertion observe that for $V_1 = \sum_i V_1^i \frac{\partial}{\partial x^i}$ we have $\left((V_1)_Y\right)_M = \left(\sum_i V_1^i \frac{\partial}{\partial y^i}\right)_M = \sum_i V_1^i \frac{\partial}{\partial x^i} = V_1$. The result for W_1 follows along the same lines. The second assertion follows due to the identity $g_Y^{(x)}(W_1, W_2)(x, y) = \sum_{i,j} g_{ij}(x) W_1^i(x, y) W_2^j(x, y) = g_M\left((W_1)_M, (W_2)_M\right)(x, y)$. The last assertion is an easy corollary of the first two statements. \blacklozenge

Since the transport operators are defined pointwise, we can extend their definition to L^2 -vector fields such that the above identities hold almost everywhere.

Using Stronger Gradient Estimates

4.2.34 Lemma.

Assume that $\{w^\varepsilon\}$ is a sequence in $W^{1,2}(M)$ which converges strongly to some $w \in W^{1,2}(M)$. Then

$$\begin{aligned} \mathcal{T}_{\mathcal{A}}^\varepsilon(w^\varepsilon) &\longrightarrow w && \text{strongly in } L^2(M \times Y) \\ \mathcal{T}_{\mathcal{A}}^\varepsilon(\nabla_M w^\varepsilon) &\longrightarrow (\nabla_M w)_Y && \text{strongly in } L^2(M; L^2TY). \end{aligned}$$

Proof. The first statement follows due to the compact embedding $W^{1,2}(M) \hookrightarrow L^2(M)$ and Lemma 4.2.27. For the second statement, note that it holds $(\nabla_M w^\varepsilon - \nabla_M w) \rightarrow 0$ in $L^2(M)$. Since $\mathcal{T}_{\mathcal{A}}^\varepsilon$ is continuous, we get that $(\mathcal{T}_{\mathcal{A}}^\varepsilon(\nabla_M w^\varepsilon) - \mathcal{T}_{\mathcal{A}}^\varepsilon(\nabla_M w)) \rightarrow 0$ in $L^2(M; L^2TY)$ as well. Thus we have to characterize $\lim_{\varepsilon \rightarrow 0} \mathcal{T}_{\mathcal{A}}^\varepsilon(\nabla_M w)$: Locally we have for a chart ϕ

$$\begin{aligned} \mathcal{T}_\phi^\varepsilon(\nabla_M w)(x, y) &= \mathcal{T}_\phi^\varepsilon\left(\sum_{i,j} g^{ij} \frac{\partial w}{\partial x^i} \frac{\partial}{\partial x^j}\right)(x, y) \\ &= \sum_{i,j} \underbrace{\mathcal{T}_\phi^\varepsilon(g^{ij})(x, y)}_{\rightarrow g^{ij}(x)} \underbrace{\mathcal{T}_\phi^\varepsilon\left(\frac{\partial w}{\partial x^i}\right)(x, y)}_{\rightarrow \frac{\partial w}{\partial x^i}} \frac{\partial}{\partial y^j} \\ &\longrightarrow \sum_{i,j} g^{ij}(x) \frac{\partial w}{\partial x^i} \frac{\partial}{\partial y^j} = (\nabla_M w)_Y, \end{aligned}$$

which gives the result. \blacklozenge

We are now able to prove the main result of this paragraph:

4.2.35 Theorem.

Let $\{w^\varepsilon\} \subset W^{1,2}(M)$ be a sequence such that

$$\begin{aligned} \|w^\varepsilon\|_{L^2(M)} &\leq C \\ \|\nabla_M w^\varepsilon\|_{L^2TM} &\leq C \end{aligned}$$

with a constant $C > 0$ independent of ε . Then there exists a $w \in W^{1,2}(M)$ and a $\hat{w} \in L^2(M; W_{\#}^{1,2}(Y))$ such that along a subsequence

$$\begin{aligned} \mathcal{T}_{\mathcal{A}}^{\varepsilon}(w^{\varepsilon}) &\longrightarrow w && \text{in } L^2(M \times Y) \\ \mathcal{T}_{\mathcal{A}}^{\varepsilon}(\nabla_M w^{\varepsilon}) &\longrightarrow (\nabla_M w)_Y + \nabla_Y^{(x)} \hat{w} && \text{in } L^2(M; L^2TY), \end{aligned}$$

where by abuse of notation we use $\nabla_Y^{(x)} w$ to denote a function $(x, y) \mapsto \nabla_Y^{(x)} w(x, y)$.

Proof. Step 0 Existence of w :

Since the bounds are equivalent to the fact that the sequence $\{w^{\varepsilon}\}$ is bounded in $W^{1,2}(M)$, we obtain the existence of a $w \in W^{1,2}(M)$ such that along a subsequence $w^{\varepsilon} \rightharpoonup w$ in $W^{1,2}(M)$. Due to the compact embedding $W^{1,2}(M) \hookrightarrow L^2(M)$, w^{ε} converges strongly in $L^2(M)$ to w .

Step 1 $(\nabla_M w)_Y \in L^2(M \times Y)$:

We have the estimate

$$\begin{aligned} \|(\nabla_M w)_Y\|_{L^2(M \times Y)} &= \|\lim \mathcal{T}_{\mathcal{A}}^{\varepsilon}(\nabla_M w)\|_{L^2(M \times Y)} \\ &\leq \lim \|\mathcal{T}_{\mathcal{A}}^{\varepsilon}(\nabla_M w)\|_{L^2(M \times Y)} \\ &\leq C \|\nabla_M w\|_{L^2(M)} \end{aligned}$$

by the continuity of $\mathcal{T}_{\mathcal{A}}^{\varepsilon}$, thus $(\nabla_M w)_Y \in L^2(M \times Y)$.

Step 2 Existence of a weak limit:

Since

$$\|\mathcal{T}_{\mathcal{A}}^{\varepsilon}(\nabla_M w^{\varepsilon})\|_{L^2(M \times Y)} \leq \|\mathcal{T}_{\mathcal{A}}^{\varepsilon}(\nabla_M w^{\varepsilon})\|_{L^2(M \times Y^{(x,\varepsilon)})} \leq C \|\nabla_M w^{\varepsilon}\|_{L^2(M)} \leq C$$

with a bound independent of ε , we obtain that $(\mathcal{T}_{\mathcal{A}}^{\varepsilon}(\nabla_M w^{\varepsilon}) - (\nabla_M w)_Y)$ is bounded in $L^2(M \times Y)$. Thus there exists a $\xi \in L^2(M \times Y)$ such that along a subsequence

$$\mathcal{T}_{\mathcal{A}}^{\varepsilon}(\nabla_M w^{\varepsilon}) - (\nabla_M w)_Y \rightharpoonup \xi.$$

It remains to show that $\xi = \nabla_Y^{(x)} \hat{w}$ for a function \hat{w} in $L^2(M; W_{\#}^{1,2}(Y))$.

Step 3 Construction of an auxiliary vector field:

Let $\phi : U \rightarrow \mathbb{R}^n$ be a chart. Choose a function $\psi \in C_0^{\infty}(M; C_{\#}^{\infty}(Y)^n)$ with $\operatorname{div}_Y^{(x)} \psi = 0$.

For $x \in U$, $\varepsilon > 0$ define locally $\hat{\psi}^{\varepsilon}(x) = \psi(x, \left\{ \frac{\phi(x)}{\varepsilon} \right\})$. We want to test $\mathcal{T}_{\mathcal{A}}^{\varepsilon}(\nabla_M w^{\varepsilon}) - (\nabla_M w)_Y$ with $\hat{\psi}^{\varepsilon}$ – however this function is a vector field in Y , not on M ! Thus we interpret $\hat{\psi}^{\varepsilon}(x)$ for fixed $x \in U$ as a constant vector field in Y and define via the tangential map $T\phi^{-1}$

$$\psi^{\varepsilon}(x) := (T_{\phi(x)}\phi^{-1})\hat{\psi}^{\varepsilon}(x).$$

This is a vector field in U . In order to determine the limit of $\mathcal{T}_{\phi}^{\varepsilon}(\psi^{\varepsilon})$, we calculate

$$(\phi_*\psi^{\varepsilon})(z) = \underbrace{(T_{\phi^{-1}(z)}\phi)(T_z\phi^{-1})}_{=\operatorname{Id}} \psi(\phi^{-1}(z), \frac{z}{\varepsilon}) = \psi(\phi^{-1}(z), \frac{z}{\varepsilon})$$

and thus $\mathcal{T}^\varepsilon(\phi_*\psi^\varepsilon)(z, y) = \psi(\phi^{-1}(\varepsilon \lfloor \frac{z}{\varepsilon} \rfloor + \varepsilon y), y)$. This finally gives the convergence property

$$\mathcal{T}_\phi^\varepsilon(\psi^\varepsilon)(x, y) = (\phi \times \text{Id})^* \mathcal{T}^\varepsilon(\phi_*\psi^\varepsilon) = \psi(\phi^{-1}(\varepsilon \lfloor \frac{\phi(x)}{\varepsilon} \rfloor + \varepsilon y), y) \longrightarrow \psi(x, y)$$

in the space of smooth functions.

For two charts ϕ_α, ϕ_β with $U_\alpha \cap U_\beta \neq \emptyset$, note that by the (UC)-condition $\hat{\psi}^\varepsilon(x) := \psi(x, \lfloor \frac{\phi_\alpha(x)}{\varepsilon} \rfloor) = \psi(x, \lfloor \frac{\phi_\beta(x)}{\varepsilon} \rfloor)$. The argument used in the proof of Lemma 4.2.4 shows (by using an arbitrary vector instead of e_i) that for the tangent maps the identity

$$T_{\phi_\alpha(x)}\phi_\alpha^{-1} = T_{\phi_\beta(x)}\phi_\beta^{-1}$$

holds. Thus $\psi^\varepsilon(x) = (T_{\phi_\alpha(x)}\phi_\alpha^{-1})\hat{\psi}^\varepsilon(x) = (T_{\phi_\beta(x)}\phi_\beta^{-1})\hat{\psi}^\varepsilon(x)$ on $U_\alpha \cap U_\beta$. By this identity, ψ^ε is well defined on the whole manifold M .

Step 4 An auxiliary integral identity:

Now consider the identity

$$\int_M g_M(\nabla_M w^\varepsilon - \nabla_M w, \psi^\varepsilon) \, \text{dvol}_M = - \int_M (w^\varepsilon - w) \, \text{div}_Y^{(x)} \psi^\varepsilon \, \text{dvol}_M.$$

By the usual arguments, we can apply the unfolding operator to both sides and obtain (in the sense of \simeq)

$$\begin{aligned} & \int_{M \times Y} g_Y^{(x, \varepsilon)} \left(\mathcal{T}_{\mathcal{A}}^\varepsilon(\nabla_M w^\varepsilon) - \mathcal{T}_{\mathcal{A}}^\varepsilon(\nabla_M w), \mathcal{T}_{\mathcal{A}}^\varepsilon(\psi^\varepsilon) \right) \mathcal{T}_{\mathcal{A}}^\varepsilon(\sqrt{|G|}) \, \text{d}y \, \text{d}x \\ &= - \int_{M \times Y} [\mathcal{T}_{\mathcal{A}}^\varepsilon(w^\varepsilon) - \mathcal{T}_{\mathcal{A}}^\varepsilon(w)] \frac{1}{\varepsilon} \, \text{div}_Y^{(x, \varepsilon)} \mathcal{T}_{\mathcal{A}}^\varepsilon(\psi^\varepsilon) \mathcal{T}_{\mathcal{A}}^\varepsilon(\sqrt{|G|}) \, \text{d}y \, \text{d}x. \end{aligned} \quad (4.9)$$

For the left hand side, we obtain the following expression and limit:

$$\begin{aligned} & \int_{M \times Y} g_Y^{(x, \varepsilon)} \left(\underbrace{\mathcal{T}_{\mathcal{A}}^\varepsilon(\nabla_M w^\varepsilon) - (\nabla_M w)_Y}_{\rightarrow \xi} + \underbrace{(\nabla_M w)_Y - \mathcal{T}_{\mathcal{A}}^\varepsilon(\nabla_M w)}_{\rightarrow 0}, \mathcal{T}_{\mathcal{A}}^\varepsilon(\psi^\varepsilon) \right) \mathcal{T}_{\mathcal{A}}^\varepsilon(\sqrt{|G|}) \, \text{d}y \, \text{d}x \\ & \longrightarrow \int_{M \times Y} g_Y^{(x)}(\xi, \psi) \, \text{d}y \, \text{dvol}_M. \end{aligned}$$

Here we used the fact that $\mathcal{T}_{\mathcal{A}}^\varepsilon(\sqrt{|G|}) \rightarrow \sqrt{|G|}$, that $g_Y^{(x, \varepsilon)}$ converges to $g_Y^{(x)}$ (see above), and the result from step 3.

For the right hand side, we will show that $\frac{1}{\varepsilon} \, \text{div}_Y^{(x, \varepsilon)} \mathcal{T}_{\mathcal{A}}^\varepsilon(\psi^\varepsilon)$ is bounded independent of ε . Since $(\mathcal{T}_{\mathcal{A}}^\varepsilon(w^\varepsilon) - \mathcal{T}_{\mathcal{A}}^\varepsilon(w)) \rightarrow 0$, the right hand side thus converges to 0, and we obtain from (4.9)

$$\boxed{\int_{M \times Y} g_Y^{(x)}(\xi, \psi) \, \text{d}y \, \text{dvol}_M = 0} \quad (4.10)$$

for all $\psi \in \mathcal{C}_0^\infty(M; \mathcal{C}_\#^\infty(Y)^n)$ with $\operatorname{div}_Y^{(x)} \psi = 0$.

In order to show the bound on $\operatorname{div}_Y^{(x,\varepsilon)} \mathcal{T}_\phi^\varepsilon(\psi^\varepsilon)$, we split the term into the following sum:

$$\operatorname{div}_Y^{(x,\varepsilon)} \mathcal{T}_\phi^\varepsilon(\psi^\varepsilon) = \underbrace{\operatorname{div}_Y^{(x,\varepsilon)} \mathcal{T}_\phi^\varepsilon(\psi^\varepsilon) - \operatorname{div}_Y^{(x)} \mathcal{T}_\phi^\varepsilon(\psi^\varepsilon)}_{=:D_1} + \underbrace{\operatorname{div}_Y^{(x)} \mathcal{T}_\phi^\varepsilon(\psi^\varepsilon) - \operatorname{div}_Y^{(x)} \psi}_{=:D_2}$$

We will need the following two arguments (A) and (B), which hold for a \mathcal{C}^1 -function $g : M \rightarrow \mathbb{R}$: By Taylor expansion of $g \circ \phi^{-1}$ we obtain

$$(A) \left\{ \begin{aligned} g(x) - \mathcal{T}_\phi^\varepsilon(g)(x, y) &= g(\phi^{-1} \circ \phi(x)) - g(\phi^{-1}(\varepsilon \left[\frac{\phi(x)}{\varepsilon} \right] + \varepsilon y)) \\ &= (g \circ \phi^{-1})'(\phi(x)) \left[\phi(x) - \varepsilon \left[\frac{\phi(x)}{\varepsilon} \right] + \varepsilon y \right] + \mathcal{O}(\varepsilon^2) \\ &= \varepsilon (g \circ \phi^{-1})'(\phi(x)) \left[- \left\{ \frac{\phi(x)}{\varepsilon} \right\} + y \right] + \mathcal{O}(\varepsilon^2) \\ &= \mathcal{O}(\varepsilon). \end{aligned} \right.$$

Similarly, by employing the chain rule, we get

$$(B) \left\{ \begin{aligned} \frac{\partial(\mathcal{T}_\phi^\varepsilon(g))}{\partial y^i} &= \frac{\partial[g(\phi^{-1}(\varepsilon \left[\frac{\phi(x)}{\varepsilon} \right] + \varepsilon y))]}{\partial y^i} \\ &= \varepsilon (g \circ \phi^{-1})'(\varepsilon \left[\frac{\phi(x)}{\varepsilon} \right] + \varepsilon y) \\ &= \mathcal{O}(\varepsilon). \end{aligned} \right.$$

In the sequel, we will indicate where to use each argument. For D_1 we obtain in local coordinates

$$\begin{aligned} -D_1 &= -\operatorname{div}_Y^{(x,\varepsilon)} \mathcal{T}_\phi^\varepsilon(\psi^\varepsilon)(x, y) + \operatorname{div}_Y^{(x)} \mathcal{T}_\phi^\varepsilon(\psi^\varepsilon)(x, y) \\ &= \underbrace{\left(\frac{1}{\sqrt{|G|(x)}} - \frac{1}{\sqrt{\mathcal{T}_\phi^\varepsilon(|G|)(x, y)}} \right)}_{(A)} \sum_i \frac{\partial}{\partial y^i} [\sqrt{|G|(x)} \mathcal{T}_\phi^\varepsilon(\psi^{\varepsilon,i})(x, y)] \\ &\quad + \frac{1}{\sqrt{\mathcal{T}_\phi^\varepsilon(|G|)(x, y)}} \left(\sum_i \frac{\partial}{\partial y^i} [\sqrt{|G|(x)} \mathcal{T}_\phi^\varepsilon(\psi^{\varepsilon,i})(x, y) - \sqrt{\mathcal{T}_\phi^\varepsilon(|G|)(x, y)} \mathcal{T}_\phi^\varepsilon(\psi^{\varepsilon,i})(x, y)] \right) \\ &= \mathcal{O}(\varepsilon) + \frac{1}{\sqrt{\mathcal{T}_\phi^\varepsilon(|G|)(x, y)}} \left(\sum_i \underbrace{(\sqrt{|G|} - \sqrt{\mathcal{T}_\phi^\varepsilon(|G|)(x, y)})}_{(A)} \frac{\partial \psi^{\varepsilon,i}}{\partial y^i} \right. \\ &\quad \left. + \sum_i \psi^{\varepsilon,i} \underbrace{\frac{\partial(\mathcal{T}_\phi^\varepsilon(\sqrt{|G|})(x, y))}{\partial y^i}}_{(B)} \right) \\ &= \mathcal{O}(\varepsilon) \end{aligned}$$

(since all other terms not covered by (A) or (B) are smooth and bounded). For D_2 we have

$$\begin{aligned}
D_2 &= \operatorname{div}_Y^{(x)} \mathcal{T}_\phi^\varepsilon(\psi^\varepsilon)(x, y) - \operatorname{div}_Y^{(x)} \psi(x, y) \\
&= \frac{1}{\sqrt{|G|(x)}} \sum_i \sqrt{|G|(x)} \frac{\partial}{\partial y^i} [\mathcal{T}_\phi^\varepsilon(\psi^{\varepsilon, i}) - \psi^i](x, y) \\
&= \frac{1}{\sqrt{|G|(x)}} \sum_i \sqrt{|G|(x)} \frac{\partial}{\partial y^i} [\psi^i(\phi^{-1}(\varepsilon \left[\frac{\phi(x)}{\varepsilon} \right] + \varepsilon y), y) - \psi^i(x, y)] \\
&= \frac{1}{\sqrt{|G|(x)}} \sum_i \sqrt{|G|(x)} \varepsilon \frac{\partial}{\partial x^i} [\psi^i \circ (\phi^{-1} \times \operatorname{Id})](\varepsilon \left[\frac{\phi(x)}{\varepsilon} \right] + \varepsilon y, y) \\
&\quad + \frac{1}{\sqrt{|G|(x)}} \sum_i \sqrt{|G|(x)} \underbrace{\left[\frac{\partial \psi^i}{\partial y^i}(\phi^{-1}(\varepsilon \left[\frac{\phi(x)}{\varepsilon} \right] + \varepsilon y), y) - \frac{\partial \psi^i}{\partial y^i}(x, y) \right]}_{(A)} \\
&= \mathcal{O}(\varepsilon).
\end{aligned}$$

Thus $\frac{D_1 + D_2}{\varepsilon} \leq C$, which is the desired bound.

Step 5 Representation as a gradient, limits:

Equation (4.10) shows that ξ is orthogonal to divergence-free functions in the variable y on the set $M \times Y$. By using Hodge theory as in the proof of Theorem 4.2.29, we obtain thus the representation

$$\xi = \nabla_Y^{(x)} \hat{w} \quad \text{for some } \hat{w} \in L^2(M; W_{\#}^{1,2}(Y)).$$

To sum up, we have obtained the existence of a $\hat{w} \in L^2(M; W_{\#}^{1,2}(Y))$ with $\mathcal{T}_{\mathcal{A}}^\varepsilon(\nabla_M w^\varepsilon) - (\nabla_M w)_Y \longrightarrow \nabla_Y^{(x)} \hat{w}$, which is equivalent to

$$\mathcal{T}_{\mathcal{A}}^\varepsilon(\nabla_M w^\varepsilon) \longrightarrow (\nabla_M w)_Y + \nabla_Y^{(x)} \hat{w}.$$

This finishes the proof of the theorem. ◆

4.3 Example for a Chart-Periodic Manifold

Up to now it is not clear whether there exist manifolds (apart from the trivial ones) which satisfy the UC-criterion from Definition 4.2.2. In this section we show how a spherical zone can be equipped with an atlas that satisfies the compatibility condition. For this we make use of polar coordinates. A reminder about the main facts is given in the next paragraph. Note that we do not distinguish between row- and column-vectors.

There is a large amount of literature available on polar and spherical coordinates. At this place, we only refer the reader to the overviews given in the encyclopedic books [Zei04] or [BSMM07].

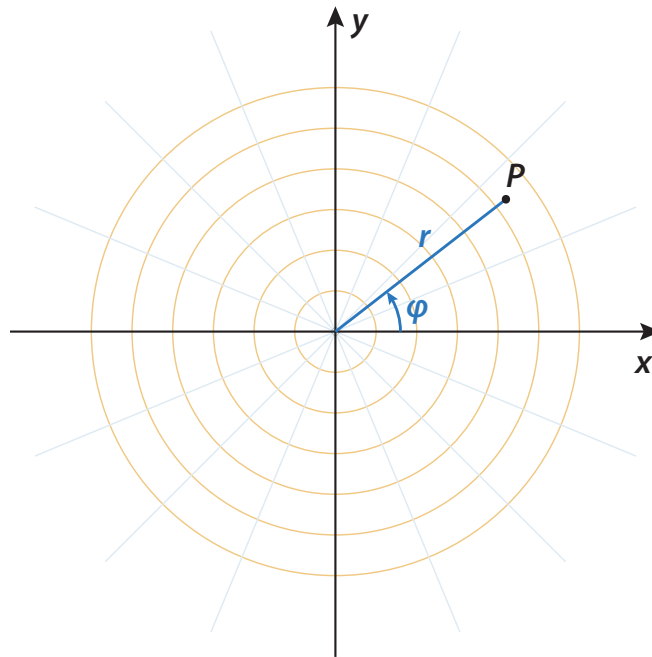


Figure 4.1: Representation of the point P in polar coordinates with radius r and angle φ .

4.3.1 Reminder on Polar Coordinates

4.3.1 Definition.

Let $(x, y) \in \mathbb{R}^2$, $(x, y) \neq 0$ be a point in the plane given in Cartesian coordinates. We call the pair $(r, \varphi) \in [0, \infty) \times [0, 2\pi)$ the representation of (x, y) in polar coordinates if

$$\begin{aligned} x &= r \cos \varphi \\ y &= r \sin \varphi. \end{aligned}$$

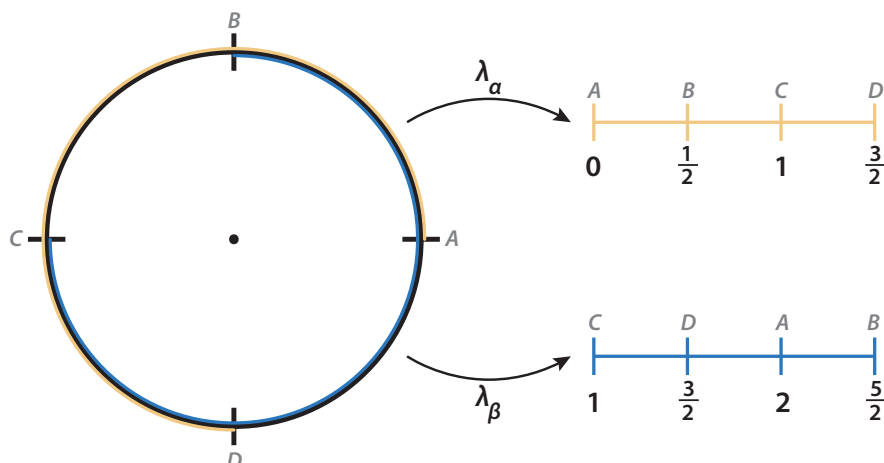
We will loosely write $r(x, y)$ and $\varphi(x, y)$ for the polar representation of a given (x, y) . Vice versa we also use $x(r, \varphi)$ and $y(r, \varphi)$. We have the following functional representation:⁴

4.3.2 Lemma.

We have the calculation rules

$$\begin{aligned} x(r, \varphi) &= r \cos \varphi \\ y(r, \varphi) &= r \sin \varphi \end{aligned} \quad \text{as well as} \quad \begin{aligned} r(x, y) &= \sqrt{x^2 + y^2} \\ \varphi(x, y) &= \begin{cases} \arccos \frac{x}{\sqrt{x^2 + y^2}} & \text{for } y \geq 0 \\ 2\pi - \arccos \frac{x}{\sqrt{x^2 + y^2}} & \text{for } y < 0 \end{cases}. \end{aligned}$$

⁴There are several ways to define a correspondence between polar and Cartesian coordinates, see the references. We chose a representation which is well suited to our subsequent application to the spherical zone.

Figure 4.2: Illustration of the charts λ_α and λ_β .

4.3.2 An Atlas for the Unit Circle

Let $S^1 := \{(x, y) \in \mathbb{R}^2; x^2 + y^2 = 1\}$ be the unit circle in \mathbb{R}^2 . We define the quadrants H_1, \dots, H_4 of the Cartesian coordinate system as

$$\begin{aligned} H_1 &:= \{(x, y) \in \mathbb{R}^2; x \geq 0, y \geq 0\}, & H_2 &:= \{(x, y) \in \mathbb{R}^2; x \leq 0, y \geq 0\}, \\ H_3 &:= \{(x, y) \in \mathbb{R}^2; x \leq 0, y \leq 0\}, & H_4 &:= \{(x, y) \in \mathbb{R}^2; x \geq 0, y \leq 0\}. \end{aligned}$$

We would like to make S^1 a manifold. Therefore we introduce the charts λ_α and λ_β defined as follows: The set $S^1 \setminus H_4$ is open; there we define the bijection

$$\begin{aligned} \lambda_\alpha : S^1 \setminus H_4 &\longrightarrow \left(0, \frac{3}{2}\right) \\ (x, y) &\longmapsto \lambda_\alpha(x, y) := \begin{cases} \frac{\arccos x}{\pi} & \text{for } y \geq 0 \\ 2 - \frac{\arccos x}{\pi} & \text{for } y < 0 \end{cases}. \end{aligned}$$

The idea is to use a polar representation of the unit circle, thus $r \equiv 1$. Moreover, in order to be able to define a periodic structure, we want the circle to correspond to the interval $[0, 2)$, thus we divide the polar angle φ by π . Analogously, we define for $S^1 \setminus H_2$

$$\begin{aligned} \lambda_\beta : S^1 \setminus H_2 &\longrightarrow \left(1, \frac{3}{2} + 1\right) \\ (x, y) &\longmapsto \lambda_\beta(x, y) := \lambda_\alpha(-x, -y) + 1. \end{aligned}$$

The idea of λ_β is to "continue" the parametrization defined on $S^1 \cap H_3$, see Figure 4.2 and the next lemma.

Keeping in mind the construction of the polar coordinates, we can easily give the inverse functions to λ_α and λ_β : With the notation of Lemma 4.3.2 one obtains

$$\begin{pmatrix} x \\ y \end{pmatrix} (\lambda_\alpha) = \begin{pmatrix} \cos(\pi\lambda_\alpha) \\ \sin(\pi\lambda_\alpha) \end{pmatrix} \quad \text{as well as} \quad \begin{pmatrix} x \\ y \end{pmatrix} (\lambda_\beta) = \begin{pmatrix} -\cos(\pi(\lambda_\beta - 1)) \\ -\sin(\pi(\lambda_\beta - 1)) \end{pmatrix}.$$

Since $S^1 \setminus H_4$ and $S^1 \setminus H_2$ cover S^1 and the charts defined above are smooth, $\mathcal{A} := \{(S^1/H_4, \lambda_\alpha), (S^1/H_2, \lambda_\beta)\}$ is an atlas for S^1 . We now show that this atlas satisfies the UC-condition:

4.3.3 Lemma.

For $(x, y) \in S^1 \cap H_3$ it holds $\lambda_\alpha(x, y) = \lambda_\beta(x, y)$, whereas for $(x, y) \in S^1 \cap H_1$ we have $\lambda_\alpha(x, y) = \lambda_\beta(x, y) - 2$.

Proof. The proof is based on the following calculation rule for the arcus cosine: It holds $\arccos(-x) = \pi - \arccos(x)$ and thus for $(x, y) \in S^1 \cap H_3$, i.e. $-y \geq 0$ we obtain

$$\begin{aligned} \lambda_\beta(x, y) &= \lambda_\alpha(-x, -y) + 1 = \frac{\arccos(-x)}{\pi} + 1 = \frac{\pi - \arccos(x)}{\pi} + 1 \\ &= 2 - \frac{\arccos(x)}{\pi} = \lambda_\alpha(x, y), \end{aligned}$$

whereas for $(x, y) \in S^1 \cap H_1$ ($\Rightarrow -y \leq 0$) it holds

$$\lambda_\beta(x, y) = \lambda_\alpha(-x, -y) + 1 = 2 - \frac{\arccos(-x)}{\pi} + 1 = 2 + \frac{\arccos(x)}{\pi} = \lambda_\alpha(x, y) + 2. \quad \blacklozenge$$

4.3.4 Lemma.

For $\varepsilon \in \{\frac{1}{n}; n \in \mathbb{N}\}$, the atlas \mathcal{A} satisfies the UC-criterion.

Proof. The assertion is more or less obvious; on $S^1 \cap H_3$ one has $\lambda_\alpha = \lambda_\beta + \varepsilon 0e_1$, whereas on $S^1 \cap H_1$ one gets

$$\lambda_\alpha = \lambda_\beta + \varepsilon \cdot \underbrace{\left(-\frac{2}{\varepsilon}e_1\right)}_{\in \mathbb{Z}}$$

(here $e_1 = 1$ is the unit vector in \mathbb{R}). \blacklozenge

4.3.3 Reminder on Spherical Coordinates

We recall the notion of spherical coordinates:⁵

4.3.5 Definition.

Let $(x, y, z) \in \mathbb{R}^3$, $(x, y, z) \neq 0$, $(x, y, z) \neq \pm(0, 0, 1)$ be a point in the 3-dimensional space given in Cartesian coordinates. We call the pair $(r, \varphi, \theta) \in [0, \infty) \times [0, 2\pi) \times (-\frac{\pi}{2}, \frac{\pi}{2})$ the

⁵Note again that different notions of these coordinate system exist in the literature. We choose one with the application in the last paragraph of this section in mind.

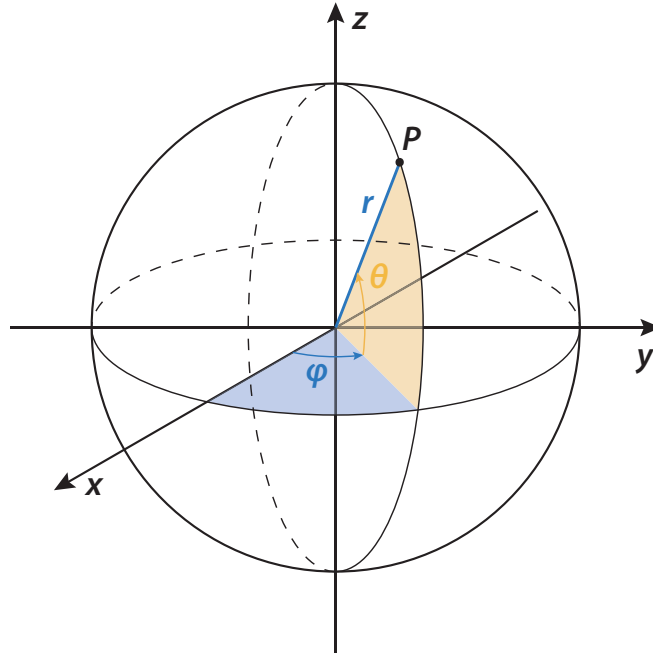


Figure 4.3: Representation of the point P in spherical coordinates with radius r and angles φ and θ .

representation of (x, y, z) in spherical coordinates if

$$\begin{aligned} x &= r \cos(\varphi) \cos(\theta) \\ y &= r \sin(\varphi) \cos(\theta) \\ z &= r \sin(\theta). \end{aligned}$$

For the inverse map, we have the representation

$$\begin{aligned} r(x, y, z) &= \sqrt{x^2 + y^2 + z^2} \\ \varphi(x, y, z) &= \begin{cases} \arccos \frac{x}{\sqrt{x^2 + y^2}} & \text{for } y \geq 0 \\ 2\pi - \arccos \frac{x}{\sqrt{x^2 + y^2}} & \text{for } y < 0 \end{cases} \\ \theta(x, y, z) &= \arcsin\left(\frac{z}{\sqrt{x^2 + y^2 + z^2}}\right). \end{aligned}$$

4.3.4 Application to a Spherical Zone

Let $S^2 := \{(x, y, z) \in \mathbb{R}^3; x^2 + y^2 + z^2 = 1\}$ be the unit sphere in \mathbb{R}^3 (hence $r \equiv 1$). Similarly to the 2-dimensional constructions we define the sets

$$\begin{aligned} H_1 &:= \{(x, y, z) \in \mathbb{R}^2; x \geq 0, y \geq 0\}, & H_2 &:= \{(x, y, z) \in \mathbb{R}^2; x \leq 0, y \geq 0\}, \\ H_3 &:= \{(x, y, z) \in \mathbb{R}^2; x \leq 0, y \leq 0\}, & H_4 &:= \{(x, y, z) \in \mathbb{R}^2; x \geq 0, y \leq 0\}. \end{aligned}$$

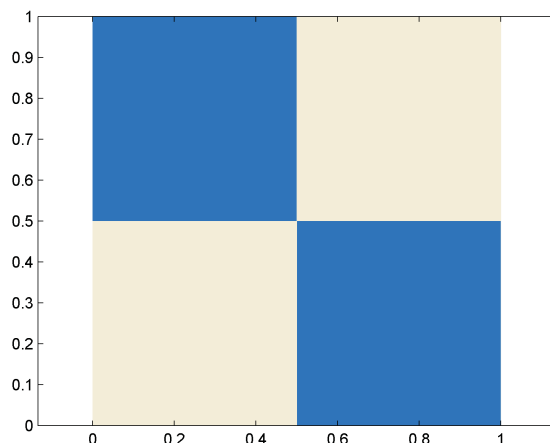


Figure 4.4: Illustration of the function D on the reference cell $[0, 1]^2$. The dark color corresponds to the value of 1, the light color to the value of 0.

We will consider the spherical zone

$$Z := \{(x, y, z) \in S^2; |z| \leq \frac{\sqrt{2}}{2}\}$$

with subsets $Z_1 := \{(x, y, z) \in Z; -\frac{1}{2} < z \leq \frac{\sqrt{2}}{2}\}$ as well as $Z_2 := \{(x, y, z) \in Z; -\frac{\sqrt{2}}{2} \leq z < \frac{1}{2}\}$. We want to give Z the structure of a manifold with boundary. Therefore we introduce the four charts $\tilde{\lambda}_{\alpha i}$ and $\tilde{\lambda}_{\beta i}$, $i = 1, 2$, as follows (see page 92 for the definition of \mathbb{R}_u^n):

$$\begin{aligned} \tilde{\lambda}_{\alpha 1} : Z_1 \setminus H_4 &\longrightarrow (0, \frac{3}{2}) \times (-\frac{2}{3} - 1, 0] \subset \mathbb{R}_{\begin{pmatrix} 0 \\ -1 \end{pmatrix}}^2 \\ (x, y, z) &\longmapsto \tilde{\lambda}_{\alpha}(x, y, z) := \begin{pmatrix} \lambda_{\alpha}(\frac{(x, y)}{\sqrt{x^2 + y^2}}) \\ \frac{\arcsin(z)}{\pi/4} - 1 \end{pmatrix}, \\ \tilde{\lambda}_{\alpha 2} : Z_2 \setminus H_4 &\longrightarrow (0, \frac{3}{2}) \times [0, \frac{2}{3} + 1) \subset \mathbb{R}_{\begin{pmatrix} 0 \\ 1 \end{pmatrix}}^2 \\ (x, y, z) &\longmapsto \tilde{\lambda}_{\alpha}(x, y, z) := \begin{pmatrix} \lambda_{\alpha}(\frac{(x, y)}{\sqrt{x^2 + y^2}}) \\ \frac{\arcsin(z)}{\pi/4} \end{pmatrix} \end{aligned}$$

as well as

$$\begin{aligned} \tilde{\lambda}_{\beta 1} : Z_1 \setminus H_1 &\longrightarrow (1, \frac{3}{2} + 1) \times (-\frac{2}{3} - 1, 0] \subset \mathbb{R}_{\begin{pmatrix} 0 \\ -1 \end{pmatrix}}^2 \\ (x, y, z) &\longmapsto \tilde{\lambda}_{\beta}(x, y, z) := \begin{pmatrix} \lambda_{\beta}(\frac{(x, y)}{\sqrt{x^2 + y^2}}) \\ \frac{\arcsin(z)}{\pi/4} - 1 \end{pmatrix}, \end{aligned}$$

$$\begin{aligned} \tilde{\lambda}_{\beta 2} : Z_2 \setminus H_1 &\longrightarrow (1, \frac{3}{2} + 1) \times [0, \frac{2}{3} + 1) \subset \mathbb{R}^2_{\binom{0}{1}} \\ (x, y, z) &\longmapsto \tilde{\lambda}_{\beta}(x, y, z) := \begin{pmatrix} \lambda_{\beta} \left(\frac{(x, y)}{\sqrt{x^2 + y^2}} \right) \\ \frac{\arcsin(z)}{\pi/4} + 1 \end{pmatrix} \end{aligned}$$

with $\lambda_{\alpha}, \lambda_{\beta}$ defined as above. The scaling is chosen in a way that the "latitude" is parametrized by $[0, 2)$ (corresponding to the unit circle case), and the "longitude" has arc length 2. In this connection, note that $\frac{\pi}{6} = \arcsin(\frac{1}{2})$ and $\frac{\pi}{4} = \arcsin(\frac{\sqrt{2}}{2})$, which accounts for the scaling factor in the second coordinate of $\tilde{\lambda}_i(x, y, z)$, $i \in \{\alpha 1, \alpha 2, \beta 1, \beta 2\}$.

Keeping the construction of the spherical coordinates as well as the inversion formulas for the unit circle in mind, one sees that the inverse maps are given by

$$\begin{aligned} \begin{pmatrix} x \\ y \\ z \end{pmatrix} \begin{pmatrix} \tilde{\lambda}_{\alpha 1}^1 \\ \tilde{\lambda}_{\alpha 1}^2 \end{pmatrix} &= \begin{pmatrix} \cos(\pi \tilde{\lambda}_{\alpha 1}^1) \cos(\frac{\pi}{4}(\tilde{\lambda}_{\alpha 1}^2 + 1)) \\ \sin(\pi \tilde{\lambda}_{\alpha 1}^1) \cos(\frac{\pi}{4}(\tilde{\lambda}_{\alpha 1}^2 + 1)) \\ \sin(\frac{\pi}{4}(\tilde{\lambda}_{\alpha 1}^2 + 1)) \end{pmatrix}, \\ \begin{pmatrix} x \\ y \\ z \end{pmatrix} \begin{pmatrix} \tilde{\lambda}_{\alpha 2}^1 \\ \tilde{\lambda}_{\alpha 2}^2 \end{pmatrix} &= \begin{pmatrix} \cos(\pi \tilde{\lambda}_{\alpha 2}^1) \cos(\frac{\pi}{4}(\tilde{\lambda}_{\alpha 2}^2 - 1)) \\ \sin(\pi \tilde{\lambda}_{\alpha 2}^1) \cos(\frac{\pi}{4}(\tilde{\lambda}_{\alpha 2}^2 - 1)) \\ \sin(\frac{\pi}{4}(\tilde{\lambda}_{\alpha 2}^2 - 1)) \end{pmatrix} \end{aligned}$$

as well as

$$\begin{aligned} \begin{pmatrix} x \\ y \\ z \end{pmatrix} \begin{pmatrix} \tilde{\lambda}_{\beta 1}^1 \\ \tilde{\lambda}_{\beta 1}^2 \end{pmatrix} &= \begin{pmatrix} -\cos(\pi(\tilde{\lambda}_{\beta 1}^1 - 1)) \cos(\frac{\pi}{4}(\tilde{\lambda}_{\beta 1}^2 + 1)) \\ -\sin(\pi(\tilde{\lambda}_{\beta 1}^1 - 1)) \cos(\frac{\pi}{4}(\tilde{\lambda}_{\beta 1}^2 + 1)) \\ \sin(\frac{\pi}{4}(\tilde{\lambda}_{\beta 1}^2 + 1)) \end{pmatrix}, \\ \begin{pmatrix} x \\ y \\ z \end{pmatrix} \begin{pmatrix} \tilde{\lambda}_{\beta 2}^1 \\ \tilde{\lambda}_{\beta 2}^2 \end{pmatrix} &= \begin{pmatrix} -\cos(\pi(\tilde{\lambda}_{\beta 2}^1 - 1)) \cos(\frac{\pi}{4}(\tilde{\lambda}_{\beta 2}^2 - 1)) \\ -\sin(\pi(\tilde{\lambda}_{\beta 2}^1 - 1)) \cos(\frac{\pi}{4}(\tilde{\lambda}_{\beta 2}^2 - 1)) \\ \sin(\frac{\pi}{4}(\tilde{\lambda}_{\beta 2}^2 - 1)) \end{pmatrix}. \end{aligned}$$

With the help of Lemma 4.3.3, one can easily see that the following identities hold:

$$\begin{aligned} \tilde{\lambda}_{\alpha 1} - \tilde{\lambda}_{\alpha 2} &= -\binom{0}{2} \quad \text{in } (Z_1 \cap Z_2) \setminus H_4 \\ \tilde{\lambda}_{\beta 1} - \tilde{\lambda}_{\beta 2} &= -\binom{0}{2} \quad \text{in } (Z_1 \cap Z_2) \setminus H_1 \\ \tilde{\lambda}_{\alpha 1} - \tilde{\lambda}_{\beta 1} &= \begin{cases} \binom{0}{0} & \text{in } Z_1 \cap H_3 \\ -\binom{2}{0} & \text{in } Z_1 \cap H_1 \end{cases} \\ \tilde{\lambda}_{\alpha 2} - \tilde{\lambda}_{\beta 2} &= \begin{cases} \binom{0}{0} & \text{in } Z_2 \cap H_3 \\ -\binom{2}{0} & \text{in } Z_2 \cap H_1 \end{cases} \\ \tilde{\lambda}_{\alpha 1} - \tilde{\lambda}_{\beta 2} &= \begin{cases} -\binom{0}{2} & \text{in } Z_1 \cap Z_2 \cap H_3 \\ -\binom{2}{2} & \text{in } Z_1 \cap Z_2 \cap H_1 \end{cases} \\ \tilde{\lambda}_{\alpha 2} - \tilde{\lambda}_{\beta 1} &= \begin{cases} -\binom{0}{2} & \text{in } Z_1 \cap Z_2 \cap H_3 \\ -\binom{2}{2} & \text{in } Z_1 \cap Z_2 \cap H_1 \end{cases}. \end{aligned}$$

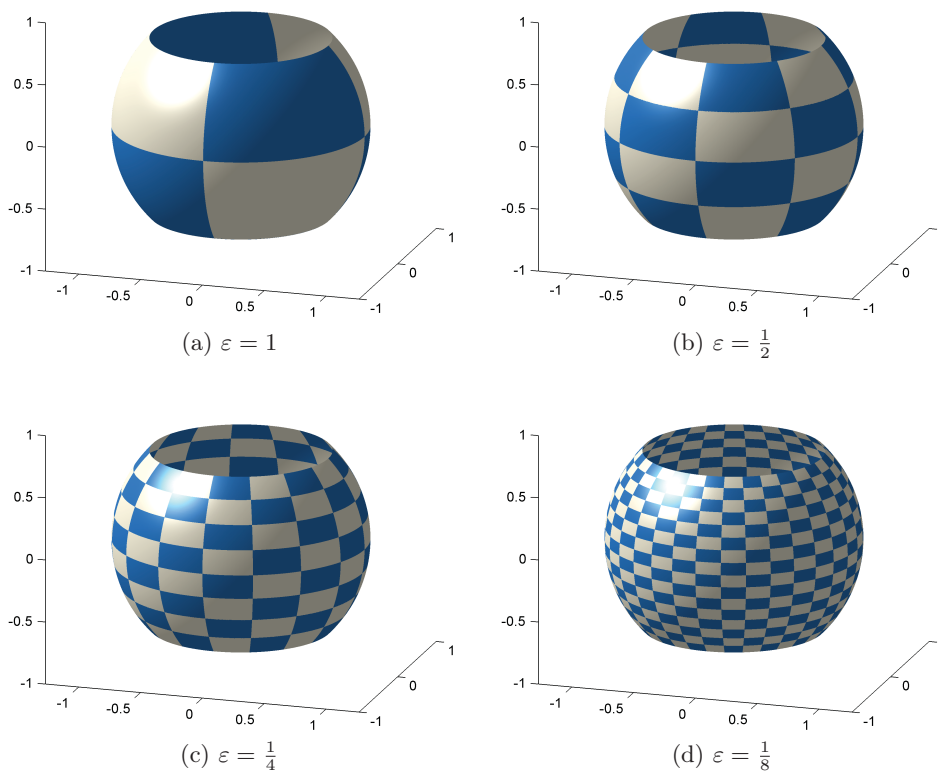


Figure 4.5: Illustration of periodicity on a spherical zone: We plot the function D^ε as defined on page 120 with respect to the atlas constructed in Section 4.3.4. The dark color corresponds to the value of 1, the light color to the value of 0.

4.3.6 Lemma.

For $\varepsilon \in \{\frac{1}{n}; n \in \mathbb{N}\}$, the atlas

$$\mathcal{A} := \{(Z_1 \setminus H_4, \tilde{\lambda}_{\alpha 1}), (Z_2 \setminus H_4, \tilde{\lambda}_{\alpha 2}), (Z_1 \setminus H_1, \tilde{\lambda}_{\beta 1}), (Z_2 \setminus H_1, \tilde{\lambda}_{\beta 2})\}$$

satisfies the UC-criterion.

Proof. The calculation from above shows that for each choice of $i, j \in \{\alpha 1, \alpha 2, \beta 1, \beta 2\}$ there exists $\delta_{ij}, \gamma_{ij} \in \{-1, 0, 1\}$ such that $\tilde{\lambda}_i = \tilde{\lambda}_j + 2\delta_{ij}e_1 + 2\gamma_{ij}e_2$ on the domain where the charts overlap. Thus

$$\tilde{\lambda}_i = \tilde{\lambda}_j + \varepsilon \cdot \frac{2\delta_{ij}}{\varepsilon} e_1 + \varepsilon \cdot \frac{2\gamma_{ij}}{\varepsilon} e_2.$$

Since $\frac{2\delta_{ij}}{\varepsilon}, \frac{2\gamma_{ij}}{\varepsilon} \in \mathbb{Z}$ for all $\varepsilon \in \{\frac{1}{n}; n \in \mathbb{N}\}$, the UC-criterion is fulfilled for the atlas \mathcal{A} . \blacklozenge

4.3.7 Remark.

As a note, we would like to point out that a consideration of a full sphere is not possible without further technicalities. This is not a limitation of the method presented in this chapter, but a limitation of the spherical coordinates itself. They do not allow a unique representation of the north- and south-poles, hence of the full sphere.

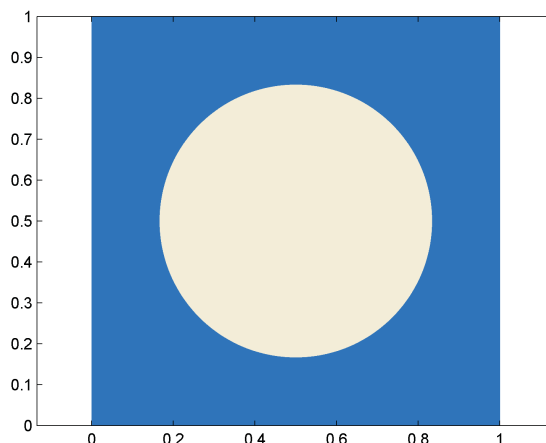


Figure 4.6: Illustration of another choice of the Function D on the reference cell $[0, 1]^2$. The dark color corresponds to the value of 1, the light color to the value of 0.

4.3.5 Example for a Periodic Function on a Spherical Zone

In order to illustrate what we mean by a function to be “periodic” in non-flat coordinates, or $\varepsilon_{\mathcal{A}}$ -periodic, choose a function $D : Y \rightarrow \mathbb{R}$ which is periodically extended (in the usual sense). For example, D might represent heat conductivity or permeability of a composite material. Then define for $\varepsilon \in \{\frac{1}{n}; n \in \mathbb{N}\}$

$$D^\varepsilon : Z \rightarrow \mathbb{R}$$

$$x \mapsto D^\varepsilon(x) = D\left(\left\{\frac{\tilde{\lambda}_i(x)}{\varepsilon}\right\}\right)$$

for x in the domain of $\tilde{\lambda}_i$, $i \in \{\alpha 1, \alpha 2, \beta 1, \beta 2\}$. Due to the UC-criterion (see Lemma 4.2.3), the function D^ε is well defined on Z . For the unfolding of that function, we obtain $\mathcal{T}_{\mathcal{A}}^\varepsilon(D^\varepsilon)(x, y) = D(y)$. This clarifies the notion that a function is periodic with respect to some chart (or atlas).

To give an even more concrete example, we specify the function D as

$$D(y) = \begin{cases} 0 & \text{for } 0 \leq y_1 < \frac{1}{2} \text{ and } 0 \leq y_2 < \frac{1}{2} \\ 0 & \text{for } \frac{1}{2} \leq y_1 < 1 \text{ and } \frac{1}{2} \leq y_2 < 1 \\ 1 & \text{for } 0 \leq y_1 < \frac{1}{2} \text{ and } \frac{1}{2} \leq y_2 < 1 \\ 1 & \text{for } \frac{1}{2} \leq y_1 < 1 \text{ and } 0 \leq y_2 < \frac{1}{2} \end{cases}.$$

This function is illustrated in Figure 4.4. Applied to the spherical zone, we obtain Figure 4.5. Another choice for D is given in Figure 4.6, with the corresponding spherical zones shown in Figure 4.7.

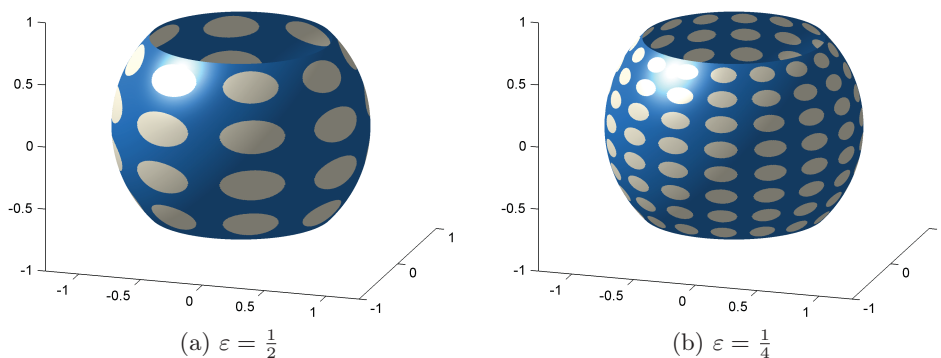


Figure 4.7: Illustration of periodicity on a spherical zone: This structure is obtained by a similar function D^ε , where the corresponding "base"-function is depicted in Figure 4.6. The dark color corresponds to the value of 1, the light color to the value of 0.

4.4 Application to a Reaction-Diffusion-Problem

In this section we show how one can apply the results for the unfolding operator $\mathcal{T}_{\mathcal{A}}^\varepsilon$ to a simple (standard) elliptic homogenization problem. One can think of this problem as the stationary solution to a heat conduction or reaction-diffusion problem on an $\varepsilon_{\mathcal{A}}$ -periodic manifold.

To fix the notation, let $M \subset \mathbb{R}^m$ be a n -dimensional Riemannian manifold (with boundary) of class \mathcal{C}^2 . We assume the boundary ∂M of M to be sufficiently smooth. Denote the atlas by

$$\mathcal{A} = \{(U_\alpha, \phi_\alpha); \alpha \in I\}$$

with some index set I and the charts $\phi_\alpha : U_\alpha \rightarrow V_\alpha$. On M , let there be given a smooth Riemannian metric $g_M \in \Gamma(TM^* \otimes TM^*)$. Moreover, denote by $Y := [0, 1]^n$ the reference cell in \mathbb{R}^n . Finally, we assume that the structure we are investigating is $\varepsilon_{\mathcal{A}}$ -periodic, where the atlas \mathcal{A} fulfills the UC-criterion.

As an example, the reader can keep the spherical zone together with the atlas from the preceding section in mind.

Let $D \in \mathcal{C}_{\#}(Y)$ be a fixed periodic function such that $0 < d_0 \leq D \leq D_0$ for some positive constants d_0 and D_0 . For $\varepsilon > 0$ we define the function $D^\varepsilon : M \rightarrow \mathbb{R}$ via $D^\varepsilon(x) := D\left(\left\{\frac{\phi_\alpha(x)}{\varepsilon}\right\}\right)$ for $x \in U_\alpha$. Due to the UC-condition we obtain $D\left(\left\{\frac{\phi_\alpha(x)}{\varepsilon}\right\}\right) = D\left(\left\{\frac{\phi_\beta(x)}{\varepsilon}\right\}\right)$ for $x \in U_\alpha \cap U_\beta$. Thus, the function D^ε is well-defined. D^ε can be interpreted as heat conductivity or diffusivity of M for fixed $\varepsilon > 0$.

Let $c > 0$ be a constant and let $f \in L^2(M)$ be a source term. We are considering the problem: Find $u^\varepsilon \in H_0^1(M)$ with

$$-\operatorname{div}_M(D^\varepsilon \nabla_M u^\varepsilon) + cu^\varepsilon = f \quad \text{in } M \quad (4.11a)$$

$$u^\varepsilon = 0 \quad \text{on } \partial M. \quad (4.11b)$$

The weak formulation of this problem reads as

$$\int_M D^\varepsilon g_M(\nabla_M u^\varepsilon, \nabla_M \varphi) \, d\text{vol}_M + \int_M c u^\varepsilon \varphi \, d\text{vol}_M = \int_M f \varphi \, d\text{vol}_M \quad \forall \varphi \in H_0^1(M). \quad (4.12)$$

Formally, the weak formulation is obtained by multiplication of Equation (4.11a) with a suitable test function φ and subsequent integration by parts, taking into account the boundary condition (4.11b). Existence of a solution for fixed $\varepsilon > 0$ is obtained easily by using the Lax-Milgram lemma.

4.4.1 A-priori Estimates and Limits

We have the following a-priori estimates:

4.4.1 Lemma.

There exists a constant $C > 0$ independent of ε such that

$$\|u^\varepsilon\|_{H^1(M)} \leq C.$$

Proof. We use $\varphi = u^\varepsilon$ as a test function in the weak formulation (4.12). Due to the bounds on D , we obtain

$$d_0 \|\nabla_M u^\varepsilon\|_{L^2(TM)}^2 + c \|u^\varepsilon\|_{L^2(M)}^2 \leq C_\delta \|f\|_{L^2(M)}^2 + \delta \|u^\varepsilon\|_{L^2(M)}^2.$$

Choosing $\delta = \frac{1}{2}c$, we obtain the desired bound with $C^2 = \frac{C_\delta \|f\|_{L^2(M)}^2}{\min\{d_0, \frac{c}{2}\}}$. \blacklozenge

Theorem 4.2.35 and the usual compactness results and embeddings now show that there exists a $u \in H^1(M)$ and a $\hat{u} \in L^2(M; H_{\#}^1(Y))$ such that along a subsequence

$$\begin{aligned} u^\varepsilon &\rightharpoonup u && \text{in } H^1(M) \\ u^\varepsilon &\rightarrow u && \text{in } L^2(M) \\ \mathcal{T}_{\mathcal{A}}^\varepsilon(u^\varepsilon) &\rightarrow u && \text{in } L^2(M \times Y) \\ \mathcal{T}_{\mathcal{A}}^\varepsilon(\nabla_M u^\varepsilon) &\rightarrow (\nabla_M u)_Y + \nabla_Y^{(x)} \hat{u} && \text{in } L^2(M; L^2TY). \end{aligned}$$

4.4.2 Lemma.

For the limit u we have $u \in H_0^1(M)$, that is $u = 0$ on ∂M .

Proof. We have the embeddings $H^1(M) \hookrightarrow H^{\frac{1}{2}}(\partial M) \hookrightarrow L^2(\partial M)$, where the last embedding is compact. This gives $u^\varepsilon \rightarrow u$ in $L^2(\partial M)$, i.e.

$$u|_{\partial M} = \lim_{\varepsilon \rightarrow 0} (u^\varepsilon|_{\partial M}) = 0$$

in the sense of $L^2(\partial M)$. \blacklozenge

4.4.2 The Limit Problem

In order to derive the limit problem, we choose two test functions $\varphi_1 \in C_0^\infty(M)$ and $\varphi_2 \in C_0^\infty(M; C_\#^\infty(Y))$ and define

$$\varphi^\varepsilon(x) := \varphi_1(x) + \varepsilon \varphi_2 \left(x, \left\{ \frac{\phi_\alpha(x)}{\varepsilon} \right\} \right) \quad \text{for } x \in U_\alpha.$$

We need the following auxiliary result:

4.4.3 Lemma.

We have

- $\mathcal{T}_{\mathcal{A}}^\varepsilon(D^\varepsilon)(x, y) = D(y)$,
- $\mathcal{T}_{\mathcal{A}}^\varepsilon(\nabla_M \varphi^\varepsilon) \longrightarrow (\nabla_M \varphi_1)_Y + \nabla_Y^{(x)} \varphi_2$ in $L^\infty(M \times Y)$,
- $\mathcal{T}_{\mathcal{A}}^\varepsilon(\varphi^\varepsilon) \longrightarrow \varphi_1$ in $L^\infty(M \times Y)$.

Proof. Keeping Remark 4.2.7 about the explicit form of $\mathcal{T}_{\phi_\alpha}^\varepsilon$ in mind, we obtain for $x \in U_\alpha$

$$\mathcal{T}_{\mathcal{A}}^\varepsilon(D^\varepsilon)(x, y) = D \left(\left(\frac{\varepsilon \left[\frac{\phi_\alpha(x)}{\varepsilon} \right] + \varepsilon y}{\varepsilon} \right) \right) = D(y).$$

Next, we have due to the unfolding rules for gradients (see Proposition 4.2.16)

$$\mathcal{T}_{\mathcal{A}}^\varepsilon(\nabla_M \varphi^\varepsilon) = \mathcal{T}_{\mathcal{A}}^\varepsilon(\nabla_M \varphi_1) + \nabla_Y^{(x, \varepsilon)} \mathcal{T}_{\mathcal{A}}^\varepsilon(\varphi_2).$$

For the first term on the right hand side we obtain for $x \in U_\alpha$ the convergence

$$\begin{aligned} \mathcal{T}_{\phi_\alpha}^\varepsilon(\nabla_M \varphi_1)(x, y) &= \mathcal{T}_{\phi_\alpha}^\varepsilon \left(\sum_{i,j} g^{ij} \frac{\partial \varphi_1}{\partial x^i} \frac{\partial}{\partial x^j} \right) (x, y) \\ &= \sum_{i,j} \underbrace{\mathcal{T}_{\phi_\alpha}^\varepsilon(g^{ij})(x, y)}_{\rightarrow g^{ij}(x)} \underbrace{\mathcal{T}_{\phi_\alpha}^\varepsilon \left(\frac{\partial \varphi_1}{\partial x^i} \right) (x, y)}_{\rightarrow \frac{\partial \varphi_1}{\partial x^i}} \frac{\partial}{\partial y^j} \\ &\longrightarrow \sum_{i,j} g^{ij}(x) \frac{\partial \varphi_1}{\partial x^i} \frac{\partial}{\partial y^j} = (\nabla_M \varphi_1)_Y \end{aligned}$$

in $\mathcal{C}(M \times Y)$. For the second term, we have due to Remark 4.2.7

$$\begin{aligned} \nabla_Y^{(x, \varepsilon)} \mathcal{T}_{\phi_\alpha}^\varepsilon(\varphi_2)(x, y) &= \nabla_Y^{(x, \varepsilon)} \varphi_2 \left(\phi_\alpha^{-1} \left(\varepsilon \left[\frac{\phi_\alpha(x)}{\varepsilon} \right] + \varepsilon y \right), y \right) \\ &= \sum_{i,j} \mathcal{T}_{\phi_\alpha}^\varepsilon(g^{ij})(x, y) \frac{\partial \varphi_2}{\partial y^i} \left(\phi_\alpha^{-1} \left(\varepsilon \left[\frac{\phi_\alpha(x)}{\varepsilon} \right] + \varepsilon y \right), y \right) \frac{\partial}{\partial y^j}, \end{aligned}$$

where $\frac{\partial \varphi_2}{\partial y^i}$ has to be understood as derivative with respect to the second variable. Since $\mathcal{T}_{\phi_\alpha}^\varepsilon(g^{ij}) \rightarrow g^{ij}$ as well as

$$\phi_\alpha^{-1}\left(\underbrace{\varepsilon \left[\frac{\phi_\alpha(x)}{\varepsilon} \right]}_{\rightarrow \phi_\alpha(x)} + \underbrace{\varepsilon y}_{\rightarrow 0}\right) \longrightarrow \phi_\alpha^{-1}(\phi_\alpha(x)) = x \quad (4.13)$$

(due to the continuity of ϕ_α), we obtain by using the continuity of $\frac{\partial \varphi_2}{\partial y^i}$ that

$$\nabla_Y^{(x,\varepsilon)} \mathcal{T}_{\phi_\alpha}^\varepsilon(\varphi_2)(x, y) \longrightarrow \sum_{i,j} g^{ij}(x) \frac{\partial \varphi_2}{\partial y^i}(x, y) \frac{\partial}{\partial y^j} = \nabla_Y^{(x)} \varphi_2(x, y).$$

The last assertion follows along the same lines by using the boundedness of φ_2 , Remark 4.2.7 and equation (4.13). \blacklozenge

We choose $\varphi = \varphi^\varepsilon$ as a test function in the weak formulation (4.12). Since all the terms appearing under the integrals in (4.12) are bounded in $L^1(M)$ independently of ε , these terms satisfy the UCM-criterion, and we can unfold the integral identity with respect to \simeq . Keeping in mind the rules for products (Lemma 4.2.9), for the unfolding of gradients (Proposition 4.2.16) and for the unfolding of the Riemannian metric (Proposition 4.2.15), we obtain the expression

$$\begin{aligned} & \frac{1}{|Y|} \int_{M \times Y} D(y) g_Y^{(x,\varepsilon)} \left(\mathcal{T}_{\mathcal{A}}^\varepsilon(\nabla_M u^\varepsilon), \mathcal{T}_{\mathcal{A}}^\varepsilon(\nabla_M \varphi^\varepsilon) \right)(x, y) \mathcal{T}_{\mathcal{A}}^\varepsilon(\sqrt{|G|})(x, y) \, dy \, dx \\ & + \frac{1}{|Y|} \int_{M \times Y} c \mathcal{T}_{\mathcal{A}}^\varepsilon(u^\varepsilon)(x, y) \mathcal{T}_{\mathcal{A}}^\varepsilon(\varphi^\varepsilon)(x, y) \mathcal{T}_{\mathcal{A}}^\varepsilon(\sqrt{|G|})(x, y) \, dy \, dx \\ & = \frac{1}{|Y|} \int_{M \times Y} \mathcal{T}_{\mathcal{A}}^\varepsilon(f)(x, y) \mathcal{T}_{\mathcal{A}}^\varepsilon(\varphi^\varepsilon)(x, y) \mathcal{T}_{\mathcal{A}}^\varepsilon(\sqrt{|G|})(x, y) \, dy \, dx + r(\varepsilon) \end{aligned}$$

with $r(\varepsilon) \rightarrow 0$ as $\varepsilon \rightarrow 0$. Taking the limit on both sides and keeping in mind the convergence statements from above, one obtains the *two-scale formulation of the limit problem*

$$\begin{aligned} & \frac{1}{|Y|} \int_{M \times Y} D(y) g_Y^{(x)} \left((\nabla_M u)_Y + \nabla_Y^{(x)} \hat{u}, (\nabla_M \varphi_1)_Y + \nabla_Y^{(x)} \varphi_2 \right) \, dy \, d\text{vol}_M \\ & + \int_M c u \varphi_1 \, dy \, d\text{vol}_M = \int_M f \varphi_1 \, dy \, d\text{vol}_M. \end{aligned} \quad (4.14)$$

By density of test functions, this holds for all $(\varphi_1, \varphi_2) \in H_0^1(M) \times L^2(M; H_{\#}^1(Y))$. Since the structure of the limit problem is not clear due to the first term, we give the strong formulation in the next theorem:

4.4.4 Theorem.

The limit function u satisfies the homogenized equation

$$\begin{aligned} -\operatorname{div}_M(B \nabla_M u) + cu &= f \quad \text{in } M \\ u &= 0 \quad \text{on } \partial M, \end{aligned} \quad (4.15)$$

where the linear operator B is constructed with the help of the following parameter-dependent cell problem: For fixed $x \in M$ and $i = 1, \dots, n$, find $w_i(x) \in H_{\#}^1(Y) \setminus \mathbb{R}$, solution of

$$\begin{aligned} -\operatorname{div}_Y^{(x)}(D(y) \nabla_Y^{(x)} w_i(x, y)) &= \operatorname{div}_Y^{(x)}(D(y) \frac{\partial}{\partial y^i}) \quad \text{in } Y \\ y &\longmapsto w_i(x, y) \quad \text{is } Y\text{-periodic.} \end{aligned}$$

Then we define a tensor A as $A_i^k(x, y) := \sum_j g^{kj}(x) \frac{\partial w_i}{\partial y^j}(x, y)$, and the linear operator B as

$$B_i^k(x) := \int_Y D(y) (\delta_i^k + A_i^k(x, y)) \, dy.$$

Moreover, the corresponding tensor \tilde{B} with lowered index, i.e. $\tilde{B}_{ki} := \sum_j g_{kj} B_i^j$ is symmetric and positive definite.

Proof. Step 1 The cell problem:

We start with the weak formulation (4.14). Choosing $\varphi_1 = 0$, one obtains $\frac{1}{|Y|} \int_{M \times Y} D(y) g_Y^{(x)} \left((\nabla_M u)_Y + \nabla_Y^{(x)} \hat{u}, \nabla_Y^{(x)} \varphi_2 \right) dy \, d\operatorname{vol}_M = 0$. Upon integration by parts, this yields

$$-\int_{M \times Y} \operatorname{div}_Y^{(x)} \left(D \left[(\nabla_M u)_Y + \nabla_Y^{(x)} \hat{u} \right] \right) \varphi_2 \, dy \, d\operatorname{vol}_M = 0 \quad \forall \varphi_2 \in L^2(M; H_{\#}^1(Y)),$$

whose strong form is given by: For fixed $x \in M$, find $\hat{u}(x) \in H_{\#}^1(Y)$ such that

$$\begin{aligned} -\operatorname{div}_Y^{(x)}(D(y) \nabla_Y^{(x)} \hat{u}(x, y)) &= \operatorname{div}_Y^{(x)}(D(y) (\nabla_M u)_Y(x, y)) \quad \text{in } M \\ y &\longmapsto \hat{u}(x, y) \quad \text{is } Y\text{-periodic.} \end{aligned} \quad (4.16)$$

To "factor out" the term $(\nabla_M u)_Y$, we construct a solution of the cell problem for $i = 1, \dots, n$, given by: Find a solution $w_i(x) \in H_{\#}^1(Y) \setminus \mathbb{R}$ of

$$\begin{aligned} -\operatorname{div}_Y^{(x)}(D(y) \nabla_Y^{(x)} w_i(x)(y)) &= \operatorname{div}_Y^{(x)}(D(y) \frac{\partial}{\partial y^i}) \quad \text{in } Y \\ y &\longmapsto w_i(x)(y) \quad \text{is } Y\text{-periodic.} \end{aligned}$$

The weak formulation of this problem

$$\int_Y D(y)g_Y^{(x)}\left(\nabla_Y^{(x)} w_i, \nabla_Y^{(x)} \varphi\right) dy = - \int_Y D(y)g_Y^{(x)}\left(\frac{\partial}{\partial y^i}, \nabla_Y^{(x)} \varphi\right) dy \quad \forall \varphi \in H_{\#}^1(Y) \setminus \mathbb{R} \quad (4.17)$$

is well defined in the indicated function space and thus a solution w^i exists, which is unique up to constants (see also Lemma 4.4.6 and Section 4.4.3 for a detailed investigation of the cell problem). Define $\hat{u}(x, y) = \sum_i w_i(x, y)(\nabla_M u(x))^i$. The following calculation shows that this \hat{u} is a solution of (4.16): While the periodicity in the variable y is obvious, we have

$$\begin{aligned} -\operatorname{div}_Y^{(x)}(D \nabla_Y^{(x)} \hat{u}) &= - \sum_{i=1}^n (\nabla_M u)^i \operatorname{div}_Y^{(x)}(D \nabla_Y^{(x)} w_i) \\ &= \operatorname{div}_Y^{(x)}\left(D \sum_{i=1}^n (\nabla_M u)^i \frac{\partial}{\partial y^i}\right) = \operatorname{div}_Y^{(x)}(D(\nabla_M u)_Y). \end{aligned}$$

Step 2 The homogenized problem:

We now choose $\varphi_2 = 0$ in (4.14) to obtain $\frac{1}{|Y|} \int_{M \times Y} D(y)g_Y^{(x)}\left((\nabla_M u)_Y + \nabla_Y^{(x)} \hat{u}, (\nabla_M \varphi_1)_Y\right) dy \operatorname{dvol}_M + \int_M c u \varphi_1 dy \operatorname{dvol}_M = \int_M f \varphi_1 dy \operatorname{dvol}_M$. Inserting \hat{u} and using Lemma 4.2.33, this is equivalent to

$$\begin{aligned} \frac{1}{|Y|} \int_{M \times Y} D(y)g_M\left(\nabla_M u + \sum_{i=1}^n (\nabla_M u)^i (\nabla_Y^{(x)} w_i)_M, \nabla_M \varphi_1\right) dy \operatorname{dvol}_M \\ + \int_M c u \varphi_1 dy \operatorname{dvol}_M = \int_M f \varphi_1 dy \operatorname{dvol}_M. \end{aligned}$$

Upon an integration by parts, we obtain the following strong form:

$$\begin{aligned} -\operatorname{div}_M\left(\int_Y D[\nabla_M u + \sum_{i=1}^n (\nabla_M u)^i (\nabla_Y^{(x)} w_i)_M] dy\right) + c u = f \quad \text{in } M \\ u = 0 \quad \text{on } \partial M. \end{aligned}$$

It remains to characterize the expression

$$K(x, y) := D(y)[\nabla_M u(x) + \sum_{i=1}^n (\nabla_M u(x))^i (\nabla_Y^{(x)} w_i(x, y))_M].$$

Written component-wise, we obtain

$$\begin{aligned} K(x, y) &= \sum_k D(y)\left((\nabla_M u(x))^k + \sum_{i,j} (\nabla_M u(x))^i g^{kj}(x) \frac{\partial w_i(x, y)}{\partial y^j}\right) \frac{\partial}{\partial x^k} \\ &= \sum_{k,i,j} D(y)\left(\delta_i^k (\nabla_M u(x))^i + (\nabla_M u(x))^i g^{kj}(x) \frac{\partial w_i(x, y)}{\partial y^j}\right) \frac{\partial}{\partial x^k} \end{aligned}$$

$$= \sum_{k,i} D(y) \left(\delta_i^k + \sum_j g^{kj}(x) \frac{\partial w_i(x,y)}{\partial y^j} \right) (\nabla_M u(x))^i \frac{\partial}{\partial x^k}.$$

Another expression is given by $K(x, y) = \sum_{k,i} D(y) (\delta_i^k + (\nabla_Y^{(x)} w_i(x, y))^k) (\nabla_M u(x))^i \frac{\partial}{\partial x^k}$. The part $x \mapsto \delta_i^k + \sum_j g^{kj}(x) \frac{\partial w_i(x,y)}{\partial y^j}$ corresponds to a linear map in tensorial notation. We set $A(x, y) := [\sum_j g^{kj}(x) \frac{\partial w_i(x,y)}{\partial y^j}]_i^k$. Since $\text{Id} = [\delta_i^k]_i^k$, we can apply $(\text{Id} + A(\cdot, y))$ to $\nabla_M u$ to obtain

$$K(\cdot, y) = D(y)(\text{Id} + A)(\nabla_M u).$$

Integrating over y , we get the expression $B \nabla_M u$ as stated in the theorem. Note however that at this point we do not know if B is a real tensor, i.e. invariant under coordinate changes. This is due to the fact that the lower index i stems from an index number (of the function w_i) and not from a tensorial expression itself. On the other hand, the upper index k stems from a tensorial expression, and thus B is contravariant in this index.

We overcome this difficulty with the result of step 3: There it is shown that the expression $\tilde{B} = [\tilde{B}_{ki}]$, corresponding to B with a lowered index k , is symmetric. Since B is contravariant in k , \tilde{B} is covariant in k and thus, due to the symmetry, also in i . Therefore B has to be covariant in i as well, and B is finally a well-defined mixed tensor corresponding to a linear map acting on vector fields.

Step 3 Properties of the homogenized linear operator:

Define $\tilde{B}_{ki} = \sum_j g_{kj} B_i^j$. In order to show that \tilde{B} is symmetric, we start with the weak formulation of the cell problem (4.17) for $i = \alpha$, where we use $\varphi = w_\beta$ as a test function ($\alpha, \beta \in \{1, \dots, n\}$),⁶

$$\int_Y D(y) g_Y^{(x)} \left(\nabla_Y^{(x)} w_\alpha, \nabla_Y^{(x)} w_\beta \right) dy = - \int_Y D(y) g_Y^{(x)} \left(\frac{\partial}{\partial y^\alpha}, \nabla_y^{(x)} w_\beta \right) dy.$$

In component notation, this reads as

$$\sum_{i,j} \int_Y D(y) g_{ij} (\nabla_Y^{(x)} w_\alpha)^i (\nabla_Y^{(x)} w_\beta)^j dy = - \sum_j \int_Y D(y) g_{\alpha j} (\nabla_Y^{(x)} w_\beta)^j dy.$$

Since $g_{\alpha j} = \sum_i \delta_\alpha^i g_{ij}$, above expression is equivalent to

$$\sum_{i,j} \int_Y D(y) g_{ij} [(\nabla_Y^{(x)} w_\alpha)^i + \delta_\alpha^i] (\nabla_Y^{(x)} w_\beta)^j dy = 0. \quad (4.18)$$

Now we have

$$\begin{aligned} \tilde{B}_{\beta\alpha} &= \sum_i g_{\beta i} \left[\int_Y D(y) (\text{Id} + A(\cdot, y)) dy \right]_\alpha^i = \sum_i \int_Y D(y) g_{\beta i} \left(\delta_\alpha^i + \sum_k g^{ik} \frac{\partial w_\alpha}{\partial y^k} \right) dy \\ &= \sum_i \int_Y D(y) g_{\beta i} \left(\delta_\alpha^i + (\nabla_Y^{(x)} w_\alpha)^i \right) dy = \sum_{i,j} \int_Y D(y) \delta_\beta^j g_{ij} \left(\delta_\alpha^i + (\nabla_Y^{(x)} w_\alpha)^i \right) dy. \end{aligned}$$

⁶We switch to greek letters for the index of the functions w in order to make the following considerations more readable.

Adding the expression (4.18), we get

$$\tilde{B}_{\beta\alpha} = \sum_{i,j} \int_Y D(y) g_{ij} \left(\delta_{\beta}^j + (\nabla_Y^{(x)} w_{\beta})^j \right) \left(\delta_{\alpha}^i + (\nabla_Y^{(x)} w_{\alpha})^i \right) dy.$$

We easily see that $\tilde{B}_{\beta\alpha} = \tilde{B}_{\alpha\beta}$. Since $\alpha, \beta \in \{1, \dots, n\}$ is arbitrary, \tilde{B} is symmetric.

Next, we show that \tilde{B} is positive. To this end, let V be a vector field on M . Then

$$\begin{aligned} \sum_{\alpha,\beta} \tilde{B}_{\alpha\beta} V^{\alpha} V^{\beta} &= \sum_{i,j,\alpha,\beta} \int_Y D(y) g_{ij} \left(\delta_{\beta}^j + (\nabla_Y^{(x)} w_{\beta})^j \right) \left(\delta_{\alpha}^i + (\nabla_Y^{(x)} w_{\alpha})^i \right) V^{\alpha} V^{\beta} dy \\ &= \sum_{i,j} \int_Y D(y) g_{ij} \sum_{\beta} V^{\beta} \left(\delta_{\beta}^j + (\nabla_Y^{(x)} w_{\beta})^j \right) \sum_{\alpha} V^{\alpha} \left(\delta_{\alpha}^i + (\nabla_Y^{(x)} w_{\alpha})^i \right) dy \quad (4.19) \\ &= \sum_{i,j} \int_Y D(y) g_{ij} \zeta^i \zeta^j dy \geq 0 \end{aligned}$$

since D is positive and the g_{ij} 's are the coefficients of a Riemannian metric. Here $\zeta^i = \sum_{\beta} V^{\beta} \left(\delta_{\beta}^j + (\nabla_Y^{(x)} w_{\beta})^j \right)$.

We show that \tilde{B} is definite: Let V again be a vector field on M and assume that $V \neq 0$. Let $\sum_{\alpha,\beta} \tilde{B}_{\alpha\beta} V^{\alpha} V^{\beta} = 0$. Keeping in mind the definition of \tilde{B} , the index-free version of the second line of the previous considerations (4.19) reads as

$$\sum_{\alpha,\beta} \tilde{B}_{\alpha\beta} V^{\alpha} V^{\beta} = \int_Y D(y) g_M((\text{Id} + A)V, V) dy = \int_Y D(y) g_M((\text{Id} + A)V, (\text{Id} + A)V) dy$$

The assumption $\sum_{\alpha,\beta} \tilde{B}_{\alpha\beta} V^{\alpha} V^{\beta} = 0$ is equivalent to $g_M((\text{Id} + A)V, (\text{Id} + A)V) = 0$ due to the positivity of D . Using the transport operator, this is equivalent to $g_Y^{(x)} \left((\widetilde{\text{Id} + A})(V)_Y, (\widetilde{\text{Id} + A})(V)_Y \right) = 0$, which in turn is equivalent to $(\widetilde{\text{Id} + A})(V)_Y = 0$.

Here $(\widetilde{\text{Id} + A})$ is a map acting on a parameter-dependent vector field W on Y via

$$\sum_i W^i(x, y) \frac{\partial}{\partial y^i} \mapsto \sum_{i,j} [\delta_i^j + (\nabla_Y^{(x)} w_i(x, y))^j] W^i(x, y) \frac{\partial}{\partial y^j}.$$

Consider for $i = 1, \dots, n$ the auxiliary functions $\eta^i : (Y \rightarrow \mathbb{R})^M$ given by $\eta^i(x, y) = \sum_j g_{ij}(x) y^j$. It holds

$$\begin{aligned} \nabla_Y^{(x)} \eta^i &= \sum_{k,l} g^{kl} \frac{\partial \eta^i}{\partial y^l} \frac{\partial}{\partial y^k} = \sum_{k,l} \sum_j g^{kl} g_{ij} \underbrace{\frac{\partial y^j}{\partial y^l}}_{=\delta_k^j} \frac{\partial}{\partial y^k} \\ &= \sum_{k,l} \underbrace{g^{kl} g_{il}}_{=\delta_k^i} \frac{\partial}{\partial y^k} = \frac{\partial}{\partial y^i}. \end{aligned}$$

Note that η^i corresponds to the function $y \mapsto y^i$ in the corresponding proof from homogenization in \mathbb{R}^n , and $\frac{\partial}{\partial y^i}$ corresponds to the unit vector e_i .

With the help of this auxiliary function η^i , we obtain

$$0 = (\widetilde{\text{Id} + A})(V)_Y = \sum_i \nabla_Y^{(x)}(\eta^i - w^i)V^i = \sum_i \nabla_Y^{(x)}[(\eta^i - w^i)V^i],$$

since V^i depends only on $x \in M$ and not on $y \in Y$. Therefore $\sum_i (\eta^i - w^i)V^i = \text{const.}$, with a constant depending on x but not on y . This amounts to saying that

$$\sum_i \eta^i(x, y)V^i(x) - \text{const}(x) = \sum_i w^i(x, y)V^i(x). \quad (4.20)$$

Since $V \neq 0$, there exists a $x \in M$ with $V(x) \neq 0$. Then (using matrix notation)

$$\begin{aligned} \sum_i \eta^i(x, y)V^i(x) &= \sum_{i,j} g_{ij}(x)y^j V^i(x) \\ &= \begin{pmatrix} V^1(x) \\ \vdots \\ V^n(x) \end{pmatrix}^T G(x) \begin{pmatrix} y^1 \\ \vdots \\ y^n \end{pmatrix} \\ &= \left(G(x) \begin{pmatrix} V^1(x) \\ \vdots \\ V^n(x) \end{pmatrix} \right)^T \cdot \begin{pmatrix} y^1 \\ \vdots \\ y^n \end{pmatrix}. \end{aligned}$$

Since $\begin{pmatrix} V^1(x) \\ \vdots \\ V^n(x) \end{pmatrix} \neq 0$ and $G(x)$ is invertible, $G(x) \begin{pmatrix} V^1(x) \\ \vdots \\ V^n(x) \end{pmatrix}$ is not equal to 0 as well and thus

$$\left(G(x) \begin{pmatrix} V^1(x) \\ \vdots \\ V^n(x) \end{pmatrix} \right)^T \cdot \begin{pmatrix} y^1 \\ \vdots \\ y^n \end{pmatrix} \neq 0$$

for some choice of $y \neq 0$. Especially, this expression is not Y -periodic in y . However, the right hand side of (4.20) is periodic in y . Thus we have reached a contradiction. This shows that $\sum_{\alpha,\beta} \tilde{B}_{\alpha\beta} V^\alpha V^\beta = 0$ implies $V = 0$ and finishes the proof of the theorem. \blacklozenge

Why is the matrix \tilde{B} so important? This is due to the fact that it appears "naturally" in the weak formulation of the homogenized problem: Upon multiplication with a test function $\varphi \in H_0^1(M)$ and integration by parts, problem (4.15) reads as

$$\int_M g_M(B \nabla_M u, \nabla_M \varphi) \, \text{dvol}_M + \int_M cu\varphi \, \text{dvol}_M = \int_M f\varphi \, \text{dvol}_M. \quad (4.21)$$

The first term can now be written in component notation as

$$\begin{aligned} g_M(B \nabla_M u, \nabla_M \varphi) &= \sum_{i,j} \sum_{\alpha} g_{ij} B_{\alpha}^j (\nabla_M u)^{\alpha} (\nabla_M \varphi)^i \\ &= \sum_{i,\alpha} \tilde{B}_{i\alpha} (\nabla_M u)^{\alpha} (\nabla_M \varphi)^i =: g_B(\nabla_M u, \nabla_M \varphi). \end{aligned}$$

Due to the properties of \tilde{B} , g_B is a symmetric and coercive bilinear form on M , and the lemma of Lax-Milgram can be applied to the weak formulation (4.21) above to obtain the existence and uniqueness of a solution u .

As a corollary to the fact that the solution of the homogenized problem is unique, we note:

4.4.5 Corollary.

The convergence properties from Section 4.4.1 hold for the whole sequence $\{u^{\varepsilon}\}$.

4.4.3 Dependence of the Cell Problem on the Parameter

We investigate the dependence of the solution of the cell problem w_i on the parameter $x \in M$. As a preparation for the subsequent Section 4.4.4, we will deal with a generalized cell problem. In order to carry out the proofs with full mathematical rigor, we need to distinguish between two different Riemannian metrics on the reference cell Y : First, the metric induced by the Euclidean scalar product on \mathbb{R}^n (i.e. with metric coefficients δ_{ij}). To indicate the use of this metric, we write the reference cell as Y in the corresponding spaces. Second, we need the reference cell with metric given by the coefficients $g_{ij}(x)$, where $x \in M$ is fixed. For this we will use $Y^{(x)}$ as notation. Note that since Y (considered as a set) is compact, both metrics are equivalent. In Lemma 4.4.7, we will show that the corresponding constants can be chosen independently of $x \in M$. Please note that we need at least \mathcal{C}^2 -regularity for the charts and the atlas in this section.

For a given vector field $Q \in L^2TY$ in Y (see Section 4.6.4 for the notation) consider the problem: Find $w_Q^x \in H_{\#}^1(Y)/\mathbb{R}$ such that for fixed $x \in M$

$$-\operatorname{div}_Y^{(x)}(D_Y \nabla_Y^{(x)} w_Q^x) = \operatorname{div}_Y^{(x)}(D_Y Q) \quad \text{in } Y \quad (4.22a)$$

$$y \mapsto w_Q^x(y) \quad \text{is } Y\text{-periodic.} \quad (4.22b)$$

We will also use the notation $w_Q(x, y) = w_Q^x(y)$. The weak formulation of this problem is given by: Find $w_Q^x \in H_{\#}^1(Y)/\mathbb{R}$ such that

$$\int_Y D(y) g_Y^{(x)}(\nabla_Y^{(x)} w_Q^x, \nabla_Y^{(x)} \phi) \, dy = - \int_Y D(y) g_Y^{(x)}(Q, \nabla_Y^{(x)} \phi) \, dy \quad (4.23)$$

for all $\phi \in H_{\#}^1(Y)/\mathbb{R}$.

We begin with some preparatory results:

4.4.6 Lemma.

There exists a unique solution of Problem (4.23) in $H_{\#}^1(Y)/\mathbb{R}$, i.e. the solution is unique up to constants in $H_{\#}^1(Y)$.

Proof. Define for $u, v \in H_{\#}^1(Y)/\mathbb{R}$ and fixed $x \in M$ the bilinear form

$$a(u, v) := \int_Y D(y) g_Y^{(x)}(\nabla_Y^{(x)} u, \nabla_Y^{(x)} v) \, dy$$

and the linear map

$$b(v) = - \int_Y D(y) g_Y^{(x)}(Q, \nabla_Y^{(x)} v) \, dy.$$

Since $0 < d_0 \leq D \leq D_0$ and $g_Y^{(x)}$ is a scalar product, we obtain by the Cauchy-Schwarz inequality

$$|b(v)| \leq D_0 \int_Y g_Y^{(x)}(Q, \nabla_Y^{(x)} v) \, dy \leq D_0 \left(\int_Y g_Y^{(x)}(Q, Q) \, dy \right)^{\frac{1}{2}} \left(\int_Y g_Y^{(x)}(\nabla_Y^{(x)} v, \nabla_Y^{(x)} v) \, dy \right)^{\frac{1}{2}}.$$

The next lemma shows that $\int_Y g_Y^{(x)}(\nabla_Y^{(x)} v, \nabla_Y^{(x)} v) \, dy \leq C \|\nabla_Y^{(x)} v\|_{L^2 TY}^2$, where TY is endowed with the standard metric induced by \mathbb{R}^n . Since $Q \in L^2 TY$, we have similarly $\int_Y g_Y^{(x)}(Q, Q) \, dy \leq C \|Q\|_{L^2 TY}^2 < \infty$. Thus b is a linear and continuous map on $H_{\#}^1(Y)/\mathbb{R}$.

Arguing similarly for a , one obtains $|a(u, v)| \leq C \|\nabla_Y^{(x)} u\|_{L^2 TY} \|\nabla_Y^{(x)} v\|_{L^2 TY}$, which shows that a is bilinear and continuous. Using the subsequent lemma again, one gets

$$c \|\nabla_Y^{(x)} u\|_{L^2 TY}^2 \leq d_0 \int_Y g_Y^{(x)}(\nabla_Y^{(x)} u, \nabla_Y^{(x)} u) \, dy \leq a(u, u).$$

Since $\|\cdot\|_{L^2 TY}$ and $\|\cdot\|_{L^2 TY(x)}$ are equivalent norms (with a constant independent of $x \in M$), we can use the Poincaré inequality $\|u\|_{H_{\#}^1(Y(x))/\mathbb{R}} \leq C \|\nabla_Y^{(x)} u\|_{L^2 TY(x)}$ to obtain that a is coercive as well. Now the Lemma of Lax-Milgram yields the existence of a weak solution of the generalized cell problem. \blacklozenge

4.4.7 Lemma.

The norms $\|\cdot\|_{L^2(Y)}$ and $\|\cdot\|_{L^2(Y(x))}$ as well as $\|\cdot\|_{L^2 TY}$ and $\|\cdot\|_{L^2 TY(x)}$ are equivalent, where the constant in the estimate does not depend on $x \in M$.

Proof. We start by showing that there exist constants $d_0, D_0 > 0$ independent of $x \in M$ such that

$$d_0 |\xi|^2 \leq \sum_{i,j} g_{ij}(x) \xi^i \xi^j \leq D_0 |\xi|^2 \quad \text{holds for } \xi \in \mathbb{R}^n.$$

To this end, set $S := \{\xi \in \mathbb{R}^n : |\xi|^2 = 1\}$. S is compact. Since M is compact as well, the set $M \times S$ is compact by Tychonov's Theorem. Define

$$\begin{aligned} \Lambda : M \times S &\longrightarrow \mathbb{R} \\ (x, \xi) &\longmapsto \sum_{i,j} g_{ij}(x) \xi^i \xi^j. \end{aligned}$$

Λ is clearly continuous on a compact set, thus there exists $d_0 := \min_{M \times S} \Lambda$ and $D_0 := \max_{M \times S} \Lambda < \infty$. Since the metric g is (pointwise) positive definite, $\Lambda > 0$ and therefore $d_0 > 0$. Replacing ξ by $\frac{\eta}{|\eta|}$, $\eta \in \mathbb{R}^n$ arbitrary, one obtains

$$d_0 |\eta|^2 \leq \sum_{i,j} g_{ij}(x) \eta^i \eta^j \leq D_0 |\eta|^2$$

with constants independent of $x \in M$. Similarly, $x \mapsto \sqrt{|\det G(x)|}$ is continuous on the compact set M with $\sqrt{\det G(x)} > 0$ for $x \in M$, thus there exist $\tilde{d}_0 := \min_{x \in M} \sqrt{\det G(x)} > 0$ and $\tilde{D}_0 := \max_{x \in M} \sqrt{\det G(x)} < \infty$.

Now for $f \in L^2(Y)$ we obtain

$$\begin{aligned} \tilde{d}_0 \|f\|_{L^2(Y)}^2 &= \tilde{d}_0 \int_Y f^2 \, dy \leq \int_Y f^2 \sqrt{|G(x)|} \, dy = \|f\|_{L^2(Y^{(x)})}^2 \\ &\leq \tilde{D}_0 \int_Y f^2 \, dy = \tilde{D}_0 \|f\|_{L^2(Y)}^2 \end{aligned} \tag{4.24}$$

and thus the equivalence of $\|\cdot\|_{L^2(Y)}$ and $\|\cdot\|_{L^2(Y^{(x)})}$ with a constant independent of $x \in M$.

Let $F \in L^2TY$, then

$$\begin{aligned} d_0 \|F\|_{L^2TY}^2 &= d_0 \int_Y \sum_i (F^i)^2 \, dy \leq \int_Y \sum_{i,j} g_{ij}(x) F^i F^j \, dy = \|F\|_{L^2TY^{(x)}}^2 \\ &\leq D_0 \int_Y \int_Y \sum_i (F^i)^2 \, dy = D_0 \|F\|_{L^2TY}^2, \end{aligned}$$

which gives the desired norm equivalence, again independent of $x \in M$. ◆

4.4.8 Remark.

Note that the correct definition of the norm in $L^2TY^{(x)}$ would be

$$\|F\|_{L^2TY^{(x)}} = \int_Y g_{ij}(x) F^i F^j \sqrt{|G(x)|} \, dy.$$

However, arguing similarly as in (4.24), one can omit the factor $\sqrt{|G(x)|}$ and still obtain equivalent norms. This is done in this work.

4.4.9 Lemma.

The constant C in the Poincaré inequality $\|u\|_{H_{\#}^1(Y^{(x)})/\mathbb{R}} \leq C \|\nabla_Y^{(x)} u\|_{L^2TY^{(x)}}$, where $u \in H_{\#}^1(Y)/\mathbb{R}$, does not depend on $x \in M$.

Proof. The inverse matrix of $G = [g_{ij}]$ is positive definite as well. Thus arguing as in the preceding proof, one obtains positive constants \hat{d}_0, \hat{D}_0 such that

$$\hat{d}_0 |\eta|^2 \leq \sum_{i,j} g^{ij}(x) \eta_i \eta_j \leq \hat{D}_0 |\eta|^2.$$

This gives for $u \in H^1(Y)$

$$\begin{aligned} \hat{d}_0 \|\nabla_Y u\|_{L^2_{TY}}^2 &= \hat{d}_0 \int_Y \sum_i \left(\frac{\partial u}{\partial y^i} \right)^2 dy \leq \int_Y g^{ij}(x) \frac{\partial u}{\partial y^i} \frac{\partial u}{\partial y^j} dy = \|\nabla_Y^{(x)} u\|_{L^2_{TY}}^2 \\ &\leq \hat{D}_0 \int_Y \sum_i \left(\frac{\partial u}{\partial y^i} \right)^2 dy = \hat{D}_0 \|\nabla_Y u\|_{L^2_{TY}}^2. \end{aligned}$$

For $u \in H^1_{\#}(Y)/\mathbb{R}$ we obtain due to Poincaré's inequality

$$\begin{aligned} \|u\|_{H^1_{\#}(Y(x))}^2 &= \|u\|_{L^2(Y(x))}^2 + \|\nabla_Y^{(x)} u\|_{L^2_{TY(x)}}^2 \leq C \|u\|_{L^2(Y)}^2 + C \|\nabla_Y u\|_{L^2_{TY}}^2 \\ &\leq C \|\nabla_Y u\|_{L^2_{TY}}^2 \leq C \|\nabla_Y^{(x)} u\|_{L^2_{TY}}^2, \end{aligned}$$

where all the appearing constants are independent of $x \in M$. \blacklozenge

We prove the following estimate for the solution of the cell problem:

4.4.10 Lemma.

There exists a constant $C > 0$, independent of $x \in M$, such that for the solution w_Q^x of (4.22) it holds

$$\|w_Q(x, \cdot)\|_{L^2(Y)} + \|\nabla_Y^{(x)} w_Q(x, \cdot)\|_{L^2_{TY}} \leq C.$$

Proof. Use $\phi = w_Q^x$ as a test function in (4.23). With the notation of the proof of Lemma 4.4.6, we obtain

$$c \|\nabla_Y^{(x)} w_Q^x\|_{L^2_{TY}}^2 \leq a(w_Q^x, w_Q^x) = b(w_Q^x) \leq D_0 \|Q\|_{L^2_{TY}} \|\nabla_Y^{(x)} w_Q^x\|_{L^2_{TY}}.$$

Using a scaled version of Young's inequality, it holds

$$\|Q\|_{L^2_{TY}} \|\nabla_Y^{(x)} w_Q^x\|_{L^2_{TY}} \leq \frac{\delta}{2} \|\nabla_Y^{(x)} w_Q^x\|_{L^2_{TY}}^2 + \frac{1}{2\delta} \|Q\|_{L^2_{TY}}^2$$

for all $\delta > 0$. Choosing $\delta = d_0$, we arrive at $\frac{d_0}{2} \|\nabla_Y^{(x)} w_Q^x\|_{L^2_{TY}}^2 \leq C \|Q\|_{L^2_{TY}}^2 \leq C$ independent of x . Now the Poincaré inequality and equivalence of norms shows that $\|w_Q^x\|_{L^2(Y)} \leq C \|\nabla_Y^{(x)} w_Q^x\|_{L^2_{TY}} \leq C$. \blacklozenge

The main idea to treat the dependence of w_Q on the parameter x is the use of the Implicit Function Theorem for Banach Spaces. Similar arguments can be found in [Dob09] or in the dissertation thesis of Heuser [Heu08]. For the convenience of the reader, we recall the main theorem here:

4.4.11 Theorem (Implicit Function Theorem).

Let X, Y and Z be Banach spaces over \mathbb{R} . Let $\mathcal{F} : U(x_0, y_0) \subseteq X \times Y \rightarrow Z$ be a mapping

defined on an open neighbourhood $U(x_0, y_0)$ of $x_0 \in X, y_0 \in Y$ with $\mathcal{F}(x_0, y_0) = 0$. Assume that the total derivative in y -direction $\mathcal{D}_y \mathcal{F}$ exists in $U(x_0, y_0)$, and $((\mathcal{D}_y \mathcal{F})(x_0, y_0))^{-1}$ exists as a continuous linear operator. Assume also that \mathcal{F} and $\mathcal{D}_y \mathcal{F}$ are continuous in (x_0, y_0) . Then the following holds:

1. There exist $r_0, r > 0$ such that: For all $x \in X$ with $\|x - x_0\|_X \leq r_0$ there exists exactly one $y(x) \in Y$ with $\mathcal{F}(x, y(x)) = 0$ and $\|y(x) - y_0\|_Y \leq r$.
2. If \mathcal{F} is m -times continuously differentiable in a neighbourhood of (x_0, y_0) , then $y(\cdot)$ is also m -times continuously differentiable in a neighborhood of x_0 .
3. For the derivative $\mathcal{D}_x y(x)$ it holds

$$\mathcal{D}_x y(x) = -\mathcal{D}_y \mathcal{F}(x, y(x))^{-1} \circ \mathcal{D}_x \mathcal{F}(x, y(x)). \quad (4.25)$$

Proof. See Zeidler [Zei86], Theorem 4.B. ◆

Since the manifold M is not a Banach space and thus no valid parameter space for the theorem above, we have to recast the problem in local coordinates: To this end, let $\varphi : U \subset M \rightarrow V$ be a chart. Considering the cell problem locally around $\varphi(x) = z$ in V , we obtain the equation

$$-\operatorname{div}_Y^{(\varphi^{-1}(z))} (D(y) \nabla_Y^{(\varphi^{-1}(z))} w_Q(\varphi^{-1}(z), y)) = \operatorname{div}_Y^{(\varphi^{-1}(z))} (D(y) Q(y)).$$

This leads to an operator \mathcal{D} with

$$\begin{aligned} \mathcal{D} : V \times H_{\#}^1(Y)/\mathbb{R} &\longrightarrow (H_{\#}^1(Y)/\mathbb{R})' \\ (z, w) &\longmapsto -\operatorname{div}_Y^{(\varphi^{-1}(z))} (D \nabla_Y^{(\varphi^{-1}(z))} w + DQ) \end{aligned}$$

such that for the solution of the cell problem $w_Q^{(\varphi^{-1}(z))}$ it holds $\mathcal{D}(\varphi^{-1}(z), w_Q^{(\varphi^{-1}(z))}) = 0$.

In order not to obfuscate the notation in the sequel, we will write $w_Q(z, \cdot)$ and $g_{ij}(z)$ etc. to express the functions locally, i.e. $w_Q(z, \cdot) := w_Q(\varphi^{-1}(z), \cdot)$, $g_{ij}(z) := g_{ij}(\varphi^{-1}(z))$ and so on. The following lemmas show that the prerequisites of Theorem 4.4.11 are fulfilled.

4.4.12 Lemma.

Choose $(z_0, w_0) \in V \times H_{\#}^1(Y)/\mathbb{R}$. The total derivative $\mathcal{D}_w \mathcal{D}$ exists, and $(\mathcal{D}_w \mathcal{D}(z_0, w_0))^{-1}$ exists as a continuous linear operator.

Proof. The operator \mathcal{D} is linear, thus its derivative is the operator itself: $\mathcal{D}_w \mathcal{D}(z_0, w_0)[w] = \mathcal{D}(z_0, w)$ for $w \in H_{\#}^1(Y)/\mathbb{R}$. For $h \in (H_{\#}^1(Y)/\mathbb{R})'$, the lemma of Lax-Milgram gives the unique solvability of $\mathcal{D}(z_0, w) = h$, see Lemma 4.4.6. Thus $(\mathcal{D}_w \mathcal{D}(z_0, w_0))^{-1}$ exists. The usual estimates show that for the solution $\|w\|_{H_{\#}^1(Y)/\mathbb{R}} \leq C \|h\|_{(H_{\#}^1(Y)/\mathbb{R})'}$, therefore $(\mathcal{D}_w \mathcal{D}(z_0, w_0))^{-1}$ is continuous as well. A similar proof with more details can be found in [Dob09]. ◆

4.4.13 Lemma.

Choose $(z_0, w_0) \in V \times H_{\#}^1(Y)/\mathbb{R}$. \mathcal{D} and $\mathcal{D}_w \mathcal{D}$ are continuous in (z_0, w_0) .

Proof. Let $z_n \rightarrow z_0$ in \mathbb{R}^n and $w_n \rightarrow w_0$ in $H_{\#}^1(Y)/\mathbb{R}$. We have to estimate the operator norm $\|\mathcal{D}(z_n, w_n) - \mathcal{D}(z_0, w_0)\|$. Now

$$\begin{aligned}
\|\mathcal{D}(z_n, w_n) - \mathcal{D}(z_0, w_0)\| &= \sup_{\|\phi\|_{H_{\#}^1(Y)/\mathbb{R}} \leq 1} \left| \int_Y Dg_Y^{(z_n)}(\nabla_Y^{z_n} w_n, \nabla_Y^{z_n} \phi) \, dy \right. \\
&\quad \left. - \int_Y Dg_Y^{(z)}(\nabla_Y^{(z)} w, \nabla_Y^{(z)} \phi) \, dy \right| \\
&= \sup_{\|\phi\|_{H_{\#}^1(Y)/\mathbb{R}} \leq 1} \left| \int_Y D \left(\sum_{i,j=1}^n g^{ij}(z_n) \frac{\partial w_n}{\partial y^i} \frac{\partial \phi}{\partial y^j} - \sum_{i,j=1}^n g^{ij}(z) \frac{\partial w_0}{\partial y^i} \frac{\partial \phi}{\partial y^j} \right) \right| \\
&\leq \sup_{\|\phi\|_{H_{\#}^1(Y)/\mathbb{R}} \leq 1} \left[\left| \int_Y D \sum_{i,j=1}^n (g^{ij}(z_n) - g^{ij}(z)) \frac{\partial w_n}{\partial y^i} \frac{\partial \phi}{\partial y^j} \, dy \right| \right. \\
&\quad \left. + \left| \int_Y D \sum_{i,j=1}^n g^{ij}(z) \left(\frac{\partial w_n}{\partial y^i} - \frac{\partial w_0}{\partial y^i} \right) \frac{\partial \phi}{\partial y^j} \, dy \right| \right] \\
&\quad \quad \quad = g_Y^{(z)} \nabla_Y^{(z)}(w_n - w_0), \nabla_Y^{(z)} \phi \\
&\leq \sup_{\|\phi\|_{H_{\#}^1(Y)/\mathbb{R}} \leq 1} \left(CD_0 \sup_{i,j} |g^{ij}(z_n) - g^{ij}(z)| \|w_n\|_{H_{\#}^1(Y)/\mathbb{R}} \|\phi\|_{L^2(Y)} \right. \\
&\quad \left. + CD_0 \left\| \nabla_Y^{(z)}(w_n - w_0) \right\|_{L^2(Y)} \left\| \nabla_Y^{(z)} \phi \right\|_{L^2(Y)} \right) \\
&\leq CD_0 \sup_{i,j} |g^{ij}(z_n) - g^{ij}(z)| \|w_n\|_{H_{\#}^1(Y)/\mathbb{R}} + CD_0 \|w_n - w_0\|_{H_{\#}^1(Y)/\mathbb{R}} \longrightarrow 0,
\end{aligned}$$

since $g^{ij} \circ \varphi^{-1}$ is continuous. This shows that \mathcal{D} is continuous. Arguing similarly for $\mathcal{D}_w \mathcal{D}$, one obtains

$$\begin{aligned}
\|\mathcal{D}_w \mathcal{D}(z_n, w_n) - \mathcal{D}_w \mathcal{D}(z_0, w_0)\| &= \sup_{\|\phi\|_{H_{\#}^1(Y)/\mathbb{R}} \leq 1} \|\mathcal{D}_w \mathcal{D}(z_n, w_n)[\phi] - \mathcal{D}_w \mathcal{D}(z_0, w_0)[\phi]\|_{(H_{\#}^1(Y)/\mathbb{R})'} \\
&= \sup_{\|\phi\|_{H_{\#}^1(Y)/\mathbb{R}} \leq 1} \|\mathcal{D}(z_n, \phi) - \mathcal{D}(z_0, \phi)\|_{(H_{\#}^1(Y)/\mathbb{R})} \\
&\leq CD_0 \sup_{i,j} |g^{ij}(z_n) - g^{ij}(z)| \longrightarrow 0.
\end{aligned}$$

Thus $\mathcal{D}_w \mathcal{D}$ is continuous as well. ◆

4.4.14 Lemma.

Choose $(z_0, w_0) \in V \times H_{\#}^1(Y)/\mathbb{R}$. \mathcal{D} is continuously differentiable in (z_0, w_0) .

Proof. We start by considering the partial derivatives in z first: Let $h \in H_{\#}^1(Y)/\mathbb{R}$ and e^l be the l -th unit vector with $l \in \{1, \dots, n\}$. Lowering the index in the vector field Q , we obtain

$$\mathcal{D}(z_0, w_0)(h) = \int_Y D \sum_{i,j=1}^n g^{ij}(z_0) \left(\frac{\partial w_0}{\partial y^i} + \sum_{k=1}^n g_{ik}(z_0) Q^k \right) \frac{\partial h}{\partial y^j} \, dy$$

and thus

$$\begin{aligned}
\frac{\partial}{\partial z^l}(\mathcal{D}(z_0, w_0)(h)) &= \lim_{\delta \rightarrow 0} \frac{\mathcal{D}(z_0 + \delta e^l, w_0) - \mathcal{D}(z_0, w_0)}{\delta} \\
&= \lim_{\delta \rightarrow 0} \int_Y D \sum_{i,j=1}^n \frac{g^{ij}(z_0 + \delta e^l) - g^{ij}(z_0)}{\delta} \left(\frac{\partial w_0}{\partial y^i} \right. \\
&\quad \left. + \sum_{k=1}^n \frac{g_{ik}(z_0 + \delta e^l) - g_{ik}(z_0)}{\delta} Q^k \right) \frac{\partial h}{\partial y^j} dy \\
&= \int_Y D \left(\sum_{i,j=1}^n (g^{ij})'(z_0) \left(\frac{\partial w_0}{\partial y^i} + \sum_{k=1}^n g_{ik}(z_0) Q^k \right) \right. \\
&\quad \left. + g^{ij}(z_0) \sum_{k=1}^n (g_{ik})'(z_0) Q^k \right) \frac{\partial h}{\partial y^j} dy.
\end{aligned}$$

by the product rule. The limit exists by Lebesgue's dominated convergence theorem, since the $g^{ij} \circ \varphi^{-1}$'s and the $g_{ij} \circ \varphi^{-1}$'s are continuously differentiable and bounded. We see that

$$\frac{\partial}{\partial z^l} \mathcal{D}(z_0, w_0) : V \times H_{\#}^1(Y)/\mathbb{R} \longrightarrow (H_{\#}^1(Y)/\mathbb{R})'.$$

Since $(g^{ij} \circ \varphi)'$ and $(g_{ij} \circ \varphi)'$ are continuous for $i, j = 1, \dots, n$, arguing as in the proof of Lemma 4.4.13 yields that $\frac{\partial}{\partial z^l} \mathcal{D}$ is continuous. l is arbitrary, thus $\mathcal{D}_z \mathcal{D}$ exists as a continuous operator. The other direction $\mathcal{D}_w \mathcal{D}$ has been treated before. \blacklozenge

We are now ready to prove the main theorem:

4.4.15 Theorem.

For the solution w_Q of the cell problem (4.22) it holds

$$w_Q \in \Omega_0^1(M, H_{\#}^1(Y)/\mathbb{R}).$$

Note that a result like $w_Q \in \mathcal{C}^1(M; H_{\#}^1(Y)/\mathbb{R})$ would not be meaningful, since it is not clear in which sense the derivative of w_Q has to be understood. Therefore we have to consider the derivatives of w_Q locally and "patch" them together in a way which is automatically independent of the actual coordinate description.

Proof. Due to Lemmas 4.4.12 and 4.4.13, we can apply the implicit function theorem to obtain that the the solution of the equation $\mathcal{D}(z, w) = 0$ can be parametrized by a function $w \in \mathcal{C}(V, H_{\#}^1(Y)/\mathbb{R})$. w is a solution of problem (4.22) for $x = \varphi^{-1}(z)$, $z \in V$ fixed. By uniqueness of this solution, it has to hold $w(z, y) = w_Q(\varphi^{-1}(z), y)$. Thus $w_Q(\varphi^{-1}(\cdot), \cdot) \in \mathcal{C}(V; H_{\#}^1(Y)/\mathbb{R})$, which leads (via pullback to the manifold) to $w_Q \in \mathcal{C}(U; H_{\#}^1(Y)/\mathbb{R})$. Since the chart (and therefore U) are arbitrary, the estimate from Lemma 4.4.10 shows that

$$w_Q \in \mathcal{C}(M; H_{\#}^1(Y)/\mathbb{R}) = \Omega_0^0(M, H_{\#}^1(Y)/\mathbb{R}).$$

We now consider the partial derivative $\frac{\partial w_Q(\varphi^{-1}(z), y)}{\partial z^l}$. Keeping in mind Lemma 4.4.14, $\frac{\partial w_Q}{\partial z^l}$ exists in $\mathcal{C}(V, H_{\#}^1(Y)/\mathbb{R})$ by the implicit function theorem. Employing equation (4.25), we get (with e^l being the l 'th unit vector)

$$\begin{aligned} \frac{\partial w_Q(\varphi^{-1}(z), y)}{\partial z^l} &= \mathcal{D}_z w_Q(\varphi^{-1}(z), y)[e^l] \\ &= -\mathcal{D}_w \mathcal{D}(z, w_Q(z, y))^{-1} \circ \mathcal{D}_z \mathcal{D}(z, w_Q)[e^l]. \end{aligned}$$

Thus $\frac{\partial w_Q}{\partial z^l}$ solves (in weak formulation)

$$\begin{aligned} \int_Y Dg_Y^{(z)}(\nabla_Y^{(z)} \frac{\partial w_Q(z)}{\partial z^l}, \nabla_Y^{(z)} \phi) dy &= - \int_Y D \left(\sum_{i,j=1}^n (g^{ij}(z))' \left(\frac{\partial w_Q}{\partial y^i} + \sum_{k=1}^n g_{ik}(z) Q^k \right) \right. \\ &\quad \left. + g^{ij}(z) \sum_{k=1}^n (g_{ik}(z))' Q^k \right) \frac{\partial h}{\partial y^j} dy \end{aligned}$$

for all $h \in H_{\#}^1(Y)/\mathbb{R}$. Using $\phi = \frac{\partial w_Q}{\partial z^l}$ as a test function, using the coercivity of the left hand side yields the estimate

$$\begin{aligned} d_0 \left\| \nabla_Y^{(z)} \frac{\partial w_Q(z, \cdot)}{\partial z^l} \right\|_{L^2_{TY}} &\leq CD_0 \sup_{\substack{x \in M \\ i,j \in \{1, \dots, n\}}} (|g^{ij}| + |(g^{ij})'| + |(g_{ij})'|) \left\| \nabla_Y^{(z)} w_Q \right\|_{L^2_Y} \\ &\quad \cdot \left\| \nabla_Y^{(z)} \frac{\partial w_Q(z)}{\partial z^l} \right\|_{L^2_{TY}}. \end{aligned}$$

Therefore (arguing similarly as in the proof of Lemma 4.4.10 with Young's inequality), by Poincaré's inequality we arrive at

$$\left\| \frac{\partial w_Q(z, \cdot)}{\partial z^l} \right\|_{L^2(Y)} + \left\| \nabla_Y^{(z)} \frac{\partial w_Q(z, \cdot)}{\partial z^l} \right\|_{L^2_{TY}} \leq C,$$

where the constant C can be chosen independent of $x \in M$.

We can now construct the exterior derivative $d_x w_Q$ locally in $\varphi(x) = z$ by setting

$$\sum_{i=1}^n \frac{\partial w_Q}{\partial z^i} dz^i = \varphi_*(d_x w_Q)|_U.$$

The representation formula in Proposition 4.6.26 shows that the left hand side defines a form in $\Omega_1^0(\varphi(U), H_{\#}^1(Y)/\mathbb{R})$. By Definition 4.6.29, the arbitrariness of the chart φ and the estimate above, this gives a form $d_x w_Q \in \Omega_1^0(M, H_{\#}^1(Y)/\mathbb{R})$. This finishes the proof. \blacklozenge

4.4.4 Equivalent Atlases

In this section we construct an equivalence relation between certain UC-atlases for M and show that all equivalent atlases lead to the same limit problem (4.15). We begin by considering the transformation behaviour of the cell problem. To this end, let Y and

Z be two rectangular subsets of \mathbb{R}^n , representing two reference cells. We assume both cells to be equipped with the chart Id and denote the local basis vectors by $\frac{\partial}{\partial y^i}$ (for Y) and $\frac{\partial}{\partial z^i}$ (for Z), $i = 1, \dots, n$. The corresponding dual forms are denoted by dy^i and dz^i , respectively.

Let there be given two scalar functions $D_Y : Y \rightarrow \mathbb{R}$ and $D_Z : Z \rightarrow \mathbb{R}$, representing e.g. material properties as above. In order to obtain the same "physical" situation, D_Y and D_Z have to be related, see the next lemma.

4.4.16 Lemma.

Let $\phi : Y \rightarrow Z$ be a coordinate transformation between the reference cells. As above, define $g_Y^{(x)} = \sum_{i,j} g_{ij}(x) dy^i \otimes dy^j$ and $g_Z^{(x)} = \sum_{i,j} g_{ij}(x) dz^i \otimes dz^j$ and assume that there exists a $\lambda > 0$ such that both metrics are related by $\lambda g_Z^{(x)} = \phi_* g_Y^{(x)}$. Furthermore, assume that $D_Z = \phi_* D_Y$.

For given vector fields $Q \in TY$ in Y and $H \in TZ$ in Z consider the generalized cell problems: Find $w_Y^Q \in H_{\#}^1(Y)/\mathbb{R}$ and $w_Z^H \in H_{\#}^1(Z)/\mathbb{R}$ such that for fixed $x \in M$

$$-\text{div}_Y^{(x)}(D_Y \nabla_Y^{(x)} w_Y^Q) = \text{div}_Y^{(x)}(D_Y Q) \quad \text{in } Y \quad (4.26a)$$

$$y \mapsto w_Y^Q(x, y) \quad \text{is } Y\text{-periodic} \quad (4.26b)$$

and

$$-\text{div}_Z^{(x)}(D_Z \nabla_Z^{(x)} w_Z^H) = \text{div}_Z^{(x)}(D_Z H) \quad \text{in } Z \quad (4.27a)$$

$$z \mapsto w_Z^H(x, z) \quad \text{is } Z\text{-periodic.} \quad (4.27b)$$

Then it holds

$$\lambda \phi_* w_Y^Q = w_Z^{\phi_* Q} \quad \text{as well as} \quad \phi_*(\nabla_Y^{(x)} w_Y^Q) = \nabla_Z^{(x)} w_Z^{\phi_* Q}.$$

Proof. Keep the relations $\text{div}_Z^{(x)} \circ \phi_* = \phi_* \circ \text{div}_Y^{(x)}$ as well as $\nabla_Z^{(x)} \circ \phi_* = \frac{1}{\lambda} \phi_* \circ \nabla_Y^{(x)}$ in mind, which hold due to the asserted relation between the metrics on Y and Z , see [AE01]. Application of ϕ_* to equation (4.26a) now yields

$$\begin{aligned} & -\phi_*[\text{div}_Y^{(x)}(D_Y \nabla_Y^{(x)} w_Y^Q)] = \phi_* \text{div}_Y^{(x)}(D_Y Q) \\ \iff & -\text{div}_Z^{(x)}(\phi_* D_Y \phi_*[\nabla_Y^{(x)} w_Y^Q]) = \text{div}_Z^{(x)}(\phi_* D_Y \phi_* Q) \\ \iff & -\text{div}_Z^{(x)}(D_Z \nabla_Z^{(x)}(\lambda \phi_* w_Y^Q)) = \text{div}_Z^{(x)}(D_Z \phi_* Q). \end{aligned}$$

Since the solution of (4.27) (with $H = \phi_* Q$) is unique (see Lemma 4.4.6), we obtain $\lambda \phi_* w_Y^Q = w_Z^{\phi_* Q}$. Application of $\nabla_Z^{(x)}$ to both sides of this identity finally gives

$$\nabla_Z^{(x)} w_Z^{\phi_* Q} = \lambda \nabla_Z^{(x)}(\phi_* w_Y^Q) = \phi_*(\nabla_Y^{(x)} w_Y^Q). \quad \blacklozenge$$

4.4.17 Remark.

An analogous argument as in the proof above shows that for $\alpha, \beta \in \mathbb{R}$ and $H_1, H_2 \in TZ$ it holds

$$\alpha w_Z^{H_1} + \beta w_Z^{H_2} = w_Z^{\alpha H_1 + \beta H_2}.$$

In the sequel, we assume the following:

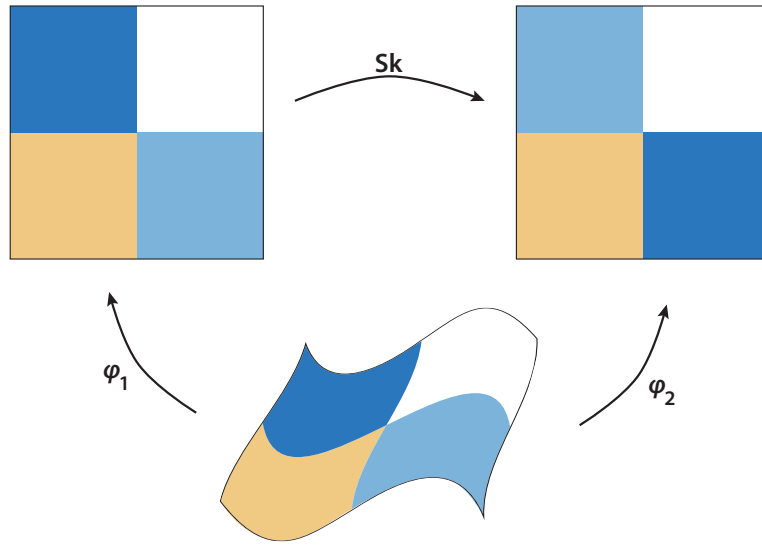


Figure 4.8: Illustration of Assumption 4.4.18. A 2-dimensional manifold (below) is mapped to the unit cube in \mathbb{R}^2 with the help of two different atlases $\mathcal{A}^1 := \{\varphi_1\}$ and $\mathcal{A}^2 := \{\varphi_2\}$. The map $Sk = \varphi_2 \circ \varphi_1^{-1}$ (see Example 4.4.25) can be extended to a linear map $\mathbb{R}^2 \rightarrow \mathbb{R}^2$.

4.4.18 Assumption.

Let the manifold M be equipped with two atlases $\mathcal{A}^1 = \{\phi_\alpha^1 : U_\alpha^1 \rightarrow V_\alpha^1; \alpha \in I\}$ and $\mathcal{A}^2 = \{\phi_\alpha^2 : U_\alpha^2 \rightarrow V_\alpha^2; \alpha \in \tilde{I}\}$, both satisfying the UC-criterium, with some finite index sets I and \tilde{I} . Assume that whenever $U_\alpha^1 \cap U_\beta^2 \neq \emptyset$ for some $\alpha \in I, \beta \in \tilde{I}$, then the coordinate transformation $\phi_\beta^2 \circ (\phi_\alpha^1)^{-1}$ is the restriction of some linear map $\tilde{F} : \mathbb{R}^n \rightarrow \mathbb{R}^n$ to V_α^1 . The next lemma shows that this map \tilde{F} is unique across different charts, thus it is not restrictive to assume the existence of one linear map $F : \mathbb{R}^n \rightarrow \mathbb{R}^n$ such that $\phi_\beta^2 \circ (\phi_\alpha^1)^{-1} = F|_{V_\alpha^1}$ for all suitable index pairs.

Furthermore, assume that $F|_Y : Y \rightarrow Z$ is a coordinate transformation between the reference cells such that for the functions D_Y and D_Z representing material properties, we have $D_Z = (F|_Y)_* D_Y$.

Examples of situations which satisfy these assumptions will be given later. An illustration is given in Figure 4.8. We now show the asserted uniqueness of the transformation F and collect further results needed for subsequent derivations:

4.4.19 Lemma.

Let $\alpha, \tilde{\alpha}$ be two indices with $V_\alpha^1 \cap V_{\tilde{\alpha}}^1 \neq \emptyset$. Choose $\beta, \tilde{\beta}$ such that $U_\alpha^1 \cap U_{\tilde{\beta}}^2 \neq \emptyset$ and $U_{\tilde{\alpha}}^1 \cap U_{\tilde{\beta}}^2 \neq \emptyset$. Then $\phi_\beta^2 \circ (\phi_\alpha^1)^{-1} = \phi_{\tilde{\beta}}^2 \circ (\phi_{\tilde{\alpha}}^1)^{-1}$ in $V_\alpha^1 \cap V_{\tilde{\alpha}}^1$. Thus the linear map \tilde{F} is unique for all index pairs.

Proof. Due to the UC-criterion, there exists $K, \tilde{K} \in \mathbb{R}^n$ such that $\phi_{\tilde{\alpha}}^1 = \phi_\alpha^1 + K$ as well as $\phi_{\tilde{\beta}}^2 = \phi_\beta^2 + \tilde{K}$. This implies $(\phi_{\tilde{\alpha}}^1)^{-1}(\cdot) = (\phi_\alpha^1)^{-1}(\cdot - K)$, see also the proof of Lemma 4.2.4.

Since $\phi_\beta^2 \circ (\phi_\alpha^1)^{-1}$ as well as $\phi_{\tilde{\beta}}^2 \circ (\phi_{\tilde{\alpha}}^1)^{-1}$ are supposed to be linear, it holds $\phi_\beta^2 \circ (\phi_\alpha^1)^{-1} = D(\phi_\beta^2 \circ (\phi_\alpha^1)^{-1})$ and $\phi_{\tilde{\beta}}^2 \circ (\phi_{\tilde{\alpha}}^1)^{-1} = D(\phi_{\tilde{\beta}}^2 \circ (\phi_{\tilde{\alpha}}^1)^{-1})$, where D denotes the total derivative.

By the chain rule, we obtain

$$D[\phi_\beta^2 \circ (\phi_\alpha^1)^{-1}] = D[\phi_\beta^2((\phi_\alpha^1)^{-1}(\cdot - K)) + \tilde{K}] = D[\phi_\beta^2 \circ (\phi_\alpha^1)^{-1}].$$

This implies the asserted equality and the uniqueness of the linear map \tilde{F} . \blacklozenge

The next lemma shows that the description of material properties is independent of the atlas:

4.4.20 Lemma.

It holds

$$D^\varepsilon(x) = D_Y\left(\frac{\phi_\alpha^1(x)}{\varepsilon}\right) = D_Z\left(\frac{\phi_\beta^2(x)}{\varepsilon}\right)$$

for $x \in U_\alpha^1 \cap U_\beta^2$.

Proof. Since $F = \phi_\beta^2 \circ (\phi_\alpha^1)^{-1}$ is linear, one has $\frac{\phi_\beta^2 \circ (\phi_\alpha^1)^{-1}(\phi_\alpha^1(x))}{\varepsilon} = \phi_\beta^2 \circ (\phi_\alpha^1)^{-1}\left(\frac{\phi_\alpha^1(x)}{\varepsilon}\right)$. This gives

$$\begin{aligned} D^\varepsilon(x) &:= D_Z\left(\frac{\phi_\beta^2(x)}{\varepsilon}\right) = D_Z\left(\frac{\phi_\beta^2 \circ (\phi_\alpha^1)^{-1}(\phi_\alpha^1(x))}{\varepsilon}\right) = D_Z\left(\underbrace{\phi_\beta^2 \circ (\phi_\alpha^1)^{-1}}_{=F}\left(\frac{\phi_\alpha^1(x)}{\varepsilon}\right)\right) \\ &= (F^* D_Z)\left(\frac{\phi_\alpha^1(x)}{\varepsilon}\right). \end{aligned}$$

Since $D_Z = F_* D_Y \Leftrightarrow D_Y = F^* D_Z$, the last expression is equal to $D_Y\left(\frac{\phi_\alpha^1(x)}{\varepsilon}\right)$, which finishes the proof. \blacklozenge

In the sequel, we will use the index notation of coordinate transformations in differential geometry (see e.g. Zeidler [Zei88] or Amann/Escher [AE01]): Let $\phi_\alpha^1 \in \mathcal{A}_1, \phi_\beta^2 \in \mathcal{A}_2$ such that $U_\alpha^1 \cap U_\beta^2 \neq \emptyset$. Writing $\phi_\alpha^1 = (x^1, \dots, x^n)$ and $\phi_\beta^2 = (\tilde{x}^1, \dots, \tilde{x}^n)$ for the components of the charts, one uses the notation $\frac{\partial \tilde{x}^i}{\partial x^j}(x)$ to denote the ij -th entry of the Jacobian matrix of $\phi_\beta^2 \circ (\phi_\alpha^1)^{-1}$ at $\phi_\alpha^1(x), x \in U_\alpha^1 \subset M$.

Note two peculiarities due to the Assumptions 4.4.18: First, $\frac{\partial \tilde{x}^i}{\partial x^j}(x)$ corresponds to the ij -th entry in the matrix representation of the linear map F ; and second, due to Lemma 4.4.19, this value is constant on all of M . Furthermore, we will "switch" between the interpretations of $\phi_\beta^2 \circ (\phi_\alpha^1)^{-1}$ being a coordinate transformation for M and for Y without using a specific notation.

4.4.21 Lemma.

It holds

$$(F|_Y)_* g_Y^{(x)} = g_Z^{(x)}.$$

Proof. By the usual transformation rules for tensor fields, the Riemannian metric g on M has the two local representations

$$g = \sum_{i,j} g_{ij} dx^i \otimes dx^j \quad \text{as well as} \quad g = \sum_{i,j} \tilde{g}_{ij} d\tilde{x}^i \otimes \tilde{x}^j,$$

where the coefficients are related via the identity $\tilde{g}_{lk} = \sum_{i,j} g_{ij} \frac{\partial x^i}{\partial \tilde{x}^l} \frac{\partial x^j}{\partial \tilde{x}^k}$. By the construction of the induced metric on the reference cell, we obtain the metrics

$$g_Y^{(x)} = \sum_{i,j} g_{ij}(x) dy^i \otimes dy^j \quad \text{and} \quad g_Z^{(x)} = \sum_{i,j} \tilde{g}_{ij}(x) dz^i \otimes dz^j.$$

Let $X \in TZ$ be a vector field in Z , with local representation $X = \sum_i X^i \frac{\partial}{\partial z^i}$. By the transformation rules for vector fields, the local representation of $F^*X \in TY$ is given by $\sum_i (\sum_l X^l \frac{\partial x^i}{\partial \tilde{x}^l}) \frac{\partial}{\partial y^i}$. We obtain for this X and a similar vector field $Y \in TZ$

$$\begin{aligned} [F_*g_Y^{(x)}](X, Y) &= g_Y^{(x)}(F^*X, F^*Y) = \sum_{i,j} \left(g_{ij}(x) \cdot \left[\sum_l X^l \frac{\partial x^i}{\partial \tilde{x}^l} \right] \cdot \left[\sum_k Y^k \frac{\partial x^j}{\partial \tilde{x}^k} \right] \right) \\ &= \sum_{l,k} \tilde{g}_{lk}(x) X^l Y^k = g_Z^{(x)}(X, Y). \end{aligned}$$

This shows that $F_*g_Y^{(x)} = g_Z^{(x)}$. ◆

4.4.22 Lemma.

For the volumes of the reference cells, the identity

$$|Y| = |\det(F^{-1})| |Z|$$

holds.

Proof. Keeping in mind that $F_*(dy^1 \dots dy^n) = |\det(F^{-1})| dz^1 \dots dz^n$, we obtain by the transformation formula for integrals that

$$\begin{aligned} |Y| &= \int_Y 1 dy^1 \dots dy^n = \int_Z |\det(F^{-1})| dz^1 \dots dz^n \\ &= |\det(F^{-1})| \int_Z 1 dz^1 \dots dz^n = |\det(F^{-1})| |Z|. \end{aligned} \quad \text{◆}$$

We now present the main result of this section:

4.4.23 Theorem.

Under the Assumptions 4.4.18, the limit problem (4.15) is independent of the atlas \mathcal{A}_i , $i = 1, 2$.

Proof. Taking a look at the proof of Theorem 4.4.4 (and especially step 2), we have to show that the expression $\frac{1}{|Y|} \int_Y D[\nabla_M u + \sum_{i=1}^n (\nabla_M u)^i (\nabla_Y^{(x)} w_i)_M] dy$ has an "appropriate" transformation behaviour. Put in the framework used in this section, we have to compare

the terms (see the expression K in the proof mentioned above)

$$\sum_{i,k} D_Y(\delta_k^i + (\nabla_Y^{(x)} w_Y^{e_i})^k)(\nabla_M u)^i \frac{\partial}{\partial x^k} \quad \text{and}$$

$$\sum_{i,k} D_Z(\delta_k^i + (\nabla_Z^{(x)} w_Z^{e_i})^k)(\nabla_M u)^i \frac{\partial}{\partial \tilde{x}^k}.$$

Note that here $(\nabla_M u)^i$ in both formulas does *not* signify the same mathematical expression! In the first formula, $(\nabla_M u)^i$ denotes the i -th component with respect to the local basis $\frac{\partial}{\partial x^k}$, whereas in the second formula the same term is the i -th component with respect to the local basis $\frac{\partial}{\partial \tilde{x}^k}$. To avoid this notational confusion, we use the representation $\nabla_M u = \sum_i X^i \frac{\partial}{\partial x^i}$. Then, by the transformation rules for vector fields, $\nabla_M u = \sum_i (\sum_l X^l \frac{\partial \tilde{x}^i}{\partial x^l}) \frac{\partial}{\partial \tilde{x}^i}$. Now we see that $(\nabla_M u)^i = X^i$ in the first expression, and $(\nabla_M u)^i = \sum_l X^l \frac{\partial \tilde{x}^i}{\partial x^l} =: \tilde{X}^i$ in the second.

Step 1 Transformation of the individual terms:

We have

$$F_* \left[\sum_{l,m} \delta_l^m (\nabla_M u)^l \frac{\partial}{\partial x^m} \right] = F_* \left[\sum_{l,m} \delta_l^m X^l \frac{\partial}{\partial x^m} \right] = \sum_{l,m,i,k} \delta_i^k X^l \frac{\partial \tilde{x}^i}{\partial x^l} \frac{\partial x^m}{\partial \tilde{x}^k} \frac{\partial}{\partial x^m} = \sum_{i,k} \delta_i^k \tilde{X}^i \frac{\partial}{\partial \tilde{x}^k}.$$

Due to Lemma 4.4.21, we can use the transformation lemma for the cell problems (with $\lambda = 1$, see Lemma 4.4.16) and Remark 4.4.17 to obtain

$$\begin{aligned} F_* \left[\sum_{i,k} (\nabla_Y^{(x)} w_Y^{e_i})^k X^i \frac{\partial}{\partial x^k} \right] &= \sum_{i,k,m} (\nabla_Y^{(x)} w_Y^{e_i})^k X^i \underbrace{\left(\frac{\partial \tilde{x}^m}{\partial x^k} \frac{\partial}{\partial \tilde{x}^m} \right)}_{= \frac{\partial}{\partial x^k}} \\ &= \sum_{i,m} \underbrace{\sum_k \frac{\partial \tilde{x}^m}{\partial x^k} (\nabla_Y^{(x)} w_Y^{e_i})^k}_{=(F_* \nabla_Y^{(x)} w_Y^{e_i})^m} X^i \frac{\partial}{\partial \tilde{x}^m} \\ &= \sum_{i,m} (\nabla_Z^{(x)} w_Z^{F_* e_i})^m X^i \frac{\partial}{\partial \tilde{x}^m} \\ &= \sum_{i,m} (\nabla_Z^{(x)} w_Z^{\sum_k \frac{\partial \tilde{x}^k}{\partial x^i} e_k})^m X^i \frac{\partial}{\partial \tilde{x}^m} \\ &= \sum_{k,m} (\nabla_Z^{(x)} w_Z^{e_k})^m \left(\sum_i X^i \frac{\partial \tilde{x}^k}{\partial x^i} \right) \frac{\partial}{\partial \tilde{x}^m} \\ &= \sum_{k,m} (\nabla_Z^{(x)} w_Z^{e_k})^m \tilde{X}^k \frac{\partial}{\partial \tilde{x}^m}. \end{aligned}$$

Step 2 Transformation of the integrals:

Keeping in mind $F_* D_Y = D_Z$, $F_*(dy^1 \dots dy^n) = |\det(F^{-1})| dz^1 \dots dz^n$ and the formulas derived in step 1, we can apply the pushforward F_* to the integral $\frac{1}{|Y|} \int_Y D_Y [\nabla_M u +$

$\sum_{i=1}^n (\nabla_M u)^i (\nabla_Y^{(x)} w_Y^{e_i})_M] dy$ to obtain

$$\begin{aligned} & F_* \left[\frac{1}{|Y|} \int_Y \left(\sum_{i,k} D_Y (\delta_k^i + (\nabla_Y^{(x)} w_Y^{e_i})^k) (\nabla_M u)^i \frac{\partial}{\partial x^k} \right) dy^1 \dots dy^n \right] \\ &= \frac{1}{|Y|} \int_Z F_* D_Y \left(F_* \left[\sum_{i,k} \delta_k^i X^i \frac{\partial}{\partial x^k} \right] + F_* \left[\sum_{i,k} (\nabla_Y^{(x)} w_Y^{e_i})^k X^i \frac{\partial}{\partial x^k} \right] \right) F_* [dy^1 \dots dy^n] \\ &= \frac{1}{|Y|} |\det(F^{-1})| \int_Z D_Z \left(\sum_{l,m} \delta_m^l \tilde{X}^m \frac{\partial}{\partial \tilde{x}^l} + (\nabla_Z^{(x)} w_Z^{e_m})^l \tilde{X}^m \frac{\partial}{\partial \tilde{x}^l} \right) dz^1 \dots dz^n. \end{aligned}$$

Since $\frac{|\det(F^{-1})|}{|Y|} = \frac{1}{|Z|}$, we finally get that the last term is equal to

$$\frac{1}{|Z|} \int_Z D_Z \left(\sum_{i,k} \delta_k^i + (\nabla_Z^{(x)} w_Z^{e_i})^k \right) \tilde{X}^i \frac{\partial}{\partial \tilde{x}^k} dz,$$

which is (written with respect to the local basis $\frac{\partial}{\partial \tilde{x}^k}$) nothing else than $\frac{1}{|Z|} \int_Z D_Z [\nabla_M u + \sum_{i=1}^n (\nabla_M u)^i (\nabla_Z^{(x)} w_Z^{e_i})_M] dz$. Thus we see that the expression constituting the homogenized problem is invariant under a change of the atlas which satisfies Assumptions 4.4.18. \blacklozenge

Before giving an example, we show that the class of atlases satisfying the assumptions given above constitutes an equivalence relation:

4.4.24 Proposition.

Let \mathcal{A} and \mathcal{B} be two atlases for M , both satisfying the UC-criterion. We write $\mathcal{A} \sim \mathcal{B}$ to denote that the couple $(\mathcal{A}, \mathcal{B})$ satisfies the Assumptions 4.4.18. Then the relation ' \sim ' is an equivalence relation on the set of UC-atlases.

This result tacitly assumes that there exist reference cells $Y_{\mathcal{A}}$ (belonging to \mathcal{A}) and $Y_{\mathcal{B}}$ (belonging to \mathcal{B}) etc. as well as "material-property" functions $D_{Y_{\mathcal{A}}}$ and $D_{Y_{\mathcal{B}}}$ as stated above.

Proof. Let $\mathcal{A}, \mathcal{B}, \mathcal{C}$ be UC-atlases. Due to Lemma 4.4.19, we only have to consider a suitable pair of charts for each atlas-combination. Therefore we are not going to consider the domains and codomains of each chart explicitly.

Denote by $F_{\mathcal{A}\mathcal{B}}$ the linear map $\phi_{\mathcal{B}} \circ \phi_{\mathcal{A}}^{-1}$, which is obtained for charts $\phi_{\mathcal{A}} \in \mathcal{A}, \phi_{\mathcal{B}} \in \mathcal{B}$. Since $\phi_{\mathcal{A}} \circ \phi_{\mathcal{A}}^{-1} = \text{Id}$, clearly $F_{\mathcal{A}\mathcal{A}} = \text{Id}$. Due to $\text{Id}_* D_{Y_{\mathcal{A}}} = D_{Y_{\mathcal{A}}}$ we have $\mathcal{A} \sim \mathcal{A}$.

Now let $\mathcal{A} \sim \mathcal{B}$. Due to the invertibility of the charts, $F_{\mathcal{A}\mathcal{B}}$ is invertible with $\phi_{\mathcal{A}} \circ \phi_{\mathcal{B}}^{-1} = (\phi_{\mathcal{B}} \circ \phi_{\mathcal{A}}^{-1})^{-1} = F_{\mathcal{A}\mathcal{B}}^{-1}$. As $F_{\mathcal{A}\mathcal{B}}$ is linear, its inverse is linear as well and therefore $F_{\mathcal{B}\mathcal{A}} = F_{\mathcal{A}\mathcal{B}}^{-1}$. If $D_{Y_{\mathcal{B}}} = (F_{\mathcal{A}\mathcal{B}})_* D_{Y_{\mathcal{A}}}$, application of $(F_{\mathcal{B}\mathcal{A}})_*$ to both sides of the equality yields $D_{Y_{\mathcal{A}}} = (F_{\mathcal{B}\mathcal{A}})_* D_{Y_{\mathcal{B}}}$. Thus $\mathcal{B} \sim \mathcal{A}$.

Finally, let $\mathcal{A} \sim \mathcal{B}$ and $\mathcal{B} \sim \mathcal{C}$. For $\phi_{\mathcal{C}} \in \mathcal{C}$ we obtain

$$\phi_{\mathcal{C}} \circ \phi_{\mathcal{A}}^{-1} = \underbrace{\phi_{\mathcal{C}} \circ \phi_{\mathcal{B}}^{-1}}_{=F_{\mathcal{B}\mathcal{C}}} \circ \underbrace{\phi_{\mathcal{B}} \circ \phi_{\mathcal{A}}^{-1}}_{=F_{\mathcal{A}\mathcal{B}}},$$

which gives the linear map $F_{\mathcal{A}\mathcal{C}} = F_{\mathcal{B}\mathcal{C}}F_{\mathcal{A}\mathcal{B}}$. Due to

$$(F_{\mathcal{A}\mathcal{C}})_*D_{Y_{\mathcal{A}}} = (F_{\mathcal{B}\mathcal{C}})_*(F_{\mathcal{A}\mathcal{B}})_*D_{Y_{\mathcal{A}}} = (F_{\mathcal{B}\mathcal{C}})_*D_{Y_{\mathcal{B}}} = D_{Y_{\mathcal{C}}},$$

we obtain $\mathcal{A} \sim \mathcal{C}$. This concludes the proof. \blacklozenge

To give an example of a periodic homogenization with different atlases, consider the following situation:

4.4.25 Example.

Let $\Omega \subset \mathbb{R}^2$ be a domain. We equip Ω with two different atlases, each consisting of one chart: $\mathcal{A}_1 := \{\text{Id} : \Omega \rightarrow \Omega\}$ as well as $\mathcal{A}_2 := \{\text{Sk} : \Omega \rightarrow \text{Sk}(\Omega)\}$, where the map Sk is given by

$$\begin{aligned} \text{Sk} : \mathbb{R}^n &\longrightarrow \mathbb{R}^n \\ \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} &\longmapsto \begin{pmatrix} x_2 \\ x_1 \end{pmatrix}. \end{aligned}$$

As reference cells, we use $Y_1 = [0, 1]^2$ (for \mathcal{A}_1) and $Y_2 = [0, 1]^2$ (for \mathcal{A}_2). Furthermore, let $D_{Y_1} : Y_1 \rightarrow \mathbb{R}$ be a function (representing material properties in the first reference cell) and set $D_{Y_2}(y_1, y_2) := D_{Y_1}(y_2, y_1)$.

Since $\text{Sk} \circ \text{Id}^{-1} = \text{Sk} : \Omega \rightarrow \text{Sk}(\Omega)$ can be trivially extended to the linear map Sk , defined on the whole of \mathbb{R}^n , and since $\text{Sk} : Y_1 \rightarrow Y_2$ is a coordinate transformation of the reference cells such that $D_{Y_2} = \text{Sk}_*D_{Y_1}$, the Assumption 4.4.18 is fulfilled. Letting $D^\varepsilon(x) = D_{Y_1}(\frac{x}{\varepsilon})$ and $f \in L^2(\Omega)$, the homogenization limit of the Problem (4.11)

$$\begin{aligned} &\text{Find } u^\varepsilon \in W_0^{1,2}(\Omega) \text{ such that:} \\ &-\text{div}(D^\varepsilon \nabla u^\varepsilon) + cu = f \quad \text{in } \Omega \\ &u^\varepsilon = 0 \quad \text{on } \partial\Omega \end{aligned}$$

is identical with respect to both distinguished atlases \mathcal{A}_1 and \mathcal{A}_2 .

4.4.26 Example.

In the situation of the preceding example, one can also consider $\mathcal{A}_1 := \{\text{Id} : \Omega \rightarrow \Omega\}$ and $\mathcal{A}_2 := \{2\text{Id} : \Omega \rightarrow 2\text{Id}(\Omega)\}$, with reference cells $Y_1 = [0, 1]^2$ as well as $Y_2 = [0, 2]^2$ and functions D_{Y_1} as above with $D_{Y_2}(y_1, y_2) = D_{Y_1}(\frac{y_1}{2}, \frac{y_2}{2})$. Here

$$\begin{aligned} 2\text{Id} : \mathbb{R}^n &\longrightarrow \mathbb{R}^n \\ \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} &\longmapsto \begin{pmatrix} 2x_1 \\ 2x_2 \end{pmatrix}. \end{aligned}$$

4.5 Application to Multiscale Problems

In this section we show that the tools we developed for the unfolding on Riemannian manifolds can be used together with the usual methods of periodic unfolding. To this end, we consider a simple multiscale setting in \mathbb{R}^2 , which is outlined in the sequel. We are

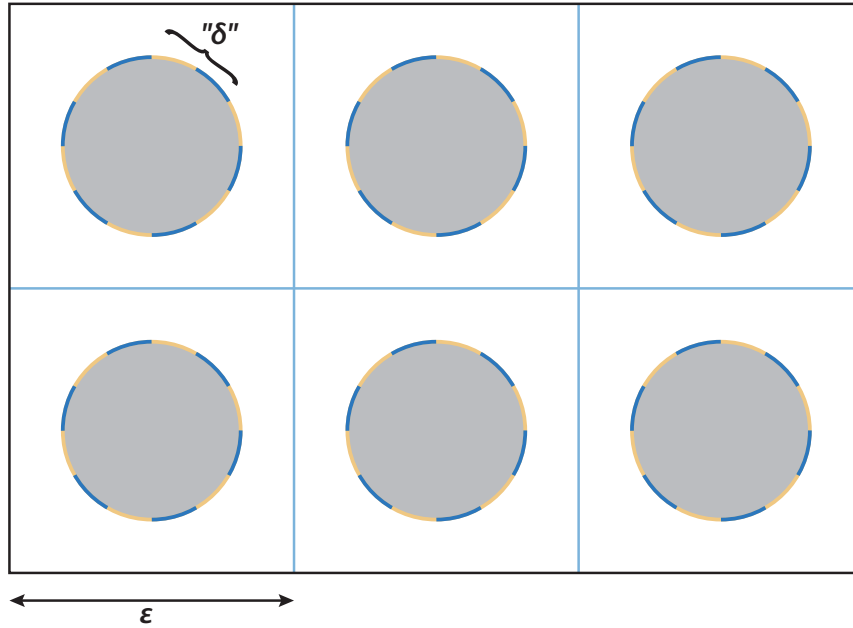


Figure 4.9: Illustration of the multi-scale setting used in this section.

not going into details with the uniqueness and existence proofs as well as the estimates for the solutions, but focus on the derivation of the effective equations.

Let $Y_1 := [0, 1]^2$ be a first reference cell, and let $Y_S := B_{\frac{1}{3}}(\frac{1}{2}, \frac{1}{2}) \subset Y_1$ be an open ball of radius $\frac{1}{3}$ around the center of Y_1 . We consider Y_S to be a solid inclusion in the reference cell and $Y_F := Y \setminus \bar{Y}_S$ to be a part of the reference cell filled with a fluid. The boundary between the two parts is denoted by $\Gamma := \partial Y_S$. Furthermore, let $Y_2 := [0, 1]$ be a second reference cell. Let $\mathcal{A} = \{\varphi_\alpha, \varphi_\beta\}$ be an atlas for Γ as follows: We use the constructions from Section 4.3.2 and define $\varphi_i(x, y) = \lambda_i(3x, 3y)$, $i = \alpha, \beta$. The inverse maps are then given by $\varphi_i^{-1} = \frac{1}{3}\lambda_i^{-1}$, $i = \alpha, \beta$. One can easily see that \mathcal{A} fulfills the UC-criterion.

Now let $\Omega \subset \mathbb{R}^2$ be the domain of interest. Choose two scaling parameters $\varepsilon > 0$ (for Y_1) and $\delta > 0$ (for Y_2). Set

$$\Omega^\varepsilon := \Omega \cap \sum_{k \in \mathbb{Z}^2} \varepsilon(Y_F + k) \quad \text{and} \quad \Gamma^\varepsilon := \bar{\Omega} \cap \sum_{k \in \mathbb{Z}^2} \varepsilon(\Gamma + k).$$

Let the two functions $D : \Omega \times Y_1 \rightarrow \mathbb{R}$ as well as $D_\Gamma : \bar{\Omega} \times Y_2 \rightarrow \mathbb{R}$ be given. (They correspond to the diffusivity in Ω and on Γ .) We assume that D and D_Γ are continuous, periodic with respect to the argument in the corresponding reference cell, and bounded in the following way: Let there exist constants $0 < d_0 < D_0$ and $0 < d_1 < D_1$ such that $d_0 \leq D \leq D_0$ as well as $d_1 \leq D_\Gamma \leq D_1$.

Define $D^\varepsilon(x) := D(x, \{\frac{x}{\varepsilon}\}_{Y_1})$ as well as

$$D_\Gamma^{\varepsilon\delta} := D_\Gamma\left(x, \left\{ \frac{\varphi_i(\{\frac{x}{\varepsilon}\}_{Y_1})}{\delta} \right\}_{Y_2} \right),$$

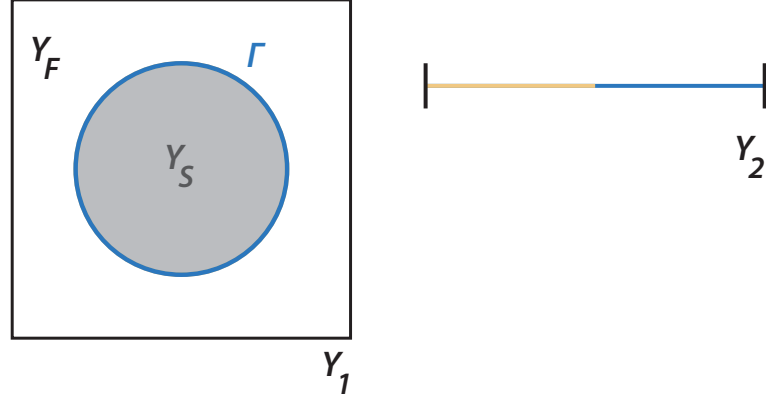


Figure 4.10: The reference cells used for the construction of the domain.

where $i \in \{\alpha, \beta\}$ is chosen such that $\{\frac{x}{\varepsilon}\}_{Y_1}$ is in the domain of φ_i . Due to the UC-criterion, the expression $\left\{ \frac{\varphi_i(\{\frac{x}{\varepsilon}\}_{Y_1})}{\delta} \right\}_{Y_2}$ is well-defined independently of i .

On Γ^ε , we use the Riemannian metric g induced by the Euclidean scalar product. Thus for the metric coefficient it holds $g_{1,1} \equiv 1$. This implies that $(g_{Y_2}^{(y_1, \delta)})_{11} \equiv 1 \equiv (g_{Y_2}^{(y_1)})_{11}$ and $\nabla_{Y_2}^{(y_1, \delta)} = \nabla_{Y_2}^{(y_1)} = \nabla_{Y_2}$ (independent of $y_1 \in Y_1$) as well.

4.5.1 Diffusion and Exchange on a Periodically Structured Boundary

We consider the following problem: For given right hand side $f \in H^1(0, T; L^2(\Omega))$, initial values $u_0 \in H^1(\Omega)$ and $u_{0, \Gamma} \in H^2(\Omega)$ and exchange coefficients $a, b > 0$ find $u^{\varepsilon\delta}$ and $u_{\Gamma}^{\varepsilon\delta}$ such that

$$\partial_t u^{\varepsilon\delta} - \operatorname{div}(D^\varepsilon \nabla u^{\varepsilon\delta}) = f \quad \text{in } \Omega^\varepsilon \quad (4.28a)$$

$$-D^\varepsilon \nabla u^{\varepsilon\delta} \cdot \nu = \varepsilon(au^{\varepsilon\delta} - bu_{\Gamma}^{\varepsilon\delta}) \quad \text{on } \Gamma^\varepsilon \quad (4.28b)$$

$$u^{\varepsilon\delta} = 0 \quad \text{on } \partial\Omega \quad (4.28c)$$

$$u^{\varepsilon\delta}(0, \cdot) = u_0 \quad \text{in } \Omega^\varepsilon \quad (4.28d)$$

as well as

$$\partial_t u_{\Gamma}^{\varepsilon\delta} - \varepsilon^2 \operatorname{div}_{\Gamma}(D_{\Gamma}^{\varepsilon\delta} \nabla_{\Gamma} u_{\Gamma}^{\varepsilon\delta}) = au^{\varepsilon\delta} - bu_{\Gamma}^{\varepsilon\delta} \quad \text{on } \Gamma^\varepsilon \quad (4.29a)$$

$$u_{\Gamma}^{\varepsilon\delta}(0, \cdot) = u_{0, \Gamma} \quad \text{on } \Gamma^\varepsilon. \quad (4.29b)$$

4.5.1 Proposition.

There exists a unique solution

$$u^{\varepsilon\delta} \in L^2(0, T; H^1(\Omega^\varepsilon)), \quad \partial_t u^{\varepsilon\delta} \in L^2(0, T; L^2(\Omega^\varepsilon))$$

$$u_{\Gamma}^{\varepsilon\delta} \in L^2(0, T; H^1(\Gamma^\varepsilon)) \quad \partial_t u_{\Gamma}^{\varepsilon\delta} \in L^2(0, T; L^2(\Gamma^\varepsilon))$$

of Problem (4.28), (4.29).

Proof. This is a special case of Theorem 3.3.9 and the results in Section 3.3 (with obvious modifications), where no evolution of the microstructure takes place (and thus $F = \text{Id}$). \blacklozenge

4.5.2 Proposition.

There exists a constant $C > 0$, independent of ε, δ , such that

$$\left. \begin{aligned} & \|u^{\varepsilon\delta}\|_{L^2(0, T; L^2(\Omega^\varepsilon))} + \|\nabla u^{\varepsilon\delta}\|_{L^2(0, T; L^2(\Omega^\varepsilon))} \leq C \\ \varepsilon \|u_\Gamma^{\varepsilon\delta}\|_{L^2(0, T; L^2(\Gamma^\varepsilon))} + \varepsilon^{\frac{3}{2}} \|\nabla^\Gamma u_\Gamma^{\varepsilon\delta}\|_{L^2(0, T; L^2(\Gamma^\varepsilon))} & \leq C \end{aligned} \right\} \quad (4.30)$$

as well as

$$\left. \begin{aligned} & \|\partial_t u^{\varepsilon\delta}\|_{L^2(0, T; L^2(\Omega^\varepsilon))} + \|\nabla \partial_t u^{\varepsilon\delta}\|_{L^2(0, T; L^2(\Omega^\varepsilon))} \leq C \\ \varepsilon \|\partial_t u_\Gamma^{\varepsilon\delta}\|_{L^2(0, T; L^2(\Gamma^\varepsilon))} + \varepsilon^{\frac{3}{2}} \|\nabla^\Gamma \partial_t u_\Gamma^{\varepsilon\delta}\|_{L^2(0, T; L^2(\Gamma^\varepsilon))} & \leq C. \end{aligned} \right\} \quad (4.31)$$

Proof. This is again a special case of the results for evolving hypersurfaces (with obvious modifications), see Section 3.3.5. Equation (4.30) follows by inserting $u^{\varepsilon\delta}$ and $u_\Gamma^{\varepsilon\delta}$ as test functions in the weak formulation of Problems (4.28) and (4.29), resp. To obtain (4.31), one can differentiate the equations defining $u^{\varepsilon\delta}$ and $u_\Gamma^{\varepsilon\delta}$, and use $\partial_t u^{\varepsilon\delta}$ as well as $\partial_t u_\Gamma^{\varepsilon\delta}$ as test functions. \blacklozenge

Using the continuity of the unfolding operators and the compactness results for $\mathcal{T}^\varepsilon, \mathcal{T}_b^\varepsilon$ and $\mathcal{T}_\mathcal{A}^\delta$ (cf. Theorems 4.2.29 and 4.2.35), we obtain that along a subsequence

$$\begin{aligned} \mathcal{T}^\varepsilon(u^{\varepsilon\delta}) &\rightharpoonup u && \text{in } L^2(0, T; L^2(\Omega \times Y_F)) \\ \mathcal{T}^\varepsilon(\nabla u^{\varepsilon\delta}) &\rightharpoonup \nabla u + \nabla_{Y_1} u_1 && \text{in } L^2(0, T; L^2(\Omega \times Y_F)) \\ \mathcal{T}_b^\varepsilon(u^{\varepsilon\delta}) &\rightharpoonup u && \text{in } L^2(0, T; L^2(\Omega \times \Gamma)) \\ \mathcal{T}_\mathcal{A}^\delta \mathcal{T}_b^\varepsilon(u_\Gamma^{\varepsilon\delta}) &\rightharpoonup u_\Gamma && \text{in } L^2(0, T; L^2(\Omega \times \Gamma)) \\ \varepsilon \mathcal{T}_\mathcal{A}^\delta \mathcal{T}_b^\varepsilon(\nabla^\Gamma u_\Gamma^{\varepsilon\delta}) &\rightharpoonup (\nabla_{Y_1, \Gamma} u_\Gamma)_{Y_2} + \nabla_{Y_2} u_{\Gamma, 1} && \text{in } L^2(0, T; L^2(\Omega \times \Gamma \times Y_2)) \\ \mathcal{T}^\varepsilon(\partial_t u^{\varepsilon\delta}) &\rightharpoonup \partial_t u && \text{in } L^2(0, T; L^2(\Omega \times Y_F)) \\ \mathcal{T}_\mathcal{A}^\delta \mathcal{T}_b^\varepsilon(\partial_t u_\Gamma^{\varepsilon\delta}) &\rightharpoonup \partial_t u_\Gamma && \text{in } L^2(0, T; L^2(\Omega \times \Gamma)) \end{aligned}$$

with functions

$$\begin{aligned} u &\in L^2(0, T; H^1(\Omega)) \\ u_1 &\in L^2(0, T; L^2(\Omega; H_\#^1(Y_F))) \\ u_\Gamma &\in L^2(0, T; L^2(\Omega; H^1(\Gamma))) \\ u_{\Gamma, 1} &\in L^2(0, T; L^2(\Omega \times \Gamma; H_\#^1(Y_2))). \end{aligned}$$

Now we choose test functions $\phi \in \mathcal{C}([0, T]; \mathcal{C}_0^\infty(\Omega))$, $\phi_1 \in \mathcal{C}([0, T]; \mathcal{C}_0^\infty(\Omega; \mathcal{C}_\#^\infty(Y_F)))$ as well as $\phi_\Gamma \in \mathcal{C}([0, T]; \mathcal{C}_0^\infty(\Omega; \mathcal{C}^\infty(\Gamma)))$, $\phi_{\Gamma, 1} \in \mathcal{C}([0, T]; \mathcal{C}_0^\infty(\Omega; \mathcal{C}^\infty(\Gamma; \mathcal{C}_\#^\infty(Y_2))))$ and construct

$$\begin{aligned} \phi^\varepsilon(t, x) &= \phi(t, x) + \varepsilon \phi_1\left(t, x, \left\{\frac{x}{\varepsilon}\right\}_{Y_1}\right) \\ \phi_\Gamma^{\varepsilon\delta}(t, x) &= \phi_\Gamma\left(t, x, \left\{\frac{x}{\varepsilon}\right\}_{Y_1}\right) + \varepsilon \phi_{\Gamma, 1}\left(t, x, \left\{\frac{x}{\varepsilon}\right\}_{Y_1}, \left\{\frac{\varphi_i(\left\{\frac{x}{\varepsilon}\right\}_{Y_1})}{\delta}\right\}_{Y_2}\right) \end{aligned}$$

with $i \in \{\alpha, \beta\}$. Note that $\mathcal{T}^\varepsilon(\phi^\varepsilon) \rightarrow \phi$, $\mathcal{T}^\varepsilon(\nabla \phi^\varepsilon) \rightarrow \nabla \phi + \nabla_{Y_1} \phi_1$. Moreover

$$\begin{aligned} \mathcal{T}_{\mathcal{A}}^\delta \mathcal{T}_b^\varepsilon(\phi_\Gamma^\varepsilon)(t, x, y_1, y_2) &= \phi_\Gamma \left(t, \varepsilon \left[\frac{x}{\varepsilon} \right] + \varepsilon \left(\varphi_i^{-1} \left(\delta \left[\frac{\varphi_i(y_1)}{\delta} \right] + \delta y_2 \right) \right), \varphi_i^{-1} \left(\delta \left[\frac{\varphi_i(y_1)}{\delta} \right] + \delta y_2 \right) \right) \\ &\quad + \varepsilon \phi_{\Gamma,1} \left(t, \varepsilon \left[\frac{x}{\varepsilon} \right] + \varepsilon \left(\varphi_i^{-1} \left(\delta \left[\frac{\varphi_i(y_1)}{\delta} \right] + \delta y_2 \right) \right), \varphi_i^{-1} \left(\delta \left[\frac{\varphi_i(y_1)}{\delta} \right] + \delta y_2 \right), y_2 \right) \\ &\rightarrow \varphi_\Gamma(t, x, y_1) \end{aligned}$$

(this convergence also holds in $\mathcal{C}([0, T] \times \Omega \times Y_1 \times Y_2)$) and

$$\begin{aligned} \varepsilon \mathcal{T}_{\mathcal{A}}^\delta \mathcal{T}_b^\varepsilon(\nabla^\Gamma \phi_\Gamma^\varepsilon)(t, x, y_1, y_2) &= \mathcal{T}_{\mathcal{A}}^\delta \left(\nabla_{\Gamma, Y_1} \mathcal{T}_b^\varepsilon(\phi_\Gamma^\varepsilon) \right)(t, x, y_1, y_2) \\ &= \mathcal{T}_{\mathcal{A}}^\delta \left(\nabla_{\Gamma, Y_1} \left[\phi_\Gamma \left(t, \varepsilon \left[\frac{x}{\varepsilon} \right] + \varepsilon y_1, y_1 \right) + \varepsilon \phi_{\Gamma,1} \left(t, \varepsilon \left[\frac{x}{\varepsilon} \right] + \varepsilon y_1, y_1, \left\{ \frac{\varphi_i(y_1)}{\delta} \right\}_{Y_2} \right) \right] \right) \\ &\rightarrow \left((\nabla_{\Gamma, Y_1} \phi_\Gamma)_{Y_2} + \nabla_{Y_2} \phi_{\Gamma,1} \right)(t, x, y_1, y_2), \end{aligned}$$

cf. Lemma 4.4.3. Here we used the notation $\nabla_{Y_2}^{(y_1)} = \nabla_{Y_2}$, since the operator on the left hand side does not depend on y_1 .

We now come to the unfolding of the bulk problem. Its weak formulation (with test function ϕ^ε) is given by

$$\begin{aligned} \int_0^T \int_{\Omega^\varepsilon} \partial_t u^{\varepsilon\delta} \phi^\varepsilon \, dx \, dt + \int_0^T \int_{\Omega^\varepsilon} D^\varepsilon \nabla u^{\varepsilon\delta} \nabla \phi^\varepsilon \, dx \, dt \\ = \int_0^T \int_{\Omega^\varepsilon} f \phi^\varepsilon \, dx \, dt - \varepsilon \int_0^T \int_{\Gamma^\varepsilon} (a u^{\varepsilon\delta} \phi^\varepsilon - b u_\Gamma^{\varepsilon\delta} \phi^\varepsilon) \, d\sigma_x \, dt. \end{aligned}$$

Unfolding of the first term of the last integral on the right hand side with $\mathcal{T}_b^\varepsilon$, the second term with $\mathcal{T}_{\mathcal{A}}^\delta \mathcal{T}_b^\varepsilon$, and unfolding of the remaining integrals with \mathcal{T}^ε (with respect to \simeq) yields

$$\begin{aligned} \frac{1}{|Y_1|} \int_0^T \int_{\Omega} \int_{Y_F} \mathcal{T}^\varepsilon(\partial_t u^{\varepsilon\delta}) \mathcal{T}^\varepsilon(\phi^\varepsilon) \, dy_1 \, dx \, dt \\ + \frac{1}{|Y_1|} \int_0^T \int_{\Omega} \int_{Y_F} \mathcal{T}^\varepsilon(D^\varepsilon) \mathcal{T}^\varepsilon(\nabla u^{\varepsilon\delta}) \mathcal{T}^\varepsilon(\nabla \phi^\varepsilon) \, dy_1 \, dx \, dt \\ = \frac{1}{|Y_1|} \int_0^T \int_{\Omega} \int_{Y_F} \mathcal{T}^\varepsilon(f) \mathcal{T}^\varepsilon(\phi^\varepsilon) \, dy_1 \, dx \, dt - \frac{1}{|Y_1|} \int_0^T \int_{\Omega} \int_{\Gamma} a \mathcal{T}_b^\varepsilon(u^{\varepsilon\delta}) \mathcal{T}_b^\varepsilon(\phi^\varepsilon) \, d\sigma_{y_1} \, dx \, dt \\ + \frac{1}{|Y_1| |Y_2|} \int_0^T \int_{\Omega} \int_{\Gamma} \int_{Y_2} b \mathcal{T}_{\mathcal{A}}^\delta \mathcal{T}_b^\varepsilon(u_\Gamma^{\varepsilon\delta}) \mathcal{T}_{\mathcal{A}}^\delta \mathcal{T}_b^\varepsilon(\phi^\varepsilon) \, dy_2 \, d\sigma_{y_1} \, dx \, dt. \end{aligned}$$

Passing to the limit, we obtain

$$\begin{aligned}
& \frac{1}{|Y_1|} \int_0^T \int_{\Omega} \int_{Y_F} \partial_t u(t, x) \phi(t, x) \, dy_1 \, dx \, dt \\
& \quad + \frac{1}{|Y_1|} \int_0^T \int_{\Omega} \int_{Y_F} D(x, y_1) (\nabla u(t, x) + \nabla_{Y_1} u_1(t, x, y_1)) \\
& \quad \quad \cdot (\nabla \phi(t, x) + \nabla_{Y_1} \phi_1(t, x, y_1)) \, dy_1 \, dx \, dt \\
& = \frac{1}{|Y_1|} \int_0^T \int_{\Omega} \int_{Y_F} f(t, x) \phi(t, x) \, dy_1 \, dx \, dt - \frac{1}{|Y_1|} \int_0^T \int_{\Omega} \int_{\Gamma} a u(t, x) \phi(t, x) \, d\sigma_{y_1} \, dx \, dt \\
& \quad + \frac{1}{|Y_1| |Y_2|} \int_0^T \int_{\Omega} \int_{\Gamma} \int_{Y_2} b u_{\Gamma}(t, x, y_1) \phi(t, x) \, dy_2 \, d\sigma_{y_1} \, dx \, dt.
\end{aligned}$$

For the surface problem, we obtain in the weak form

$$\begin{aligned}
& \int_0^T \int_{\Gamma^\varepsilon} \partial_t u_{\Gamma}^{\varepsilon\delta} \phi_{\Gamma}^{\varepsilon\delta} \, d\sigma_x \, dt + \int_0^T \int_{\Gamma^\varepsilon} D_{\Gamma}^{\varepsilon\delta} \nabla^{\Gamma} u_{\Gamma}^{\varepsilon\delta} \nabla^{\Gamma} \phi_{\Gamma}^{\varepsilon\delta} \, d\sigma_x \, dt \\
& \quad = \int_0^T \int_{\Gamma^\varepsilon} a u^{\varepsilon\delta} \phi_{\Gamma}^{\varepsilon\delta} \, d\sigma_x \, dt - \int_0^T \int_{\Gamma^\varepsilon} b u_{\Gamma}^{\varepsilon\delta} \phi_{\Gamma}^{\varepsilon\delta} \, d\sigma_x \, dt,
\end{aligned}$$

which upon multiplication with ε and unfolding with $\mathcal{T}_{\mathcal{A}}^{\delta} \mathcal{T}_b^{\varepsilon}$ yields

$$\begin{aligned}
& \frac{1}{|Y_1| |Y_2|} \int_0^T \int_{\Omega} \int_{\Gamma} \int_{Y_2} \mathcal{T}_{\mathcal{A}}^{\delta} \mathcal{T}_b^{\varepsilon} (\partial_t u_{\Gamma}^{\varepsilon\delta}) \mathcal{T}_{\mathcal{A}}^{\delta} \mathcal{T}_b^{\varepsilon} (\phi_{\Gamma}^{\varepsilon\delta}) \, dy_2 \, d\sigma_{y_1} \, dx \, dt \\
& \quad + \frac{1}{|Y_1| |Y_2|} \int_0^T \int_{\Omega} \int_{\Gamma} \int_{Y_2} \mathcal{T}_{\mathcal{A}}^{\delta} \mathcal{T}_b^{\varepsilon} (D_{\Gamma}^{\varepsilon\delta}) g_{Y_2} \left(\mathcal{T}_{\mathcal{A}}^{\delta} (\nabla_{Y_1, \Gamma} \mathcal{T}_b^{\varepsilon} (u_{\Gamma}^{\varepsilon\delta})), \right. \\
& \quad \quad \quad \left. \mathcal{T}_{\mathcal{A}}^{\delta} (\nabla_{Y_1, \Gamma} \mathcal{T}_b^{\varepsilon} (\phi_{\Gamma}^{\varepsilon\delta})) \right) \, dy_2 \, d\sigma_{y_1} \, dx \, dt \\
& = \frac{1}{|Y_1| |Y_2|} \int_0^T \int_{\Omega} \int_{\Gamma} \int_{Y_2} a \mathcal{T}_{\mathcal{A}}^{\delta} \mathcal{T}_b^{\varepsilon} (u^{\varepsilon\delta}) \mathcal{T}_{\mathcal{A}}^{\delta} \mathcal{T}_b^{\varepsilon} (\phi_{\Gamma}^{\varepsilon\delta}) \, dy_2 \, d\sigma_{y_1} \, dx \, dt \\
& \quad - \frac{1}{|Y_1| |Y_2|} \int_0^T \int_{\Omega} \int_{\Gamma} \int_{Y_2} b \mathcal{T}_{\mathcal{A}}^{\delta} \mathcal{T}_b^{\varepsilon} (u_{\Gamma}^{\varepsilon\delta}) \mathcal{T}_{\mathcal{A}}^{\delta} \mathcal{T}_b^{\varepsilon} (\phi_{\Gamma}^{\varepsilon\delta}) \, dy_2 \, d\sigma_{y_1} \, dx \, dt.
\end{aligned}$$

Passing to the limit, we obtain

$$\begin{aligned}
& \frac{1}{|Y_1||Y_2|} \int_0^T \int_{\Omega} \int_{\Gamma} \int_{Y_2} \partial_t u_{\Gamma}(t, x, y_1) \phi_{\Gamma}(t, x, y_1) \, dy_2 \, d\sigma_{y_1} \, dx \, dt \\
& + \frac{1}{|Y_1||Y_2|} \int_0^T \int_{\Omega} \int_{\Gamma} \int_{Y_2} D_{\Gamma}(x, y_2) g_{Y_2} \left((\nabla_{Y_1, \Gamma} u_{\Gamma}(t, x, y_1))_{Y_2} + \nabla_{Y_2} u_{\Gamma, 1}(t, x, y_1, y_2), \right. \\
& \quad \left. (\nabla_{Y_1, \Gamma} \phi_{\Gamma}(t, x, y_1))_{Y_2} + \nabla_{Y_2} \phi_{\Gamma, 1}(t, x, y_1, y_2) \right) \, dy_2 \, d\sigma_{y_1} \, dx \, dt \\
& = \frac{1}{|Y_1||Y_2|} \int_0^T \int_{\Omega} \int_{\Gamma} \int_{Y_2} au(t, x) \phi_{\Gamma}(t, x, y_1) \, dy_2 \, d\sigma_{y_1} \, dx \, dt \\
& + \frac{1}{|Y_1||Y_2|} \int_0^T \int_{\Omega} \int_{\Gamma} \int_{Y_2} bu_{\Gamma}(t, x, y_1) \phi_{\Gamma}(t, x, y_1) \, dy_2 \, d\sigma_{y_1} \, dx \, dt.
\end{aligned}$$

Using the techniques outlined previously in this work, we arrive at the following strong form of the limit problem:

4.5.3 Theorem.

The limit functions u, u_{Γ} satisfy the following problem:

$$\begin{aligned}
P \partial_t u(t, x) - \frac{1}{|Y_1|} \operatorname{div}(\tilde{D}(x) \nabla u(t, x)) &= P f(t, x) - \frac{|\Gamma|}{|Y_1|} au(t, x) \\
&+ \frac{1}{|Y_1|} \int_{\Gamma} bu_{\Gamma}(t, x, y_1) \, d\sigma_{y_1} \quad \text{in } \Omega \\
u &= 0 \quad \text{on } \partial\Omega \\
u(0, \cdot) &= u_0 \quad \text{in } \Omega
\end{aligned}$$

with the matrix $(\tilde{D}(x))_{ij} = (\int_{Y_F} D(x, y_1) (\delta_{ij} + \frac{\partial w_i}{\partial y_{1,j}}(x, y_1)) \, dy_1)$, $P = \frac{|Y_F|}{|Y_1|}$ and the cell problem

$$\begin{aligned}
-\operatorname{div}_{Y_1}(D(x, y_1) \nabla_{Y_1} w_i(x, y_1)) &= \operatorname{div}_{Y_1}(D(x, y_1) e_i) \quad \text{in } Y_F \\
D(x, y_1) \nabla_{Y_1} w_i(x, y_1) \cdot \nu &= 0 \quad \text{on } \Gamma \\
y_1 &\mapsto w_i(x, y_1) \quad \text{is } Y_1\text{-periodic,}
\end{aligned}$$

together with

$$\begin{aligned}
\partial_t u_{\Gamma}(t, x, y_1) - \operatorname{div}_{Y_1, \Gamma}(\tilde{D}_{\Gamma}(x) \nabla_{Y_1, \Gamma} u_{\Gamma}(t, x, y_1)) &= au(t, x) - bu_{\Gamma}(t, x, y_1) \quad \text{on } \Gamma \\
u_{\Gamma}(0, x, \cdot) &= u_{0, \Gamma}(x),
\end{aligned}$$

where $\tilde{D}_\Gamma(x) = (\int_{Y_2} D_\Gamma(x, y_2)(1 + \frac{\partial w}{\partial y_2}(x, y_2)) dy_2)$ and w fulfills

$$\begin{aligned} -\operatorname{div}_{Y_2}(D_\Gamma(x, y_2) \nabla_{Y_2} w) &= \operatorname{div}_{Y_2}(D_\Gamma(x, y_2) \cdot 1) \quad \text{in } Y_2 \\ y_2 &\longmapsto w(x, y_2) \quad \text{is } Y_2\text{-periodic.} \end{aligned}$$

4.5.2 Periodic Exchange Coefficient

In addition to the assumptions and constructions at the beginning of this section, let $h : \Omega \times Y_2 \rightarrow \mathbb{R}$ be continuous. Define

$$h^{\varepsilon\delta}(x) = h(x, \left\{ \frac{\phi_i(\{\frac{x}{\varepsilon}\}_{Y_1})}{\delta} \right\}_{Y_2}).$$

We consider the following problem with a periodic exchange coefficient: Find $u^{\varepsilon\delta}$ such that

$$\partial_t u^{\varepsilon\delta} - \operatorname{div}(D^\varepsilon \nabla u^{\varepsilon\delta}) = f \quad \text{in } \Omega^\varepsilon \quad (4.32a)$$

$$D^\varepsilon \nabla u^{\varepsilon\delta} \cdot \nu = \varepsilon D_\Gamma^{\varepsilon\delta}(u^{\varepsilon\delta} - h^{\varepsilon\delta}) \quad \text{on } \Gamma^\varepsilon \quad (4.32b)$$

$$u^{\varepsilon\delta} = 0 \quad \text{on } \partial\Omega \quad (4.32c)$$

$$u^{\varepsilon\delta}(0, \cdot) = u_0 \quad \text{in } \Omega^\varepsilon. \quad (4.32d)$$

The following result can be obtained by standard methods:

4.5.4 Proposition.

Assume $f \in H^1(0, T; L^2(\Omega))$ and $u_0 \in H^1(\Omega)$. Let D^ε and $D_\Gamma^{\varepsilon\delta}$ be given as above. Then there exists a unique weak solution $u^{\varepsilon\delta} \in L^2(0, T; H^1(\Omega^\varepsilon)) \cap H^1(0, T; L^2(\Omega^\varepsilon))$ of Problem (4.32), and the estimate

$$\|u^{\varepsilon\delta}\|_{L^2(0, T; H^1(\Omega^\varepsilon))} + \|\partial_t u^{\varepsilon\delta}\|_{L^2(0, T; L^2(\Omega^\varepsilon))} \leq C$$

holds with a constant $C > 0$ independent of ε, δ .

Due to the compactness results, we obtain the following convergences (along subsequences):

$$\begin{aligned} \mathcal{T}^\varepsilon(u^{\varepsilon\delta}) &\longrightarrow u && \text{in } L^2(0, T; L^2(\Omega \times Y_F)) \\ \mathcal{T}^\varepsilon(\nabla u^{\varepsilon\delta}) &\longrightarrow \nabla u + \nabla_{Y_1} u_1 && \text{in } L^2(0, T; L^2(\Omega \times Y_F)) \\ \mathcal{T}^\varepsilon(\partial_t u^{\varepsilon\delta}) &\longrightarrow \partial_t u && \text{in } L^2(0, T; L^2(\Omega \times Y_F)), \end{aligned}$$

where $u \in L^2(0, T; H^1(\Omega))$, $u_1 \in L^2(0, T; L^2(\Omega; H_{\#}^1(Y_F)))$. Note that

$$\begin{aligned} \mathcal{T}_{\mathcal{A}}^\delta \mathcal{T}_b^\varepsilon(D_\Gamma^{\varepsilon\delta})(t, x, y_1, y_2) &\longrightarrow D_\Gamma(x, y_2) \\ \mathcal{T}_{\mathcal{A}}^\delta \mathcal{T}_b^\varepsilon(h^{\varepsilon\delta})(t, x, y_1, y_2) &\longrightarrow h(x, y_2) \end{aligned}$$

uniformly. Using the test function ϕ^ε as above, we obtain in the weak formulation

$$\begin{aligned} & \int_0^T \int_\Omega \partial_t u^{\varepsilon\delta} \, dx \, dt + \int_0^T \int_\Omega D^\varepsilon \nabla u^{\varepsilon\delta} \nabla \phi^\varepsilon \, dx \, dt \\ &= \int_0^T \int_\Omega f \phi^\varepsilon \, dx \, dt + \varepsilon \int_0^T \int_{\Gamma^\varepsilon} D_{\Gamma^\varepsilon}^{\varepsilon\delta} (u^{\varepsilon\delta} - h^{\varepsilon\delta}) \phi^\varepsilon \, d\sigma_x \, dt. \end{aligned}$$

Upon unfolding, we obtain with respect to \simeq

$$\begin{aligned} & \frac{1}{|Y_1|} \int_0^T \int_\Omega \int_{Y_F} \mathcal{T}^\varepsilon(\partial_t u^{\varepsilon\delta}) \mathcal{T}^\varepsilon(\phi^\varepsilon) \, dy_1 \, dx \, dt \\ &+ \frac{1}{|Y_1|} \int_0^T \int_\Omega \int_{Y_F} \mathcal{T}^\varepsilon(D^\varepsilon) \mathcal{T}^\varepsilon(\nabla u^{\varepsilon\delta}) \mathcal{T}^\varepsilon(\nabla \phi^\varepsilon) \, dy_1 \, dx \, dt \\ &= \frac{1}{|Y_1|} \int_0^T \int_\Omega \int_{Y_F} \mathcal{T}^\varepsilon(f) \mathcal{T}^\varepsilon(\phi^\varepsilon) \, dy_1 \, dx \, dt + \frac{1}{|Y_1||Y_2|} \int_0^T \int_\Omega \int_\Gamma \int_{Y_2} \mathcal{T}_{\mathcal{A}}^\delta \mathcal{T}_b^\varepsilon(D^{\varepsilon\delta}) \left(\mathcal{T}_{\mathcal{A}}^\delta \mathcal{T}_b^\varepsilon(u^{\varepsilon\delta}) \right. \\ &\quad \left. - \mathcal{T}_{\mathcal{A}}^\delta \mathcal{T}_b^\varepsilon(h^{\varepsilon\delta}) \right) \mathcal{T}_{\mathcal{A}}^\delta \mathcal{T}_b^\varepsilon(\phi^\varepsilon) \, dy_2 \, dy_1 \, dx \, dt. \end{aligned}$$

Passing to the limit yields

$$\begin{aligned} & \frac{1}{|Y_1|} \int_0^T \int_\Omega \int_{Y_F} \partial_t u(t, x) \phi(t, x) \, dy_1 \, dx \, dt \\ &+ \frac{1}{|Y_1|} \int_0^T \int_\Omega \int_{Y_F} D(x, y_1) (\nabla u(t, x) + \nabla_{Y_1} u_1(t, x, y_1)) \\ &\quad \cdot (\nabla \phi(t, x) + \nabla_{Y_1} \phi_1(t, x, y_1)) \, dy_1 \, dx \, dt \\ &= \frac{1}{|Y_1|} \int_0^T \int_\Omega \int_{Y_F} f(t, x) \phi(t, x) \, dy_1 \, dx \, dt \\ &+ \frac{1}{|Y_1||Y_2|} \int_0^T \int_\Omega \int_\Gamma \int_{Y_2} D_\Gamma(x, y_2) (u(t, x) - h(x, y_2)) \phi(t, x) \, dy_2 \, d\sigma_{y_1} \, dx \, dt. \end{aligned}$$

If we recast this formulation into the strong form, we obtain the following:

4.5.5 Theorem.

The limit function u satisfies the following problem:

$$\begin{aligned}
 P\partial_t u(t, x) - \frac{1}{|Y_1|} \operatorname{div}(\tilde{D}(x) \nabla u(t, x)) &= Pf(t, x) + \frac{|\Gamma|}{|Y_2|} \int_{Y_2} D_\Gamma(x, y_2) \left(u(t, x) \right. \\
 &\quad \left. - h(x, y_2) \right) dy_2 \quad \text{in } \Omega \\
 u &= 0 \quad \text{on } \partial\Omega \\
 u(0, \cdot) &= u_0 \quad \text{in } \Omega,
 \end{aligned}$$

where P, \tilde{D} and the cell problem are the same as in Theorem 4.5.3.

4.6 Appendix: Function Spaces on Manifolds

In this section we collect some results about Lebesgue and Sobolev spaces on manifolds, with a focus on the constructions used for the unfolding on manifolds and the application treated in Section 4.4. In the sequel, let $M \subset \mathbb{R}^m$ be a n -dimensional compact Riemannian manifold of class \mathcal{C}^1 with metric $g \in \Gamma(TM^* \otimes TM^*)$. Further assumptions on the smoothness of M will be imposed later. Note that the compactness of M facilitates a lot of results and proofs – thus the reader should keep in mind that noncompact situations require special attention!

Although there is a large amount of literature available on Sobolev-spaces on domains (see e.g. the classical references Maz'ja [Maz85], Adams and Fournier [AF03] or Kufner, John, and Fučík [KJF77]), there is no concise treatise of Sobolev spaces on manifolds available which covers the results needed for the unfolding theory. Therefore we point the reader to the following works: Emmanuel Hebey considers the spaces for different classes of Riemannian manifolds, with a strong emphasis on embeddings and best constants, see [Heb96], [Heb99] and especially [HR08]. Additional results can also be found in the book of Rosenberg [Ros97] or other literature on global analysis (see also Jost [Jos98]). Sobolev spaces on manifolds with applications to partial differential equations in mind are treated in Wloka [Wlo92] and Taylor [Tay97].

4.6.1 Lebesgue-Spaces

We follow the derivations in [AE01], where the proof of the following statements can be found as well: A subset $A \subset M$ is called (Lebesgue-)measurable, if for all $x \in A$ there exists a chart (ϕ, U) with $x \in U$ such that $\phi(A \cap U)$ is Lebesgue-measurable in \mathbb{R}^n . The set \mathcal{M} of all measurable subsets of M is called the Lebesgue σ -Algebra of M .

Let $\mathcal{A} = \{(\phi_i, U_i), i \in \{1, \dots, k\}\}$ be a finite atlas for M . Let $\{\pi_i, i = 1, \dots, k\}$ be a partition of unity, subordinate to $\{U_i, i = 1, \dots, k\}$. For $A \in \mathcal{M}$, one can define the measure

$$\operatorname{vol}_M(A) := \int_A 1 \, d\operatorname{vol}_M := \sum_{i=1}^k \int_{\phi_i(A \cap U_i)} (\phi_i)_* \pi_i \cdot (\phi_i)_* \sqrt{|G|} \, d\lambda^n.$$

4.6.1 Lemma.

A function $f : M \rightarrow \mathbb{R}$ is measurable iff $\phi_* f : \phi(U) \rightarrow \mathbb{R}$ is measurable for all charts $(\phi, U) \in \mathcal{A}$.

4.6.2 Proposition.

A measurable function $f : M \rightarrow \mathbb{R}$ is in $L^p(M)$ for $1 \leq p < \infty$ iff $(\phi_* |f|^p) \phi_* \sqrt{|G|}$ is in $L^1(\phi(U))$ for all charts $(\phi, U) \in \mathcal{A}$. We have the identity

$$\int_M f \, d\text{vol}_M = \sum_{i=1}^k \int_{U_i} \pi_i f \, d\text{vol}_M = \sum_{i=1}^k \int_{\phi_i(U_i)} (\phi_i)_* \pi_i \cdot (\phi_i)_* f \cdot (\phi_i)_* \sqrt{|G|} \, d\lambda^n$$

for all $f \in L^1(M)$.

4.6.3 Lemma.

It holds

- Each continuous scalar function on M is measurable.
- The set $\mathcal{C}_0(M)$ is dense in $L^p(M)$ for all $1 \leq p < \infty$.

4.6.2 Sobolev-Spaces for Scalar Functions

Here we require more regularity for the manifold: Let M be of class $\mathcal{C}^{l,\kappa}$. Again, let $\mathcal{A} = \{(\phi_i, U_i), i \in \{1, \dots, k\}\}$ be a finite atlas for M , and let $\{\pi_i, i = 1, \dots, k\}$ be a partition of unity, subordinate to $\{U_i, i = 1, \dots, k\}$. We will follow the derivations in [Wlo92] and prove some results needed for the unfolding on manifolds and its applications. To this end, fix $l \in \mathbb{R}_{\geq 0}$ and $\kappa \in [0, 1)$. Choose an order of differentiability $r \leq l + \kappa$ if $l + \kappa$ is an integer; or $r < l + \kappa$ otherwise. Let $p \in [1, \infty)$ be an order of integration.

4.6.4 Definition.

Let $u : M \rightarrow \mathbb{R}$ be measurable. u belongs to the Sobolev space $W^{r,p}(M)$ if

$$(\phi_i)_*(u \cdot \pi_i) : \phi_i(U_i) \rightarrow \mathbb{R}$$

is an element of $W^{r,p}(\phi_i(U_i))$ for all $i \in \{1, \dots, k\}$.

4.6.5 Lemma.

$W^{r,p}(M)$ is a Banach space with the norm

$$\|u\|_{W^{r,p}(M)}^p = \sum_{i=1}^k \|(\phi_i)_*(u \cdot \pi_i)\|_{W^{r,p}(\phi_i(U_i))}^p.$$

For $p = 2$, this norm is induced by a scalar product

$$(u, w)_r = \sum_{i=1}^k ((\phi_i)_*(u \cdot \pi_i), (\phi_i)_*(w \cdot \pi_i))_{W^{r,2}(\phi_i(U_i))},$$

and hence $W^{r,2}(M)$ is a Hilbert space.

The reader is pointed to the fact that we are not going to use these norms in the sequel, but we will endow the Sobolev-spaces with an equivalent norm, see below.

4.6.6 Proposition.

The space $\mathcal{C}^{l,\kappa}(M)$ is dense in $W^{r,p}(M)$.

Proof. Let $u \in W^{r,p}(M)$. Set $u_i = u \cdot \pi_i$ for $i = 1, \dots, k$, i.e. $u = \sum_i u_i$ and $(\phi_i)_* u_i \in W_0^{r,p}(\phi_i(U_i))$. Since $\mathcal{C}_0^\infty(\phi_i(U_i))$ is dense in $W_0^{r,p}(\phi_i(U_i))$, for each $n \in \mathbb{N}$ there exists a $w_{i,n} \in \mathcal{C}_0^\infty(\phi_i(U_i))$ such that

$$\|(\phi_i)_* u_i + w_{i,n}\|_{W^{r,p}(\phi_i(U_i))} \leq \frac{1}{n \cdot k}.$$

Extend the $w_{i,n}$ by 0 and define $w = \sum_{i=1}^k w_{i,n} \circ \phi_i$. Then clearly $w \in \mathcal{C}^{l,\kappa}(M)$ and by the definition of the norm

$$\|u - w\|_{W^{r,p}(M)} \leq \frac{1}{n}. \quad \blacklozenge$$

Note that the smoothness of the charts ϕ_i limits the smoothness of the functions $w_{i,n}$.

The following result is crucial in a lot of proofs and constructions:

4.6.7 Proposition.

On a compact manifold, all Riemannian metrics are mutually equivalent.

Proof. See e.g. [HR08]. \blacklozenge

Thanks to this proposition, we can introduce an equivalent norm on $W^{r,p}(M)$ by carrying out all the integrations with respect to the volume measure vol_M on M , i.e. one integrates in $\phi_i(U_i)$ with respect to $(\phi_i)_* \sqrt{|G|} \lambda^n$. The case $p = 2, r = 1$ is considered in the following lemma:

4.6.8 Lemma.

For the Hilbert space $W^{1,2}(M)$, an equivalent scalar product is given by

$$(u, w)_1 = \int_M u \cdot w \, \text{dvol}_M + \int_M g(\nabla_M u, \nabla_M w) \, \text{dvol}_M. \quad (4.33)$$

Epecially, $u \in W^{1,2}(M)$ if and only if $u \in L^2(M)$ and $\nabla_M u \in L^2 TM$ (see the next section).

Proof. The norm given in Lemma 4.6.5 can be written as

$$\|u\|_{W^{1,2}(M)}^2 = \sum_{i=1}^k \int_{\phi_i(U_i)} ((\phi_i)_* u)^2 + \tilde{g}(\nabla(\phi_i)_* u, \nabla(\phi_i)_* u) \, \text{dvol}_M,$$

where \tilde{g} denotes the Riemannian metric induced by the Euclidean scalar product with metric coefficients $\tilde{g}_{ij} = \delta_{ij}$. We first show that the inner product in (4.33) induces an equivalent norm for $g = \tilde{g}$.

To this end, denote by $W^{1,2}(M)$ the Hilbert space as defined in Lemma 4.6.5, and let $\tilde{W}^{1,2}(M)$ be the completion of $\mathcal{C}^{l,\kappa}(M)$ with respect to the norm induced by the scalar product (4.33) (where we use $g = \tilde{g}$). To see that $\tilde{W}^{1,2}(M)$ is a well-defined Hilbert space, we refer the reader to the works of Hebey cited above. We show that there exists a constant $C > 0$ such that $\|\cdot\|_{W^{1,2}(M)} \leq C \|\cdot\|_{\tilde{W}^{1,2}(M)}$, thus the injection $j : \tilde{W}^{1,2}(M) \rightarrow W^{1,2}(M)$ is linear and continuous: Let $u \in \mathcal{C}^\infty(M)$, then

$$\begin{aligned} & \int_M (\pi_i u)^2 \, d\text{vol}_M + \int_M \nabla(\pi_i u) \cdot \nabla(\pi_i u) \, d\text{vol}_M \\ & \leq C \int_M u^2 \, d\text{vol}_M + \int_M (\nabla u \cdot \nabla u + u^2 \nabla \pi_i \cdot \nabla \pi_i + 2u \nabla \pi_i \cdot \nabla u) \, d\text{vol}_M \\ & \leq C \int_M u^2 \, d\text{vol}_M + C \int_M \nabla u \cdot \nabla u \, d\text{vol}_M, \end{aligned}$$

where we used the fact that the functions π_i are continuously differentiable and bounded and Young's inequality on the last summand. Upon summation over i , we obtain the norm inequality for smooth functions. By density of $\mathcal{C}^\infty(M)$ in both spaces, the estimate follows.

Now we show that the range of j is closed. Choose a sequence $u_n \in \tilde{W}^{1,2}(M)$ such that $ju_n \rightarrow w$ for some $w \in W^{1,2}(M)$. Since ju_n is a bounded set in $W^{1,2}(M)$, we see that for all $i = 1, \dots, k$ the functions $\pi_i u_n$ and $\nabla(\pi_i u_n)$ are bounded independent of $n \in \mathbb{N}$ in $L^2(M)$ and $L^2(TM)$, resp. Upon summation over the index i , we obtain that u_n is bounded in $L^2(M)$ and that ∇u_n is bounded in $L^2(TM)$ – thus $\{u_n\}$ is a bounded set in $\tilde{W}^{1,2}(M)$. Since $\tilde{W}^{1,2}$ is reflexive (see [Heb96]), we can extract a subsequence (still denoted by u_n) such that $u_n \rightharpoonup u$ for some $u \in \tilde{W}^{1,2}(M)$. Since j is continuous and linear, it is also weakly continuous, thus $ju_n \rightharpoonup ju$. By the uniqueness of the limits, we obtain $ju = w$, i.e. the range of j is closed. The open mapping theorem now yields that j is surjective and has a continuous inverse. This amounts to saying that $\|\cdot\|_{\tilde{W}^{1,2}(M)} \leq C \|\cdot\|_{W^{1,2}(M)}$, which shows that both norms are equivalent.

Due to Proposition 4.6.7, we can now choose any Riemannian metric on M to obtain a norm equivalent to $\|\cdot\|_{\tilde{W}^{1,2}(M)}$. This finishes the proof of the lemma. \blacklozenge

4.6.9 Remark.

Analogously, we can define Sobolev spaces for functions with values in \mathbb{R}^n . This is done component-wise via the identification $W^{r,p}(M; \mathbb{R}^n) = (W^{r,p}(M))^n$.

In applications, one also needs generalizations of Sobolev spaces with vanishing trace on the boundary of a domain. This is considered next:

Denote by $\mathcal{C}_0^{l,\kappa}(M)$ the set of functions $u \in \mathcal{C}^{l,\kappa}(M)$ such that $\text{supp}(u) \subset M^0$.

4.6.10 Definition.

The function space $W_0^{r,p}(M)$ is defined to be the completion of $\mathcal{C}_0^{l,\kappa}(M)$ with respect to the $W^{r,p}(M)$ -norm.

4.6.3 Embeddings, Traces and the Poincaré Inequality

In this section, we cite some results for Sobolev spaces on manifolds with boundary. Since for our applications (see Section 4.4) we only need the Hilbert space case, we focus on the exponent $p = 2$ and on compact manifolds, following Taylor [Tay97]. Results for arbitrary exponents $p \in [1, \infty]$, for noncompact manifolds or for manifolds without boundary can be found in the books of Hebey [Heb96], [Heb99] and in the classical reference Aubin [Aub82]. In short, most of the well-known results for Sobolev spaces on domains in \mathbb{R}^n also hold for compact Riemannian manifolds with or without boundary. Note that the compactness plays a crucial role!

We use the same assumptions as in the previous section.

4.6.11 Theorem.

Let M have dimension $n \in \mathbb{N}$. Then for $k \in \mathbb{N}_0$, the space $W^{r,2}(M)$ is continuously embedded in

$$\begin{aligned} \mathcal{C}(\bar{M}) & \text{ if } r > \frac{n}{2}, \\ \mathcal{C}^k(\bar{M}) & \text{ if } r > \frac{n}{2} + k, \\ \mathcal{C}^{k,\alpha}(\bar{M}) & \text{ if } r = \frac{n}{2} + k + \alpha \quad \text{with } \alpha \in (0, 1). \end{aligned}$$

4.6.12 Theorem.

For any $r \geq 0$ and $\sigma > 0$, the embedding $W^{r+\sigma,2}(M) \hookrightarrow W^{r,2}(M)$ is compact.

4.6.13 Theorem.

Assume that the boundary ∂M of M is not empty and of class \mathcal{C}^1 . Then for $r > \frac{1}{2}$ there exists a linear and continuous map

$$\tau : W^{r,2}(M) \longrightarrow W^{r-\frac{1}{2},2}(\partial M),$$

the trace map, such that $\tau u = u|_{\partial M}$ for smooth functions u .

4.6.14 Proposition.

We have the characterization

$$W_0^{1,2}(M) = \{u \in W^{1,2}(M) : \tau u = 0\}.$$

4.6.15 Theorem (Poincaré inequality).

Assume that the boundary ∂M of the compact manifold M is not empty. Then there exists a constant $C > 0$ (depending on M) such that $\|u\|_{L^2(M)} \leq C \|du\|_{L^2 T^*M}$ for all $u \in W_0^{1,2}(M)$. Since $\|du\|_{L^2 T^*M} = \|\nabla_M u\|_{L^2 TM}$, this is equivalent to the inequality

$$\|u\|_{L^2(M)} \leq C \|\nabla_M u\|_{L^2 TM} \quad \text{for all } u \in W_0^{1,2}(M).$$

4.6.16 Remark.

The last theorem states that $\|\nabla u\|_{L^2 TM}$ induces an equivalent norm on $W_0^{1,2}(M)$. The spaces $L^2 TM$ and $L^2 T^*M$ are defined in the next section.

4.6.4 L^2 -spaces of Vector Fields, Tensor Fields, and Forms

We follow [AE01]: Let $\Theta_g : \mathfrak{X}(M) \rightarrow \Omega^1(M)$ be the Riesz isomorphism induced by the metric g . The expression

$$(u, w) = \int_M g(u, w) \, d\text{vol}_M$$

defines a scalar product for vector fields $u, w \in \mathfrak{X}(M)$, i.e. for smooth sections of the tangent bundle TM . Via the Riesz isomorphism, one can define an induced scalar product for 1-forms $\alpha, \beta \in \Omega^1(M)$, that is smooth sections of the cotangent bundle T^*M by letting

$$(\alpha, \beta)_* = \int_M g_*(\alpha, \beta) \, d\text{vol}_M := \int_M g(\Theta_g^{-1}\alpha, \Theta_g^{-1}\beta) \, d\text{vol}_M.$$

Similarly, one obtains induced metrics for tensor products: Let $\tilde{u} = u_1 \otimes \cdots \otimes u_l$ and $\tilde{w} = w_1 \otimes \cdots \otimes w_l$ for $l \in \mathbb{N}$ be smooth sections of the product bundle $\bigotimes^l TM$, then set

$$(\tilde{u}, \tilde{w})^l = \int_M g^l(\tilde{u}, \tilde{w}) \, d\text{vol}_M := \int_M \det[g(u_i, w_j)]_{i,j=1,\dots,l} \, d\text{vol}_M.$$

Similarly, for $\tilde{\alpha} = \alpha_1 \otimes \cdots \otimes \alpha_l$, $\tilde{\beta} = \beta_1 \otimes \beta_l$ smooth sections of $\bigotimes^l T^*M$ we define

$$(\tilde{\alpha}, \tilde{\beta})_*^l = \int_M g_*^l(\tilde{\alpha}, \tilde{\beta}) \, d\text{vol}_M := \int_M \det[g_*(\alpha_i, \beta_j)]_{i,j=1,\dots,l} \, d\text{vol}_M.$$

Since the set $\bigwedge^l T^*M$ is a closed vector subspace of $\bigotimes^l T^*M$, we can also define the induced inner product for two l -forms $\alpha_1 \wedge \cdots \wedge \alpha_l$ and $\beta_1 \wedge \cdots \wedge \beta_l$ in $\Omega^l(M)$ as

$$(\alpha_1 \wedge \cdots \wedge \alpha_l, \beta_1 \wedge \cdots \wedge \beta_l)_*^l = \int_M \det[g_*(\alpha_i, \beta_j)]_{i,j=1,\dots,l} \, d\text{vol}_M.$$

4.6.17 Definition.

Let \mathcal{M} be any of the sets $TM, T^*M, \bigotimes^l TM, \bigotimes^l T^*M, \bigwedge^l T^*M$ with $l \in \mathbb{N}$. Similar to Rosenberg [Ros97], denote by $\mathcal{C}_0\mathcal{M}$ the set of continuous sections of \mathcal{M} with compact support. The set $L^2\mathcal{M}$ is defined to be the completion of $\mathcal{C}_0\mathcal{M}$ with respect to the induced scalar product on \mathcal{M} as defined above (where – as usual – maps are identified which coincide except on a set of measure 0).

We finish this paragraph with a result concerning the local behaviour of vector fields in L^2 :

4.6.18 Lemma.

Let $X \in L^2TM$ and let (ϕ, U) be a chart with $\phi = (x^1, \dots, x^n)$. Assume that X can be represented in U as $X = \sum_{i=1}^n X^i \frac{\partial}{\partial x^i}$. Then $X^i \in L^2(U)$ for $i = 1, \dots, n$.

Proof. Due to Proposition 4.6.7, we can endow M with an equivalent metric \tilde{g} induced by the Euclidean metric in \mathbb{R}^m with metric coefficients δ_{ij} . Then we obtain

$$\int_U (X^i)^2 dx \leq \int_U \sum_{j=1}^n (X^j)^2 dx = \int_U \tilde{g}(X, X) dx \leq C \int_M g(X, X) d\text{vol}_M < \infty,$$

which gives the desired result. \blacklozenge

4.6.5 Sobolev-Spaces of Sections of a Vector Bundle

For the manifold M with Riemannian metric g let (E, π, M) be a vector bundle over M . We denote by $\mathcal{C}^{l,\kappa}E$ the space of $\mathcal{C}^{l,\kappa}$ -smooth sections of E . Again, we assume that M is of class $\mathcal{C}^{l,\kappa}$. We use the same definitions for r, p as in Section 4.6.2.

Let (ϕ, U) be a bundle chart; note that $\phi : \pi^{-1}(U) \rightarrow U \times \mathbb{R}^s$ for some (fixed) $s \in \mathbb{N}$. Denote by pr_1 and pr_2 the projections on the first and second component of the image of ϕ .

Since E is a manifold, E can be equipped with a σ -Algebra as in Section 4.6.1. Hence the notion of a measurable section $s : M \rightarrow E$ makes sense. Following Jost [Jos98], we can give the following definition:

4.6.19 Definition.

A measurable section $s : M \rightarrow E$ is contained in the Sobolev space $W^{r,p}E$ if for all bundle charts (ϕ, U) it holds

$$\text{pr}_2 \circ \phi \circ s|_U \in W^{r,p}(U; \mathbb{R}^s).$$

Let $\{(\phi_i, U_i), i = 1, \dots, k\}$ be a finite bundle atlas (with corresponding partition of unity $\{\pi_i, i = 1, \dots, k\}$). The norm on $W^{r,p}E$ is defined as

$$\|s\|_{W^{r,p}E}^p = \sum_{i=1}^k \|\pi_i \cdot \text{pr}_2 \circ \phi \circ s\|_{W^{r,p}(U; \mathbb{R}^s)}^p.$$

This definition makes sense, since we obtain with the help the bundle projection π that $\pi \circ s|_U : U \rightarrow U$. Due to $\pi = \text{pr}_1 \circ \phi$, we have $\text{pr}_1 \circ \phi \circ s|_U : U \rightarrow U$ and thus $\phi \circ s|_U : U \rightarrow U \times \mathbb{R}^s$.

4.6.20 Proposition.

Assume that all bundle charts are of class $\mathcal{C}^{l,\kappa}$. Let $r \leq l + \kappa$ if $l + \kappa$ is an integer; let $r < l + \kappa$ otherwise. Then the set $\mathcal{C}^{l,\kappa}E$ is dense in $W^{r,p}E$.

Proof. For $u \in W^{r,p}E$, we construct a local approximation as in the proof of Proposition 4.6.6. By density of $\mathcal{C}^\infty(U; \mathbb{R}^s)$ in $W^{r,p}(U; \mathbb{R}^s)$, there exists a $w_n \in \mathcal{C}^\infty(U; \mathbb{R}^s)$ such that

$$\|\text{pr}_2 \circ \phi \circ s|_U - w_n\|_{W^{r,p}(U; \mathbb{R}^s)} \leq \frac{1}{n}$$

for $n \in \mathbb{N}$. Set $\tilde{w}_n(z) = \phi^{-1}(z, w_n(z))$ for $z \in M$, then $\text{pr}_2 \circ \phi \circ \tilde{w}_n = w_n$ and

$$\|s|_U - \tilde{w}_n\|_{W^{r,p}(U;E)} \leq \frac{1}{n}. \quad \blacklozenge$$

4.6.6 Forms with Values in a Banach Space

In this section we present a generalization of the concept of differential forms (i.e. multilinear maps taking values in \mathbb{R}) to Banach-space valued forms. They are needed for an exact treatment of the dependence of the cell-problem on the parameter $x \in M$, see Section 4.4.3. We will mostly follow Cartan [Car70], to which the reader is also referred for proofs and further results.

In this section, let E, F, G, H be Banach spaces. Denote by $\mathcal{L}_k(E; F)$, $k \in \mathbb{N}$, the set of all multilinear antisymmetric maps

$$f : \underbrace{E \times \cdots \times E}_{k\text{-times}} \longrightarrow F$$

such that $f(x_1, \dots, x_k) = 0$ if $x_i = x_j$ for some index pair $i, j \in \{1, \dots, k\}$, $i \neq j$. $\mathcal{L}_k(E; F)$ is a closed linear subspace of the Banach space of multilinear maps from E^k to F .

Basic Notions

4.6.21 Definition (Exterior Product).

Assume that there exists a continuous bilinear map $\Phi : F \times G \longrightarrow H$. Let $f \in \mathcal{L}_k(E; F)$ and $g \in \mathcal{L}_l(E; G)$ with $k, l \in \mathbb{N}$. There exists a unique form

$$f \underset{\Phi}{\wedge} g \in \mathcal{L}_{k+l}(E; H)$$

defined by

$$f \underset{\Phi}{\wedge} g(x_1, \dots, x_{k+l}) = \sum_{\sigma} \epsilon(\sigma) \Phi(f(x_{\sigma(1)}, \dots, x_{\sigma(k)}), g(x_{\sigma(k+1)}, \dots, x_{\sigma(k+l)})),$$

where the sum is taken over all permutations σ of $\{1, \dots, k+l\}$ such that $\sigma(1) < \cdots < \sigma(k)$ and $\sigma(k+1) < \cdots < \sigma(k+l)$. The map $(f, g) \mapsto f \underset{\Phi}{\wedge} g$ is bilinear, anticommutative and associative.

4.6.22 Definition (Differential Forms).

Let $U \subset E$ be open. A map

$$\omega : U \longrightarrow \mathcal{L}_k(E; F)$$

is called a differential form in U of degree $k \in \mathbb{N}$ with values in F . If ω is n -times continuously differentiable (as a map between Banach spaces), we call ω of class C^n and write $\omega \in \Omega_k^n(U, F)$.

4.6.23 Remark.

Defined to operate pointwise, the exterior product generalises to a map

$$\wedge: \Omega_k^n(U, F) \times \Omega_l^n(U, G) \longrightarrow \Omega_{k+l}^n(U, H).$$

4.6.24 Definition (Exterior Derivative).

Let $\omega \in \Omega_k^n(U, F)$ with $n \geq 1$. The form $d\omega \in \Omega_{k+1}^{n-1}(U; F)$ defined by

$$d\omega(x)(x_1, \dots, x_n) = \sum_{i=0}^k (-1)^i \mathcal{D}\omega(x)[x_i](x_1, \dots, \hat{x}_i, \dots, x_k)$$

is called exterior derivative of ω . Here $x \in U$, $(x_0, x_1, \dots, x_k) \in E^{k+1}$. $\mathcal{D}\omega : U \longrightarrow L(E; \mathcal{L}_k(E; F))$ denotes the total derivative of ω , $L(E; G)$ being the set of linear maps from E to G , and $(x_0, \dots, \hat{x}_i, \dots, x_k) = (x_0, \dots, x_{i-1}, x_{i+1}, \dots, x_k)$ is the vector with the i -th component removed.

4.6.25 Proposition (Coordinate Transformations).

Let U be an open subset of the Banach space E , and let U' be an open subset of a Banach space E' . Assume that there exists a map $\phi'_U \longrightarrow U$ of class \mathcal{C}^{n+1} . Then for $\omega \in \Omega_k^n(U, F)$, the pullback $\phi^*\omega$ (defined as in the case of \mathbb{R}^m) is a form $\phi^*\omega \in \Omega_k^n(U', F)$, and ϕ^* is a linear mapping

$$\phi^* : \Omega_k^n(U, F) \longrightarrow \Omega_k^n(U', F).$$

Moreover, ϕ^* commutes with the exterior product and the exterior derivative.

Representation Formulas for $E = \mathbb{R}^m$

In the case of a finite dimensional Banach space E , one obtains special representation formulas. We will tacitly identify E with \mathbb{R}^m , $m \in \mathbb{N}$ in the results that follow.

4.6.26 Proposition.

Let $U \subset \mathbb{R}^m$ and $\omega \in \Omega_k^n(U, F)$. Then ω can be uniquely written as

$$\omega = \sum_{1 \leq i_1 \leq \dots \leq i_k \leq m} c_{i_1, \dots, i_k}(\cdot) dx_{i_1} \wedge \dots \wedge dx_{i_k},$$

where \wedge denotes the usual wedge-product in \mathbb{R}^m and $c_{i_1, \dots, i_k} \in \mathcal{C}^n(U; F)$.

4.6.27 Proposition.

Let $f : U \longrightarrow F$ be a scalar \mathcal{C}^1 -function, i.e. $f \in \Omega_0^1(U, F)$. Then

$$df = \sum_{i=1}^m \frac{\partial f}{\partial x_i} dx_i.$$

4.6.28 Lemma.

Let $\omega \in \Omega_k^1(U, F)$ be represented as in Proposition 4.6.26. Then

$$d\omega = \sum_{1 \leq i_1 \leq \dots \leq i_k \leq m} dc_{i_1, \dots, i_k} \wedge dx_{i_1} \wedge \dots \wedge dx_{i_k}.$$

Forms on Manifolds

The constructions in [Car70] do not treat forms defined on manifolds (with values in a Banach space). We give the corresponding generalizations in the sequel: Let M be a compact manifold of dimension $m \in \mathbb{N}$ with corresponding atlas \mathcal{A} of class \mathcal{C}^l , $l \in \mathbb{N}$.

4.6.29 Definition.

Let $k \in \mathbb{N}$, $k < l$. A map $\omega : \bigcup_{\{x\} \in M} \{x\} \times T_x M^k \rightarrow F$ is said to be a differential form of degree k over M with values in F (Notation: $\omega \in \Omega_k^n(M, F)$), if for all charts $\phi : U \rightarrow \mathbb{R}^m$ for the restriction $\omega|_U$ of ω to U it holds

$$\phi_* \omega|_U \in \Omega_k^n(\phi(U), F),$$

where $\phi_* \omega|_U$ is understood as a map $\phi(U) \times (\mathbb{R}^m)^k \rightarrow F$.

4.6.30 Lemma.

The definition above is independent of the coordinate representation ϕ and thus well-defined.

Proof. Let $\phi : U \rightarrow \mathbb{R}^m$ and $\tilde{\phi} : \tilde{U} \rightarrow \mathbb{R}^m$ be two charts with $V := U \cap \tilde{U} \neq \emptyset$. Note that $\tilde{\phi} \circ \phi^{-1} : \phi(V) \rightarrow \tilde{\phi}(V)$ is a \mathcal{C}^l -coordinate transformation. Assuming that $\phi_* \omega|_V \in \Omega_k^n(\phi(V), F)$, we can apply Proposition 4.6.25 to obtain that

$$\tilde{\phi}_* \omega|_V = (\tilde{\phi} \circ \phi^{-1})_* \circ \phi_* \omega|_V = [(\tilde{\phi} \circ \phi^{-1})^{-1}]^* \circ \phi_* \omega|_V \in \Omega_k^n(\tilde{\phi}(V), F). \quad \blacklozenge$$

4.6.31 Lemma.

For $F = \mathbb{R}$, Definition 4.6.29 yields the usual well-known differential forms on manifolds.

Proof. For $\phi_* \omega|_U \in \Omega_k^n(\phi(U), \mathbb{R})$ we obtain a representation due to Proposition 4.6.26 of the form

$$\phi_* \omega|_U = \sum_{1 \leq i_1 \leq \dots \leq i_k \leq m} c_{i_1, \dots, i_k} dx_{i_1} \wedge \dots \wedge dx_{i_k}$$

with coefficient functions $c_{i_1, \dots, i_k} \in \mathcal{C}^n(\phi(U))$. Taking a look at the usual definition of a differential form on a manifold, the right hand side is simply the local representation of the form $\omega \in \Omega_k^n(M)$ in U . Thus the two definitions coincide. \blacklozenge

5 Numerical Simulations

In this chapter, we describe a numerical simulation of the results obtained in Section 4.5. We implement a variant of the multiscale problem (4.28) and (4.29) (diffusion and exchange on a periodically structured boundary) in COMSOL MULTIPHYSICS for $(\varepsilon, \delta) = (0.1, 0.5)$ and $(\varepsilon, \delta) = (0.2, 0.5)$. Moreover, we simulate the homogenized problem given in Theorem 4.5.3 for comparison. This is done to show the efficiency and effectiveness of the homogenization method. Note, however, that this chapter serves an illustrational purpose – an independent contribution to the field of numerical analysis is not aspired.

Other implementations of effective equations and upscaling methods can be found in the literature: Arbogast proposes in [Arb89] a finite element scheme for a double porosity model, see also [Arb88] for the background of the model. Newer developments in this direction can be found in chapter 10 "Computational Aspects of Dual Porosity Models" in Hornung [Hor97]. In [EKK02], Eck and his coworkers derive a two-scale model for dendritic growth. Numerical simulations are carried out by imposing a cell problem on each node of the domain. See also [Eck04] and the unpublished work of Magnus Redeker (Stuttgart). Simulations of homogenization models with evolving microstructure can be found in Peter and Böhm [PB09], with applications to carbonation in concrete. For a more detailed exposition, the reader is referred to Peter [Pet06]. Finally, newer Galerkin schemes for nonlinear reaction diffusion problems, which might lead to corresponding numerical techniques, can be found in the work of Muntean and Neuss-Radu [MNR10] (see also [ML10] for corresponding convergence results).

Related numerical methods can also be found under the key words *heterogeneous multiscale method* (see e.g. E, Ming, and Zhang [EMZ04]) and *XFEM- or FE²-methods* (see for instance Feyel [Fey03] and the works cited therein). In this connection, the reader is also referred to the book by Efendiev and Hou [EH09].

5.1 Formulation of the Problems

We consider a rectangular domain $\Omega = [0, 0.8] \times [0, 0.6]$ in \mathbb{R}^2 . Denote the reference cell for the domain by $Y_F := [0, 1]^2 \setminus Y_S$, where $Y_S = B_{\frac{1}{4}}(\frac{1}{2}, \frac{1}{2})$ is a solid inclusion with boundary $\Gamma = \partial Y_S$. The reference cell for the boundary is given by $Y_2 := [0, 1]$. Set $\Omega^\varepsilon := \Omega \cap \sum_{k \in \mathbb{Z}^2} \varepsilon(Y_F + k)$, and $\Gamma^\varepsilon := \bar{\Omega} \cap \sum_{k \in \mathbb{Z}^2} \varepsilon(\Gamma + k)$.

The Periodic Problem is given by: Find $u^{\varepsilon\delta}$ and $u_{\Gamma}^{\varepsilon\delta}$, solution of

$$\begin{aligned} \partial_t u^{\varepsilon\delta} - \operatorname{div}(D^\varepsilon \nabla u^{\varepsilon\delta}) &= 0 && \text{in } [0, 1] \times \Omega^\varepsilon \\ -D^\varepsilon \nabla u^{\varepsilon\delta} \cdot \nu &= \varepsilon(au^{\varepsilon\delta} - bu_{\Gamma}^{\varepsilon\delta}) && \text{on } [0, 1] \times \Gamma^\varepsilon \\ -D^\varepsilon \nabla u^{\varepsilon\delta} \cdot \nu &= 0 && \text{on } [0, 1] \times \partial\Omega \\ u^{\varepsilon\delta}(0, \cdot) &= u_0 && \text{in } \Omega \end{aligned}$$

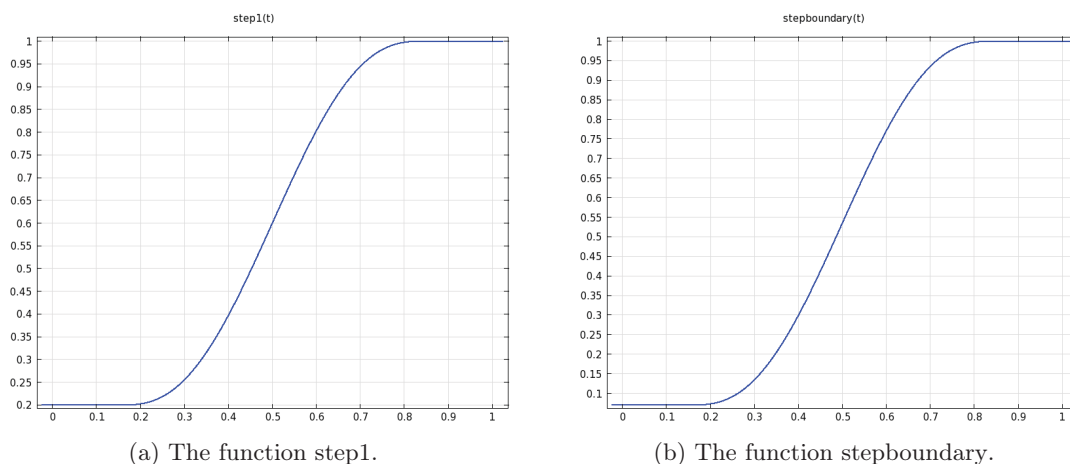


Figure 5.1: The auxiliary functions used in the construction of the periodic diffusion coefficients.

as well as

$$\begin{aligned} \partial_t u_\Gamma^{\varepsilon\delta} - \varepsilon^2 \operatorname{div}_\Gamma(D_\Gamma^{\varepsilon\delta} \nabla_\Gamma u_\Gamma^{\varepsilon\delta}) &= a u_\Gamma^{\varepsilon\delta} - b u_\Gamma^{\varepsilon\delta} && \text{on } [0, 1] \times \Gamma^\varepsilon \\ u_\Gamma^{\varepsilon\delta}(0, \cdot) &= u_{0,\Gamma} && \text{on } \Gamma^\varepsilon. \end{aligned}$$

We make the following choices for the coefficients etc.: We choose $a = b = \frac{1}{2}$, the initial value in the bulk as the constant $u_0 \equiv 1$ and the initial value on the boundary as the linear function $u_{0,\Gamma}(x_1, x_2) = 4x_1x_2$.

For the diffusion coefficients, we construct the auxiliary step functions step1 (having range $[0.2, 1]$) and stepboundary (having range $[0.07, 0.5]$); see Figure 5.1. Then choose $D(y_1, y_2) = 10^{-1} \text{step1}(y_1) \text{step1}(y_2)$ and $D_\Gamma(z) = \text{stepboundary}(z)$ and construct the periodic coefficients D^ε as well as D_Γ^ε as in Section 4.5 on page 145.

The Cell Problems are given by: Find w_1, w_2 and w , solutions of

$$\begin{aligned} -\operatorname{div}_y(D(y) \nabla_Y w_i(y)) &= \operatorname{div}_y(D(y) e_i) && \text{in } Y_F \\ D(y) \nabla_y w_i(y) \cdot \nu &= 0 && \text{on } \Gamma \\ y \longmapsto w_i(y) & \text{ is } Y_1\text{-periodic,} \end{aligned}$$

for $i = 1, 2$ as well as

$$\begin{aligned} -\operatorname{div}_z(D_\Gamma(z) \nabla_z w(z)) &= \operatorname{div}_z(D_\Gamma(z)) && \text{in } Y_2 \\ z \longmapsto w(z) & \text{ is } Y_2\text{-periodic.} \end{aligned}$$

The diffusion coefficients are the same as constructed above.

Periodic Problems	$\varepsilon = 0.2$	$\varepsilon = 0.1$
# Elements in the domain	3724	16074
# Elements in each hole model	50	50

Table 5.1: Number of mesh elements for the periodic problems.

The Homogenized Problem is given by: Find u and u_Γ , solution of

$$\begin{aligned}
 P\partial_t u(t, x) - \operatorname{div}(\tilde{D}(x) \nabla u(t, x)) &= |\Gamma|au(t, x) - \int_{\Gamma} bu_\Gamma(t, x, y_1) \, d\sigma_{y_1} && \text{in } [0, 1] \times \Omega \\
 \tilde{D}(x) \nabla u(t, x) \cdot \nu &= 0 && \text{on } [0, 1] \times \partial\Omega \\
 u(0, \cdot) &= u_0 && \text{in } \Omega
 \end{aligned}$$

as well as

$$\begin{aligned}
 \partial_t u_\Gamma(t, x, y) - \operatorname{div}_{y,\Gamma}(\tilde{D}_\Gamma(x) \nabla_{y,\Gamma} u_\Gamma(t, x, y)) \\
 = |\Gamma|au(t, x) - bu_\Gamma(t, x, y) &&& \text{on } [0, 1] \times \Omega \times \Gamma && (5.3a)
 \end{aligned}$$

$$u_\Gamma(0, x, \cdot) = u_{0,\Gamma}(x) \quad \text{on } \Gamma, \quad (5.3b)$$

Here $P = |Y_F| = 1 - \frac{1}{16}\pi$, $|\Gamma| = \frac{\pi}{2}$, and the effective diffusion tensors are given by $\tilde{D} = (\tilde{D}_{ij})_{i,j=1,2}$ with $\tilde{D}_{ij} = (\int_{Y_F} D(y)(\delta_{ij} - \frac{\partial w_i}{\partial y_j}(y)) \, dy)$ and $\tilde{D}_\Gamma = (\int_{Y_2} D_\Gamma(z)(1 + \frac{\partial w}{\partial z}(z)) \, dz)$. The other terms have already been described above.

5.2 Numerical Implementation

We solve the problems above by the Method of Finite Elements, using COMSOL MULTIPHYSICS. COMSOL is a commercial PDE-solver with strong emphasis on the treatment of complex coupled physical and engineering problems, see e.g. the manual [COM10] or Zimmerman [Zim06].

All problems are solved on a triangular Delaunay-mesh of element size "fine" (details can be found below). The mesh is fixed, i.e. no adaptive mesh refinement or remeshing is used. The time-dependent problems are discretized in time by using a backward differentiation formula (BDF) with time step 0.1. Initialization takes place by using a step with the backward Euler method. Finally, the resulting algebraic equations are solved by using PARDISO, an explicit solver for large sparse linear systems of equations, see Schenk and Gärtner [SG04]. This also applies to the stationary cell problems.

The Periodic Problems are implemented using the "Transport of Diluted Species"-module. We construct a 2D-domain with the periodic arrangement of holes and add a 1D-model for each hole boundary, representing a parametrization in arc length normalized to the interval $[0, 1]$. The problems are then coupled using a "General Extrusion"-operator. Informations on the mesh and the running time can be found in Tables 5.1 and 5.2. The latter refers (in all simulations) to an Intel Core2Duo processor with 2GHz, being supplied with 1GB RAM.

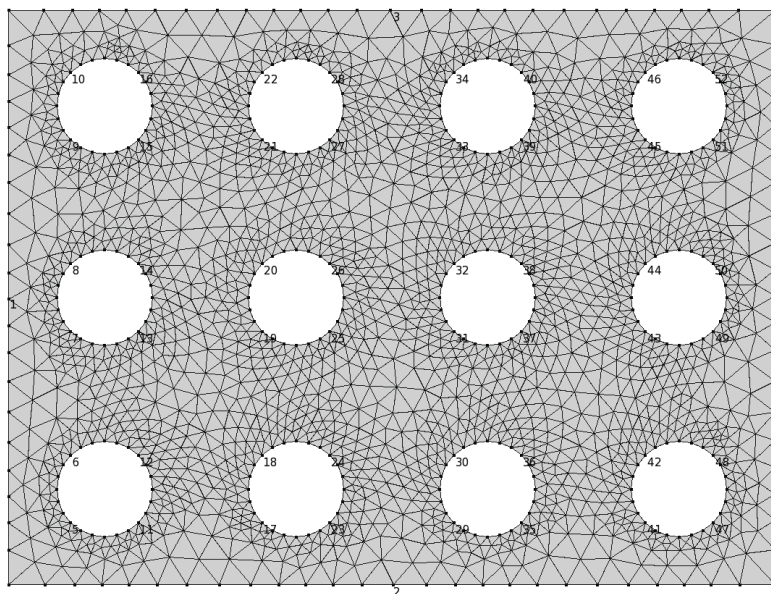


Figure 5.2: The triangulation of the domain for the periodic problem for $\varepsilon = 0.2$.

Periodic Problems	$\varepsilon = 0.2$	$\varepsilon = 0.1$
# Degrees of freedom	2653	11112
Running Time	42s	405s

Table 5.2: Number of degrees of freedom and running time for the periodic problems.

The Cell Problems use the 2D reference geometry Y_F and the 1D interval Y_2 . The implementation is based on the "Convection-Diffusion"-module, where the mean value property of the solutions is ensured by using an integration operator and imposing a pointwise constraint. All cell problems are solved simultaneously. Further information can be found in Tables 5.3 and 5.4.

By using the "derived values" feature in COMSOL, one can calculate the effective diffusion tensors by using a 4th order numerical integration scheme. This yields

$$\tilde{D} = \begin{bmatrix} 0.02615 & 6.103 \cdot 10^{-4} \\ 6.103 \cdot 10^{-4} & 0.02615 \end{bmatrix} \quad \text{as well as} \quad \tilde{D}_\Gamma = 0.1364.$$

The Homogenized Problem is implemented on the 2D-domain Ω using the "Convection-Diffusion"-module for the function u . In order to implement the parameter-dependent boundary equation, we need the following Lemma:

Cell Problems	
# Elements in Y_F	558
# Elements in Y_2	50

Table 5.3: Number of mesh elements for the cell problems.

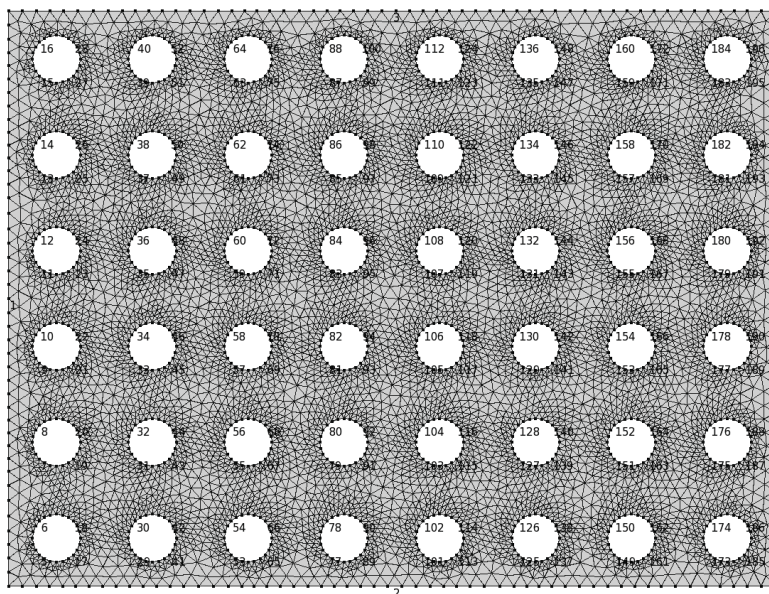


Figure 5.3: The triangulation of the domain for the periodic problem for $\varepsilon = 0.1$.

Cell Problems	
# Degrees of freedom	2501
Running Time	16s

Table 5.4: Number of degrees of freedom and running time for the cell problems.

5.2.1 Lemma.

Let $u_\Gamma : [0, 1] \times \Omega \rightarrow \mathbb{R}$ be a solution of the following parameter-dependent ODE: For fixed $x \in \Omega$ solve

$$\begin{aligned} \partial_t u_\Gamma(t, x) &= |\Gamma| a u(t, x) - |\Gamma| b u_\Gamma(t, x) \\ u_\Gamma(0, x) &= u_{0,\Gamma}(x). \end{aligned}$$

By defining $\tilde{u}_\Gamma(t, x, y) := u_\Gamma(t, x)$ for $y \in \Gamma$, the function \tilde{u}_Γ is a solution of (5.3).

Proof. Consider \tilde{u}_Γ as given above. Since clearly $\nabla_{y,\Gamma} \tilde{u}_\Gamma = 0$, this function satisfies equation (5.3). Since the solution of this parabolic problem is unique, we obtain the assertion. \blacklozenge

This result means that the solution of problem (5.3) is constant in y ! Therefore, we solve the boundary problem by implementing an ODE-problem in each point of the domain via the "General-Form-PDE"-module. Details on the mesh and the running time can be found in Tables 5.5 and 5.6. Note that the problem is solved again fully coupled.

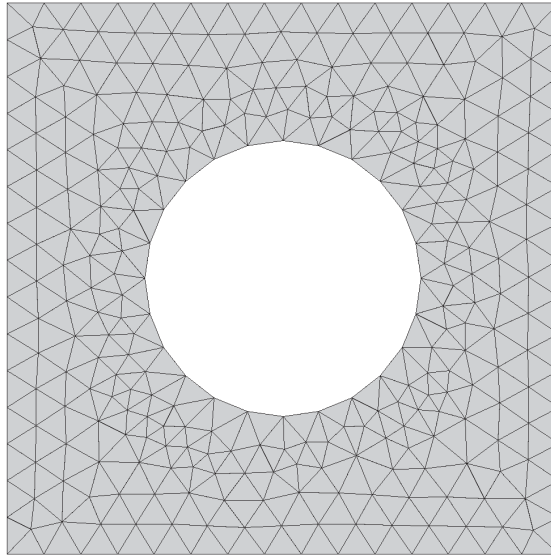


Figure 5.4: The triangulation for the cell problem.

Homogenized Problem	
# Elements in the domain	692

Table 5.5: Number of mesh elements for the homogenized problem.

5.3 Results

5.3.1 The Periodic Problems

The results of the simulation of the periodic problem for $\varepsilon = 0.2$ can be found in Figures 5.10 and 5.11 (see page 173 f). The first figure shows the bulk concentration at times $t = 0, 0.2, 0.5, 0.7, 1$. At $t = 0$, the concentration is given by the uniform initial concentration. Then, an exchange between the domain and the boundaries of the solid parts starts, leading to a loss of substance in the lower and left part of the domain and a gain in the upper right part. Investigating the part $[0, 0.2] \times [0, 0.2]$ of the domain Ω at time $t = 0.5$, one sees that the concentration gradients are higher in the lower left part of that subdomain and smaller in the upper right part. This is due to the fact that the diffusivity is small in the former subset of the subdomain, whereas the high diffusivity in the latter parts leads to a more evenly distributed concentration. Of course, the same applies basically to the surrounding of each solid part.

Homogenized Problem	
# Degrees of freedom	2902
Running Time	6s

Table 5.6: Number of degrees of freedom and running time for the homogenized problem.

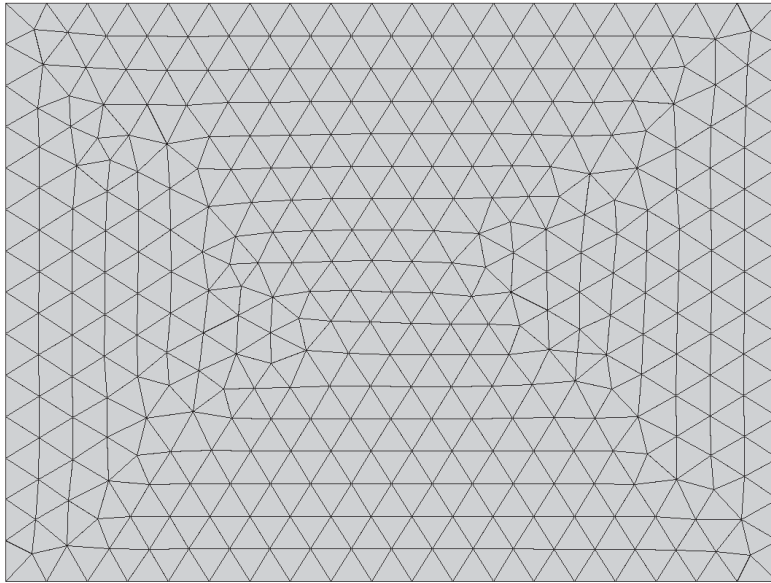


Figure 5.5: The triangulation of the domain for the homogenized problem.

Concerning the concentration on the boundary, the evolution of it is shown in Figure 5.11. Note that the position of the graph in the diagram corresponds to the position of the boundary in the domain. For an interpretation of these graphs, we exemplarily refer to Figure 5.6: Since the initial concentration on the boundary (the lowest curve) has a range in $[0.05, 0.32]$, which is lower than the initial concentration in the domain, substance flows from the bulk to the boundary. Thus, the concentration there is increasing as seen in the graph. Moreover, boundary diffusion has a smoothing effect on the concentration profile. Since the diffusion coefficient $D_{\Gamma}^{\varepsilon\delta}$ is especially low in the arc-length range $[0, 0.2] \cup [0.5, 0.7]$ and high in $[0.3, 0.5] \cup [0.8, 1]$, we see that the "steepness" of the concentration profile changes only little on the former set, but is leveled out on the latter. If one considers the boundary in the upper left corner of the domain (cf. Figure 5.11), one sees that an exchange from the boundary to the domain takes place, since the initial concentration on the boundary is higher than the initial concentration in the bulk.

Analogous results for $\varepsilon = 0.1$ can be found in Figures 5.12 and 5.13, see page 175 f.

5.3.2 The Cell Problems

The solution of the bulk cell problems w_1 and w_2 in Y_F is depicted in Figure 5.7. The solution of the cell problem w on Y_2 is given in Figure 5.8.

5.3.3 The Homogenized Problem

Simulation results obtained for the homogenized problem are depicted in Figures 5.14 and 5.15, cf. page 177 f.

Comparing the solutions of the homogenized with the periodic problems, one sees that the qualitative behaviour is captured quite well, and the maxima and minima of the

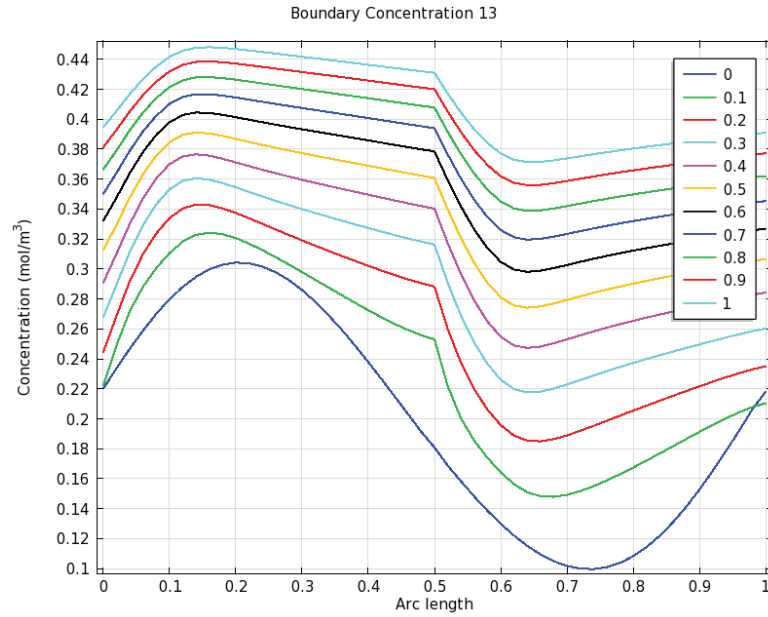


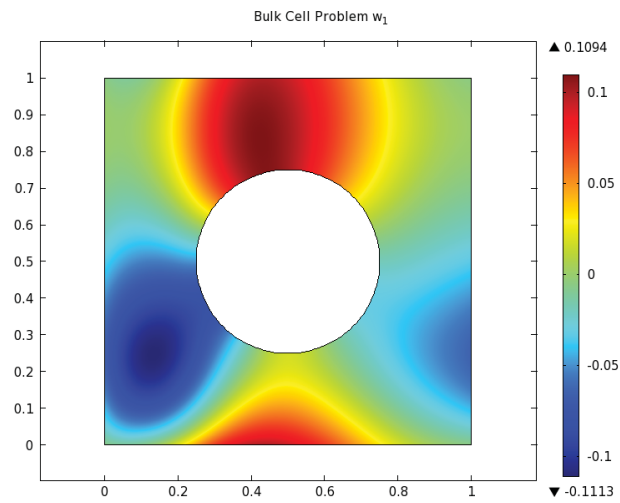
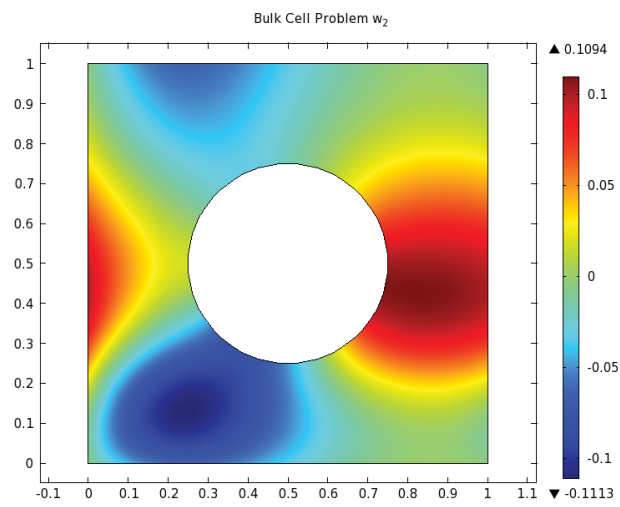
Figure 5.6: The evolution of the the boundary concentration of the third boundary in the last row.

solutions differ in the order of 10^{-2} . Here, one should keep in mind that the values of ε are chosen rather large to ensure computational feasibility. For a more detailed comparison, we compute the integral over the bulk concentrations for fixed time. Since $\mathcal{T}^\varepsilon(u^\varepsilon) \rightarrow u$ strongly in $L^2(\Omega \times Y_F)$ and thus also in $L^1(\Omega \times Y_F)$, we obtain

$$\int_{\Omega^\varepsilon} u^\varepsilon \, dx = \int_{\Omega \times Y_F} \mathcal{T}^\varepsilon(u^\varepsilon) \, dy \, dx \longrightarrow \int_{\Omega \times Y_F} u \, dy \, dx = |Y_F| \int_{\Omega} u \, dx.$$

Thus for a reasonable analysis, we have to compare the integral over the concentration of the periodic problems with a scaled integral over the bulk concentration of the homogenized problem. This is done in Figure 5.9. Taking into account the scaling of the axis of ordinates, one finds a good agreement of the quantity taken into consideration, with a possible tendency of the homogenized concentration to underestimate those of the periodic problems.

The big advantage of the homogenized model is the fast computational time: Computing both the cell problems and the homogenized solution needs 22s, compared to 42s and 405s for the periodic problems.

(a) Solution of the cell problem w_1 .(b) Solution of the cell problem w_2 .Figure 5.7: Solutions of the cell problems for the reference cell Y_F .

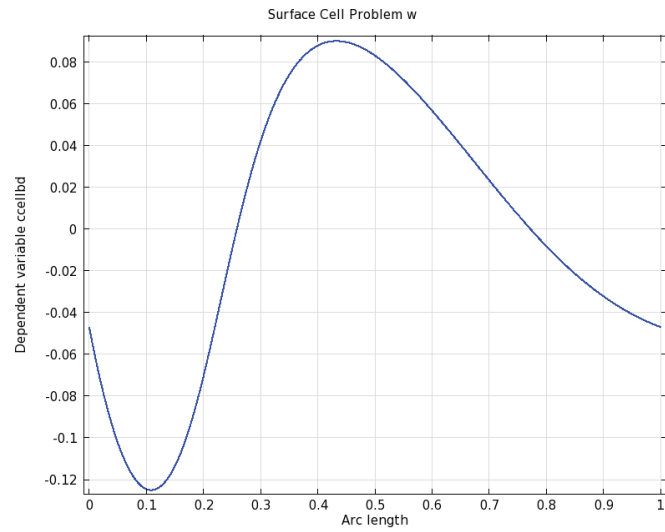


Figure 5.8: Solution of the cell problem for the reference cell Y_2 .

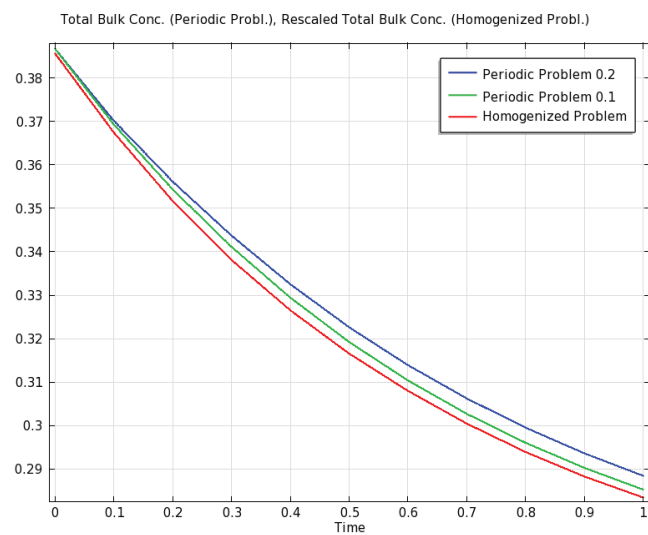
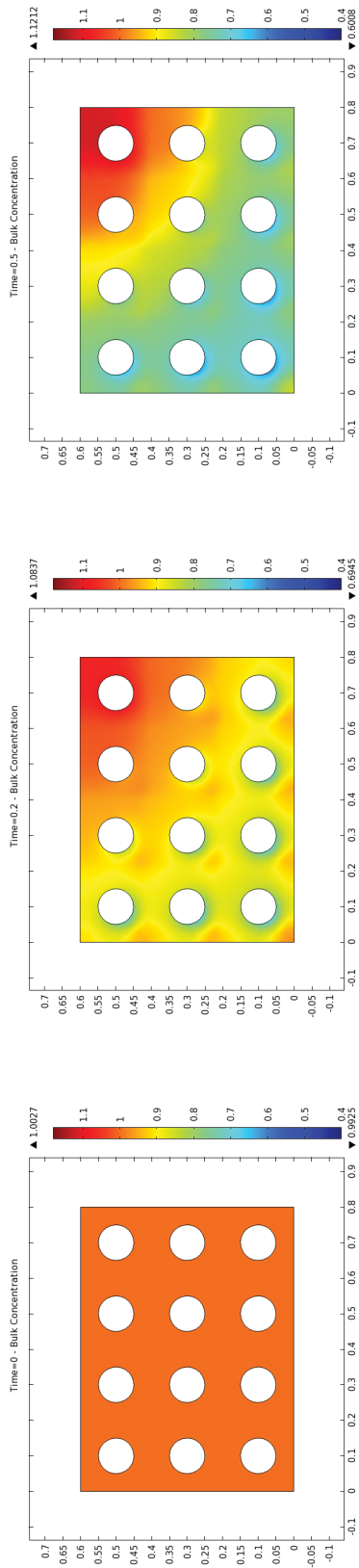
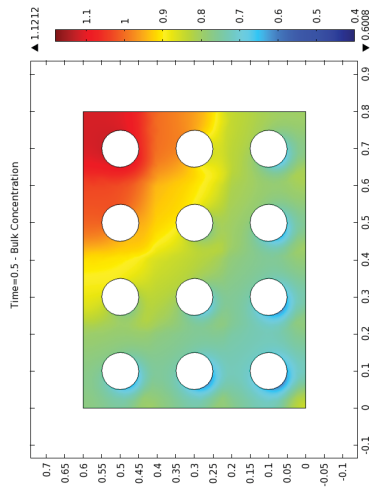


Figure 5.9: Comparison of the total substance in the domain.

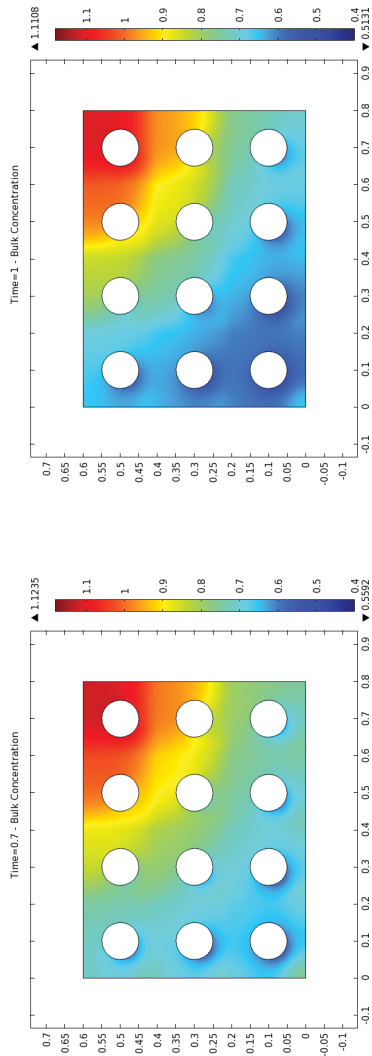


(a) $t = 0$

(b) $t = 0.2$



(c) $t = 0.5$



(d) $t = 0.7$

(e) $t = 1$

Figure 5.10: The concentrations in the domain for the indicated time steps for $\epsilon = 0.2$.

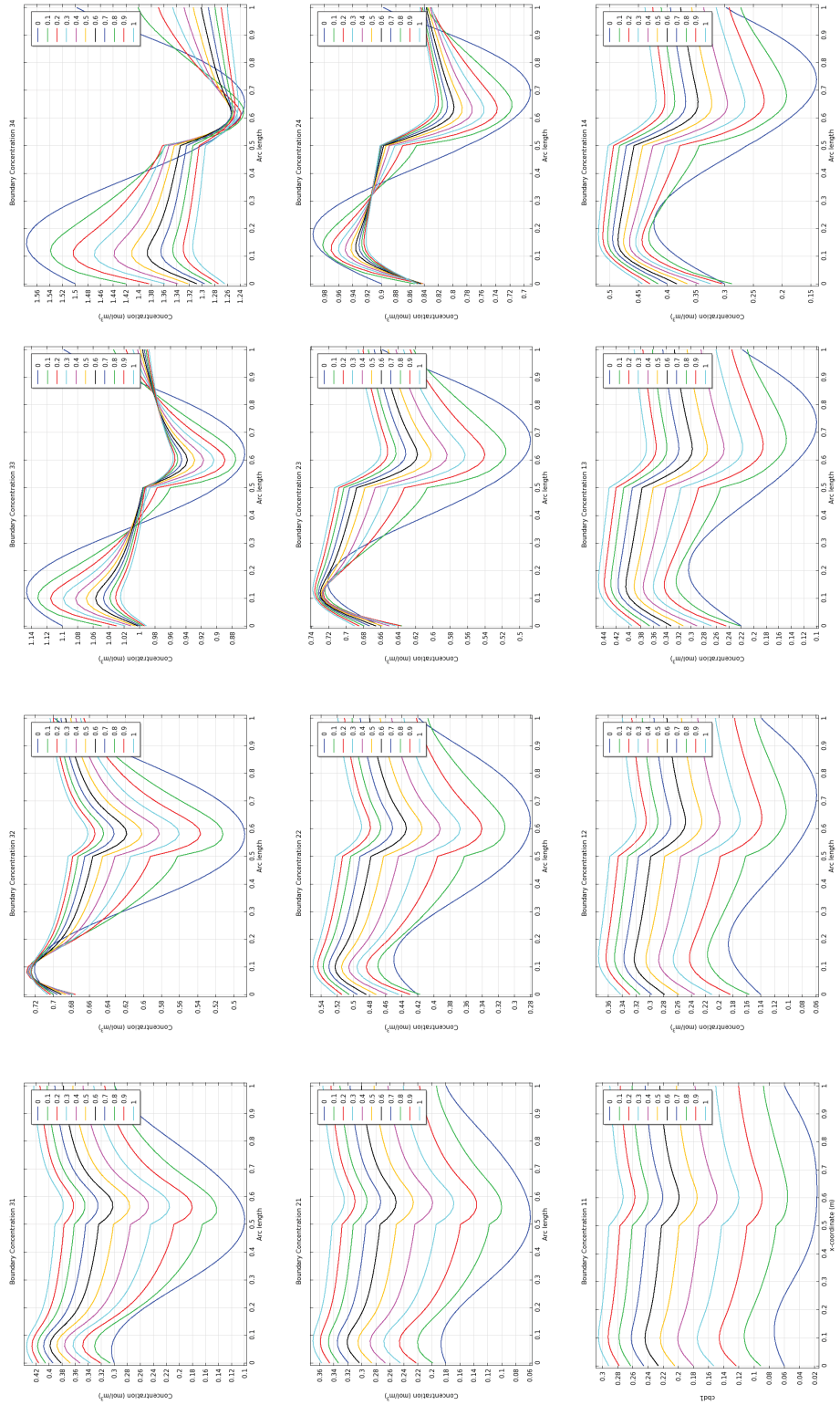
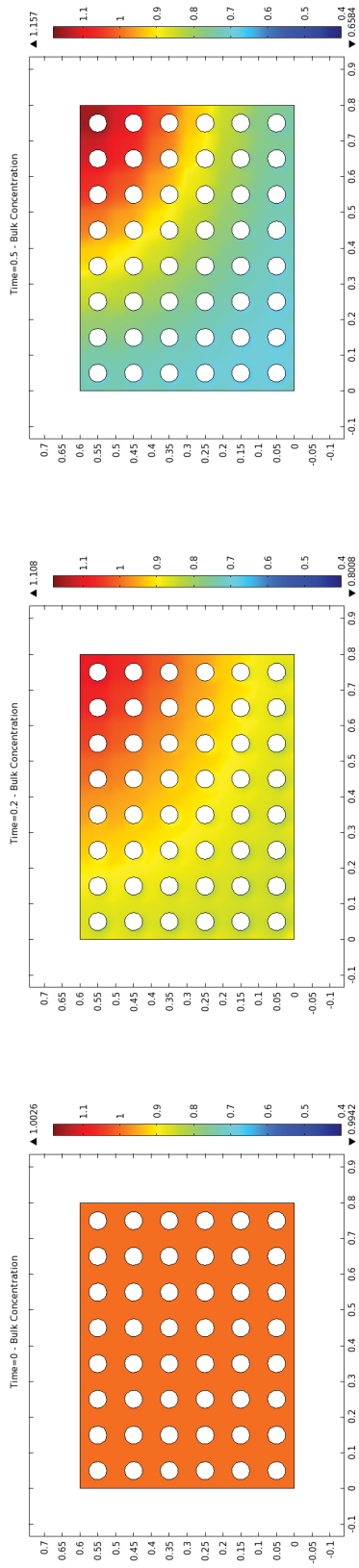


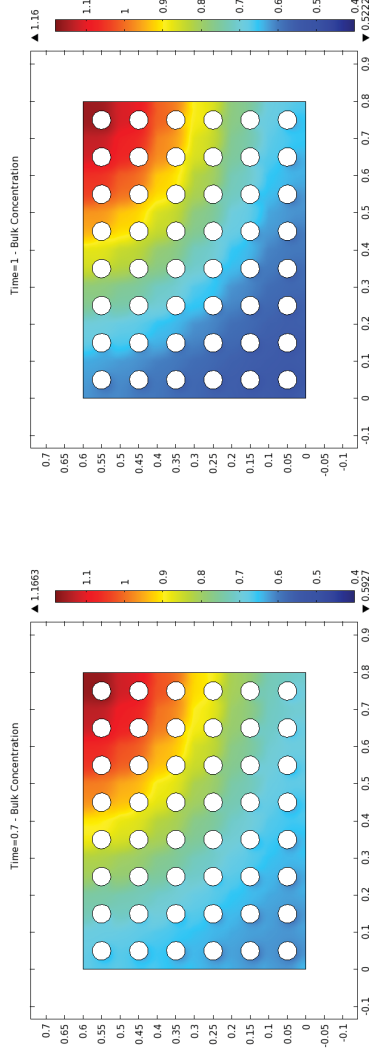
Figure 5.11: The concentrations on the boundary of the solid inclusions for $\epsilon = 0.2$. The position of the graph in this figure corresponds to the position of the boundary in the domain.



(a) $t = 0$

(b) $t = 0.2$

(c) $t = 0.5$



(d) $t = 0.7$

(e) $t = 1$

Figure 5.12: The concentrations in the domain for the indicated time steps for $\epsilon = 0.1$.

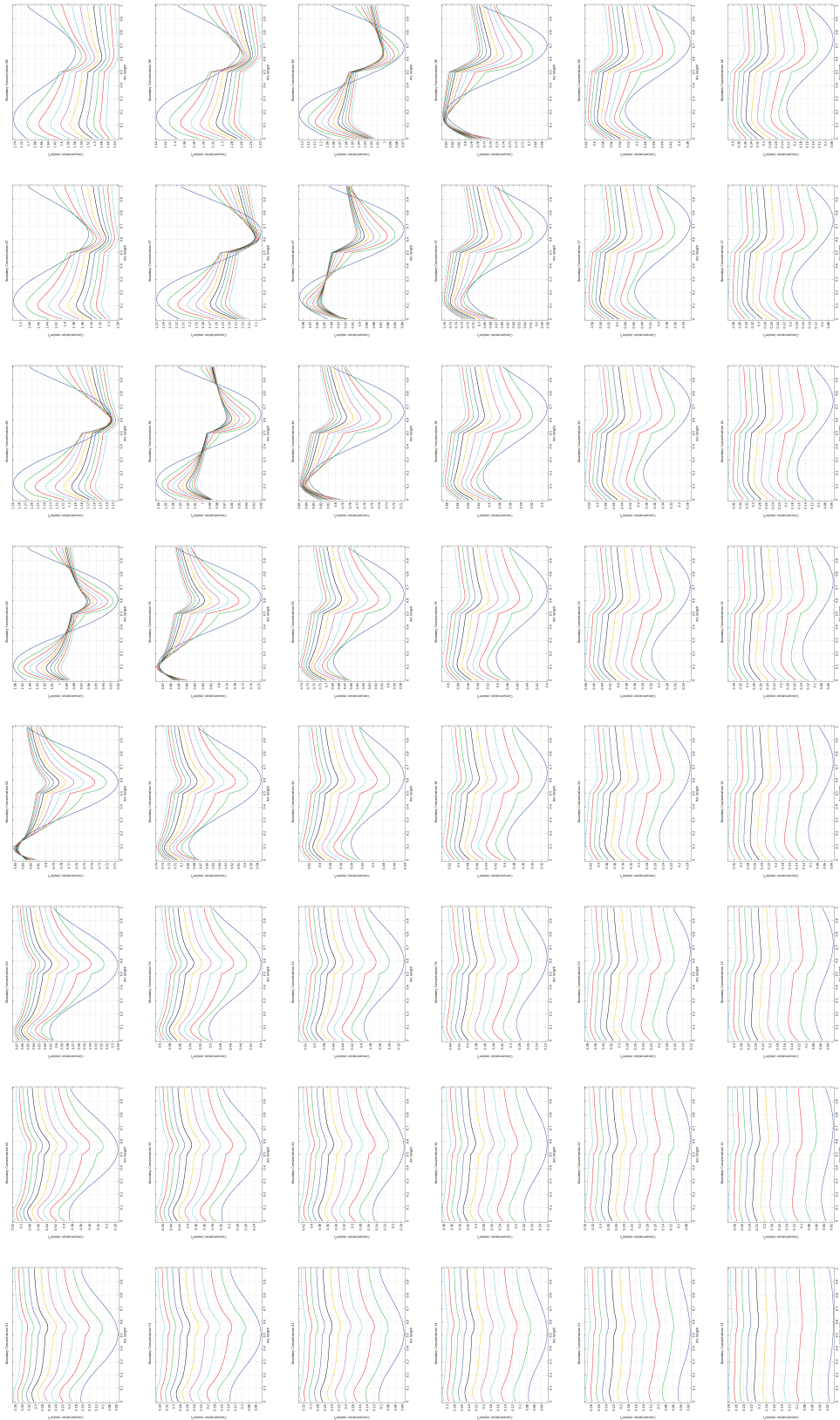


Figure 5.13: The concentrations on the boundary of the solid inclusions for $\varepsilon = 0.1$. The position of the graph in this figure corresponds to the position of the boundary in the domain. Note that the color for the different timesteps corresponds to those used in Figure 5.11.

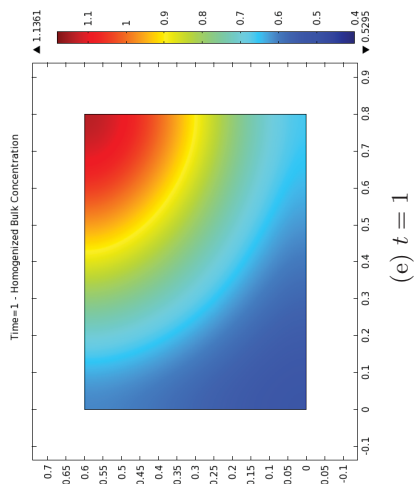
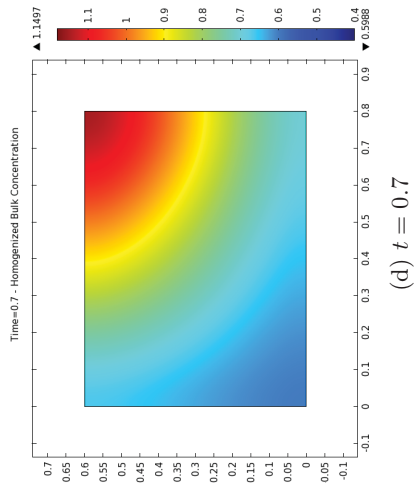
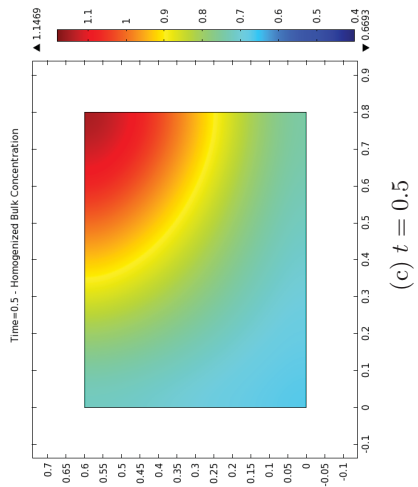
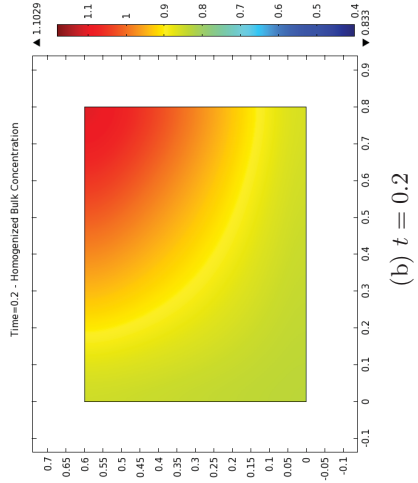
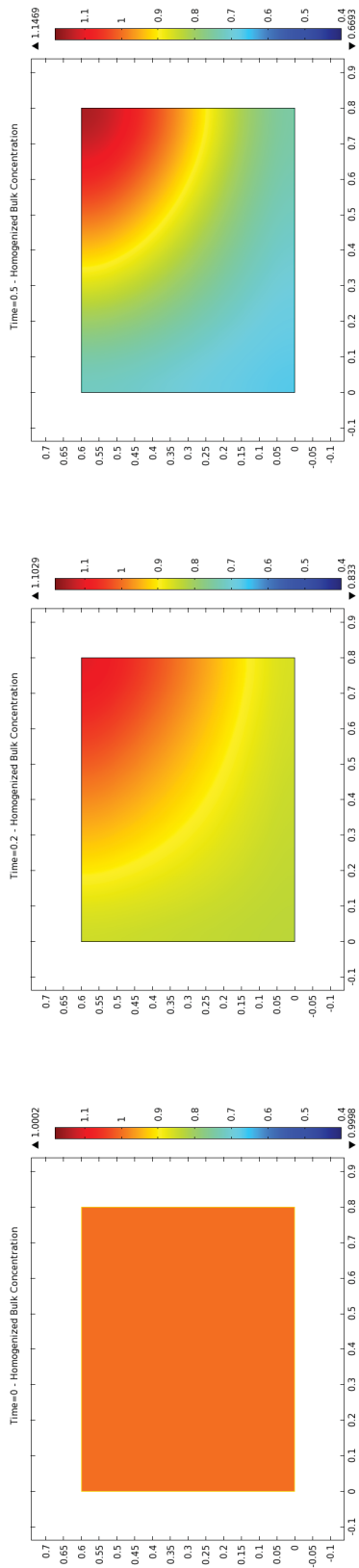


Figure 5.14: The concentrations in the domain for the indicated time steps.

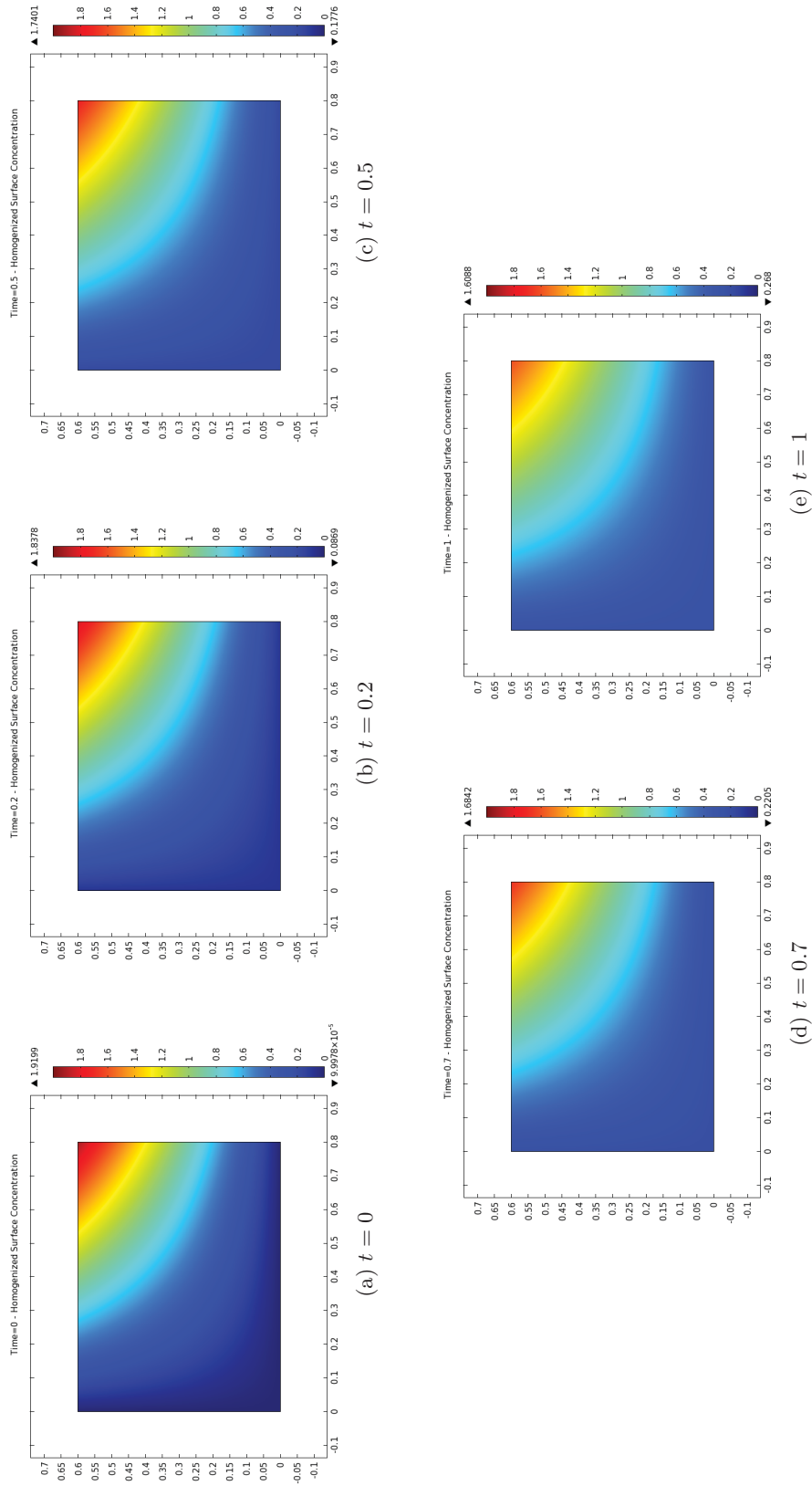


Figure 5.15: The concentration on the boundary for the indicated time steps. Since for fixed $x \in \Omega$ the concentration for each cell boundary is constant, this constant is depicted for each point in the domain.

6 Conclusions

In this work we extended the methods and techniques of (mathematical) homogenization. This was done with a focus on biological and chemical reaction-diffusion processes as outlined in Chapter 2: Some important modeling aspects of these applications have not been considered in the literature so far as outlined in Section 2.3. Out of these, we chose to further investigate the case of an evolution of microstructure combined with surface reaction and diffusion, as well as the treatment of processes on structured surfaces and other "nonflat" objects. These problems were treated in subsequent chapters:

In Chapter 3, we first collected some necessary mathematical tools for the modeling and analysis of processes on evolving domains. In this work, we used the framework of homogenization after transformation to a fixed setting, developed by Peter and Meier (see the references given in the corresponding chapter): Formal application of the transformation rules given in Section 3.1.3 lead to a system of transformed equations in Section 3.3.3. After proving existence and uniqueness results together with appropriate a-priori estimates, we applied the method of homogenization to obtain (in the limit) a macroscopic problem coupled with a family of problems posed on the microstructure, in which also the evolution of the domain takes place. These results can be found in Section 3.4.3.

The case of a "periodic surface" is considered in Chapter 4. We developed a notion of periodicity on Riemannian manifolds whose atlas satisfies a specific compatibility condition. This allowed for the construction of generalized unfolding operators, see Section 4.2. There it was also shown that well-known properties (in the case of the "usual" operator), integral identities and compactness results generalise to Riemannian manifolds. As an application, we considered an elliptic model problem (e.g. stationary heat conduction) on a manifold in Section 4.4. In this connection, we were able to show additional properties of the cell problem and to construct an equivalence relation for different atlases. It turned out that the limit problem is independent of the choice of an atlas with respect to this relation. Finally, we showed that unfolding in domains of \mathbb{R}^n and on manifolds is "compatible" and can be applied together in one problem. This was illustrated in Section 4.5 with the help of a multiscale problem.

Finally, as a demonstration of homogenization techniques, we numerically implemented this multiscale problem in COMSOL for two choices of the scale parameter. The simulations showed a fair agreement of the complex problems with the homogenized one.

6.1 Overview of New Results

We give an overview of the most important results which – to the knowledge of the author – have not appeared in the mathematical literature so far:

Concerning the case of an evolution of the microstructure, we point the reader to the following aspects:

- The **system of equations** (3.9) and (3.10) has not been considered so far in the context of periodic homogenization. Note especially the appearance of terms involving the normal velocity and the mean curvature of the surface. This also applies to the set of transformed equations (3.11), (3.12).
- In **Theorem 3.4.7** we give the limit system which is obtained by homogenization of the previous equations. The result that in this case the surface evolution takes place in the microstructure is new.

The treatment of Riemannian manifolds is new in the field of homogenization. We consider the following results as the most important aspects:

- The **Definitions 4.2.1** of periodicity on a manifold and **4.2.2** of the UC-criterion.
- **Definition 4.2.20** of a global unfolding operator on the manifold together with its **properties**.
- The compactness **Theorems 4.2.29 and 4.2.35**. In the proof, we rely on a variant of the Helmholtz decomposition and thus avoid the use of scale-splitting operators as in most part of the literature (see e.g. [CDG08]).
- The **application** to an elliptic model problem in **Theorem 4.4.4**.
- The construction of an **equivalence relation for different atlases** (see Assumption 4.4.18) which shows that homogenization is "robust" with respect to parametrizations.

6.2 Open Problems

In this section we collect possible extensions of the current work: Concerning both main subjects of this thesis, a next step could be to apply the techniques to real world applications. For the case of porous catalysts, a good starting point might be the paper by Pfafferoth, Heidebrecht et. al. [PHS⁺08], where material parameters are presented. In this connection, see also the conclusions in Heidebrecht, Pfafferoth and Sundmacher [HPS11], where the need for a sound mathematical treatment of application problems in catalysis is expressed.

For the field of homogenization with evolving microstructure, we suggest the following extensions:

- The idea of a locally periodic structure (see the works of Fatima, van Noorden, and Muntean [FAZM11] and [vNM10]) seems to be related to our construction of the domain in Section 3.2. While in the papers cited above the homogenization is carried out only formally, our method could lead to a rigorous proof.
- In this work, the evolution of the domain was assumed to be given. A more realistic setting would include a coupling between the evolution of the domain and the processes in the bulk and on the boundary (similar to [Mei08] and [Pet06]).
- All methods developed so far do not allow a change of the topology of the domain. However, in real world situations, phenomena like coalescence (e.g., of air bubbles) happen frequently. We expect that such processes cannot be treated by coordinate transformations, but would recommend an investigation of phase field and level set methods in the context of homogenization.

Concerning homogenization on Riemannian manifolds, we propose to investigate the following subjects:

- We only treated stationary problems in this work – thus it seems reasonable to extend the method to time-dependent (e.g. parabolic) problems as well. Since time appears in the context of periodic unfolding as an additional parameter (see for example [NR92]), it should be relatively easy to include. In this context, one can also try to work out the case of time-dependent Riemannian metrics, or metrics depending on other parameters (as in the field of gradient flows, see Chill and Fasangova [CF10] for an introduction).
- We only proved compactness results for gradients in the Hilbert space $W^{1,2}(M)$, see Theorems 4.2.29 and 4.2.35. Especially for nonlinear problems, one needs similar results for functions in $W^{1,p}(M)$ with $1 \leq p \leq \infty$, $p \neq 2$. A proof could be based on a version of the Hodge- or Helmholtz decomposition in $L^p(M)$ -spaces.
- The manifold M was assumed to be compact. For the case of non-compact manifolds, one would have to control the "overlap" of the partition of unity in a reasonable way to get corresponding results.
- Finally, we constructed an equivalence relation for atlases leading to the same limit problem. It would be interesting to investigate the case of non-equivalent atlases: Up to now, it is not clear what happens in this case. Do such atlases lead to different limit problems? Moreover, what is the *maximal* class of atlases leading to the same limit?

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