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Transient Numerical Simulation of Sublimation Growth of SiC Bulk Single Crystals

Modeling, Finite Volume Method, Results

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Transient Numerical Simulation of Sublimation Growth of SiC Bulk Single Crystals

Modeling, Finite Volume Method, Results

Doctoral Thesis

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Abstract

This work treats transient numerical simulation of growth of silicon carbide (SiC) bulk single crystals by physical vapor transport (also called the modified Lely method). A transient mathematical model of the growth process is presented. Subsequently, the finite volume method for the discretization of evolution equations, which constitutes the basis for the numerical simulations presented in this work, is studied mathematically, proving the existence of discrete solutions. All material data used for numerical simulations in this work are collected in the appendix.

Starting with a description of the physical growth procedure, problems arising during the growth process are discussed as well as techniques that are used for process control. It is explained why numerical simulation is an important tool for control, and the advantages of a transient approach are considered.

Within the presented transient model, continuous mixture theory is used to obtain balance equations for energy, mass, and momentum inside the gas phase. In particular, reaction-diffusion equations are deduced. Heat conduction is treated inside solid materials. Heat transport by radiation is modeled via the net radiation method for diffuse-gray radiation to allow for radiative heat transfer between the surfaces of cavities. The model includes the semi-transparency of the single crystal via a band approximation. Induction heating is modeled by an axisymmetric complex-valued magnetic scalar potential that is determined as the solution of an elliptic problem. The resulting heat source distribution is calculated from the magnetic potential. The heat sources are updated continuously during the solution of the transient problem for the temperature evolution to allow for changes in the electrical conductivity depending on temperature and for changes due to a moving induction coil.

The finite volume method is treated in a rigorous mathematical framework. It allows the discretization of parabolic, hyperbolic, and elliptic partial differential equations, as they arise from the mathematical model of the growth process, including nonlocal contributions due to radiative heat transfer. The general abstract setting consists of a system of nonlinear evolution equations in arbitrary finite space dimension, each evolution equation living on a different polytope domain. In general, each evolution equation has diffusive and convective contributions as well as source and sink terms. Each contribution is permitted to depend on the solution. Discontinuities of the solution are allowed at domain interfaces. Interface conditions in terms of the solution and its flux are considered. Moreover, nonlocal interface conditions are considered. Outer boundary conditions include Dirichlet conditions, flux conditions, emission conditions, and nonlocal conditions. Time discretization is performed by an implicit Euler scheme, where an explicit discretization is allowed in certain dependencies such that the temperature-dependent emissivities can be taken from the previous time step. As usual, the space discretization is performed by integrating the evolution equations over control volumes and then using quadrature formulas. As an axisymmetric setting and cylindrical coordinates are used in the simulations, a treatment of change of variables is included in the abstract considerations.

For the case that the evolution equations constitute nonlinear heat equations, still allowing nonlinear diffusion, convection, and source and sink terms, as well as nonlocal interface and boundary conditions as they arise from modeling radiative heat transfer, discrete L^∞-L^1 a priori estimates are established for the system resulting from the finite volume discretization. A fixed point argument is then used to prove the existence and uniqueness of discrete solutions.

The presented numerical simulations are conducted in an axisymmetric setting. They constitute transient investigations of control parameters affecting the temperature evolution during the heating of the growth apparatus. A cylindrically symmetric finite volume scheme provides the discretization for both the transient nonlinear heat problem and the stationary magnetic potential problem.

For different heating powers and different vertical coil positions, the temperature evolution is monitored at the surface of the crystal and at the surface of the source powder as well as at the top and at the bottom of the growth apparatus. It is studied how the temperature difference between source and seed, which is highly relevant to the growth process, is related to the measurable temperature difference between bottom and top. Results concerning the time lack between the heating of the surface of the source powder and the heating of its interior are considered. Finally, the global evolution of temperature and heat sources is investigated.

Preface

Foreword

A few words might be in order on how this work came about. In September 1997, I took a research position at the *Weierstrass Institute for Applied Analysis and Stochastics (WIAS)*, Berlin, to join the recently created research team for the topic of numerical simulation of sublimation growth of SiC bulk single crystals, at the time consisting of Prof. Dr. Jürgen Sprekels (head person), Dr. Nikolaus Bubner, Dr. Olaf Klein, and Prof. Dr. Krzysztof Wilmański. The *Bundesministerium für Bildung, Wissenschaft, Forschung und Technologie*[1] *(BMBF)* had granted funding for my position due to a successful application of the research team.

The goal was to create a physical model and to use numerical mathematics to develop software that can be employed to control and optimize the SiC sublimation growth process. The project was to be done in cooperation with the *Institute of Crystal Growth (IKZ)*, Berlin, where SiC bulk single crystals are produced using the sublimation growth method.

As, especially in the early stages of the project, my main task lay less with the modeling than with the numerical discretization of the model equations and the succeeding implementation, my initial inclination was to restrict this work to these aspects. However, I now think (not the least thanks to my advisor's and coworkers' suggestions) that a more comprehensive presentation of the subject is much more valuable to the reader. So the intention of this work is to give such a presentation. Section 1.2 describes the extend and limits of the scope of this work.

Acknowledgments

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[1]German Ministry for Education, Science, Research, and Technology

[2]New Mathematical Methods in Manufacturing and Service Industry

zur Lösung von Problemstellungen in Industrie und Wirtschaft[3] # 03SP7FV1/6. The author is responsible for the contents of this publication.

Large parts of the material presented in Chapters 2 and 4 have been joint work with Dr. Nikolaus Bubner, Dr. Olaf Klein, Prof. Dr. Jürgen Sprekels, and Prof. Dr. Krzysztof Wilmański of the *WIAS* (cf. [BKP+99], [KP99], [KPSW01], [KP01], [KP02]). In particular, the ideas for the gas model as published in [BKP+99] are mainly due to Prof. Dr. Krzysztof Wilmański, and Dr. Olaf Klein has contributed many ideas concerning the models for radiation and for induction heating as published in [KPSW01], [KP01], and [KP02], respectively. Dr. Volker Weiß provided most of the references for material data from the literature presented in App. A. However, I am solely responsible for the compilation of the material in this work and for the implementation of the computer code used to perform the numerical simulations presented in Ch. 4. The entire material of Ch. 3 is my original work.

My advisor Prof. Dr. Jürgen Sprekels supervised and guided my work, which I gratefully acknowledge. From the very beginning, the cooperative work with my coworker Dr. Olaf Klein has been very intensive and productive. I am particularly indebted for his patient proofreading and productive criticism.

Working in modeling and numerical simulation, it is extremely important to get feedback from experimenters working with the physical system. I thank Dr. Klaus Böttcher, Dr. Thomas Müller, Dr. Detlev Schulz, and Dr. Dietmar Siche of the *IKZ* for giving that feedback and for providing material and experimental data. I also thank Michael Rasp of *SiCrystal*, Erlangen, for bringing to my attention some of the particular aspects relevant to the commercial producer.

I thank my coworkers and former coworkers of the *WIAS*. I am grateful to my dear friends Ingrid Philip[4], Ortrun Schermeier, and Andrea Warnke for being precisely that. Last but not least, I thank all my friends and family, and I don't think that I can say it any better than with the words of Dr. Peter Råback [Råb96]: "Maybe you didn't speed up the process [of this work], but you certainly made the time much more worthwhile." In particular, I would like to mention my grandmother Else Ritter, who muchly would have liked to see this work completed, but unfortunately died too early.

[3]Mathematical Methods Solving Problems in Industry and Business

[4]Ingrid is also my mom - being a good parent is responsible, also being a good friend is more.

Curriculum Vitae

Personal Data

Peter Philip
born on December 15, 1971 in Hillerød, Denmark

Education

1978 – 1984	Grundschule[5] der Evangelischen Schule Neukölln in Berlin, Germany
1984 – 1991	Albert-Schweitzer-Oberschule (Gymnasium[6]) in Berlin, Germany Graduation examination: Abitur[7]
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1994 – 1995	Graduate studies at the mathematics department of the University of Maryland at College Park, USA, due to an exchange program of the Free Universtiy of Berlin
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Positions

1994 – 1995	Teaching assistant at the mathematics department of the University of Maryland at College Park, USA
since 1997	Research position as a member of the research group Partial Differential Equations and Variational Equations at the Weierstrass Institute for Applied Analysis and Stochastics (WIAS), Berlin

[5] elementary school
[6] German high school
[7] German qualification for university entrance
[8] German university degree

Abbreviations and Notation

Numbered environments are capitalized and are abbreviated except at the beginning of sentences (e.g. Fig. 1, Ch. 1). The abbreviations used for Appendix, Chapter, Claim, Definition, Equation, Example, Figure, Notation, Remark, Section, Table, Theorem and their respective plurals are App., Apps, Ch., Chs, Cl., Cls, Def., Defs, Eq., Eqs, Ex., Exs, Fig., Figs, Not., Nots, Rem., Rems, Sec., Secs, Tab., Tabs, Th., Ths.

To enhance readability, a centered dash is sometimes used to mark the end of a definition, example, etc.:

—

Equations and environments are numbered within sections. References in parentheses (e.g. (1.1.1)) *always* refer to equations whereas references without parentheses *never* refer to equations, but to sections, theorems etc. (e.g. Th. 1.1.1).

As it is common in the mathematical literature, the word "iff" is used to express "if and only if".

To avoid confusion and to make formulas more readable, parentheses are only used to group terms, whereas brackets are used to enclose function arguments: $a \cdot (b + c)$, but $f[x]$.

The quantifiers $\bigwedge$ (for all) and $\bigvee$ (there exists) are used:

$$\bigwedge_x \phi[x], \qquad \bigvee_x \phi[x]. \tag{0.1}$$

The left-hand expression in (0.1) means that the formula ϕ holds for all x, whereas the right-hand expression in (0.1) means that there exists at least one x such that the formula ϕ holds for x.

The symbol $\mathbb{N}$ denotes the set $\{1, 2, \dots\}$, whereas $\mathbb{N}_0 := \{0\} \cup \mathbb{N}$. If the set $\mathbb{K}$ is used in a statement, then the statement is meant to hold for both $\mathbb{K} = \mathbb{R}$ and $\mathbb{K} = \mathbb{C}$.

Variables in boldface (e.g. $\mathbf{u}$, $\mathbf{T}$) always denote vectorial or tensorial quantities. However, in the mathematical chapters Ch. 3 and App. C, boldface is used only for matrices and for vectorial physical quantities.

The terms *function*, *map*, and *operator* are used synonymously, but operator is preferred for cases, where the domain consists of functions or vectors.

Contents

Chapter 1

Introduction

1.1 Application and Growth of SiC Bulk Single Crystals

Due to its advantageous physical properties, silicon carbide (SiC) is used in numerous industrial applications. As a semiconductor substrate material, SiC is utilized in electronic and optoelectronic devices such as MESFETs, MOSFETs, thyristors, P-i-N diodes, Schottky diodes, blue and green LEDs, lasers, and sensors. Its chemical and thermal stability enable SiC to be used in high temperature applications as well as in intensive radiation environments. Moreover, SiC is especially suitable for usage in high power and high frequency applications. Figure 1.1 shows an SiC wafer grown at the *Institute of Crystal Growth (IKZ)*, Berlin.

An economically profitable use of SiC requires the availability of low-defect SiC boules

Figure 1.1: 1 inch diameter SiC boule grown at the IKZ, Berlin.

with large diameter. At the same time, a high growth rate is desirable to reduce production time and cost. Even though there has been substantial progress in SiC manufacturing in recent years, satisfying all of the aforementioned demands remains challenging, as only partial solutions exist (cf. e.g. [GHTC97], [CTG+99], [MGH+00]).

Several fundamentally different growth techniques for the production of SiC single crystals are described in the literature. Even though SiC single crystals have been grown from melt (cf. [HMW98]), currently this does not constitute a growth method suitable for large scale industrial production. More practical techniques are given by chemical vapor deposition (CVD), the sublimation sandwich method (SSM), and physical vapor transport (PVT). An overview of SiC single crystal growth by CVD is found in [Nis95b] which also includes a large number of further references on the subject. For descriptions of SSM one can consult e.g. [VMRR79] and [VRR+97]. Both CVD and SSM are mainly used to grow thin crystalline layers, even though variants of these methods have been successfully applied to SiC bulk single crystal growth (cf. [EKI+98] for CVD and [MRRV97] for SSM). Large SiC single crystals are usually grown by PVT according to the modified Lely method. Since modeling and simulation of PVT is the major concern of this work, this method is now considered in more detail.

The original Lely method dates back to [Lel55]. In its initial form, the procedure used a resistance heated thermally insulated graphite crucible, containing a polycrystalline SiC source enclosing a cavity. The system was heated to some 2800 K in an inert gas (e.g. Ar) atmosphere at 10^5 Pa (normal pressure). Due to the high temperatures, SiC from the source sublimates and crystallizes in places of lower temperature, e.g. inside the cavity, resulting in transparent SiC single crystals of up to 1 cm diameter.

The original Lely method had many drawbacks such as uncontrolled nucleation and dendritic growth. The introduction of seeded sublimation growth using single crystals grown by the original Lely method as seed crystals, led to substantial improvements in size and quality of the produced SiC crystals (cf. [TT78] and [TT81]). In this form, the technique became known as the modified Lely method and PVT.

Usually, modern PVT growth systems consist of a graphite crucible containing polycrystalline SiC source powder and a single-crystalline SiC seed. The crucible is heated e.g. by induction or resistance heating. The source powder is placed in the hot zone of the growth apparatus, whereas the seed crystal is cooled by means of a blind hole, establishing a temperature difference between source and seed. To this end, different geometrical setups have been proposed, the main types being drawn schematically in [Nis95a, Fig. 1(a), 1(b)]. In the first configuration ([Nis95a, Fig. 1(a)]), the source and the seed are placed inside a single chamber with the source at the bottom and the seed at the top. For numerical simulations of this type of setup presented subsequently in Sec. 4.3, the growth apparatus displayed in [PAC+99, Fig. 2] is used. It is reproduced in Fig. 1.2. In the second configuration ([Nis95a, Fig. 1(b)]), the source and the seed are placed in different chambers, separated by a thin porous graphite wall, the seed being located at the bottom of the inner chamber. The corresponding structure that we used for numerical simulations of the second type of setup presented in [KPSW01] is a modified version of [Nis95a, Fig. 1(b)]. It is depicted in Fig. 1.3. On its outside, the growth apparatus is thermally insulated, typically with graphite felt or foam.

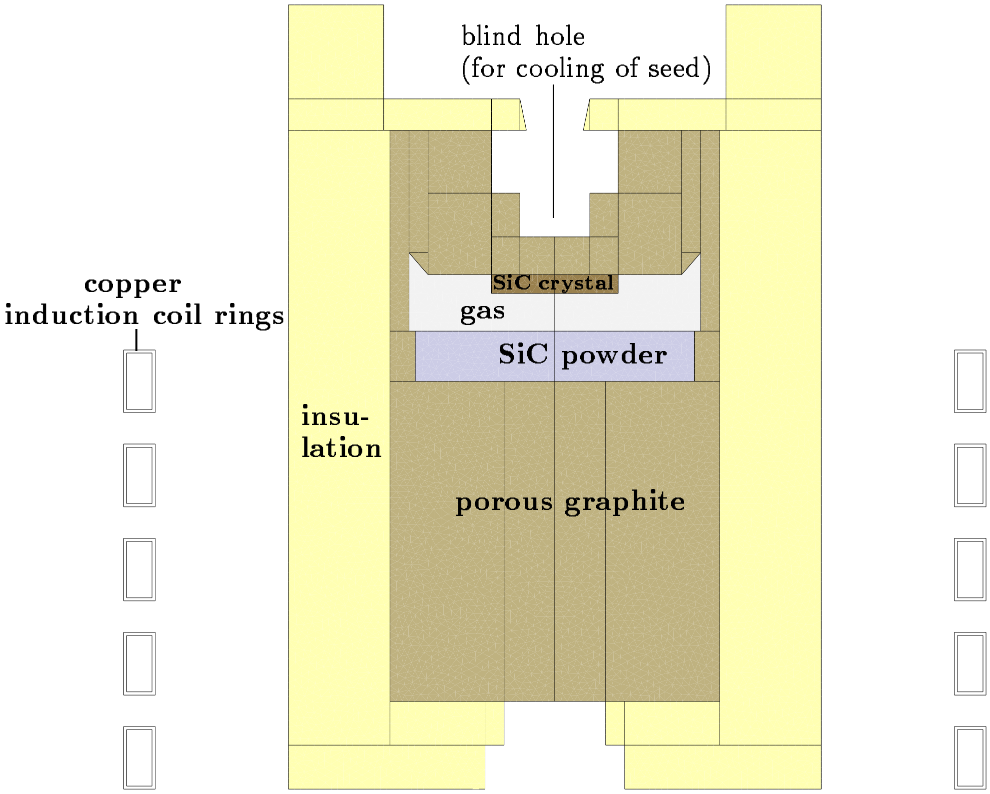

Figure 1.2: Setup of growth apparatus according to [PAC+99, Fig. 2].

To eliminate contaminants such as S, B, and metallic elements from the growth system, in a first heating stage, the apparatus is degassed at some 10^{-3} Pa and heated to about 1200 K. After the contaminant bakeout phase has been completed, a high-purity argon atmosphere is established at 10^5 Pa, and the temperature is further increased. At growth temperature, which can reach up to 3000 K for growth of the SiC polytype 6H, pressure is reduced to about $2 \cdot 10^3$ Pa (cf. [BMH+93]).

The high temperature and the low pressure cause the source powder to sublimate, adding molecules made up of silicon and carbon to the gas phase. The composition of the gas mixture has been analysized both experimentally and by thermodynamical theorectical considerations, showing that, apart from the inert gas, Si, Si_2C and SiC_2 constitute the predominant species (cf. e.g. [DMI58], [RCB96], [GHTC97], and [ABEP98]). As the SiC source is kept at a higher temperature than the cooled SiC seed, sublimation is encouraged at the source and crystallization is encouraged at the

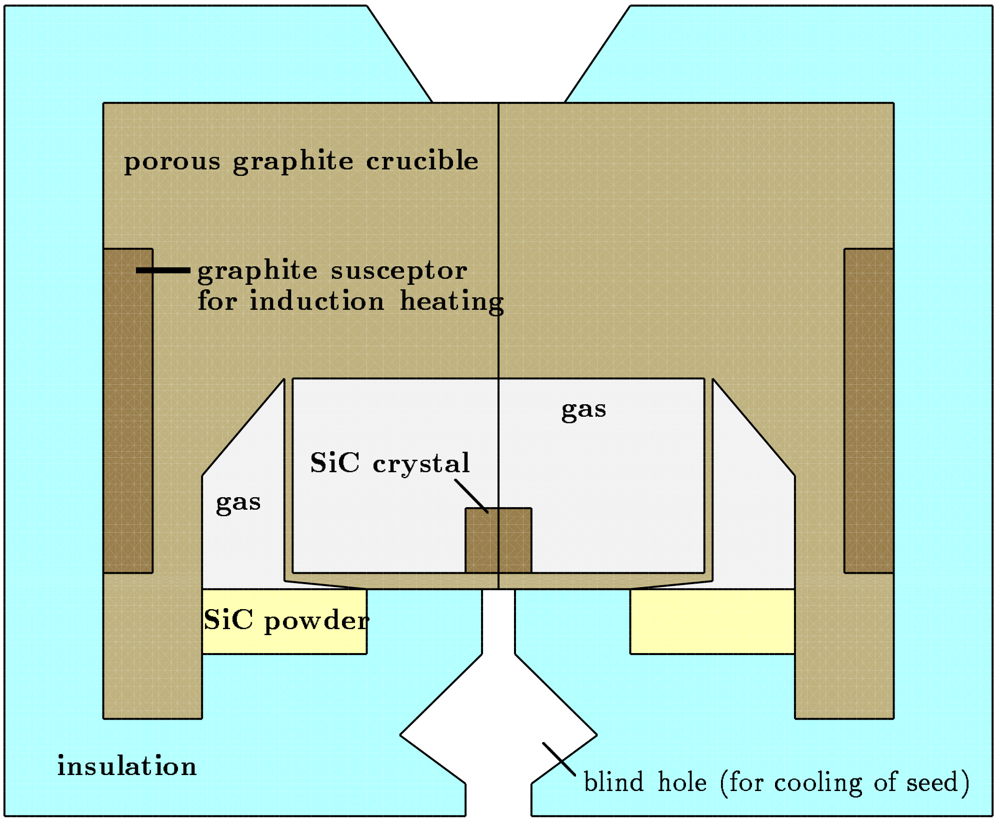

Figure 1.3: Setup of growth apparatus with source powder and seed crystal in separate chambers, seed at bottom.

seed, causing the partial pressures of Si, Si_2C and SiC_2 to be higher in the neighborhood of the source and lower in the neighborhood of the seed. As the system tries to equalize the partial pressures, source material is transported to the seed which grows into the reaction chamber. In the setup with two different chambers for source and seed as depicted in Fig. 1.3, the molecules originating from the source diffuse through the pores of the graphite wall into the growth chamber.

According to the aforementioned requirements, the growth process needs to be optimized in order to lower the defect rate of the grown crystal, and simultaneously to increase its size and growth rate.

Typical defects are the growth of unwanted polytypes, micropipes (tiny tubelike cavities), vacancies, dislocations, and impurities. A selection of published results on boule size, defect densities, and growth rates may give an idea of the current possibilities of SiC single crystal growth by PVT. Reference [MGH+00] reports the growth of a 2.5 cm (diameter) micropipe-free 4H-SiC wafer, a 5 cm 4H-SiC wafer with a micropipe density of 1.1 cm^{-2}, and a 7.5 cm 4H-SiC wafer (no information on defects). The authors report impurities of less than 0.1 parts per million. Growth rates from 0.2 to 4 mm/h are reported by [BMH+93].

It is found (cf. e.g. [SBP98], [RSD+99], and [SVK+00]) that the crystal's defect density and growth rate are strongly influenced by the temperature distribution (especially the temperature at the seed and the temperature difference between source and seed), the mass transport, and the pressure and concentrations of gas species. These *internal control parameters* can only be tuned indirectly by varying *external control parameters* such as the geometrical configuration of the setup, the power of the RF heater, the position of the induction coil, and the inert gas pressure.

Due to the high temperatures, experimental verification of the correlation between the properties of the grown crystal and both internal and external control parameters is very intricate and costly. Hence, theoretical modeling and numerical simulation play an essential role in the investigation and determination of the relation between controllable quantities and advantageous growth conditions. In consequence, the development of numerical models and software and their application to PVT growth of SiC crystals has been an active field of research in recent years. Papers on stationary models include [HHW+95], [PBD+96], [KMR97], [EGG+98], [CAB+99], [PAC+99], [RMD+99], [KKZ+00], [SKM+00]. In [Råb96], a transient model is stated, but the numerical considerations are restricted to the stationary case. Results of transient numerical simulations of the heat transfer during PVT are presented in [CZP+99], [KPSW01], and [KP01]. Results similar to the ones presented in [KP01] are included in Ch. 4.

For a number of reasons, it is not sufficient to restrict one's attention to the quasi-stationary state at the end of the heating process, but it is also important to monitor and control the temperature field evolution during the heating process itself: Crystal growth can already occur during the heating-up stage, possibly causing micropipes or the growth of unwanted polytypes. Moreover, thermal stresses in the seed crystal due to temperature gradients during heating can initiate crystal defects.

Results of transient simulations can help to gauge the time one has to allow for the contaminant bakeout phase described above, and it can be an important tool to verify the validity of using temperatures measured at the blind holes to estimate temperatures (or temperature differences) in the growth chamber (s. Sec. 4.3.3).

1.2 Scope and Structure of this Work

1.2.1 Modeling and Simulation

It is the goal of this work to present a rather comprehensive treatment of transient modeling and numerical simulation of SiC bulk single crystal growth by PVT. It is comprehensive in the sense that it treats all aspects of the numerical simulation process, from the experimental setup (as decribed above), the compilation of relevant material data (App. A), the formulation of a physical model (Ch. 2), a treatment of the numerical methods including a description of the discretization and mathematical analysis (Ch. 3), and the presentation and discussion of numerical results (Ch. 4).

However, the subject is so vast that striving for completeness is impossible at the current stage of research and far beyond the scope of this work. Actually, further research is warranted in virtually all of the aforementioned aspects of the numerical simulation process. The following paragraphs describe this work's scope and indicate some fields where further research seems desirable.

The physical properties of the materials used in the PVT growth system are very difficult to control e.g. due to the high temperatures and the chemical reactivity and the porosity of the involved substances such as SiC powder, graphite crucible and insulation. One goal of research is to find materials and setups of growth systems where the physical properties are more stable or at least where their change is more predictable. This would also help to provide more accurate material data to be used in numerical simulations. I tried to use material data typical for real growth systems for the numerical simulations presented in Ch. 4, but in some cases the available data are probably merely crude approximations of the real situation (cf. App. A).

The gas model based on continuous mixture theory described in Sec. 2.1 covers heat transport as well as gas dynamics and chemical reactions. The deduced system (2.1.28) consists of simplified transient balance equations for mass, momentum, and energy as well as of reaction-diffusion equations for the gas mixture in three space dimensions. The material laws of an ideal gas (2.1.31) are used, which are valid in a low pressure or high temperature setting.

Transient and temperature-dependent heat conduction according to (2.2.1) is considered in solid materials, but no mechanical or chemical reactions in solid bodies are accounted for. In particular, neither graphitizing or sintering of the SiC source nor Si accumulation in the insulation is included in the model, even though these processes do occur in real growth systems. A possibility to improve the modeling of solid components in future research is the application of the theory of porous media to the SiC source powder, the graphite crucible, and the insulation.

Models for crystal growth, source powder sublimation, and thermal stress in the single crystal are not treated in this work, but should certainly be included in more complete future models. References on these subjects are e.g. [KMR97], [KKZ+00], [SVK+00].

Heat transport by radiation inside solid materials is included in the respective temperature-dependent laws of thermal conductivity. Radiative heat transfer between surfaces of cavities is modeled in Sec. 2.4. Using a diffuse-gray model is justified, since the involved surfaces are generally non-smooth. The semi-transparency of the SiC single crystal is modeled via a band approximation model in Sec. 2.4.4; all other solids are treated as opaque. Volumetric coupling of surface radiation with the interiors of either the single crystal or the gas phase is neglected. The resulting numerical expenditure from including volumetric coupling is not justified by the expected gain in accuracy, since at higher temperatures, the temperature variations in the crystal and in the gas regions is in the order of 100 K.

Even though the radiation model of Sec. 2.4 is valid in three space dimensions, the numerical methods described in Sec. 3.7.8 assume cylindrical symmetry, thereby reducing the problems to two space dimensions. For example, computing visibility factors in three space dimensions without cylindrical symmetry is much more complicated (cf. e.g. [SH93], [Kel96]).

In Sec. 2.5, induction heating is modeled assuming cylindrical symmetry of fields and domains, sinusoidal time dependence, and independence of the magnetic permeability of the magnetic field. The sinusoidal time dependence allows to reduce the transient electo-magnetic problem to a stationary problem (s. Sec. 2.5.6). Since the time scale of changes in the electo-magnetic fields is at least five orders of magnitude faster than the time scale of changes in the temperature field, it is reasonable to solve quasi-stationary electro-magnetic problems in each time step of the solution of the transient heat transport problem (accounting for temperature-dependent material data or changing coil positions). The assumption of cylindrical symmetry, however, is somewhat crude, replacing the induction coil by disjoint cylindrical rings. Still, this drawback seems almost unavoidable, since the solution of Maxwell's equations (2.5.2) in three space dimensions is much more difficult.

Only transient heat transport is simulated for the numerical results discussed in Ch. 4, i.e. in the gas phase, only the energy balance (2.1.28c) is considered. To include the other equations describing the gas phase, i.e. the mass balance (2.1.28a), the momentum balance (2.1.28b), and the reaction-diffusion equations (2.1.28d), one still needs to set up appropriate boundary conditions, and additional material functions such as the diffusion coefficients $D^{(\alpha_\iota)}$ in (2.1.28d) need to be determined.

The restriction to simulations of heat transport allows another significant simplification without considerable loss of accuracy. Since for lower temperatures, only argon is present in the gas phase, and for higher temperatures, heat is mainly conveyed by radiation, argon can be considered as the only constituent of the gas phase. This allows to use the simplified model of Sec. 2.1.4.

As cylindrical symmetry is an essential assumption for both the induction heating model and the numerical methods used to calculate radiation terms, cylindrical symmetry is presumed in all the presented numerical simulations, i.e. the equations (2.1.34c) and (2.2.1) describing heat transport in gas and solid, respectively, are also considered in an axisymmetric setting, even though the equations are equally valid in three space dimensions.

The numerical results presented in Ch. 4 are similar to the results shown in [KP01], studying the evolution of the temperature distribution depending on the heating power and the coil position. In contrast to [KP01], where a constant heating voltage is prescribed, in Ch. 4 the power is prescribed and it is increased gradually from 0 to its maximum. Some new results concerning the temperature evolution in the SiC source powder are discussed in Sec. 4.3.3. Moreover, Sec. 4.3.3 contains some new results bearing on the validity of using the temperature differences between lower and upper blind hole as an indicator for the temperature differences between SiC source and seed. As mentioned in Sec. 1.1, in a stationary setting there are many articles in the literature presenting numerical simulations including phenomena other than heat transport.

1.2.2 Finite Volume Method

In Ch. 3, time and space discretization of coupled partial differential equations is treated mathematically, using the finite volume method. The partial differential equations have the general form of nonlinear evolution equations. The coupling is across interfaces between different space domains, not between different equations on the same domain (approaches for the latter situation can be found in [EGH00, Ch. VII]). The setting was chosen sufficiently general to include the situations occurring during the discretizations for the simulations of Ch. 4, [BKP+99], and [KPSW01], in particular, allowing for nonlinear diffusive and convective contributions as well as source and sink terms. Interface conditions in terms of the solution and its flux are considered, and nonlocal coupling is treated, as it occurs owing to radiative heat tranfer through cavities. Outer boundary conditions include Dirichlet conditions, flux conditions, and emission conditions as well as nonlocal conditions.

To avoid further complications in the formulation of the finite volume discretization, input functions as well as solutions are assumed to be continuous within each space domain. However, discontinuities of the solution and of the input functions are allowed across interfaces, such as to include the situation of temperature steps between solid and gas, and to allow jumps in material parameters.

Only polytope domains are considered to avoid the introduction of further notions and notation when treating more general manifolds. As convergence of the discrete scheme to continuous solutions is not the subject of this work, it presents no complication to admit an arbitrary finite space dimension.

In Secs 3.3.2 and 3.4.3, time discretization is performed by an implicit Euler scheme, where an explicit discretization is allowed in certain dependencies such that the temperature-dependent emissivities can be taken from the previous time step. The space discretization is performed by integrating the evolution equations over control volumes (Sec. 3.5) and then using quadrature formulas (Sec. 3.7). It is shown in Sec. 3.6, how a change of variables (e.g. cylindrical coordinates) can be handled within this framework.

For the case that the evolution equations constitute nonlinear heat equations, still allowing nonlinear diffusion, convection, and source and sink terms, as well as nonlocal interface and boundary conditions as they arise from modeling radiative heat transfer, discrete L^∞-L^1 a priori estimates are established for the system resulting from the finite volume discretization (s. Sec. 3.7.13). Using a fixed point argument, it is shown that the discrete system then has a unique solution (Sec. 3.8).

An analytic mathematical treatment of the existence theory (let alone the regularity theory, approximation theory, and control theory) of the complete model including nonlocally coupled nonlinear heat equations with discontinuous coefficients and different types of boundary conditions, coupled with Euler equations and reaction-diffusion equations, including free boundaries at least on the surfaces of the SiC source and the seed crystal, also coupled to an electro-magnetic induction heating problem, (in two, let alone in three, space dimensions) seems completely hopeless at the current state of research.

Promising starting points for further analytical research might be given by [LT00], where an existence theory of heat equations with nonlocal coupling due to radiation operators is treated.

In my own forthcoming work, I plan to use the discrete existence and uniqueness results of Sec. 3.8 together with discrete L^∞-L^2 a priori estimates similar to [MR01], to establish convergence results for the finite volume scheme defined in Sec. 3.7.12 (s. Def. 3.7.41). The strategy is outlined in Sec. 3.9.

Chapter 2

Modeling

2.1 Model of the Gas Phase

The purpose of this section is to present a transient model describing the processes in gas regions of the growth apparatus during SiC bulk single crystal growth by PVT. As explained in Sec. 1.1, the gas regions contain a mixture made up of several constituents, where Ar, Si, Si_2C, and SiC_2 are the predominant species. The model needs to account for the interchange of mass and momentum between the different constituents, in addition to chemical reactions and thermomechanical processes such as motion and heat transfer.

The model developed below has been published in a similar form in [BKP+99]. In the framework of a continuous mixture theory of A constituents, the model starts out from general partial balance equations for mass and momentum, and another balance equation for the total energy. The system of balance equations is then algebraically transformed into a system of field equations, followed by simplifications and the addition of material laws. It is noted that there exist mixtures (e.g. plasmas), where it is necessary to consider a different temperature for each constituent. However, in the following treatment it is always assumed that the constituents of the mixture exchange energy sufficiently rapidly so that a single temperature can be assigned to the mixture at all times.

2.1.1 General Balance and Field Equations

A gas mixture consisting of A constituents is considered, the different constituents being denoted by (α_ι), $\iota \in \{1, \dots, A\}$. As mentioned above, the application one should have in mind is the gas mixture consisting of the predominant species occurring during SiC growth by PVT, where $A = 4$ and

$$\big\{\alpha_\iota : \iota \in \{1, \dots, 4\}\big\} = \{\mathrm{Ar}, \mathrm{Si}, \mathrm{Si_2C}, \mathrm{SiC_2}\}. \tag{2.1.1}$$

The following symbols are used, where the superscript (α_ι), $\iota \in \{1, \dots, A\}$, indicates quantities inside the gas species α_ι (e.g. $\rho^{(\mathrm{Ar})}$, $\mathbf{v}^{(\mathrm{Si})}$, etc., see below), and where boldface denotes vectorial or tensorial quantities:

$\rho^{(\alpha_\iota)}$ – partial mass density,

$\mathbf{v}^{(\alpha_\iota)}$ – partial local mean velocity of gas particles,

$\rho^{*(\alpha_\iota)}$ – partial mass source, $\mathbf{T}^{(\alpha_\iota)} = \left(t_{i,j}^{(\alpha_\iota)}\right)$ – partial stress tensor,

$\mathbf{b}^{(\alpha_\iota)}$ – partial force density, e.g. gravimetric acceleration,

$\mathbf{p}^{*(\alpha_\iota)}$ – partial momentum source, $\varepsilon^{(\alpha_\iota)}$ – partial internal energy,

$\mathbf{q}^{(\alpha_\iota)}$ – partial heat flux, $\varepsilon^{*(\alpha_\iota)}$ – partial energy source,

$r^{(\alpha_\iota)}$ – partial radiaton.

Partial mass sources, partial momentum sources, and partial energy sources allow for the exchange of mass, momentum, and energy between the different gas constituents, which can occur e.g. due to diffusion, chemical reactions, and phase transitions.

It is noted that the stress tensors $\mathbf{T}^{(\alpha_\iota)}$ are symmetric (cf. [Mül85, p. 66 (3.53)] and [Wil98, p. 63 (4.71)]), i.e.

$$\bigwedge_{\iota \in \{1,\dots,A\}} \bigwedge_{(i,j) \in \{1,2,3\}^2} t_{i,j}^{(\alpha_\iota)} = t_{j,i}^{(\alpha_\iota)}. \tag{2.1.2}$$

In the following, vector and tensor notation is employed. Some definitions and relations are provided in App. B.1.

Balance Equations

Equations (2.1.3) and (2.1.7) below can be found in [Mül85, p. 69 (3.65), p. 173 (6.2) and (6.6)]. Equations (2.1.3a) and (2.1.3b) constitute partial balance equations for mass and momentum written for each constituent α_ι, $\iota \in \{1, \dots, A\}$. Following [Mül85, (6.2)], the total energy balance is written in (2.1.3c) (using the slightly different form [Mül85, (3.76)]). Equations (2.1.7) form the global conservation laws of mass and momentum. The total energy balance (2.1.3c) employs a number of quantities defined subsequently in (2.1.4) and (2.1.6). For completeness and since it is often customary (cf. [Mül85, p. 68 (3.61)] and [Wil98, p. 191 (10.4)]), partial energy balances are formulated in (2.1.9). However, in this work no subsequent use is made of the partial energy balances.

As usual, t denotes time.

- Partial Mass Balance:

$$\bigwedge_{\iota \in \{1,\dots,A\}} \frac{\partial \rho^{(\alpha_\iota)}}{\partial t} + \operatorname{div}\left(\rho^{(\alpha_\iota)} \mathbf{v}^{(\alpha_\iota)}\right) = \rho^{*(\alpha_\iota)}. \tag{2.1.3a}$$

- Partial Momentum Balance:

$$\bigwedge_{\iota\in\{1,\dots,A\}} \left(\begin{array}{c} \dfrac{\partial\left(\rho^{(\alpha_\iota)}\mathbf{v}^{(\alpha_\iota)}\right)}{\partial t} + \operatorname{div}\left(\rho^{(\alpha_\iota)}\mathbf{v}^{(\alpha_\iota)} \otimes \mathbf{v}^{(\alpha_\iota)} - \mathbf{T}^{(\alpha_\iota)}\right) \\ = \mathbf{p}^{*\,(\alpha_\iota)} + \rho^{(\alpha_\iota)}\mathbf{b}^{(\alpha_\iota)} \end{array} \right). \tag{2.1.3b}$$

  Using (B.1.3) and (B.1.6d) yields (2.1.3b) in components:

$$\bigwedge_{\substack{\iota\in\{1,\dots,A\},\\ i\in\{1,2,3\}}} \left(\begin{array}{c} \dfrac{\partial\left(\rho^{(\alpha_\iota)}v_i^{(\alpha_\iota)}\right)}{\partial t} + \displaystyle\sum_{j=1}^{3}\frac{\partial}{\partial x_j}\left(\rho^{(\alpha_\iota)}v_i^{(\alpha_\iota)}v_j^{(\alpha_\iota)} - t_{i,j}^{(\alpha_\iota)}\right) \\ = p_i^{*\,(\alpha_\iota)} + \rho^{(\alpha_\iota)}b_i^{(\alpha_\iota)} \end{array} \right). \tag{2.1.3b'}$$

- Total Energy Balance (using quantities defined in (2.1.4) and (2.1.6)):

$$\begin{aligned} &\frac{\partial}{\partial t}\left(\rho_{\text{gas}}\left(\varepsilon_{\text{gas}} + \frac{1}{2}\left(\mathbf{v}_{\text{gas}}\right)^2\right)\right) \\ &+ \operatorname{div}\left(\rho_{\text{gas}}\left(\varepsilon_{\text{gas}} + \frac{1}{2}\left(\mathbf{v}_{\text{gas}}\right)^2\right)\mathbf{v}_{\text{gas}} + \mathbf{q}_{\text{gas}} - \mathbf{T}_{\text{gas}}\mathbf{v}_{\text{gas}}\right) \\ &= \rho_{\text{gas}}\mathbf{b}_{\text{gas}} \bullet \mathbf{v}_{\text{gas}} + \rho_{\text{gas}} r_{\text{gas}}. \end{aligned} \tag{2.1.3c}$$

Now the promised definitions needed in the formulation of (2.1.3c): Let

$$\rho_{\text{gas}} := \sum_{\iota=1}^{A}\rho^{(\alpha_\iota)}, \tag{2.1.4a}$$

$$\mathbf{v}_{\text{gas}} := \frac{1}{\rho_{\text{gas}}}\sum_{\iota=1}^{A}\rho^{(\alpha_\iota)}\mathbf{v}^{(\alpha_\iota)}, \tag{2.1.4b}$$

and for each $\iota \in \{1,\dots,A\}$

$$c^{(\alpha_\iota)} := \frac{\rho^{(\alpha_\iota)}}{\rho_{\text{gas}}}, \tag{2.1.4c}$$

$$\mathbf{u}^{(\alpha_\iota)} := \mathbf{v}^{(\alpha_\iota)} - \mathbf{v}_{\text{gas}}. \tag{2.1.4d}$$

The meaning of the quantities is as follows: ρ_{gas} is the total mass density of the gas mixture, $\mathbf{v}_{\text{gas}}$ is the local mean velocity of all constituents, $c^{(\alpha_\iota)}$ is the concentration of the species α_ι, and $\mathbf{u}^{(\alpha_\iota)}$ is the diffusion velocity of the species α_ι. As immediate consequences of the definitions one gets

$$\sum_{\iota=1}^{A} c^{(\alpha_\iota)} = 1, \qquad \sum_{\iota=1}^{A} c^{(\alpha_\iota)}\mathbf{u}^{(\alpha_\iota)} = 0. \tag{2.1.5}$$

It still remains to define the total stress tensor $\mathbf{T}_{\mathbf{gas}}$, the total force density $\mathbf{b}_{\mathbf{gas}}$, the total internal energy $\varepsilon_{\mathbf{gas}}$, the total radiation $r_{\mathbf{gas}}$, and the total heat flux $\mathbf{q}_{\mathbf{gas}}$, which is now done in (2.1.6):

$$\mathbf{T}_{\mathbf{gas}} := \sum_{\iota=1}^{A} \left(\mathbf{T}^{(\alpha_\iota)} - \rho^{(\alpha_\iota)}\mathbf{u}^{(\alpha_\iota)} \otimes \mathbf{u}^{(\alpha_\iota)}\right), \tag{2.1.6a}$$

$$\mathbf{b}_{\mathbf{gas}} := \frac{1}{\rho_{\mathbf{gas}}} \sum_{\iota=1}^{A} \rho^{(\alpha_\iota)}\mathbf{b}^{(\alpha_\iota)}, \tag{2.1.6b}$$

$$\varepsilon_{\mathbf{gas}} := \frac{1}{\rho_{\mathbf{gas}}} \sum_{\iota=1}^{A} \rho^{(\alpha_\iota)} \left(\varepsilon^{(\alpha_\iota)} + \frac{1}{2}\left(\mathbf{u}^{(\alpha_\iota)}\right)^2\right), \tag{2.1.6c}$$

$$r_{\mathbf{gas}} := \frac{1}{\rho_{\mathbf{gas}}} \sum_{\iota=1}^{A} \rho^{(\alpha_\iota)} \left(r^{(\alpha_\iota)} + \mathbf{b}^{(\alpha_\iota)} \bullet \mathbf{u}^{(\alpha_\iota)}\right), \tag{2.1.6d}$$

$$\mathbf{q}_{\mathbf{gas}} := \sum_{\iota=1}^{A} \left(\mathbf{q}^{(\alpha_\iota)} + \left(\rho^{(\alpha_\iota)} \left(\varepsilon^{(\alpha_\iota)} + \frac{1}{2}\left(\mathbf{u}^{(\alpha_\iota)}\right)^2\right) - \mathbf{T}^{(\alpha_\iota)}\right) \mathbf{u}^{(\alpha_\iota)}\right). \tag{2.1.6e}$$

In addition to the balance equations (2.1.3), the following global conservation laws hold:

- Global Mass Conservation:

$$\sum_{\iota=1}^{A} \rho^{*(\alpha_\iota)} = 0. \tag{2.1.7a}$$

- Global Momentum Conservation:

$$\sum_{\iota=1}^{A} \mathbf{p}^{*\,(\alpha_\iota)} = 0. \tag{2.1.7b}$$

For each instant in time the state of the gas mixture is determined by the $2A+1$ quantities

$$\left\{\rho^{(\alpha_1)}, \dots, \rho^{(\alpha_A)}, \mathbf{v}^{(\alpha_1)}, \dots, \mathbf{v}^{(\alpha_A)}, T_{\mathbf{gas}}\right\}, \tag{2.1.8}$$

where $T_{\mathbf{gas}}$ denotes the (common) absolute temperature in the gas mixture. In the formulations of (2.1.3) and (2.1.7), the dependence on $T_{\mathbf{gas}}$ is implicit. Equations (2.1.3) and (2.1.7) are further coupled by material laws which are provided subsequently in Sec. 2.1.3, where the variable T_{gas} occurs explicitly.

As mentioned above, one can also write partial energy balance equations for each constituent:

- Partial Energy Balance:

$$\bigwedge_{\iota\in\{1,\dots,A\}} \begin{pmatrix} \dfrac{\partial}{\partial t}\left(\rho^{(\alpha_\iota)}\left(\varepsilon^{(\alpha_\iota)}+\dfrac{1}{2}\left(\mathbf{v}^{(\alpha_\iota)}\right)^2\right)\right) \\ +\operatorname{div}\left(\rho^{(\alpha_\iota)}\left(\varepsilon^{(\alpha_\iota)}+\dfrac{1}{2}\left(\mathbf{v}^{(\alpha_\iota)}\right)^2\right)\mathbf{v}^{(\alpha_\iota)}+\mathbf{q}^{(\alpha_\iota)}-\mathbf{T}^{(\alpha_\iota)}\mathbf{v}^{(\alpha_\iota)}\right) \\ =\varepsilon^{*(\alpha_\iota)}+\rho^{(\alpha_\iota)}\mathbf{b}^{(\alpha_\iota)}\bullet\mathbf{v}^{(\alpha_\iota)}+\rho^{(\alpha_\iota)}r^{(\alpha_\iota)} \end{pmatrix}. \tag{2.1.9}$$

Equations (2.1.9) can be viewed as defining equations for the partial energy sources $\varepsilon^{*(\alpha_\iota)}$. Then summing (2.1.9) over ι, and using (B.2.8), the linearity of ∂_t, (B.2.9), Rem. B.1.7, (B.2.2), and (2.1.3c) yields

- Global Energy Conservation:

$$\sum_{\iota=1}^{A}\varepsilon^{*(\alpha_\iota)}=0. \tag{2.1.10}$$

Conversely, (2.1.9) and (2.1.10) imply (2.1.3c).

Analogous to the total energy balance (2.1.3c), one can write total balance equations for mass and momentum:

- Total Mass Balance:

$$\frac{\partial\rho_{\mathrm{gas}}}{\partial t}+\operatorname{div}\left(\rho_{\mathrm{gas}}\mathbf{v}_{\mathrm{gas}}\right)=0. \tag{2.1.11a}$$

- Total Momentum Balance:

$$\frac{\partial\left(\rho_{\mathrm{gas}}\mathbf{v}_{\mathrm{gas}}\right)}{\partial t}+\operatorname{div}\left(\rho_{\mathrm{gas}}\mathbf{v}_{\mathrm{gas}}\otimes\mathbf{v}_{\mathrm{gas}}-\mathbf{T}_{\mathrm{gas}}\right)=\rho_{\mathrm{gas}}\mathbf{b}_{\mathrm{gas}}. \tag{2.1.11b}$$

Lemma 2.1.1. *The partial balance equations* (2.1.3) *together with the global conservation laws* (2.1.7) *imply the total balance equations* (2.1.11).

Proof. Summing (2.1.3a) over ι, and using (2.1.4a), (2.1.4b), (2.1.7a), the linearity of ∂_t, and Rem. B.1.7 gives (2.1.11a); summing (2.1.3b) over ι, and using (2.1.4b), (2.1.6a), (B.2.7), (2.1.7b), (2.1.6b), the linearity of ∂_t, and Rem. B.1.7 gives (2.1.11b). ∎

Field Equations

For each time instant, the state of the gas mixture is determined by the $2A+3$ quantities

$$\left\{\rho_{\mathbf{gas}}, \mathbf{v}_{gas}, c^{(\alpha_1)}, \dots, c^{(\alpha_A)}, \mathbf{u}^{(\alpha_1)}, \dots, \mathbf{u}^{(\alpha_A)}, T_{\mathbf{gas}}\right\}, \tag{2.1.12}$$

which can be used alternatively to the $2A+1$ quantities (2.1.8). The combination of the following field equations (2.1.14) together with (2.1.5)[1] is equivalent to the system consisting of (2.1.3) and (2.1.7) (s. Apps B.2.2 and B.2.3). Moreover, one also has that (2.1.11a), (2.1.11b), and (2.1.3c) are equivalent to (2.1.14a), (2.1.14c), and (2.1.14d) (s. App. B.2.4). Let $\frac{d}{dt}$ denote the *material derivative* , i.e.

$$\frac{d}{dt} := \frac{\partial}{\partial t} + \mathbf{v}_{\mathbf{gas}} \bullet \nabla\,. \tag{2.1.13}$$

The field equations read

$$\rho_{\mathbf{gas}} \frac{d\,\mathbf{v}_{\mathbf{gas}}}{dt} = \operatorname{div} \mathbf{T}_{\mathbf{gas}} + \rho_{\mathbf{gas}} \mathbf{b}_{\mathbf{gas}}, \tag{2.1.14a}$$

$$\bigwedge_{\iota\in\{1,\dots,A\}} \begin{pmatrix} c^{(\alpha_\iota)} \dfrac{d\,\mathbf{u}^{(\alpha_\iota)}}{dt} + \left(\nabla\,\mathbf{u}^{(\alpha_\iota)} + \nabla\,\mathbf{v}_{\mathbf{gas}}\right) \bullet \left(c^{(\alpha_\iota)}\,\mathbf{u}^{(\alpha_\iota)}\right) \\ = \dfrac{1}{\rho_{\mathbf{gas}}} \left(\operatorname{div} \mathbf{T}^{(\alpha_\iota)} - c^{(\alpha_\iota)} \operatorname{div} \mathbf{T}_{\mathbf{gas}}\right) \\ + \dfrac{1}{\rho_{\mathbf{gas}}} \left(\mathbf{p}^{*(\alpha_\iota)} - \rho^{*(\alpha_\iota)} \mathbf{v}^{(\alpha_\iota)}\right) + c^{(\alpha_\iota)} \left(\mathbf{b}^{(\alpha_\iota)} - \mathbf{b}_{\mathbf{gas}}\right) \end{pmatrix}, \tag{2.1.14b}$$

$$\frac{d\,\varepsilon_{\mathbf{gas}}}{dt} + \frac{1}{\rho_{\mathbf{gas}}} \operatorname{div} \mathbf{q}_{\mathbf{gas}} = \frac{1}{\rho_{\mathbf{gas}}}\, \mathbf{T}_{\mathbf{gas}} \bullet \left(\nabla\,\mathbf{v}_{\mathbf{gas}}\right) + r_{\mathbf{gas}}, \tag{2.1.14c}$$

$$\frac{d\,\rho_{\mathbf{gas}}}{dt} + \rho_{\mathbf{gas}} \operatorname{div} \mathbf{v}_{\mathbf{gas}} = 0, \tag{2.1.14d}$$

$$\bigwedge_{\iota\in\{1,\dots,A\}} \frac{d\,c^{(\alpha_\iota)}}{dt} + \frac{1}{\rho_{\mathbf{gas}}} \operatorname{div}\left(\rho_{\mathbf{gas}} c^{(\alpha_\iota)} \mathbf{u}^{(\alpha_\iota)}\right) = \frac{1}{\rho_{\mathbf{gas}}}\, \rho^{*(\alpha_\iota)}. \tag{2.1.14e}$$

2.1.2 Simplifications

Fick's Law

One of the standard simplifications in the theory of gas mixtures is to replace (2.1.14b) by

$$\bigwedge_{\iota\in\{1,\dots,A\}} \nabla\,p^{(\alpha_\iota)} - c^{(\alpha_\iota)}\,\nabla\,p_{\mathbf{gas}} = -D^{(\alpha_\iota)} \mathbf{u}^{(\alpha_\iota)}, \tag{2.1.15}$$

[1]To ensure $0 \le \rho^{(\alpha_\iota)} \le \rho_{\mathbf{gas}}$ for each ι, one needs the additional assumption $c^{(\alpha_\iota)} \ge 0$ for each ι.

where the $D^{(\alpha_\iota)}$ denote diffusion coefficients, the $p^{(\alpha_\iota)}$ denote the partial pressures, and p_{gas} is the total pressure:

$$p_{\mathrm{gas}} = \sum_{\iota=1}^{A} p^{(\alpha_\iota)}. \tag{2.1.16}$$

Equation (2.1.15) is known as *Fick's Law.*

In the setting of SiC growth by the PVT method, Fick's Law can be justified by the following reasoning, divided into points (i) – (v).

(i) The viscosity of the gas constituents is sufficiently small to neglect its contributions to the partial stress tensors. So the stress tensors are presumed to be given by

$$\bigwedge_{\iota\in\{1,\dots,A\}} \mathbf{T}^{(\alpha_\iota)} = -p^{(\alpha_\iota)}\mathbf{1}, \tag{2.1.17}$$

where $\mathbf{1}$ denotes the unit matrix. In consequence, using (B.1.6), one has

$$\bigwedge_{\iota\in\{1,\dots,A\}} \operatorname{div}\mathbf{T}^{(\alpha_\iota)} = -\nabla p^{(\alpha_\iota)}. \tag{2.1.18}$$

(ii) For each $\iota \in \{1,\dots,A\}$ the term $\rho^{(\alpha_\iota)}\mathbf{u}^{(\alpha_\iota)} \otimes \mathbf{u}^{(\alpha_\iota)}$ is neglected in the total stress tensor $\mathbf{T}_{\mathrm{gas}}$, since the components of $\rho^{(\alpha_\iota)}\mathbf{u}^{(\alpha_\iota)} \otimes \mathbf{u}^{(\alpha_\iota)}$ are orders of magnitude smaller than $p^{(\alpha_\iota)}$ (see App. A.2.2). Together with (2.1.6a), (2.1.16), and (2.1.17), this leads to

$$\mathbf{T}_{\mathrm{gas}} = -p_{\mathrm{gas}}\mathbf{1}, \tag{2.1.19}$$

and then (B.1.6) yields

$$\operatorname{div}\mathbf{T}_{\mathrm{gas}} = -\nabla p_{\mathrm{gas}}. \tag{2.1.20}$$

Remark 2.1.2. Even though (2.1.18) and (2.1.20) do follow logically from (2.1.17) and (2.1.19), respectively, in general $f \ll g$ does not imply the same relation for derivatives of f and g. Thus, (2.1.17) and (2.1.19) are only justified under the implicit assumption that changes of the neglected quantities are small if the quantities themselves are small.

(iii) It is assumed that there are diffusion coefficients $D^{(\alpha_\iota)}$ relating the mass and momentum exchange to the diffusion velocities via

$$\bigwedge_{\iota\in\{1,\dots,A\}} \mathbf{p}^{*(\alpha_\iota)} - \rho^{*(\alpha_\iota)}\mathbf{v}^{(\alpha_\iota)} = -D^{(\alpha_\iota)}\mathbf{u}^{(\alpha_\iota)}. \tag{2.1.21}$$

(iv) The diffusion processes change slowly in the sense that

$$\bigwedge_{\iota\in\{1,\dots,A\}} \frac{d\,\mathbf{u}^{(\alpha_\iota)}}{dt} \approx 0. \tag{2.1.22}$$

(v) Gravimetric acceleration $\mathbf{g}$ is the only force density acting on the gas species, i.e.

$$\bigwedge_{\iota\in\{1,\ldots,A\}} \mathbf{b}^{(\alpha_\iota)} = \mathbf{g}, \tag{2.1.23}$$

which implies

$$\mathbf{b}_{\mathbf{gas}} = \mathbf{g} \tag{2.1.24}$$

according to (2.1.6b) and (2.1.4a).

Using (2.1.22), (2.1.4c), (2.1.18), (2.1.20), (2.1.21), (2.1.23), and (2.1.24) in (2.1.14b) yields

$$\bigwedge_{\iota\in\{1,\ldots,A\}} \begin{pmatrix} \left(\nabla\, \mathbf{u}^{(\alpha_\iota)} + \nabla\, \mathbf{v}_{\mathbf{gas}}\right) \bullet \left(\rho^{(\alpha_\iota)}\, \mathbf{u}^{(\alpha_\iota)}\right) \\ = -\nabla\, p^{(\alpha_\iota)} + c^{(\alpha_\iota)}\, \nabla\, p_{\mathbf{gas}} - D^{(\alpha_\iota)} \mathbf{u}^{(\alpha_\iota)} \end{pmatrix}. \tag{2.1.25}$$

One now obtains Fick's Law by the usual linearization assumption of classical fluid dynamics, neglecting the left-hand side term in (2.1.25).

Neglecting Nonlinear Velocity Terms

As justified in App. A.2.2, $\frac{1}{2}\left(\mathbf{u}^{(\alpha_\iota)}\right)^2$ can be neglected in comparison with $\varepsilon^{(\alpha_\iota)}$, $\frac{1}{2}\left(\mathbf{v}_{\mathbf{gas}}\right)^2$ can be neglected in comparison with $\varepsilon_{\mathbf{gas}}$, and $\rho_{\mathbf{gas}}\mathbf{v}_{\mathbf{gas}} \otimes \mathbf{v}_{\mathbf{gas}}$ can be neglected in comparison with $\mathbf{T}_{\mathbf{gas}}$, i.e.

$$\bigwedge_{\iota\in\{1,\ldots,A\}} \varepsilon^{(\alpha_\iota)} + \frac{1}{2}\left(\mathbf{u}^{(\alpha_\iota)}\right)^2 \quad \text{is replaced by} \quad \varepsilon^{(\alpha_\iota)}, \tag{2.1.26a}$$

$$\varepsilon_{\mathbf{gas}} + \frac{1}{2}\left(\mathbf{v}_{\mathbf{gas}}\right)^2 \quad \text{is replaced by} \quad \varepsilon_{\mathbf{gas}}, \tag{2.1.26b}$$

$$\rho_{\mathbf{gas}}\mathbf{v}_{\mathbf{gas}} \otimes \mathbf{v}_{\mathbf{gas}} - \mathbf{T}_{\mathbf{gas}} \quad \text{is replaced by} \quad p_{\mathbf{gas}}\mathbf{1}. \tag{2.1.26c}$$

As the approximations (2.1.26) are also to be used under derivatives, notes analogous to Rem. 2.1.2 apply.

Consequences

Thanks to the above simplifications, (2.1.6) now become (2.1.27), and the field equations (2.1.14) can now be formulated in the form (2.1.28) (s. App. B.2.5 for details):

Simplified Quantities in the Gas Mixture:

$$\mathbf{T}_{\mathbf{gas}} = -p_{\mathbf{gas}}\mathbf{1}, \tag{2.1.27a}$$

$$\mathbf{b}_{\mathbf{gas}} = \mathbf{g}, \tag{2.1.27b}$$

$$\varepsilon_{\text{gas}} = \sum_{\iota=1}^{A} c^{(\alpha_\iota)} \varepsilon^{(\alpha_\iota)}, \tag{2.1.27c}$$

$$r_{\text{gas}} = \sum_{\iota=1}^{A} c^{(\alpha_\iota)} r^{(\alpha_\iota)}, \tag{2.1.27d}$$

$$\mathbf{q}_{\text{gas}} = \sum_{\iota=1}^{A} \Big(\mathbf{q}^{(\alpha_\iota)} - \left(\rho_{\text{gas}} c^{(\alpha_\iota)} \varepsilon^{(\alpha_\iota)} + p^{(\alpha_\iota)}\right) \cdot \left(D^{(\alpha_\iota)}\right)^{-1} \left(\nabla p^{(\alpha_\iota)} - c^{(\alpha_\iota)} \nabla p_{\text{gas}}\right)\Big). \tag{2.1.27e}$$

Simplified Field Equations:

- Simplified Total Mass Balance:

$$\frac{\partial \rho_{\text{gas}}}{\partial t} + \operatorname{div}\left(\rho_{\text{gas}} \mathbf{v}_{\text{gas}}\right) = 0. \tag{2.1.28a}$$

- Simplified Total Momentum Balance:

$$\frac{\partial\left(\rho_{\text{gas}} \mathbf{v}_{\text{gas}}\right)}{\partial t} + \operatorname{div}\left(p_{\text{gas}} \mathbf{1}\right) = \rho_{\text{gas}} \mathbf{g}. \tag{2.1.28b}$$

- Simplified Total Energy Balance:

$$\frac{\partial}{\partial t}\left(\rho_{\text{gas}} \varepsilon_{\text{gas}}\right) + \operatorname{div}\left(\rho_{\text{gas}} \varepsilon_{\text{gas}} \mathbf{v}_{\text{gas}} + \mathbf{q}_{\text{gas}} + p_{\text{gas}} \mathbf{v}_{\text{gas}}\right) = \rho_{\text{gas}} \mathbf{g} \bullet \mathbf{v}_{\text{gas}} + \rho_{\text{gas}} r_{\text{gas}}. \tag{2.1.28c}$$

- Reaction-Diffusion Equations:

$$\bigwedge_{\iota \in \{1,\dots,A\}} \frac{d\, c^{(\alpha_\iota)}}{dt} - \frac{1}{\rho_{\text{gas}}} \operatorname{div}\Big(\rho_{\text{gas}} c^{(\alpha_\iota)} \left(D^{(\alpha_\iota)}\right)^{-1} \left(\nabla p^{(\alpha_\iota)} - c^{(\alpha_\iota)} \nabla p_{\text{gas}}\right)\Big) = \frac{1}{\rho_{\text{gas}}} \rho^{*(\alpha_\iota)}. \tag{2.1.28d}$$

2.1.3 Material Laws

In the equivalent systems ((2.1.3) & (2.1.7)) and ((2.1.14) & (2.1.5)) as well as in the simplified system (2.1.28), the equations are further coupled by material laws.

The partial mass sources have the form (cf. [Mül85, p. 70 (3.66)])

$$\bigwedge_{\iota \in \{1,\dots,A\}} \rho^{*(\alpha_\iota)} = \sum_{a=1}^{n} \gamma_a^{(\alpha_\iota)} M^{(\alpha_\iota)} M^{(\mathrm{H})} \Lambda_a, \tag{2.1.29}$$

where $\gamma_a^{(\alpha_\iota)}$ are stoichiometric coefficients, $M^{(\alpha_\iota)}$ denotes the molecular mass (in particular, $M^{(\mathrm{H})}$ is the molecular mass of hydrogen), and Λ_a are rates of chemical reactions or phase transitions, respectively.

The heat flux is presumed to satisfy Fourier's Law:

$$\sum_{\iota=1}^{A} \mathbf{q}^{(\alpha_\iota)} = -\kappa_{\mathrm{gas}} \nabla T_{\mathrm{gas}}, \tag{2.1.30}$$

κ_{gas} denoting the thermal conductivity of the gas mixture.

If the gas mixture behaves according to the laws of an ideal gas, then the material laws read for each $\iota \in \{1, \ldots, A\}$:

$$p^{(\alpha_\iota)} = \rho_{\mathrm{gas}} c^{(\alpha_\iota)} \frac{R}{M^{(\alpha_\iota)}} T_{\mathrm{gas}}, \tag{2.1.31a}$$

$$\varepsilon^{(\alpha_\iota)} = z^{(\alpha_\iota)} \frac{R}{M^{(\alpha_\iota)}} T_{\mathrm{gas}}, \tag{2.1.31b}$$

where R is the universal gas constant, $z^{(\alpha_\iota)} = \frac{3}{2}$ for single-, $z^{(\alpha_\iota)} = \frac{5}{2}$ for double-, and $z^{(\alpha_\iota)} = 3$ for multi-atomic gas molecules.

Using the material laws, and (2.1.16) together with (2.1.27), one gets

$$p_{\mathrm{gas}} = R\,\rho_{\mathrm{gas}}\,T_{\mathrm{gas}} \sum_{\iota=1}^{A} \frac{c^{(\alpha_\iota)}}{M^{(\alpha_\iota)}}, \tag{2.1.32a}$$

$$\varepsilon_{\mathrm{gas}} = R\,T_{\mathrm{gas}} \sum_{\iota=1}^{A} z^{(\alpha_\iota)} \frac{c^{(\alpha_\iota)}}{M^{(\alpha_\iota)}}, \tag{2.1.32b}$$

$$\begin{aligned} \mathbf{q}_{\mathrm{gas}} &= -\kappa_{\mathrm{gas}} \nabla T_{\mathrm{gas}} \\ &\quad - R^2 \rho_{\mathrm{gas}} T_{\mathrm{gas}} \sum_{\iota=1}^{A} \frac{c^{(\alpha_\iota)} \left(z^{(\alpha_\iota)} + 1\right)}{\left(M^{(\alpha_\iota)}\right)^2} \cdot \left(D^{(\alpha_\iota)}\right)^{-1} \nabla \left(\rho_{\mathrm{gas}} c^{(\alpha_\iota)} T_{\mathrm{gas}}\right) \\ &\quad + R^2 \rho_{\mathrm{gas}} T_{\mathrm{gas}} \sum_{\iota,\iota'=1}^{A} \frac{\left(c^{(\alpha_\iota)}\right)^2 \left(z^{(\alpha_\iota)} + 1\right)}{M^{(\alpha_\iota)} M^{(\alpha_{\iota'})}} \cdot \left(D^{(\alpha_\iota)}\right)^{-1} \nabla \left(\rho_{\mathrm{gas}} T_{\mathrm{gas}} c^{(\alpha_{\iota'})}\right). \end{aligned} \tag{2.1.32c}$$

2.1.4 Simplifications Assuming the Gas Consists of One Constituent Only

Equations (2.1.28) and (2.1.32) simplify considerably if the gas mixture is reduced to a gas made up of merely a single constituent. The simplified forms are formulated in the present section.

As mentioned in Sec. 1.1, Ar, Si, Si_2C, and SiC_2 are the predominant gas species in the PVT growth system. For temperatures above 2500 K, species other than Ar make up a significant portion of the gas mixture. However, for lower temperatures only Ar is present, and for higher temperatures heat is mainly transported via radiation (cf. Sec. 2.4). So e.g. if one is mainly interested in the temperature distribution and its evolution, assuming a pure Ar gas phase can be a reasonable approximation.

If $\mathrm{Ar} = \alpha_1$ is the only gas constituent present, then $A = 1$, leading to

$$
\begin{aligned}
\rho_{\mathrm{gas}} &= \rho^{(\mathrm{Ar})} && \text{(from (2.1.4a))}, && (2.1.33a)\\
\mathbf{v}_{\mathrm{gas}} &= \mathbf{v}^{(\mathrm{Ar})} && \text{(from (2.1.4b))}, && (2.1.33b)\\
c^{(\mathrm{Ar})} &= 1 && \text{(from (2.1.4c))}, && (2.1.33c)\\
p^{(\mathrm{Ar})} &= \rho^{(\mathrm{Ar})} \frac{R}{M^{(\mathrm{Ar})}} T_{\mathrm{gas}} && \text{(from (2.1.31a))}, && (2.1.33d)\\
p_{\mathrm{gas}} &= p^{(\mathrm{Ar})} && \text{(from (2.1.32a))}, && (2.1.33e)\\
\varepsilon^{(\mathrm{Ar})} &= z^{(\mathrm{Ar})} \frac{R}{M^{(\mathrm{Ar})}} T_{\mathrm{gas}} && \text{(from (2.1.31b))}, && (2.1.33f)\\
\varepsilon_{\mathrm{gas}} &= \varepsilon^{(\mathrm{Ar})} && \text{(from (2.1.32b))}, && (2.1.33g)\\
\mathbf{q}_{\mathrm{gas}} &= -\kappa_{\mathrm{gas}} \nabla T_{\mathrm{gas}} = -\kappa^{(\mathrm{Ar})} \nabla T_{\mathrm{gas}} && \text{(from (2.1.32c))}, && (2.1.33h)\\
r_{\mathrm{gas}} &= r^{(\mathrm{Ar})} && \text{(from (2.1.27d))}. && (2.1.33i)
\end{aligned}
$$

Now (2.1.33) is substituted into (2.1.28) (in spite of (2.1.33a) and (2.1.33b) the notation ρ_{gas} and $\mathbf{v}_{\mathrm{gas}}$ is kept to underscore ρ_{gas} and $\mathbf{v}_{\mathrm{gas}}$ being unknown functions to be determined as solutions to the system (2.1.34)), resulting in

$$\frac{\partial \rho_{\mathrm{gas}}}{\partial t} + \operatorname{div}\left(\rho_{\mathrm{gas}} \mathbf{v}_{\mathrm{gas}}\right) = 0, \tag{2.1.34a}$$

$$\frac{\partial\left(\rho_{\mathrm{gas}} \mathbf{v}_{\mathrm{gas}}\right)}{\partial t} + \frac{R}{M^{(\mathrm{Ar})}} \nabla\left(\rho_{\mathrm{gas}} T_{\mathrm{gas}}\right) = \rho_{\mathrm{gas}} \mathbf{g}, \tag{2.1.34b}$$

$$
\begin{aligned}
\frac{z^{(\mathrm{Ar})} R}{M^{(\mathrm{Ar})}} \frac{\partial}{\partial t}\left(\rho_{\mathrm{gas}} T_{\mathrm{gas}}\right) + \operatorname{div}\left(\frac{\left(z^{(\mathrm{Ar})}+1\right) R}{M^{(\mathrm{Ar})}} \rho_{\mathrm{gas}} T_{\mathrm{gas}} \mathbf{v}_{\mathrm{gas}} - \kappa^{(\mathrm{Ar})} \nabla T_{\mathrm{gas}}\right)& \\
= \rho_{\mathrm{gas}} \mathbf{g} \bullet \mathbf{v}_{\mathrm{gas}} + \rho_{\mathrm{gas}} r^{(\mathrm{Ar})}.& \qquad (2.1.34c)
\end{aligned}
$$

The reaction-diffusion equations (2.1.28d) no longer occur in (2.1.34) owing to (2.1.33c) and (2.1.33e).

2.2 Heat Conduction in Solid Materials

The PVT growth system comprises several solid material components. Quantities in the solid material β_j, $j \in \{1, \dots, N\}$, will carry the superscript $[\beta_j]$. For the setups depicted in Fig. 1.2 on p. 3 and Fig. 1.3 on p. 4, the solid materials are given by the SiC source powder, the SiC seed crystal, the graphite crucible, and the graphite felt insulation.

These materials will be referred to using the superscripts [SiC-Powder], [SiC-Crystal], [Crucible], and [Insulation], respectively. Additional and/or different materials occur in many real growth systems.

Heat conduction in the copper induction coil is not considered, as in real growth systems the coil is cooled very effectively, e.g. by water flowing inside the coil rings. Thereby the coil is kept virtually at room temperature.

The mechanisms of heat transport inside solid materials considered in this work are heat conduction according to (2.2.1a) and radiative heat transfer through semi-transparent materials as treated in Sec. 2.4.4. It is also noted that radiative heat transfer due to radiation which is both emitted and absorbed inside the same material β_j is included in the current model via using an appropriate temperature-depending law for the thermal conductivity of the material β_j.

However, the current model neglects any mechanical or chemical interactions inside the solid materials. In particular, it does not account for certain effects observed in real growth systems such as porosity changes, sintering and graphitization of the source powder, and accumulation of Si in the graphite felt insulation.

Heat conduction in the solid material β_j, $j \in \{1, \dots, N\}$, obeys

$$\rho^{[\beta_j]} c_{\mathrm{sp}}^{[\beta_j]} \frac{\partial T^{[\beta_j]}}{\partial t} + \operatorname{div} \mathbf{q}^{[\beta_j]} = f^{[\beta_j]}, \tag{2.2.1a}$$

$$\mathbf{q}^{[\beta_j]} = -\kappa^{[\beta_j]} \nabla T^{[\beta_j]}, \tag{2.2.1b}$$

where

t – time,	$T^{[\beta_j]}$ – absolute temperature,
$\rho^{[\beta_j]}$ – mass density,	$c_{\mathrm{sp}}^{[\beta_j]}$ – specific heat,
$\mathbf{q}^{[\beta_j]}$ – heat flux,	$\kappa^{[\beta_j]}$ – thermal conductivity,
$f^{[\beta_j]}$ – power density (per volume).	

The power density $f^{[\beta_j]}$ is caused in conducting materials β_j due to induction heating. It is determined according to the sinusoidal RF-heating model in Sec. 2.5.

2.3 Interface, Boundary, and Initial Conditions

To complete the heat transport model inside the entire growth apparatus, the heat equation of the gas phase (2.1.34c) (assuming only one constituent) and the different heat equations (2.2.1) for the solid materials β_j, $j \in \{1, \dots, N\}$, need to be coupled by appropriate interface conditions, and suitable outer boundary conditions have to be set.

The interface conditions are provided in terms of the heat flux by (2.3.1) and in terms of the absolute temperature by (2.3.2), where it is presumed that the respective locations of all solid components of the growth apparatus do not change with time.

Let $\{\beta, \beta'\} \subseteq \{\beta_1, \ldots, \beta_N\}$. The normal heat flux is assumed to be continuous on an interface $\gamma_{\beta,\beta'}$ between two solid materials β and β', i.e. the interface condition is given by (2.3.1a). If the solid material β is semi-transparent, or on an interface $\gamma_{\beta',\mathbf{gas}}$ between the solid material β' and the gas phase, one needs to account for radiosity R and for irradiation J, resulting in interface conditions (2.3.1b) and (2.3.1c), respectively. The modeling of R and J is the subject of Sec. 2.4.

$$
\begin{aligned}
\mathbf{q}^{[\beta]} \bullet \mathbf{n}^{[\beta]} & & = \quad & \mathbf{q}^{[\beta']} \bullet \mathbf{n}^{[\beta]} & \text{on } \gamma_{\beta,\beta'}, & \qquad (2.3.1a)\\
\mathbf{q}^{[\beta]} \bullet \mathbf{n}^{[\beta]} & -R+J & = \quad & \mathbf{q}^{[\beta']} \bullet \mathbf{n}^{[\beta]} & \text{on } \gamma_{\beta,\beta'}, & \qquad (2.3.1b)\\
\mathbf{q}_{\mathbf{gas}} \bullet \mathbf{n}_{\mathbf{gas}} & -R+J & = \quad & \mathbf{q}^{[\beta]} \bullet \mathbf{n}_{\mathbf{gas}} & \text{on } \gamma_{\beta,\mathbf{gas}}, & \qquad (2.3.1c)
\end{aligned}
$$

where $\mathbf{n}^{[\beta]}$ is the outer unit normal vector to the solid material β, and $\mathbf{n}_{\mathbf{gas}}$ is the outer unit normal vector to the gas phase.

The temperature is always assumed to be continuous between solid materials, i.e. on an interface $\gamma_{\beta,\beta'}$ between two solid materials β and β' one has (2.3.2a). Even though in reality the temperature is also continuous across an interface $\gamma_{\beta,\mathbf{gas}}$ between a solid material β and the gas phase as stated in (2.3.2b), the temperature gradient can be extremely steep inside an interface layer. If the size of the interface layer is much less than typical lengths of the system to be modeled, then it is reasonable to assume a temperature jump on the interface. In this case, if the heat flux in the gas phase satisfies (2.1.33h), then the temperature discontinuity depends linearly on the normal heat flux through the interface, with a positive factor of proportionality ξ_β. Thus, (2.3.2b) is then replaced by (2.3.2b$'$). It is noted that in heat transport problems where a solid surface is sourrounded by a gas of known temperature, (2.3.2b$'$) often arises in the form of an outer boundary condition of third kind, written in terms of the normal heat flux of the solid. Here, however, it is more natural to use $\kappa_{\mathbf{gas}} \nabla T_{\mathbf{gas}}$, as otherwise the radiation terms R and J occurred explicitly in (2.3.2b$'$) according to (2.3.1c).

$$
\begin{aligned}
T^{[\beta]} &= T^{[\beta']} & \text{on } \gamma_{\beta,\beta'}, & \qquad (2.3.2a)\\
T^{[\beta]} &= T_{\mathbf{gas}} & \text{on } \gamma_{\beta,\mathbf{gas}}, & \qquad (2.3.2b)\\
-(\kappa_{\mathbf{gas}} \nabla T_{\mathbf{gas}}) \bullet \mathbf{n}_{\mathbf{gas}} &= \xi_\beta \left(T_{\mathbf{gas}} - T^{[\beta]}\right) & \text{on } \gamma_{\beta,\mathbf{gas}}. & \qquad (2.3.2b')
\end{aligned}
$$

The Stefan-Boltzmann law together with (2.2.1b) provides the outer boundary condition

$$
-\left(\kappa^{[\beta]} \nabla T^{[\beta]}\right) \bullet \mathbf{n}^{[\beta]} = \sigma \epsilon^{[\beta]} \left[T^{[\beta]}\right] \left(\left(T^{[\beta]}\right)^4 - T_{\mathrm{room}}^4 \right). \qquad (2.3.3)
$$

Here $\sigma = 5.6696 \cdot 10^{-8} \frac{\mathrm{W}}{\mathrm{m^2 K^4}}$ denotes the Boltzmann radiation constant, and $\epsilon^{[\beta]}$ denotes the (temperature-dependent) emissivity of the surface. Condition (2.3.3) means that the growth apparatus is exposed to a black body environment (e.g. a large isothermal room) radiating at room temperature $T_{\text{room}} = 293$ K.

On outer boundaries receiving radiation from other parts of the apparatus, the situation is more complicated. On such boundaries, it does not suffice to use just the Stefan-Boltzmann law according to (2.3.3), but, as in (2.3.1b) and (2.3.1c), one has to account for radiosity R and irradiation J, leading to the boundary condition

$$\mathbf{q}^{[\beta]} \bullet \mathbf{n}^{[\beta]} - R + J = 0, \tag{2.3.4}$$

where, as before, the modeling of R and J is deferred to Sec. 2.4.

Condition (2.3.4) is used on outer boundaries representing surfaces adjacent to the upper and lower blind hole in Fig. 4.1 on p. 195. To allow for radiative interactions between such open cavities and the ambient environment, including reflections at the cavity's surfaces, black body phantom closures are used, emitting radiation at T_{room}. In Fig. 4.1, the phantom closures are the dashed lines labeled Γ_{top} and Γ_{bottom}.

Finally, in the case of transient simulations, one needs to prescribe a temperature distribution at the initial time. For the simulations presented in Sec. 4, it is assumed that the initial temperature distribution is homogeneous at T_{room}.

2.4 Model of Diffuse-Gray Radiation Including Semi-Transparency

2.4.1 Model Assumptions

The model does not consider any interaction between gas and radiation. In particular, radiation is assumed to travel unperturbed between surfaces of solid components throughout cavities inside the growth apparatus. All solids except the SiC single crystal are treated as opaque media (Sec. 2.4.2). For the SiC single crystal, semi-transparency is included via the band approximation model (Sec. 2.4.4).

Reflection and emittance are supposed to be diffuse-gray , i.e. independent of the angle of incidence and independent of the wavelength. Since the solid surfaces inside the growth apparatus (including the surface of the SiC single crystal) are generally non-smooth, the effect of specular reflections is expected to be negligible.

The heat flux due to radiosity R and the heat flux due to irradiation J have to be included in the interface conditions between a solid and a semi-transparent material and between a solid material and the gas phase, resulting in the interface conditions (2.3.1b) and (2.3.1c). Similarly, the heat fluxes due to R and J have to be taken into account on outer boundaries being in mutual radiative interaction, resulting in the outer boundary condition (2.3.4).

The model employs the net radiation method as described in [Jär96, Chapter 3.3] and, with a different notation, in [DNR+90]. More general treatments of this standard model can be found in textbooks such as [SC78] and [Mod93].

2.4.2 Opaque Case

In the present section, it is assumed that all solid materials adjacent to the cavity under consideration are opaque, i.e. no radiation is transmitted through a solid's suface.

Let Γ consist of the union of all surfaces of solid materials adjacent to the considered cavity. Let Γ_{sin} denote the singular part of Γ, consisting of the set of all points of Γ where Γ has a corner (i.e. where Γ has no unique normal vector), united with the set of all points of Γ belonging to interfaces between different solids. The set $\Gamma_{\text{reg}} := \Gamma \setminus \Gamma_{\text{sin}}$ is called the regular part of Γ.

On Γ_{sin} the emissivity or the normal vector might be discontinuous. To avoid problems arising in such situations, the following considerations are carried out on Γ_{reg}. This is legitimate, since in applications, the functions defined below will always occur under integrals with respect to which Γ_{sin} constitutes a null set, thus giving no contribution.

At each point $\mathbf{x} \in \Gamma_{\text{reg}}$, the radiosity R is the sum of the contribution from emitted radiation E and of the contribution from reflected radiation J_{ref}:

$$\bigwedge_{\mathbf{x}\in\Gamma_{\text{reg}}} R[\mathbf{x}] = E[\mathbf{x}] + J_{\text{ref}}[\mathbf{x}]. \tag{2.4.1}$$

It is convenient to write the material dependence of the emissivity as a dependence on the space variable $\mathbf{x}$:

$$\bigwedge_{\mathbf{x}\in\Gamma_{\text{reg}}} \begin{pmatrix} \epsilon\big[(T_{\text{solid}}[\mathbf{x}], \mathbf{x})\big] := \epsilon^{[\beta]}\big[T_{\text{solid}}[\mathbf{x}]\big] \\ \text{for each } \mathbf{x} \text{ in the domain of the solid } \beta \end{pmatrix}, \tag{2.4.2}$$

where T_{solid} denotes the absolute temperature in the respective solid material adjacent to the considered cavity. While due to the possible temperature jump between solid and gas (cf. (2.3.2b$'$)), one needs to distinguish between the corresponding temperatures, such a distinction is not necessary between the temperatures in different solids, as continuity is assumed on solid-solid interfaces.

According to the Stefan-Boltzmann law, the emitted radiation is given by

$$\bigwedge_{\mathbf{x}\in\Gamma_{\text{reg}}} E[\mathbf{x}] = \sigma\epsilon\big[(T_{\text{solid}}[\mathbf{x}], \mathbf{x})\big]\,(T_{\text{solid}}[\mathbf{x}])^4. \tag{2.4.3}$$

The reflective term in (2.4.1) can be expressed using the reflectivity ϱ, i.e. the ratio of reflected radiation and irradiation J:

$$\bigwedge_{\mathbf{x}\in\Gamma_{\text{reg}}} J_{\text{ref}}[\mathbf{x}] = \varrho\big[(T_{\text{solid}}[\mathbf{x}], \mathbf{x})\big] \cdot J. \tag{2.4.4}$$

If α denotes the absorptivity, i.e. the ratio of absorbed radiation and irradiation, then opaqueness implies

$$\alpha + \varrho = 1, \tag{2.4.5}$$

and by Kirchhoff's law

$$\alpha = \epsilon. \tag{2.4.6}$$

Due to diffuseness, J can be calculated using the integral operator $\mathcal{J}$ defined by

$$\bigwedge_{\mathbf{x}\in\Gamma_{\text{reg}}} \quad J[\mathbf{x}] = \mathcal{J}[R][\mathbf{x}] := \int_\Gamma \Lambda[(\mathbf{x},\mathbf{y})]\,\omega[(\mathbf{x},\mathbf{y})]\,R[\mathbf{y}]\,\mathrm{d}\mathbf{y}\,, \tag{2.4.7}$$

where Λ is the visibility factor defined by

$$\bigwedge_{(\mathbf{x},\mathbf{y})\in(\Gamma_{\text{reg}})^2} \quad \Lambda[(\mathbf{x},\mathbf{y})] := \begin{cases} 1 & \text{iff } \mathbf{x},\, \mathbf{y} \text{ are mutually visible,} \\ 0 & \text{iff } \mathbf{x},\, \mathbf{y} \text{ are mutually invisible,} \end{cases} \tag{2.4.8}$$

and where ω is the view factor defined by

$$\bigwedge_{\substack{(\mathbf{x},\mathbf{y})\in(\Gamma_{\text{reg}})^2:\\ \mathbf{x}\neq\mathbf{y}}} \quad \omega[(\mathbf{x},\mathbf{y})] := \frac{\big(\mathbf{n}_{\text{gas}}[\mathbf{y}] \bullet (\mathbf{x}-\mathbf{y})\big)\,\big(\mathbf{n}_{\text{gas}}[\mathbf{x}] \bullet (\mathbf{y}-\mathbf{x})\big)}{\pi\big((\mathbf{y}-\mathbf{x}) \bullet (\mathbf{y}-\mathbf{x})\big)^2}, \tag{2.4.9}$$

$\mathbf{n}_{\text{gas}}$ denoting the unit normal vector on Γ_{reg} pointing from gas to solid.

For later use, it is noted that for a closed surface Γ:

$$\bigwedge_{\mathbf{x}\in\Gamma_{\text{reg}}} \quad \int_\Gamma \Lambda[(\mathbf{x},\mathbf{y})]\,\omega[(\mathbf{x},\mathbf{y})]\,\mathrm{d}\mathbf{y} \,= 1. \tag{2.4.10}$$

See [Tii97, Lem. 1] for a proof of (2.4.10). The physical meaning of (2.4.10) is the conservation of radiation energy: Radiation emitted from a point $\mathbf{x}$ on the boundary Γ of a cavity enclosed by Γ must be absorbed somewhere on Γ (as it is assumed that no radiation is absorbed in the interior of the cavity).

Combining Eqs (2.4.1) through (2.4.7) provides the following non-local equation for the radiosity R:

$$\bigwedge_{\mathbf{x}\in\Gamma_{\text{reg}}} \quad R[\mathbf{x}] - \big(1 - \epsilon\big[(T_{\text{solid}}[\mathbf{x}],\mathbf{x})\big]\big)\mathcal{J}[R][\mathbf{x}] = \sigma\epsilon\big[(T_{\text{solid}}[\mathbf{x}],\mathbf{x})\big]\,\big(T_{\text{solid}}[\mathbf{x}]\big)^4. \tag{2.4.11}$$

It is often useful to have (2.4.11) written in operator form

$$\mathcal{G}[T_{\text{solid}}][R] = \mathcal{E}[T_{\text{solid}}], \tag{2.4.12}$$

where the operators $\mathcal{G}$ and $\mathcal{E}$ are defined by

$$\bigwedge_{T,R} \bigwedge_{\mathbf{x}\in\Gamma_{\text{reg}}} \big(\mathcal{G}[T][R]\big)[\mathbf{x}] := R[\mathbf{x}] - \big(1 - \epsilon\big[(T[\mathbf{x}], \mathbf{x})\big]\big)\mathcal{J}[R][\mathbf{x}], \tag{2.4.13a}$$

$$\bigwedge_{T} \bigwedge_{\mathbf{x}\in\Gamma_{\text{reg}}} \mathcal{E}[T][\mathbf{x}] := \sigma\epsilon\big[(T[\mathbf{x}], \mathbf{x})\big]\,(T[\mathbf{x}])^4. \tag{2.4.13b}$$

If $\epsilon[(T[\mathbf{x}], \mathbf{x})] > 0$ for each $\mathbf{x} \in \Gamma$, then $\mathcal{G}[T]$ is invertible for each T (see [LT00, Lem. 2]), such that one can let

$$\bigwedge_{T} \mathcal{R}[T] := \big(\mathcal{G}[T]\big)^{-1}\big[\mathcal{E}[T]\big], \tag{2.4.13c}$$

and (2.4.12) can be stated as

$$R = \mathcal{R}[T_{\text{solid}}]. \tag{2.4.14}$$

Finally, as it is needed in the interface conditions (2.3.1b) and (2.3.1c), and in the outer boundary condition (2.3.4), the expression $-R + J$ is computed from (2.4.11) and (2.4.7):

$$\bigwedge_{\mathbf{x}\in\Gamma_{\text{reg}}} -R[\mathbf{x}] + J[\mathbf{x}] = \epsilon\big[(T_{\text{solid}}[\mathbf{x}], \mathbf{x})\big]\cdot\big(\mathcal{J}[R][\mathbf{x}] - \sigma\,(T_{\text{solid}}[\mathbf{x}])^4\big). \tag{2.4.15}$$

While the new formulation of (2.3.1b) and (2.3.1c) will be given in Sec. 2.4.4 (see (2.4.38) and (2.4.39), respectively), the open cavities of the setup in Fig. 4.1 on p. 195 do not involve semi-transparent materials, allowing to rewrite the outer boundary condition (2.3.4) as

$$\mathbf{q}^{[\beta]} \bullet \mathbf{n}^{[\beta]} + \epsilon\cdot\big(\mathcal{J}[R] - \sigma T_{\text{solid}}^4\big) = 0 \tag{2.4.16}$$

on each outer boundary of solid material β adjacent to an open radiation region. Using the operator $\mathcal{R}$, (2.4.16) reads

$$\mathbf{q}^{[\beta]} \bullet \mathbf{n}^{[\beta]} + \epsilon\cdot\big(\mathcal{J}\big[\mathcal{R}[T_{\text{solid}}]\big] - \sigma T_{\text{solid}}^4\big) = 0. \tag{2.4.17}$$

2.4.3 Axisymmetric Model

Assuming cylindrical symmetry of the growth apparatus and of the relevant physical quantities, the model of the previous section can be reduced from three to two dimensions. The axisymmetric model is later used for the discretization in Sec. 3.7.8 and the numerical simulations discussed in Ch. 4.

In the following, (r, ϑ, z) denote cylindrical coordinates (cf. App. B.3).

As in the previous section, let Γ denote the radiating surface of the cavity under consideration, and let Γ_{reg} be its regular part. The visibility factor Λ and the view factor

ω were defined in (2.4.8) and (2.4.9), respectively. In an axisymmetric situation, Λ and ω are invariant with respect to rotations around the symmetry axis (s. (2.4.18)) as well as with respect to reflections through planes with $\vartheta =$ const. (s. (2.4.19)):

$$\bigwedge_{\substack{\left((r,\vartheta,z),(\tilde r,\tilde\vartheta,\tilde z),\vartheta'\right)\\ \in(\Gamma_{\text{reg}})^2\times[0,2\pi]}} \begin{pmatrix} \Lambda\left[\left((r,\vartheta,z),(\tilde r,\tilde\vartheta,\tilde z)\right)\right] \\ = \Lambda\left[\left((r,(\vartheta+\vartheta')\bmod 2\pi,z),(\tilde r,(\tilde\vartheta+\vartheta')\bmod 2\pi,\tilde z)\right)\right] \end{pmatrix}, \tag{2.4.18a}$$

$$\bigwedge_{\substack{\left((r,\vartheta,z),(\tilde r,\tilde\vartheta,\tilde z),\vartheta'\right)\\ \in(\Gamma_{\text{reg}})^2\times[0,2\pi]}} \begin{pmatrix} \omega\left[\left((r,\vartheta,z),(\tilde r,\tilde\vartheta,\tilde z)\right)\right] \\ = \omega\left[\left((r,(\vartheta+\vartheta')\bmod 2\pi,z),(\tilde r,(\tilde\vartheta+\vartheta')\bmod 2\pi,\tilde z)\right)\right] \end{pmatrix}, \tag{2.4.18b}$$

$$\bigwedge_{\substack{\left((r,\vartheta,z),(\tilde r,\vartheta',\tilde z)\right)\\ \in(\Gamma_{\text{reg}})^2}} \begin{pmatrix} \Lambda\left[\left((r,\vartheta,z),(\tilde r,(\vartheta+\vartheta')\bmod 2\pi,\tilde z)\right)\right] \\ = \Lambda\left[\left((r,\vartheta,z),(\tilde r,(\vartheta-\vartheta')\bmod 2\pi,\tilde z)\right)\right] \end{pmatrix}, \tag{2.4.19a}$$

$$\bigwedge_{\substack{\left((r,\vartheta,z),(\tilde r,\vartheta',\tilde z)\right)\\ \in(\Gamma_{\text{reg}})^2}} \begin{pmatrix} \omega\left[\left((r,\vartheta,z),(\tilde r,(\vartheta+\vartheta')\bmod 2\pi,\tilde z)\right)\right] \\ = \omega\left[\left((r,\vartheta,z),(\tilde r,(\vartheta-\vartheta')\bmod 2\pi,\tilde z)\right)\right] \end{pmatrix}. \tag{2.4.19b}$$

The following notation is introduced: The *circular projection* π_{circ} discards the angular coordinate ϑ. It can be viewed as a rotation into the $\vartheta = 0$ plane. More precisely,

$$\pi_{\text{circ}} : \mathbb{R}_0^+ \times [0,2\pi] \times \mathbb{R} \longrightarrow \mathbb{R}_0^+ \times \mathbb{R}, \quad \pi_{\text{circ}}[(r,\vartheta,z)] := (r,z). \tag{2.4.20}$$

Furthermore, for a function f defined on an axisymmetric set $A \subseteq \mathbb{R}_0^+ \times [0,2\pi] \times \mathbb{R}$, $f : A \longrightarrow \mathbb{R}$, let $f_{\text{circ}} := f\restriction_{\pi_{\text{circ}}A}$.

Using (2.4.18) and (2.4.19), one can write (2.4.11) in axisymmetric form:

$$\bigwedge_{\substack{(r,z)\\ \in\pi_{\text{circ}}\Gamma_{\text{reg}}}} \begin{pmatrix} R_{\text{circ}}[(r,z)] - \left(1-\epsilon_{\text{circ}}\left[\left(T_{\text{solid,circ}}[(r,z)],(r,z)\right)\right]\right)\mathcal{J}_{\text{circ}}[R_{\text{circ}}][(r,z)] \\ = \sigma\epsilon_{\text{circ}}\left[\left(T_{\text{solid,circ}}[(r,z)],(r,z)\right)\right]\left(T_{\text{solid,circ}}[(r,z)]\right)^4 \end{pmatrix}, \tag{2.4.21}$$

where

$$\bigwedge_{(r,z)\in\pi_{\text{circ}}\Gamma_{\text{reg}}} \mathcal{J}_{\text{circ}}[R_{\text{circ}}][(r,z)] := \int_{\pi_{\text{circ}}\Gamma_{\text{reg}}} \Lambda_{\text{circ}}\left[\left((r,z),(\tilde r,\tilde z)\right)\right] R_{\text{circ}}[(\tilde r,\tilde z)]\,\tilde r \,\mathrm{d}(\tilde r,\tilde z), \tag{2.4.22}$$

$$\bigwedge_{((r,z),(\tilde{r},\tilde{z}))\in(\pi_{\mathrm{circ}}\Gamma_{\mathrm{reg}})^2} \begin{pmatrix} \Lambda_{\mathrm{circ}}\big[\big((r,z),(\tilde{r},\tilde{z})\big)\big] \\ := 2\displaystyle\int_0^{\pi} \Lambda\big[\big((r,0,z),(\tilde{r},\vartheta,\tilde{z})\big)\big]\ \omega\big[\big((r,0,z),(\tilde{r},\vartheta,\tilde{z})\big)\big]\ \mathrm{d}\vartheta \end{pmatrix}. \quad (2.4.23)$$

One can combine (2.4.10), (2.4.18), (2.4.19), and (2.4.23) to express the conservation of radiation energy in the axisymmetric case: If Γ denotes a cylindrically symmetric closed surface, then

$$\bigwedge_{(r,z)\in\pi_{\mathrm{circ}}\Gamma_{\mathrm{reg}}} \int_{\pi_{\mathrm{circ}}\Gamma_{\mathrm{reg}}} \Lambda_{\mathrm{circ}}\big[\big((r,z),(\tilde{r},\tilde{z})\big)\big]\ \tilde{r}\ \mathrm{d}(\tilde{r},\tilde{z}) = 1. \quad (2.4.24)$$

Proceeding analogously as after (2.4.11), one can write (2.4.21) in operator form

$$\mathcal{G}_{\mathrm{circ}}[T_{\mathrm{solid,circ}}][R_{\mathrm{circ}}] = \mathcal{E}_{\mathrm{circ}}[T_{\mathrm{solid,circ}}], \quad (2.4.25)$$

where

$$\bigwedge_{T,R}\ \bigwedge_{\mathbf{x}\in\pi_{\mathrm{circ}}\Gamma_{\mathrm{reg}}} \big(\mathcal{G}_{\mathrm{circ}}[T][R]\big)[\mathbf{x}] := R[\mathbf{x}] - \big(1-\epsilon_{\mathrm{circ}}\big[(T[\mathbf{x}],\mathbf{x})\big]\big)\mathcal{J}_{\mathrm{circ}}[R][\mathbf{x}], \quad (2.4.26a)$$

$$\bigwedge_{T}\ \bigwedge_{\mathbf{x}\in\pi_{\mathrm{circ}}\Gamma_{\mathrm{reg}}} \mathcal{E}_{\mathrm{circ}}[T][\mathbf{x}] := \sigma\epsilon_{\mathrm{circ}}\big[(T[\mathbf{x}],\mathbf{x})\big](T[\mathbf{x}])^4. \quad (2.4.26b)$$

If $\epsilon_{\mathrm{circ}}[(T[\mathbf{x}],\mathbf{x})] > 0$ for each $\mathbf{x}\in\pi_{\mathrm{circ}}\Gamma$, then $\mathcal{G}_{\mathrm{circ}}[T]$ is invertible for each T, such that one can let

$$\bigwedge_{T} \mathcal{R}_{\mathrm{circ}}[T] := \big(\mathcal{G}_{\mathrm{circ}}[T]\big)^{-1}\big[\mathcal{E}_{\mathrm{circ}}[T]\big], \quad (2.4.26c)$$

and (2.4.21) can be stated as

$$R_{\mathrm{circ}} = \mathcal{R}_{\mathrm{circ}}[T_{\mathrm{solid,circ}}]. \quad (2.4.27)$$

The axisymmetric version of (2.4.15) reads

$$\bigwedge_{\mathbf{x}\in\pi_{\mathrm{circ}}\Gamma_{\mathrm{reg}}} \begin{pmatrix} -R_{\mathrm{circ}}[\mathbf{x}] + J_{\mathrm{circ}}[\mathbf{x}] \\ = \epsilon_{\mathrm{circ}}\big[(T_{\mathrm{solid,circ}}[\mathbf{x}],\mathbf{x})\big]\cdot\big(\mathcal{J}_{\mathrm{circ}}[R_{\mathrm{circ}}][\mathbf{x}] - \sigma\,(T_{\mathrm{solid,circ}}[\mathbf{x}])^4\big) \end{pmatrix}. \quad (2.4.28)$$

2.4.4 Semi-Transparent Case

This section contains a description of the band approximation model to account for the semi-transparency of the SiC single crystal.

According to the band approximation model, the spectrum decomposes into a *reflective* band of wavelengths I_{r} and a *transmittive* band of wavelengths I_{t}. Radiation corresponding to I_{r} interacts with the surface of the semi-transparent material, i.e. it is emitted, reflected and absorbed by the surface. Radiation corresponding to I_t does not interact with the material at all, i.e. it is transmitted unperturbed through the medium. Thus, the band model neglects radiation transmitted between the interior and the exterior of the semi-transparent material. This is an accurate approximation if the range of wavelengths in which the spectral optical thickness (penetration depth devided by material thickness) is close to one, is sufficiently small (cf. [DNR+90, Sec. 3.4]). As mentioned before, radiation-driven heat transport staying inside a solid component is assumed to be accounted for by the corresponding temperature-dependent law of thermal conductivity.

The contributions from the two bands of wavelengths are computed separately. While the radiation region for the reflective band consists of the actual cavity, the radiation region for the transmittive band is made up of the cavity united with the semi-transparent body. Consequently, the boundary Γ_t of the transmittive radiation region is different from the boundary Γ from the opaque case, Γ_t containing the interfaces between semi-transparent material and opaque solids instead of interfaces between semi-transparent body and gas. Analogous to the definition of Γ_{reg} in Sec. 2.4.2, let $\Gamma_{t,reg}$ denote the regular part of Γ_t.

On Γ, let R_r, E_r, $J_{ref,r}$, and J_r denote the respective contributions to the radiosity, emitted radiation, reflected radiation, and irradiation, stemming from wavelengths in the reflective band I_r. The corresponding contributions from the transmittive band are defined on Γ_t and are written as R_t, E_t, $J_{ref,t}$, and J_t. Analogous to the opaque case (cf. (2.4.1)), one now has

$$\bigwedge_{x\in\Gamma_{reg}} R_r[x] = E_r[x] + J_{ref,r}[x], \tag{2.4.29a}$$

$$\bigwedge_{x\in\Gamma_{t,reg}} R_t[x] = E_t[x] + J_{ref,t}[x]. \tag{2.4.29b}$$

According to Planck's law of black body radiation, to get the analogue of (2.4.3) for the reflective and for the transmittive band, one needs to replace the total emissivity by the respective band contribution:

$$\bigwedge_{x\in\Gamma_{reg}} E_r[x] = \sigma\epsilon_r\left[(T_{solid}[x], x)\right](T_{solid}[x])^4, \tag{2.4.30a}$$

$$\bigwedge_{x\in\Gamma_{t,reg}} E_t[x] = \sigma\epsilon_t\left[(T_{solid}[x], x)\right](T_{solid}[x])^4, \tag{2.4.30b}$$

where

$$\bigwedge_{x\in\Gamma_{reg}} \epsilon_r\left[(T_{solid}[x], x)\right] = \int_{I_r} \epsilon\left[(T_{solid}[x], x, \lambda)\right] I_{b,\lambda}[T_{solid}[x]]\, d\lambda\,, \tag{2.4.31a}$$

$$\bigwedge_{x\in\Gamma_{t,reg}} \epsilon_t\left[(T_{solid}[x], x)\right] = \int_{I_t} \epsilon\left[(T_{solid}[x], x, \lambda)\right] I_{b,\lambda}[T_{solid}[x]]\, d\lambda\,, \tag{2.4.31b}$$

$$I_{\mathrm{b},\lambda}[T] := \frac{15C^4}{\pi^4 \lambda^5 T^4 \left(e^{\frac{C}{\lambda T}} - 1\right)}, \tag{2.4.32}$$

λ denoting the wavelength, $\epsilon\left[(T_{\mathrm{solid}}[\mathbf{x}], \mathbf{x}\lambda)\right]$ denoting the emissivity for monochromatic radiation of wavelength λ, and $C := 1.4388 \cdot 10^{-2}\,\mathrm{mK}$.

Planck's law and Kirchhoff's law yield the bandwise analogues of (2.4.4):

$$\bigwedge_{\mathbf{x}\in\Gamma_{\mathrm{reg}}} J_{\mathrm{ref,r}}[\mathbf{x}] = \varrho_{\mathrm{r}}\left[(T_{\mathrm{solid}}[\mathbf{x}], \mathbf{x})\right] \cdot J_{\mathrm{r}}, \tag{2.4.33a}$$

$$\bigwedge_{\mathbf{x}\in\Gamma_{\mathrm{t,reg}}} J_{\mathrm{ref,t}}[\mathbf{x}] = \varrho_{\mathrm{t}}\left[(T_{\mathrm{solid}}[\mathbf{x}], \mathbf{x})\right] \cdot J_{\mathrm{t}}, \tag{2.4.33b}$$

where

$$\bigwedge_{\mathbf{x}\in\Gamma_{\mathrm{reg}}} \varrho_{\mathrm{r}}\left[(T_{\mathrm{solid}}[\mathbf{x}], \mathbf{x})\right] = 1 - \frac{\epsilon_{\mathrm{r}}\left[(T_{\mathrm{solid}}[\mathbf{x}], \mathbf{x})\right]}{\int_{I_r} I_{\mathrm{b},\lambda}[T_{\mathrm{solid}}[\mathbf{x}]]\,\mathrm{d}\lambda}, \tag{2.4.34a}$$

$$\bigwedge_{\mathbf{x}\in\Gamma_{\mathrm{t,reg}}} \varrho_{\mathrm{t}}\left[(T_{\mathrm{solid}}[\mathbf{x}], \mathbf{x})\right] = 1 - \frac{\epsilon_{\mathrm{t}}\left[(T_{\mathrm{solid}}[\mathbf{x}], \mathbf{x})\right]}{\int_{I_t} I_{\mathrm{b},\lambda}[T_{\mathrm{solid}}[\mathbf{x}]]\,\mathrm{d}\lambda}. \tag{2.4.34b}$$

Again, one writes the irradiation via an integral operator acting on the radiosity (cf. (2.4.7)):

$$\bigwedge_{\mathbf{x}\in\Gamma_{\mathrm{reg}}} J_{\mathrm{r}}[\mathbf{x}] = \mathcal{J}_{\mathrm{r}}[R_{\mathrm{r}}][\mathbf{x}] := \int_{\Gamma} \Lambda[(\mathbf{x},\mathbf{y})]\,\omega[(\mathbf{x},\mathbf{y})]\,R_{\mathrm{r}}[\mathbf{y}]\,\mathrm{d}\mathbf{y}\,, \tag{2.4.35a}$$

$$\bigwedge_{\mathbf{x}\in\Gamma_{\mathrm{t,reg}}} J_{\mathrm{t}}[\mathbf{x}] = \mathcal{J}_{\mathrm{t}}[R_{\mathrm{t}}][\mathbf{x}] := \int_{\Gamma_{\mathrm{t}}} \Lambda[(\mathbf{x},\mathbf{y})]\,\omega[(\mathbf{x},\mathbf{y})]\,R_{\mathrm{t}}[\mathbf{y}]\,\mathrm{d}\mathbf{y}\,. \tag{2.4.35b}$$

As in the opaque case, combining (2.4.29) through (2.4.35) one can derive non-local equations for R_{r} and R_{t}, similar to (2.4.11):

$$\bigwedge_{\mathbf{x}\in\Gamma_{\mathrm{reg}}} R_{\mathrm{r}}[\mathbf{x}] - \left(1 - \epsilon_{\mathrm{r}}\left[(T_{\mathrm{solid}}[\mathbf{x}], \mathbf{x})\right]\right)\mathcal{J}_{\mathrm{r}}[R_{\mathrm{r}}][\mathbf{x}] = \sigma\epsilon_{\mathrm{r}}\left[(T_{\mathrm{solid}}[\mathbf{x}], \mathbf{x})\right]\left(T_{\mathrm{solid}}[\mathbf{x}]\right)^4, \tag{2.4.36a}$$

$$\bigwedge_{\mathbf{x}\in\Gamma_{\mathrm{t,reg}}} R_{\mathrm{t}}[\mathbf{x}] - \left(1 - \epsilon_{\mathrm{t}}\left[(T_{\mathrm{solid}}[\mathbf{x}], \mathbf{x})\right]\right)\mathcal{J}_{\mathrm{t}}[R_{\mathrm{t}}][\mathbf{x}] = \sigma\epsilon_{\mathrm{t}}\left[(T_{\mathrm{solid}}[\mathbf{x}], \mathbf{x})\right]\left(T_{\mathrm{solid}}[\mathbf{x}]\right)^4. \tag{2.4.36b}$$

Moreover, one has the following analogues of (2.4.15):

$$\bigwedge_{\mathbf{x}\in\Gamma_{\mathrm{reg}}} -R_{\mathrm{r}}[\mathbf{x}] + J_{\mathrm{r}}[\mathbf{x}] = \epsilon_{\mathrm{r}}\left[(T_{\mathrm{solid}}[\mathbf{x}], \mathbf{x})\right] \cdot \left(\mathcal{J}_{\mathrm{r}}[R_{\mathrm{r}}][\mathbf{x}] - \sigma\left(T_{\mathrm{solid}}[\mathbf{x}]\right)^4\right), \tag{2.4.37a}$$

$$\bigwedge_{\mathbf{x}\in\Gamma_{\mathrm{t,reg}}} \quad -R_{\mathrm{t}}[\mathbf{x}] + J_{\mathrm{t}}[\mathbf{x}] = \epsilon_{\mathrm{t}}\big[(T_{\mathrm{solid}}[\mathbf{x}],\mathbf{x})\big]\cdot\big(\mathcal{J}_{\mathrm{t}}[R_{\mathrm{t}}][\mathbf{x}] - \sigma\,(T_{\mathrm{solid}}[\mathbf{x}])^4\big). \tag{2.4.37b}$$

One is now in the position to rewrite (2.3.1b) and (2.3.1c) depending on which of the following three cases occurs at the respective interface:

Case (i): The interface is part of $\Gamma_{\mathrm{t}}\setminus\Gamma$, i.e. it is an interface between a semi-transparent material (here: the SiC single crystal) and an opaque solid β. Let the interface be denoted by $\gamma_{\text{SiC-Crystal},\beta}$. Since only transmittive contributions are present on $\gamma_{\text{SiC-Crystal},\beta}$, the interface condition reads

$$\begin{aligned}\mathbf{q}^{[\text{SiC-Crystal}]}\bullet\mathbf{n}^{[\text{SiC-Crystal}]} + \epsilon_{\mathrm{t}}\cdot\big(\mathcal{J}_{\mathrm{t}}[R_{\mathrm{t}}] - \sigma T_{\mathrm{solid}}^4\big) &= \mathbf{q}^{[\beta]}\bullet\mathbf{n}^{[\text{SiC-Crystal}]}\\ &\text{on } \gamma_{\text{SiC-Crystal},\beta}.\end{aligned}\tag{2.4.38a}$$

Case (ii): The interface is part of $\Gamma_{\mathrm{t}}\cap\Gamma$, i.e. it lies between an opaque solid β and the gas phase. Let the interface be called $\gamma_{\beta,\mathrm{gas}}$. On $\gamma_{\beta,\mathrm{gas}}$, one obtains contributions from both bands I_{r} and I_{t}, which then are incorporated additively into the corresponding interface condition, yielding

$$\mathbf{q}_{\mathrm{gas}}\bullet\mathbf{n}_{\mathrm{gas}} + \epsilon_{\mathrm{r}}\cdot\big(\mathcal{J}_{\mathrm{r}}[R_{\mathrm{r}}] - \sigma T_{\mathrm{solid}}^4\big) + \epsilon_{\mathrm{t}}\cdot\big(\mathcal{J}_{\mathrm{t}}[R_{\mathrm{t}}] - \sigma T_{\mathrm{solid}}^4\big) = \mathbf{q}^{[\beta]}\bullet\mathbf{n}_{\mathrm{gas}} \quad \text{on } \gamma_{\beta,\mathrm{gas}}. \tag{2.4.38b}$$

Case (iii): The interface is part of $\Gamma\setminus\Gamma_{\mathrm{t}}$, i.e. the interface is between the SiC crystal and the gas phase. Hence, it will be denoted by $\gamma_{\text{SiC-Crystal,gas}}$. On $\gamma_{\text{SiC-Crystal,gas}}$, only contributions from the reflective band are present, resulting in

$$\mathbf{q}_{\mathrm{gas}}\bullet\mathbf{n}_{\mathrm{gas}} + \epsilon_{\mathrm{r}}\cdot\big(\mathcal{J}_{\mathrm{r}}[R_{\mathrm{r}}] - \sigma T_{\mathrm{solid}}^4\big) = \mathbf{q}^{[\text{SiC-Crystal}]}\bullet\mathbf{n}_{\mathrm{gas}} \quad \text{on } \gamma_{\text{SiC-Crystal,gas}}. \tag{2.4.38c}$$

Finally, this section is concluded by the reformulation of interface conditions (2.4.38) using operators for the radiation terms. Analogously to the procedure carried out after (2.4.11), where $\mathcal{J}$ and ϵ are used to define $\mathcal{R}$, one can use $\mathcal{J}_{\mathrm{r}}$ and ϵ_{r} to define $\mathcal{R}_{\mathrm{r}}$, and one can use $\mathcal{J}_{\mathrm{t}}$ and ϵ_{t} to define $\mathcal{R}_{\mathrm{t}}$. Then (2.4.38) become

$$\begin{aligned}\mathbf{q}^{[\text{SiC-Crystal}]}\bullet\mathbf{n}^{[\text{SiC-Crystal}]} + \epsilon_{\mathrm{t}}\cdot\big(\mathcal{J}_{\mathrm{t}}\big[\mathcal{R}_{\mathrm{t}}[T_{\mathrm{solid}}]\big] - \sigma T_{\mathrm{solid}}^4\big) &= \mathbf{q}^{[\beta]}\bullet\mathbf{n}^{[\text{SiC-Crystal}]}\\ &\text{on } \gamma_{\text{SiC-Crystal},\beta},\end{aligned}\tag{2.4.39a}$$

$$\begin{aligned}\mathbf{q}_{\mathrm{gas}}\bullet\mathbf{n}_{\mathrm{gas}} &+ \epsilon_{\mathrm{r}}\cdot\big(\mathcal{J}_{\mathrm{r}}\big[\mathcal{R}_{\mathrm{r}}[T_{\mathrm{solid}}]\big] - \sigma T_{\mathrm{solid}}^4\big)\\ &+ \epsilon_{\mathrm{t}}\cdot\big(\mathcal{J}_{\mathrm{t}}\big[\mathcal{R}_{\mathrm{t}}[T_{\mathrm{solid}}]\big] - \sigma T_{\mathrm{solid}}^4\big) = \mathbf{q}^{[\beta]}\bullet\mathbf{n}_{\mathrm{gas}} \quad \text{on } \gamma_{\beta,\mathrm{gas}},\end{aligned}\tag{2.4.39b}$$

$$\begin{aligned}\mathbf{q}_{\mathrm{gas}}\bullet\mathbf{n}_{\mathrm{gas}} + \epsilon_{\mathrm{r}}\cdot\big(\mathcal{J}_{\mathrm{r}}\big[\mathcal{R}_{\mathrm{r}}[T_{\mathrm{solid}}]\big] - \sigma T_{\mathrm{solid}}^4\big) &= \mathbf{q}^{[\text{SiC-Crystal}]}\bullet\mathbf{n}_{\mathrm{gas}}\\ &\text{on } \gamma_{\text{SiC-Crystal,gas}}.\end{aligned}\tag{2.4.39c}$$

In (2.4.39) as well as throughout Sec. 2.4, T_{solid} was written independently of the particular solid material. It is reiterated that this is justified, since no temperature step is considered between different solid materials.

Proceeding in the same manner as in Sec. 2.4.3, it is straightforward to write the equations of the semi-transparent case in axisymmetric form.

2.5 Modeling Induction Heating

2.5.1 Model Assumptions

In this section, a model for the radio frequency (RF) induction heating of the PVT growth system is presented. The basic ideas are taken from [CRS94] and [RS96].

The crucible is placed inside a copper induction coil as depicted in Fig. 1.2 on p. 3. An alternating current is imposed in the coil, generating a rapidly oscillating magnetic field, inducing eddy currents in the conducting materials of the growth apparatus. The values for the frequencies used vary in the literature, e.g. 10 kHz in [BSG+91] and 125 kHz in [PAC+99]. The eddy currents cause heat sources due to the Joule effect, giving rise to the term $f^{[\beta]} := f^{[\beta j]}$ on the right-hand side of (2.2.1a). For each time instant t and for each point $\mathbf{x}$ inside the conducting material β, one can calculate $f^{[\beta]}$ from the current density j according to

$$f^{[\beta]}[(t, \mathbf{x})] = \frac{j^2[(t, \mathbf{x})]}{\sigma_c^{[\beta]}}, \tag{2.5.1}$$

where $\sigma_c^{[\beta]}$ is the electrical conductivity of the material β.

The difficulty now lies in computing the current density j from known input data, such as the heating power, the heating voltage, or the heating current. The following model allows one to choose either the power, the voltage, or the current as known (s. Sec. 2.5.7).

The strategy is to use Maxwell's equations together with the following simplifying assumptions **(indHeat)** to get a formula for j. Let $\{\mathbf{e}_r, \mathbf{e}_\vartheta, \mathbf{e}_z\}$ denote the space-dependent standard basis for the cylindrical coordinates (r, ϑ, z). Some background material on cylindrical coordinates can be found in App. B.3.

(indHeat-i) The growth system is cylindrically symmetric; in particular, the induction coil is approximated by a number of disjoint rings.

(indHeat-ii) The electric field $\mathbf{E}$, the magnetic induction $\mathbf{B}$, the magnetic field $\mathbf{H}$, and the current density vector $\mathbf{j}$ are cylindrically symmetric. Finally, $\mathbf{j}$ is perpendicular with respect to the r-z-plane, i.e. $\mathbf{j} = j[(t, r, z)]\mathbf{e}_\vartheta$.

(indHeat-iii) The magnetic permeability μ is independent of the magnetic field $\mathbf{H}$.

(indHeat-iv) No rapid movements of conducting materials occur in the growth system, and displacement currents are neglected.

(indHeat-v) Time dependence is sinusoidal.

Hypothesis (indHeat-i) is somewhat subtle as it changes the topology of the coil. Replacing each turn of the coil by a cylindrical ring means that the start and the end of the turn now coincide. However, one has to think about the start and the end of the turn as still being insulated against each other, such that the voltage present in the three-dimensional turn is also present between the start and the end of the corresponding ring. The sum of the voltages in the different rings must equal the actual voltage imposed in the three-dimensional coil (cf. (2.5.42)). Moreover, even though the coil rings are now disjoint, to model the three-dimensional situation one needs to make sure that the total current is always the same in each ring (cf. 2.5.38a). To take these aspects into account is the subject of Sec. 2.5.7.

Even though the hypothesis (indHeat-v) will play an essential role when the transient model will be reduced to a stationary one (used in each of the numerical simulations presented in Ch. 4), the following considerations up to Sec. 2.5.6 do not make use of the assumption of sinusoidal time dependence.

2.5.2 Consequences of Maxwell's Equations

If there is no displacement current, then Maxwell's equations take the form

$$\operatorname{div}\mathbf{B} = 0, \tag{2.5.2a}$$

$$\operatorname{curl}\mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t}, \tag{2.5.2b}$$

$$\operatorname{curl}\mathbf{H} = \mathbf{j}, \tag{2.5.2c}$$

$$\nu\mathbf{B} = \mathbf{H}, \tag{2.5.2d}$$

where ν denotes the magnetic reluctivity, i.e. the reciprocal of the magnetic permeability μ.

According to Ohm's law,

$$\mathbf{j} = \sigma_c^{[\beta]}\mathbf{E} \qquad \text{in each conducting material } \beta, \tag{2.5.3a}$$

$$\mathbf{j} = 0 \qquad \text{in each insulating material.} \tag{2.5.3b}$$

Using (2.5.2c), (B.3.8) from App. B.3, and continuity of $\mathbf{H}$ at $r = 0$, the assumption (indHeat-ii) on $\mathbf{H}$ and $\mathbf{j}$ implies

$$\mathbf{H}[(t,r,\vartheta,z)] = \mathbf{H}[(t,r,z)] = H_r[(t,r,z)]\mathbf{e}_r + H_z[(t,r,z)]\mathbf{e}_z \tag{2.5.4}$$

and

$$\frac{\partial H_r[(t,r,z)]}{\partial z} - \frac{\partial H_z[(t,r,z)]}{\partial r} = j[(t,r,z)]. \tag{2.5.5}$$

Then (2.5.4) together with (2.5.2d) and (indHeat-ii) gives

$$\mathbf{B}[(t,r,\vartheta,z)] = \mathbf{B}[(t,r,z)] = B_r[(t,r,z)]\mathbf{e}_r + B_z[(t,r,z)]\mathbf{e}_z, \tag{2.5.6a}$$

$$B_r[(t,r,z)] = \mu[(t,r,z)]H_r[(t,r,z)], \tag{2.5.6b}$$

$$B_z[(t,r,z)] = \mu[(t,r,z)]H_z[(t,r,z)]. \tag{2.5.6c}$$

Next, (2.5.6a), (2.5.2a), and (B.3.7) lead to

$$\frac{1}{r}\frac{\partial(rB_r)}{\partial r} + \frac{\partial B_z}{\partial z} = 0. \tag{2.5.7}$$

As usual, (2.5.2a) gives rise to a magnetic vector potential $\mathbf{A}$ such that

$$\mathbf{B} = \operatorname{curl}\mathbf{A}. \tag{2.5.8}$$

Due to (2.5.6a) and its consequence (2.5.7), one can even find a magnetic scalar potential ϕ_A: As shown in App. B.4, if (2.5.7) is satisfied, then one can choose $\phi_A[(t,r,z)]$ such that the two equations

$$B_r = -\frac{\partial\phi_A}{\partial z}, \quad B_z = \frac{1}{r}\frac{\partial(r\phi_A)}{\partial r} \tag{2.5.9}$$

hold. If one now lets

$$\mathbf{A} := \phi_A\mathbf{e}_\vartheta, \tag{2.5.10}$$

then (2.5.8) holds according to (B.3.8), (2.5.9), and (2.5.6a). It is noted as an aside that the Coulomb condition $\operatorname{div}\mathbf{A} = 0$ is also fulfilled, as is implied by (2.5.10), (B.3.7), and ϕ_A being independent of ϑ.

Combining (2.5.5), (2.5.6b), (2.5.6c), and (2.5.9), one gets

$$j = -\frac{\partial}{\partial z}\left(\nu\frac{\partial\phi_A}{\partial z}\right) - \frac{\partial}{\partial r}\left(\frac{\nu}{r}\frac{\partial(r\phi_A)}{\partial r}\right). \tag{2.5.11}$$

For the discretization by means of a finite volume method (cf. Ch. 3), it is desirable to rewrite the right-hand side of (2.5.11) in divergence form. This can be achieved easily in space domains where ν is constant. Using (B.3.6) and (B.3.7), one gets

$$\begin{aligned}\operatorname{div}\frac{\nabla(r\phi_A)}{r^2} &= \operatorname{div}\left(\frac{\partial_r(r\phi_A)}{r^2},\ 0,\ \frac{\partial_z(r\phi_A)}{r^2}\right) = \frac{1}{r}\partial_r\left(\frac{\partial_r(r\phi_A)}{r}\right) + \frac{\partial_z^2(r\phi_A)}{r^2}\\ &= -\frac{\partial_r(r\phi_A)}{r^3} + \frac{\partial_r^2(r\phi_A)}{r^2} + \frac{\partial_z^2(r\phi_A)}{r^2}.\end{aligned} \tag{2.5.12}$$

One verifies that if ν is constant, then carrying out the outer differentiation with respect to r in the right-hand side of (2.5.11) and multiplying by $1/r$ yields the negative of the ν-fold of the right-hand side of (2.5.12). Thus, (2.5.11) can be written in the divergence form

$$\frac{j}{r} = -\nu\operatorname{div}\frac{\nabla(r\phi_A)}{r^2}. \tag{2.5.13}$$

If ϕ_A is sufficiently smooth, such that time and space derivatives commute, then (2.5.8) implies

$$\frac{\partial \mathbf{B}}{\partial t} = \operatorname{curl} \frac{\partial \mathbf{A}}{\partial t}. \tag{2.5.14}$$

Finally, (2.5.14) and (2.5.2b) imply

$$\operatorname{curl}\left(\mathbf{E} + \frac{\partial \mathbf{A}}{\partial t}\right) = \mathbf{0}. \tag{2.5.15}$$

2.5.3 Magnetic Scalar Potential Equation in Insulators

The current density vanishes in insulating materials, i.e. (2.5.3b) holds. This, together with (2.5.13), yields

$$-\nu \operatorname{div} \frac{\nabla(r\phi_A)}{r^2} = 0 \quad \text{in each insulating material.} \tag{2.5.16}$$

2.5.4 Magnetic Scalar Potential Equation in Conductors

In the material β (2.5.3a), the form of $\mathbf{j}$, and (2.5.10) can be used to get

$$\mathbf{E} + \frac{\partial \mathbf{A}}{\partial t} = \left(\frac{j}{\sigma_c^{[\beta]}} + \frac{\partial \phi_A}{\partial t}\right) \mathbf{e}_\vartheta. \tag{2.5.17}$$

If ϕ_A is sufficiently smooth in the domain $\Omega^{[\beta]}$ of the material β, such that (2.5.15) holds, then one can use (2.5.17) in (2.5.15) to get

$$\operatorname{curl}\left(\left(\frac{j}{\sigma_c^{[\beta]}} + \frac{\partial \phi_A}{\partial t}\right) \mathbf{e}_\vartheta\right) = \mathbf{0}. \tag{2.5.18}$$

Using (2.5.18), and the cylindrical symmetry of j and ϕ_A, one sees from (B.3.6) and (B.3.8) in App. B.3.2 that

$$\nabla\left(r\left(\frac{j}{\sigma_c^{[\beta]}} + \frac{\partial \phi_A}{\partial t}\right)\right) = \mathbf{0}. \tag{2.5.19}$$

In particular, if $\Omega^{[\beta]}$ is connected, then the expression $r(j/\sigma_c^{[\beta]} + \partial_t \phi_A)$ does not depend on the space coordinates (r, ϑ, z) in $\Omega^{[\beta]}$. That means there is a time-dependent function $C^{[\beta]}[t]$ such that

$$r\left(\frac{j[(t,r,z)]}{\sigma_c^{[\beta]}[(t,r,z)]} + \frac{\partial \phi_A[(t,r,z)]}{\partial t}\right) = C^{[\beta]}[t] \quad \text{in } \Omega^{[\beta]}. \tag{2.5.20}$$

To identify the function $C^{[\beta]}[t]$, voltages in the material β are computed. Two phenomena contribute to the existence of a voltage along a path Γ, namely the presence of the field $\mathbf{E}$, and the field $\mathbf{B}$ changing in time owing to induction. Let $V^{[\beta]}[\Gamma]$ be the voltage resulting from integrating $\mathbf{E}+\partial_t\mathbf{A}$ over the closed circular path Γ of radius r, contained in $\Omega^{[\beta]}$. Using (2.5.17), (2.5.20), and that the tangent unit vector $\mathbf{t}_\Gamma$ of Γ is identical to $\mathbf{e}_\vartheta$ on Γ, one calculates

$$\begin{aligned} V^{[\beta]}[\Gamma] &= \int_\Gamma \left(\mathbf{E} + \frac{\partial \mathbf{A}}{\partial t}\right) \bullet \mathbf{t}_\Gamma = \int_\Gamma \left(\frac{j}{\sigma_c^{[\beta]}} + \frac{\partial \phi_A}{\partial t}\right) \mathbf{e}_\vartheta \bullet \mathbf{e}_\vartheta \\ &= \int_0^{2\pi} \left(\frac{j}{\sigma_c^{[\beta]}} + \frac{\partial \phi_A}{\partial t}\right) r \,\mathrm{d}\vartheta \; = 2\pi C^{[\beta]}, \end{aligned} \tag{2.5.21}$$

showing that $V^{[\beta]}[\Gamma] =: V^{[\beta]}$ is actually independent of Γ. Now there are two different situations to consider, depending on whether the path Γ is contained in one of the coil rings or in the growth apparatus.

Let the induction coil consist of N rings, and let $\Omega_k^{[\mathrm{ring}]}$, $k \in \{1, \dots, N\}$, denote their respective domains. As described in Sec. 2.5.1, each coil ring needs to be considered as the two-dimensional model of a three-dimensional coil turn. In particular, the voltage between the start and the end of the k-th coil turn is represented by the voltage $V_k^{[\mathrm{ring}]}[t]$ in the k-th coil ring. If Γ lies in $\Omega_k^{[\mathrm{ring}]}$, then (2.5.21) implies

$$C^{[\beta]}[t] = \frac{V_k^{[\mathrm{ring}]}[t]}{2\pi} \qquad \text{in } \Omega_k^{[\mathrm{ring}]}. \tag{2.5.22a}$$

If the path Γ lies in the domain $\Omega^{[\beta]}_{\mathrm{appCon}}$ of some conducting material β in the growth apparatus, then

$$C^{[\beta]}[t] = 0 \qquad \text{in } \Omega^{[\beta]}_{\mathrm{appCon}}, \tag{2.5.22b}$$

since there is no voltage imposed in the growth apparatus.

Assuming that ν is constant in $\Omega^{[\beta]}$, one can plug (2.5.13) and (2.5.22) into (2.5.20) to conclude

$$-\nu \operatorname{div} \frac{\nabla(r\phi_A)}{r^2} + \frac{\sigma_c^{[\mathrm{ring}]}}{r}\frac{\partial \phi_A}{\partial t} = \frac{\sigma_c^{[\mathrm{ring}]} V_k^{[\mathrm{ring}]}[t]}{2\pi r^2} \qquad \text{in } \Omega_k^{[\mathrm{ring}]}, \tag{2.5.23a}$$

$$-\nu \operatorname{div} \frac{\nabla(r\phi_A)}{r^2} + \frac{\sigma_c^{[\beta]}}{r}\frac{\partial \phi_A}{\partial t} = 0 \qquad \text{in } \Omega^{[\beta]}_{\mathrm{appCon}}. \tag{2.5.23b}$$

The voltages $V_k^{[\mathrm{ring}]}[t]$ have to be determined from the input voltage, the input current, or the input power. How this can be done in the case of sinusoidal time dependence is described in Secs 2.5.6 and 2.5.7.

2.5.5 Interface and Boundary Conditions

The magnetic scalar potential ϕ_A is determined from (2.5.16) and (2.5.23), completed by the following interface and boundary conditions.

It is assumed that ϕ_A is continuous throughout the considered domain. If there are no surface currents, then on interfaces $\gamma_{\gamma_1,\gamma_2}$ between a material γ_1 and a material γ_2 (the materials can be either solid or gas), one has the flux interface condition

$$\frac{\nu_{\gamma_1}}{r}\,\nabla(r\phi_A) \bullet \mathbf{n}_{\gamma_1} = \frac{\nu_{\gamma_2}}{r}\,\nabla(r\phi_A) \bullet \mathbf{n}_{\gamma_1}. \tag{2.5.24}$$

As for the boundary condition on ϕ_A, it follows from the continuity of $\mathbf{A}$ and (2.5.10), that $\phi_A = 0$ on the symmetry axis $r = 0$. It is also assumed that ϕ_A vanishes on outer boundaries sufficiently far from the growth apparatus (cf. [KP01, Sec. 3.2] and Sec. 4.1 for more information on what distance may be considered "sufficiently far").

2.5.6 Sinusoidal Time Dependence

It is now assumed that (indHeat-v) holds, i.e. that the time dependence of the functions $V_k^{[\text{ring}]}$, $k \in \{1, \dots, N\}$, j, and ϕ_A is sinusoidal. In addition to (indHeat-iii), this includes the implicit assumption that μ and σ_c do not depend on time, since otherwise sinusoidal time dependence can generally not be expected.

Sinusoidal time dependence means there are an angular frequency ω, voltages $V_{k,0}^{[\text{ring}]}$, a current density $j_0[(r,z)]$, a magnetic scalar potential $\phi_{A,0}[(r,z)]$, and times $t_{V,k,0}$, $k \in \{1,\dots,N\}$, $t_{j,0}[(r,z)]$, $t_{\phi_A,0}[(r,z)]$ such that

$$V_k^{[\text{ring}]}[t] = V_{k,0}^{[\text{ring}]} \sin\left[\omega(t + t_{V,k,0})\right], \quad k \in \{1,\dots,N\}, \tag{2.5.25a}$$

$$j[(t,r,z)] = j_0[(r,z)] \sin\left[\omega(t + t_{j,0}[(r,z)])\right], \tag{2.5.25b}$$

$$\phi_A[(t,r,z)] = \phi_{A,0}[(r,z)] \sin\left[\omega(t + t_{\phi_A,0}[(r,z)])\right]. \tag{2.5.25c}$$

As is customary, the functions $V_k^{[\text{ring}]}$, j, and ϕ_A are extended into the complex plane by letting

$$V_k^{[\text{ring}],\text{complex}}[t] := iV_k^{[\text{ring}]}[t] + V_k^{[\text{ring}]}\left[t + \frac{\pi}{2\omega}\right], \quad k \in \{1,\dots,N\}, \tag{2.5.26a}$$

$$j^{\text{complex}}[(t,r,z)] := ij[(t,r,z)] + j\left[\left(t + \frac{\pi}{2\omega}, r, z\right)\right], \tag{2.5.26b}$$

$$\phi_A^{\text{complex}}[(t,r,z)] := i\phi_A[(t,r,z)] + \phi_A\left[\left(t + \frac{\pi}{2\omega}, r, z\right)\right]. \tag{2.5.26c}$$

Then

$$V_k^{[\text{ring}]}[t] = \operatorname{Im}\left[V_k^{[\text{ring}],\text{complex}}[t]\right], \quad k \in \{1,\dots,N\}, \tag{2.5.27a}$$

$$j[(t,r,z)] = \operatorname{Im}\left[j^{\text{complex}}[(t,r,z)]\right], \tag{2.5.27b}$$

$$\phi_A[(t,r,z)] = \operatorname{Im}\left[\phi_A^{\text{complex}}[(t,r,z)]\right]. \tag{2.5.27c}$$

Define

$$V_{k,0}^{[\mathrm{ring}],\mathrm{complex}} := V_{k,0}^{[\mathrm{ring}]} e^{i\omega t_{V,k,0}}, \quad k \in \{1, \dots, N\}, \tag{2.5.28a}$$

$$j_0^{\mathrm{complex}}[(r,z)] := j_0[(r,z)] e^{i\omega t_{j,0}[(r,z)]}, \tag{2.5.28b}$$

$$\phi_{A,0}^{\mathrm{complex}}[(r,z)] := \phi_{A,0}[(r,z)] e^{i\omega t_{\phi_A,0}[(r,z)]}. \tag{2.5.28c}$$

From (2.5.25), (2.5.26), (2.5.28), and the relation $e^{i\varphi} = \cos[\varphi] + i\sin[\varphi]$, it follows that

$$V_k^{[\mathrm{ring}],\mathrm{complex}}[t] = V_{k,0}^{[\mathrm{ring}]} e^{i\omega(t+t_{V,k,0})} = V_{k,0}^{[\mathrm{ring}],\mathrm{complex}} e^{i\omega t}, \quad k \in \{1, \dots, N\}, \tag{2.5.29a}$$

$$j^{\mathrm{complex}}[(t,r,z)] = j_0[(r,z)] e^{i\omega(t+t_{j,0}[(r,z)])} = j_0^{\mathrm{complex}}[(r,z)] e^{i\omega t}, \tag{2.5.29b}$$

$$\phi_A^{\mathrm{complex}}[(t,r,z)] = \phi_{A,0}[(r,z)] e^{i\omega(t+t_{\phi_A,0}[(r,z)])} = \phi_{A,0}^{\mathrm{complex}}[(r,z)] e^{i\omega t}. \tag{2.5.29c}$$

One then gets the formula

$$\frac{j_0^{\mathrm{complex}}[(r,z)]}{r} = -\nu \operatorname{div} \frac{\nabla\left(r\phi_{A,0}^{\mathrm{complex}}[(r,z)]\right)}{r^2}, \tag{2.5.30}$$

which follows from (2.5.26) and (2.5.29) by writing (2.5.13) once for $t + \frac{\pi}{2\omega}$ and once for t multiplied by i, adding, and multiplying by $e^{-i\omega t}$.

One of the main simplifications achieved by the assumption of sinusoidal time dependence is the possible reduction of the transient problem for ϕ_A to a stationary problem for $\phi_{A,0}^{\mathrm{complex}}$ in the presence of time-independent material parameters ν and σ_c (see (2.5.32)). Since the quantities of the electromagnetic problem change orders of magnitude faster than the quantities of the heat problem, the heat sources $f^{[\beta]}$ in (2.5.1) can be computed by taking the average of j^2 over one period:

$$\begin{aligned} f^{[\beta]}[(r,z)] &= \frac{\int_{\mathrm{period}} j^2[(t,r,z)]\,\mathrm{d}t}{\sigma_c^{[\beta]} \cdot |\mathrm{period}|} = \frac{j_0^2[(r,z)]}{\sigma_c^{[\beta]}} \cdot \frac{\int_0^{\frac{\pi}{\omega}} \sin^2\left[\omega(t + t_{j,0}[(r,z)])\right]\mathrm{d}t}{\frac{\omega}{\pi}} \\ &= \frac{j_0^{\mathrm{complex}}[(r,z)]\,\overline{j_0^{\mathrm{complex}}[(r,z)]}}{2\sigma_c^{[\beta]}}. \end{aligned} \tag{2.5.31}$$

The function j_0^{complex} in (2.5.31) can be computed from (2.5.33) below.

It is noted that in order to account for the temperature dependence of the electrical conductivity and for changing coil positions when solving the transient heat problem, the quasi-stationary problem for $\phi_{A,0}^{\mathrm{complex}}$ has to be solved after each time step (or at least after each significant change of the electrical conductivity or the coil positions) of the time-discretized heat problem.

Now the stationary problem for $\phi_{A,0}^{\mathrm{complex}}$ is going to be formulated. For easy reference, the system of partial differential equations for ϕ_A, consisting of (2.5.16) and (2.5.23) with the interface and boundary conditions written in Sec. 2.5.5, is given the name

(PDE: ϕ_A). Analogously, let (PDE: $\phi_{A,0}^{\text{complex}}$) be the system consisting of the following Equations and Conditions (2.5.32):

$$-\nu \operatorname{div} \frac{\nabla\left(r\phi_{A,0}^{\text{complex}}\right)}{r^2} = 0 \quad \text{in each insulating material,} \tag{2.5.32a}$$

$$-\nu \operatorname{div} \frac{\nabla\left(r\phi_{A,0}^{\text{complex}}\right)}{r^2} + \frac{i\omega\sigma_{\text{c}}^{[\text{ring}]}\phi_{A,0}^{\text{complex}}}{r} = \frac{\sigma_{\text{c}}^{[\text{ring}]}V_{k,0}^{[\text{ring}],\text{complex}}}{2\pi r^2} \quad \text{in } \Omega_k^{[\text{ring}]}, \tag{2.5.32b}$$

$$-\nu \operatorname{div} \frac{\nabla\left(r\phi_{A,0}^{\text{complex}}\right)}{r^2} + \frac{i\omega\sigma_{\text{c}}^{[\beta]}\phi_{A,0}^{\text{complex}}}{r} = 0 \quad \text{in } \Omega_{\text{appCon}}^{[\beta]}, \tag{2.5.32c}$$

$$\frac{\nu_{\gamma_1}}{r}\nabla\left(r\phi_{A,0}^{\text{complex}}\right) \bullet \mathbf{n}_{\gamma_1} = \frac{\nu_{\gamma_2}}{r}\nabla\left(r\phi_{A,0}^{\text{complex}}\right) \bullet \mathbf{n}_{\gamma_1} \quad \text{on each interface } \gamma_{\gamma_1,\gamma_2}, \tag{2.5.32d}$$

$$\phi_{A,0}^{\text{complex}} \text{ is continuous on each interface,} \tag{2.5.32e}$$

$$\phi_{A,0}^{\text{complex}} = 0 \quad \text{on each outer boundary.} \tag{2.5.32f}$$

It is easily verified that ϕ_A satisfies (PDE: ϕ_A) if $\phi_{A,0}^{\text{complex}}$ satisfies (PDE: $\phi_{A,0}^{\text{complex}}$): Using (2.5.27) and (2.5.29), (2.5.32a) implies (2.5.16), (2.5.32b) implies (2.5.23a), (2.5.32c) implies (2.5.23b), (2.5.32d) implies (2.5.24), and (2.5.32f) implies $\phi_A = 0$ on outer boundaries, simply by multiplying the assumed equation by $e^{i\omega t}$ and taking the imaginary part. The continuity of ϕ_A on interfaces follows from (2.5.32e), since multiplication by $e^{i\omega t}$ and taking the imaginary part are both continuous operations.

One can combine (2.5.30) with (2.5.32b) and (2.5.32c), respectively, to determine the stationary complex current density needed for (2.5.31):

$$j_0^{\text{complex}}[(r,z)] = -i\omega\sigma_{\text{c}}^{[\text{ring}]}\phi_{A,0}^{\text{complex}} + \frac{\sigma_{\text{c}}^{[\text{ring}]}V_{k,0}^{[\text{ring}],\text{complex}}}{2\pi r} \quad \text{in } \Omega_k^{[\text{ring}]}, \tag{2.5.33a}$$

$$j_0^{\text{complex}}[(r,z)] = -i\omega\sigma_{\text{c}}^{[\beta]}\phi_{A,0}^{\text{complex}} \quad \text{in } \Omega_{\text{appCon}}^{[\beta]}. \tag{2.5.33b}$$

Substituting (2.5.33) in (2.5.31) yields

$$f^{[\text{ring}]}[(r,z)] = \frac{\omega^2\sigma_{\text{c}}^{[\text{ring}]}}{2r^2}\left(\left(\frac{\operatorname{Re}\left[V_{k,0}^{[\text{ring}],\text{complex}}\right]}{2\pi\omega} + \operatorname{Im}\left[r\phi_{A,0}^{\text{complex}}\right]\right)^2 + \left(\frac{\operatorname{Im}\left[V_{k,0}^{[\text{ring}],\text{complex}}\right]}{2\pi\omega} - \operatorname{Re}\left[r\phi_{A,0}^{\text{complex}}\right]\right)^2\right) \quad \text{in } \Omega_k^{[\text{ring}]}, \tag{2.5.34a}$$

$$f^{[\beta]}[(r,z)] = \frac{\omega^2\sigma_{\text{c}}^{[\beta]}}{2r^2}\left(\left(\operatorname{Re}\left[r\phi_{A,0}^{\text{complex}}\right]\right)^2 + \left(\operatorname{Im}\left[r\phi_{A,0}^{\text{complex}}\right]\right)^2\right) \quad \text{in } \Omega_{\text{appCon}}^{[\beta]}. \tag{2.5.34b}$$

2.5.7 Prescribing Current, Voltage, or Power

In order to solve the system of partial differential equations (PDE: $\phi_{A,0}^{\text{complex}}$) for $\phi_{A,0}^{\text{complex}}$, one still has to determine the quantities $V_{k,0}^{[\text{ring}],\text{complex}}$ in (2.5.32b), i.e. the voltages in the different coil rings. The goal of the present section is to compute the $V_{k,0}^{[\text{ring}],\text{complex}}$ from a given total current, a given total voltage, or a given total power imposed in the induction coil. The approach presented here has been published in [KP02].

The circular projection π_{circ} that was defined in (2.4.20) is used again in the following. The total current J_k in the k-th coil ring corresponding to $\phi_{A,0}^{\text{complex}}$ and $V_{k,0}^{[\text{ring}],\text{complex}}$ is computed from (2.5.27b), (2.5.29b), and (2.5.33a):

$$\begin{aligned}
&J_k\left[(\phi_{A,0}^{\text{complex}}, V_{k,0}^{[\text{ring}],\text{complex}}, t)\right] = \int_{\pi_{\text{circ}}\Omega_k^{[\text{ring}]}} j[(t,r,z)]\,\mathrm{d}r\ \mathrm{d}z \\
&= \operatorname{Im}\left[e^{i\omega t}\int_{\pi_{\text{circ}}\Omega_k^{[\text{ring}]}} j_0^{\text{complex}}[(r,z)]\,\mathrm{d}r\ \mathrm{d}z\right] \\
&= \operatorname{Im}\left[e^{i\omega t}\left(\frac{V_{k,0}^{[\text{ring}],\text{complex}}}{2\pi}\int_{\pi_{\text{circ}}\Omega_k^{[\text{ring}]}}\frac{\sigma_{\text{c}}^{[\text{ring}]}}{r}\,\mathrm{d}r\ \mathrm{d}z - i\omega\int_{\pi_{\text{circ}}\Omega_k^{[\text{ring}]}}\sigma_{\text{c}}^{[\text{ring}]}\phi_{A,0}^{\text{complex}}\,\mathrm{d}r\ \mathrm{d}z\right)\right] \\
&= \operatorname{Im}\left[e^{i\omega t}\left(V_{k,0}^{[\text{ring}],\text{complex}}\sigma_{\text{c},k} - i\omega\int_{\pi_{\text{circ}}\Omega_k^{[\text{ring}]}}\sigma_{\text{c}}^{[\text{ring}]}\phi_{A,0}^{\text{complex}}\,\mathrm{d}r\ \mathrm{d}z\right)\right] \\
&= \operatorname{Im}\left[e^{i\omega t}J_{k,0}^{\text{complex}}\left[(\phi_{A,0}^{\text{complex}}, V_{k,0}^{[\text{ring}],\text{complex}})\right]\right],
\end{aligned} \tag{2.5.35}$$

where

$$\sigma_{\text{c},k} := \frac{1}{2\pi}\int_{\pi_{\text{circ}}\Omega_k^{[\text{ring}]}}\frac{\sigma_{\text{c}}^{[\text{ring}]}}{r}\,\mathrm{d}r\ \mathrm{d}z\,, \tag{2.5.36}$$

$$\begin{aligned}
&J_{k,0}^{\text{complex}}\left[(\phi_{A,0}^{\text{complex}}, V_{k,0}^{[\text{ring}],\text{complex}})\right] \\
&:= V_{k,0}^{[\text{ring}],\text{complex}}\sigma_{\text{c},k} - i\omega\int_{\pi_{\text{circ}}\Omega_k^{[\text{ring}]}}\sigma_{\text{c}}^{[\text{ring}]}\phi_{A,0}^{\text{complex}}\,\mathrm{d}r\ \mathrm{d}z\,.
\end{aligned} \tag{2.5.37}$$

If the cylindrically symmetric approximation of the coil by disjoint rings is supposed to reflect the three-dimensional situation, then the total current must be the same in each coil ring and for each point in time, i.e.

$$\begin{aligned}
J_{\text{total}}[t] &:= J_1\left[(\phi_{A,0}^{\text{complex}}, V_{1,0}^{[\text{ring}],\text{complex}}, t)\right] \\
&= \cdots = J_N\left[(\phi_{A,0}^{\text{complex}}, V_{N,0}^{[\text{ring}],\text{complex}}, t)\right]
\end{aligned} \quad \text{for each time } t \tag{2.5.38a}$$

or, equivalently,

$$\begin{aligned}
J_{\text{total},0}^{\text{complex}} &:= J_{1,0}^{\text{complex}}\left[(\phi_{A,0}^{\text{complex}}, V_{1,0}^{[\text{ring}],\text{complex}})\right] \\
&= \cdots = J_{N,0}^{\text{complex}}\left[(\phi_{A,0}^{\text{complex}}, V_{N,0}^{[\text{ring}],\text{complex}})\right].
\end{aligned} \tag{2.5.38b}$$

One can now formulate a joint determining system for $\phi_{A,0}^{\text{complex}}$ and the $V_{k,0}^{[\text{ring}],\text{complex}}$, $k \in \{1,\ldots,N\}$, consisting of (2.5.40) or (2.5.45) together with (PDE: $\phi_{A,0}^{\text{complex}}$), depending on whether the total current or the total voltage is to be prescribed. Scaling of the solution to (PDE: $\phi_{A,0}^{\text{complex}}$) and (2.5.45) allows to prescribe the total power.

Prescription of Total Current: Suppose the sinusoidal total current

$$J_{\text{given}}[t] = J_{\text{given},0}\sin[\omega t] = \operatorname{Im}[J_{\text{given},0}e^{i\omega t}] \tag{2.5.39}$$

is to be prescribed. Then $\phi_{A,0}^{\text{complex}}$ and the $V_{k,0}^{[\text{ring}],\text{complex}}$ must satisfy the system

$$J_{\text{given},0} = J_{k,0}^{\text{complex}}\big[(\phi_{A,0}^{\text{complex}}, V_{k,0}^{[\text{ring}],\text{complex}})\big], \quad k \in \{1,\ldots,N\}. \tag{2.5.40}$$

Prescription of Total Voltage: Suppose the sinusoidal total voltage

$$V_{\text{total}}[t] = V_{\text{total},0}\sin[\omega t] = \operatorname{Im}[V_{\text{total},0}e^{i\omega t}] \tag{2.5.41}$$

is to be prescribed. The sum of the voltages in the coil rings equals the total voltage, i.e.

$$V_{\text{total}}[t] = \sum_{k=1}^{N} V_k^{[\text{ring}]}[t]. \tag{2.5.42}$$

The equivalent complex equation reads

$$V_{\text{total}}^{\text{complex}}[t] = \sum_{k=1}^{N} V_k^{[\text{ring}],\text{complex}}[t], \tag{2.5.43}$$

where

$$V_{\text{total}}^{\text{complex}}[t] = iV_{\text{total}}[t] + V_{\text{total}}\left[t + \frac{\pi}{2\omega}\right] = V_{\text{total},0}e^{i\omega t}. \tag{2.5.44}$$

Moreover, (2.5.43) is equivalent to the stationary equation

$$V_{\text{total},0} = \sum_{k=1}^{N} V_{k,0}^{[\text{ring}],\text{complex}}. \tag{2.5.45a}$$

So in the present case, $\phi_{A,0}^{\text{complex}}$ and the $V_{k,0}^{[\text{ring}],\text{complex}}$ must satisfy the system consisting of (2.5.45a) and

$$\begin{aligned} &J_{k,0}^{\text{complex}}\big[(\phi_{A,0}^{\text{complex}}, V_{k,0}^{[\text{ring}],\text{complex}})\big] \\ &= J_{k+1,0}^{\text{complex}}\big[(\phi_{A,0}^{\text{complex}}, V_{k+1,0}^{[\text{ring}],\text{complex}})\big], \end{aligned} \quad k \in \{1,\ldots,N-1\}, \tag{2.5.45b}$$

which is (2.5.38b) rewritten. It is noted that instead of solving (PDE: $\phi_{A,0}^{\text{complex}}$) and (2.5.45) one can also solve (PDE: $\phi_{A,0}^{\text{complex}}$) and (2.5.40) for a reference current, and then scale the solution to the prescribed voltage.

Prescription of Total Power: The electrical power P_k in the k-th coil ring is

$$P_k[t] = V_k^{[\text{ring}]}[t]\, J_k[t], \tag{2.5.46}$$

and the average over one period is

$$\overline{P_k} = \frac{\omega}{2\pi} \int_0^{\frac{2\pi}{\omega}} P_k[t]\, \mathrm{d}t\,. \tag{2.5.47}$$

Summing over all coil rings, one gets the total electrical power

$$P_{\text{total}}[t] = \sum_{k=1}^{N} P_k[t] = \sum_{k=1}^{N} V_k^{[\text{ring}]}[t]\, J_k[t] \tag{2.5.48}$$

and the corresponding average power

$$\overline{P_{\text{total}}} = \frac{\omega}{2\pi} \int_0^{\frac{2\pi}{\omega}} P_{\text{total}}[t]\, \mathrm{d}t = \sum_{k=1}^{N} \overline{P_k}. \tag{2.5.49}$$

Assuming (2.5.38a) and using (2.5.42), (2.5.48) implies

$$P_{\text{total}}[t] = V_{\text{total}}[t]\, J_{\text{total}}[t]. \tag{2.5.50}$$

If $(\phi_{A,0}^{\text{complex}}, V_{1,0}^{[\text{ring}],\text{complex}}, \dots, V_{N,0}^{[\text{ring}],\text{complex}})$ is the solution to (PDE: $\phi_{A,0}^{\text{complex}}$) and (2.5.45), then for each $\lambda \in \mathbb{R}$, it is

$$\left(\lambda \phi_{A,0}^{\text{complex}}, \lambda V_{1,0}^{[\text{ring}],\text{complex}}, \dots, \lambda V_{N,0}^{[\text{ring}],\text{complex}}\right) \tag{2.5.51}$$

the solution to (PDE: $\phi_{A,0}^{\text{complex}}$) and (2.5.45) with $V_{\text{total},0}$ replaced by $\lambda V_{\text{total},0}$.

Using (2.5.50), (2.5.41), (2.5.35), and (2.5.45b), the total power of the scaled solution (2.5.51) can be computed as

$$\begin{aligned} P_{\text{total},\lambda}[t] &= \lambda^2 V_{\text{total},0} \sin[\omega t] \cdot \operatorname{Im}\left[e^{i\omega t} J_{1,0}^{\text{complex}}\big[(\phi_{A,0}^{\text{complex}}, V_{1,0}^{[\text{ring}],\text{complex}})\big]\right] \\ &= \lambda^2 V_{\text{total},0} \operatorname{Re}\left[J_{1,0}^{\text{complex}}\big[(\phi_{A,0}^{\text{complex}}, V_{1,0}^{[\text{ring}],\text{complex}})\big]\right] (\sin[\omega t])^2 \\ &\quad + \lambda^2 V_{\text{total},0} \operatorname{Im}\left[J_{1,0}^{\text{complex}}\big[(\phi_{A,0}^{\text{complex}}, V_{1,0}^{[\text{ring}],\text{complex}})\big]\right] \sin[\omega t] \cos[\omega t]. \end{aligned} \tag{2.5.52}$$

Combining (2.5.49) and (2.5.52) provides the average power of the scaled solution:

$$\overline{P_{\text{total},\lambda}} = \frac{\lambda^2 V_{\text{total},0} \operatorname{Re}\left[J_{1,0}^{\text{complex}}\big[(\phi_{A,0}^{\text{complex}}, V_{1,0}^{[\text{ring}],\text{complex}})\big]\right]}{2}. \tag{2.5.53}$$

Thus, to prescribe the average total power P, one solves (PDE: $\phi_{A,0}^{\text{complex}}$) and (2.5.45) with arbitrary $V_{\text{total},0} \neq 0$ and then scales the solution with

$$\lambda_P := \sqrt{\frac{2P}{V_{\text{total},0} \operatorname{Re}\left[J_{1,0}^{\text{complex}}\big[(\phi_{A,0}^{\text{complex}}, V_{1,0}^{[\text{ring}],\text{complex}})\big]\right]}}. \tag{2.5.54}$$

Decomposition for Numerical Solution

As the system (PDE: $\phi_{A,0}^{\text{complex}}$) is linear, (PDE: $\phi_{A,0}^{\text{complex}}$) plus either (2.5.40) or (2.5.45) can be decomposed into $N+1$ (numerically) simpler problems: N reference problems of the form (PDE: $\phi_{A,0}^{\text{complex}}$) and one problem of the form (2.5.40) or (2.5.45), respectively.

To that end, choose an arbitrary reference voltage $V_{\text{ref}} \neq 0$ ($V_{\text{ref}} = 1\text{V}$ is used during the simulations presented in Ch. 4). Then for each $l \in \{1, \ldots, N\}$, one can solve the problem (PDE$_l$: $\phi_{A,0}^{\text{complex}}$) which consists of (PDE: $\phi_{A,0}^{\text{complex}}$) with

$$V_{k,0}^{[\text{ring}],\text{complex}} = V_{l,k,0}^{[\text{ring}],\text{complex}} := \begin{cases} V_{\text{ref}} & \text{for } k = l, \\ 0 & \text{for } k \in \{1, \ldots, N\} \setminus \{l\}. \end{cases} \tag{2.5.55}$$

It is noted that for each (PDE$_l$: $\phi_{A,0}^{\text{complex}}$), the matrix $\mathcal{M}$ of the linear discrete problem arising from a fixed spatial discretization is the same. Hence the numerically costly procedure of inverting $\mathcal{M}$ (rank($\mathcal{M}$)¿10 000 not being unusual in applications) has to be performed only once.

Let $\phi_{A,l,0}^{\text{complex}}$ denote the solution to the problem (PDE$_l$: $\phi_{A,0}^{\text{complex}}$). Then according to (2.5.35) and (2.5.37) the corresponding total current $J_{l,k,\text{ref}}$ in the k-th coil ring is given by

$$J_{l,k,\text{ref}}[t] := J_k\left[(\phi_{A,l,0}^{\text{complex}}, V_{l,k,0}^{[\text{ring}],\text{complex}}, t)\right] = \operatorname{Im}\left[e^{i\omega t} J_{l,k,\text{ref},0}^{\text{complex}}\right], \tag{2.5.56}$$

where

$$\begin{aligned} J_{l,k,\text{ref},0}^{\text{complex}} &:= J_{k,0}^{\text{complex}}\left[(\phi_{A,l,0}^{\text{complex}}, V_{l,k,0}^{[\text{ring}],\text{complex}})\right] \\ &= \begin{cases} V_{\text{ref}}\sigma_{\text{c},k} - i\omega \int_{\pi_{\text{circ}}\Omega_k^{[\text{ring}]}} \sigma_{\text{c}}^{[\text{ring}]} \phi_{A,l,0}^{\text{complex}} \, \mathrm{d}r \; \mathrm{d}z & \text{for } k = l, \\ \qquad\qquad - i\omega \int_{\pi_{\text{circ}}\Omega_k^{[\text{ring}]}} \sigma_{\text{c}}^{[\text{ring}]} \phi_{A,l,0}^{\text{complex}} \, \mathrm{d}r \; \mathrm{d}z & \text{for } k \neq l. \end{cases} \end{aligned} \tag{2.5.57}$$

Now for arbitrary complex numbers c_l^{complex}, $l \in \{1, \ldots, N\}$, the function $\phi_{A,0}^{\text{complex}}$ defined by

$$\phi_{A,0}^{\text{complex}} := \sum_{l=1}^{N} c_l^{\text{complex}} \phi_{A,l,0}^{\text{complex}} \tag{2.5.58}$$

is the solution to the problem (PDE: $\phi_{A,0}^{\text{complex}}$) with $V_{k,0}^{[\text{ring}],\text{complex}} = c_k^{\text{complex}} V_{\text{ref}}$, $k \in \{1, \ldots, N\}$. According to (2.5.35), (2.5.37), (2.5.56), (2.5.57), and (2.5.58), the corresponding total current in the k-th coil ring is given by

$$J_k\left[(\phi_{A,0}^{\text{complex}}, c_k^{\text{complex}} V_{\text{ref}}, t)\right] = \operatorname{Im}\left[e^{i\omega t} \sum_{l=1}^{N} c_l^{\text{complex}} J_{l,k,\text{ref},0}^{\text{complex}}\right]. \tag{2.5.59}$$

It remains to determine the numbers c_l^{complex}, $l \in \{1, \ldots, N\}$, such that

$$(\phi_{A,0}^{\text{complex}}, c_1^{\text{complex}} V_{\text{ref}}, \ldots, c_N^{\text{complex}} V_{\text{ref}})$$

is a solution to (2.5.40) or (2.5.45), respectively.

Prescription of Total Current: The numbers c_l^{complex} must satisfy the linear system

$$J_{\text{given},0} = \sum_{l=1}^{N} c_l^{\text{complex}} J_{l,k,\text{ref},0}^{\text{complex}}, \quad k \in \{1,\dots,N\}. \tag{2.5.60}$$

Prescription of Total Voltage: The numbers c_l^{complex} must satisfy the linear system

$$V_{\text{total},0} = \sum_{l=1}^{N} c_l^{\text{complex}} V_{\text{ref}}, \tag{2.5.61a}$$

$$\sum_{l=1}^{N} c_l^{\text{complex}} J_{l,k,\text{ref},0}^{\text{complex}} = \sum_{l=1}^{N} c_l^{\text{complex}} J_{l,k+1,\text{ref},0}^{\text{complex}}, \quad k \in \{1,\dots,N-1\}. \tag{2.5.61b}$$

Prescription of Total Power: Assume that $(c_{1,\text{ref}}^{\text{complex}},\dots,c_{N,\text{ref}}^{\text{complex}})$ denotes the solution to (2.5.61) with $V_{\text{total},0} = V_{\text{ref}}$, i.e. to (2.5.61b) combined with $\sum_{l=1}^{N} c_l^{\text{complex}} = 1$. Then for each $\lambda \in \mathbb{R}$, it is

$$(\lambda c_{1,\text{ref}}^{\text{complex}},\dots,\lambda c_{N,\text{ref}}^{\text{complex}}) \tag{2.5.62}$$

the solution to (2.5.61) with $V_{\text{total},0} = \lambda V_{\text{ref}}$, and

$$\phi_{A,0}^{\lambda,\text{complex}} := \lambda \sum_{l=1}^{N} c_l^{\text{complex}} \phi_{A,l,0}^{\text{complex}} \tag{2.5.63}$$

is the solution to (PDE: $\phi_{A,0}^{\text{complex}}$) with $V_{k,0}^{[\text{ring}],\text{complex}} = \lambda c_k^{\text{complex}} V_{\text{ref}}$, $k \in \{1,\dots,N\}$. A computation analogous to the one preceding (2.5.53) yields the corresponding average total power:

$$\overline{P_{\text{total,ref},\lambda}} = \frac{\lambda^2 V_{\text{ref}} \operatorname{Re}\left[\sum_{l=1}^{N} c_l^{\text{complex}} J_{l,1,\text{ref},0}^{\text{complex}}\right]}{2}. \tag{2.5.64}$$

Thus, to prescribe the average total power P, one has to set

$$\lambda = \sqrt{\frac{2P}{V_{\text{ref}} \operatorname{Re}\left[\sum_{l=1}^{N} c_l^{\text{complex}} J_{l,1,\text{ref},0}^{\text{complex}}\right]}}. \tag{2.5.65}$$

Chapter 3

Finite Volume Method

In Ch. 2, boldface is used to denote vector- and matrix-valued quantities. Accordingly, in the present chapter, boldface denotes matrices and vectorial *physical* quantities occurring in examples. However, to avoid an overuse of boldfaced symbols, vectors occurring in abstract mathematical settings are *not* set in boldface.

3.1 The Considered Problem Class and Scope of the Treatment

Chapter 3 contains a mathematical treatment of the finite volume method, which is used for the discretization of partial differential equations such as occurring in (2.1.34), (2.2.1), and (2.5.32). The first main objective is the rigorous formulation of a finite volume scheme in a setting suitable to be used for the transient numerical simulations of temperature field evolutions presented in Ch. 4. The second main objective is to prove discrete a priori estimates for the resulting finite volume scheme, leading to the existence and uniqueness of a discrete solution. In future work, the goal is to proceed to establish the convergence of the finite volume scheme; however, this is outside the scope of the material presented here.

Even though the contents of this chapter is dedicated to transient problems of the form (3.1.1), the formulation of the finite volume discretization for stationary prolems lacking the term $\partial_t b_j[(u_j, t, x)]$ in (3.1.1) (such as (2.5.32)) can be done analogously. Omitting the time discretization step, one ends up with the finite volume discretization (3.7.122) without the first summand (3.7.122a) which involves the time step $t_\nu - t_{\nu-1}$. However, the proof of the existence and uniqueness of a discrete solution makes essential use of the presence of the time derivative or, more precisely, of the presence of the term involving the time step in the discrete scheme.

Similar remarks apply to other features of (3.1.1): The formulation of the finite volume discretization is done in a more general setting than the proof of discrete existence and uniqueness, e.g. since different mathematical techniques are needed depending on the type of (3.1.1). For example, during the formulation of the discretization, the range of the unknown u is allowed to be some arbitrary subset of $\mathbb{C}$, but for the mathematical results in Secs 3.7.13 and 3.8, the range is assumed to be of the form $[m, \infty[$. Furthermore, boundedness and regularity conditions are added in Ths 3.7.50 and 3.8.35.

The setting of (3.1.1) is rather general in the sense that each term is allowed to depend nonlinearly on the solution u_j as well as on the space variable x and the time variable t. In its full generality, (3.1.1) comprehends a vast abundance of interesting examples, including those enumerated in Ex. 3.1.1. However, since the mathematical results of Secs 3.7.13 and 3.8 are restricted to the transient case and to a solution range of the form $[m, \infty[$, in Ex. 3.1.1, it only applies to (b) and the first case of (a). In Ex. 3.1.1(b), Eq. (3.1.1) plays the role of a heat transport equation including the time derivative of an internal energy term, diffusion, convection, and source and sink terms.

Even though different equations on different space domains coupled via spatial interfaces are allowed in this treatment, only a single equation is considered on the same space domain. For example, (3.1.1) can represent either one of the equations in (2.1.34), but the discretization of the coupled system (2.1.34) is beyond the scope of this work. Systems are treated e.g. in [EGH00, Ch. VII].

The interface and boundary conditions allow for nonlocal terms as they arise during radiation modeling (s. Exs 3.1.2(c) and 3.1.3(e)).

Section 3.6 addresses the problem of dimension reduction by a change of variables in the case the problem at hand displays an exploitable symmetry. This is relevant to the simulation application in Ch. 4, where cylindrical coordinates are used to take advantage of the cylindrical symmetry of the problem.

Now the problem class will be stated and some examples will be considered. As described above, the objects of interest are rather general nonlinear partial differential equations of the form

$$\partial_t b_j[(u_j, t, x)] - \operatorname{div}\left(k_j[(u_j, t, x)]\, \nabla u_j\right) + \operatorname{div} v_j[(u_j, t, x)] - f_j[(u_j, t, x)] = 0 \quad (3.1.1)$$

for the unknown function u_j defined on the time-space domain

$$\tau \times \Omega_j = [t_0, t_{\mathrm{f}}] \times \Omega_j, \quad (3.1.2)$$

where Ω_j is a d-dimensional space domain, $d \in \mathbb{N}$. For the major part of the sequel, it is assumed that the set Ω_j is polyhedral, in which case it is denoted by p_j. It is assumed that there is a finite number of domains Ω_j, i.e. there is a finite index set J such that the set of domains is $\{\Omega_j : j \in J\}$. If there is no time dependence in (3.1.1) and if b_j vanishes, then one deals with the corresponding stationary problem.

Example 3.1.1. Except in the second case of (b), the index $j \in J$ plays no role in the present example. Thus, except in the second case of (b), the index j is suppressed, i.e. u, b, k, v, and f is written instead of u_j, b_j, k_j, v_j, and f_j.

(a) *Hyperbolic Balance Equations*: For example, one can get (2.1.34a) by setting $u := \rho_{\mathrm{gas}}$, $b[(u,t,x)] := u$, $k[(u,t,x)] := 0$, $v[(u,t,x)] := u\,\mathbf{v}_{\mathrm{gas}}[(t,x)]$, and $f[(u,t,x)] := 0$.

To get the i-th component of (2.1.34b), $i \in \{1,2,3\}$, set $u := (\mathbf{v}_{\mathrm{gas}})_i$, $b[(u,t,x)] := \rho_{\mathrm{gas}}[(t,x)]\,u$, $k[(u,t,x)] := 0$, $v[(u,t,x)] := \frac{R}{M^{(\mathrm{Ar})}}\,\rho_{\mathrm{gas}}[(t,x)]\,T_{\mathrm{gas}}[(t,x)]\,\mathbf{e}_i$, where $\mathbf{e}_i$ denotes the unit vector in the i-th coordinate direction, and $f[(u,t,x)] := \rho_{\mathrm{gas}}[(t,x)]\,g_i$.

(b) *Transient Heat Equations*: For example, one can get (2.1.34c) by setting $u := T_{\mathrm{gas}}$, $b[(u,t,x)] := \frac{z^{(\mathrm{Ar})}R}{M^{(\mathrm{Ar})}}\rho_{\mathrm{gas}}[(t,x)]\,u$, $k[(u,t,x)] := \kappa^{(\mathrm{Ar})}[(u,t,x)]$, $v[(u,t,x)] := \frac{\left(z^{(\mathrm{Ar})}+1\right)R}{M^{(\mathrm{Ar})}}\,\rho_{\mathrm{gas}}[(t,x)]\,u\,\mathbf{v}_{\mathrm{gas}}[(t,x)]$, and $f[(u,t,x)] := \rho_{\mathrm{gas}}[(t,x)]\,\mathbf{g} \bullet \mathbf{v}_{\mathrm{gas}}[(t,x)]$. Here, the radiation term $r^{(\mathrm{Ar})}$ is neglected, as it typically shows a nonlocal volumetric space dependence inside the gas region, and the detailed modeling of this term is outside the scope of this work.

One can get (2.2.1) by setting $u_j := T^{[\beta_j]}$, $b_j[(u_j,t,x)] := \rho^{[\beta_j]}[(t,x)]\,\varepsilon[(u_j,t,x)]$, where $\varepsilon[(u_j,t,x)] = \int_0^{u_j} c_{\mathrm{sp}}^{[\beta_j]}[(y,t,x)]\,\mathrm{d}y$, $k_j[(u_j,t,x)] := \kappa^{[\beta_j]}[(u_j,t,x)]$, $v_j[(u_j,t,x)] := 0$, and $f_j[(u_j,t,x)] := f^{[\beta_j]}[(u_j,t,x)]$.

As another example consider the slightly different form of the gas energy balance (where, as above, the volumetric radiation term $\rho_{\mathrm{gas}} r_{\mathrm{gas}}$ has been dropped)

$$\rho_{\mathrm{gas}}\,\partial_t \varepsilon_{\mathrm{gas}} + \rho_{\mathrm{gas}}\mathbf{v}_{\mathrm{gas}} \bullet \nabla\,\varepsilon_{\mathrm{gas}} - \operatorname{div}(\kappa_{\mathrm{gas}}\,\nabla\,T_{\mathrm{gas}}) + p_{\mathrm{gas}}\operatorname{div}\mathbf{v}_{\mathrm{gas}} = 0, \tag{3.1.3}$$

that was used in [BKP+99, (2.18c)], also cf. (2.1.14c).

Equation (3.1.3) can be written in the form (3.1.1) by using

$$\rho_{\mathrm{gas}}\mathbf{v}_{\mathrm{gas}} \bullet \nabla\,\varepsilon_{\mathrm{gas}} = \operatorname{div}(\varepsilon_{\mathrm{gas}}\,\rho_{\mathrm{gas}}\mathbf{v}_{\mathrm{gas}}) - \varepsilon_{\mathrm{gas}}\operatorname{div}(\rho_{\mathrm{gas}}\mathbf{v}_{\mathrm{gas}}), \tag{3.1.4}$$

and then letting $u := T_{\mathrm{gas}}$, $b[(u,t,x)] := \rho_{\mathrm{gas}}[(t,x)]\,\varepsilon_{\mathrm{gas}}[(u,t,x)]$, $k[(u,t,x)] := \kappa_{\mathrm{gas}}[(u,t,x)]$, $v[(u,t,x)] := \varepsilon_{\mathrm{gas}}[(u,t,x)]\,\rho_{\mathrm{gas}}[(t,x)]\,\mathbf{v}_{\mathrm{gas}}[(t,x)]$, and

$$f[(u,t,x)] := \varepsilon_{\mathrm{gas}}[(u,t,x)]\,\operatorname{div}\left(\rho_{\mathrm{gas}}[(t,x)]\,\mathbf{v}_{\mathrm{gas}}[(t,x)]\right) - p_{\mathrm{gas}}[(t,x)]\,\operatorname{div}\mathbf{v}_{\mathrm{gas}}[(t,x)].$$

(c) *Stationary Heat Equations*: By setting $b[(u,t,x)] := 0$ and $b_j[(u_j,t,x)] := 0$, respectively, in the examples in (b) and assuming all functions to be time-independent.

(d) *Elliptic Equations*: For example, one can get (2.5.32b) by setting $u := r\phi_{A,0}^{\mathrm{complex}}$, $b\big[\big(u,t,(r,z)\big)\big] := 0$, $k\big[\big(u,t,(r,z)\big)\big] := \frac{\nu}{r^2}$, $v\big[\big(u,t,(r,z)\big)\big] := 0$, and

$$\begin{aligned} f\big[\big(u,t,(r,z)\big)\big] := & \frac{\sigma_{\mathrm{c}}^{[\mathrm{ring}]}\big[\big(t,(r,z)\big)\big]\,V_{k,0}^{[\mathrm{ring}],\mathrm{complex}}\big[\big(t,(r,z)\big)\big]}{2\pi r^2} \\ & - \frac{i\,\omega\,\sigma_{\mathrm{c}}^{[\mathrm{ring}]}\big[\big(t,(r,z)\big)\big]\,u}{r^2}. \end{aligned}$$

(e) *Richards Equation*: It reads

$$\partial_t \theta[(u,x)] - \operatorname{div}\big(K[(u,x)]\,(\nabla u - \mathbf{g})\big) = 0, \tag{3.1.5}$$

where θ denotes the saturation, K denotes permeability, u denotes the capillary pressure, and $\mathbf{g}$ denotes gravity. Richards Equation describes saturated-unsaturated fluid transport in porous media (cf. [Ric31]). To fit (3.1.5) into the framework of (3.1.1), one lets

$$\begin{aligned} b[(u,t,x)] &:= \theta[(u,x)], & k[(u,t,x)] &:= K[(u,x)], \\ v[(u,t,x)] &:= K[(u,x)]\,\mathbf{g}[x], & f[(u,t,x)] &:= 0. \end{aligned}$$

Also cf. [FL01, Sec. 6.6].

—

On $(d-1)$-dimensional interfaces $\gamma = \gamma_{j_1,j_2}$ between adjacent domains Ω_{j_1} and Ω_{j_2}, *interface conditions* for the unknown functions u_{j_1} and u_{j_2} and the fluxes $F_{j_1} := k_{j_1}[(u_{j_1},t,x)]\,\nabla u_{j_1}$ and $F_{j_2} := k_{j_2}[(u_{j_2},t,x)]\,\nabla u_{j_2}$ are considered. The unknown functions either satisfy the *continuity interface condition*

$$u_{j_1}\restriction_{\tau\times\gamma} = u_{j_2}\restriction_{\tau\times\gamma} \tag{3.1.6a}$$

or a *jump interface condition* of the form

$$F_{j_1} \bullet n_{\Omega_{j_1}} + a^{\gamma,1}_{\text{jump}}[(u_{j_1},t,x)] - a^{\gamma,2}_{\text{jump}}[(u_{j_2},t,x)] = 0 \quad \text{on} \quad \tau\times\gamma, \tag{3.1.6b}$$

where n denotes the outer unit normal vector. The fluxes satisfy an interface condition of the form

$$\begin{aligned} F_{j_1} \bullet n_{\Omega_{j_1}} - F_{j_2} \bullet n_{\Omega_{j_1}} - \mathcal{A}_\gamma\left[\left(u_j\restriction_{\{t\}\times\Omega_j}\right)_{j\in J}\right][x] \\ - a^{\gamma,1}_{\text{flux}}[(u_{j_1},t,x)] + a^{\gamma,2}_{\text{flux}}[(u_{j_2},t,x)] = 0 \quad \text{on} \quad \tau\times\gamma. \end{aligned} \tag{3.1.7}$$

Conditions (3.1.6) are similar to condition [EGH00, (11.14)], which occurs in a time-independent setting and has the form $u_{j_2}\restriction_\gamma - u_{j_1}\restriction_\gamma = a^{(\gamma)}_{\text{jump}}[x]$. However, in contrast to [EGH00, (11.14)], according to (3.1.6) the solution is either continuous at γ or satisfies a jump condition *involving the flux*, where a nonlinear dependence on the solution is allowed in the functions $a^{\gamma,1}_{\text{jump}}$ and $a^{\gamma,2}_{\text{jump}}$. For applications involving (3.1.6) see Exs 3.1.2(a),(b) below.

Condition (3.1.7) is in generalization of [EGH00, (11.13)], where [EGH00, (11.13)] is a time-independent condition of the same form as (3.1.7), but only admitting positive real numbers instead of the potentially nonlinear functions k_{j_1} and k_{j_2}, and without a nonlocal coupling term $\mathcal{A}_\gamma$. The introduction of the operator $\mathcal{A}_\gamma$ into (3.1.7) allows to account for nonlocal radiation operators such as $\epsilon_{\mathrm{r}}(\mathcal{J}_{\mathrm{r}} \circ \mathcal{R}_{\mathrm{r}})$ and $\epsilon_{\mathrm{t}}(\mathcal{J}_{\mathrm{t}} \circ \mathcal{R}_{\mathrm{t}})$ in (2.4.39). Thus, in practice, the operator $\mathcal{A}_\gamma$ merely depends on the functions u_j defined on domains adjacent to the radiation region under consideration (more precisely, it depends on the restrictions of such functions u_j to the respective interfaces).

Example 3.1.2 shows how the interface conditions arising in Secs 2.3, 2.4.4, and 2.5.6 fit into the framework of (3.1.6) and (3.1.7).

Example 3.1.2. (a) *Continuous Temperature*: It is seen immediately that (2.3.2a), (2.3.2b), and (2.5.32e) are of the form (3.1.6a).

(b) *Temperature Jump*: To write (2.3.2b′) in the form (3.1.6b), let $u_{j_1} := T_{\mathrm{gas}}$, $u_{j_2} := T^{[\beta]}$, $k_{j_1} := \kappa^{(\mathrm{Ar})}$, $n_{\Omega_{j_1}} := \mathbf{n}_{\mathrm{gas}}$, $a^{\gamma,1}_{\mathrm{jump}}[(u_{j_1}, t, x)] := \xi_\beta u_{j_1}$, and $a^{\gamma,2}_{\mathrm{jump}}[(u_{j_2}, t, x)] := \xi_\beta u_{j_2}$, $\xi \in \mathbb{R}^+$.

(c) *Heat Flux Including Radiation*: If (2.1.33h) and (2.2.1b) hold, then each of the Eqs (2.4.39) can be written in the form (3.1.7), as is demonstrated below. In the considered cases, the operator $\mathcal{A}_\gamma$ acting on the family $\left[(u_j\restriction_{\{t\}\times\Omega_j})_{j\in J}\right]$ is defined in terms of a radiation operator acting on T_{solid}. The precise meaning of such a definition is the following: The radiation operator acts on all temperature functions $u_j := T_{\mathrm{solid}}\restriction_{\Omega_j}$, $j \in J_\gamma$, where J_γ is such that the family $(\Omega_j)_{j\in J_\gamma}$ includes all solid domains adjacent to the same radiation region as γ (s. Fig. 3.1).

For (2.4.39a), let $u_{j_1} := T_{\mathrm{solid}}\restriction_{\Omega^{[\mathrm{SiC-Crystal}]}}$, $u_{j_2} := T_{\mathrm{solid}}\restriction_{\Omega^{[\beta]}}$, $k_{j_1} := \kappa^{[\mathrm{SiC-Crystal}]}$, $k_{j_2} := \kappa^{[\beta]}$, $n_{\Omega_{j_1}} := \mathbf{n}^{[\mathrm{SiC-Crystal}]} = -\mathbf{n}^{[\beta]}$,

$$\mathcal{A}_\gamma\left[\left(u_j\restriction_{\{t\}\times\Omega_j}\right)_{j\in J}\right] := \epsilon_{\mathrm{t}}[(u_{j_2}, x)]\,\mathcal{J}_{\mathrm{t}}\left[\mathcal{R}_{\mathrm{t}}[T_{\mathrm{solid}}]\right],$$

$a^{\gamma,1}_{\mathrm{flux}} := 0$, and $a^{\gamma,2}_{\mathrm{flux}}[(u_{j_2}, t, x)] := \epsilon_{\mathrm{t}}[(u_{j_2}, x)]\,\sigma\,u^4_{j_2}$.

For (2.4.39b), let $u_{j_1} := T_{\mathrm{gas}}$, $u_{j_2} := T_{\mathrm{solid}}\restriction_{\Omega^{[\beta]}}$, $k_{j_1} := \kappa_{\mathrm{gas}}$, $k_{j_2} := \kappa^{[\beta]}$, $n_{\Omega_{j_1}} := \mathbf{n}_{\mathrm{gas}} = -\mathbf{n}^{[\beta]}$,

$$\mathcal{A}_\gamma\left[\left(u_j\restriction_{\{t\}\times\Omega_j}\right)_{j\in J}\right] := \epsilon_{\mathrm{r}}[(u_{j_2}, x)]\,\mathcal{J}_{\mathrm{r}}\left[\mathcal{R}_{\mathrm{r}}[T_{\mathrm{solid}}]\right] + \epsilon_{\mathrm{t}}[(u_{j_2}, x)]\,\mathcal{J}_{\mathrm{t}}\left[\mathcal{R}_{\mathrm{t}}[T_{\mathrm{solid}}]\right],$$

$a^{\gamma,1}_{\mathrm{flux}} := 0$, and $a^{\gamma,2}_{\mathrm{flux}}[(u_{j_2}, t, x)] := (\epsilon_{\mathrm{r}} + \epsilon_{\mathrm{t}})[(u_{j_2}, x)]\,\sigma\,u^4_{j_2}$.

For (2.4.39c), let $u_{j_1} := T_{\mathrm{gas}}$, $u_{j_2} := T_{\mathrm{solid}}\restriction_{\Omega^{[\mathrm{SiC-Crystal}]}}$, $k_{j_1} := \kappa_{\mathrm{gas}}$, $k_{j_2} := \kappa^{[\mathrm{SiC-Crystal}]}$, $n_{\Omega_{j_1}} := \mathbf{n}_{\mathrm{gas}} = -\mathbf{n}^{[\mathrm{SiC-Crystal}]}$,

$$\mathcal{A}_\gamma\left[\left(u_j\restriction_{\{t\}\times\Omega_j}\right)_{j\in J}\right] := \epsilon_{\mathrm{r}}[(u_{j_2}, x)]\,\mathcal{J}_{\mathrm{r}}\left[\mathcal{R}_{\mathrm{r}}[T_{\mathrm{solid}}]\right],$$

$a^{\gamma,1}_{\mathrm{flux}} := 0$, and $a^{\gamma,2}_{\mathrm{flux}}[(u_{j_2}, t, x)] := \epsilon_{\mathrm{r}}[(u_{j_2}, x)]\,\sigma\,u^4_{j_2}$.

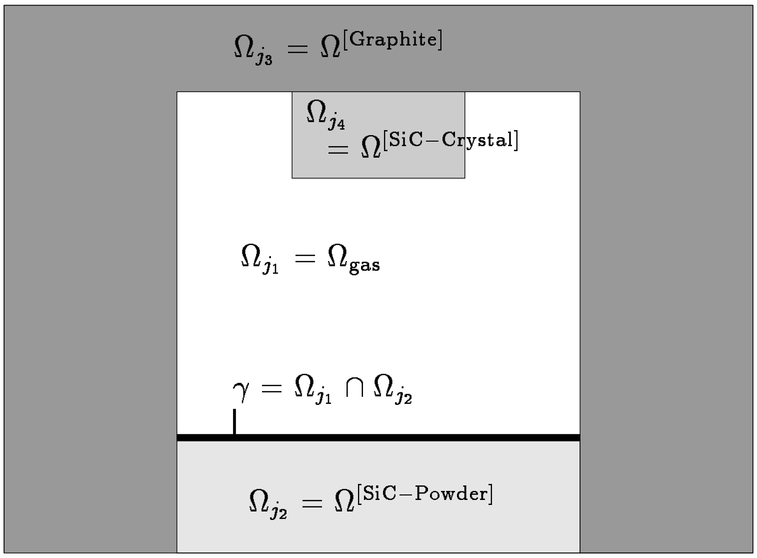

Figure 3.1: If the radiation region is given by Ω_{gas}, then the set of indices corresponding to the adjacent solid domains is given by $J_\gamma = \{j_2, j_3, j_4\}$.

(d) *Magnetic Scalar Potential Flux*: To verify that (2.5.32d) is of the form (3.1.7), let $u_{j_1} := u_{j_2} := r\,\phi_{A,0}^{\text{complex}}$, $k_{j_1} := \frac{\nu_{\gamma_1}}{r}$, $k_{j_2} := \frac{\nu_{\gamma_2}}{r}$, $n_{\Omega_{j_1}} := \mathbf{n}_{\gamma_1}$, $\mathcal{A}_\gamma := 0$, and $a_{\text{flux}}^{\gamma,1} := a_{\text{flux}}^{\gamma,2} := 0$.

—

In general, the outer boundary of Ω_j (i.e. the part of the boundary that is not an interface) is partitioned into disjoint $(d-1)$-dimensional parts $\Gamma_{j,\text{Dir}}$ and $\Gamma_{j,\iota}$, $\iota \in J_j$, where different types of *outer boundary conditions* are considered. Outer boundary conditions are either of *Dirichlet type* or of *non-Dirichlet type*. Outer boundary conditions of Dirichlet type have the form

$$u_j[(t,x)] = u_{j,\text{Dir}}[(t,x)] \quad \text{on} \quad \tau \times \Gamma_{j,\text{Dir}}. \tag{3.1.8}$$

Outer boundary conditions of non-Dirichlet type have the form

$$F_j \bullet n_{\Omega_j} - \mathcal{B}_{j,\iota}\left[\left(u_j\restriction_{\{t\}\times\Omega_j}\right)_{j\in J}\right] + a_{\text{out}}^{j,\iota}[(u_j,t,x)] = 0 \quad \text{on} \quad \tau \times \Gamma_{j,\iota}. \tag{3.1.9}$$

Conditions (3.1.8) and (3.1.9) are in generalization of [EGH00, (11.10) – (11.12)]. Some important special cases are considered in Ex. 3.1.3, where [EGH00, (11.10) – (11.12)] are actually special cases of Exs 3.1.3 (a), (b), and (c).

Example 3.1.3. (a) *Zero Dirichlet Condition*: This is the case $u_{j,\text{Dir}} = 0$ as in (2.5.32f).

(b) *Neumann Condition*: Condition (3.1.9), where $\mathcal{B}_{j,\iota} = 0$ and $a_{\text{out}}^{j,\iota}$ does not depend on u_j. A Neumann condition is called a *zero flux condition* iff $a_{\text{out}}^{j,\iota} = 0$.

(c) *Condition of Third Kind*: Condition (3.1.9), where $\mathcal{B}_{j,\iota} = 0$ and $a^{j,\iota}_{\text{out}}$ has the form $a^{j,\iota}_{\text{out}}[(u_j, t, x)] = \xi \left(u_j - u_{\text{ext},j,\iota}[(t, x)]\right)$, $\xi \in \mathbb{R}^+$.

(d) *Emission Condition*: This is the type of outer boundary condition written in (2.3.3), where $\mathcal{B}_{j,\iota} = 0$ and $a^{j,\iota}_{\text{out}}[(u_j, t, x)] = \sigma\, \epsilon^{[\beta]}[(u_j, x)]\, \left(u_j^4 - T^4_{\text{room}}\right)$ with $u_j := T^{[\beta]}$.

(e) *Nonlocal Radiation Condition*: This is the type of outer boundary condition written in (2.4.17), where

$$\mathcal{B}_{j,\iota}\left[\left(u_{\underline{j}}\restriction_{\{t\}\times\Omega_{\underline{j}}}\right)_{\underline{j}\in J}\right] := \epsilon[(u_j, x)] \cdot \mathcal{J}\left[\mathcal{R}[T_{\text{solid}}]\right]$$

and $a^{j,\iota}_{\text{out}}[(u_j, t, x)] = \epsilon[(u_j, x)]\, \sigma\, u_j^4$ with $u_j := T_{\text{solid}}$. An analogous note as made at the beginning of Ex. 3.1.2(c) applies to the present situation.

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Finally, an initial condition

$$u_j[(t_0, x)] = u_j^{(0)}[x] \tag{3.1.10}$$

prescribes the solution u_j at time t_0 in the transient case.

3.2 Literature Review

Finite volume techniques for the solution of partial differential equations have been used in the literature at least since [Mac53], where the method is used to discretize the elliptic equation $-\operatorname{div}\left(k[(t, x)]\, \nabla u\right) - f[(u, t, x)] = 0$, allowing linear dependence of f on u. Finite volume schemes for more general linear elliptic problems are studied in [Hei87] and [Hei88], including results on convergence of the scheme. Finite volume discretizations for linear elliptic problems are also treated in [Bey98], focussing on aspects of adaptive grid refinement and multi-grid methods.

An extensive survey on the finite volume method can be found in [EGH00]. In [EGH00], elliptic problems ([EGH00, Chs II and III]) are considered as well as hyperbolic problems ($b_j[(u, t, x)] = u$, $k_j = 0$, $v \not\equiv 0$, [EGH00, Chs V – VII]), and parabolic problems ($b_j[(u, t, x)] = u$, $k_j > 0$, [EGH00, Ch. IV]). Convergence results and error estimates are presented for both linear and nonlinear cases.

Even though, in the following Secs 3.3 – 3.7, the finite volume discretization is developed for the general form of (3.1.1), in view of the numerical applications in Ch. 4, the main focus of this work is the fully nonlinear parabolic case of (3.1.1), allowing mixed, nonlinear and nonlocal boundary and interface conditions. In particular, the discrete a priori estimates of Sec. 3.7.13 and the proof of discrete existence and uniqueness in Sec. 3.8 are mainly designed for the parabolic case, even though certain hyperbolic cases (such as the first case of Ex. 3.1.1(a)) are included as well. Special cases are considered in [FL01] and in [EGH00, Ch. IV], and these situations are now briefly discussed.

In [FL01], a finite volume discretization is considered for equations $\partial_t b_j[(u_j, x)] - \operatorname{div}\left(k_j[(u_j, x)]\,\nabla u_j\right) + \operatorname{div} v_j[(u_j, x)] = 0$, where the solution is supposed to be continuous across interfaces. In [FL01], the equations are completed by special mixed boundary conditions of Dirichlet form (3.1.8) and non-Dirichlet form (3.1.9) ($\mathcal{B}_{j,\iota} = 0$), and discrete existence and uniqueness results are proved as well as a maximum principle and stability. The structure of the treatment in [FL01] is completely different from the structure of the treatment in this work: Whereas the hypotheses in this work are usually formulated in terms of properties of the input functions b_j, k_j, etc., the hypotheses in [FL01] are provided in terms of (monotonicity) properties of the finite volume discretization, which have to be verified for a given concrete class of problems. Moreover, the existence theory in [FL01] is based on matrix theory rather than on L^∞-L^1 a priori estimates and the Banach Fixed Point Theorem. Neither time dependence of the input functions, nor source and sink terms f_j, nor jump interface conditions, nor nonlocal interface or boundary conditions are considered in [FL01].

In [EGH00, Sec. 17], error estimates are proved for a finite volume scheme for the linear parabolic equation $\partial_t u - \operatorname{div}\nabla u + \operatorname{div}(u\,v[(t,x)] - f[(u,t,x)] = 0$, where f depends linearly on u, with Dirichlet boundary conditions. In [EGH00, Sec. 18], a maximum principle and a convergence result are established for a finite volume scheme for the (degenerate) nonlinear parabolic equation $\partial_t u - \operatorname{div}\left(k[(u,t,x)]\,\nabla u\right) - f[(t,x)] = 0$ with a zero flux boundary condition (cf. Ex. 3.1.3(b)).

In this work, (3.1.1) is always considered in the context of an initial-boundary value problem, i.e. the evolution equation is completed by initial conditions and boundary conditions. However, in the literature, the finite volume method is also used as a discretization procedure for initial value problems, where the evolution equation is completed by initial conditions together with so-called entropy conditions. For literature on this subject, it is referred to [Krö97], [Ohl01], and references therein.

The continuous solution theory of initial-boundary value problems for evolution equations is studied in a vast number of papers and textbooks, e.g. [GGZ74, Chs IV – VII], [Wlo82, Ch. IV], [Zei90, Ch. 23], [RR96, Ch. 10], and [CH98], just to mention a few. However, especially for nonlinear problems, nonsmooth domains, and for problems with mixed, nonlinear, and/or nonlocal boundary and interface conditions, there are still many open problems concerning existence, uniqueness, and regularity questions. Existence, uniqueness, and regularity results for linear parabolic problems with mixed boundary conditions of Dirichlet and Neumann type (cf. (3.1.8) and Ex. 3.1.3(b)) on Lipschitz domains are provided in [Gri99, Ch. 2]. In [Tii97], existence and uniqueness is proved for an elliptic diffusion-convection problem ($b_j = 0$) with nonlinear and nonlocal interface and boundary conditions arising from radiative heat transfer as described in Exs 3.1.2(c) and 3.1.3(d),(e). In [LT00] results of [Tii97] are proved with weaker hypotheses and existence and uniqueness are also established for the corresponding parabolic case ($b[(u,t,x)] = u$). References for the existence of a solution for the problem class studied in [EGH00, Sec. 18] (see above) are provided therein.

3.3 The Evolution Equation

The subject of the present Sec. 3.3 and also of the following Sec. 3.4 is to provide the mathematical setting for the subsequent study of partial differential equations of the form (3.1.1), subsequently called *evolution equations*, by means of the finite volume method.

First, in the present section, the case of a single evolution equation is considered: the continuous setting in Sec. 3.3.1 and the time discretization in Sec. 3.3.2.

Then, in Sec. 3.4, the case of several evolution equations (3.1.1) is treated, each equation living on a different spatial domain, where coupling occurs via local and nonlocal interface conditions. Outer boundary conditions are also treated in Sec. 3.4. Analogous to Sec. 3.3, Sec. 3.4 covers both the continuous and the time-discrete case.

In preparation of the space discretization and the formulation of a finite volume scheme in Sec. 3.7, Sec. 3.5 provides an integral formulation of coupled systems of evolution equations (3.1.1) including interface and boundary conditions.

3.3.1 Continuous Setting

Since only a single equation is considered in the current section, the subscript j occurring in (3.1.1) is dropped:

$$\partial_t b[(u,t,x)] - \operatorname{div}\big(k[(u,t,x)]\,\nabla u\big) + \operatorname{div} v[(u,t,x)] - f[(u,t,x)] = 0. \tag{3.3.1}$$

As described in Sec. 3.1, it is the purpose of (3.3.1) to determine the *unknown function* u, defined on a *time-space domain* $\tau \times p$, where τ is a *time domain* and p is a d-dimensional polyhedral *space domain*, $d \in \mathbb{N}$. It is assumed that u has its range in the set $v \subseteq \mathbb{K}$, where $\mathbb{K} = \mathbb{R}$ or $\mathbb{K} = \mathbb{C}$.

Throughout Ch. 3, τ denotes the compact time interval $\tau := [t_0, t_{\mathrm{f}}]$ with *initial time* t_0 and *final time* t_{f}. Moreover, d always denotes the dimension of the space domain, and v always denotes the range of the unknown.

In the sequel, space domains are always (closed) polytopes, i.e. bounded polyhedral sets, cf. App. C.4.2. Most of the theory could also be developed for more general domains having sufficiently regular boundaries. The restriction to polytopes avoids certain difficulties, not the least being of notational and technical nature, arising in the case that e.g. the boundaries of the domains are more general manifolds of codimension one.

As the constituent functions b, k, v, and f of (3.3.1) are allowed to depend on the unknown, they are typically defined on a domain of the form $\upsilon \times \tau \times p$. To include Ex. 3.1.1(d), b, k, and f are allowed to be $\mathbb{C}$-valued. However, to allow the use of an upwind function according to Def. 3.7.14 in the formulation of the finite volume discretization in Sec. 3.7, v is assumed to be $\mathbb{R}^d$-valued. For the proof of the discrete a priori estimate in Sec. 3.7.13 and of the existence and uniqueness of a discrete solution in Sec. 3.8, b, k, and f are also assumed to be real-valued.

In its full generality, the question of what regularity one can expect for a solution u of (3.3.1) is very difficult. The answer depends on the particular type of the equation, on the regularity of input functions, on the boundary and interface conditions, and on the regularity of the domains. Hence, the final choice of solution spaces is inexorably linked with the continuous solution theory (for details, it is referred to the literature, see the last paragraph of Sec. 3.2). Since the continuous solution theory is not the subject of this work, matters concerning regularity and weak differentiability are not considered in detail, except where needed in the formulation of the finite volume scheme, the discrete existence theory, and the discrete a priori estimates. Naturally, regularity and weak differentiability questions have to be investigated in more depth to consider the convergence of the finite volume schemes.

Even though detailed regularity and differentiability questions are not the main objective of this work, some words on the meaning of (3.3.1) in a rigorous framework are in order. In general, each of the functions b, v, k, and f can depend on the time coordinate t, on the spatial location x, and on the value of the unknown at (t, x). The regularity of b, v, k, f, and of the unknown u need to be such that each term in (3.3.1) has meaning, at least in a certain weak sense (cf. Rem. 3.3.2 below). In addition, solutions to (3.3.1) are assumed to be continuous in this work, notwithstanding the fact that, especially for higher values of d, the existence of continuous solutions can not be guaranteed in general, and weaker requirements for the solution can be mathematically reasonable. In the case where different equations of the form (3.1.1) are coupled via spatial interfaces (cf. Sec. 3.4), the solutions u_j are not always assumed to fit together continuously, but discontinuities between the u_j are required at jump interfaces according to condition (3.1.6b).

In this work, continuity of the given functions b, v, k, and f is assumed, except at interfaces. It is known that in many cases less regularity suffices, e.g. f being square integrable with respect to time and space variables. However, continuity of the given functions is present for the simulation applications in Ch. 4, and its assumption allows considerable simplifications in the formulation of time and space discretization: It is used in (3.3.9) that b, v, k, and f can be evaluated at discrete times $t_\nu \in \tau$, and it is used in Def. 3.7.41 that b, v, k, and f can be evaluated at points $y \in \upsilon$ and $x \in p$. Otherwise, more complicated approximations have to be used (cf. Rems 3.3.6 and 3.7.37).

For later reference, the setting for (3.3.1) is now summarized in Def. 3.3.1. Moreover, Def. 3.3.1 introduces an operator formulation of (3.3.1).

Definition 3.3.1. Let τ be the closed time interval, let p be a d-dimensional polytope, and let $\upsilon \subseteq \mathbb{K}$. Given

$$b \in C(\upsilon \times \tau \times p, \mathbb{K}), \tag{3.3.2a}$$
$$v \in C(\upsilon \times \tau \times p, \mathbb{R}^d), \tag{3.3.2b}$$
$$k \in C(\upsilon \times \tau \times p, \mathbb{K}), \tag{3.3.2c}$$
$$f \in C(\upsilon \times \tau \times p, \mathbb{K}), \tag{3.3.2d}$$

the *evolution operator* $H_{b,v,k,f}$ is defined by

$$\begin{aligned} H_{b,v,k,f}[u][(t,x)] :=& \partial_t b\big[(u[(t,x)],t,x)\big] + \operatorname{div}\big(v\big[(u[(t,x)],t,x)\big]\big) \\ &- \operatorname{div}\big(k\big[(u[(t,x)],t,x)\big]\,\nabla u[(t,x)]\big) - f\big[(u[(t,x)],t,x)\big]. \end{aligned} \tag{3.3.3}$$

Thus, $H_{b,v,k,f}$ maps a suitable subset $\mathcal{U}$ of $C(\tau \times p, \upsilon)$ into the set of all $\mathbb{K}$-valued functions on $\tau \times p$: $H_{b,v,k,f} : \mathcal{U} \longrightarrow \mathcal{F}(\tau \times p, \mathbb{K})$.

Then the corresponding *evolution equation* is defined by

$$H_{b,v,k,f}[u] = 0. \tag{3.3.4}$$

—

In a more concise form, (3.3.3) reads

$$H_{b,v,k,f}[u] = \partial_t(b \circ u^{\text{t.-sp.}}) + \operatorname{div}(v \circ u^{\text{t.-sp.}}) - \operatorname{div}\big((k \circ u^{\text{t.-sp.}})\,\nabla u\big) - f \circ u^{\text{t.-sp.}}, \tag{3.3.5}$$

where given $u : \tau \times p \longrightarrow \mathbb{K}$, the function $u^{\text{t.-sp.}}$ is defined by

$$u^{\text{t.-sp.}} : \tau \times p \longrightarrow \upsilon \times \tau \times p, \quad u^{\text{t.-sp.}}[(t,x)] := \big(u[(t,x)],t,x\big). \tag{3.3.6}$$

The use of $u^{\text{t.-sp.}}$ allows more concise and more precise formulations. However, in order not to burden the reader with this nonstandard notation, formulations of the form (3.3.3) are generally preferred in the sequel.

As a caveat, it is pointed out that (3.3.4) might be an equality of function classes (e.g. of elements of $L^2(\tau \times p, \mathbb{K})$) such that writing arguments means picking representatives from the classes.

Even though the right-hand side of (3.3.4) is 0, it does allow for source and sink terms by means of the function f.

Remark 3.3.2. In addition to the regularity assumptions on u, b, v, k, and f listed in Def. 3.3.1, these functions need to be such that the terms $\partial_t b[(u,t,x)]$, $\operatorname{div}\big(v[(u,t,x)]\big)$, $\operatorname{div}\big(k[(u,t,x)]\,\nabla u\big)$, and $f[(u,t,x)]$ are meaningful, e.g. in terms of weak differentiability, and such that these terms belong to the same space, e.g. $L^2(\tau \times p, \mathbb{K})$. To handle boundary and interface conditions, $k[(u,t,x)]\,\nabla u$ is required to have a trace on $\tau \times \partial p$. As $v[(u,t,x)]$ is continuous, it can simply be restricted to $\tau \times \partial p$.

Example 3.3.3. If the evolution equation (3.3.4) is interpreted as a transient heat equation as in Ex. 3.1.1(b), then b plays the role of an internal energy, v constitutes a convection, k constitutes a diffusion, and f represents heat sources or sinks.

3.3.2 Time Discretization

This section begins the task of formulating discretized versions of evolution equations, treating the time discretization of a single evolution equation (3.3.4). The time discretization of coupled systems of evolution equations including the time discretization of interface and boundary conditions is carried out in Sec. 3.4.3.

The description of the subsequent space discretization is more involved and is the subject of Sec. 3.5.

Discretization in time means to discretize the time domain τ into a strictly increasing sequence of discrete times $(t_\nu)_{\nu\in\{0,\dots,n\}} = (t_0, \dots, t_n = t_{\mathrm{f}})$. The positive real number

$$\Delta := \max\left\{t_\nu - t_{\nu-1} : \nu \in \{1,\dots,n\}\right\} \tag{3.3.7}$$

is called the *fineness* of the time discretization.

The discretization $(t_\nu)_{\nu\in\{0,\dots,n\}}$ of τ with fineness Δ is kept fixed for the rest of the chapter.

For each time step, the time derivative in the evolution equation (3.3.4) is replaced by a difference quotient (s. (3.3.8)), and each term of the evolution equation is either evaluated at the current time t_ν (so-called *implicit* discretization) or at the previous time $t_{\nu-1}$ (so-called *explicit* discretization). The result is a scheme of equations, one equation for each discrete time $t_\nu > t_0$. Starting from the initial condition, the equation at time t_ν is used to determine a solution $u^{(\nu)}$ at t_ν, treating the solution $u^{(\nu-1)}$ at $t_{\nu-1}$ as known.

In this work, only implicit time discretization is considered (with the exception of the nonlocal interface and boundary conditions, where a semi-implicit method is used, s. Secs 3.4.3, 3.4.3). In the context of evolution equations, an implicit time discretization is known to be advantageous, due to properties such as unconditional stability. In case of an explicit time discretization, it is known that to get stability even for simple examples, the dependence of the finess of the time discretization on the fineness of the space discretization is such that the time step has to be chosen impracticably small (s. e.g. [GO92, Secs 8.2, 8.3], [GKO95, Secs 2.1, 2.3, and p. 279], and [PTVF96, Sec. 19.2]).

Definition 3.3.4. The *implicit time discretization* of the evolution operator $H_{b,v,k,f}$ is defined as the family $(H^{(\nu)}_{b,v,k,f})_{\nu\in\{1,\dots,n\}}$, where

$$\begin{aligned} H^{(\nu)}_{b,v,k,f}[(u,\tilde{u})][x] :=& (t_\nu - t_{\nu-1})^{-1}\left(b^{(\nu)}\left[(u[x],x)\right] - b^{(\nu-1)}\left[(\tilde{u}[x],x)\right]\right) \\ &+ \operatorname{div}\left(v^{(\nu)}\left[(u[x],x)\right]\right) - \operatorname{div}\left(k^{(\nu)}\left[(u[x],x)\right]\nabla u[x]\right) \\ &- f^{(\nu)}\left[(u[x],x)\right] \end{aligned} \tag{3.3.8}$$

for each $\nu \in \{1,\dots,n\}$, and

$$b^{(\nu)} \in C(v \times p, \mathbb{K}), \qquad b^{(\nu)}[(y,x)] := b[(y,t_\nu,x)], \tag{3.3.9a}$$

$$v^{(\nu)} \in C(v \times p, \mathbb{R}^d), \qquad v^{(\nu)}[(y,x)] := v[(y,t_\nu,x)], \tag{3.3.9b}$$

$$k^{(\nu)} \in C(v \times p, \mathbb{K}), \qquad k^{(\nu)}[(y,x)] := k[(y,t_\nu,x)], \tag{3.3.9c}$$

$$f^{(\nu)} \in C(v \times p, \mathbb{K}), \qquad f^{(\nu)}[(y,x)] := f[(y,t_\nu,x)] \tag{3.3.9d}$$

for each $\nu \in \{0,\dots,n\}$.

Thus, each $H^{(\nu)}_{b,v,k,f}$ maps a suitable subset $\mathcal{U}^{(\nu)} \times \mathcal{U}^{(\nu-1)}$ of $C(p,v) \times C(p,v)$ into the set of all $\mathbb{K}$-valued functions on p:

$$H^{(\nu)}_{b,v,k,f} : \mathcal{U}^{(\nu)} \times \mathcal{U}^{(\nu-1)} \longrightarrow \mathcal{F}(p,\mathbb{K}). \tag{3.3.10}$$

The *implicit Euler scheme* of the evolution equation $H_{b,v,k,f}[u] = 0$ is given by

$$\bigwedge_{\nu \in \{1,\dots,n\}} H^{(\nu)}_{b,v,k,f}[(u^{(\nu)}, u^{(\nu-1)})] = 0. \tag{3.3.11}$$

—

In a manner similar to (3.3.5), one can write (3.3.8) in the more concise form

$$\begin{aligned} H^{(\nu)}_{b,v,k,f}[(u,\tilde{u})] =& (t_\nu - t_{\nu-1})^{-1} \left(b^{(\nu)} \circ u^{\mathrm{sp.}} - b^{(\nu-1)} \circ \tilde{u}^{\mathrm{sp.}}\right) + \operatorname{div}\left(v^{(\nu)} \circ u^{\mathrm{sp.}}\right) \\ &- \operatorname{div}\left(\left(k^{(\nu)} \circ u^{\mathrm{sp.}}\right) \nabla u\right) - f^{(\nu)} \circ u^{\mathrm{sp.}}, \end{aligned} \tag{3.3.12}$$

where given $u : p \longrightarrow \mathbb{K}$, the function $u^{\mathrm{sp.}}$ is defined by

$$u^{\mathrm{sp.}} : p \longrightarrow \mathbb{K} \times p, \quad u^{\mathrm{sp.}}[x] := (u[x], x). \tag{3.3.13}$$

Once more, conforming to standard notation, the formulation (3.3.8) is mostly used instead of (3.3.12).

Remark 3.3.5. Analogous to Rem. 3.3.2, in addition to the regularity assumptions on $u^{(\nu)}$, $b^{(\nu)}$, $v^{(\nu)}$, $k^{(\nu)}$, and $f^{(\nu)}$ listed in Def. 3.3.4, these functions need to be such that the terms in (3.3.8) are meaningful in a suitable sense.

Remark 3.3.6. As mentioned in Sec. 3.3.1, for the mathematical theory it is often not necessary to assume continuity of f. For example, if one just had square integrability of f with respect to t, then one would replace $f^{(\nu)}\big[(u[x],x)\big]$ with $(t_\nu - t_{\nu-1})^{-1} \int_{t_{\nu-1}}^{t_\nu} f\big[(u[x],t,x)\big]\,\mathrm{d}t$ in (3.3.8).

3.4 Evolution Equation Complexes

As described in Sec. 3.1, the goal is to study different evolution equations (3.1.1) on different domains, coupled by interface conditions. The contents of the present section provides the setting and the notation for this situation, which is then kept fixed for the remainder of Ch. 3.

In the language of Def. 3.3.1, one considers a family of evolution equations $H_{b_j,v_j,k_j,f_j}[u_j] = 0$, $j \in J$, where J is a finite nonempty index set and each $H_{b_j,v_j,k_j,f_j} : \mathcal{U}_j \longrightarrow \mathcal{F}(\tau \times p_j, \mathbb{K})$ is an evolution operator. Thus, the evolution equations all share the same time domain τ as well as the same solution range v; they just differ in their space domains p_j.

The *total space domain* p is the union of the spatial subdomains p_j, and, moreover, $(p_j)_{j\in J}$ is assumed to form a partition of p in the sense of Def. C.1.3. A nontrivial example is depicted in Fig. 3.2, where further notation used in Fig. 3.2 is explained below.

3.4.1 Interface, Boundary, and Initial Conditions

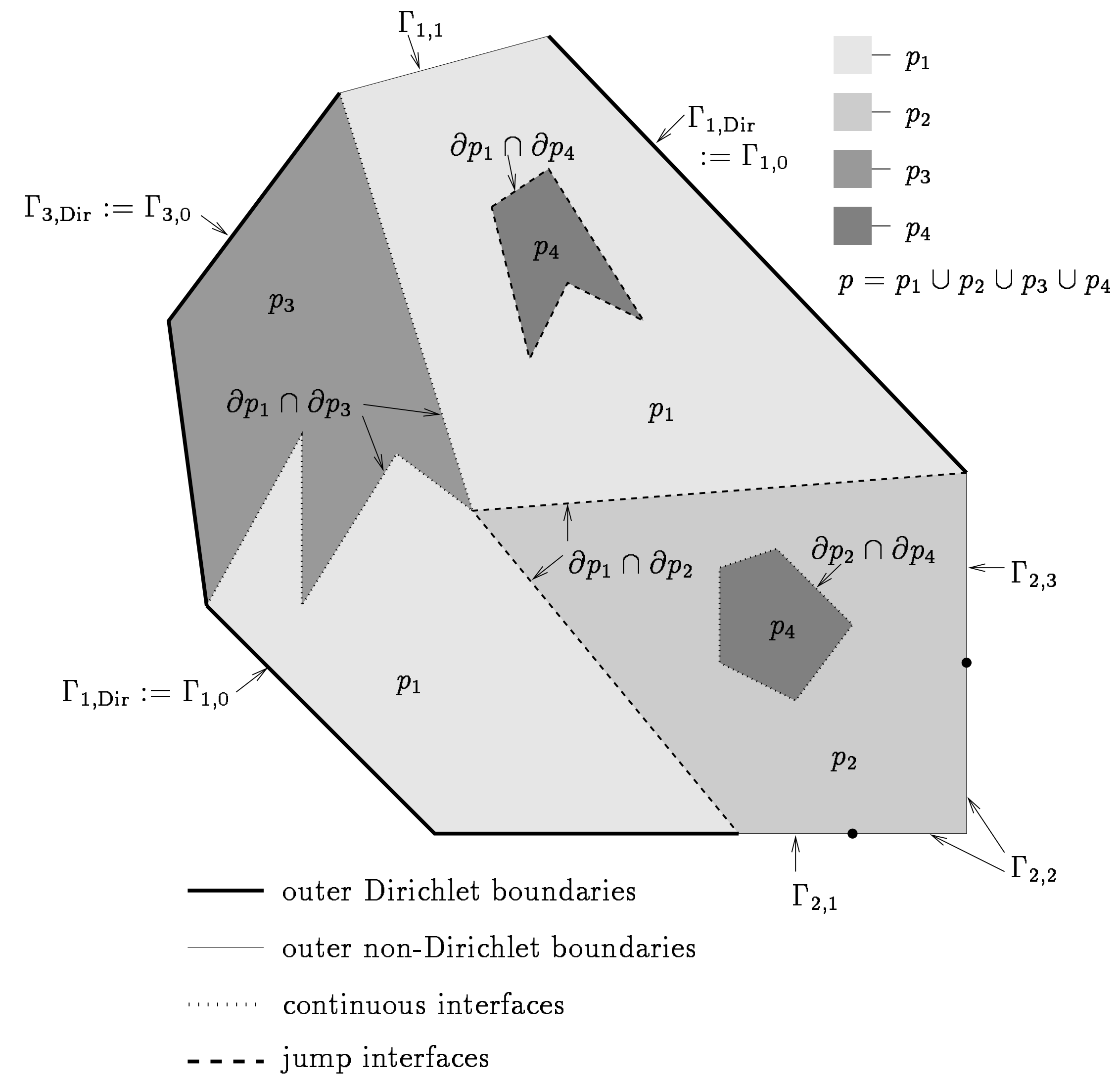
An evolution equation (cf. (3.3.1) and (3.3.4)) does not determine a unique solution u. In many cases, a unique solution can be selected by prescribing the unknown's behaviour at the boundary of the domain via boundary and interface conditions. An initial condition, prescribing the solution at the initial time, can be viewed as a special case, but in the following, the terms boundary and interface conditions are reserved for conditions on the boundaries of *space* domains.

As described in Sec. 3.1, boundary conditions in terms of the unknown itself and in terms of its flux are considered in this work (cf. (3.1.8), (3.1.9)).

If evolution equations (3.3.4) are considered on several space domains having common interfaces, then on such interfaces, boundary conditions are replaced by interface conditions. Analogously to the case of the boundary conditions, the interface conditions of interest here are given in terms of the unknowns and their fluxes (cf. (3.1.6a), (3.1.6b), (3.1.7), and also (3.4.6), (3.4.7) below).

In case the boundaries of two spatial subdomains p_{j_1} and p_{j_2} did not intersect in an interface, one would provide one boundary condition on ∂p_{j_1} and one boundary condition on ∂p_{j_2}. Accordingly, one needs two conditions at an interface between p_{j_1} and p_{j_2}. Here, one condition is always given as a relationship between the two adjacent fluxes, i.e. in the form (3.1.7). It might or might not involve the values of the unknowns u_{j_1} and u_{j_2} at the interface (or even at other interfaces e.g. due to radiation), but it always involves the values of the fluxes. On the other hand, the second interface condition involves the fluxes if and only if the unknown is allowed to have a discontinuity at the interface (cf. (3.1.6)).

During the discretization process described in the succeeding sections, interface and boundary operators are used to deal with flux terms on surfaces of polyhedral control volumes. It is noted that due to the fact that derivatives might exist only in a weak



$N = 4,\ J = \{1,2,3,4\}$,

$E_{\mathrm{con}} = \big\{\{1,3\},\{2,4\}\big\}$, $\mathrm{IF}_{\mathrm{con}} = \{\partial_{\mathrm{reg}} p_1 \cap \partial_{\mathrm{reg}} p_3, \partial_{\mathrm{reg}} p_2 \cap \partial_{\mathrm{reg}} p_4\}$,

$E_{\mathrm{jump}} = \big\{\{1,2\},\{1,4\}\big\}$, $\mathrm{IF}_{\mathrm{jump}} = \{\partial_{\mathrm{reg}} p_1 \cap \partial_{\mathrm{reg}} p_2, \partial_{\mathrm{reg}} p_1 \cap \partial_{\mathrm{reg}} p_4\}$,

$J_1 = \{0,1\},\ J_2 = \{1,2,3\},\ J_3 = \{0\},\ J_4 = \emptyset$.

Figure 3.2: Space domain p of a $(2,4)$-dimensional domain complex $\big(v, \tau, (p_j)_{j\in J}, E_{\mathrm{IF}}, E_{\mathrm{con}}, (i_e)_{e\in E_{\mathrm{IF}}}, (J_j)_{j\in J}, (\Gamma_{j,\iota})_{(j,\iota)\in J\times J_j}\big)$ (s. Def. 3.4.5).

sense, in general, the flux must be interpreted as the trace of a weakly differentiable function:

Notation 3.4.1. Let $j \in J$, and let $\omega \subseteq p_j$ be a d-dimensional polytope. Then the flux $F_{j,\partial\omega}$ through the boundary of ω is defined by

$$F_{j,\partial\omega}[(t,x)] := \mathrm{tr}_{\tau\times\partial\omega}\left(k_j\left[(u_j[(t,x)],t,x)\right]\nabla u_j[(t,x)]\right), \tag{3.4.1}$$

or, more precisely, using (3.3.6), by

$$F_{j,\partial\omega} := \mathrm{tr}_{\tau\times\partial\omega}\left((k_j \circ u_j^{\text{t.-sp.}})\nabla u_j\right). \tag{3.4.2}$$

Interface Conditions

Given two distinct indices $j_1 \in J$ and $j_2 \in J$, the spatial subdomains p_{j_1} and p_{j_2} are said to have an *interface* iff $\partial_{\text{reg}} p_{j_1} \cap \partial_{\text{reg}} p_{j_2} \neq \emptyset$. The regular boundary of a polytope is defined and illustrated in App. C.4.2, cf. Def. C.4.11 and Fig. C.3. Since interfaces are supposed to have dimension $d-1$, it does not suffice to require $\partial p_{j_1} \cap \partial p_{j_2} \neq \emptyset$. For example in Fig. 3.2, p_2 and p_3 do not have a common interface, even though $\partial p_2 \cap \partial p_3 \neq \emptyset$.

Given the family $(p_j)_{j\in J}$, the set off *all* interfaces is given by

$$\mathrm{IF} := \left\{\partial_{\text{reg}} p_{j_1} \cap \partial_{\text{reg}} p_{j_2} : \partial_{\text{reg}} p_{j_1} \cap \partial_{\text{reg}} p_{j_2} \neq \emptyset,\ j_1 \neq j_2\right\}. \tag{3.4.3}$$

Remark 3.4.2. It is implied by Rem. C.4.13 that at most two spatial subdomains intersect at an interface, i.e. for each $\gamma \in \mathrm{IF}$, there is precisely one two-elementic index set $\{j_1, j_2\} \subseteq J$ such that $\gamma = \partial_{\text{reg}} p_{j_1} \cap \partial_{\text{reg}} p_{j_2}$.

—

In consequence of Rem. 3.4.2, instead of by IF, the set of all interfaces is also characterized by

$$E_{\mathrm{IF}} := \left\{\{j_1, j_2\} \subseteq J : \partial_{\text{reg}} p_{j_1} \cap \partial_{\text{reg}} p_{j_2} \in \mathrm{IF}\right\}. \tag{3.4.4}$$

Then one has the bijective map $e : \mathrm{IF} \longrightarrow E_{\mathrm{IF}}$, that assigns each $\gamma \in \mathrm{IF}$ the unique two-elementic subset $e[\gamma] := \{j_1, j_2\}$ of J such that $\gamma = \partial_{\text{reg}} p_{j_1} \cap \partial_{\text{reg}} p_{j_2}$.

It was described in Sec. 3.1 that given the interface $\gamma = \partial_{\text{reg}} p_{j_1} \cap \partial_{\text{reg}} p_{j_2} \in \mathrm{IF}$, the unknowns $u_{j_1} \in \mathcal{U}_{j_1}$ and $u_{j_2} \in \mathcal{U}_{j_2}$ are supposed to satisfy either the continuity interface condition (3.1.6a) or the jump interface condition (3.1.6b). Therefore, the set IF is decomposed into the disjoint union of the sets IF_{con} and $\mathrm{IF}_{\text{jump}}$: $\mathrm{IF} = \mathrm{IF}_{\text{con}} \dot\cup \mathrm{IF}_{\text{jump}}$, where a continuity interface condition is prescribed for each $\gamma \in \mathrm{IF}_{\text{con}}$ and a jump interface condition is prescribed for each $\gamma \in \mathrm{IF}_{\text{jump}}$. The corresponding decomposition of E_{IF} reads $E_{\mathrm{IF}} = E_{\text{con}} \dot\cup E_{\text{jump}}$, where $E_{\text{con}} := \{e[\gamma] : \gamma \in \mathrm{IF}_{\text{con}}\}$, $E_{\text{jump}} := \{e[\gamma] : \gamma \in \mathrm{IF}_{\text{jump}}\}$. Equivalently, one can also treat the set E_{con} as given, subsequently defining $\mathrm{IF}_{\text{con}} := \{\gamma \in \mathrm{IF} : e[\gamma] \in E_{\text{con}}\}$. The latter point of view is taken in Def. 3.4.5 of a domain complex, since two-elementic index sets are simpler objects than the actual interfaces. In particular, E_{con} can be prescribed without first defining IF or E_{IF}.

Remark 3.4.3. The sets E_{IF}, E_{con}, and E_{jump} can be interpreted as sets of edges of a graph (cf. App. C.5 for some basics about graphs), namely of the graph having the subdomains as vertices that are connected by an edge if and only if they have a common interface. Then each $e[\gamma]$ corresponds to an edge in that graph.

—

A flux interface condition (3.1.7) is assumed to hold at both continuous and jump interfaces, i.e. at each $\gamma \in \mathrm{IF}$.

Both jump interface conditions and flux interface conditions are asymmetric with respect to the adjacent subdomains, i.e. they are not invariant under a switch of j_1 and j_2. Ordering the two subdomains adjacent to an interface allows to write jump interface conditions and flux interface conditions in a normalized manner by introducing the following conventions:

If the jump interface condition at $\gamma = \partial_{\mathrm{reg}} p_{j_1} \cap \partial_{\mathrm{reg}} p_{j_2}$ is given as

$$F_{j_1,\partial p_{j_1}} \bullet n_{p_{j_1}} + a^{\gamma,1}_{\mathrm{jump}}[(u_{j_1}, t, x)] - a^{\gamma,2}_{\mathrm{jump}}[(u_{j_2}, t, x)] = 0 \quad \text{on} \quad \tau \times \gamma, \tag{3.4.5}$$

i.e. in terms of the flux $F_{j_1,\partial p_{j_1}}$ through the boundary of p_{j_1}, then p_{j_1} is called the *first* subdomain at γ and p_{j_2} is called the *second* subdomain at γ. In the following, $i_1[\gamma]$ is written for the index of the first subdomain, and $i_2[\gamma]$ is written for the index of the second subdomain. For the purpose of subsequent reference, (3.4.5) is restated in terms of $i_1[\gamma]$ and $i_2[\gamma]$:

$$F_{i_1[\gamma],\partial p_{i_1[\gamma]}} \bullet n_{p_{i_1[\gamma]}} + a^{\gamma,1}_{\mathrm{jump}}[(u_{i_1[\gamma]}, t, x)] - a^{\gamma,2}_{\mathrm{jump}}[(u_{i_2[\gamma]}, t, x)] = 0 \quad \text{on} \quad \tau \times \gamma. \tag{3.4.6}$$

Moreover, the flux interface condition at γ is always assumed to be given in the form

$$\begin{aligned} F_{i_1[\gamma],\partial p_{i_1[\gamma]}} \bullet n_{p_{i_1[\gamma]}} - F_{i_2[\gamma],\partial p_{i_2[\gamma]}} \bullet n_{p_{i_1[\gamma]}} - \mathcal{A}_\gamma \left[\left(u_j \restriction_{\{t\} \times p_j} \right)_{j \in J} \right] [x] \\ - a^{\gamma,1}_{\mathrm{flux}}[(u_{i_1[\gamma]}, t, x)] + a^{\gamma,2}_{\mathrm{flux}}[(u_{i_2[\gamma]}, t, x)] = 0 \quad \text{on} \quad \tau \times \gamma. \end{aligned} \tag{3.4.7}$$

Thus, both i_1 and i_2 are maps from IF into J such that

$$\bigwedge_{\gamma \in \mathrm{IF}} \quad \{i_1[\gamma], i_2[\gamma]\} = e[\gamma]. \tag{3.4.8}$$

In particular, given i_1, the map i_2 is uniquely determined by (3.4.8).

The following Ex. 3.4.4 treats a situation arising from the model of Ch. 2.

Example 3.4.4. In Fig. 3.1 on p. 50, γ denotes the interface between $p_{j_1} := \Omega_{j_1} = \Omega_{\mathrm{gas}}$ and $p_{j_2} := \Omega_{j_2} = \Omega^{[\mathrm{SiC-Powder}]}$. If the jump interface condition (2.3.2b′) and the flux interface condition (2.4.39b) both hold at γ, then the situation of Ex. 3.1.2(b) is combined with the situation of the second case of Ex. 3.1.2(c):

$$\begin{gathered}
u_{j_1} := T_{\mathrm{gas}}, \quad u_{j_2} := T_{\mathrm{solid}}\restriction_{p_{j_2}}, \quad k_{j_1} := \kappa_{\mathrm{gas}}, \quad k_{j_2} := \kappa^{[\mathrm{SiC-Powder}]}, \\
n_{p_{j_1}} = \mathbf{n}_{\mathrm{gas}} = -\mathbf{n}^{[\mathrm{SiC-Powder}]} = -n_{p_{j_2}}, \\
a^{\gamma,1}_{\mathrm{jump}}[(u_{j_1}, t, x)] := \xi_{\mathrm{SiC-Powder}} u_{j_1}, \quad a^{\gamma,2}_{\mathrm{jump}}[(u_{j_2}, t, x)] := \xi_{\mathrm{SiC-Powder}} u_{j_2}, \\
a^{\gamma,1}_{\mathrm{flux}} := 0, \qquad a^{\gamma,2}_{\mathrm{flux}}[(u_{j_2}, t, x)] := (\epsilon_{\mathrm{r}} + \epsilon_{\mathrm{t}})[(u_{j_2}, x)]\,\sigma\,u_{j_2}^4, \\
\mathcal{A}_\gamma\Big[\big(u_j\restriction_{\{t\}\times p_j}\big)_{j\in J}\Big] := \epsilon_{\mathrm{r}}[(u_{j_2}, x)]\,\mathcal{J}_{\mathrm{r}}\big[\mathcal{R}_{\mathrm{r}}[T_{\mathrm{solid}}]\big] + \epsilon_{\mathrm{t}}[(u_{j_2}, x)]\,\mathcal{J}_{\mathrm{t}}\big[\mathcal{R}_{\mathrm{t}}[T_{\mathrm{solid}}]\big].
\end{gathered}$$

According to the above convention, one has $i_1[\gamma] = j_1$ and $i_2[\gamma] = j_2$ in the present situation.

—

As in (3.3.2), continuity of the given functions is assumed:

$$\bigwedge_{\gamma\in\mathrm{IF}_{\mathrm{jump}}} \quad a^{\gamma,1}_{\mathrm{jump}} \in C(\upsilon\times\tau\times\gamma,\mathbb{K}), \qquad a^{\gamma,2}_{\mathrm{jump}} \in C(\upsilon\times\tau\times\gamma,\mathbb{K}), \tag{3.4.9a}$$

$$\bigwedge_{\gamma\in\mathrm{IF}} \quad a^{\gamma,1}_{\mathrm{flux}} \in C(\upsilon\times\tau\times\gamma,\mathbb{K}), \qquad a^{\gamma,2}_{\mathrm{flux}} \in C(\upsilon\times\tau\times\gamma,\mathbb{K}). \tag{3.4.9b}$$

The precise setting for the *nonlocal interface operators* $\mathcal{A}_\gamma$, $\gamma \in \mathrm{IF}$, is the following:

$$\mathcal{A}_\gamma : \prod_{j\in J} C(p_j, \upsilon) \longrightarrow C_{\mathrm{pw}}(\gamma, \mathbb{K}), \tag{3.4.10}$$

assigning a $\mathbb{K}$-valued piecewise continuous function on the interface to a family of υ-valued space-dependent continuous functions.

In the following, as in (3.4.7), $\mathcal{A}_\gamma$ is always applied to a family of unknowns restricted to the time instant $t \in \tau$: $\mathcal{A}_\gamma[\mathfrak{u}\restriction_{\{t\}}]$, where the symbol $\mathfrak{u}$ always denotes the family $(u_j)_{j\in J}$, and $\mathfrak{u}\restriction_{\{t\}} := \big(u_j\restriction_{\{t\}\times p_j}\big)_{j\in J}$ denotes its restriction to the time instant $t \in \tau$.

At a jump interface $\gamma \in \mathrm{IF}_{\mathrm{jump}}$, the jump interface condition and the flux interface condition can be combined to yield a different jump interface condition in terms of the flux in the second subdomain at γ: Using (3.4.6) to replace $F_{i_1[\gamma],\partial p_{i_1[\gamma]}} \bullet n_{p_{i_1[\gamma]}}$ in (3.4.7) together with $n_{p_{i_1[\gamma]}} = -n_{p_{i_2[\gamma]}}$, results in

$$\begin{aligned}
F_{i_2[\gamma],\partial p_{i_2[\gamma]}} \bullet n_{p_{i_2[\gamma]}} - \mathcal{A}_\gamma\Big[\big(u_j\restriction_{\{t\}\times p_j}\big)_{j\in J}\Big]\,[x] \\
- a^{\gamma,1}_{\mathrm{flux}}[(u_{i_1[\gamma]}, t, x)] + a^{\gamma,2}_{\mathrm{flux}}[(u_{i_2[\gamma]}, t, x)] \\
- a^{\gamma,1}_{\mathrm{jump}}[(u_{i_1[\gamma]}, t, x)] + a^{\gamma,2}_{\mathrm{jump}}[(u_{i_2[\gamma]}, t, x)] = 0 \quad \text{on} \quad \tau\times\gamma.
\end{aligned} \tag{3.4.11}$$

Boundary Conditions

As described at the end of Sec. 3.1, several different outer boundary conditions of Dirichlet type (3.1.8) and non-Dirichlet type (3.1.9) are considered on outer boundaries $\partial p \cap \partial p_j$. The notation for outer boundaries introduced in the following is illustrated in Fig. 3.2 on p. 59.

Let $\mathcal{O}_j$ denote the relative topology on $\partial p \cap \partial p_j$ with respect to the norm topology on $\mathbb{R}^d$. Subsequently, it is always assumed that for each $j \in J$, the family $(\Gamma_{j,\iota})_{\iota \in J_j}$ forms a partition of $\partial p \cap \partial p_j$ with respect to $\mathcal{O}_j$, where J_j is a nonempty finite index set. Moreover, each $\Gamma_{j,\iota}$ is required to be a $(d-1)$-polytope. In particular, each $\Gamma_{j,\iota}$ has nonempty interior with respect to $\mathcal{O}_j$.

The index $\iota = 0$ is reserved for Dirichlet boundaries: $\Gamma_{j,\mathrm{Dir}} := \Gamma_{j,0}$. That means p_j has a Dirichlet boundary if and only if $0 \in J_j$.

Thus, for each $j \in J$, the Dirichlet condition (3.1.8) is presumed to hold on $\Gamma_{j,\mathrm{Dir}}$ (if it exists), and a non-Dirichlet condition (3.1.9) is presumed to hold on each $\Gamma_{j,\iota}$, $\iota \in J_j \setminus \{0\}$, where once again continuity of the given functions is supposed:

$$\bigwedge_{j \in J:\, 0 \in J_j} \quad u_{j,\mathrm{Dir}} \in C(\tau \times \Gamma_{j,\mathrm{Dir}}, \upsilon), \tag{3.4.12a}$$

$$\bigwedge_{(j,\iota) \in J \times \left(J_j \setminus \{0\}\right)} \quad a_{\mathrm{out}}^{j,\iota} \in C(\upsilon \times \tau \times \Gamma_{j,\iota}, \mathbb{K}). \tag{3.4.12b}$$

The $u_{j,\mathrm{Dir}}$ are called *Dirichlet functions.*

In analogy with (3.4.10), the setting for the *nonlocal boundary operators* $\mathcal{B}_{j,\iota}$, $(j,\iota) \in J \times \left(J_j \setminus \{0\}\right)$ is

$$\mathcal{B}_{j,\iota} : \prod_{\underline{j} \in J} C(p_{\underline{j}}, \upsilon) \longrightarrow C_{\mathrm{pw}}(\Gamma_{j,\iota}, \mathbb{K}). \tag{3.4.13}$$

As the solution is known a priori at Dirichlet boundaries, there is a conceptual difference in the subsequent handling of Dirichlet and non-Dirichlet boundaries (s. Sec. 3.7).

Initial Conditions

For each $j \in J$, the initial condition is given by (3.1.10), where the *initial distributions* $u_j^{(0)}$ satisfy

$$\bigwedge_{j \in J} \quad u_j^{(0)} \in C(p_j, \upsilon). \tag{3.4.14}$$

3.4.2 Domain Complex and Evolution Equation Complex

The domain complex (Def. 3.4.5) and the evolution equation complex (Def. 3.4.6) are structures combining all the previous ingredients of Sec. 3.4. The evolution equation complex contains all information needed to describe a problem of coupled evolution equations on several domains, where the domain-related data is collected in the domain complex.

Definition 3.4.5. Let $(d, N) \in \mathbb{N}^2$, and let J be an index set with $\#J = N$. A (d, N)-dimensional *domain complex*

$$\mathfrak{D} = \big(\upsilon, \tau, (p_j)_{j\in J}, E_{\text{con}}, i_1, (J_j)_{j\in J}, (\Gamma_{j,\iota})_{(j,\iota)\in J\times J_j}\big) \tag{3.4.15}$$

is an 8-tuple consisting of the solution range $\upsilon \subseteq \mathbb{K}$, the time domain τ, a finite family of d-polytopes $(p_j)_{j\in J}$, a set E_{con} of two-elementic subsets of J, a map i_1, a finite family of nonempty finite index sets $(J_j)_{j\in J}$, and a finite family $(\Gamma_{j,\iota})_{(j,\iota)\in J\times J_j}$ of $(d-1)$-polytopes $\Gamma_{j,\iota} \subseteq \partial p \cap \partial p_j$, satisfying the following conditions (i) – (iii). Given the objects collected in (3.4.15), the sets IF, E_{IF}, IF_{con}, IF_{jump}, E_{jump}, and the maps e and i_2 can be defined as described in Sec. 3.4.1.

(i) $(p_j)_{j\in J}$ is a partition of $p := \bigcup_{j\in J} p_j$.

(ii) It is $i_1 : \text{IF} \longrightarrow J$ such that $i_1[\gamma] \in e[\gamma]$ for each $\gamma \in \text{IF}$.

(iii) For each $j \in J$, the family $(\Gamma_{j,\iota})_{\iota\in J_j}$ is a partition of $\partial p \cap \partial p_j$ with respect to the relative topology on $\partial p \cap \partial p_j$.

—

Figure 3.2 on p. 59 illustrates the $(2, 4)$-dimensional domain complex that was already used for examples in Sec. 3.4.1.

A problem of coupled evolution equations on several domains is given via a domain complex together with the information about given functions, leading to the following notion of an evolution equation complex:

Definition 3.4.6. Let $(d, N) \in \mathbb{N}^2$, and let J be an index set with $\#J = N$. A (d, N)-dimensional *evolution equation complex*

$$\begin{aligned}\mathfrak{C} = \Big(&\mathfrak{D}, \big(H_{b_j,v_j,k_j,f_j}\big)_{j\in J}, \big((a^{\gamma,1}_{\text{jump}}, a^{\gamma,2}_{\text{jump}})\big)_{\gamma\in \text{IF}_{\text{jump}}}, \big((a^{\gamma,1}_{\text{flux}}, a^{\gamma,2}_{\text{flux}}, \mathcal{A}_\gamma)\big)_{\gamma\in\text{IF}}, \\ &\big(u_{j,\text{Dir}}\big)_{j\in J:\, 0\in J_j}, \big((a^{j,\iota}_{\text{out}}, \mathcal{B}_{j,\iota})\big)_{(j,\iota)\in J\times(J_j\setminus\{0\})}, \big(u^{(0)}_j\big)_{j\in J}\Big),\end{aligned} \tag{3.4.16}$$

consists of a (d, N)-dimensional domain complex $\mathfrak{D}$ (s. Def. 3.4.5), an evolution operator H_{b_j,v_j,k_j,f_j} for each spatial subdomain p_j (cf. Def. 3.3.1), two continuous functions $a^{\gamma,1}_{\text{jump}}$

and $a^{\gamma,2}_{\text{jump}}$ for each jump interface γ (cf. (3.4.6) and (3.4.9a)), two continuous functions $a^{\gamma,1}_{\text{flux}}$ and $a^{\gamma,2}_{\text{flux}}$ and one nonlocal operator $\mathcal{A}_\gamma$ for each interface γ (cf. (3.4.7), (3.4.9b), and (3.4.10)), a Dirichlet function $u_{j,\text{Dir}}$ for each Dirichlet boundary $\Gamma_{j,\text{Dir}}$ (cf. (3.1.8) and (3.4.12a)), a continuous function $a^{j,\iota}_{\text{out}}$ and a nonlocal operator $\mathcal{B}_{j,\iota}$ for each non-Dirichlet boundary $\Gamma_{j,\iota}$ (cf. (3.1.9), (3.4.12b), and (3.4.13)), and an initial distribution on each spatial subdomain p_j (cf. (3.1.10) and (3.4.14)), satisfying the *compatibility conditions* (i) – (iii).

(i) $u^{(0)}_{i_1[\gamma]}\restriction_\gamma = u^{(0)}_{i_2[\gamma]}\restriction_\gamma$ for each $\gamma \in \text{IF}_{\text{con}}$.

(ii) For each $\gamma \in \text{IF}_{\text{con}}$ such that $0 \in J_{i_1[\gamma]} \cap J_{i_2[\gamma]}$ and such that $q := \overline{\gamma} \cap \Gamma_{i_1[\gamma],\text{Dir}} \cap \Gamma_{i_2[\gamma],\text{Dir}} \neq \emptyset$, it holds that $u_{i_1[\gamma],\text{Dir}}\restriction_{\tau\times q} = u_{i_2[\gamma],\text{Dir}}\restriction_{\tau\times q}$, where $\overline{\gamma}$ is the closure of γ with respect to the relative topology on $p_{i_1[\gamma]} \cap p_{i_2[\gamma]}$. Confer Fig. 3.3.

(iii) $u_{j,\text{Dir}}\restriction_{\{t_0\}\times\Gamma_{j,0}} = u^{(0)}_j\restriction_{\Gamma_{j,0}}$ for each $j \in J$ such that $0 \in J_j$.

—

In Def. 3.4.6, condition (i) ensures that different initial distributions agree where they are defined on common continuous interfaces, and condition (ii) does likewise for Dirichlet functions. Condition (iii) guarantees the consistency of the Dirichlet functions with the initial distributions. The compatibility conditions (i), (ii), and (iii) of Def. 3.4.6 are the most elementary, and it is trivial that they are necessary for the existence of discrete solutions (cf. Th. 3.8.35 in Sec. 3.8). However, if one wants to proceed to prove the existence of continuous solutions, then, in general, more complicated compatibility conditions related to interface and boundary conditions are needed.

A solution to an evolution equation complex is a family of functions $(u_j)_{j\in J}$, satisfying all corresponding evolution equations, interface conditions, boundary conditions, and the initial conditions:

Definition 3.4.7. Given an evolution equation complex $\mathfrak{C}$ as defined in Def. 3.4.6, a family $\mathfrak{u} := (u_j)_{j\in J} \in \prod_{j\in J} \mathcal{U}_j$ is called a *solution* to $\mathfrak{C}$ iff it satisfies the following conditions (i) – (vii).

(i) Each u_j, $j \in J$, satisfies the initial condition $u_j\restriction_{\{t_0\}\times p_j} = u^{(0)}_j$.

(ii) $H_{b_j,v_j,k_j,f_j}[u_j] = 0$ for each $j \in J$.

(iii) For each $\gamma \in \text{IF}_{\text{con}}$, the functions $u_{i_1[\gamma]}$ and $u_{i_2[\gamma]}$ satisfy the continuity interface condition $u_{i_1[\gamma]}\restriction_{\tau\times\gamma} = u_{i_2[\gamma]}\restriction_{\tau\times\gamma}$.

(iv) For each $\gamma \in \text{IF}_{\text{jump}}$, the functions $u_{i_1[\gamma]}$ and $u_{i_2[\gamma]}$ satisfy the jump interface condition (3.4.6).

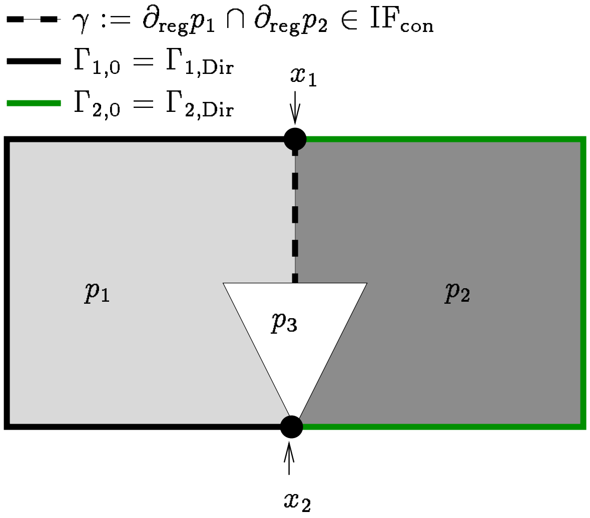


Figure 3.3: Subdomains p_1 and p_2 have the continuous interface γ. One has $x_1 \notin \gamma$, but $\{x_1\} = q := \overline{\gamma} \cap \Gamma_{1,\text{Dir}} \cap \Gamma_{2,\text{Dir}}$. Moreover, $x_2 \in \Gamma_{1,\text{Dir}} \cap \Gamma_{2,\text{Dir}}$, but $x_2 \notin q$. Thus, $u_{1,\text{Dir}}$ and $u_{2,\text{Dir}}$ must agree on x_1, but not necessarily on x_2.

(v) For each $\gamma \in \text{IF}$, the family $\mathfrak{u}$ satisfies the flux interface condition (3.4.7).

(vi) For each $j \in J$ such that $0 \in J_j$, the function u_j satisfies the Dirichlet boundary condition (3.1.8) on $\Gamma_{j,\text{Dir}} = \Gamma_{j,0}$.

(vii) For each $(j, \iota) \in J \times \big(J_j \setminus \{0\}\big)$, the function u_j satisfies the non-Dirichlet boundary condition (3.1.9) on $\Gamma_{j,\iota}$.

A domain complex $\mathfrak{D}$ as defined in Def. 3.4.5 and an evolution equation complex $\mathfrak{C}$ as defined in Def. 3.4.6 is now kept fixed for the remainder of Ch. 3.

3.4.3 Time Discretization

The goal of this section is to discretize the evolution equation complex $\mathfrak{C}$ in time. This includes the time discretization of evolution equations and of the several interface and boundary conditions considered in the previous sections.

The time discretization of an evolution equation has already been performed in Sec. 3.3.2. Now a similar procedure is used to deal with interface and boundary conditions. It is recalled that the time domain $\tau = [t_0, t_{\text{f}}]$ is discretized into $(t_0, \ldots, t_n = t_{\text{f}})$. As in Sec. 3.3.2, implicit discretization is used. The only exceptions are the nonlocal operators $\mathcal{A}_\gamma$ and $\mathcal{B}_{j,\iota}$ in the flux interface conditions (3.4.7) and the boundary conditions (3.1.9), respectively, where some of the dependencies on the solution are discretized explicitly (cf. Nots 3.4.9, 3.4.11, and Eqs (3.4.24), (3.4.31) below). In the application to heat equations, where the $\mathcal{A}_\gamma$ and $\mathcal{B}_{j,\iota}$ represent nonlocal radiation operators (cf. Exs 3.1.2(c), 3.1.3(e) and Exs 3.4.10, 3.4.12 below), this allows to evaluate the emissivities at the temperature of the previous time $t_{\nu-1}$, which considerably simplifies the solution of the nonlinear system resulting after space discretization, given by Def. 3.7.42(iii), by means of Newton's method.

The result of the time discretization is a scheme of systems of equations and conditions, one system for each discrete time t_ν. Starting from the initial condition, the system at time t_ν is supposed to be a determining system for the solution family $\mathfrak{u}^{(\nu)} = (u_j^{(\nu)})_{j\in J}$ at t_ν, treating the solution family $\mathfrak{u}^{(\nu-1)}$ at $t_{\nu-1}$ as known.

Interface Conditions

For each continuous interface $\gamma \in \mathrm{IF}_{\mathrm{con}}$, the continuity interface condition in Def. 3.4.7(iii) is replaced by the time-discrete scheme

$$\bigwedge_{\nu\in\{0,\dots,n\}} u^{(\nu)}_{i_1[\gamma]}\restriction_\gamma = u^{(\nu)}_{i_2[\gamma]}\restriction_\gamma . \tag{3.4.17}$$

To discretize the jump interface conditions (3.4.6), the time-discrete analogue of Not. 3.4.1 is provided:

Notation 3.4.8. Let $j \in J$, and let $\omega \subseteq p_j$ be a d-dimensional polytope. Then the flux $F^{(\nu)}_{j,\partial\omega}$ through the boundary of ω at time t_ν is defined by

$$F^{(\nu)}_{j,\partial\omega}[x] := \mathrm{tr}_{\partial\omega}\left(k_j^{(\nu)}\left[(u_j^{(\nu)}[x], x)\right] \nabla u_j^{(\nu)}[x]\right), \tag{3.4.18}$$

i.e. in function notation using (3.3.13)

$$F^{(\nu)}_{j,\partial\omega} = \mathrm{tr}_{\partial\omega}\left((k_j^{(\nu)} \circ (u_j^{(\nu)})^{\mathrm{sp.}}) \nabla u_j^{(\nu)}\right), \tag{3.4.19}$$

where the $k_j^{(\nu)}$ are given according to (3.3.9c).

—

For each jump interface $\gamma \in \mathrm{IF}_{\mathrm{jump}}$, the jump interface condition (3.4.6) is replaced by the time-discrete scheme

$$\bigwedge_{\nu\in\{0,\dots,n\}} F^{(\nu)}_{i_1[\gamma],\partial p_{i_1[\gamma]}} \bullet n_{p_{i_1[\gamma]}} + a^{\gamma,1,\nu}_{\mathrm{jump}}[(u^{(\nu)}_{i_1[\gamma]}, x)] - a^{\gamma,2,\nu}_{\mathrm{jump}}[(u^{(\nu)}_{i_2[\gamma]}, x)] = 0 \quad \text{on} \quad \gamma, \tag{3.4.20}$$

where for each $(\gamma, \alpha, \nu) \in \mathrm{IF}_{\mathrm{jump}} \times \{1, 2\} \times \{0, \dots, n\}$:

$$a^{\gamma,\alpha,\nu}_{\mathrm{jump}} \in C(v \times \gamma, \mathbb{K}), \qquad a^{\gamma,\alpha,\nu}_{\mathrm{jump}}[(y, x)] = a^{\gamma,\alpha}_{\mathrm{jump}}[(y, t_\nu, x)]. \tag{3.4.21}$$

In order to formulate the time-discrete version of the flux interface conditions (3.4.7), the possible dependencies of the nonlocal interface operators $\mathcal{A}_\gamma$ on the family of unknowns $\mathfrak{u}$ is artificially divided into dependencies that are to be discretized explicitly and into dependencies that are to be discretized implicitly:

Notation 3.4.9. For each interface $\gamma \in \mathrm{IF}$, an operator

$$(\mathcal{A}_\gamma)^{\text{ex.-im.}} : \left(\prod_{j\in J} C(p_j, v)\right)^2 \longrightarrow C_{\mathrm{pw}}(\gamma, \mathbb{K}) \tag{3.4.22a}$$

is called a *dependency splitting* of $\mathcal{A}_\gamma$ iff

$$\bigwedge_{\mathfrak{u}\in\prod_{j\in J} C(p_j,v)} (\mathcal{A}_\gamma)^{\text{ex.-im.}}[(\mathfrak{u},\mathfrak{u})] = \mathcal{A}_\gamma[\mathfrak{u}]. \tag{3.4.22b}$$

Analogously, for each $\alpha \in \{1, 2\}$, a function

$$(a_{\text{flux}}^{\gamma,\alpha})^{\text{ex.-im.}} \in C(v^2 \times \tau \times \gamma, \mathbb{K}) \tag{3.4.23a}$$

is called a *dependency splitting* of $a_{\text{flux}}^{\gamma,\alpha}$ iff

$$\bigwedge_{(y,t,x)\in v\times\tau\times\gamma} (a_{\text{flux}}^{\gamma,\alpha})^{\text{ex.-im.}}\big[\big((y,y),t,x\big)\big] = a_{\text{flux}}^{\gamma,\alpha}[(y,t,x)]. \tag{3.4.23b}$$

—

The first argument of a dependency splitting is to be discretized explicitly, whereas the second argument of a dependency splitting is to be discretized implicitly.

Example 3.4.10. When applied to Ex. 3.1.2(c), the dependency splittings allow one to separate the temperature dependence of the emissivity into the first argument. One is then in the position to discretize the emissivity explicitly in an otherwise implicit discretization.

The following dependency splittings are actually used for the numerical simulation applications in Ch. 4. The precise relation between the temperature T_{solid} and the family of unknowns $(u_j)_{j\in J}$ was explained in Ex. 3.1.2(c). Here, to simplify notation, the family $(u_j)_{j\in J}$ is always hidden behind the symbols T_{solid} and S_{solid}.

Dependency splittings in the first case of Ex. 3.1.2(c):

$$\begin{aligned}
(\mathcal{A}_\gamma)^{\text{ex.-im.}}[(S_{\text{solid}}, T_{\text{solid}})] &:= \epsilon_{\mathrm{t}}[(S_{\text{solid}}, x)]\, \mathcal{J}_{\mathrm{t}}\big[\mathcal{R}_{\mathrm{t}}[T_{\text{solid}}]\big],\\
(a_{\text{flux}}^{\gamma,2})^{\text{ex.-im.}}\big[\big((S_{\text{solid}}, T_{\text{solid}}), t, x\big)\big] &:= \epsilon_{\mathrm{t}}[(S_{\text{solid}}, x)]\, \sigma\, T_{\text{solid}}^4.
\end{aligned}$$

Dependency splittings in the second case of Ex. 3.1.2(c):

$$\begin{aligned}
(\mathcal{A}_\gamma)^{\text{ex.-im.}}[(S_{\text{solid}}, T_{\text{solid}})] &:= \epsilon_{\mathrm{r}}[(S_{\text{solid}}, x)]\, \mathcal{J}_{\mathrm{r}}\big[\mathcal{R}_{\mathrm{r}}[T_{\text{solid}}]\big]\\
&\quad + \epsilon_{\mathrm{t}}[(S_{\text{solid}}, x)]\, \mathcal{J}_{\mathrm{t}}\big[\mathcal{R}_{\mathrm{t}}[T_{\text{solid}}]\big],\\
(a_{\text{flux}}^{\gamma,2})^{\text{ex.-im.}}\big[\big((S_{\text{solid}}, T_{\text{solid}}), t, x\big)\big] &:= (\epsilon_{\mathrm{r}} + \epsilon_{\mathrm{t}})[(S_{\text{solid}}, x)]\, \sigma\, T_{\text{solid}}^4.
\end{aligned}$$

Dependency splittings in the third case of Ex. 3.1.2(c):

$$(\mathcal{A}_\gamma)^{\text{ex.-im.}}[(S_{\text{solid}}, T_{\text{solid}})] := \epsilon_{\text{r}}[(S_{\text{solid}}, x)]\, \mathcal{J}_{\text{r}}\big[\mathcal{R}_{\text{r}}[T_{\text{solid}}]\big],$$
$$(a^{\gamma,2}_{\text{flux}})^{\text{ex.-im.}}\big[\big((S_{\text{solid}}, T_{\text{solid}}), t, x\big)\big] := \epsilon_{\text{r}}[(S_{\text{solid}}, x)]\, \sigma\, T^4_{\text{solid}}.$$

In each of the three cases, one recovers the original situation by setting $S_{\text{solid}} = T_{\text{solid}}$:

$$(\mathcal{A}_\gamma)^{\text{ex.-im.}}[(T_{\text{solid}}, T_{\text{solid}})] = \mathcal{A}_\gamma[T_{\text{solid}}],$$
$$(a^{\gamma,2}_{\text{flux}})^{\text{ex.-im.}}\big[\big((T_{\text{solid}}, T_{\text{solid}}), t, x\big)\big] = a^{\gamma,2}_{\text{flux}}[T_{\text{solid}}].$$

—

It is recalled that $\mathfrak{u}^{(\nu)} = (u^{(\nu)}_j)_{j\in J}$. For each interface $\gamma \in \text{IF}$, the (semi-implicit) time-discrete scheme for the flux interface condition (3.4.7) is formulated:

$$\bigwedge_{\nu\in\{1,\dots,n\}} \begin{pmatrix} F^{(\nu)}_{i_1[\gamma],\partial p_{i_1[\gamma]}} \bullet n_{p_{i_1[\gamma]}} - F^{(\nu)}_{i_2[\gamma],\partial p_{i_2[\gamma]}} \bullet n_{p_{i_1[\gamma]}} \\ - (\mathcal{A}_\gamma)^{\text{ex.-im.}}\big[\big(\mathfrak{u}^{(\nu-1)}, \mathfrak{u}^{(\nu)}\big)\big][x] \\ - (a^{\gamma,1,\nu}_{\text{flux}})^{\text{ex.-im.}}\big[\big((u^{(\nu-1)}_{i_1[\gamma]}, u^{(\nu)}_{i_1[\gamma]}), x\big)\big] \\ + (a^{\gamma,2,\nu}_{\text{flux}})^{\text{ex.-im.}}\big[\big((u^{(\nu-1)}_{i_2[\gamma]}, u^{(\nu)}_{i_2[\gamma]}), x\big)\big] = 0 \end{pmatrix} \quad \text{on } \gamma, \tag{3.4.24}$$

where for each $(\gamma, \alpha, \nu) \in \text{IF} \times \{1, 2\} \times \{0, \dots, n\}$:

$$(a^{\gamma,\alpha,\nu}_{\text{flux}})^{\text{ex.-im.}} \in C(v^2 \times \gamma, \mathbb{K}),$$
$$(a^{\gamma,\alpha,\nu}_{\text{flux}})^{\text{ex.-im.}}\big[\big((y, y'), x\big)\big] = (a^{\gamma,\alpha}_{\text{flux}})^{\text{ex.-im.}}\big[\big((y, y'), t_\nu, x\big)\big]. \tag{3.4.25}$$

Finally, combining (3.4.20) and (3.4.24) yields the time-discrete analogue of (3.4.11) for each $\gamma \in \text{IF}_{\text{jump}}$:

$$\bigwedge_{\nu\in\{1,\dots,n\}} \begin{pmatrix} F^{(\nu)}_{i_2[\gamma],\partial p_{i_2[\gamma]}} \bullet n_{p_{i_2[\gamma]}} - (\mathcal{A}_\gamma)^{\text{ex.-im.}}\big[\big(\mathfrak{u}^{(\nu-1)}, \mathfrak{u}^{(\nu)}\big)\big][x] \\ - (a^{\gamma,1,\nu}_{\text{flux}})^{\text{ex.-im.}}\big[\big((u^{(\nu-1)}_{i_1[\gamma]}, u^{(\nu)}_{i_1[\gamma]}), x\big)\big] \\ + (a^{\gamma,2,\nu}_{\text{flux}})^{\text{ex.-im.}}\big[\big((u^{(\nu-1)}_{i_2[\gamma]}, u^{(\nu)}_{i_2[\gamma]}), x\big)\big] \\ - a^{\gamma,1,\nu}_{\text{jump}}[(u^{(\nu)}_{i_1[\gamma]}, x)] + a^{\gamma,2,\nu}_{\text{jump}}[(u^{(\nu)}_{i_2[\gamma]}, x)] = 0 \end{pmatrix} \quad \text{on } \gamma. \tag{3.4.26}$$

Boundary Conditions

For each $j \in J$ such that $0 \in J_j$, the Dirichlet boundary condition (3.1.8) is replaced by the time-discrete scheme

$$\bigwedge_{\nu\in\{0,\dots,n\}} \quad u^{(\nu)}_j[x] = u^{(\nu)}_{j,\text{Dir}}[x] \quad \text{on} \quad \Gamma_{j,\text{Dir}}, \tag{3.4.27}$$

where for each $(j,\nu) \in J \times \{0,\dots,n\}$ such that $0 \in J_j$:

$$u^{(\nu)}_{j,\mathrm{Dir}} \in C(\Gamma_{j,\mathrm{Dir}}, \mathbb{K}), \quad u^{(\nu)}_{j,\mathrm{Dir}}[x] = u_{j,\mathrm{Dir}}[(t_\nu, x)]. \tag{3.4.28}$$

To state the time-discrete version of the non-Dirichlet boundary conditions (3.1.9), the strategy is analogous to the case of the flux interface conditions, introducing dependency splittings of the $\mathcal{B}_{j,\iota}$ and the $a^{j,\iota}_{\mathrm{out}}$:

Notation 3.4.11. For each $(j,\iota) \in J \times \big(J_j \setminus \{0\}\big)$, the operator $(\mathcal{B}_{j,\iota})^{\text{ex.-im.}}$ and the function $(a^{j,\iota}_{\mathrm{out}})^{\text{ex.-im.}}$ are *dependency splittings* of $\mathcal{B}_{j,\iota}$ and $a^{j,\iota}_{\mathrm{out}}$, respectively, iff

$$(\mathcal{B}_{j,\iota})^{\text{ex.-im.}} : \left(\prod_{j\in J} C(p_j, \upsilon)\right)^2 \longrightarrow C_{\mathrm{pw}}(\Gamma_{j,\iota}, \mathbb{K}), \tag{3.4.29a}$$

$$\bigwedge_{\mathfrak{u}\in\prod_{j\in J} C(p_j,\upsilon)} (\mathcal{B}_{j,\iota})^{\text{ex.-im.}}[(\mathfrak{u},\mathfrak{u})] = \mathcal{B}_{j,\iota}[\mathfrak{u}], \tag{3.4.29b}$$

$$(a^{j,\iota}_{\mathrm{out}})^{\text{ex.-im.}} \in C(\upsilon^2 \times \tau \times \Gamma_{j,\iota}, \mathbb{K}), \tag{3.4.30a}$$

$$\bigwedge_{(y,t,x)\in\upsilon\times\tau\times\Gamma_{j,\iota}} (a^{j,\iota}_{\mathrm{out}})^{\text{ex.-im.}}\big[\big((y,y),t,x\big)\big] = a^{j,\iota}_{\mathrm{out}}[(y,t,x)]. \tag{3.4.30b}$$

Example 3.4.12. The present example is analogous to Ex. 3.4.10, where dependency splittings were used to separate the temperature dependence of the emissivity occurring in the interface conditions of Ex. 3.1.2(c) into the first argument. Now the same is done in the case of boundary conditions by applying dependency splittings to Ex. 3.1.3(e), where, as in Ex. 3.4.10, T_{solid} and S_{solid} is written instead of $(u_j)_{j\in J}$:

$$(\mathcal{B}_{j,\iota})^{\text{ex.-im.}}[(S_{\mathrm{solid}}, T_{\mathrm{solid}})] := \epsilon[(S_{\mathrm{solid}}, x)] \cdot \mathcal{J}\big[\mathcal{R}[T_{\mathrm{solid}}]\big],$$
$$(a^{j,\iota}_{\mathrm{out}})^{\text{ex.-im.}}\big[\big((S_{\mathrm{solid}}, T_{\mathrm{solid}}), t, x\big)\big] := \epsilon[(S_{\mathrm{solid}}, x)]\, \sigma\, T^4_{\mathrm{solid}}.$$

As in Ex. 3.4.10, setting $S_{\mathrm{solid}} = T_{\mathrm{solid}}$ yields the original situation.

—

For each $(j,\iota) \in J \times \big(J_j \setminus \{0\}\big)$, the non-Dirichlet boundary condition (3.1.9) is replaced by the time-discrete scheme

$$\bigwedge_{\nu\in\{1,\dots,n\}} \begin{pmatrix} F^{(\nu)}_{j,\partial p_j} \bullet n_{p_j} - (\mathcal{B}_{j,\iota})^{\text{ex.-im.}}\big[\big(\mathfrak{u}^{(\nu-1)}, \mathfrak{u}^{(\nu)}\big)\big][x] \\ + (a^{j,\iota,\nu}_{\mathrm{out}})^{\text{ex.-im.}}\big[\big((u^{(\nu-1)}_j, u^{(\nu)}_j), x\big)\big] = 0 \end{pmatrix} \quad \text{on } \Gamma_{j,\iota}, \tag{3.4.31}$$

where for each $(j,\iota,\nu) \in J \times \big(J_j \setminus \{0\}\big) \times \{0,\dots,n\}$:

$$\begin{gathered} (a^{j,\iota,\nu}_{\mathrm{out}})^{\text{ex.-im.}} \in C(\upsilon^2 \times \Gamma_{j,\iota}, \mathbb{K}), \\ (a^{j,\iota,\nu}_{\mathrm{out}})^{\text{ex.-im.}}\big[\big((\tilde{y}, y), x\big)\big] = (a^{j,\iota}_{\mathrm{out}})^{\text{ex.-im.}}\big[\big((\tilde{y}, y), t_\nu, x\big)\big]. \end{gathered} \tag{3.4.32}$$

Evolution Equation Complex

The time discretization of an evolution equation complex (3.4.16) includes the time discretization of the evolution equations (Sec. 3.3.2) as well as of the interface and boundary conditions (Sec. 3.4.3). The structure $\mathfrak{T}$ defined in the following Def. 3.4.13 contains all the resulting data.

Definition 3.4.13. Given an evolution equation complex $\mathfrak{C}$, a *time discretization* $\mathfrak{T}$ of $\mathfrak{C}$ (implicit except in some interface and boundary condition dependencies),

$$
\begin{aligned}
\mathfrak{T} = \Big(& (t_\nu)_{\nu\in\{0,\dots,n\}}, \big(\mathcal{U}_j^{(\nu)}\big)_{(j,\nu)\in J\times\{0,\dots,n\}}, \big(H^{(\nu)}_{b_j,v_j,k_j,f_j}\big)_{(j\times\nu)\in J\times\{0,\dots,n\}}, \\
& \big((a^{\gamma,1,\nu}_{\text{jump}}, a^{\gamma,2,\nu}_{\text{jump}})\big)_{(\gamma,\nu)\in \mathrm{IF}_{\text{jump}}\times\{0,\dots,n\}}, \\
& \big(((a^{\gamma,1}_{\text{flux}})^{\text{ex.-im.}}, (a^{\gamma,2}_{\text{flux}})^{\text{ex.-im.}}, (\mathcal{A}_\gamma)^{\text{ex.-im.}})\big)_{\gamma\in\mathrm{IF}}, \\
& \big(((a^{\gamma,1,\nu}_{\text{flux}})^{\text{ex.-im.}}, (a^{\gamma,2,\nu}_{\text{flux}})^{\text{ex.-im.}})\big)_{(\gamma,\nu)\in\mathrm{IF}\times\{0,\dots,n\}}, \\
& \big(u^{(\nu)}_{j,\text{Dir}}\big)_{(j,\nu)\in J\times\{0,\dots,n\}:0\in J_j}, \\
& \big(((a^{j,\iota}_{\text{out}})^{\text{ex.-im.}}, (\mathcal{B}_{j,\iota})^{\text{ex.-im.}})\big)_{(j,\iota)\in J\times(J_j\setminus\{0\})}, \\
& \big((a^{j,\iota,\nu}_{\text{out}})^{\text{ex.-im.}}\big)_{(j,\iota,\nu)\in J\times(J_j\setminus\{0\})\times\{0,\dots,n\}}\Big),
\end{aligned}
\tag{3.4.33}
$$

consists of a discretization $(t_\nu)_{\nu\in\{0,\dots,n\}}$ of τ, sets $\mathcal{U}_j^{(\nu)} \subseteq C(p_j, v)$, an implicit time discretization $\big(H^{(\nu)}_{b_j,v_j,k_j,f_j}\big)_{\nu\in\{0,\dots,n\}}$ of each H_{b_j,v_j,k_j,f_j}, where $H^{(\nu)}_{b_j,v_j,k_j,f_j}$ is defined on $\mathcal{U}_j^{(\nu)} \times \mathcal{U}_j^{(\nu-1)}$ (cf. Def. 3.3.4), functions $a^{\gamma,\alpha,\nu}_{\text{jump}}$ satisfying (3.4.21), dependency splittings $(a^{\gamma,\alpha}_{\text{flux}})^{\text{ex.-im.}}$ and $(\mathcal{A}_\gamma)^{\text{ex.-im.}}$ of $a^{\gamma,\alpha}_{\text{flux}}$ and $\mathcal{A}_\gamma$, respectively (cf. Not. 3.4.9), functions $(a^{\gamma,\alpha,\nu}_{\text{flux}})^{\text{ex.-im.}}$ satisfying (3.4.25), functions $u^{(\nu)}_{j,\text{Dir}}$ satisfying (3.4.28), dependency splittings $(a^{j,\iota}_{\text{out}})^{\text{ex.-im.}}$ and $(\mathcal{B}_{j,\iota})^{\text{ex.-im.}}$ of $a^{j,\iota}_{\text{out}}$ and $\mathcal{B}_{j,\iota}$, respectively (cf. Not. 3.4.11), and functions $(a^{j,\iota,\nu}_{\text{out}})^{\text{ex.-im.}}$ satisfying (3.4.32).

Definition 3.4.14. A *solution* to a time discretization $\mathfrak{T}$ of an evolution equation complex $\mathfrak{C}$, where $\mathfrak{T}$ is given by (3.4.33), is a sequence of families

$$
(\mathfrak{u}^{(0)}, \dots, \mathfrak{u}^{(n)}) = \big(u_j^{(\nu)}\big)_{(j,\nu)\in J\times\{0,\dots,n\}} \in \prod_{(j,\nu)\in J\times\{0,\dots,n\}} \mathcal{U}_j^{(\nu)},
\tag{3.4.34}
$$

satisfying the time-discrete schemes for the evolution equations, for the interface conditions, and for the boundary conditions. That means, (3.4.34) is a solution to $\mathfrak{T}$ iff it satisfies the following conditions (i) – (vii):

(i) For each $j \in J$, $u_j^{(0)}$ is identical to the initial distribution.

(ii) $H^{(\nu)}_{b_j,v_j,k_j,f_j}\big[(u_j^{(\nu)}, u_j^{(\nu-1)})\big] = 0$ for each $(j,\nu) \in J \times \{1,\dots,n\}$.

(iii) For each $\gamma \in \mathrm{IF}_{\mathrm{con}}$, the functions $u^{(\nu)}_{i_1[\gamma]}$ and $u^{(\nu)}_{i_2[\gamma]}$, $\nu \in \{0, \dots, n\}$, satisfy (3.4.17), i.e. the time-discrete scheme for the continuity interface condition on γ.

(iv) For each $\gamma \in \mathrm{IF}_{\mathrm{jump}}$, the functions $u^{(\nu)}_{i_1[\gamma]}$ and $u^{(\nu)}_{i_2[\gamma]}$, $\nu \in \{0, \dots, n\}$, satisfy (3.4.20), i.e. the time-discrete scheme for the jump interface condition on γ.

(v) For each $\gamma \in \mathrm{IF}$, the families $\mathfrak{u}^{(\nu)}$, $\nu \in \{0, \dots, n\}$, satisfy (3.4.24), i.e. the time-discrete scheme for the flux interface condition on γ.

(vi) For each $j \in J$ such that $0 \in J_j$, the functions $u^{(\nu)}_j$, $\nu \in \{0, \dots, n\}$, satisfy (3.4.27), i.e. the time-discrete scheme for the Dirichlet boundary condition on $\Gamma_{j,\mathrm{Dir}} = \Gamma_{j,0}$.

(vii) For each $(j, \iota) \in J \times \big(J_j \setminus \{0\}\big)$, the functions $u^{(\nu)}_j$, $\nu \in \{0, \dots, n\}$, satisfy (3.4.31), i.e. the time-discrete scheme for the non-Dirichlet boundary condition on $\Gamma_{j,\iota}$.

3.5 Integral Formulation

The subject of the present Sec. 3.5 is to deduce an integral formulation of coupled systems of evolution equations including interface and boundary conditions that have previously been subject to a time discretization according to the description in Sec. 3.4.3. The strategy is a follows:

Each d-dimensional space domain p_j is discretized into a finite number of control volumes, where each control volume consists of a d-polytope (cf. Sec. 3.5.1).

Each time-discrete evolution equation is then integrated over control volumes contained inside the space domain where the respective evolution equation is defined (cf. Sec. 3.5.2). The Gauss-Green Integration Th. C.8.2 is used to transform volume integrals into boundary integrals.

In Sec. 3.5.3, the time-discrete interface conditions (3.4.17), (3.4.20), and (3.4.24) are used to link equations on adjacent domains, and the time-discrete boundary conditions (3.4.31) are used to deal with terms on outer boundaries.

Towards the end of Sec. 3.5.3, everything is put together to yield the final integral formulation (3.5.24). In Sec. 3.7, (3.5.24) is discretized in space, providing the finite volume scheme (3.7.5) using the operators (3.7.122). The discretization is achieved by approximating the integrals occurring in (3.5.24) using quadrature formulas, assuming the integrands to be constant inside their respective domains of integration. Since the integration domains are either control volumes or flat pieces of control volume surfaces, the approximation should become better as the partition into control volumes gets finer and the control volumes become smaller, provided that the integrands are sufficiently regular.

3.5.1 Polytope Discretization of Space Domains

To commence with the program outlined above, let $\mathfrak{C}$ be the usual evolution equation complex (3.4.16), and let $\mathfrak{D}$ be the corresponding domain complex (3.4.15).

Each d-dimensional space domain p_j, $j \in J$, is to be discretized into finitely many d-polytopes $\omega_k^{(j)}$. To that end, for each $j \in J$, consider a partition $\Pi^{(j)} := (\omega_k^{(j)})_{k\in I^{(j)}}$ of p_j, where each $\omega_k^{(j)}$ is a d-dimensional polytope, and each $I^{(j)}$ is a finite set. The polytopes $\omega_k^{(j)}$ are called *control volumes*. An example is depicted in Fig. 3.4.

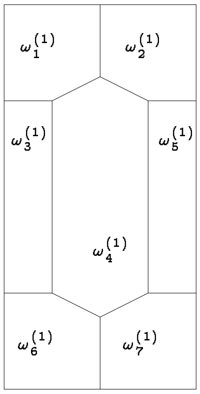


Figure 3.4: Partition of space domain p_1 into control volumes $\omega_1^{(1)}, \dots, \omega_7^{(1)}$.

Notation 3.5.1. Let $A \subseteq \mathbb{R}^d$. Then

$$\operatorname{diam} A := \sup \left\{ \|a-b\|_2 : (a,b) \in A^2 \right\} \in [0,\infty] \tag{3.5.1}$$

is called the *diameter* of the set A.

—

The number

$$h^{(j)} := \max \left\{ \operatorname{diam} \omega_k^{(j)} : k \in I^{(j)} \right\} \tag{3.5.2}$$

is called the *fineness* of the partition $\Pi^{(j)}$.

3.5.2 Integral Formulation of Time-Discrete Evolution Equations

Fix a time discretization $\mathfrak{T}$ of $\mathfrak{C}$ according to (3.4.33). Moreover, fix a solution

$$\left(\mathfrak{u}^{(0)}, \dots, \mathfrak{u}^{(n)}\right) = \left(u_j^{(\nu)}\right)_{(j,\nu)\in J\times\{0,\dots,n\}}$$

to $\mathfrak{T}$ according to Def. 3.4.14.

Of course, in general, a solution to $\mathfrak{T}$ might not exist, and its existence is not claimed here. It is just shown in the following, that each solution to $\mathfrak{T}$ (if it exists) also satisfies an integral formulation of the problem. This is the standard approach when passing from strong solutions (of the original problem) to weak solutions (of the integral problem), where the term "weak solutions" is used, since the integral problem can have a solution even if the original problem has none.

The time-discrete evolution equations from Def. 3.4.14(ii) are to be integrated over each control volume $\omega_k^{(j)}$. As $H^{(\nu)}_{b_j,v_j,k_j,f_j}$ is computed according to (3.3.8), integrating

$$H^{(\nu)}_{b_j,v_j,k_j,f_j}\left[(u_j^{(\nu)}, u_j^{(\nu-1)})\right] = 0$$

over $\omega_k^{(j)}$, $k \in I^{(j)}$, results in

$$\begin{aligned}
0 = (t_\nu - t_{\nu-1})^{-1} &\left(\int_{\omega_k^{(j)}} b_j^{(\nu)}\left[(u_j^{(\nu)}[x], x)\right] \mathrm{d}\lambda_d[x] - \int_{\omega_k^{(j)}} b_j^{(\nu-1)}\left[(u_j^{(\nu-1)}[x], x)\right] \mathrm{d}\lambda_d[x] \right) \\
&+ \int_{\omega_k^{(j)}} \operatorname{div}\left(v_j^{(\nu)}\left[(u_j^{(\nu)}[x], x)\right]\right) \mathrm{d}\lambda_d[x] - \int_{\omega_k^{(j)}} \operatorname{div}\left(k_j^{(\nu)}\left[(u_j^{(\nu)}[x], x)\right] \nabla u_j^{(\nu)}[x]\right) \mathrm{d}\lambda_d[x] \\
&- \int_{\omega_k^{(j)}} f_j^{(\nu)}\left[(u_j^{(\nu)}[x], x)\right] \mathrm{d}\lambda_d[x] ,
\end{aligned} \tag{3.5.3}$$

where λ_d denotes d-dimensional Lebesgue measure, and $\mathrm{d}\lambda_d[x]$ indicates integration with respect to the variable x.

Now the Gauss-Green Integration Th. C.8.2 can be applied if the arguments of the divergence terms in (3.5.3) are sufficiently regular. In that case, one gets

$$\begin{aligned}
&\int_{\omega_k^{(j)}} \operatorname{div}\left(v_j^{(\nu)}\left[(u_j^{(\nu)}[x], x)\right]\right) \mathrm{d}\lambda_d[x] \\
&= \int_{\partial\omega_k^{(j)}} \left(v_j^{(\nu)}\left[(u_j^{(\nu)}[x], x)\right]\right) \bullet n_{\omega_k^{(j)}}[x] \, \mathrm{d}\lambda_{d-1}[x] ,
\end{aligned} \tag{3.5.4a}$$

$$\begin{aligned}
&\int_{\omega_k^{(j)}} \operatorname{div}\left(k_j^{(\nu)}\left[(u_j^{(\nu)}[x], x)\right] \nabla u_j^{(\nu)}[x]\right) \mathrm{d}\lambda_d[x] \\
&= \int_{\partial\omega_k^{(j)}} F^{(\nu)}_{j,\partial\omega_k^{(j)}}[x] \bullet n_{\omega_k^{(j)}}[x] \, \mathrm{d}\lambda_{d-1}[x] .
\end{aligned} \tag{3.5.4b}$$

Decomposition of the Boundary Integrals

With respect to the relative topology on $\partial\omega_k^{(j)}$,

$$\left(\partial\omega_k^{(j)} \cap \operatorname{int}[p_j],\ \ \partial\omega_k^{(j)} \cap \partial p,\ \ \partial\omega_k^{(j)} \cap (\partial p_j \setminus \partial p)\right) \tag{3.5.5}$$

is a partition of $\partial\omega_k^{(j)}$ (s. Figs 3.5 and 3.6). Thus,

$$\int_{\partial\omega_k^{(j)}} = \int_{\partial\omega_k^{(j)}\cap\mathrm{int}[p_j]} + \int_{\partial\omega_k^{(j)}\cap\partial p} + \int_{\partial\omega_k^{(j)}\cap(\partial p_j\setminus\partial p)} . \tag{3.5.6}$$

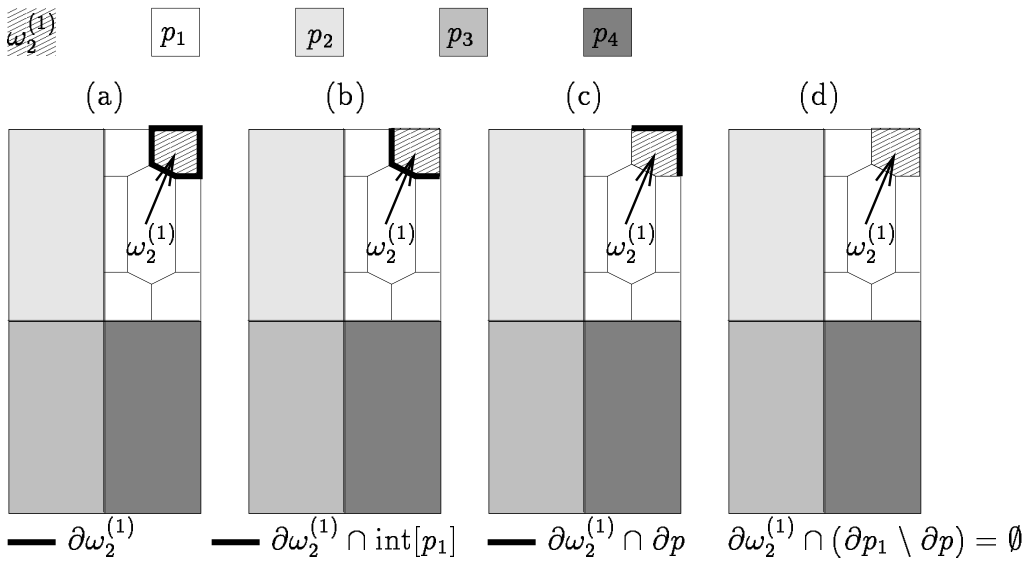


Figure 3.5: Partition of $\partial\omega_2^{(1)}$ according to (3.5.5).

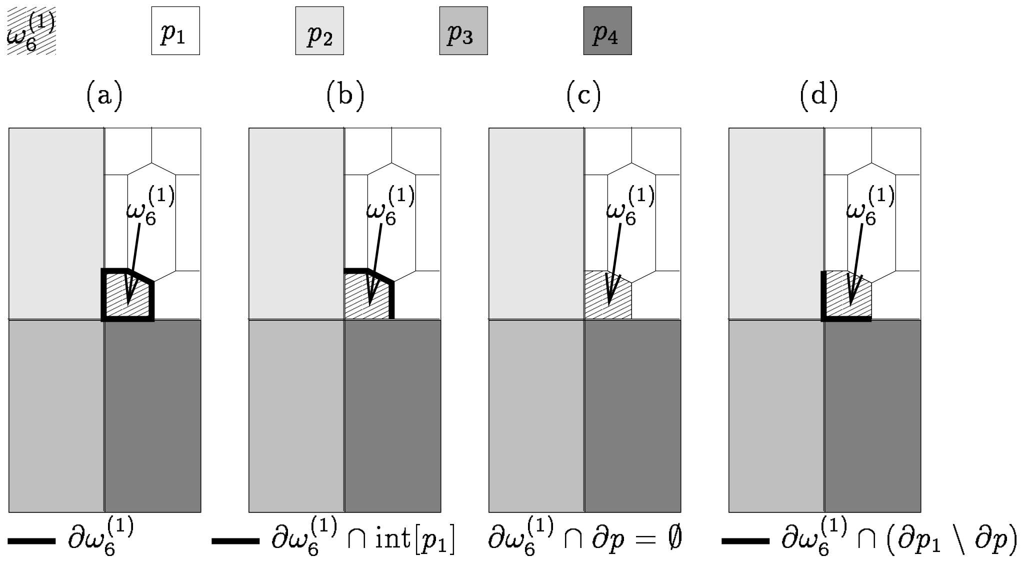


Figure 3.6: Partition of $\partial\omega_6^{(1)}$ according to (3.5.5).

With respect to the relative topology on $\partial\omega_k^{(j)} \cap \partial p$,

$$\left(\partial\omega_k^{(j)} \cap \Gamma_{j,\iota}\right)_{\iota\in J_j} \tag{3.5.7}$$

is a partition of $\partial\omega_k^{(j)} \cap \partial p$ (s. Fig. 3.7), i.e. in consequence,

$$\int_{\partial\omega_k^{(j)}\cap\partial p} = \sum_{\iota\in J_j} \int_{\partial\omega_k^{(j)}\cap\Gamma_{j,\iota}} . \tag{3.5.8}$$

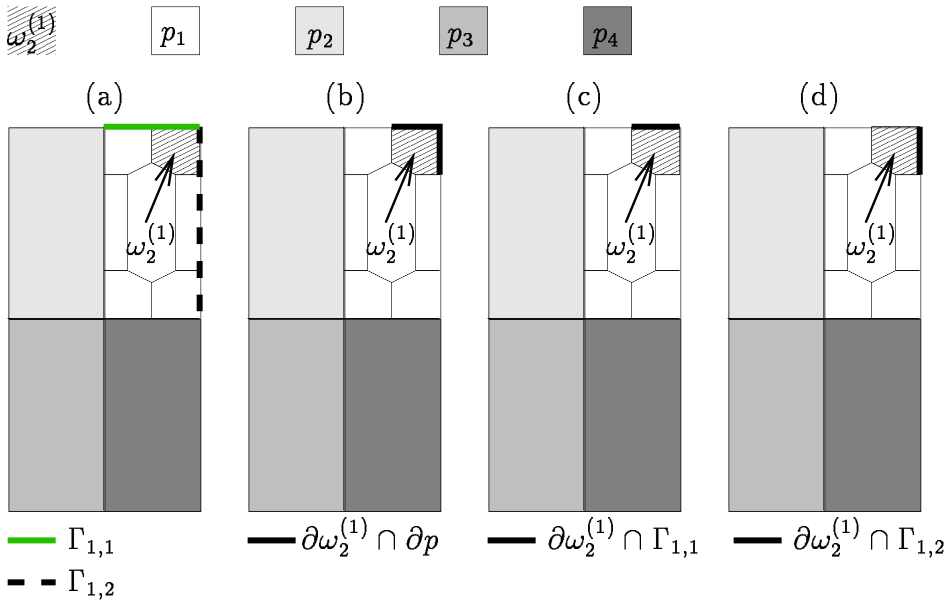


Figure 3.7: Partition of $\partial\omega_2^{(1)} \cap \partial p$ according to (3.5.7).

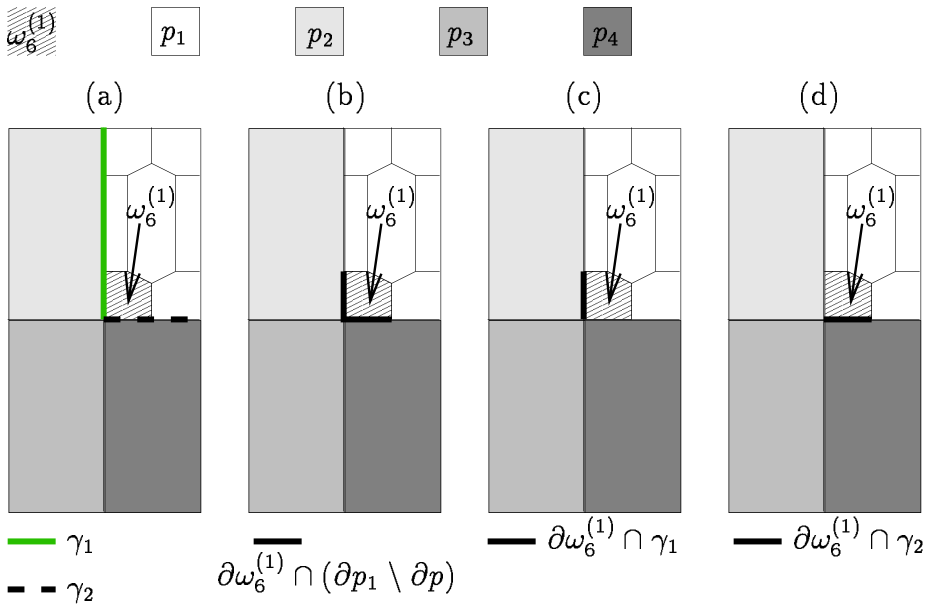


Figure 3.8: Partition of $\partial\omega_6^{(1)} \cap (\partial p_1 \setminus \partial p)$ according to (3.5.9).

With respect to the relative topology on $\partial\omega_k^{(j)} \cap (\partial p_j \setminus \partial p)$,

$$(\partial\omega_k^{(j)} \cap \gamma)_{\gamma \in \mathrm{IF}} \tag{3.5.9}$$

is a partition of $\partial\omega_k^{(j)} \cap (\partial p_j \setminus \partial p)$ (s. Fig. 3.8), resulting in

$$\int_{\partial\omega_k^{(j)} \cap (\partial p_j \setminus \partial p)} = \sum_{\gamma \in \mathrm{IF}} \int_{\partial\omega_k^{(j)} \cap \gamma}. \tag{3.5.10}$$

Combining (3.5.6), (3.5.8), and (3.5.10) yields:

$$\int_{\partial\omega_k^{(j)}} = \int_{\partial\omega_k^{(j)} \cap \mathrm{int}[p_j]} + \sum_{\iota \in J_j} \int_{\partial\omega_k^{(j)} \cap \Gamma_{j,\iota}} + \sum_{\gamma \in \mathrm{IF}} \int_{\partial\omega_k^{(j)} \cap \gamma}. \tag{3.5.11}$$

Now using (3.5.4) and (3.5.11), (3.5.3) can be written as

$$0 = (t_\nu - t_{\nu-1})^{-1} \left(\int_{\omega_k^{(j)}} b_j^{(\nu)}\left[(u_j^{(\nu)}[x], x)\right] \mathrm{d}\lambda_d[x] - \int_{\omega_k^{(j)}} b_j^{(\nu-1)}\left[(u_j^{(\nu-1)}[x], x)\right] \mathrm{d}\lambda_d[x] \right) \tag{3.5.12a}$$

$$+ \int_{\partial\omega_k^{(j)} \cap \mathrm{int}[p_j]} \left(v_j^{(\nu)}\left[(u_j^{(\nu)}[x], x)\right]\right) \bullet n_{\omega_k^{(j)}}[x] \, \mathrm{d}\lambda_{d-1}[x] \tag{3.5.12b}$$

$$+ \int_{\partial\omega_k^{(j)} \cap \partial p} \left(v_j^{(\nu)}\left[(u_j^{(\nu)}[x], x)\right]\right) \bullet n_{\omega_k^{(j)}}[x] \, \mathrm{d}\lambda_{d-1}[x] \tag{3.5.12c}$$

$$+ \sum_{\gamma \in \mathrm{IF}} \int_{\partial\omega_k^{(j)} \cap \gamma} \left(v_j^{(\nu)}\left[(u_j^{(\nu)}[x], x)\right]\right) \bullet n_{\omega_k^{(j)}}[x] \, \mathrm{d}\lambda_{d-1}[x] \tag{3.5.12d}$$

$$- \int_{\partial\omega_k^{(j)} \cap \mathrm{int}[p_j]} F_{j,\partial\omega_k^{(j)}}^{(\nu)}[x] \bullet n_{\omega_k^{(j)}}[x] \, \mathrm{d}\lambda_{d-1}[x] \tag{3.5.12e}$$

$$- \sum_{\iota \in J_j} \int_{\partial\omega_k^{(j)} \cap \Gamma_{j,\iota}} F_{j,\partial\omega_k^{(j)}}^{(\nu)}[x] \bullet n_{\omega_k^{(j)}}[x] \, \mathrm{d}\lambda_{d-1}[x] \tag{3.5.12f}$$

$$- \sum_{\gamma \in \mathrm{IF}} \int_{\partial\omega_k^{(j)} \cap \gamma} F_{j,\partial\omega_k^{(j)}}^{(\nu)}[x] \bullet n_{\omega_k^{(j)}}[x] \, \mathrm{d}\lambda_{d-1}[x] \tag{3.5.12g}$$

$$- \int_{\omega_k^{(j)}} f_j^{(\nu)}\left[(u_j^{(\nu)}[x], x)\right] \mathrm{d}\lambda_d[x]. \tag{3.5.12h}$$

On non-Dirichlet boundaries, the boundary conditions (3.4.31) are used to replace

(3.5.12f):

$$
\begin{aligned}
&-\sum_{\iota\in J_j\setminus\{0\}}\int_{\partial\omega_k^{(j)}\cap\Gamma_{j,\iota}} F^{(\nu)}_{j,\partial\omega_k^{(j)}}[x]\bullet n_{\omega_k^{(j)}}[x]\,\mathrm{d}\lambda_{d-1}[x]\\
&=-\sum_{\iota\in J_j\setminus\{0\}}\int_{\partial\omega_k^{(j)}\cap\Gamma_{j,\iota}} (\mathcal{B}_{j,\iota})^{\text{ex.-im.}}\big[\big(\mathfrak{u}^{(\nu-1)},\mathfrak{u}^{(\nu)}\big)\big][x]\,\mathrm{d}\lambda_{d-1}[x]\\
&\quad+\sum_{\iota\in J_j\setminus\{0\}}\int_{\partial\omega_k^{(j)}\cap\Gamma_{j,\iota}} \big(a^{j,\iota,\nu}_{\text{out}}\big)^{\text{ex.-im.}}\big[\big((u_j^{(\nu-1)}[x],u_j^{(\nu)}[x]),x\big)\big]\,\mathrm{d}\lambda_{d-1}[x]\,.
\end{aligned}
\tag{3.5.13}
$$

3.5.3 Using Interface Conditions to Replace Terms Involving the Flux across Interfaces

The interface conditions (3.4.17), (3.4.20), and (3.4.24) are to be used to replace (3.5.12g). Therefore, one needs to have a relationship between the partitions $\Pi^{(j_1)}$ and $\Pi^{(j_2)}$ whenever p_{j_1} and p_{j_2} share a common interface, i.e. whenever $\{j_1,j_2\}\in\mathrm{IF}$.

The idea is to start with a finite partition $\Pi=(\omega_k)_{k\in I_\Pi}$ of the total space domain p. As before, the ω_k are assumed to be d-dimensional polytopes that will be referred to as control volumes. The partition Π is used to construct the partitions $\Pi^{(j)}=(\omega_k^{(j)})_{k\in I^{(j)}}$ by letting

$$\omega_k^{(j)} := \overline{\mathrm{int}[\omega_k\cap p_j]}, \tag{3.5.14}$$

$$I^{(j)} := \big\{k\in I_\Pi : \omega_k^{(j)}\neq\emptyset\big\}. \tag{3.5.15}$$

Indeed, if $\omega_k^{(j)}$ is not empty, then it is a d-polytope according to Rem. C.4.10. Moreover, as Π is a partition of p and $(p_j)_{j\in J}$ is a partition of p by Def. 3.4.5(i), $(\omega_k^{(j)})_{j\in J:\,k\in I^{(j)}}$ is a partition of ω_k, and $\Pi^{(j)}$ is a partition of p_j. An example is illustrated in Fig. 3.9.

In general, (3.5.14) can not be replaced by $\omega_k^{(j)} := \omega_k\cap p_j$, since $\omega_k\cap p_j$ can have dimension less than d (cf. Fig. 3.10).

According to the considerations of Sec. 3.5.2, (3.5.12) holds for each $\omega_k^{(j)}$. The term (3.5.12g) can only yield a nonzero contribution if $\partial\omega_k^{(j)}\cap\gamma$ has dimension $d-1$. This is precisely the case where the interface conditions are to be used on (3.5.12g). For that reason, ω_k needs to lie on both sides of its $(d-1)$-dimensional intersections with an interface γ (if any). In the language of the following Def. 3.5.2, ω_k needs to be nontangent to interfaces.

Definition 3.5.2. If $\omega\subseteq p$ is a d-dimensional polytope, and for each $j\in J$, $\omega^{(j)} := \overline{\mathrm{int}[\omega\cap p_j]}$, then ω is called *nontangent* to interfaces iff

$$\bigwedge_{\gamma\in\mathrm{IF}} \quad \partial_{\mathrm{reg}}\omega^{(i_1[\gamma])}\cap\gamma=\partial_{\mathrm{reg}}\omega^{(i_2[\gamma])}\cap\gamma, \tag{3.5.16}$$

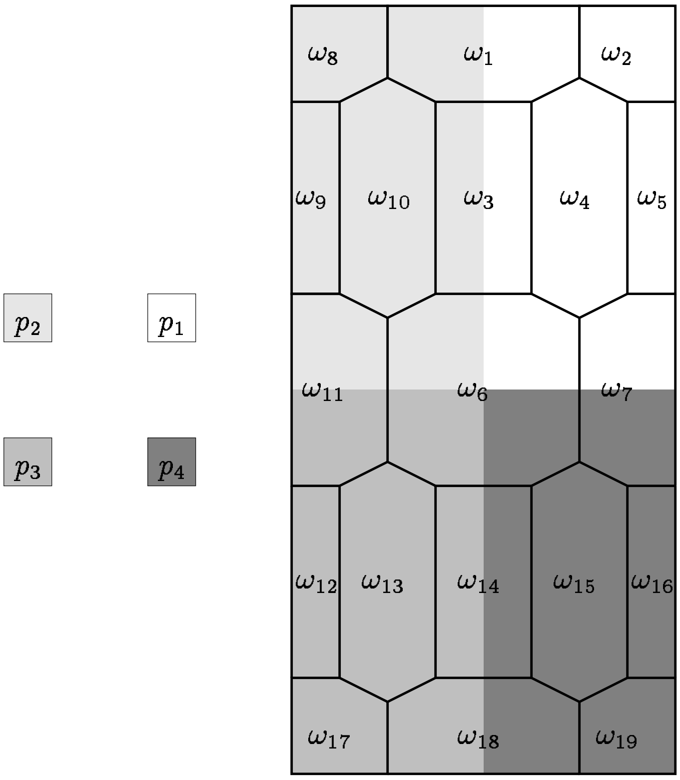


Figure 3.9: The domain $p := p_1 \cup p_2 \cup p_3 \cup p_4$ is partitioned into $\omega_1, \ldots, \omega_{19}$. If for each $j \in \{1, \ldots, 4\}$, one lets $\omega_k^{(j)} := \omega_k \cap p_j$, $k \in \{1, \ldots, 19\}$, then for each j, $\Pi^{(j)} := (\omega_k^{(j)})_{k \in I^{(j)}}$ forms a partition of p_j, where e.g. $I^{(1)} = \{1, \ldots, 7\}$, $I^{(2)} = \{1, 3, 6, 8, 9, 10, 11\}$. The ω_k are numbered such that $\Pi^{(1)}$ recovers the partition of Fig. 3.4. For example, one also has that $(\omega_1^{(1)}, \omega_1^{(2)})$ is a partition of ω_1, and that $(\omega_6^{(1)}, \omega_6^{(2)}, \omega_6^{(3)}, \omega_6^{(4)})$ is a partition of ω_6.

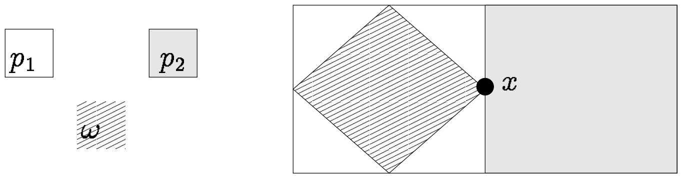


Figure 3.10: The intersection of the control volume ω with p_2 is the 0-polytope $\{x\}$.

where i_1 and i_2 are the maps introduced after (3.4.5).

The polytope ω is called *tangent* to interfaces iff it fails to satisfy (3.5.16).

—

Examples of polytopes being nontangent (respectively tangent) to interfaces are given in Fig. 3.11 (respectively Fig. 3.12). All the control volumes occurring in Fig. 3.9 are nontangent to interfaces.

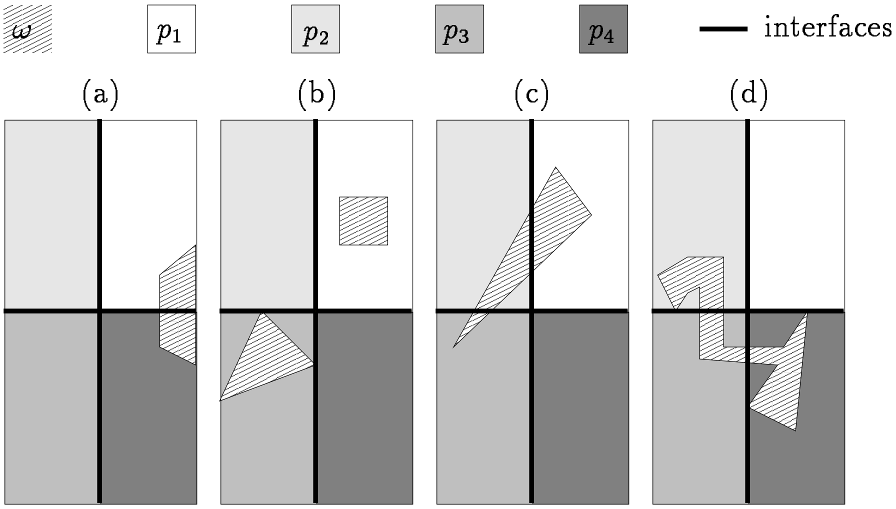


Figure 3.11: Examples of the polytope ω being *nontangent* to interfaces according to Def. 3.5.2.

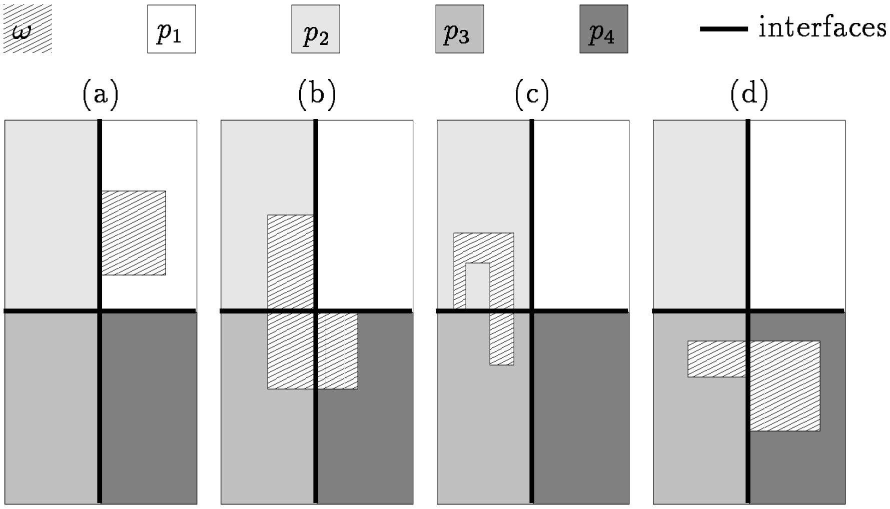


Figure 3.12: Examples of the polytope ω being *tangent* to interfaces according to Def. 3.5.2.

Due to the different situations found at continuous interfaces as compared to jump interfaces, another preparatory step is taken before the interface conditions are applied to (3.5.12g).

To ensure that in the finite volume discretization (3.7.5) the number of equations is the same as the number of degrees of freedom of the solution due to discontinuities at jump interfaces (cf. the paragraph after (3.5.24)), equations (3.5.12) are combined by summation if and only if the corresponding $\omega_k^{(j)}$ are connected via a sequence of continuous interfaces. To that end, an equivalence relation is defined on the set

$$V_{\omega_k} := \{ j \in J : \text{int}\,[\omega_k \cap p_j] \neq \emptyset \}, \tag{3.5.17}$$

by defining j_1 and j_2 to be equivalent (denoted $j_1 \sim j_2$) if and only if $\partial_{\text{reg}}\omega_k^{(j_1)} \cap \partial_{\text{reg}}\omega_k^{(j_2)} \neq \emptyset$ and $\partial_{\text{reg}} p_{j_1} \cap \partial_{\text{reg}} p_{j_2} \in \text{IF}_{\text{con}}$ ($\{j_1, j_2\} \in E_{\text{con}}$). To obtain an equivalence relation, the closure of the relation "$\sim$" with respect to transitivity is taken. Then each equivalence class can be identified with the connected component of a graph (cf. Def. C.5.3 in App. C.5):

Definition 3.5.3. For each d-dimensional polytope $\omega \subseteq p$, define the *associated graph* $\mathcal{G}_\omega = (V_\omega, E_\omega)$, where the set of vertices $V := V_\omega$ is defined analogous to the set V_{ω_k} in (3.5.17), and the set of edges E_ω is defined by

$$E_\omega := \{ \{j_1, j_2\} \subseteq V_\omega : \partial_{\text{reg}}\omega_k^{(j_1)} \cap \partial_{\text{reg}}\omega_k^{(j_2)},\ \{j_1, j_2\} \in E_{\text{con}} \neq \emptyset \}. \tag{3.5.18}$$

Example 3.5.4. Figure 3.13 depicts three examples differing in the way the jump interfaces and the continuous interfaces are distributed. In each case, the associated graph of the polytope ω is drawn below the respecive space domain. In case (a), $\mathcal{G} := \mathcal{G}_\omega$ has the single connected component $\{1, 2, 3, 4\}$. In (b) and (c), $\mathcal{G}$ has two connected components, $\text{CoCmp}[\mathcal{G}] = \{\{1, 2\}, \{2, 3\}\}$ in (b) and $\text{CoCmp}[\mathcal{G}] = \{\{1\}, \{2, 3, 4\}\}$ in (c).

—

In a natural way, the connected components $\mathcal{C} \in \text{CoCmp}[\mathcal{G}_\omega]$ are again graphs, and the vertex set of $\mathcal{C}$ is denoted by $V[\mathcal{C}]$ (cf. App. C.5). These vertex sets are identical to the equivalence classes defined above.

Lemma 3.5.5. *As before, let* $\Pi = (\omega_k)_{k \in I_\Pi}$ *be a partition of* p *into control volumes, and let the* $\omega_k^{(j)}$ *be defined by* (3.5.14). *Moreover, let* $\mathcal{C} \in \text{CoCmp}[\mathcal{G}_{\omega_k}]$, *and let* $\gamma \in \text{IF}$ *such that*

$$\gamma \cap \bigcup_{j \in V[\mathcal{C}]} \partial_{\text{reg}}\omega_k^{(j)} \neq \emptyset. \tag{3.5.19}$$

If ω_k *is nontangent to interfaces, then precisely one of the following three situations occurs:*

(a) $\gamma \in \text{IF}_{\text{con}}$ *and* $\{i_1[\gamma], i_2[\gamma]\} \subseteq V[\mathcal{C}]$.

(b) $\gamma \in \text{IF}_{\text{jump}}$ *and* $i_1[\gamma] \in V[\mathcal{C}]$.

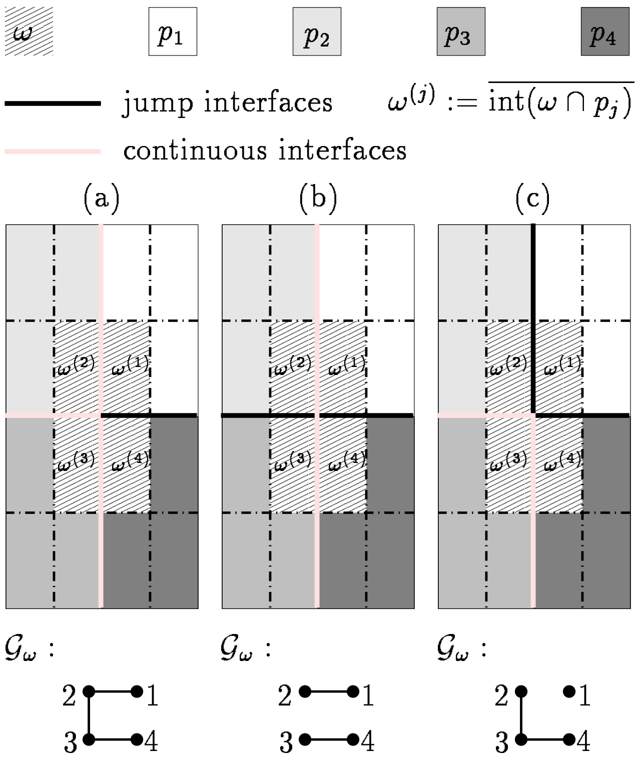


Figure 3.13: Three examples showing the associated graph of a polytope ω for different distributions of jump interfaces and continuous interfaces (s. Exs 3.5.4 and 3.5.8).

(c) $\gamma \in \mathrm{IF}_{\mathrm{jump}}$ *and* $i_2[\gamma] \in V[\mathcal{C}]$.

Proof. According to (3.4.8), one has $\gamma = \partial_{\mathrm{reg}} p_{i_1[\gamma]} \cap \partial_{\mathrm{reg}} p_{i_2[\gamma]}$. Combining (3.5.19) with (3.5.16) yields $\partial_{\mathrm{reg}} \omega^{(i_1[\gamma])} \cap \gamma = \partial_{\mathrm{reg}} \omega^{(i_2[\gamma])} \cap \gamma \neq \emptyset$ with either $i_1[\gamma] \in V[\mathcal{C}]$ or $i_2[\gamma] \in V[\mathcal{C}]$, which proves the lemma for $\gamma \in \mathrm{IF}_{\mathrm{jump}}$. If $\gamma \in \mathrm{IF}_{\mathrm{con}}$, then $\{i_1[\gamma], i_2[\gamma]\} \subseteq V[\mathcal{C}]$ by (3.5.18). ■

Notation 3.5.6. If ω_k is nontangent to interfaces, then, bearing in mind Lem. 3.5.5, for each $\alpha \in \{1, 2\}$ define

$$\begin{aligned} G_{\mathrm{jump},\alpha} &: \mathrm{CoCmp}[\mathcal{G}_{\omega_k}] \longrightarrow \mathcal{P}[\mathrm{IF}_{\mathrm{jump}}], \\ G_{\mathrm{jump},\alpha}[\mathcal{C}] &:= \big\{\gamma \in \mathrm{IF}_{\mathrm{jump}} : i_\alpha[\gamma] \in V[\mathcal{C}]\big\}. \end{aligned} \tag{3.5.20}$$

Remark 3.5.7. For each $\mathcal{C} \in \mathrm{CoCmp}[\mathcal{G}_{\omega_k}]$, $\alpha \in \{1, 2\}$, and $\gamma \in \mathrm{IF}_{\mathrm{jump}}$, one has $i_\alpha[\gamma] \in V[\mathcal{C}] \Leftrightarrow \mathcal{C} = \mathrm{CoCmp}_{\mathcal{G}_{\omega_k}}[i_\alpha[\gamma]]$, as each connected component is the connected component of all its vertices.

Example 3.5.8. Consider case (c) of Fig. 3.13. It is clear that ω is nontangent to interfaces. Let the four interfaces be denoted by $\gamma_{1,2} := \partial_{\mathrm{reg}} p_1 \cap \partial_{\mathrm{reg}} p_2$, $\gamma_{2,3} := \partial_{\mathrm{reg}} p_2 \cap \partial_{\mathrm{reg}} p_3$, $\gamma_{3,4} := \partial_{\mathrm{reg}} p_3 \cap \partial_{\mathrm{reg}} p_4$, and $\gamma_{1,4} := \partial_{\mathrm{reg}} p_1 \cap \partial_{\mathrm{reg}} p_4$. Then $\mathrm{IF}_{\mathrm{con}} = \{\gamma_{2,3}, \gamma_{3,4}\}$ and

$\mathrm{IF}_{\mathrm{jump}} = \{\gamma_{1,2}, \gamma_{1,4}\}$. As illustrated in Fig. 3.13(c), the associated graph of ω has the two connected components $\mathcal{C}_1 = (V[\mathcal{C}_1], E[\mathcal{C}_1])$ and $\mathcal{C}_2 = (V[\mathcal{C}_2], E[\mathcal{C}_2])$, where $V[\mathcal{C}_1] = \{1\}$, $E[\mathcal{C}_1] = \emptyset$, $V[\mathcal{C}_2] := \{2, 3, 4\}$, and $E[\mathcal{C}_2] = \big\{\{2, 3\}, \{3, 4\}\big\}$.

A typical application resulting in the picture shown in Fig. 3.13(c) is given by the following situation: Let p_1 be the domain of a gas phase, and let p_2, p_3, and p_4 denote the domains of different solid materials. Between different solids, assume continuity of both heat flux and temperature according to (2.3.1a) and (2.3.2a). Between solid and gas assume the jump interface condition (2.3.2b′) and the flux interface condition (2.4.39b).

As the interface conditions (2.3.1a) and (2.3.2a) are completely symmetric with respect to the materials adjacent to the respective continuous interface, one still has a choice when defining i_1 and i_2 on $\gamma_{2,3}$ and $\gamma_{3,4}$. For definiteness, let $i_1[\gamma_{2,3}] := 2$, $i_2[\gamma_{2,3}] := 3$, $i_1[\gamma_{3,4}] := 3$, $i_2[\gamma_{3,4}] := 4$. However, (2.3.2b′) and (2.4.39b) are not symmetric with respect to the materials adjacent to the respective jump interface. To conform to the conventions introduced in (3.4.6) and (3.4.7), respecitvely, one has to define $i_1[\gamma_{1,2}] := 1$, $i_2[\gamma_{1,2}] := 2$, $i_1[\gamma_{1,4}] := 1$, $i_2[\gamma_{1,4}] := 4$ (cf. Ex. 3.4.4).

Consider the case $\mathcal{C} := \mathcal{C}_1$. Then the condition (3.5.19) is satisfied if and only if $\gamma \in \mathrm{IF}_{\mathrm{jump}}$. For both the choices of $\gamma \in \mathrm{IF}_{\mathrm{jump}}$, one is in the case of Lem. 3.5.5(b). In particular, $G_{\mathrm{jump},1}[\mathcal{C}_1] = \mathrm{IF}_{\mathrm{jump}}$ and $G_{\mathrm{jump},2}[\mathcal{C}_1] = \emptyset$.

Consider the case $\mathcal{C} := \mathcal{C}_2$. Then the condition (3.5.19) is satisfied for each $\gamma \in \mathrm{IF}$. For $\gamma \in \mathrm{IF}_{\mathrm{con}}$, one is in case (a) of Lem. 3.5.5. For both the choices of $\gamma \in \mathrm{IF}_{\mathrm{jump}}$, one is in the case of Lem. 3.5.5(c). In particular, $G_{\mathrm{jump},1}[\mathcal{C}_2] = \emptyset$ and $G_{\mathrm{jump},2}[\mathcal{C}_2] = \mathrm{IF}_{\mathrm{jump}}$.

—

For the rest of Sec. 3.5.3, assume that for each $k \in I_\Pi$, ω_k is nontangent to interfaces, and let $\mathcal{G}_k := \mathcal{G}_{\omega_k}$ be the associated graph of ω_k.

Fix $k \in I_\Pi$ and $\mathcal{C} \in \mathrm{CoCmp}[\mathcal{G}_k]$. Sum (3.5.12g) over $j \in V[\mathcal{C}]$. If $\gamma \in \mathrm{IF}_{\mathrm{con}}$ and $\gamma \cap \bigcup_{j \in V[\mathcal{C}]} \partial_{\mathrm{reg}}\omega_k^{(j)} \neq \emptyset$, then $\{i_1[\gamma], i_2[\gamma]\} \subseteq V[\mathcal{C}]$ according to Lem. 3.5.5(a). Hence, (3.4.24) can be applied to yield

$$\begin{aligned}
&- \sum_{j \in V[\mathcal{C}]} \sum_{\gamma \in \mathrm{IF}_{\mathrm{con}}} \int_{\partial\omega_k^{(j)} \cap \gamma} F^{(\nu)}_{j, \partial\omega_k^{(j)}}[x] \bullet n_{\omega_k^{(j)}}[x] \, \mathrm{d}\lambda_{d-1}[x] \\
&= - \sum_{\gamma \in \mathrm{IF}_{\mathrm{con}}} \int_{\gamma \cap \bigcup_{j \in V[\mathcal{C}]} \partial_{\mathrm{reg}}\omega_k^{(j)}} (\mathcal{A}_\gamma)^{\text{ex.-im.}} \big[\big(\mathrm{u}^{(\nu-1)}, \mathrm{u}^{(\nu)}\big) \big] [x] \, \mathrm{d}\lambda_{d-1}[x] \\
&\quad - \sum_{\gamma \in \mathrm{IF}_{\mathrm{con}}} \int_{\gamma \cap \bigcup_{j \in V[\mathcal{C}]} \partial_{\mathrm{reg}}\omega_k^{(j)}} (a_{\mathrm{flux}}^{\gamma,1,\nu})^{\text{ex.-im.}} \Big[\big((u_{i_1[\gamma]}^{(\nu-1)}[x], u_{i_1[\gamma]}^{(\nu)}[x]), x \big) \Big] \, \mathrm{d}\lambda_{d-1}[x] \\
&\quad + \sum_{\gamma \in \mathrm{IF}_{\mathrm{con}}} \int_{\gamma \cap \bigcup_{j \in V[\mathcal{C}]} \partial_{\mathrm{reg}}\omega_k^{(j)}} (a_{\mathrm{flux}}^{\gamma,2,\nu})^{\text{ex.-im.}} \Big[\big((u_{i_2[\gamma]}^{(\nu-1)}[x], u_{i_2[\gamma]}^{(\nu)}[x]), x \big) \Big] \, \mathrm{d}\lambda_{d-1}[x] \,. \qquad (3.5.21)
\end{aligned}$$

If $\gamma \in \mathrm{IF}_{\mathrm{jump}}$ and $\gamma \cap \bigcup_{j \in V[\mathcal{C}]} \partial_{\mathrm{reg}} \omega_k^{(j)} \neq \emptyset$, then according to Lem. 3.5.5 and Not. 3.5.6 either $\gamma \in G_{\mathrm{jump},1}[\mathcal{C}]$ or $\gamma \in G_{\mathrm{jump},2}[\mathcal{C}]$.

If $\gamma \in G_{\mathrm{jump},1}[\mathcal{C}]$, then $i_1[\gamma] \in V[\mathcal{C}]$, and one can use (3.4.20) to get

$$\begin{aligned}
&- \sum_{j \in V[\mathcal{C}]} \sum_{\gamma \in G_{\mathrm{jump},1}[\mathcal{C}]} \int_{\partial \omega_k^{(j)} \cap \gamma} F^{(\nu)}_{j, \partial \omega_k^{(j)}}[x] \bullet n_{\omega_k^{(j)}}[x] \, \mathrm{d}\lambda_{d-1}[x] \\
&= \sum_{\gamma \in G_{\mathrm{jump},1}[\mathcal{C}]} \int_{\partial \omega_k^{(i_1[\gamma])} \cap \gamma} \Big(a^{\gamma,1,\nu}_{\mathrm{jump}}\big[(u^{(\nu)}_{i_1[\gamma]}[x], x)\big] - a^{\gamma,2,\nu}_{\mathrm{jump}}\big[(u^{(\nu)}_{i_2[\gamma]}[x], x)\big]\Big) \, \mathrm{d}\lambda_{d-1}[x]\,. \qquad (3.5.22)
\end{aligned}$$

If $\gamma \in G_{\mathrm{jump},2}[\mathcal{C}]$, then $i_2[\gamma] \in V[\mathcal{C}]$, and one can use (3.4.26) to get

$$\begin{aligned}
&- \sum_{j \in V[\mathcal{C}]} \sum_{\gamma \in G_{\mathrm{jump},2}[\mathcal{C}]} \int_{\partial \omega_k^{(j)} \cap \gamma} F^{(\nu)}_{j, \partial \omega_k^{(j)}}[x] \bullet n_{\omega_k^{(j)}}[x] \, \mathrm{d}\lambda_{d-1}[x] \\
&= - \sum_{\gamma \in G_{\mathrm{jump},2}[\mathcal{C}]} \int_{\partial \omega_k^{(i_2[\gamma])} \cap \gamma} (\mathcal{A}_\gamma)^{\text{ex.-im.}}\Big[\big(\mathrm{u}^{(\nu-1)}, \mathrm{u}^{(\nu)}\big)\Big][x] \, \mathrm{d}\lambda_{d-1}[x] \\
&\quad - \sum_{\gamma \in G_{\mathrm{jump},2}[\mathcal{C}]} \int_{\partial \omega_k^{(i_2[\gamma])} \cap \gamma} (a^{\gamma,1,\nu}_{\mathrm{flux}})^{\text{ex.-im.}}\Big[\big((u^{(\nu-1)}_{i_1[\gamma]}[x], u^{(\nu)}_{i_1[\gamma]}[x]), x\big)\Big] \, \mathrm{d}\lambda_{d-1}[x] \\
&\quad + \sum_{\gamma \in G_{\mathrm{jump},2}[\mathcal{C}]} \int_{\partial \omega_k^{(i_2[\gamma])} \cap \gamma} (a^{\gamma,2,\nu}_{\mathrm{flux}})^{\text{ex.-im.}}\Big[\big((u^{(\nu-1)}_{i_2[\gamma]}[x], u^{(\nu)}_{i_2[\gamma]}[x]), x\big)\Big] \, \mathrm{d}\lambda_{d-1}[x] \\
&\quad + \sum_{\gamma \in G_{\mathrm{jump},2}[\mathcal{C}]} \int_{\partial \omega_k^{(i_2[\gamma])} \cap \gamma} \Big(- a^{\gamma,1,\nu}_{\mathrm{jump}}\big[(u^{(\nu)}_{i_1[\gamma]}[x], x)\big] + a^{\gamma,2,\nu}_{\mathrm{jump}}\big[(u^{(\nu)}_{i_2[\gamma]}[x], x)\big]\Big) \, \mathrm{d}\lambda_{d-1}[x]\,.
\end{aligned}$$

(3.5.23)

Putting Everything Together

Summing (3.5.12) over $j \in V[\mathcal{C}]$, and using (3.5.13) to replace (3.5.12f), and (3.5.21), (3.5.22), and (3.5.23) to replace (3.5.12g), results in

$$\begin{aligned}
&(t_\nu - t_{\nu-1})^{-1} \sum_{j \in V[\mathcal{C}]} \Bigg(\int_{\omega_k^{(j)}} b_j^{(\nu)}\big[(u_j^{(\nu)}[x], x)\big] \, \mathrm{d}\lambda_d[x] \\
&\qquad\qquad - \int_{\omega_k^{(j)}} b_j^{(\nu-1)}\big[(u_j^{(\nu-1)}[x], x)\big] \, \mathrm{d}\lambda_d[x] \Bigg) \qquad (3.5.24a) \\
&+ \sum_{j \in V[\mathcal{C}]} \int_{\partial \omega_k^{(j)} \cap \operatorname{int}[p_j]} \Big(v_j^{(\nu)}\big[(u_j^{(\nu)}[x], x)\big]\Big) \bullet n_{\omega_k^{(j)}}[x] \, \mathrm{d}\lambda_{d-1}[x] \qquad (3.5.24b) \\
&+ \sum_{j \in V[\mathcal{C}]} \int_{\partial \omega_k^{(j)} \cap \partial p} \Big(v_j^{(\nu)}\big[(u_j^{(\nu)}[x], x)\big]\Big) \bullet n_{\omega_k^{(j)}}[x] \, \mathrm{d}\lambda_{d-1}[x] \qquad (3.5.24c)
\end{aligned}$$

$$+ \sum_{j \in V[\mathcal{C}]} \sum_{\gamma \in \mathrm{IF}} \int_{\partial\omega_k^{(j)} \cap \gamma} \left(v_j^{(\nu)} \left[(u_j^{(\nu)}[x], x) \right] \right) \bullet n_{\omega_k^{(j)}}[x] \, \mathrm{d}\lambda_{d-1}[x] \tag{3.5.24d}$$

$$- \sum_{j \in V[\mathcal{C}]} \int_{\partial\omega_k^{(j)} \cap \mathrm{int}[p_j]} F^{(\nu)}_{j, \partial\omega_k^{(j)}}[x] \bullet n_{\omega_k^{(j)}}[x] \, \mathrm{d}\lambda_{d-1}[x] \tag{3.5.24e}$$

$$- \sum_{j \in V[\mathcal{C}] : 0 \in J_j} \int_{\partial\omega_k^{(j)} \cap \Gamma_{j,0}} F^{(\nu)}_{j, \partial\omega_k^{(j)}}[x] \bullet n_{\omega_k^{(j)}}[x] \, \mathrm{d}\lambda_{d-1}[x]$$

$$- \sum_{j \in V[\mathcal{C}]} \sum_{\iota \in J_j \setminus \{0\}} \int_{\partial\omega_k^{(j)} \cap \Gamma_{j,\iota}} (\mathcal{B}_{j,\iota})^{\text{ex.-im.}} \left[\left(\mathfrak{u}^{(\nu-1)}, \mathfrak{u}^{(\nu)} \right) \right] [x] \, \mathrm{d}\lambda_{d-1}[x] \tag{3.5.24f}$$

$$+ \sum_{j \in V[\mathcal{C}]} \sum_{\iota \in J_j \setminus \{0\}} \int_{\partial\omega_k^{(j)} \cap \Gamma_{j,\iota}} (a_{\text{out}}^{j,\iota,\nu})^{\text{ex.-im.}} \left[\left((u_j^{(\nu-1)}[x], u_j^{(\nu)}[x]), x \right) \right] \mathrm{d}\lambda_{d-1}[x] \tag{3.5.24g}$$

$$- \sum_{\gamma \in \mathrm{IF}_{\mathrm{con}}} \int_{\gamma \cap \bigcup_{j \in V[\mathcal{C}]} \partial\omega_k^{(j)}} (\mathcal{A}_\gamma)^{\text{ex.-im.}} \left[\left(\mathfrak{u}^{(\nu-1)}, \mathfrak{u}^{(\nu)} \right) \right] [x] \, \mathrm{d}\lambda_{d-1}[x] \tag{3.5.24h}$$

$$+ \sum_{\gamma \in \mathrm{IF}_{\mathrm{con}}} \left(- \int\limits_{\gamma \cap \bigcup_{j \in V[\mathcal{C}]} \partial_{\mathrm{reg}}\omega_k^{(j)}} (a_{\text{flux}}^{\gamma,1,\nu})^{\text{ex.-im.}} \left[\left((u_{i_1[\gamma]}^{(\nu-1)}[x], u_{i_1[\gamma]}^{(\nu)}[x]), x \right) \right] \mathrm{d}\lambda_{d-1}[x] \right.$$

$$\left. + \int\limits_{\gamma \cap \bigcup_{j \in V[\mathcal{C}]} \partial_{\mathrm{reg}}\omega_k^{(j)}} (a_{\text{flux}}^{\gamma,2,\nu})^{\text{ex.-im.}} \left[\left((u_{i_2[\gamma]}^{(\nu-1)}[x], u_{i_2[\gamma]}^{(\nu)}[x]), x \right) \right] \mathrm{d}\lambda_{d-1}[x] \right) \tag{3.5.24i}$$

$$+ \sum_{\gamma \in G_{\mathrm{jump},1}[\mathcal{C}]} \int_{\partial\omega_k^{(i_1[\gamma])} \cap \gamma} \left(a_{\text{jump}}^{\gamma,1,\nu} \left[(u_{i_1[\gamma]}^{(\nu)}[x], x) \right] - a_{\text{jump}}^{\gamma,2,\nu} \left[(u_{i_2[\gamma]}^{(\nu)}[x], x) \right] \right) \mathrm{d}\lambda_{d-1}[x] \tag{3.5.24j}$$

$$- \sum_{\gamma \in G_{\mathrm{jump},2}[\mathcal{C}]} \int_{\partial\omega_k^{(i_2[\gamma])} \cap \gamma} (\mathcal{A}_\gamma)^{\text{ex.-im.}} \left[\left(\mathfrak{u}^{(\nu-1)}, \mathfrak{u}^{(\nu)} \right) \right] [x] \, \mathrm{d}\lambda_{d-1}[x] \tag{3.5.24k}$$

$$+ \sum_{\gamma \in G_{\mathrm{jump},2}[\mathcal{C}]} \left(- \int_{\partial\omega_k^{(i_2[\gamma])} \cap \gamma} (a_{\text{flux}}^{\gamma,1,\nu})^{\text{ex.-im.}} \left[\left((u_{i_1[\gamma]}^{(\nu-1)}[x], u_{i_1[\gamma]}^{(\nu)}[x]), x \right) \right] \mathrm{d}\lambda_{d-1}[x] \right.$$

$$\left. + \int_{\partial\omega_k^{(i_2[\gamma])} \cap \gamma} (a_{\text{flux}}^{\gamma,2,\nu})^{\text{ex.-im.}} \left[\left((u_{i_2[\gamma]}^{(\nu-1)}[x], u_{i_2[\gamma]}^{(\nu)}[x]), x \right) \right] \mathrm{d}\lambda_{d-1}[x] \right) \tag{3.5.24l}$$

$$+ \sum_{\gamma \in G_{\mathrm{jump},2}[\mathcal{C}]} \int\limits_{\partial\omega_k^{(i_2[\gamma])} \cap \gamma} \left(- a_{\text{jump}}^{\gamma,1,\nu} \left[(u_{i_1[\gamma]}^{(\nu)}[x], x) \right] + a_{\text{jump}}^{\gamma,2,\nu} \left[(u_{i_2[\gamma]}^{(\nu)}[x], x) \right] \right) \mathrm{d}\lambda_{d-1}[x] \tag{3.5.24m}$$

$$- \sum_{j \in V[\mathcal{C}]} \int_{\omega_k^{(j)}} f_j^{(\nu)} \left[(u_j^{(\nu)}[x], x) \right] \mathrm{d}\lambda_d[x] \quad = \quad 0. \tag{3.5.24n}$$

As mentioned above, Eqs (3.5.24) form the basis for the subsequent space discretization of evolution equation complexes, resulting in a finite volume scheme (cf. the description in Sec. 3.7.1 and Def. 3.7.41). The idea is to replace the integrands in (3.5.24) by their values at certain points inside the respective domain of integration. For each connected component $\mathcal{C}$ of the graph $\mathcal{G}_k$, (3.5.24) provides precisely one equation. In the finite volume discretization (3.7.5), this ensures that the number of equations is the same as the number of degrees of freedom of the solution due to discontinuities at jump interfaces. Dirichlet boundaries play a special role, since there the solution is known a priori, i.e. it is not to be determined using (3.5.24). This leads to an exceptional handling of Dirichlet boundaries in Sec. 3.7.

3.6 Change of Variables

In many applications, time and space discretization are not applied directly to the equations of some problem, but only after the equations have been simplified by reducing the dimension of the space domain. This kind of simplification is possible if the space dependence of the original problem contains symmetries that can be exploited by a suitable change of variables. Here a "suitable" change of variables is one such that the symmetries cause the transformed problem to be independent of one or more of the new variables, thereby allowing the dimension reduction.

A typical example is given by the situation considered during the simulations presented in Ch. 4, where the assumption of cylindrical symmetry allows to reduce the space dimension of the problem from three to two. More precisely, instead of considering Eqs (4.2.1) in cartesian coordinates (x_1, x_2, x_3), they are considered in cylindrical coordinates (r, ϑ, z), in which they are independent of the angular coordinate ϑ.

The purpose of the present section is to show how a dimension reduction by change of variables can be treated within the framework of the preceding sections; in particular, this section describes the modifications that have to be made in the deduction of the integral formulation in Sec. 3.5. If one starts out with equations having the form (3.3.3) with respect to the original variables, one then performs a change of variables, carries out considerations analogous to Sec. 3.5, and finally reduces the dimension using symmetry conditions, then one ends up with equations (3.6.22). Comparing (3.6.22) to (3.5.24), one finds that there is a (lower dimensional) problem in the new variables leading to the same equations (3.6.22) by the prodedure of Sec. 3.5. The evolution operators of the new problem still have the form (3.3.3), but in general, the functions k_j are no longer scalar-valued as was required in (3.3.2c), but matrix-valued. However, for cylindrical coordinates the new functions k_j are scalar-valued, showing that the setting of Secs 3.1 – 3.5 is sufficiently general to apply to the simulations of Ch. 4.

In the present section, the polytope domains p_j are the domains of the new variables, whereas the domains of the original variables no longer need to be polytopes (e.g. in the case of cylindrical symmetry, a polygon in the r-z-plane rotated around the symmetry axis is no longer a polytope). Due to this reason, the restriction made in the preceding sections of Ch. 3, that space domains must be polyhedral, is lifted within the remainder of the current section. In consequence, when used in this section, some definitions of ealier sections are implicitly extended to the situation where the space domain is no polytope. For instance in the situation treated below, $\overline{T(\text{int}[p \times q])}$ is considered a space domain, even though it is not polyhedral in general.

3.6.1 Coordinate Transformations

Coordinate transformations and change of variables are first defined in general terms, followed by the application to cylindrical coordinates.

Definition 3.6.1. Let Ω be an open subset of $\mathbb{R}^d$, $d \in \mathbb{N}$. A map $T : \Omega \longrightarrow T\Omega \subseteq \mathbb{R}^d$ is called a *coordinate transformation* iff T is a diffeomorphism, i.e. iff T is bijective, and both T and T^{-1} are differentiable.

Definition 3.6.2. Let $(d, d') \in \mathbb{N}^2$. Suppose p is a d-dimensional polytope, and $q = \prod_{i\in\{1,\dots,d'\}}[\lambda_i, \mu_i]$ is a cartesian product of d' intervals. Suppose O is an open subset of $\mathbb{R}^d$, and let $\Omega := O \times \text{int}[q]$. Moreover, let $T : \Omega \longrightarrow T\Omega \subseteq \mathbb{R}^{d+d'}$ be a coordinate transformation and $\text{int}[p] \subseteq O$ (s. Fig. 3.14 for an example of how p and O can be situated in the case of cylindrical coordinates). Define

$$\bigwedge_{A\subseteq p} \quad \bar{T}[A \times q] := \overline{T((A \cap O) \times \text{int}[q])}. \tag{3.6.1}$$

The map T is then called a *change of variables* between the space domains $p \times q$ and $\bar{T}[p \times q]$, where the *new variables* are elements of $p \times q$ and the *old variables* are elements of $\bar{T}[p \times q]$.

—

It is assumed that the symmetry of the problem is such that the solution is expected to be independent of the variable $x_q \in q$.

Example 3.6.3. In the case of cylindrical symmetry, assumed for the simulations of Ch. 4, the solution is supposedly independent of the angular coordinate ϑ. The usage of cylindrical coordinates means choosing $T = T_{\text{cyl}}$ (s. Def. B.3.1), where the polytope p is a subset of $\mathbb{R}_0^+ \times \mathbb{R}$ and $q = [0, 2\pi]$ ($d = 2$, $d' = 1$). For O one can choose each open set $O \subseteq \mathbb{R}^d$ that is sufficiently large. More precisely, O needs to be large enough to contain the parts of the boundary of p not lying on the axis $r = 0$ (e.g. each $]0, r_{\max}[\times]z_{\min}, z_{\max}[$ with $r_{\max} > \max\{r : (r,z) \in p\}$, $z_{\min} < \min\{z : (r,z) \in p\}$, $z_{\max} > \max\{z : (r,z) \in p\}$, will do for O, s. Fig. 3.14). According to Rem. B.3.2(b),(c),

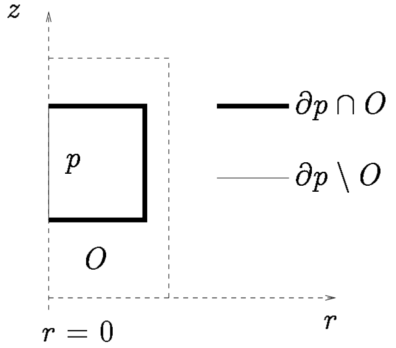


Figure 3.14: The relation between the polytope p and the open set O is illustrated in the r-z-plane of cylindrical coordinates.

T_{cyl} restricted to $\Omega = O \times]0, 2\pi[$ is a coordinate transformation in the sense of Def. 3.6.1.

—

To proceed in the general situation, using the notation of Def. 3.6.2, it is assumed that T is a change of variables between $p \times q$ and $\bar{T}[p \times q]$. The strategy now is as follows: Starting with an evolution equation complex in the old variables (i.e. with total space domain $\bar{T}[p \times q]$), the arguments of Sec. 3.5 are used to deduce the analogue of (3.5.24), which is then transformed into the new variables.

Let the (d, N)-dimensional evolution equation complex in the old variables be denoted by

$$\underline{\mathfrak{C}} = \Big(\underline{\mathfrak{D}}, \big(H_{\underline{b}_j, \underline{v}_j, \underline{k}_j, \underline{f}_j}\big)_{j \in J}, \big((\underline{a}^{\gamma,1}_{\mathrm{jump}}, \underline{a}^{\gamma,2}_{\mathrm{jump}})\big)_{\underline{\gamma} \in \underline{\mathrm{IF}}_{\mathrm{jump}}}, \big((\underline{a}^{\gamma,1}_{\mathrm{flux}}, \underline{a}^{\gamma,2}_{\mathrm{flux}}, \underline{\mathcal{A}}_{\underline{\gamma}})\big)_{\underline{\gamma} \in \underline{\mathrm{IF}}}, \\ \big(\underline{u}_{j,\mathrm{Dir}}\big)_{j \in J : 0 \in \underline{J}_j}, \big((\underline{a}^{j,\iota}_{\mathrm{out}}, \underline{\mathcal{B}}_{j,\iota})\big)_{(j,\iota) \in J \times (\underline{J}_j \setminus \{0\})}, \big(\underline{u}^{(0)}_j\big)_{j \in J}\Big),$$

and assume that in the new variables, there is a domain complex

$$\mathfrak{D} = \big(v, \tau, (p_j)_{j \in J}, E_{\mathrm{con}}, i_1, (J_j)_{j \in J}, (\Gamma_{j,\iota})_{(j,\iota) \in J \times J_j}\big)\,,$$

such that

$$\underline{\mathfrak{D}} = \Big(v, \tau, \big(\bar{T}[p_j \times q]\big)_{j \in J}, E_{\mathrm{con}}, i_1, (\underline{J}_j)_{j \in J}, \big(\bar{T}[\Gamma_{j,\iota} \times q]\big)_{(j,\iota) \in J \times \underline{J}_j}\Big),$$

where J_j is the disjoint union of the sets $\underline{J}_j$ and $J_{j,0}$: $J_j = \underline{J}_j \,\dot{\cup}\, J_{j,0}$,

$$\bigwedge_{j \in J} \quad J_{j,0} := \begin{cases} \emptyset & \text{if } (\partial p_j) \setminus O = \emptyset, \\ \{\iota_{j,0}\} & \text{if } (\partial p_j) \setminus O \neq \emptyset, \end{cases} \tag{3.6.2}$$

$(\Gamma_{j,\iota})_{\iota \in \underline{J}_j}$ is a partition of $\overline{O \cap \partial p_j}$ with respect to the relative topology, and $\Gamma_{j,\iota_{j,0}} = (\partial p_j) \setminus O$ in the case $(\partial p_j) \setminus O \neq \emptyset$.

The introduction of $J_{j,0}$ is necessary, since the case of cylindrical coordinates shows that the boundary of the domain p in the new variables can have some part $\partial p \setminus O$ that does not correspond to a boundary in the old variables (cf. Fig. 3.14).

In analogy with Sec. 3.5, fix a time discretization $\underline{\mathfrak{T}}$ of $\underline{\mathfrak{C}}$ according to Def. 3.4.13,

$$\begin{aligned}\underline{\mathfrak{T}} = \Big(& (t_\nu)_{\nu\in\{0,\dots,n\}}, \big(\underline{\mathcal{U}}_j^{(\nu)}\big)_{(j,\nu)\in J\times\{0,\dots,n\}}, \big(H^{(\nu)}_{\underline{b}_j,\underline{v}_j,\underline{k}_j,\underline{f}_j}\big)_{(j\times\nu)\in J\times\{0,\dots,n\}}, \\ & \big((\underline{a}^{\underline{\gamma},1,\nu}_{\text{jump}}, \underline{a}^{\underline{\gamma},2,\nu}_{\text{jump}})\big)_{(\underline{\gamma},\nu)\in\underline{\mathrm{IF}}_{\text{jump}}\times\{0,\dots,n\}}, \\ & \big(((\underline{a}^{\underline{\gamma},1}_{\text{flux}})^{\text{ex.-im.}}, (\underline{a}^{\underline{\gamma},2}_{\text{flux}})^{\text{ex.-im.}}, (\underline{\mathcal{A}}_{\underline{\gamma}})^{\text{ex.-im.}})\big)_{\underline{\gamma}\in\underline{\mathrm{IF}}}, \\ & \big(((\underline{a}^{\underline{\gamma},1,\nu}_{\text{flux}})^{\text{ex.-im.}}, (\underline{a}^{\underline{\gamma},2,\nu}_{\text{flux}})^{\text{ex.-im.}})\big)_{(\underline{\gamma},\nu)\in\underline{\mathrm{IF}}\times\{0,\dots,n\}}, \\ & \big(\underline{u}^{(\nu)}_{j,\text{Dir}}\big)_{(j,\nu)\in J\times\{0,\dots,n\}:\, 0\in\underline{J}_j}, \\ & \big(((\underline{a}^{j,\iota}_{\text{out}})^{\text{ex.-im.}}, (\underline{\mathcal{B}}_{j,\iota})^{\text{ex.-im.}})\big)_{(j,\iota)\in J\times(\underline{J}_j\setminus\{0\})}, \\ & \big((\underline{a}^{j,\iota,\nu}_{\text{out}})^{\text{ex.-im.}}\big)_{(j,\iota,\nu)\in J\times(\underline{J}_j\setminus\{0\})\times\{0,\dots,n\}}\Big),\end{aligned}$$

and fix a solution $(\underline{\mathrm{u}}^{(0)}, \dots, \underline{\mathrm{u}}^{(n)}) = \big(\underline{u}_j^{(\nu)}\big)_{(j,\nu)\in J\times\{0,\dots,n\}}$ to $\underline{\mathfrak{T}}$ according to Def. 3.4.14.

3.6.2 Integral Formulation

Continuing to follow Sec. 3.5, let $\Pi = (\omega_k)_{k\in I_\Pi}$ be a finite partition of p (in the new variables) and define partitions $\Pi^{(j)}$ of each p_j: $\Pi^{(j)} := (\omega_k^{(j)})_{k\in I^{(j)}}$, $\omega_k^{(j)} := \overline{\mathrm{int}[\omega_k \cap p_j]}$, $I^{(j)} := \{k \in I_\Pi : \omega_k^{(j)} \neq \emptyset\}$. As in Sec. 3.5, the ω_k, $k \in I_\Pi$, are assumed to be nontangent to interfaces (cf. Def. 3.5.2 and Lem. 3.5.5). The time-discrete evolution equations

$$H_{\underline{b}_j,\underline{v}_j,\underline{k}_j,\underline{f}_j}\big[(\underline{u}_j^{(\nu)}, \underline{u}_j^{(\nu-1)})\big] = 0 \tag{3.6.3}$$

are integrated over $\bar{T}[\omega_k^{(j)} \times q]$.

As in Sec. 3.5.3, let $\mathcal{G}_k := \mathcal{G}_{\omega_k}$ be the associated graph of ω_k for each $k \in I_\Pi$. Fix $k \in I_\Pi$ and $\mathcal{C} \in \mathrm{CoCmp}[\mathcal{G}_k]$.

Analogous to (3.5.4), the Gauss-Green Integration Th. C.8.2 is used to transform integrals over $\bar{T}[\omega_k^{(j)} \times q]$ involving divergence terms into integrals over $\partial\big(\bar{T}[\omega_k^{(j)} \times q]\big)$. Decomposing the resulting boundary integrals followed by an applications of interface conditions analogous to Sec. 3.5.2, and finally using interface conditions analogous to Sec. 3.5.3, leads to (3.6.6) which is analogous to (3.5.24).

In the formulation of (3.6.6) as well as in the entire rest of Sec. 3.6, the function notation introduced in (3.3.12) and (3.3.13) is used. Consistently writing function compositions and avoiding writing arguments makes the following integral formulas much more concise. It seems especially suitable in the context of the application of the Change of Variables Th. C.8.3 in Sec. 3.6.4. For the terms involving the functions $(\underline{a}_{\mathrm{out}}^{j,\iota,\nu})^{\text{ex.-im.}}$ and $(\underline{a}_{\mathrm{flux}}^{\gamma,\alpha,\nu})^{\text{ex.-im.}}$, respectively, it becomes necessary to extend (3.3.13) to two functions: Given $(u_1,u_2) \in \mathcal{F}(A,\mathbb{K}) \times \mathcal{F}(A,\mathbb{K})$, where A is either a subset of $\mathbb{R}^d$ or a subset of $\mathbb{R}^{d+d'}$, define

$$(u_1,u_2)^{\text{sp.}}: \; A \longrightarrow \mathbb{K} \times \mathbb{K} \times A, \quad (u_1,u_2)^{\text{sp.}}[x] := (u_1[x], u_2[x], x). \tag{3.6.4}$$

For each $(j,\nu) \in J \times \{1,\dots,n\}$, let $\underline{F}^{(\nu)}_{j,\partial\left(\bar{T}[\omega_k^{(j)} \times q]\right)}$ denote the flux through the boundary of $\bar{T}[\omega_k^{(j)} \times q]$ at time t_ν, i.e.

$$\underline{F}^{(\nu)}_{j,\partial\left(\bar{T}[\omega_k^{(j)} \times q]\right)} := \operatorname{tr}_{\partial\left(\bar{T}[\omega_k^{(j)} \times q]\right)} \left(\left(\underline{k}_j^{(\nu)} \circ (\underline{u}_j^{(\nu)})^{\text{sp.}} \right) \nabla \underline{u}_j^{(\nu)} \right). \tag{3.6.5}$$

After these preparations, the promised analogue of (3.5.24) is written:

$$(t_\nu - t_{\nu-1})^{-1} \sum_{j \in V[\mathcal{C}]} \int_{\bar{T}[\omega_k^{(j)} \times q]} \left(\underline{b}_j^{(\nu)} \circ \left(\underline{u}_j^{(\nu)}\right)^{\text{sp.}} - \underline{b}_j^{(\nu-1)} \circ \left(\underline{u}_j^{(\nu-1)}\right)^{\text{sp.}} \right) \tag{3.6.6a}$$

$$+ \sum_{j \in V[\mathcal{C}]} \int_{\mathrm{int}\left[\bar{T}[p_j \times q]\right] \cap \partial\left(\bar{T}[\omega_k^{(j)} \times q]\right)} \left(\underline{v}_j^{(\nu)} \circ \left(\underline{u}_j^{(\nu)}\right)^{\text{sp.}} \right) \bullet n_{\bar{T}[\omega_k^{(j)} \times q]} \tag{3.6.6b}$$

$$+ \sum_{j \in V[\mathcal{C}]} \int_{\partial\left(\bar{T}[p \times q]\right) \cap \partial\left(\bar{T}[\omega_k^{(j)} \times q]\right)} \left(\underline{v}_j^{(\nu)} \circ \left(\underline{u}_j^{(\nu)}\right)^{\text{sp.}} \right) \bullet n_{\bar{T}[\omega_k^{(j)} \times q]} \tag{3.6.6c}$$

$$+ \sum_{j \in V[\mathcal{C}]} \sum_{\underline{\gamma} \in \underline{\mathrm{IF}}} \int_{\underline{\gamma} \cap \partial\left(\bar{T}[\omega_k^{(j)} \times q]\right)} \left(\underline{v}_j^{(\nu)} \circ \left(\underline{u}_j^{(\nu)}\right)^{\text{sp.}} \right) \bullet n_{\bar{T}[\omega_k^{(j)} \times q]} \tag{3.6.6d}$$

$$- \sum_{j \in V[\mathcal{C}]} \int_{\mathrm{int}\left[\bar{T}[p_j \times q]\right] \cap \partial\left(\bar{T}[\omega_k^{(j)} \times q]\right)} \underline{F}^{(\nu)}_{j,\partial\left(\bar{T}[\omega_k^{(j)} \times q]\right)} \bullet n_{\bar{T}[\omega_k^{(j)} \times q]} \tag{3.6.6e}$$

$$- \sum_{j \in V[\mathcal{C}] : 0 \in \underline{J}_j} \int_{\bar{T}[\Gamma_{j,0} \times q] \cap \partial\left(\bar{T}[\omega_k^{(j)} \times q]\right)} \underline{F}^{(\nu)}_{j,\partial\left(\bar{T}[\omega_k^{(j)} \times q]\right)} \bullet n_{\bar{T}[\omega_k^{(j)} \times q]}$$

$$- \sum_{j \in V[\mathcal{C}]} \sum_{\iota \in \underline{J}_j \setminus \{0\}} \int_{\bar{T}[\Gamma_{j,\iota} \times q] \cap \partial\left(\bar{T}[\omega_k^{(j)} \times q]\right)} (\underline{\mathcal{B}}_{j,\iota})^{\text{ex.-im.}} \left[\left(\underline{\mathfrak{u}}^{(\nu-1)}, \underline{\mathfrak{u}}^{(\nu)} \right) \right] \tag{3.6.6f}$$

$$+ \sum_{j \in V[\mathcal{C}]} \sum_{\iota \in \underline{J}_j \setminus \{0\}} \int_{\bar{T}[\Gamma_{j,\iota} \times q] \cap \partial\left(\bar{T}[\omega_k^{(j)} \times q]\right)} (\underline{a}_{\mathrm{out}}^{j,\iota,\nu})^{\text{ex.-im.}} \circ \left(\underline{u}_j^{(\nu-1)}, \underline{u}_j^{(\nu)} \right)^{\text{sp.}} \tag{3.6.6g}$$

$$- \sum_{\underline{\gamma} \in \underline{\mathrm{IF}}_{\mathrm{con}}} \int_{\underline{\gamma} \cap \bigcup_{j \in V[\mathcal{C}]} \partial\left(\bar{T}[\omega_k^{(j)} \times q]\right)} (\underline{\mathcal{A}}_{\underline{\gamma}})^{\text{ex.-im.}} \left[\left(\underline{\mathfrak{u}}^{(\nu-1)}, \underline{\mathfrak{u}}^{(\nu)} \right) \right] \tag{3.6.6h}$$

$$+\sum_{\underline{\gamma}\in\underline{\mathrm{IF}}_{\mathrm{con}}}\int_{\underline{\gamma}\cap\bigcup_{j\in V[\mathcal{C}]}\partial\left(\bar{T}[\omega_k^{(j)}\times q]\right)}\Bigg(-\left(\underline{a}_{\mathrm{flux}}^{\underline{\gamma},1,\nu}\right)^{\mathrm{ex.\text{-}im.}}\circ\left(\underline{u}_{i_1[\underline{\gamma}]}^{(\nu-1)},\underline{u}_{i_1[\underline{\gamma}]}^{(\nu)}\right)^{\mathrm{sp.}}$$
$$+\left(\underline{a}_{\mathrm{flux}}^{\underline{\gamma},2,\nu}\right)^{\mathrm{ex.\text{-}im.}}\circ\left(\underline{u}_{i_2[\underline{\gamma}]}^{(\nu-1)},\underline{u}_{i_2[\underline{\gamma}]}^{(\nu)}\right)^{\mathrm{sp.}}\Bigg) \tag{3.6.6i}$$

$$+\sum_{\underline{\gamma}\in\underline{G}_{\mathrm{jump},1}[\mathcal{C}]}\int_{\underline{\gamma}\cap\partial\left(\bar{T}[\omega_k^{(i_1[\underline{\gamma}])}\times q]\right)}\left(\underline{a}_{\mathrm{jump}}^{\underline{\gamma},1,\nu}\circ\left(\underline{u}_{i_1[\underline{\gamma}]}^{(\nu)}\right)^{\mathrm{sp.}}-\underline{a}_{\mathrm{jump}}^{\underline{\gamma},2,\nu}\circ\left(\underline{u}_{i_2[\underline{\gamma}]}^{(\nu)}\right)^{\mathrm{sp.}}\right) \tag{3.6.6j}$$

$$-\sum_{\underline{\gamma}\in\underline{G}_{\mathrm{jump},2}[\mathcal{C}]}\int_{\underline{\gamma}\cap\partial\left(\bar{T}[\omega_k^{(i_2[\underline{\gamma}])}\times q]\right)}\left(\underline{\mathcal{A}}_{\underline{\gamma}}\right)^{\mathrm{ex.\text{-}im.}}\left[\left(\underline{\mathrm{u}}^{(\nu-1)},\underline{\mathrm{u}}^{(\nu)}\right)\right] \tag{3.6.6k}$$

$$+\sum_{\underline{\gamma}\in\underline{G}_{\mathrm{jump},2}[\mathcal{C}]}\int_{\underline{\gamma}\cap\partial\left(\bar{T}[\omega_k^{(i_2[\underline{\gamma}])}\times q]\right)}\Bigg(-\left(\underline{a}_{\mathrm{flux}}^{\underline{\gamma},1,\nu}\right)^{\mathrm{ex.\text{-}im.}}\circ\left(\underline{u}_{i_1[\underline{\gamma}]]}^{(\nu-1)},\underline{u}_{i_1[\underline{\gamma}]}^{(\nu)}\right)^{\mathrm{sp.}}$$
$$+\left(\underline{a}_{\mathrm{flux}}^{\underline{\gamma},2,\nu}\right)^{\mathrm{ex.\text{-}im.}}\circ\left(\underline{u}_{i_2[\underline{\gamma}]}^{(\nu-1)},\underline{u}_{i_2[\underline{\gamma}]}^{(\nu)}\right)^{\mathrm{sp.}}\Bigg) \tag{3.6.6l}$$

$$+\sum_{\underline{\gamma}\in\underline{G}_{\mathrm{jump},2}[\mathcal{C}]}\int_{\underline{\gamma}\cap\partial\left(\bar{T}[\omega_k^{(i_2[\underline{\gamma}])}\times q]\right)}\left(-\underline{a}_{\mathrm{jump}}^{\underline{\gamma},1,\nu}\circ\left(\underline{u}_{i_1[\underline{\gamma}]}^{(\nu)}\right)^{\mathrm{sp.}}+\underline{a}_{\mathrm{jump}}^{\underline{\gamma},2,\nu}\circ\left(\underline{u}_{i_2[\underline{\gamma}]}^{(\nu)}\right)^{\mathrm{sp.}}\right) \tag{3.6.6m}$$

$$-\sum_{j\in V[\mathcal{C}]}\int_{\bar{T}[\omega_k^{(j)}\times q]}\underline{f}_j^{(\nu)}\circ\left(\underline{u}_j^{(\nu)}\right)^{\mathrm{sp.}} \quad = \quad 0. \tag{3.6.6n}$$

3.6.3 Writing the Domains of Integration as Images of the Coordinate Transformation

In Sec. 3.6.4, the Change of Variables Th. C.8.3 is going to be used to transform (3.6.6) into the new variables. In preparation, the domains of integration in (3.6.6) are to be written as images of the coordinate transformation T.

For the volume integrals, this can be done noting that

$$\begin{aligned}\bar{T}[\omega_k^{(j)}\times q] &\supseteq T\big((\omega_k^{(j)}\cap O)\times\mathrm{int}[q]\big),\\ \lambda_{d+d'}\big[\bar{T}[\omega_k^{(j)}\times q]\big] &= \lambda_{d+d'}\big[T\big((\omega_k^{(j)}\cap O)\times\mathrm{int}[q]\big)\big].\end{aligned} \tag{3.6.7}$$

Analogously, one also has

$$\begin{aligned}\mathrm{int}\,\big[\bar{T}[\omega_k^{(j)}\times q]\big] &\supseteq \mathrm{int}\,\big[T\big((O\cap\omega_k^{(j)})\times\mathrm{int}[q]\big)\big],\\ \lambda_{d+d'}\Big[\mathrm{int}\,\big[\bar{T}[\omega_k^{(j)}\times q]\big]\Big] &= \lambda_{d+d'}\Big[\mathrm{int}\,\big[T\big((O\cap\omega_k^{(j)})\times\mathrm{int}[q]\big)\big]\Big].\end{aligned} \tag{3.6.8}$$

The following formulas are used below. They hold for each $A\subseteq\mathbb{R}^d$ and each $B\subseteq\mathbb{R}^{d'}$:

$$\mathrm{int}[A\times B]=\mathrm{int}[A]\times\mathrm{int}[B], \tag{3.6.9a}$$

$$\partial(A \times B) = (\partial A \times B) \cup (A \times \partial B). \tag{3.6.9b}$$

Let $\omega \subseteq p$ be an arbitrary d-polytope.

One can use the Domain Invariance Th. C.1.11(b) to get

$$\begin{aligned} &\operatorname{int}\left[T\big((\omega \cap O) \times \operatorname{int}[q]\big)\right] \overset{\text{Th. C.1.11(b)}}{=} T\big(\operatorname{int}\left[(\omega \cap O) \times \operatorname{int}[q]\right]\big) \\ &\overset{(3.6.9a),\,\operatorname{int}[\omega]\subseteq O}{=} T\big(\operatorname{int}[\omega] \times \operatorname{int}[q]\big), \end{aligned} \tag{3.6.10}$$

which together with (3.6.8) allows to replace $\operatorname{int}\left[\bar{T}[p_j \times q]\right]$ in (3.6.6b) and (3.6.6e) by $T\big(\operatorname{int}[p_j] \times \operatorname{int}[q]\big)$.

As a consequence of the Domain Invariance Th. C.1.11(c), one gets

$$\begin{aligned} &T\big((\omega \cap O) \times \operatorname{int}[q]\big) \cap \partial\Big(T\big((\omega \cap O) \times \operatorname{int}[q]\big)\Big) \\ &\overset{\text{Th. C.1.11(c)}}{=} T\Big(\big((\omega \cap O) \times \operatorname{int}[q]\big) \cap \partial\big((\omega \cap O) \times \operatorname{int}[q]\big)\Big) \\ &\overset{(3.6.9b)}{=} T\Big(\Big(\omega \cap O \cap \big(\partial(\omega \cap O)\big)\Big) \times \operatorname{int}[q]\Big) = T\big((O \cap \partial\omega) \times \operatorname{int}[q]\big), \end{aligned} \tag{3.6.11}$$

where the last equality in (3.6.11) holds since $\operatorname{int}[\omega] \subseteq O$, O is open, and ω is closed.

Assumption 3.6.4. It is assumed that for each d-polytope $\omega \subseteq p$, it holds that

$$\lambda_{d+d'-1}\Big[\partial\big(\bar{T}[\omega \times q]\big)\Big] = \lambda_{d+d'-1}\Big[\partial\big(\bar{T}[\omega \times q]\big) \cap T\big((\omega \cap O) \times \operatorname{int}[q]\big)\Big] \tag{3.6.12a}$$

and

$$\begin{aligned} &\partial\big(\bar{T}[\omega \times q]\big) \cap T\big((\omega \cap O) \times \operatorname{int}[q]\big) \\ &= \partial\Big(T\big((\omega \cap O) \times \operatorname{int}[q]\big)\Big) \cap T\big((\omega \cap O) \times \operatorname{int}[q]\big). \end{aligned} \tag{3.6.12b}$$

Example 3.6.5. Assumption 3.6.4 is satisfied in the case of cylindrical coordinates if O is chosen sufficiently large in the sense of Ex. 3.6.3: In that case, $\partial\big(\bar{T}[\omega \times q]\big)$ is the disjoint union of $T\big((O \cap \partial\omega) \times \operatorname{int}[q]\big)$ and the one-dimensional set $\big\{(x_1, 0, x_3) : (x_1, x_3) \in O \cap \partial\omega\big\}$, which yields (3.6.12a). Moreover, $\partial\Big(T\big((\omega \cap O) \times \operatorname{int}[q]\big)\Big)$ is the disjoint union of $T\big((O \cap \partial\omega) \times \operatorname{int}[q]\big)$ and $\big\{(x_1, 0, x_3) : (x_1, x_3) \in \partial\omega\big\}$, which yields (3.6.12b).

—

Now, (3.6.6) is rewritten as (3.6.14), where the domains of integration are written as images of the coordinate transformation T.

Combining (3.6.10), (3.6.11), and (3.6.12) with the bijectiveness of T yields (3.6.14b) and (3.6.14e).

(3.6.14c) follows from (3.6.6c), (3.6.11), and the bijectiveness of T.

Since $\mathrm{int}[p] \subseteq O$, one has $\gamma \subseteq O$ for each $\gamma \in \mathrm{IF}$. Moreover,

$$\bigwedge_{\gamma \in \mathrm{IF}} \begin{pmatrix} \bar{T}[\gamma \times q] \supseteq T\big(\gamma \times \mathrm{int}[q]\big), \\ \lambda_{d+d'-1}\big[\bar{T}[\gamma \times q]\big] = \lambda_{d+d'-1}\big[T\big(\gamma \times \mathrm{int}[q]\big)\big] \end{pmatrix}, \tag{3.6.13a}$$

$$\bigwedge_{(j,\iota) \in J \times \underline{J}_j} \begin{pmatrix} \bar{T}[\Gamma_{j,\iota} \times q] \supseteq T\big((O \cap \Gamma_{j,\iota}) \times \mathrm{int}[q]\big), \\ \lambda_{d+d'-1}\big[\bar{T}[\Gamma_{j,\iota} \times q]\big] = \lambda_{d+d'-1}\big[T\big((O \cap \Gamma_{j,\iota}) \times \mathrm{int}[q]\big)\big] \end{pmatrix}, \tag{3.6.13b}$$

which together with (3.6.11) and the bijectiveness of T allows to replace the domains of integration in (3.6.6d) and (3.6.6f) – (3.6.6m) by the domains of integration in (3.6.14d) and (3.6.14f) – (3.6.14m). The same holds for the Dirichlet term between (3.6.6d) and (3.6.6f).

$$(t_\nu - t_{\nu-1})^{-1} \sum_{j \in V[\mathcal{C}]} \int_{T\left((O \cap \omega_k^{(j)}) \times \mathrm{int}[q]\right)} \left(\underline{b}_j^{(\nu)} \circ \left(\underline{u}_j^{(\nu)}\right)^{\mathrm{sp.}} - \underline{b}_j^{(\nu-1)} \circ \left(\underline{u}_j^{(\nu-1)}\right)^{\mathrm{sp.}} \right) \tag{3.6.14a}$$

$$+ \sum_{j \in V[\mathcal{C}]} \int_{T\left((\partial\omega_k^{(j)} \cap \mathrm{int}[p_j]) \times \mathrm{int}[q]\right)} \left(\underline{v}_j^{(\nu)} \circ \left(\underline{u}_j^{(\nu)}\right)^{\mathrm{sp.}} \right) \bullet n_{\bar{T}[\omega_k^{(j)} \times q]} \tag{3.6.14b}$$

$$+ \sum_{j \in V[\mathcal{C}]} \int_{T\left((O \cap \partial\omega_k^{(j)} \cap \partial p) \times \mathrm{int}[q]\right)} \left(\underline{v}_j^{(\nu)} \circ \left(\underline{u}_j^{(\nu)}\right)^{\mathrm{sp.}} \right) \bullet n_{\bar{T}[\omega_k^{(j)} \times q]} \tag{3.6.14c}$$

$$+ \sum_{j \in V[\mathcal{C}]} \sum_{\gamma \in \mathrm{IF}} \int_{T\left((\partial\omega_k^{(j)} \cap \gamma) \times \mathrm{int}[q]\right)} \left(\underline{v}_j^{(\nu)} \circ \left(\underline{u}_j^{(\nu)}\right)^{\mathrm{sp.}} \right) \bullet n_{\bar{T}[\omega_k^{(j)} \times q]} \tag{3.6.14d}$$

$$- \sum_{j \in V[\mathcal{C}]} \int_{T\left((\partial\omega_k^{(j)} \cap \mathrm{int}[p_j]) \times \mathrm{int}[q]\right)} \underline{F}^{(\nu)}_{j,\partial\left(\bar{T}[\omega_k^{(j)} \times q]\right)} \bullet n_{\bar{T}[\omega_k^{(j)} \times q]} \tag{3.6.14e}$$

$$- \sum_{j \in V[\mathcal{C}] : 0 \in \underline{J}_j} \int_{T\left((O \cap \partial\omega_k^{(j)} \cap \Gamma_{j,0}) \times \mathrm{int}[q]\right)} \underline{F}^{(\nu)}_{j,\partial\left(\bar{T}[\omega_k^{(j)} \times q]\right)} \bullet n_{\bar{T}[\omega_k^{(j)} \times q]}$$

$$- \sum_{j \in V[\mathcal{C}]} \sum_{\iota \in \underline{J}_j \setminus \{0\}} \int_{T\left((O \cap \partial\omega_k^{(j)} \cap \Gamma_{j,\iota}) \times \mathrm{int}[q]\right)} \left(\underline{\mathcal{B}}_{j,\iota}\right)^{\mathrm{ex.\text{-}im.}} \left[\left(\underline{\mathfrak{u}}^{(\nu-1)}, \underline{\mathfrak{u}}^{(\nu)}\right)\right] \tag{3.6.14f}$$

$$+ \sum_{j \in V[\mathcal{C}]} \sum_{\iota \in \underline{J}_j \setminus \{0\}} \int_{T\left((O \cap \partial\omega_k^{(j)} \cap \Gamma_{j,\iota}) \times \mathrm{int}[q]\right)} \left(\underline{a}_{\mathrm{out}}^{j,\iota,\nu}\right)^{\mathrm{ex.\text{-}im.}} \circ \left(\underline{u}_j^{(\nu-1)}, \underline{u}_j^{(\nu)}\right)^{\mathrm{sp.}} \tag{3.6.14g}$$

$$- \sum_{\gamma \in \mathrm{IF}_{\mathrm{con}}} \int_{T\left((\gamma \cap \bigcup_{j \in V[\mathcal{C}]} \partial\omega_k^{(j)}) \times \mathrm{int}[q]\right)} \left(\underline{\mathcal{A}}_{\bar{T}[\gamma \times q]}\right)^{\mathrm{ex.\text{-}im.}} \left[\left(\underline{\mathfrak{u}}^{(\nu-1)}, \underline{\mathfrak{u}}^{(\nu)}\right)\right] \tag{3.6.14h}$$

$$+ \sum_{\gamma \in \mathrm{IF}_{\mathrm{con}}} \int_{T\left((\gamma \cap \bigcup_{j \in V[\mathcal{C}]} \partial\omega_k^{(j)}) \times \mathrm{int}[q]\right)} \Bigg(- \left(\underline{a}_{\mathrm{flux}}^{\bar{T}[\gamma\times q],1,\nu}\right)^{\text{ex.-im.}} \circ \left(\underline{u}_{i_1[\bar{T}[\gamma\times q]]}^{(\nu-1)}, \underline{u}_{i_1[\bar{T}[\gamma\times q]]}^{(\nu)}\right)^{\text{sp.}} + \left(\underline{a}_{\mathrm{flux}}^{\bar{T}[\gamma\times q],2,\nu}\right)^{\text{ex.-im.}} \circ \left(\underline{u}_{i_2[\bar{T}[\gamma\times q]]}^{(\nu-1)}, \underline{u}_{i_2[\bar{T}[\gamma\times q]]}^{(\nu)}\right)^{\text{sp.}} \Bigg) \tag{3.6.14i}$$

$$+ \sum_{\gamma \in G_{\mathrm{jump},1}[\mathcal{C}]} \int_{T\left((\partial\omega_k^{(i_1[\gamma])} \cap \gamma) \times \mathrm{int}[q]\right)} \Bigg(\underline{a}_{\mathrm{jump}}^{\bar{T}[\gamma\times q],1,\nu} \circ \left(\underline{u}_{i_1[\bar{T}[\gamma\times q]]}^{(\nu)}\right)^{\text{sp.}} - \underline{a}_{\mathrm{jump}}^{\bar{T}[\gamma\times q],2,\nu} \circ \left(\underline{u}_{i_2[\bar{T}[\gamma\times q]]}^{(\nu)}\right)^{\text{sp.}} \Bigg) \tag{3.6.14j}$$

$$- \sum_{\gamma \in G_{\mathrm{jump},2}[\mathcal{C}]} \int_{T\left((\partial\omega_k^{(i_2[\gamma])} \cap \gamma) \times \mathrm{int}[q]\right)} \left(\underline{\mathcal{A}}_{\bar{T}[\gamma\times q]}\right)^{\text{ex.-im.}} \left[\left(\underline{u}^{(\nu-1)}, \underline{u}^{(\nu)}\right)\right] \tag{3.6.14k}$$

$$+ \sum_{\gamma \in G_{\mathrm{jump},2}[\mathcal{C}]} \int_{T\left((\partial\omega_k^{(i_2[\gamma])} \cap \gamma) \times \mathrm{int}[q]\right)} \Bigg(- \left(\underline{a}_{\mathrm{flux}}^{\bar{T}[\gamma\times q],1,\nu}\right)^{\text{ex.-im.}} \circ \left(\underline{u}_{i_1[\bar{T}[\gamma\times q]]}^{(\nu-1)}, \underline{u}_{i_1[\bar{T}[\gamma\times q]]}^{(\nu)}\right)^{\text{sp.}} + \left(\underline{a}_{\mathrm{flux}}^{\bar{T}[\gamma\times q],2,\nu}\right)^{\text{ex.-im.}} \circ \left(\underline{u}_{i_2[\bar{T}[\gamma\times q]]}^{(\nu-1)}, \underline{u}_{i_2[\bar{T}[\gamma\times q]]}^{(\nu)}\right)^{\text{sp.}} \Bigg) \tag{3.6.14l}$$

$$+ \sum_{\gamma \in G_{\mathrm{jump},2}[\mathcal{C}]} \int_{T\left((\partial\omega_k^{(i_2[\gamma])} \cap \gamma) \times \mathrm{int}[q]\right)} \Bigg(- \underline{a}_{\mathrm{jump}}^{\bar{T}[\gamma\times q],1,\nu} \circ \left(\underline{u}_{i_1[\bar{T}[\gamma\times q]]}^{(\nu)}\right)^{\text{sp.}} + \underline{a}_{\mathrm{jump}}^{\bar{T}[\gamma\times q],2,\nu} \circ \left(\underline{u}_{i_2[\bar{T}[\gamma\times q]]}^{(\nu)}\right)^{\text{sp.}} \Bigg) \tag{3.6.14m}$$

$$- \sum_{j \in V[\mathcal{C}]} \int_{T\left((O \cap \omega_k^{(j)}) \times \mathrm{int}[q]\right)} \underline{f}_j^{(\nu)} \circ \left(\underline{u}_j^{(\nu)}\right)^{\text{sp.}} = 0. \tag{3.6.14n}$$

3.6.4 Change of Variables

Equation (3.6.14) is to be transformed into the new variables using the Change of Variables Th. C.8.3. Since Th. C.8.3 does not apply directly to the boundary integrals of (3.6.14), some preparatory remarks are needed. Let $S \subseteq p$ be a $(d-1)$-dimensional polytope such that $\mathrm{int}[S] \subseteq p \cap O$. Since S is piecewise affine, by decomposition one can assume that S already lies in a $(d-1)$-dimensional affine subspace of $\mathbb{R}^d$. Thus, there is a $(d-1)$-dimensional polytope $\tilde{S} \subseteq \mathbb{R}^{d-1}$ and an affine parametrization $\Phi : \tilde{S} \times q \longrightarrow \mathbb{R}^{d+d'}$ of $S \times q$ such that $\mathrm{gr}\,\Phi' = 1$, where Φ' denotes the derivative of Φ, and $\mathrm{gr}\,\Phi' := \det[(\Phi')^\top \Phi']$ denotes its Gram determinant. Then $T \circ \Phi$ is a parametrization of $T(S \times \mathrm{int}[q])$, and by the chain rule $\mathrm{gr}(T \circ \Phi)' = \mathrm{gr}((T' \circ \Phi) \cdot \Phi') = (J_T \circ \Phi)^2\,\mathrm{gr}\,\Phi' = (J_T \circ \Phi)^2$, where $J_T := \det[T']$ denotes the Jacobian of T. Thus, for each integrable function $g : T(S \times \mathrm{int}[q]) \longrightarrow \mathbb{K}$:

$$\begin{aligned}\int_{T(S\times\mathrm{int}[q])} g &= \int_{\tilde{S}\times\mathrm{int}[q]} (g\circ T\circ\Phi)\sqrt{\mathrm{gr}(T\circ\Phi)'}\\ &= \int_{\tilde{S}\times\mathrm{int}[q]} (g\circ T\circ\Phi)\cdot(|J_T|\circ\Phi) = \int_{S\times\mathrm{int}[q]} (g\circ T)\cdot|J_T|.\end{aligned} \tag{3.6.15}$$

Combining Th. C.8.3 with (3.6.15) produces the the new variable version of (3.6.14):

$$(t_\nu - t_{\nu-1})^{-1}\sum_{j\in V[\mathcal{C}]}\int_{(O\cap\omega_k^{(j)})\times\mathrm{int}[q]}\left(\left(\underline{b}_j^{(\nu)}\circ\left(\underline{u}_j^{(\nu)}\right)^{\mathrm{sp.}} - \underline{b}_j^{(\nu-1)}\circ\left(\underline{u}_j^{(\nu-1)}\right)^{\mathrm{sp.}}\right)\circ T\right)\cdot|J_T| \tag{3.6.16a}$$

$$+\sum_{j\in V[\mathcal{C}]}\int_{(\partial\omega_k^{(j)}\cap\mathrm{int}[p_j])\times\mathrm{int}[q]}\left(\left(\left(\underline{v}_j^{(\nu)}\circ\left(\underline{u}_j^{(\nu)}\right)^{\mathrm{sp.}}\right)\bullet n_{\bar{T}[\omega_k^{(j)}\times q]}\right)\circ T\right)\cdot|J_T| \tag{3.6.16b}$$

$$+\sum_{j\in V[\mathcal{C}]}\int_{(O\cap\partial\omega_k^{(j)}\cap\partial p)\times\mathrm{int}[q]}\left(\left(\left(\underline{v}_j^{(\nu)}\circ\left(\underline{u}_j^{(\nu)}\right)^{\mathrm{sp.}}\right)\bullet n_{\bar{T}[\omega_k^{(j)}\times q]}\right)\circ T\right)\cdot|J_T| \tag{3.6.16c}$$

$$+\sum_{j\in V[\mathcal{C}]}\sum_{\gamma\in\mathrm{IF}}\int_{(\partial\omega_k^{(j)}\cap\gamma)\times\mathrm{int}[q]}\left(\left(\left(\underline{v}_j^{(\nu)}\circ\left(\underline{u}_j^{(\nu)}\right)^{\mathrm{sp.}}\right)\bullet n_{\bar{T}[\omega_k^{(j)}\times q]}\right)\circ T\right)\cdot|J_T| \tag{3.6.16d}$$

$$-\sum_{j\in V[\mathcal{C}]}\int_{(\partial\omega_k^{(j)}\cap\mathrm{int}[p_j])\times\mathrm{int}[q]}\left(\left(\underline{F}^{(\nu)}_{j,\partial\left(\bar{T}[\omega_k^{(j)}\times q]\right)}\bullet n_{\bar{T}[\omega_k^{(j)}\times q]}\right)\circ T\right)\cdot|J_T| \tag{3.6.16e}$$

$$-\sum_{j\in V[\mathcal{C}]:0\in\underline{J}_j}\int_{(O\cap\partial\omega_k^{(j)}\cap\Gamma_{j,0})\times\mathrm{int}[q]}\left(\left(\underline{F}^{(\nu)}_{j,\partial\left(\bar{T}[\omega_k^{(j)}\times q]\right)}\bullet n_{\bar{T}[\omega_k^{(j)}\times q]}\right)\circ T\right)\cdot|J_T|$$

$$-\sum_{j\in V[\mathcal{C}]}\sum_{\iota\in\underline{J}_j\setminus\{0\}}\int_{(O\cap\partial\omega_k^{(j)}\cap\Gamma_{j,\iota})\times\mathrm{int}[q]}\left((\underline{\mathcal{B}}_{j,\iota})^{\mathrm{ex.\text{-}im.}}\left[\left(\underline{u}^{(\nu-1)},\underline{u}^{(\nu)}\right)\right]\circ T\right)\cdot|J_T| \tag{3.6.16f}$$

$$+\sum_{j\in V[\mathcal{C}]}\sum_{\iota\in\underline{J}_j\setminus\{0\}}\int_{(O\cap\partial\omega_k^{(j)}\cap\Gamma_{j,\iota})\times\mathrm{int}[q]}\left(\left(\left(\underline{a}_{\mathrm{out}}^{j,\iota,\nu}\right)^{\mathrm{ex.\text{-}im.}}\circ\left(\underline{u}_j^{(\nu-1)},\underline{u}_j^{(\nu)}\right)^{\mathrm{sp.}}\right)\circ T\right)\cdot|J_T| \tag{3.6.16g}$$

$$-\sum_{\gamma\in\mathrm{IF}_{\mathrm{con}}}\int_{(\gamma\cap\bigcup_{j\in V[\mathcal{C}]}\partial\omega_k^{(j)})\times\mathrm{int}[q]}\left((\underline{\mathcal{A}}_{\bar{T}[\gamma\times q]})^{\mathrm{ex.\text{-}im.}}\left[\left(\underline{u}^{(\nu-1)},\underline{u}^{(\nu)}\right)\right]\circ T\right)\cdot|J_T| \tag{3.6.16h}$$

$$\begin{aligned}+\sum_{\gamma\in\mathrm{IF}_{\mathrm{con}}}\int_{(\gamma\cap\bigcup_{j\in V[\mathcal{C}]}\partial\omega_k^{(j)})\times\mathrm{int}[q]}&\Bigg(\Bigg(-\left(\underline{a}_{\mathrm{flux}}^{\bar{T}[\gamma\times q],1,\nu}\right)^{\mathrm{ex.\text{-}im.}}\circ\left(\underline{u}^{(\nu-1)}_{i_1[\bar{T}[\gamma\times q]]},\underline{u}^{(\nu)}_{i_1[\bar{T}[\gamma\times q]]}\right)^{\mathrm{sp.}}\\ &+\left(\underline{a}_{\mathrm{flux}}^{\bar{T}[\gamma\times q],2,\nu}\right)^{\mathrm{ex.\text{-}im.}}\circ\left(\underline{u}^{(\nu-1)}_{i_2[\bar{T}[\gamma\times q]]},\underline{u}^{(\nu)}_{i_2[\bar{T}[\gamma\times q]]}\right)^{\mathrm{sp.}}\Bigg)\circ T\Bigg)\cdot|J_T|\end{aligned} \tag{3.6.16i}$$

$$+ \sum_{\gamma \in G_{\text{jump},1}[\mathcal{C}]} \int_{(\partial\omega_k^{(i_1[\gamma])} \cap \gamma) \times \text{int}[q]} \Bigg(\bigg(\underline{a}_{\text{jump}}^{\bar{T}[\gamma\times q],1,\nu} \circ \Big(\underline{u}^{(\nu)}_{i_1[\bar{T}[\gamma\times q]]} \Big)^{\text{sp.}}$$
$$- \underline{a}_{\text{jump}}^{\bar{T}[\gamma\times q],2,\nu} \circ \Big(\underline{u}^{(\nu)}_{i_2[\bar{T}[\gamma\times q]]} \Big)^{\text{sp.}} \bigg) \circ T \Bigg) \cdot |J_T| \tag{3.6.16j}$$

$$- \sum_{\gamma \in G_{\text{jump},2}[\mathcal{C}]} \int_{(\partial\omega_k^{(i_2[\gamma])} \cap \gamma) \times \text{int}[q]} \Big((\underline{\mathcal{A}}_{\bar{T}[\gamma\times q]})^{\text{ex.-im.}} \big[(\underline{u}^{(\nu-1)}, \underline{u}^{(\nu)}) \big] \circ T \Big) \cdot |J_T| \tag{3.6.16k}$$

$$+ \sum_{\gamma \in G_{\text{jump},2}[\mathcal{C}]} \int_{(\partial\omega_k^{(i_2[\gamma])} \cap \gamma) \times \text{int}[q]} \Bigg(\bigg(- \Big(\underline{a}_{\text{flux}}^{\bar{T}[\gamma\times q],1,\nu} \Big)^{\text{ex.-im.}} \circ \Big(\underline{u}^{(\nu-1)}_{i_1[\bar{T}[\gamma\times q]]}, \underline{u}^{(\nu)}_{i_1[\bar{T}[\gamma\times q]]} \Big)^{\text{sp.}}$$
$$+ \Big(\underline{a}_{\text{flux}}^{\bar{T}[\gamma\times q],2,\nu} \Big)^{\text{ex.-im.}} \circ \Big(\underline{u}^{(\nu-1)}_{i_2[\bar{T}[\gamma\times q]]}, \underline{u}^{(\nu)}_{i_2[\bar{T}[\gamma\times q]]} \Big)^{\text{sp.}} \bigg) \circ T \Bigg) \cdot |J_T| \tag{3.6.16l}$$

$$+ \sum_{\gamma \in G_{\text{jump},2}[\mathcal{C}]} \int_{(\partial\omega_k^{(i_2[\gamma])} \cap \gamma) \times \text{int}[q]} \Bigg(\bigg(- \underline{a}_{\text{jump}}^{\bar{T}[\gamma\times q],1,\nu} \circ \Big(\underline{u}^{(\nu)}_{i_1[\bar{T}[\gamma\times q]]} \Big)^{\text{sp.}}$$
$$+ \underline{a}_{\text{jump}}^{\bar{T}[\gamma\times q],2,\nu} \circ \Big(\underline{u}^{(\nu)}_{i_2[\bar{T}[\gamma\times q]]} \Big)^{\text{sp.}} \bigg) \circ T \Bigg) \cdot |J_T| \tag{3.6.16m}$$

$$- \sum_{j \in V[\mathcal{C}]} \int_{(O \cap \omega_k^{(j)}) \times \text{int}[q]} \Bigg(\bigg(\underline{f}_j^{(\nu)} \circ \Big(\underline{u}_j^{(\nu)} \Big)^{\text{sp.}} \bigg) \circ T \Bigg) \cdot |J_T| \quad = \quad 0. \tag{3.6.16n}$$

3.6.5 Symmetry Assumptions and Dimension Reduction

Finally, in this section, the assumed symmetry of the problem is used to achieve a dimension reduction from $d + d'$ to d in (3.6.16).

Definition 3.6.6. Given a subset $A \subseteq O$, a continuous function $\underline{g} : T(A \times \text{int}[q]) \longrightarrow \mathbb{K}$ is called *q-independent* iff there is a continuous function $g : \overline{A} \longrightarrow \mathbb{K}$ such that $g[x_O] = (\underline{g} \circ T)[(x_O, x_q)]$ for each $(x_O, x_q) \in A \times \text{int}[q]$. The function g is called the *dependent part* of $\underline{g}$.

Assumption 3.6.7. The coordinate transformation T is *compatible with q-independence* in the sense that there exists a matrix $\tilde{T} = (\tilde{t}_{i,i'})_{(i,i') \in \{1,\dots,d\}^2}$, $\tilde{t}_{i,i'} \in C(p, \mathbb{K})$, such that for each sufficiently smooth q-independent function $\underline{w} : T(p_j \times \text{int}[q]) \longrightarrow \mathbb{K}$ with dependent part w and for each d-polytope $\omega \subseteq p_j$, $j \in J$:

$$\bigwedge_{\substack{(x_p, x_q) \\ \in ((\partial\omega) \times q) \cap \Omega}} \left(\begin{array}{l} \Big(\nabla\, w[x_p] \cdot \tilde{T}[x_p] \Big) \bullet n_\omega[x_p] \\ = \Big(\nabla(\underline{w} \circ T)[(x_p, x_q)] \cdot (T')^{-1}[(x_p, x_q)] \Big) \bullet n_{\bar{T}[\omega\times q]} \big[T[(x_p, x_q)] \big] \end{array} \right). \tag{3.6.17}$$

Basically, the following Assumptions 3.6.8, 3.6.10, and 3.6.12 say that all relevant quantities of the considered problem are assumed to be q-independent for each fixed time $t \in \tau$. The solution functions are treated first:

Assumption 3.6.8. It is assumed that for each $j \in J$, there exist functions $u_j \in C(\tau \times p_j, \upsilon)$ such that

$$\bigwedge_{\left(t,(x_p,x_q)\right)\in\tau\times\left((p_j\times q)\cap\Omega\right)} u_j[(t,x_p)] = \left(\underline{u}_j\restriction_{\{t\}\times T(p_j\times\mathrm{int}[q])}\circ T\right)[(x_p,x_q)] = \underline{u}_j\left[\left(t, T[(x_p,x_q)]\right)\right]. \tag{3.6.18a}$$

Remark 3.6.9. Since according to Assumption 3.6.8, for each $j \in J$ and each $t \in \tau$, $\underline{u}_j\restriction_{\{t\}\times T(p_j\times\mathrm{int}[q])}$ is q-independent, and T is compatible with q-independence by Assumption 3.6.7, the chain rule yields for each d-polytope $\omega \subseteq p_j$, $j \in J$:

$$\bigwedge_{\substack{\left(t,(x_p,x_q)\right)\\ \in\tau\times\left(((\partial\omega)\times q)\cap\Omega\right)}} \begin{pmatrix} \left(\nabla u_j[(t,x_p)]\cdot\tilde{T}[x_p]\right)\bullet n_\omega[x_p] \\ = \left((\nabla\underline{u}_j\restriction_{\{t\}\times T(p_j\times\mathrm{int}[q])})\circ T\right)[(x_p,x_q)]\bullet n_{\bar{T}[\omega\times q]}\left[T[(x_p,x_q)]\right] \end{pmatrix}. \tag{3.6.18b}$$

Assumption 3.6.10. The functions $\underline{b}_j$, $\underline{v}_j$, $\underline{k}_j$, $\underline{f}_j$, $\underline{a}^{\gamma,\alpha}_{\mathrm{jump}}$, $\underline{a}^{\gamma,\alpha}_{\mathrm{flux}}$, and $\underline{a}^{j,\iota}_{\mathrm{out}}$ are also presumed to be independent of $x_q \in q$, i.e. there are functions $b_j \in C(\upsilon\times\tau\times p_j,\mathbb{K})$, $v_j \in C(\upsilon\times\tau\times p_j,\mathbb{R}^d)$, $k_j \in C(\upsilon\times\tau\times p_j,\mathbb{K})$, $f_j \in C(\upsilon\times\tau\times p_j,\mathbb{K})$, $a^{\gamma,\alpha}_{\mathrm{jump}} \in C(\upsilon\times\tau\times\gamma,\mathbb{K})$, $a^{\gamma,\alpha}_{\mathrm{flux}} \in C(\upsilon\times\tau\times\gamma,\mathbb{K})$, and $a^{j,\iota}_{\mathrm{out}} \in C(\upsilon\times\tau\times\Gamma_{j,\iota},\mathbb{K})$, such that

$$\bigwedge_{j\in J}\ \bigwedge_{\left(y,t,(x_p,x_q)\right)\in\upsilon\times\tau\times\left((p_j\times q)\cap\Omega\right)} b_j\left[\left(y,t,x_p\right)\right] = \underline{b}_j\left[\left(y,t,T[(x_p,x_q)]\right)\right], \tag{3.6.18c}$$

for each d-polytope $\omega \subseteq p_j$:

$$\bigwedge_{j\in J}\ \bigwedge_{\substack{\left(t,(x_p,x_q)\right)\\ \in\tau\times\left(((\partial\omega)\times q)\cap\Omega\right)}} \begin{pmatrix} v_j\left[\left(y,t,x_p\right)\right]\bullet n_\omega[x_p] \\ = \underline{v}_j\left[\left(y,t,T[(x_p,x_q)]\right)\right]\bullet n_{\bar{T}[\omega\times q]}\left[T[(x_p,x_q)]\right] \end{pmatrix}, \tag{3.6.18d}$$

$$\bigwedge_{j\in J}\ \bigwedge_{\left(y,t,(x_p,x_q)\right)\in\upsilon\times\tau\times\left((p_j\times q)\cap\Omega\right)} k_j\left[\left(y,t,x_p\right)\right] = \underline{k}_j\left[\left(y,t,T[(x_p,x_q)]\right)\right], \tag{3.6.18e}$$

$$\bigwedge_{j\in J}\ \bigwedge_{\left(y,t,(x_p,x_q)\right)\in\upsilon\times\tau\times\left((p_j\times q)\cap\Omega\right)} f_j\left[\left(y,t,x_p\right)\right] = \underline{f}_j\left[\left(y,t,T[(x_p,x_q)]\right)\right], \tag{3.6.18f}$$

$$\bigwedge_{\substack{(\gamma,\alpha)\\ \in \mathrm{IF}_{\mathrm{jump}}\times\{1,2\}}} \quad \bigwedge_{\left(y,t,(x_p,x_q)\right)\in\upsilon\times\tau\times\left((\gamma\times q)\cap\Omega\right)} a^{\gamma,\alpha}_{\mathrm{jump}}\left[\left(y,t,x_p\right)\right] = \underline{a}^{\bar{T}[\gamma\times q],\alpha}_{\mathrm{jump}}\left[\left(y,t,T[(x_p,x_q)]\right)\right], \tag{3.6.18g}$$

$$\bigwedge_{\substack{(\gamma,\alpha)\\ \in \mathrm{IF}\times\{1,2\}}} \quad \bigwedge_{\left(y,t,(x_p,x_q)\right)\in\upsilon\times\tau\times\left((\gamma\times q)\cap\Omega\right)} a^{\gamma,\alpha}_{\mathrm{flux}}\left[\left(y,t,x_p\right)\right] = \underline{a}^{\bar{T}[\gamma\times q],\alpha}_{\mathrm{flux}}\left[\left(y,t,T[(x_p,x_q)]\right)\right], \tag{3.6.18h}$$

$$\bigwedge_{\substack{(j,\iota)\\ \in J\times \underline{J}_j\setminus\{0\}}} \quad \bigwedge_{\left(y,t,(x_p,x_q)\right)\in\upsilon\times\tau\times\left((\Gamma_{j,\iota}\times q)\cap\Omega\right)} a^{j,\iota}_{\mathrm{out}}\left[\left(y,t,x_p\right)\right] = \underline{a}^{j,\iota}_{\mathrm{out}}\left[\left(y,t,T[(x_p,x_q)]\right)\right]. \tag{3.6.18i}$$

Moreover, it is also assumed that analogous symmetry conditions hold for the chosen dependency splittings $(\underline{a}^{\gamma,\alpha}_{\mathrm{flux}})^{\text{ex.-im.}}$, $(\underline{a}^{j,\iota}_{\mathrm{out}})^{\text{ex.-im.}}$, and $(a^{\gamma,\alpha}_{\mathrm{flux}})^{\text{ex.-im.}}$, $(a^{j,\iota}_{\mathrm{out}})^{\text{ex.-im.}}$, respectively.

Remark 3.6.11. If the symmetry conditions of Assumptions 3.6.8 and 3.6.10 hold, then the analogous symmetry conditions also hold for the corresponding time-discrete functions $\underline{u}^{(\nu)}_j$, $\underline{b}^{(\nu)}_j$, $\underline{v}^{(\nu)}_j$, $\underline{k}^{(\nu)}_j$, $\underline{f}^{(\nu)}_j$, $\underline{a}^{\gamma,\alpha,\nu}_{\mathrm{jump}}$, $(\underline{a}^{\gamma,\alpha,\nu}_{\mathrm{flux}})^{\text{ex.-im.}}$, $(\underline{a}^{j,\iota,\nu}_{\mathrm{out}})^{\text{ex.-im.}}$, and $u^{(\nu)}_j$, $b^{(\nu)}_j$, $v^{(\nu)}_j$, $k^{(\nu)}_j$, $f^{(\nu)}_j$, $a^{\gamma,\alpha,\nu}_{\mathrm{jump}}$, $(a^{\gamma,\alpha,\nu}_{\mathrm{flux}})^{\text{ex.-im.}}$, $(a^{j,\iota,\nu}_{\mathrm{out}})^{\text{ex.-im.}}$, $\nu \in \{0,\dots,n\}$.

—

Next, the symmetry conditions for the nonlocal operators are formulated:

Assumption 3.6.12. It is assumed that for each $\gamma \in \mathrm{IF}$, there is a nonlocal interface operator $\mathcal{A}_\gamma$, and that for each $(j,\iota) \in J \times \underline{J}_j \setminus \{0\}$, there is a nonlocal boundary operator $\mathcal{B}_{j,\iota}$ such that for each family of q-independent functions $\underline{\mathfrak{w}} = (\underline{w}_j)_{j\in J}$, it holds that

$$\bigwedge_{(x_p,x_q)\in(\gamma\times q)\cap\Omega} \mathcal{A}_\gamma[\mathfrak{w}][x_p] = \underline{\mathcal{A}}_{\bar{T}[\gamma\times q]}[\underline{\mathfrak{w}}]\left[T[(x_p,x_q)]\right], \tag{3.6.19a}$$

$$\bigwedge_{(x_p,x_q)\in(\Gamma_{j,\iota}\times q)\cap\Omega} \mathcal{B}_{j,\iota}[\mathfrak{w}][x_p] = \underline{\mathcal{B}}_{j,\iota}[\underline{\mathfrak{w}}]\left[T[(x_p,x_q)]\right], \tag{3.6.19b}$$

where $\mathfrak{w} = (w_j)_{j\in J}$, w_j being the dependent part of $\underline{w}_j$, $j \in J$.

As before, it is also assumed that analogous relations hold for the chosen dependency splittings $(\underline{\mathcal{A}}_{\bar{T}[\gamma\times q]})^{\text{ex.-im.}}$, $(\underline{\mathcal{B}}_{j,\iota})^{\text{ex.-im.}}$, and $(\mathcal{A}_\gamma)^{\text{ex.-im.}}$, $(\mathcal{B}_{j,\iota})^{\text{ex.-im.}}$.

Assumption 3.6.13. Assume that J_T factorizes into functions $J_{T,p} : O \longrightarrow \mathbb{R}$, $J_{T,q} : \mathrm{int}[q] \longrightarrow \mathbb{R}$, i.e.

$$\bigwedge_{(x_p,x_q)\in\Omega} J_T[(x_p,x_q)] = J_{T,p}[x_p]\cdot J_{T,q}[x_q]. \tag{3.6.20}$$

Moreover, assume that $J_{T,p}$ is continuous and extends to the whole set p continuously: $J_{T,p} \in C(p,\mathbb{R})$.

—

If $T = T_{\mathrm{cyl}}$ with p and q as in Ex. 3.6.3, then according to Rem. B.3.2(c) one has $J_{T_{\mathrm{cyl}}}[(r,\vartheta,z)] = r$, i.e. one can let $J_{T_{\mathrm{cyl}},p}[(r,z)] = r$ and $J_{T_{\mathrm{cyl}},q}[\vartheta] = 1$.

Presuming that the unknown is sufficiently regular, it is

$$\begin{aligned}&\left(\mathrm{tr}_{T\left((O\cap\partial\omega_k^{(j)})\times\mathrm{int}[q]\right)}\left(\left(\underline{k}_j^{(\nu)}\circ\left(\underline{u}_j^{(\nu)}\right)^{\mathrm{sp.}}\right)\nabla\,\underline{u}_j^{(\nu)}\right)\right)\circ T\\ &= \mathrm{tr}_{(O\cap\partial\omega_k^{(j)})\times\mathrm{int}[q]}\left(\left(\left(\underline{k}_j^{(\nu)}\circ\left(\underline{u}_j^{(\nu)}\right)^{\mathrm{sp.}}\right)\nabla\,\underline{u}_j^{(\nu)}\right)\circ T\right).\end{aligned} \tag{3.6.21}$$

Define the following families consisting of the dependent parts of the q-independent time-discrete solutions:

$$\bigwedge_{\nu\in\{0,\dots,n\}} \quad \mathfrak{u}^{(\nu)} := \left(u_j^{(\nu)}\right)_{j\in J}.$$

Putting everything together, i.e. using (3.6.5), (3.6.21), (3.6.8), Rem. 3.6.11, (3.6.19), (3.6.20), and the Fubini Th. C.8.3 in (3.6.16), then dividing the equation by $\int_{\mathrm{int}[q]}|J_{T,q}|$, results in

$$(t_\nu - t_{\nu-1})^{-1}\sum_{j\in V[\mathcal{C}]}\int_{\omega_k^{(j)}}\left(b_j^{(\nu)}\circ\left(u_j^{(\nu)}\right)^{\mathrm{sp.}} - b_j^{(\nu-1)}\circ\left(u_j^{(\nu-1)}\right)^{\mathrm{sp.}}\right)\cdot|J_{T,p}| \tag{3.6.22a}$$

$$+\sum_{j\in V[\mathcal{C}]}\int_{\partial\omega_k^{(j)}\cap\mathrm{int}[p_j]}\left(\left(v_j^{(\nu)}\circ\left(u_j^{(\nu)}\right)^{\mathrm{sp.}}\right)\bullet n_{\omega_k^{(j)}}\right)\cdot|J_{T,p}| \tag{3.6.22b}$$

$$+\sum_{j\in V[\mathcal{C}]}\int_{\partial\omega_k^{(j)}\cap\partial p}\left(\left(v_j^{(\nu)}\circ\left(u_j^{(\nu)}\right)^{\mathrm{sp.}}\right)\bullet n_{\omega_k^{(j)}}\right)\cdot|J_{T,p}| \tag{3.6.22c}$$

$$+\sum_{j\in V[\mathcal{C}]}\sum_{\gamma\in\mathrm{IF}}\int_{\partial\omega_k^{(j)}\cap\gamma}\left(\left(v_j^{(\nu)}\circ\left(u_j^{(\nu)}\right)^{\mathrm{sp.}}\right)\bullet n_{\omega_k^{(j)}}\right)\cdot|J_{T,p}| \tag{3.6.22d}$$

$$-\sum_{j\in V[\mathcal{C}]}\int_{\partial\omega_k^{(j)}\cap\mathrm{int}[p_j]}\left(\mathrm{tr}_{O\cap\partial\omega_k^{(j)}}\left(\left(k_j^{(\nu)}\circ\left(u_j^{(\nu)}\right)^{\mathrm{sp.}}\right)\nabla\,u_j^{(\nu)}\cdot\tilde{T}\right)\bullet n_{\omega_k^{(j)}}\right)\cdot|J_{T,p}| \tag{3.6.22e}$$

$$-\sum_{j\in V[\mathcal{C}]:\,0\in\underline{J}_j}\int_{\partial\omega_k^{(j)}\cap\Gamma_{j,0}}\left(\mathrm{tr}_{O\cap\partial\omega_k^{(j)}}\left(\left(k_j^{(\nu)}\circ\left(u_j^{(\nu)}\right)^{\mathrm{sp.}}\right)\nabla\,u_j^{(\nu)}\cdot\tilde{T}\right)\bullet n_{\omega_k^{(j)}}\right)\cdot|J_{T,p}|$$

$$-\sum_{j\in V[\mathcal{C}]}\sum_{\iota\in\underline{J}_j\setminus\{0\}}\int_{\partial\omega_k^{(j)}\cap\Gamma_{j,\iota}}(\mathcal{B}_{j,\iota})^{\mathrm{ex.\text{-}im.}}\left[\left(\mathfrak{u}^{(\nu-1)},\mathfrak{u}^{(\nu)}\right)\right]\cdot|J_{T,p}| \tag{3.6.22f}$$

$$+\sum_{j\in V[\mathcal{C}]}\sum_{\iota\in\underline{J}_j\setminus\{0\}}\int_{\partial\omega_k^{(j)}\cap\Gamma_{j,\iota}}\left(\left(a_{\mathrm{out}}^{j,\iota,\nu}\right)^{\mathrm{ex.\text{-}im.}}\circ\left(u_j^{(\nu-1)},u_j^{(\nu)}\right)^{\mathrm{sp.}}\right)\cdot|J_{T,p}| \tag{3.6.22g}$$

$$-\sum_{\gamma\in\mathrm{IF}_{\mathrm{con}}}\int_{\gamma\cap\bigcup_{j\in V[\mathcal{C}]}\partial\omega_k^{(j)}}(\mathcal{A}_\gamma)^{\mathrm{ex.\text{-}im.}}\left[\left(\mathfrak{u}^{(\nu-1)},\mathfrak{u}^{(\nu)}\right)\right]\cdot|J_{T,p}| \tag{3.6.22h}$$

$$+ \sum_{\gamma \in \mathrm{IF}_{\mathrm{con}}} \int_{\gamma \cap \bigcup_{j \in V[\mathcal{C}]} \partial \omega_k^{(j)}} \Big(- \left(a_{\mathrm{flux}}^{\gamma,1,\nu}\right)^{\mathrm{ex.-im.}} \circ \left(u_{i_1[\gamma]}^{(\nu-1)}, u_{i_1[\gamma]}^{(\nu)}\right)^{\mathrm{sp.}} + \left(a_{\mathrm{flux}}^{\gamma,2,\nu}\right)^{\mathrm{ex.-im.}} \circ \left(u_{i_2[\gamma]}^{(\nu-1)}, u_{i_2[\gamma]}^{(\nu)}\right)^{\mathrm{sp.}} \Big) \cdot |J_{T,p}| \tag{3.6.22i}$$

$$+ \sum_{\gamma \in G_{\mathrm{jump},1}[\mathcal{C}]} \int_{\partial \omega_k^{(i_1[\gamma])} \cap \gamma} \left(a_{\mathrm{jump}}^{\gamma,1,\nu} \circ \left(u_{i_1[\gamma]}^{(\nu)}\right)^{\mathrm{sp.}} - a_{\mathrm{jump}}^{\gamma,2,\nu} \circ \left(u_{i_2[\gamma]}^{(\nu)}\right)^{\mathrm{sp.}} \right) \cdot |J_{T,p}| \tag{3.6.22j}$$

$$- \sum_{\gamma \in G_{\mathrm{jump},2}[\mathcal{C}]} \int_{\partial \omega_k^{(i_2[\gamma])} \cap \gamma} (\mathcal{A}_\gamma)^{\mathrm{ex.-im.}} \left[(\mathfrak{u}^{(\nu-1)}, \mathfrak{u}^{(\nu)}) \right] \cdot |J_{T,p}| \tag{3.6.22k}$$

$$+ \sum_{\gamma \in G_{\mathrm{jump},2}[\mathcal{C}]} \int_{\partial \omega_k^{(i_2[\gamma])} \cap \gamma} \Big(- \left(a_{\mathrm{flux}}^{\gamma,1,\nu}\right)^{\mathrm{ex.-im.}} \circ \left(u_{i_1[\gamma]}^{(\nu-1)}, u_{i_1[\gamma]}^{(\nu)}\right)^{\mathrm{sp.}} + \left(a_{\mathrm{flux}}^{\gamma,2,\nu}\right)^{\mathrm{ex.-im.}} \circ \left(u_{i_2[\gamma]}^{(\nu-1)}, u_{i_2[\gamma]}^{(\nu)}\right)^{\mathrm{sp.}} \Big) \cdot |J_{T,p}| \tag{3.6.22l}$$

$$+ \sum_{\gamma \in G_{\mathrm{jump},2}[\mathcal{C}]} \int_{\partial \omega_k^{(i_2[\gamma])} \cap \gamma} \left(- a_{\mathrm{jump}}^{\gamma,1,\nu} \circ \left(u_{i_1[\gamma]}^{(\nu)}\right)^{\mathrm{sp.}} + a_{\mathrm{jump}}^{\gamma,2,\nu} \circ \left(u_{i_2[\gamma]}^{(\nu)}\right)^{\mathrm{sp.}} \right) \cdot |J_{T,p}| \tag{3.6.22m}$$

$$- \sum_{j \in V[\mathcal{C}]} \int_{\omega_k^{(j)}} \left(f_j^{(\nu)} \circ \left(u_j^{(\nu)}\right)^{\mathrm{sp.}} \right) \cdot |J_{T,p}| \quad = \quad 0. \tag{3.6.22n}$$

Comparing (3.6.22) with (3.5.24), one finds that one also ends up with (3.6.22) when starting out with a (d, N)-dimensional evolution equation complex

$$\mathfrak{C} = \Big(\mathfrak{D}, \left(H_{|J_{T,p}| \cdot b_j, |J_{T,p}| \cdot v_j, |J_{T,p}| \cdot k_j \cdot \tilde{T}, |J_{T,p}| \cdot f_j}\right)_{j \in J}, \left((a_{\mathrm{jump}}^{\gamma,1}, a_{\mathrm{jump}}^{\gamma,2})\right)_{\gamma \in \mathrm{IF}_{\mathrm{jump}}}, \left((a_{\mathrm{flux}}^{\gamma,1}, a_{\mathrm{flux}}^{\gamma,2}, \mathcal{A}_\gamma)\right)_{\gamma \in \mathrm{IF}}, \left(u_{j,\mathrm{Dir}}\right)_{j \in J: 0 \in J_j}, \left((a_{\mathrm{out}}^{j,\iota}, \mathcal{B}_{j,\iota})\right)_{(j,\iota) \in J \times (J_j \setminus \{0\})}, \left(u_j^{(0)}\right)_{j \in J} \Big),$$

$$\bigwedge_{(j,\iota) \in J \times J_{j,0}} \begin{pmatrix} a_{\mathrm{out}}^{j,\iota} = 0, \\ \mathcal{B}_{j,\iota} = 0, \\ v_j \restriction_{\Gamma_{j,\iota}} \bullet n_{p_j} = 0 \end{pmatrix}, \tag{3.6.23}$$

and then proceeding as in Sec. 3.5 (without change of variables). This shows that the general setting of an evolution equation complex as defined in Def. 3.4.6 is almost sufficiently general to include all situations arising from dimension reductions via a change of variables as described in the present section. To make clear what is meant by "almost sufficiently general", the evolution equations in the new variables are written:

$$\begin{aligned} &\partial_t(|J_{T,p}| \cdot b_j \circ u_j^{\mathrm{t.-sp.}}) + \mathrm{div}(|J_{T,p}| \cdot v_j \circ u_j^{\mathrm{t.-sp.}}) \\ &- \mathrm{div}\left((\nabla u_j) \cdot (|J_{T,p}| k_j \tilde{T} \circ u_j^{\mathrm{t.-sp.}})\right) - |J_{T,p}| \cdot f_j \circ u_j^{\mathrm{t.-sp.}} = 0. \end{aligned} \tag{3.6.24}$$

If $|J_{T,p}|$ is sufficiently regular, then (3.6.24) has the same form as (3.3.4) with the exception of the diffusion term. While the diffusion was assumed to be scalar-valued in (3.3.2c), it needs to be matrix-valued to include the generic situation of (3.6.24).

However, the case of cylindrical coordinates, that is used for the simulation applications of this work, is more benign than the generic case of (3.6.24). By (B.3.4) in App. B.3, one has $J_{T_{\mathrm{cyl}},p} = r$ which is C^∞, and by Rem. B.3.3, $\tilde{T}_{\mathrm{cyl}}$ is the identity matrix.

It just remains to mention the symmetry conditions for the Dirichlet functions and for the initial distributions: It is assumed that for each $j \in J$ where $0 \in J_j$ and for each $\nu \in \{0, \dots, n\}$, it is $u^{(\nu)}_{j,\mathrm{Dir}} \in C(\Gamma_{j,0}, \mathbb{K})$ such that

$$\bigwedge_{(x_p,x_q)\in(\Gamma_{j,0}\times q)\cap\Omega} u^{(\nu)}_{j,\mathrm{Dir}}[x_p] = \underline{u}^{(\nu)}_{j,\mathrm{Dir}}\big[T[(x_p, x_q)]\big]; \tag{3.6.25}$$

and for each $j \in J$, it is $u^{(0)}_j \in C(p_j, \mathbb{K})$ such that

$$\bigwedge_{(x_p,x_q)\in(p_j\times q)\cap\Omega} u^{(0)}_j[x_p] = \underline{u}^{(0)}_j\big[T[(x_p, x_q)]\big]. \tag{3.6.26}$$

3.7 Finite Volume Discretization and Discrete A Priori Estimates

The contents of Sec. 3.7 consists of the formulation of a space discretization of (3.5.24) and of the supply of discrete a priori estimates. The discrete a priori estimates are used in Sec. 3.8 in the prove of existence and uniqueness of discrete solutions.

The discretization strategy is outlined in Sec. 3.7.1, followed by a detailed treatment of each term of (3.5.24) in the subsequent Secs 3.7.2 – 3.7.11. The discretization is summarized in the definitions of Sec. 3.7.12, and the discrete a priori estimates are provided in Sec. 3.7.13.

3.7.1 Outline of Discretization Strategy

As already mentioned in Sec. 3.5, it is assumed that the control volumes introduced in Sec. 3.5.1 are small, such that the functions occurring in the integrands of (3.5.24) can be approximated as being constant inside their respective domains of integration. More precisely, for each $k \in I_\Pi$ (where $\Pi = (\omega_k)_{k\in I_\Pi}$ is the partition of p into control volumes), associate a *discretization point* x_k with the control volume ω_k, such that (cf. Fig. 3.15)

$$\bigwedge_{k\in I_\Pi} x_k \in \omega_k. \tag{3.7.1}$$

Moreover, it is assumed that the discretization points are chosen such that for each integral in (3.5.24), there is always precisely one discretization point inside the respective domain of integration. The only exceptions are the integrals involving interior fluxes, i.e. the integrals in (3.5.24b) and (3.5.24e), where the domain of integration is perpendicular to the line segment joining neighboring discretization points (s. condition (dispt-(i)) below). All integrands in (3.5.24), except the ones occurring in (3.5.24b) and (3.5.24e), and except the ones occurring in the nonlocal terms (3.5.24f), (3.5.24h), and (3.5.24k), are then replaced by their values at the respective discretization points (see the following Secs 3.7.2 – 3.7.11 for details, where the discretization of the nonlocal terms (3.5.24f), (3.5.24h), and (3.5.24k) is the subject of Secs 3.7.7 and 3.7.8).

The integrands in (3.5.24b) and (3.5.24e) involve the normal fluxes through regular interfaces $\partial_{\text{reg}}\omega_k \cap \partial_{\text{reg}}\omega_l$ between neighboring control volumes ω_k and ω_l (see Sec. 3.7.3). For the approximation of these terms in Secs 3.7.3 and 3.7.4, it is assumed that the partition Π is such that the line segment joining the neighboring discretization points x_k and x_l is always perpendicular to the interface $\partial_{\text{reg}}\omega_k \cap \partial_{\text{reg}}\omega_l$, i.e.

$$\bigwedge_{\{k,l\}\in E_{\text{IF}}[\Pi]} x_k \neq x_l \quad \text{and} \quad \frac{x_l - x_k}{\|x_k - x_l\|_2} = n_{\omega_k}\restriction_{\partial_{\text{reg}}\omega_k \cap \partial_{\text{reg}}\omega_l}, \tag{dispt-(i)}$$

where the set $E_{\text{IF}}[\Pi]$ is defined in (3.7.11) below. In Fig. 3.15, the discretization points are chosen such that (dispt-(i)) is satisfied.

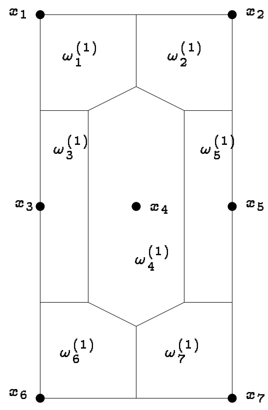


Figure 3.15: The partition of Fig. 3.4 including discretization points $x_1, \dots, x_7$.

As described in Sec. 3.5.3, the partition Π gives rise to partitions $\Pi^{(j)} = (\omega_k^{(j)})_{k\in I^{(j)}}$ of p_j, $j \in J$. Now, the value $u_{(k,j)}^{(\nu)} := u_j^{(\nu)}[x_k]$ is to be used as an approximation of the time-discrete solution $u_j^{(\nu)}$ in $\omega_k^{(j)}$ at time t_ν. Therefore, (3.7.1) is strengthened to

$$\bigwedge_{k\in I_\Pi} \bigwedge_{j\in V_{\omega_k}} x_k \in \omega_k^{(j)} \tag{dispt-(ii)}$$

(cf. (3.5.17) for the definition of V_{ω_k}). For example in the situations depicted in Fig. 3.16, the chosen position for the discretization point x_ω is the only one possible to satisfy (dispt-(ii)).

The vector $U^{(\nu)}_{\text{long}} := (u^{(\nu)}_{(k,j)})_{(k,j)\in I_\Pi\times V_{\omega_k}}$ constitutes a time- and space-discrete approximation of the family of time-discrete solutions $(u^{(\nu)}_j)_{j\in J}$ at time t_ν. Suitable interpolations of the $U^{(\nu)}_{\text{long}}$ should converge to the $(u^{(\nu)}_j)_{j\in J}$ as the size of the control volumes tends to zero; and suitable interpolations of the $(u^{(\nu)}_j)_{j\in J}$ should converge to a solution $(u_j)_{j\in J}$ to $\mathfrak{C}$ (cf. Def. 3.4.7) as the size of the time steps tends to zero.

As will be explained shortly, the approximation $U^{(\nu)}_{\text{long}}$ is also represented by the smaller vector $U^{(\nu)} := U^{(\nu)}_{\text{short}} := (u^{(\nu)}_{(k,\mathcal{C})})_{(k,\mathcal{C})\in I_{\Pi,\mathfrak{D}}}$, where

$$I_{\Pi,\mathfrak{D}} := \big\{(k,\mathcal{C}) : \, k \in I_\Pi, \; \mathcal{C} \in \operatorname{CoCmp}[\mathcal{G}_{\omega_k}]\big\}. \tag{3.7.2}$$

The index $\mathfrak{D}$ in $I_{\Pi,\mathfrak{D}}$ is used to indicate that the set depends on the domain complex $\mathfrak{D}$, as it needs the information about the distribution of continuous interfaces and jump interfaces (cf. the definition of $\mathcal{G}_{\omega_k}$ according to Def. 3.5.3). The reason for passing from the vector $U^{(\nu)}_{\text{long}}$ to the vector $U^{(\nu)}$ is the fact that values $u^{(\nu)}_{k,j_1}$ and $u^{(\nu)}_{k,j_2}$ must be the same whenever p_{j_1} and p_{j_2} are connected via continuous interfaces, i.e. whenever j_1 and j_2 lie in the same connected component of the graph $\mathcal{G}_{\omega_k}$. For example in case (a) of Fig. 3.16, $u^{(\nu)}_1[x_\omega], \dots, u^{(\nu)}_4[x_\omega]$ can have four different values, whereas in case (b) of Fig. 3.16, $u^{(\nu)}_2[x_\omega]$, $u^{(\nu)}_3[x_\omega]$, and $u^{(\nu)}_4[x_\omega]$ all have the same value, which can be different from $u^{(\nu)}_1[x_\omega]$.

It was shown in Sec. 3.5, that, if $(u^{(\nu)}_j)$ is a solution to the time discretization $\mathfrak{T}$ of $\mathfrak{C}$, then Eqs (3.5.24) are satisfied, i.e. precisely one equation for each discrete time t_ν and for each $(k,\mathcal{C}) \in I_{\Pi,\mathfrak{D}}$ (cf. the remarks immediately after the formulation of (3.5.24)). The strategy is to determine $U^{(\nu)}$ using discretized versions of (3.5.24). However, if $x_k \in \Gamma_{j,0}$, $j \in V[\mathcal{C}]$, then

$$u^{(\nu)}_{(k,\mathcal{C})} = u_{j,\text{Dir}}[(t_\nu, x_k)] \tag{3.7.3}$$

is known a priori. This actuates the introduction of the index sets

$$I_{\Pi,\mathfrak{D},\text{Dir}} := \{(k,\mathcal{C}) \in I_{\Pi,\mathfrak{D}} : \, 0 \in J_j, \; \Gamma_{j,0} \cap \partial_{\text{reg}}\omega_k \neq \emptyset \text{ for some } j \in V[\mathcal{C}]\}, \tag{3.7.4a}$$
$$I_{\Pi,\mathfrak{D},\neg\text{Dir}} := I_{\Pi,\mathfrak{D}} \setminus I_{\Pi,\mathfrak{D},\text{Dir}}. \tag{3.7.4b}$$

Here, and also in the following, the handling of the boundary conditions makes use of the assumption that one can find a discretization point in each $(d-1)$-dimensional intersection between a control volume and an outer boundary $\Gamma_{j,\iota}$:

$$\bigwedge_{k\in I_\Pi} \; \bigwedge_{(j,\iota)\in J\times J_j} \quad \Gamma_{j,\iota} \cap \partial_{\text{reg}}\omega_k \neq \emptyset \quad \Rightarrow \quad x_k \in \Gamma_{j,\iota}. \tag{dispt-(iii)}$$

In Fig. 3.17(a), (dispt-(iii)) is satisfied, whereas the condition is violated in Fig. 3.17(b) for $k \in \{3, 5, 7\}$.

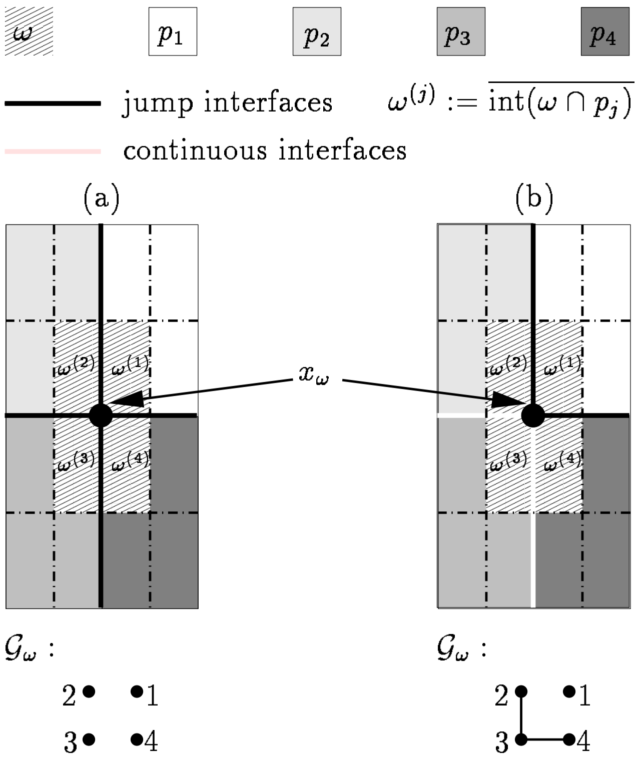


Figure 3.16: Control volume ω with discretization point x_ω for two different disributions of jump and continuous interfaces.

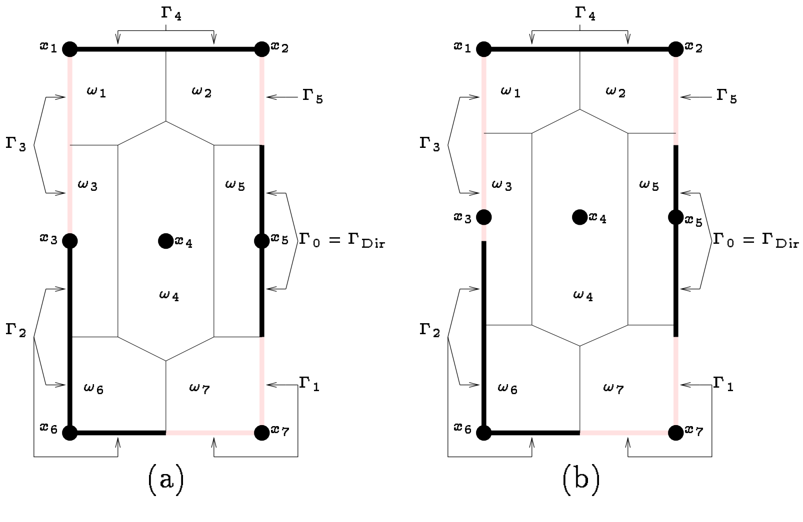


Figure 3.17: Illustration of Condition (dispt-(iii)).

As the vector $(u^{(\nu)}_{(k,\mathcal{C})})_{(k,\mathcal{C})\in I_{\Pi,\mathfrak{D},\mathrm{Dir}}}$ is known a priori, only $(u^{(\nu)}_{(k,\mathcal{C})})_{(k,\mathcal{C})\in I_{\Pi,\mathfrak{D},\neg\mathrm{Dir}}}$ is determined using discretized versions of (3.5.24), where it will suffice to discretize (3.5.24) for

$(k, \mathcal{C}) \in I_{\Pi,\mathfrak{D},\neg\mathrm{Dir}}$.

The discretization of the $(k, \mathcal{C})$-th equation of (3.5.24) at time t_ν, $(k, \mathcal{C}) \in I_{\Pi,\mathfrak{D},\neg\mathrm{Dir}}$, according to the strategy described above and as carried out in the following sections, has the form

$$\mathfrak{h}^{(\nu)}_{(k,\mathcal{C})}[(U^{(\nu-1)}, U^{(\nu)})] = 0, \tag{3.7.5a}$$

$$\mathfrak{h}^{(\nu)}_{(k,\mathcal{C})} : \upsilon^{I_{\Pi,\mathfrak{D},\neg\mathrm{Dir}}} \times \upsilon^{I_{\Pi,\mathfrak{D},\neg\mathrm{Dir}}} \longrightarrow \mathbb{K}, \tag{3.7.5b}$$

which can be combined to

$$\mathfrak{h}^{(\nu)}[(U^{(\nu-1)}, U^{(\nu)})] = 0, \tag{3.7.6a}$$

$$\mathfrak{h}^{(\nu)} : \upsilon^{I_{\Pi,\mathfrak{D},\neg\mathrm{Dir}}} \times \upsilon^{I_{\Pi,\mathfrak{D},\neg\mathrm{Dir}}} \longrightarrow \mathbb{K}^{I_{\Pi,\mathfrak{D},\neg\mathrm{Dir}}}. \tag{3.7.6b}$$

Each operator $\mathfrak{h}^{(\nu)}_{(k,\mathcal{C})}$ in (3.7.5) is a sum of operators

$$\mathfrak{h}^{(\nu)}_{(k,\mathcal{C})} = \mathfrak{h}^{(\nu)}_{(k,\mathcal{C}),(a)} + \cdots + \mathfrak{h}^{(\nu)}_{(k,\mathcal{C}),(n)}, \tag{3.7.7}$$

where the operator $\mathfrak{h}^{(\nu)}_{(k,\mathcal{C}),(a)}$ represents the space discretization of (3.5.24a) etc. It is noted that the summand between (3.5.24e) and (3.5.24f) vanishes for $(k, \mathcal{C}) \in I_{\Pi,\mathfrak{D},\neg\mathrm{Dir}}$. The operators $\mathfrak{h}^{(\nu)}_{(k,\mathcal{C}),(a)}, \dots, \mathfrak{h}^{(\nu)}_{(k,\mathcal{C}),(n)}$ are defined in the succeeding Secs 3.7.2 - 3.7.11 .

A discrete solution will have to satisfy (3.7.6a) for each $\nu \in \{1, \dots, n\}$ (cf. Def. 3.7.42(iii)).

On the way to establish discrete a priori estimates in Th. 3.7.50, it is an important auxiliary result to prove an upper bound for the operators $\mathfrak{s}^{(\nu)}$ defined by

$$\bigwedge_{\nu \in \{0,\dots,n\}} \left(\begin{array}{l} \mathfrak{s}^{(\nu)} : \upsilon^{I_{\Pi,\mathfrak{D},\neg\mathrm{Dir}}} \times \upsilon^{I_{\Pi,\mathfrak{D},\neg\mathrm{Dir}}} \longrightarrow \mathbb{K}, \\ \mathfrak{s}^{(\nu)} := - \displaystyle\sum_{(k,\mathcal{C}) \in I_{\Pi,\mathfrak{D},\neg\mathrm{Dir}}} \left(\mathfrak{h}^{(\nu)}_{(k,\mathcal{C})} - \mathfrak{h}^{(\nu)}_{(k,\mathcal{C}),(a)} \right) \end{array} \right). \tag{3.7.8}$$

Subtracting $\mathfrak{h}^{(\nu)}_{(k,\mathcal{C}),(a)}$ in (3.7.8) eliminates the time-step-dependent terms from $\mathfrak{s}^{(\nu)}$ (cf. (3.7.9)). The proof of the upper bound for the $\mathfrak{s}^{(\nu)}$ involves estimating upper bounds of the terms

$$- \sum_{(k,\mathcal{C}) \in I_{\Pi,\mathfrak{D},\neg\mathrm{Dir}}} \mathfrak{h}^{(\nu)}_{(k,\mathcal{C}),(b)}, \quad \dots, \quad - \sum_{(k,\mathcal{C}) \in I_{\Pi,\mathfrak{D},\neg\mathrm{Dir}}} \mathfrak{h}^{(\nu)}_{(k,\mathcal{C}),(n)},$$

which is accomplished in the subsequent Secs 3.7.3 – 3.7.11 succeeding the definitions of the respective operators. The result is then summarized in Lem. 3.7.45.

3.7.2 Terms Involving the Time Step

(3.5.24a) is discretized by replacing the integrand by its value at x_k, i.e. (3.5.24a) is replaced by

$$\mathfrak{h}^{(\nu)}_{(k,\mathcal{C}),(a)}\left[(U^{(\nu-1)},U^{(\nu)})\right] := (t_\nu - t_{\nu-1})^{-1}\left(\mathfrak{b}^{(\nu)}_{(k,\mathcal{C})}[U^{(\nu)}_{(k,\mathcal{C})}] - \mathfrak{b}^{(\nu-1)}_{(k,\mathcal{C})}[U^{(\nu-1)}_{(k,\mathcal{C})}]\right), \qquad (3.7.9)$$

where the $\mathfrak{b}^{(\nu)}_{(k,\mathcal{C})} : v \longrightarrow \mathbb{K}$ are defined by:

$$\bigwedge_{\substack{\nu\in\{0,\dots,n\},\\ (k,\mathcal{C})\in I_{\Pi,\mathfrak{D},\neg\mathrm{Dir}}}} \mathfrak{b}^{(\nu)}_{(k,\mathcal{C})}[y] := \sum_{j\in V[\mathcal{C}]} b^{(\nu)}_j[(y,x_k)]\cdot\lambda_d[\omega^{(j)}_k]. \qquad (3.7.10)$$

3.7.3 Terms Involving Interior Diffusion Flux

(3.5.24e) is to be discretized.

First, the domain of integration $\partial\omega^{(j)}_k \cap \mathrm{int}[p_j]$ is partitioned further: For that purpose define

$$E_{\mathrm{IF}}[\Pi] := \big\{\{k,l\} \subseteq I_\Pi : \partial_{\mathrm{reg}}\omega_k \cap \partial_{\mathrm{reg}}\omega_l \neq \emptyset,\ k\neq l\big\}, \qquad (3.7.11)$$

where it is noted that (3.7.11) is analogous to (3.4.4). A control volume ω_l, $l \in I^{(j)}$ (cf. (3.5.15)), is called a *j-neighbor* of ω_k iff $\{k,l\} \in E_{\mathrm{IF}}[\Pi]$. The set of corresponding indices is defined by

$$\bigwedge_{k\in I_\Pi} \mathrm{nb}_j[k] := \big\{l \in I^{(j)} : \{k,l\} \in E_{\mathrm{IF}}[\Pi]\big\}. \qquad (3.7.12)$$

Remark 3.7.1. The family $(\partial\omega^{(j)}_k \cap \partial\omega^{(j)}_l)_{l\in\mathrm{nb}_j[k]}$ forms a partition of $\partial\omega^{(j)}_k \cap \mathrm{int}[p_j]$ with respect to the relative topology (see Fig. 3.18).

—

In the following, one frequently needs to determine the index in $I_{\Pi,\mathfrak{D}}$ that corresponds to $(l,j) \in I_\Pi \times J$. To that end, define

$$\bigwedge_{(l,j)\in I_\Pi\times J} \mathcal{C}[(l,j)] := \mathrm{CoCmp}_{\mathcal{G}_{\omega_l}}[j]. \qquad (3.7.13)$$

Now for $l \in \mathrm{nb}_j[k]$, there is a difference depending on $\big(l,\mathcal{C}[(l,j)]\big)$ being an element of $I_{\Pi,\mathfrak{D},\mathrm{Dir}}$ or not. Define

$$\bigwedge_{k\in I_\Pi} \begin{pmatrix} \mathrm{nb}_{j,\mathrm{Dir}}[k] := \big\{l \in \mathrm{nb}_j[k] : \big(l,\mathcal{C}[(l,j)]\big) \in I_{\Pi,\mathfrak{D},\mathrm{Dir}}\big\}, \\ \mathrm{nb}_{j,\neg\mathrm{Dir}}[k] := \mathrm{nb}_j[k] \setminus \mathrm{nb}_{j,\mathrm{Dir}}[k] \end{pmatrix}. \qquad (3.7.14)$$

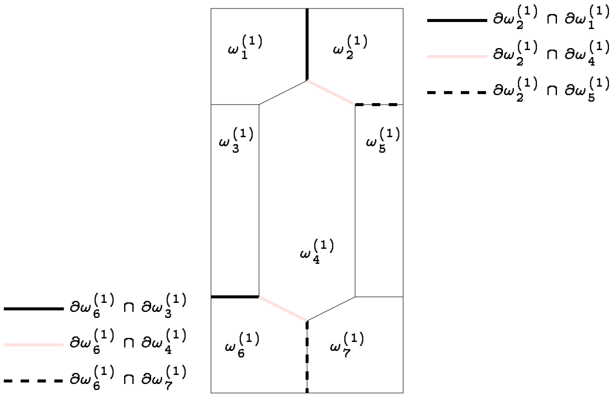


Figure 3.18: Enlargement of p_1 of Figs 3.5 and 3.6 on p. 75, illustrating the partition of $\partial\omega_2^{(1)} \cap \operatorname{int}[p_1]$ into $\partial\omega_2^{(1)} \cap \partial\omega_1^{(1)}$, $\partial\omega_2^{(1)} \cap \partial\omega_4^{(1)}$, and $\partial\omega_2^{(1)} \cap \partial\omega_5^{(1)}$; and of $\partial\omega_6^{(1)} \cap \operatorname{int}[p_1]$ into $\partial\omega_6^{(1)} \cap \partial\omega_3^{(1)}$, $\partial\omega_6^{(1)} \cap \partial\omega_4^{(1)}$, and $\partial\omega_6^{(1)} \cap \partial\omega_7^{(1)}$. One has $\mathrm{nb}_1[2] = \{1,4,5\}$ and $\mathrm{nb}_1[6] = \{3,4,7\}$.

Example 3.7.2. (a) In Fig. 3.17(a) (where the index $j = 1$ has been discarded), it is $\mathrm{nb}_{1,\mathrm{Dir}}[2] = \mathrm{nb}_{1,\mathrm{Dir}}[4] = \mathrm{nb}_{1,\mathrm{Dir}}[7] = \{5\}$, and $\mathrm{nb}_{1,\mathrm{Dir}}[k] = \emptyset$ for $k \in \{1,3,5,6\}$.

(b) If the interface $\gamma = \partial_{\mathrm{reg}}p_1 \cap \partial_{\mathrm{reg}}p_2$ in Fig. 3.19 is a jump interface, then $\mathrm{nb}_{1,\mathrm{Dir}}[3] = \{1\}$, and $\mathrm{nb}_{2,\mathrm{Dir}}[3] = \emptyset$.

(c) If the interface $\gamma = \partial_{\mathrm{reg}}p_1 \cap \partial_{\mathrm{reg}}p_2$ in Fig. 3.19 is a continuous interface, then $\mathrm{nb}_{1,\mathrm{Dir}}[3] = \{1\}$, and $\mathrm{nb}_{2,\mathrm{Dir}}[3] = \{1\}$ (even though $x_1 \notin \Gamma_{2,\mathrm{Dir}}$ which might not even exist).

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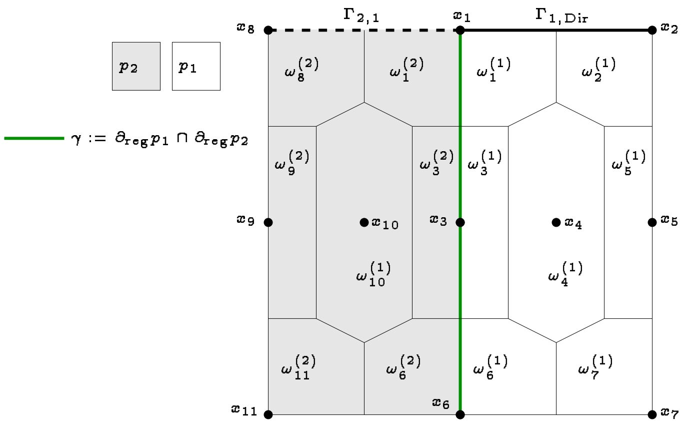


Figure 3.19: Illustration of (3.7.14), cf. Ex. 3.7.2 (b),(c)

If $l \in \mathrm{nb}_{j,\mathrm{Dir}}[k]$, then $u^{(\nu)}_{(l,\mathcal{C}[(l,j)])}$ is known a priori from

$$u^{(\nu)}_{(l,\mathcal{C}[(l,j)])} = u_{j_{\mathrm{Dir}},\mathrm{Dir}}[(t_\nu, x_l)],$$

where j_{Dir} is an element of $V\big[\mathcal{C}[(l,j)]\big]$ such that $0 \in J_{j_{\mathrm{Dir}}}$. Example 3.7.2(c) shows that one can not expect $j = j_{\mathrm{Dir}}$ in general. To avoid the ambiguity in the choice of j_{Dir}, the following Not. 3.7.3 is introduced.

Notation 3.7.3. For each (l,j) such that $(l,\mathcal{C}[(l,j)]) \in I_{\Pi,\mathfrak{D},\mathrm{Dir}}$, let $j_{\mathrm{Dir}}[(l,j)]$ be an element of $V\big[\mathcal{C}[(l,j)]\big]$ such that $0 \in J_{j_{\mathrm{Dir}}}$. The element $j_{\mathrm{Dir}}[(l,j)]$ is kept fixed for the remainder of Ch. 3.

If $l \in \mathrm{nb}_{j,\neg\mathrm{Dir}}[k]$, then $u^{(\nu)}_{(l,\mathcal{C}[(l,j)])}$ has to be determined using the discretization of (3.5.24).

To proceed with the discretization of (3.5.24e), it is recalled that according to (3.4.18):

$$F^{(\nu)}_{j,\partial\omega^{(j)}_k}[x] = \mathrm{tr}_{\partial\omega^{(j)}_k}\left(k^{(\nu)}_j\big[(u^{(\nu)}_j[x], x)\big]\,\nabla\, u^{(\nu)}_j[x]\right).$$

As mentioned in Sec. 3.7.1, for $\{k,l\} \in E_{\mathrm{IF}}[\Pi]$, it is assumed that the line segment joining x_k and x_l is perpendicular to $\partial_{\mathrm{reg}}\omega_k \cap \partial_{\mathrm{reg}}\omega_l$, i.e. (dispt-(i)) holds. The normal vector in (3.5.24e) is replaced using (dispt-(i)). The gradient of $u^{(\nu)}_j$ on $\partial_{\mathrm{reg}}\omega_k \cap \partial_{\mathrm{reg}}\omega_l$ in the normal direction is approximated by the difference quotient $\frac{u^{(\nu)}_{(l,j)} - u^{(\nu)}_{(k,j)}}{x_l - x_k}$, and the value of $k^{(\nu)}_j$ on $\partial_{\mathrm{reg}}\omega_k \cap \partial_{\mathrm{reg}}\omega_l$ is approximated by the arithmetic mean of $k^{(\nu)}_j$ evaluated at x_k and x_l, respectively.

At this point, all the preparations are in place to write the discretization of (3.5.24e), where (3.5.24e) is replaced by

$$\mathfrak{h}^{(\nu)}_{(k,\mathcal{C}),(e)}[U^{(\nu)}] := -\mathfrak{k}^{(\nu)}_{\neg\mathrm{Dir},(k,\mathcal{C})}[U^{(\nu)}] - \mathfrak{k}^{(\nu)}_{\mathrm{Dir},(k,\mathcal{C})}[U^{(\nu)}_{(k,\mathcal{C})}], \tag{3.7.15}$$

where the $\mathfrak{k}^{(\nu)}_{\neg\mathrm{Dir},(k,\mathcal{C})} : \upsilon^{I_{\Pi,\mathfrak{D},\neg\mathrm{Dir}}} \longrightarrow \mathbb{K}$ are defined by

$$\bigwedge_{\substack{\nu\in\{0,\dots,n\},\\ (k,\mathcal{C})\in I_{\Pi,\mathfrak{D},\neg\mathrm{Dir}}}} \left(\begin{aligned} &\mathfrak{k}^{(\nu)}_{\neg\mathrm{Dir},(k,\mathcal{C})}[U] \\ &:= \sum_{\substack{j\in V[\mathcal{C}],\\ l\in\mathrm{nb}_{j,\neg\mathrm{Dir}}[k]}} \frac{k^{(\nu)}_j[(U_{(k,\mathcal{C})}, x_k)] + k^{(\nu)}_j\left[\left(U_{(l,\mathcal{C}[(l,j)])}, x_l\right)\right]}{2} \\ &\qquad\qquad \cdot \frac{U_{(l,\mathcal{C}[(l,j)])} - U_{(k,\mathcal{C})}}{\|x_k - x_l\|_2} \cdot \lambda_{d-1}\big[\omega^{(j)}_k \cap \omega^{(j)}_l\big] \end{aligned} \right), \tag{3.7.16}$$

and the $\mathfrak{k}^{(\nu)}_{\mathrm{Dir},(k,\mathcal{C})} : v \longrightarrow \mathbb{K}$ are defined by

$$\bigwedge_{\substack{\nu\in\{0,\dots,n\},\\ (k,\mathcal{C})\in I_{\Pi,\mathfrak{D},\neg\mathrm{Dir}}}} \left(\begin{array}{l} \mathfrak{k}^{(\nu)}_{\mathrm{Dir},(k,\mathcal{C})}[y] \\ \displaystyle := \sum_{\substack{j\in V[\mathcal{C}],\\ l\in \mathrm{nb}_{j,\mathrm{Dir}}[k]}} \frac{k^{(\nu)}_j\big[(y,x_k)\big] + k^{(\nu)}_j\big[\big(u_{j_{\mathrm{Dir}}[(l,j)],\mathrm{Dir}}[(t_\nu,x_l)],x_l\big)\big]}{2} \\ \displaystyle \qquad\qquad \cdot \frac{u_{j_{\mathrm{Dir}}[(l,j)],\mathrm{Dir}}[(t_\nu,x_l)] - y}{\|x_k - x_l\|_2} \cdot \lambda_{d-1}\big[\omega^{(j)}_k \cap \omega^{(j)}_l\big] \end{array} \right). \tag{3.7.17}$$

The estimates provided in the following Lems 3.7.4 and 3.7.6 are steps towards proving an upper bound for the $\mathfrak{s}^{(\nu)}$ according to the remarks at the end of Sec. 3.7.1.

Lemma 3.7.4. *The following holds:*

$$\bigwedge_{\nu\in\{0,\dots,n\}} \sum_{(k,\mathcal{C})\in I_{\Pi,\mathfrak{D},\neg\mathrm{Dir}}} \mathfrak{k}^{(\nu)}_{\neg\mathrm{Dir},(k,\mathcal{C})} = 0. \tag{3.7.18}$$

—

The main ingredient to the proof of Lem. 3.7.4 is the following Lem. 3.7.5 that constitutes a purely combinatorial result to the effect that a certain sum vanishes if the summands satisfy the symmetry condition (3.7.21). Lemma 3.7.5 is also used in the proof of Lem. 3.7.16 below.

Lemma 3.7.5. *Consider a function*

$$F:\ I_{\Pi,\mathfrak{D},\mathrm{nb},\neg\mathrm{Dir}} \longrightarrow \mathbb{K}, \tag{3.7.19}$$

$$I_{\Pi,\mathfrak{D},\mathrm{nb},\neg\mathrm{Dir}} := \Big\{ \big(j,(k,\mathcal{C}),(l,\tilde{\mathcal{C}})\big) \in J \times I_{\Pi,\mathfrak{D},\neg\mathrm{Dir}} \times I_{\Pi,\mathfrak{D},\neg\mathrm{Dir}} :\ \{k,l\} \in E_{\mathrm{IF}}[\Pi],\ j \in V[\mathcal{C}] \cap V[\tilde{\mathcal{C}}] \Big\}, \tag{3.7.20}$$

satisfying the symmetry condition

$$\bigwedge_{\big(j,(k,\mathcal{C}),(l,\tilde{\mathcal{C}})\big)\in I_{\Pi,\mathfrak{D},\mathrm{nb},\neg\mathrm{Dir}}} F\Big[\big(j,(k,\mathcal{C}),(l,\tilde{\mathcal{C}})\big)\Big] = -F\Big[\big(j,(l,\tilde{\mathcal{C}}),(k,\mathcal{C})\big)\Big]. \tag{3.7.21}$$

Then

$$\sum_{\substack{(k,\mathcal{C})\in I_{\Pi,\mathfrak{D},\neg\mathrm{Dir}},\\ j\in V[\mathcal{C}],\\ l\in \mathrm{nb}_{j,\neg\mathrm{Dir}}[k]}} F\Big[\Big(j,\big(k,\mathcal{C}\big),\big(l,\mathcal{C}[(l,j)]\big)\Big)\Big] = 0. \tag{3.7.22}$$

Proof. It is shown how the order of summation on the left-hand side of (3.7.22) can be changed such that (3.7.21) can be applied. The index set for the sum in (3.7.22) is given by

$$A := \Big\{ \big((k,\mathcal{C}),j,l\big) \in I_{\Pi,\mathfrak{D},\neg\mathrm{Dir}} \times J \times I_\Pi :\ j \in V[\mathcal{C}],\ l \in \mathrm{nb}_{j,\neg\mathrm{Dir}}[k] \Big\}. \tag{3.7.23}$$

Instead, one can use the index set

$$B := \Big\{(k,j,l) \in I_\Pi \times J \times I_\Pi : \Big(j, \big(k, \mathcal{C}[(k,j)]\big), \big(l, \mathcal{C}[(l,j)]\big)\Big) \in I_{\Pi,\mathfrak{D},\mathrm{nb},\neg\mathrm{Dir}}\Big\}, \quad (3.7.24)$$

as the following map $\mathcal{I}$ establishes a bijection between A and B:

$$\begin{aligned} \mathcal{I} : A \longrightarrow B, \qquad & \mathcal{I}\big[((k,\mathcal{C}),j,l)\big] := (k,j,l),\\ \mathcal{I}^{-1} : B \longrightarrow A, \qquad & \mathcal{I}^{-1}\big[(k,j,l)\big] = \big(\big(k,\mathcal{C}[(k,j)]\big),j,l\big). \end{aligned}$$

Since $(k,j,l) \in B$ if and only if $(l,j,k) \in B$, condition (3.7.21) finishes the proof. ■

Proof of Lem. 3.7.4. Fix $\nu \in \{0,\dots,n\}$. To apply Lem. 3.7.5, define

$$\begin{aligned} F : I_{\Pi,\mathfrak{D},\mathrm{nb},\neg\mathrm{Dir}} &\longrightarrow \mathbb{K},\\ F\Big[\big(j,(k,\mathcal{C}),(l,\tilde{\mathcal{C}})\big)\Big] &:= \frac{k_j^{(\nu)}\big[(U_{(k,\mathcal{C})},x_k)\big] + k_j^{(\nu)}\big[(U_{(l,\tilde{\mathcal{C}})},x_l)\big]}{2}\\ &\quad \cdot \frac{U_{(l,\tilde{\mathcal{C}})} - U_{(k,\mathcal{C})}}{\|x_k - x_l\|_2} \cdot \lambda_{d-1}\big[\omega_k^{(j)} \cap \omega_l^{(j)}\big]. \end{aligned} \quad (3.7.25)$$

Then (3.7.21) is satisfied, and (3.7.22) together with (3.7.16) yields (3.7.18). ■

Lemma 3.7.6. *Assume that the range of the unknowns u_j is a real interval of the form $v = [m_v, \infty[$. Moreover, assume that k_j and $u_{j,\mathrm{Dir}}$ are real-valued and k_j is nonnegative for each $j \in J$. Then*

$$\bigwedge_{\nu\in\{0,\dots,n\}} \left(\begin{aligned} &-\sum_{(k,\mathcal{C})\in I_{\Pi,\mathfrak{D},\neg\mathrm{Dir}}} \mathfrak{h}^{(\nu)}_{(k,\mathcal{C}),(e)} = \sum_{(k,\mathcal{C})\in I_{\Pi,\mathfrak{D},\neg\mathrm{Dir}}} \mathfrak{k}^{(\nu)}_{\mathrm{Dir},(k,\mathcal{C})}\\ &\le B_{k,\mathrm{Dir}}[\mathfrak{C}] \cdot \big(B_{\mathrm{Dir}}[\mathfrak{C}] - m_v\big) \cdot d_{\mathrm{Dir}}[\Pi] \end{aligned} \right), \quad (3.7.26)$$

where

$$B_{\mathrm{Dir}}[\mathfrak{C}] := \max\big\{\|u_{j,\mathrm{Dir}}\|_{\max} : j \in J,\ 0 \in J_j\big\}, \quad (3.7.27)$$

$$B_{k,\mathrm{Dir}}[\mathfrak{C}] := \max\big\{k_j[(y,t,x)] : y \in [m_v, B_{\mathrm{Dir}}[\mathfrak{C}]],\ t \in \tau,\ x \in p_j,\ j \in J\big\}, \quad (3.7.28)$$

$$d_{\mathrm{Dir}}[\Pi] := \sum_{\substack{(k,\mathcal{C})\in I_{\Pi,\mathfrak{D},\mathrm{Dir}},\ j\in V[\mathcal{C}],\\ l\in \mathrm{nb}_{j,\neg\mathrm{Dir}}[k]}} \frac{\lambda_{d-1}\big[\omega_k^{(j)} \cap \omega_l^{(j)}\big]}{\|x_k - x_l\|_2}. \quad (3.7.29)$$

Proof. The equality in (3.7.26) is (3.7.15) combined with Lem. 3.7.4. To verify the estimate, it is noted that by the nonnegativity of the k_j, $\mathfrak{k}^{(\nu)}_{\mathrm{Dir},(k,\mathcal{C})}[y] \le 0$ whenever $u_{j_{\mathrm{Dir}}[(l,j)],\mathrm{Dir}}[(t_\nu,x_l)] - y \le 0$. Moreover,

$$\sup\big\{k_j^{(\nu)}[(y,x_k)] : u_{j_{\mathrm{Dir}}[(l,j)],\mathrm{Dir}}[(t_\nu,x_l)] - y > 0,$$

$$(k,\mathcal{C}) \in I_{\Pi,\mathfrak{D},\neg\mathrm{Dir}},\ j \in V[\mathcal{C}],\ l \in \mathrm{nb}_{j,\mathrm{Dir}}[k]\big\}$$
$$\leq \max\big\{k_j^{(\nu)}[(y,x)] : m_v \leq y \leq B_{\mathrm{Dir}}[\mathfrak{C}],\ x \in p_j,\ j \in J\big\} \leq B_{k,\mathrm{Dir}}[\mathfrak{C}],$$

which, together with $k_j^{(\nu)}\big[\big(u_{j_{\mathrm{Dir}}[(l,j)],\mathrm{Dir}}[(t_\nu, x_l)], x_l\big)\big] \leq B_{k,\mathrm{Dir}}[\mathfrak{C}]$, establishes the case. Using a correspondence similar to the one established in the proof of Lem. 3.7.5, the sum in (3.7.29) is written in terms of $I_{\Pi,\mathfrak{D},\mathrm{Dir}}$, whereas the sums in (3.7.26) are witten in terms of $I_{\Pi,\mathfrak{D},\neg\mathrm{Dir}}$. ■

Remark 3.7.7. The number $d_{\mathrm{Dir}}[\Pi]$ measures the size of the surface consisting of the collection of all interfaces between control volumes at Dirichlet vertices and control volumes at non-Dirichlet vertices in relation to its distance from the outer boundary. Unfortunately, the following Ex. 3.7.8 shows that $d_{\mathrm{Dir}}[\Pi]$ can not be expected to stay bounded as Π becomes finer. Thus, to prove convergence in the presence of Dirichlet boundaries, the estimate (3.7.26) needs to be improved, e.g. by first establishing a bound for the discrete gradients $\frac{u_j^{(\nu)}[x_l]-u_j^{(\nu)}[x_k]}{x_l-x_k}$.

Example 3.7.8. For the polytope discretizations depicted in Fig. 3.20, one has $\lambda_1[\omega_k \cap \omega_l] = a$ for a control volume ω_k adjacent to Γ_{Dir} and a control volume ω_l directly underneath ω_k, except at the right side and at the left side, where $\lambda_1[\omega_k \cap \omega_l] = \frac{a}{2}$. Moreover, $\|x_k - x_l\|_2 = h$ for the corresponding discretization points. Thus $d_{\mathrm{Dir}} = \frac{d}{h}$, which tends to infinity if h tends to zero.

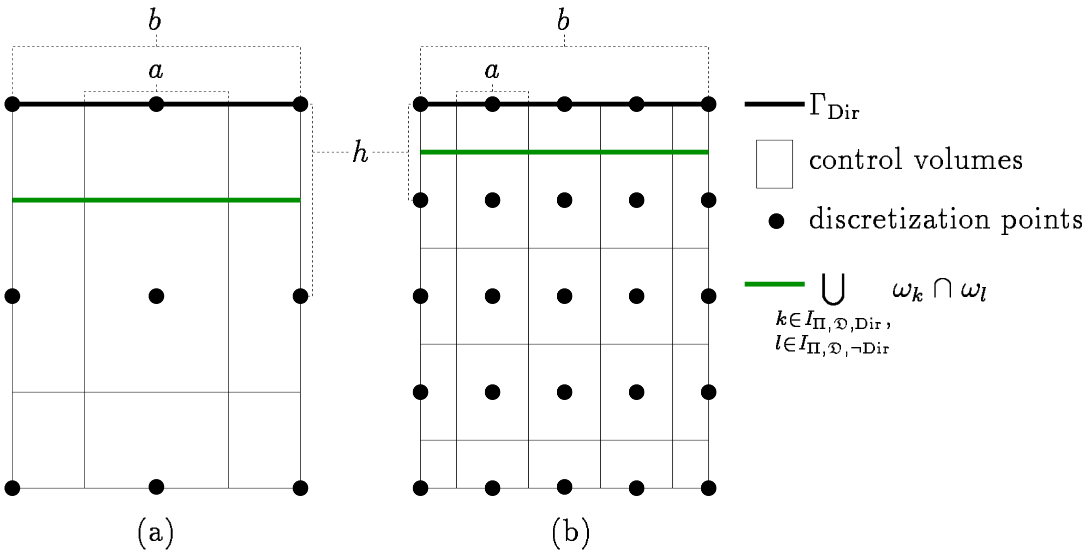


Figure 3.20: Polytope discretizations illustrating the definition of d_{Dir} according to (3.7.29). For the depicted discretizations, one has $d_{\mathrm{Dir}} = \frac{b}{h}$ (s. Ex. 3.7.8).

Example 3.7.9. In Ex. 3.1.1(b) and in the first case of 3.1.1(a), the hypotheses of Lem. 3.7.6 are satisfied, as the unknown is either mass density or absolute temperature, i.e. $\upsilon = [0, \infty[$, and the k_j are nonnegative, since they either vanish or they represent thermal conductivity.

3.7.4 Terms Involving Interior Convection Flux; Upwind

(3.5.24b) is to be discretized. The discretization is similar to the discretization of (3.5.24e) in Sec. 3.7.3, but some new complications arise from the $v_j^{(\nu)}$ being vector-valued. For the discretization of (3.5.24e) in Sec. 3.7.3, resulting in (3.7.16) and (3.7.17), it sufficed to approximate $k_j^{(\nu)}$ on $\partial_{\text{reg}}\omega_k \cap \partial_{\text{reg}}\omega_l$ by taking the arithmetic mean of $k_j^{(\nu)}$ evaluated at x_k and x_l. However, to guarantee certain monotonicity properties of the finite volume discretization that are used to prove the existence of a discrete solution in Th. 3.8.35 (cf. Lem. 3.8.12), choosing an appropriate average of the $v_j^{(\nu)}$ evaluated at x_k and x_l is more subtle.

The general idea is to choose the average depending on the directions of the vectors $v_j^{(\nu)}\big[(u_j^{(\nu)}[x_k], x_k)\big]$ and $v_j^{(\nu)}\big[(u_j^{(\nu)}[x_l], x_l)\big]$. Unfortunately, due to the dependence on the solution, the directions are a priori unknown. To circumvent this problem, the simplifying assumption is made that the solution dependence of the v_j can be decoupled from their vector-valuedness in the sense that v_j can be decomposed into two factors, one factor being scalar, but allowed to depend on the solution, the other factor being vector-valued, but independent of the solution. In other words, the v_j are assumed to have a scalar-vector-splitting in the sense of the following Def. 3.7.10:

Definition 3.7.10. Let $A \subseteq \mathbb{R}^d$. A pair $(v_{\text{sca}}, v_{\text{vec}})$ is called a *scalar-vector-splitting* of a function $v \in C(\upsilon \times \tau \times A, \mathbb{R}^d)$ iff $v_{\text{sca}} \in C(\upsilon \times \tau \times A, \mathbb{R})$, $v_{\text{vec}} \in C(\tau \times A, \mathbb{R}^d)$, and

$$\bigwedge_{(y,t,x)\in \upsilon\times\tau\times A} v[(y,t,x)] = v_{\text{sca}}[(y,t,x)] \cdot v_{\text{vec}}[(t,x)]. \tag{3.7.30}$$

—

Example 3.7.11 shows that scalar-vector-splittings exist for all the cases considered in Ex. 3.1.1.

Example 3.7.11. Scalar-vector-splittings of nonzero functions v_j occurring in Ex. 3.1.1 are considered. The potential time dependence present in Ex. 3.1.1 is disregarded in the present example to simplify notation. It poses no difficulty if time dependence is indeed present. In each of the following examples, the functions v_{sca} and v_{vec} are chosen such that they constitute a scalar-vector-splitting of the function under consideration.

In the first case of Ex. 3.1.1(a), $v_j[(y,x)] = y\mathbf{v}_{\text{gas}}[x]$. One can set $v_{\text{sca}}[(y,x)] := y$, $v_{\text{vec}}[x] := \mathbf{v}_{\text{gas}}[x]$. In the second case of Ex. 3.1.1(a), $v_j[(y,x)] = \frac{R}{M^{(\text{Ar})}}\rho_{\text{gas}}[x]T_{\text{gas}}[x]\mathbf{e}_i$. One can set $v_{\text{sca}}[(y,x)] := 1$, $v_{\text{vec}}[x] := \frac{R}{M^{(\text{Ar})}}\rho_{\text{gas}}[x]T_{\text{gas}}[x]\mathbf{e}_i$. One can also set $v_{\text{sca}}[(y,x)] := \frac{R}{M^{(\text{Ar})}}\rho_{\text{gas}}[x]T_{\text{gas}}[x]$, $v_{\text{vec}}[x] := \mathbf{e}_i$. It is seen that scalar-vector-splittings are not unique.

In the first case of Ex. 3.1.1(b), $v_j[(y,x)] = \frac{(z^{(\mathrm{Ar})}+1)R}{M^{(\mathrm{Ar})}} \rho_{\mathrm{gas}}[x] y \mathbf{v}_{\mathrm{gas}}[x]$. One can set $v_{\mathrm{sca}}[(y,x)] := \frac{(z^{(\mathrm{Ar})}+1)R}{M^{(\mathrm{Ar})}} \rho_{\mathrm{gas}}[x] y$, $v_{\mathrm{vec}}[x] := \mathbf{v}_{\mathrm{gas}}[x]$. In the second case of Ex. 3.1.1(b), $v_j = 0$. In the third case, $v_j[(y,x)] = \varepsilon_{\mathrm{gas}}[(y,x)]\, \rho_{\mathrm{gas}}[x] \mathbf{v}_{\mathrm{gas}}[x]$. One can set $v_{\mathrm{sca}}[(y,x)] := \varepsilon_{\mathrm{gas}}[(y,x)]\, \rho_{\mathrm{gas}}[x]$, $v_{\mathrm{vec}}[x] := \mathbf{v}_{\mathrm{gas}}[x]$.

In Ex. 3.1.1(e), $v_j[(y,x)] = K[(y,x)]\mathbf{g}[x]$. One can set $v_{\mathrm{sca}}[(y,x)] := K[(y,x)]$, $v_{\mathrm{vec}}[x] := \mathbf{g}[x]$.

Definition 3.7.12. A family

$$\mathfrak{V} = \big((v_{j,\mathrm{sca}}, v_{j,\mathrm{vec}})\big)_{j \in J} \tag{3.7.31}$$

is called a *family of scalar-vector-splittings* for the evolution equation complex $\mathfrak{C}$ iff $(v_{j,\mathrm{sca}}, v_{j,\mathrm{vec}})$ is a solution-vector-splitting of v_j for each $j \in J$.

The *time discretization* of $\mathfrak{V}$ is defined as the family

$$\left((v^{(\nu)}_{j,\mathrm{sca}}, v^{(\nu)}_{j,\mathrm{vec}})\right)_{(j,\nu) \in J \times \{0,\dots,n\}}, \tag{3.7.32}$$

where for each $(j,\nu) \in J \times \{0,\dots,n\}$:

$$v^{(\nu)}_{j,\mathrm{sca}} \in C(\upsilon \times p_j, \mathbb{R}), \qquad v^{(\nu)}_{j,\mathrm{sca}}[(y,x)] := v_{j,\mathrm{sca}}[(y,t_\nu,x)], \tag{3.7.33a}$$

$$v^{(\nu)}_{j,\mathrm{vec}} \in C(p_j, \mathbb{R}^d), \qquad v^{(\nu)}_{j,\mathrm{vec}}[x] := v_{j,\mathrm{vec}}[(t_\nu,x)]. \tag{3.7.33b}$$

For each $\nu \in \{0,\dots,n\}$, the pair $(v^{(\nu)}_{j,\mathrm{sca}}, v^{(\nu)}_{j,\mathrm{vec}})$ is called a *scalar-vector-splitting* of $v^{(\nu)}_j$ (cf. Rem. 3.7.13 below). The context should always make clear, if a scalar-vector-splitting belongs to a time-dependent or to a time-discrete function.

Remark 3.7.13. If $\mathfrak{V}$ as given by (3.7.31) is a family of scalar-vector-splittings for $\mathfrak{C}$ with time discretization (3.7.32), then

$$\bigwedge_{(j,\nu) \in J \times \{0,\dots,n\}} \quad \bigwedge_{(y,x) \in \upsilon \times p_j} \quad v^{(\nu)}_j[(y,x)] = v^{(\nu)}_{j,\mathrm{sca}}[(y,x)] \cdot v^{(\nu)}_{j,\mathrm{vec}}[x]. \tag{3.7.34}$$

—

For the remainder of Ch. 3, fix a family of scalar-vector-splittings $\mathfrak{V}$ for $\mathfrak{C}$ according to (3.7.31).

A direction-dependent average of $v^{(\nu)}_j\big[(u^{(\nu)}_j[x_k], x_k)\big]$ and $v^{(\nu)}_j\big[(u^{(\nu)}_j[x_l], x_l)\big]$ can now be selected by taking the arithmetic mean of $v^{(\nu)}_{j,\mathrm{vec}}[x_k]$ and $v^{(\nu)}_{j,\mathrm{vec}}[x_l]$ multiplied by a convex combination $w^{(\nu)}_j[(k,l)] v^{(\nu)}_{j,\mathrm{sca}}[x_l] + \left(1 - w^{(\nu)}_j[(k,l)]\right) v^{(\nu)}_{j,\mathrm{sca}}[x_k]$, where $w^{(\nu)}_j$ is the so-called *upwind function* for $\Pi^{(j)}$ and $v^{(\nu)}_{j,\mathrm{vec}}$, the value of $w^{(\nu)}_j$ depending on the direction of $v^{(\nu)}_{j,\mathrm{vec}}[x_k] + v^{(\nu)}_{j,\mathrm{vec}}[x_l]$ according to the following Def. 3.7.14.

One finds different kinds of upwind functions in the literature. If the upwind function is defined as in Def. 3.7.14, then one usually speaks of *full* upwinding. Since special properties of full upwinding are used to prove the existence of a discrete solution in Th. 3.8.35, no other upwind functions are considered here.

Definition 3.7.14. Define the ordered analogues of the set $E_{\mathrm{IF}}[\Pi]$ for the $\Pi^{(j)}$, $j \in J$, (cf. (3.7.11)):

$$E_{\mathrm{IF,pairs}}[\Pi^{(j)}] := \big\{(k,l) \in (I^{(j)})^2 : \{k,l\} \in E_{\mathrm{IF}}[\Pi]\big\}. \tag{3.7.35}$$

Moreover, given a function $v \in C(p_j, \mathbb{R}^d)$, define auxiliary quantities

$$\bigwedge_{(k,l)\in E_{\mathrm{IF,pairs}}[\Pi^{(j)}]} \bar{v}_{(k,l)} := (v[x_l] + v[x_k]) \bullet n_{\omega_k}\restriction_{\partial_{\mathrm{reg}}\omega_k \cap \partial_{\mathrm{reg}}\omega_l}. \tag{3.7.36}$$

The *upwind function* w for $\Pi^{(j)}$ and v is defined by

$$w : E_{\mathrm{IF,pairs}}[\Pi^{(j)}] \longrightarrow [0,1], \quad w[(k,l)] := \begin{cases} 0 & \text{for} \quad \bar{v}_{(k,l)} > 0, \\ \frac{1}{2} & \text{for} \quad \bar{v}_{(k,l)} = 0, \\ 1 & \text{for} \quad \bar{v}_{(k,l)} < 0. \end{cases} \tag{3.7.37}$$

—

Using the value $\frac{1}{2}$ for the upwind function in the case where $\bar{v}_{(k,l)} = 0$ is not essential, since the corresponding term in the discretization of (3.5.24b) vanishes anyway (s. (3.7.40) and (3.7.41)). Using $\frac{1}{2}$ has the advantage that some assertions about w can be stated more concisely, as e.g. in the following Rem. 3.7.15.

Remark 3.7.15. For each $v \in C(p_j, \mathbb{R}^d)$, the upwind function w for $\Pi^{(j)}$ and v satisfies the symmetry condition

$$\bigwedge_{(k,l)\in E_{\mathrm{IF,pairs}}[\Pi^{(j)}]} w[(k,l)] = 1 - w[(l,k)], \tag{3.7.38}$$

which is immediate from $n_{\omega_k}\restriction_{\partial_{\mathrm{reg}}\omega_k \cap \partial_{\mathrm{reg}}\omega_l} = -n_{\omega_l}\restriction_{\partial_{\mathrm{reg}}\omega_k \cap \partial_{\mathrm{reg}}\omega_l}$, (3.7.36), and (3.7.37).

—

For the rest of Ch. 3, $w_j^{(\nu)}$ denotes the upwind function for $\Pi^{(j)}$ and $v_{j,\mathrm{vec}}^{(\nu)}$, $j \in J$, $\nu \in \{0, \dots, n\}$.

Finally, the discretization of (3.5.24b) can be carried out, replacing (3.5.24b) by

$$\mathfrak{h}^{(\nu)}_{(k,\mathcal{C}),(b)}[U^{(\nu)}] := \mathfrak{v}^{(\nu)}_{\mathrm{int},\neg\mathrm{Dir},(k,\mathcal{C})}[U^{(\nu)}] + \mathfrak{v}^{(\nu)}_{\mathrm{int,Dir},(k,\mathcal{C})}[U^{(\nu)}_{(k,\mathcal{C})}], \tag{3.7.39}$$

where the $\mathfrak{v}^{(\nu)}_{\mathrm{int},\neg\mathrm{Dir},(k,\mathcal{C})} : v^{I_{\Pi,\mathfrak{D},\neg\mathrm{Dir}}} \longrightarrow \mathbb{R}$ are defined by

$$\bigwedge_{\substack{\nu\in\{0,\dots,n\},\\ (k,\mathcal{C})\in I_{\Pi,\mathfrak{D},\neg\mathrm{Dir}}}} \left(\begin{aligned} &\mathfrak{v}^{(\nu)}_{\mathrm{int},\neg\mathrm{Dir},(k,\mathcal{C})}[U] \\ &:= \sum_{\substack{j\in V[\mathcal{C}],\\ l\in \mathrm{nb}_{j,\neg\mathrm{Dir}}[k]}} \Bigg(w^{(\nu)}_j[(k,l)]\cdot v^{(\nu)}_{j,\mathrm{sca}}\left[\left(U_{(l,\mathcal{C}[(l,j)])}, x_l\right)\right] \\ &\qquad\qquad + \left(1-w^{(\nu)}_j[(k,l)]\right)\cdot v^{(\nu)}_{j,\mathrm{sca}}[(U_{(k,\mathcal{C})}, x_k)]\Bigg) \\ &\qquad\qquad \cdot \frac{\left(v^{(\nu)}_{j,\mathrm{vec}}[x_l] + v^{(\nu)}_{j,\mathrm{vec}}[x_k]\right)\bullet(x_l-x_k)}{2\|x_k-x_l\|_2} \\ &\qquad\qquad \cdot \lambda_{d-1}\left[\omega^{(j)}_k\cap\omega^{(j)}_l\right] \end{aligned} \right), \tag{3.7.40}$$

and the $\mathfrak{v}^{(\nu)}_{\mathrm{int},\mathrm{Dir},(k,\mathcal{C})} : v \longrightarrow \mathbb{R}$ are defined by

$$\bigwedge_{\substack{\nu\in\{0,\dots,n\},\\ (k,\mathcal{C})\in I_{\Pi,\mathfrak{D},\neg\mathrm{Dir}}}} \left(\begin{aligned} &\mathfrak{v}^{(\nu)}_{\mathrm{int},\mathrm{Dir},(k,\mathcal{C})}[y] \\ &:= \sum_{\substack{j\in V[\mathcal{C}],\\ l\in \mathrm{nb}_{j,\mathrm{Dir}}[k]}} \Bigg(w^{(\nu)}_j[(k,l)]\cdot v^{(\nu)}_{j,\mathrm{sca}}\left[\left(u_{j_{\mathrm{Dir}}[(l,j)],\mathrm{Dir}}[(t_\nu, x_l)], x_l\right)\right] \\ &\qquad\qquad + \left(1-w^{(\nu)}_j[(k,l)]\right)\cdot v^{(\nu)}_{j,\mathrm{sca}}\left[(y, x_k)\right]\Bigg) \\ &\qquad\qquad \cdot \frac{\left(v^{(\nu)}_{j,\mathrm{vec}}[x_l] + v^{(\nu)}_{j,\mathrm{vec}}[x_k]\right)\bullet(x_l-x_k)}{2\|x_k-x_l\|_2} \\ &\qquad\qquad \cdot \lambda_{d-1}\left[\omega^{(j)}_k\cap\omega^{(j)}_l\right] \end{aligned} \right). \tag{3.7.41}$$

The following Lems 3.7.16 and 3.7.18 are analogous to Lems 3.7.4 and 3.7.6 and are used in proving an upper bound for the $\mathfrak{s}^{(\nu)}$.

Lemma 3.7.16. *The following holds:*

$$\bigwedge_{\nu\in\{0,\dots,n\}} \sum_{(k,\mathcal{C})\in I_{\Pi,\mathfrak{D},\neg\mathrm{Dir}}} \mathfrak{v}^{(\nu)}_{\mathrm{int},\neg\mathrm{Dir},(k,\mathcal{C})} = 0. \tag{3.7.42}$$

Proof. Fix $\nu\in\{0,\dots,n\}$. To apply Lem. 3.7.5, define

$$\begin{aligned} F &: I_{\Pi,\mathfrak{D},\mathrm{nb},\neg\mathrm{Dir}} \longrightarrow \mathbb{R}, \\ F\left[\left(j,(k,\mathcal{C}),(l,\tilde{\mathcal{C}})\right)\right] &:= \Bigg(w^{(\nu)}_j[(k,l)]\cdot v^{(\nu)}_{j,\mathrm{sca}}\left[\left(U_{(l,\tilde{\mathcal{C}})}, x_l\right)\right] \\ &\qquad + \left(1-w^{(\nu)}_j[(k,l)]\right)\cdot v^{(\nu)}_{j,\mathrm{sca}}[(U_{(k,\mathcal{C})}, x_k)]\Bigg) \\ &\quad \cdot \frac{\left(v^{(\nu)}_{j,\mathrm{vec}}[x_l] + v^{(\nu)}_{j,\mathrm{vec}}[x_k]\right)\bullet(x_l-x_k)}{2\|x_k-x_l\|_2}\cdot\lambda_{d-1}\left[\omega^{(j)}_k\cap\omega^{(j)}_l\right]. \end{aligned} \tag{3.7.43}$$

Then (3.7.21) is satisfied using (3.7.38), and (3.7.22) together with (3.7.40) yields (3.7.42). ■

Definition 3.7.17. Let A be a set. A function $F : A \longrightarrow \mathbb{R}$ is called *bounded from above* iff $\sup F := \sup\{F[a] : a \in A\} < \infty$ and *bounded from below* iff $\inf F := \inf\{F[a] : a \in A\} > -\infty$.

Lemma 3.7.18. *If the family of scalar-vector-splittings $\mathfrak{V} = \big((v_{j,\mathrm{sca}}, v_{j,\mathrm{vec}})\big)_{j\in J}$ is such that each $v_{j,\mathrm{sca}}$ is bounded from below, then*

$$\bigwedge_{\nu\in\{0,\dots,n\}} \left(\begin{array}{l} -\displaystyle\sum_{(k,\mathcal{C})\in I_{\Pi,\mathfrak{D},\neg\mathrm{Dir}}} \mathfrak{h}^{(\nu)}_{(k,\mathcal{C}),(b)} = -\sum_{(k,\mathcal{C})\in I_{\Pi,\mathfrak{D},\neg\mathrm{Dir}}} \mathfrak{v}^{(\nu)}_{\mathrm{int},\mathrm{Dir},(k,\mathcal{C})} \\ \le \max\big\{B_{v,\mathrm{Dir}}[(\mathfrak{C},\mathfrak{V})],\ B_{v,\mathrm{sca},\mathrm{Dir}}[(\mathfrak{C},\mathfrak{V})]\big\}\cdot l_{\mathrm{Dir}}[\Pi] \end{array}\right), \tag{3.7.44}$$

where

$$\begin{aligned} B_{v,\mathrm{Dir}}[(\mathfrak{C},\mathfrak{V})] &:= \max\Big\{v_{j,\mathrm{sca}}\big[\big(u_{j,\mathrm{Dir}}[(t,x)],t,x\big)\big]\cdot\big\|v_{\underline{j},\mathrm{vec}}[(t,\underline{x})]\big\|_2 : \\ &\qquad (j,\underline{j},t,x,\underline{x}) \in J\times J\times\tau\times\Gamma_{j,0}\times p_{\underline{j}},\ 0\in J_j\Big\}, \end{aligned} \tag{3.7.45}$$

$$\begin{aligned} B_{v,\mathrm{sca},\mathrm{Dir}}[(\mathfrak{C},\mathfrak{V})] &:= \max\Big\{-v_{j,\mathrm{sca}}\big[(y,t,x)\big]\cdot\big\|v_{j,\mathrm{vec}}[(t,\underline{x})]\big\|_2 : \\ &\qquad (j,y,t,x,\underline{x}) \in J\times\upsilon\times\tau\times p_j\times p_j,\Big\}, \end{aligned} \tag{3.7.46}$$

$$l_{\mathrm{Dir}}[\Pi] := \sum_{\substack{(k,\mathcal{C})\in I_{\Pi,\mathfrak{D},\mathrm{Dir}},\ j\in V[\mathcal{C}],\\ l\in \mathrm{nb}_{j,\neg\mathrm{Dir}}[k]}} \lambda_{d-1}\big[\omega^{(j)}_k\cap\omega^{(j)}_l\big]. \tag{3.7.47}$$

Proof. The equality in (3.7.44) is (3.7.15) combined with Lem. 3.7.16. To verify the estimate, it is recalled that $w^{(\nu)}_j$ is the upwind function for $\Pi^{(j)}$ and $v^{(\nu)}_{j,\mathrm{vec}}$. Thus, according to (3.7.37), if $\big(v^{(\nu)}_{j,\mathrm{vec}}[x_l]+v^{(\nu)}_{j,\mathrm{vec}}[x_k]\big)\bullet(x_l-x_k)<0$, then $v^{(\nu)}_{j,\mathrm{sca}}\big[\big(u_{j_{\mathrm{Dir}}[(l,j)],\mathrm{Dir}}[(t_\nu,x_l)],x_l\big)\big]$ is selected in (3.7.41). Then by the Cauchy-Schwarz Inequality (Rem. C.2.2), the negative of the corresponding summand has the upper bound $B_{v,\mathrm{Dir}}[(\mathfrak{C},\mathfrak{V})]\cdot\lambda_{d-1}\big[\omega^{(j)}_k\cap\omega^{(j)}_l\big]$. On the other hand, if $\big(v^{(\nu)}_{j,\mathrm{vec}}[x_l]+v^{(\nu)}_{j,\mathrm{vec}}[x_k]\big)\bullet(x_l-x_k)>0$, then $v^{(\nu)}_{j,\mathrm{sca}}\big[(y,x_k)\big]$ is selected in (3.7.41), and, according to the hypothesis of Lem. 3.7.18 and the Cauchy-Schwarz Inequality, the negative of the corresponding summand has the upper bound $B_{v,\mathrm{sca},\mathrm{Dir}}[(\mathfrak{C},\mathfrak{V})]\cdot\lambda_{d-1}\big[\omega^{(j)}_k\cap\omega^{(j)}_l\big]$. Analogous to Lem. 3.7.6, the sum in (3.7.47) is written in terms of $I_{\Pi,\mathfrak{D},\mathrm{Dir}}$, whereas the sums in (3.7.41) are witten in terms of $I_{\Pi,\mathfrak{D},\neg\mathrm{Dir}}$. ■

Remark and Example 3.7.19. The number $l_{\mathrm{Dir}}[\Pi]$ measures the size of the surface consisting of the collection of all interfaces between control volumes at Dirichlet vertices and control volumes at non-Dirichlet vertices. For the type of polytope discretizations depicted in Fig. 3.20 on p. 111, one has $l_{\mathrm{Dir}}[\Pi]=b$ independently of h.

Example 3.7.20. It is verified for the cases considered in Ex. 3.7.11 that correspond to Ex. 3.1.1(b) and to the first case of Ex. 3.1.1(a), that under natural hypotheses, v_{sca} is bounded from below, as is required in Lem. 3.7.18.

If $v_{\text{sca}}[(y,x)] = y$, then $\inf v_{\text{sca}} = m_v$. If $v_{\text{sca}}[(y,x)] := \frac{(z^{(\text{Ar})}+1)R}{M^{(\text{Ar})}}\,\rho_{\text{gas}}[x]y$, then $\inf v_{\text{sca}} \geq \min\{0, \frac{(z^{(\text{Ar})}+1)R}{M^{(\text{Ar})}}\,\|\rho_{\text{gas}}\|_{\max}\cdot m_v\}$, since $\rho_{\text{gas}} \geq 0$.
If $v_{\text{sca}}[(y,x)] = \varepsilon_{\text{gas}}[(y,x)]\,\rho_{\text{gas}}[x]$, then v_{sca} is bounded from below assuming ε_{gas} is bounded from below, again using $\rho_{\text{gas}} \geq 0$.

3.7.5 Terms on Outer Boundaries

In this section, (3.5.24c) and (3.5.24g) are discretized, whereas the discretization of (3.5.24f) is postponed to Sec. 3.7.7.

Approximating the integrand of (3.5.24c) as being constant on $\partial\omega_k^{(j)}\cap\partial p$, both functions in the scalar-vector-splitting of $v_j^{(\nu)}$ are evaluated at x_k, where $x_k \in \partial\omega_k^{(j)}\cap\partial p$ is guaranteed by (dispt-(iii)). In contrast to the cases of the discretizations of (3.5.24e) and (3.5.24b) in Secs 3.7.3 and 3.7.4, respectively, the remaining integrals involving the normal vector are *not* evaluated using (dispt-(i)), since the normal vector does not have to be constant on the entire domain of integration (cf. Fig. 3.21).

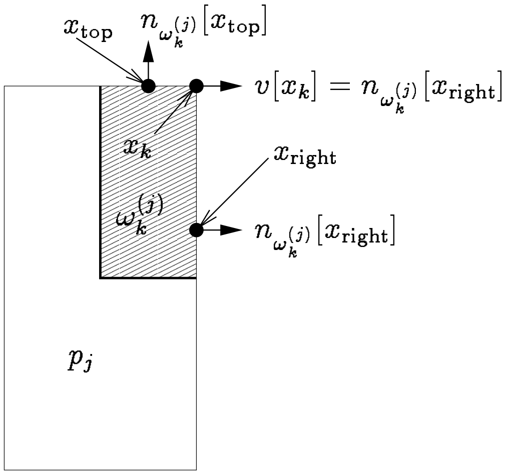


Figure 3.21: In this example, $v[x_k]\bullet n_{\omega_k^{(j)}}$ is not constant on $\partial\omega_k^{(j)}$ as it is 0 on the part of the boundary facing upwards and 1 on the part of the boundary facing right.

Thus, (3.5.24c) is replaced by

$$\mathfrak{h}^{(\nu)}_{(k,\mathcal{C}),(c)}[U^{(\nu)}] := \mathfrak{v}^{(\nu)}_{\text{out},(k,\mathcal{C})}[U^{(\nu)}_{(k,\mathcal{C})}], \tag{3.7.48}$$

where the $\mathfrak{v}^{(\nu)}_{\text{out},(k,\mathcal{C})} : v \longrightarrow \mathbb{R}$ are defined by

$$\bigwedge_{\substack{\nu\in\{0,\dots,n\},\\ (k,\mathcal{C})\in I_{\Pi,\mathfrak{D},\neg\text{Dir}}}} \mathfrak{v}^{(\nu)}_{\text{out},(k,\mathcal{C})}[y] := \sum_{j\in V[\mathcal{C}]} v^{(\nu)}_{j,\text{sca}}[(y,x_k)] \int_{\partial\omega_k^{(j)}\cap\partial p} v^{(\nu)}_{j,\text{vec}}[x_k]\bullet n_{\omega_k^{(j)}}. \tag{3.7.49}$$

Approximating the integrand of (3.5.24g) as being constant on $\partial\omega_k^{(j)} \cap \Gamma_{j,\iota}$, it is evaluated at x_k, where $x_k \in \partial\omega_k^{(j)} \cap \Gamma_{j,\iota}$ is guaranteed by (dispt-(iii)). Thus, (3.5.24g) is replaced by

$$\mathfrak{h}^{(\nu)}_{(k,\mathcal{C}),(g)}[(U^{(\nu-1)}, U^{(\nu)})] := \mathfrak{a}^{(\nu)}_{\mathrm{out},(k,\mathcal{C})}[(U^{(\nu-1)}_{(k,\mathcal{C})}, U^{(\nu)}_{(k,\mathcal{C})})], \tag{3.7.50}$$

where the $\mathfrak{a}^{(\nu)}_{\mathrm{out},(k,\mathcal{C})} : v \times v \longrightarrow \mathbb{K}$ are defined by

$$\bigwedge_{\substack{\nu\in\{0,\dots,n\},\\ (k,\mathcal{C})\in I_{\Pi,\mathfrak{D},\neg\mathrm{Dir}}}} \mathfrak{a}^{(\nu)}_{\mathrm{out},(k,\mathcal{C})}[(\tilde{y}, y)] := \sum_{\substack{(j,\iota)\in V[\mathcal{C}]\times J_j\setminus\{0\}:\\ \lambda_{d-1}[\partial\omega_k^{(j)}\cap\Gamma_{j,\iota}]>0}} \left(a^{j,\iota,\nu}_{\mathrm{out}}\right)^{\mathrm{ex.\text{-}im.}}\left[\left((\tilde{y}, y), x_k\right)\right] \cdot \lambda_{d-1}[\partial\omega_k^{(j)} \cap \Gamma_{j,\iota}]. \tag{3.7.51}$$

3.7.6 Terms on Interfaces

In this section, (3.5.24d), (3.5.24i), (3.5.24j), (3.5.24l), and (3.5.24m) are discretized, whereas the discretization of (3.5.24h) and (3.5.24k) is postponed to Sec. 3.7.7.

Throughout this section, $x_k \in \overline{\partial\omega_k^{(j)} \cap \gamma}$ is guaranteed by

$$\bigwedge_{k\in I_\Pi}\ \bigwedge_{j\in V_{\omega_k}}\ \bigwedge_{\gamma\in\mathrm{IF}} \quad \gamma \cap \partial_{\mathrm{reg}}\omega_k^{(j)} \neq \emptyset \quad \Rightarrow \quad x_k \in \overline{\gamma}, \tag{3.7.52}$$

which is a consequence of (dispt-(ii)) and of the ω_k being nontangent to interfaces.

The discretization of (3.5.24d) is analogous to the discretization of (3.5.24c) in Sec. 3.7.5, and the term (3.5.24d) is replaced by

$$\mathfrak{h}^{(\nu)}_{(k,\mathcal{C}),(d)}[U^{(\nu)}] := \mathfrak{v}^{(\nu)}_{\mathrm{con},(k,\mathcal{C})}[U^{(\nu)}_{(k,\mathcal{C})}] + \mathfrak{v}^{(\nu)}_{\mathrm{jump},(k,\mathcal{C})}[U^{(\nu)}_{(k,\mathcal{C})}], \tag{3.7.53}$$

where the $\mathfrak{v}^{(\nu)}_{\mathrm{con},(k,\mathcal{C})} : v \longrightarrow \mathbb{R}$ are defined by

$$\bigwedge_{\substack{\nu\in\{0,\dots,n\},\\ (k,\mathcal{C})\in I_{\Pi,\mathfrak{D},\neg\mathrm{Dir}}}} \mathfrak{v}^{(\nu)}_{\mathrm{con},(k,\mathcal{C})}[y] := \sum_{\substack{j\in V[\mathcal{C}],\\ \gamma\in\mathrm{IF}_{\mathrm{con}}}} v^{(\nu)}_{j,\mathrm{sca}}[(y, x_k)] \int_{\partial\omega_k^{(j)}\cap\gamma} v^{(\nu)}_{j,\mathrm{vec}}[x_k] \bullet n_{\omega_k^{(j)}}, \tag{3.7.54}$$

and the $\mathfrak{v}^{(\nu)}_{\mathrm{jump},(k,\mathcal{C})} : v \longrightarrow \mathbb{R}$ are defined by

$$\bigwedge_{\substack{\nu\in\{0,\dots,n\},\\ (k,\mathcal{C})\in I_{\Pi,\mathfrak{D},\neg\mathrm{Dir}}}} \mathfrak{v}^{(\nu)}_{\mathrm{jump},(k,\mathcal{C})}[y] := \sum_{\substack{j\in V[\mathcal{C}],\\ \gamma\in\mathrm{IF}_{\mathrm{jump}}}} v^{(\nu)}_{j,\mathrm{sca}}[(y, x_k)] \int_{\partial\omega_k^{(j)}\cap\gamma} v^{(\nu)}_{j,\mathrm{vec}}[x_k] \bullet n_{\omega_k^{(j)}}. \tag{3.7.55}$$

The reason for decomposing $\mathfrak{h}^{(\nu)}_{(k,\mathcal{C}),(d)}$ into one operator for continuous interfaces and one operator for jump interfaces is their different treatment in the estimates in Lems 3.7.31 and 3.7.33, respectively.

Approximating the integrands of (3.5.24i) as being constant on $\gamma \cap \bigcup_{j\in V[\mathcal{C}]} \partial_{\mathrm{reg}}\omega_k^{(j)}$, they are evaluated at x_k, where it is noted that $u_{i_1[\gamma]}^{(\nu-1)}[x_k] = u_{i_2[\gamma]}^{(\nu-1)}[x_k]$ and $u_{i_1[\gamma]}^{(\nu)}[x_k] = u_{i_2[\gamma]}^{(\nu)}[x_k]$, since γ is a continuous interface. Thus, (3.5.24i) is replaced by

$$\mathfrak{h}^{(\nu)}_{(k,\mathcal{C}),(i)}[(U^{(\nu-1)}, U^{(\nu)})] := \mathfrak{a}^{(\nu)}_{\mathrm{flux,con},(k,\mathcal{C})}[(U^{(\nu-1)}_{(k,\mathcal{C})}, U^{(\nu)}_{(k,\mathcal{C})})], \tag{3.7.56}$$

where the $\mathfrak{a}^{(\nu)}_{\mathrm{flux,con},(k,\mathcal{C})} : \upsilon \times \upsilon \longrightarrow \mathbb{K}$ are defined by

$$\bigwedge_{\substack{\nu\in\{0,\dots,n\},\\ (k,\mathcal{C})\in I_{\Pi,\mathfrak{D},\neg\mathrm{Dir}}}} \left(\begin{array}{l} \mathfrak{a}^{(\nu)}_{\mathrm{flux,con},(k,\mathcal{C})}[(\tilde{y}, y)] := \displaystyle\sum_{\substack{\gamma\in\mathrm{IF}_{\mathrm{con}}:\\ \lambda_{d-1}\left[\gamma\cap\bigcup_{j\in V[\mathcal{C}]}\partial_{\mathrm{reg}}\omega_k^{(j)}\right]>0}} \Big(-(a^{\gamma,1,\nu}_{\mathrm{flux}})^{\text{ex.-im.}}\big[\big((\tilde{y},y),x_k\big)\big] \\ \qquad\qquad\qquad\qquad\qquad\qquad\qquad + (a^{\gamma,2,\nu}_{\mathrm{flux}})^{\text{ex.-im.}}\big[\big((\tilde{y},y),x_k\big)\big]\Big) \\ \qquad\qquad\qquad\qquad\qquad\qquad\qquad \cdot\, \lambda_{d-1}\left[\gamma \cap \displaystyle\bigcup_{j\in V[\mathcal{C}]} \partial_{\mathrm{reg}}\omega_k^{(j)}\right] \end{array} \right). \tag{3.7.57}$$

The discretization of the terms (3.5.24j), (3.5.24l), and (3.5.24m) is similar to the discretization of the term (3.5.24i). However, since γ is now a jump interface, $u_{i_1[\gamma]}^{(\nu-1)}$ and $u_{i_2[\gamma]}^{(\nu-1)}$ can have different values at x_k and likewise for $u_{i_1[\gamma]}^{(\nu)}[x_k]$ and $u_{i_2[\gamma]}^{(\nu)}[x_k]$. Moreover, x_k can be a non-Dirichlet vertex on one side of the interface and a Dirichlet vertex on the other side of the interface (s. Fig. 3.19 on p. 107 and consider $x_k = x_1$). In this case, the solution value is known a priori at the Dirichlet vertex, which has to be taken into account in the following discretizations.

The term (3.5.24j) is replaced by

$$\mathfrak{h}^{(\nu)}_{(k,\mathcal{C}),(j)}[U^{(\nu)}] := \mathfrak{a}^{(\nu)}_{\mathrm{jump},1,\neg\mathrm{Dir},(k,\mathcal{C})}[U^{(\nu)}] + \mathfrak{a}^{(\nu)}_{\mathrm{jump},1,\mathrm{Dir},(k,\mathcal{C})}[U^{(\nu)}_{(k,\mathcal{C})}], \tag{3.7.58}$$

where the $\mathfrak{a}^{(\nu)}_{\mathrm{jump},1,\neg\mathrm{Dir},(k,\mathcal{C})} : \upsilon^{I_{\Pi,\mathfrak{D},\neg\mathrm{Dir}}} \longrightarrow \mathbb{K}$ are defined by

$$\bigwedge_{\substack{\nu\in\{0,\dots,n\},\\ (k,\mathcal{C})\in I_{\Pi,\mathfrak{D},\neg\mathrm{Dir}}}} \left(\begin{array}{l} \mathfrak{a}^{(\nu)}_{\mathrm{jump},1,\neg\mathrm{Dir},(k,\mathcal{C})}[U] \\ := \displaystyle\sum_{\substack{\gamma\in G_{\mathrm{jump},1}[\mathcal{C}]:\\ \left(k,\mathcal{C}[(k,i_2[\gamma])]\right)\in I_{\Pi,\mathfrak{D},\neg\mathrm{Dir}},\\ \lambda_{d-1}\left[\partial\omega_k^{(i_1[\gamma])}\cap\gamma\right]>0}} \Big(a^{\gamma,1,\nu}_{\mathrm{jump}}\big[\big(U_{(k,\mathcal{C})}, x_k\big)\big] - a^{\gamma,2,\nu}_{\mathrm{jump}}\big[\big(U_{\left(k,\mathcal{C}[(k,i_2[\gamma])]\right)}, x_k\big)\big]\Big) \\ \qquad\qquad\qquad\qquad\qquad \cdot\, \lambda_{d-1}\left[\partial\omega_k^{(i_1[\gamma])} \cap \gamma\right] \end{array} \right), \tag{3.7.59}$$

and the $\mathfrak{a}^{(\nu)}_{\text{jump},1,\text{Dir},(k,\mathcal{C})} : \upsilon \longrightarrow \mathbb{K}$ are defined by

$$\bigwedge_{\substack{\nu\in\{0,\dots,n\},\\ (k,\mathcal{C})\in I_{\Pi,\mathfrak{D},\neg\text{Dir}}}} \left(\begin{array}{l} \mathfrak{a}^{(\nu)}_{\text{jump},1,\text{Dir},(k,\mathcal{C})}[y] \\ := \displaystyle\sum_{\substack{\gamma\in G_{\text{jump},1}[\mathcal{C}]: \\ \left(k,\mathcal{C}[(k,i_2[\gamma])]\right)\in I_{\Pi,\mathfrak{D},\text{Dir}}, \\ \lambda_{d-1}\left[\partial\omega_k^{(i_1[\gamma])}\cap\gamma\right]>0}} \Big(a^{\gamma,1,\nu}_{\text{jump}}[(y,x_k)] \\ \qquad - a^{\gamma,2,\nu}_{\text{jump}}\left[\left(u_{j_{\text{Dir}}[(k,i_2[\gamma])],\text{Dir}}[(t_\nu,x_k)],x_k\right)\right]\Big) \\ \qquad \cdot \lambda_{d-1}\left[\partial\omega_k^{(i_1[\gamma])}\cap\gamma\right] \end{array} \right). \tag{3.7.60}$$

The term (3.5.24l) is replaced by

$$\begin{aligned} \mathfrak{h}^{(\nu)}_{(k,\mathcal{C}),(l)}[(U^{(\nu-1)},U^{(\nu)})] :=& \mathfrak{a}^{(\nu)}_{\text{flux},\text{jump},2,\neg\text{Dir},(k,\mathcal{C})}[(U^{(\nu-1)},U^{(\nu)})] \\ &+ \mathfrak{a}^{(\nu)}_{\text{flux},\text{jump},2,\text{Dir},(k,\mathcal{C})}[(U^{(\nu-1)}_{(k,\mathcal{C})},U^{(\nu)}_{(k,\mathcal{C})})], \end{aligned} \tag{3.7.61}$$

where the $\mathfrak{a}^{(\nu)}_{\text{flux},\text{jump},2,\neg\text{Dir},(k,\mathcal{C})} : \upsilon^{I_{\Pi,\mathfrak{D},\neg\text{Dir}}} \times \upsilon^{I_{\Pi,\mathfrak{D},\neg\text{Dir}}} \longrightarrow \mathbb{K}$ are defined by

$$\bigwedge_{\substack{\nu\in\{0,\dots,n\},\\ (k,\mathcal{C})\in I_{\Pi,\mathfrak{D},\neg\text{Dir}}}} \left(\begin{array}{l} \mathfrak{a}^{(\nu)}_{\text{flux},\text{jump},2,\neg\text{Dir},(k,\mathcal{C})}[(\tilde{U},U)] \\ := \displaystyle\sum_{\substack{\gamma\in G_{\text{jump},2}[\mathcal{C}]: \\ \left(k,\mathcal{C}[(k,i_1[\gamma])]\right)\in I_{\Pi,\mathfrak{D},\neg\text{Dir}}, \\ \lambda_{d-1}\left[\partial\omega_k^{(i_2[\gamma])}\cap\gamma\right]>0}} \Big(-(a^{\gamma,1,\nu}_{\text{flux}})^{\text{ex.-im.}}\left[\left((\tilde{U}_{\left(k,\mathcal{C}[(k,i_1[\gamma])]\right)},U_{\left(k,\mathcal{C}[(k,i_1[\gamma])]\right)}),x_k\right)\right] \\ \qquad + (a^{\gamma,2,\nu}_{\text{flux}})^{\text{ex.-im.}}\left[\left((\tilde{U}_{(k,\mathcal{C})},U_{(k,\mathcal{C})}),x_k\right)\right]\Big) \\ \qquad \cdot \lambda_{d-1}\left[\partial\omega_k^{(i_2[\gamma])}\cap\gamma\right] \end{array} \right), \tag{3.7.62}$$

and the $\mathfrak{a}^{(\nu)}_{\text{flux},\text{jump},2,\text{Dir},(k,\mathcal{C})} : \upsilon\times\upsilon \longrightarrow \mathbb{K}$ are defined by

$$\bigwedge_{\substack{\nu\in\{0,\dots,n\},\\ (k,\mathcal{C})\in I_{\Pi,\mathfrak{D},\neg\text{Dir}}}} \left(\begin{array}{l} \mathfrak{a}^{(\nu)}_{\text{flux},\text{jump},2,\text{Dir},(k,\mathcal{C})}[(\tilde{y},y)] \\ := \displaystyle\sum_{\substack{\gamma\in G_{\text{jump},2}[\mathcal{C}]: \\ \left(k,\mathcal{C}[(k,i_1[\gamma])]\right)\in I_{\Pi,\mathfrak{D},\text{Dir}}, \\ \lambda_{d-1}\left[\partial\omega_k^{(i_2[\gamma])}\cap\gamma\right]>0}} \Big(-(a^{\gamma,1,\nu}_{\text{flux}})^{\text{ex.-im.}}\Big[\Big(\big(u_{j_{\text{Dir}}[(k,i_1[\gamma])],\text{Dir}}[(t_{\nu-1},x_k)], \\ \qquad\qquad u_{j_{\text{Dir}}[(k,i_1[\gamma])],\text{Dir}}[(t_\nu,x_k)]\big),x_k\Big)\Big] \\ \qquad + (a^{\gamma,2,\nu}_{\text{flux}})^{\text{ex.-im.}}\left[\left((\tilde{y},y),x_k\right)\right]\Big) \\ \qquad \cdot \lambda_{d-1}\left[\partial\omega_k^{(i_2[\gamma])}\cap\gamma\right] \end{array} \right). \tag{3.7.63}$$

The term (3.5.24m) is replaced by

$$\mathfrak{h}^{(\nu)}_{(k,\mathcal{C}),(m)}[U^{(\nu)}] := \mathfrak{a}^{(\nu)}_{\text{jump},2,\neg\text{Dir},(k,\mathcal{C})}[U^{(\nu)}] + \mathfrak{a}^{(\nu)}_{\text{jump},2,\text{Dir},(k,\mathcal{C})}[U^{(\nu)}_{(k,\mathcal{C})}], \tag{3.7.64}$$

where the $\mathfrak{a}^{(\nu)}_{\text{jump},2,\neg\text{Dir},(k,\mathcal{C})} : \upsilon^{I_{\Pi,\mathfrak{D},\neg\text{Dir}}} \longrightarrow \mathbb{K}$ are defined by

$$\bigwedge_{\substack{\nu\in\{0,\dots,n\},\\ (k,\mathcal{C})\in I_{\Pi,\mathfrak{D},\neg\text{Dir}}}} \left(\begin{array}{l} \mathfrak{a}^{(\nu)}_{\text{jump},2,\neg\text{Dir},(k,\mathcal{C})}[U] \\ := \displaystyle\sum_{\substack{\gamma\in G_{\text{jump},2}[\mathcal{C}]: \\ \left(k,\mathcal{C}[(k,i_1[\gamma])]\right)\in I_{\Pi,\mathfrak{D},\neg\text{Dir}}, \\ \lambda_{d-1}\left[\partial\omega_k^{(i_2[\gamma])}\cap\gamma\right]>0}} \Big(-a^{\gamma,1,\nu}_{\text{jump}}\left[\left(U_{\left(k,\mathcal{C}[(k,i_1[\gamma])]\right)},x_k\right)\right] \\ \qquad + a^{\gamma,2,\nu}_{\text{jump}}\left[\left(U_{(k,\mathcal{C})},x_k\right)\right]\Big) \\ \qquad \cdot \lambda_{d-1}\left[\partial\omega_k^{(i_2[\gamma])}\cap\gamma\right] \end{array} \right), \tag{3.7.65}$$

and the $\mathfrak{a}^{(\nu)}_{\text{jump},2,\text{Dir},(k,\mathcal{C})} : v \longrightarrow \mathbb{K}$ are defined by

$$\bigwedge_{\substack{\nu\in\{0,\dots,n\},\\(k,\mathcal{C})\in I_{\Pi,\mathfrak{D},\neg\text{Dir}}}} \left(\begin{aligned} &\mathfrak{a}^{(\nu)}_{\text{jump},2,\text{Dir},(k,\mathcal{C})}[y] \\ &:= \sum_{\substack{\gamma\in G_{\text{jump},2}[\mathcal{C}]:\\ \left(k,\mathcal{C}[(k,i_1[\gamma])]\right)\in I_{\Pi,\mathfrak{D},\text{Dir}},\\ \lambda_{d-1}\left[\partial\omega_k^{(i_2[\gamma])}\cap\gamma\right]>0}} \Big(- a^{\gamma,1,\nu}_{\text{jump}}\big[(u_{j_{\text{Dir}}[(k,i_1[\gamma])],\text{Dir}}[(t_\nu, x_k)], x_k)\big] \\ &\qquad\qquad + a^{\gamma,2,\nu}_{\text{jump}}\big[(y, x_k)\big]\Big) \\ &\qquad\qquad \cdot \lambda_{d-1}\left[\partial\omega_k^{(i_2[\gamma])}\cap\gamma\right] \end{aligned} \right). \tag{3.7.66}$$

3.7.7 Terms Involving Nonlocal Operators

The subject of this section is the discretization of (3.5.24f), (3.5.24h), and (3.5.24k). In contrast to the discretization of the remaining terms of (3.5.24) described in other parts of Sec. 3.7, the discretization procedure for the nonlocal terms described in the following is less concrete. If at all feasible, the determination of a universal discretization method for general nonlocal operators seems to need an investigation of the continuous solution theory (s. Rem. 3.7.21 below). Since the continuous solution theory is not the subject of this work, certain aspects of the discretization procedure are left open. However, in Sec. 3.7.8, it is shown, how a concrete discretization of the terms (3.5.24f), (3.5.24h), and (3.5.24k) can be constructed, if the nonlocal interface and boundary operators represent nonlocal radiative heat transport between surfaces, i.e. for the cases considered in Exs 3.1.2(c) and 3.1.3(e) (also see Exs 3.4.10 and 3.4.12).

The terms (3.5.24f), (3.5.24h), and (3.5.24k) are replaced by

$$\mathfrak{h}^{(\nu)}_{(k,\mathcal{C}),(f)}[(U^{(\nu-1)}, U^{(\nu)})] := -\mathfrak{B}^{(\nu)}_{(k,\mathcal{C})}[(U^{(\nu-1)}, U^{(\nu)})], \tag{3.7.67a}$$

$$\mathfrak{h}^{(\nu)}_{(k,\mathcal{C}),(h)}[(U^{(\nu-1)}, U^{(\nu)})] := -\mathfrak{A}^{(\nu)}_{\text{con},(k,\mathcal{C})}[(U^{(\nu-1)}, U^{(\nu)})], \tag{3.7.67b}$$

$$\mathfrak{h}^{(\nu)}_{(k,\mathcal{C}),(k)}[(U^{(\nu-1)}, U^{(\nu)})] := -\mathfrak{A}^{(\nu)}_{\text{jump},(k,\mathcal{C})}[(U^{(\nu-1)}, U^{(\nu)})], \tag{3.7.67c}$$

respectively, where for each $\nu \in \{1,\dots,n\}$ and for each $(k,\mathcal{C}) \in I_{\Pi,\mathfrak{D},\neg\text{Dir}}$, the $\mathfrak{B}^{(\nu)}_{(k,\mathcal{C})}$, $\mathfrak{A}^{(\nu)}_{\text{con},(k,\mathcal{C})}$, and $\mathfrak{A}^{(\nu)}_{\text{jump},(k,\mathcal{C})}$ are functions from $v^{I_{\Pi,\mathfrak{D},\neg\text{Dir}}} \times v^{I_{\Pi,\mathfrak{D},\neg\text{Dir}}}$ into $\mathbb{K}$ such that the right-hand sides of (3.7.67) are suitable approximations of (3.5.24f), (3.5.24h), and (3.5.24k), respectively.

The nonlocal interface operators $\mathcal{A}_\gamma$, $\gamma \in \text{IF}$, and the nonlocal boundary operators $\mathcal{B}_{j,\iota}$, $(j,\iota) \in J \times \big(J_j \setminus \{0\}\big)$, can depend nonlocally on (potentially) all unknowns u_j. Correspondingly, the same holds for the dependency splittings $(\mathcal{A}_\gamma)^{\text{ex.-im.}}$ and $(\mathcal{B}_{j,\iota})^{\text{ex.-im.}}$ with respect to the time-discrete unknowns $u_j^{(\nu)}$. Thus, the approximations on the right-hand sides of (3.7.67) can depend on the entire vectors $U^{(\nu-1)}$ and $U^{(\nu)}$, i.e. they can depend on all solution values at discretization points of control volumes of Π.

Remark 3.7.21. In a suitable sense, the approximations on the right-hand sides of (3.7.67) should become better as Π becomes finer (i.e. as $h^{(j)}$ decreases, s. (3.5.2)). However, to make this more precise, one needs an analysis of the continuous solution and convergence theory, which is not considered here.

3.7.8 Example: Discretization of Nonlocal Radiation Terms

The subject of this section is the concrete construction of the discretization operators on the right-hand sides of (3.7.67) for the special case described in Exs 3.1.2(c) and 3.1.3(e) (also see Exs 3.4.10 and 3.4.12), i.e. if the nonlocal interface and boundary operators represent nonlocal radiative heat transport between surfaces.

Using the model of diffuse-gray radiation as described in Sec. 2.4 together with the assumed cylindrical symmetry (cf. Sec. 2.4.3), the discretization strategy follows the same paradigm used so far in this work: The relevant equations are integrated over control elements (more precisely, over boundary elements on interfaces, compatible with the control volumes of the polytope discretization Π), followed by quadratures, where functions are approximated as constant in the respective domains of integration (see Sec. 3.5 and the description in Sec. 3.7.1 for the case of evolution equations in general).

Let p_{rad} be a 2-dimensional polytope that constitutes the circular projection (cf. (2.4.20)) of some cylindrically symmetric radiation region. One should have in mind that p_{rad} typically represents (the circular projection of) a gas-filled cavity inside a complex apparatus. Thus, there are usually several $p_{\mathrm{rad},j}$ within a domain complex. However, to simplify notation, the index j is dropped, and the considerations are performed for just one radiation region p_{rad}. Moreover, as in the case of Ex. 3.1.3(e), where the nonlocal boundary operator represents radiative interactions between surfaces inside the upper and lower blind hole in Fig. 4.1 on p. 195, it can happen that p_{rad} lies outside the total space domain p, i.e. no evolution equation is solved on p_{rad}.

The case of Ex. 3.1.3(e) is the one considered in the following. The three cases of nonlocal radiation operators on interfaces considered in Ex. 3.1.2(c) can be treated analogously. The operator $\mathcal{B} := \mathcal{B}_{j,\iota}$ of Ex. 3.1.3(e) in axisymmetric form (cf. Sec. 2.4.3) reads

$$\mathcal{B}[T_{\mathrm{solid,circ}}] := \epsilon_{\mathrm{circ}}[(T_{\mathrm{solid,circ}}, x)] \cdot \mathcal{J}_{\mathrm{circ}}\big[\mathcal{R}_{\mathrm{circ}}[T_{\mathrm{solid,circ}}]\big]. \tag{3.7.68}$$

Once again, the precise meaning of $\mathcal{R}_{\mathrm{circ}}$ acting on $T_{\mathrm{solid,circ}}$ is according to the remark made at the beginning of Ex. 3.1.2(c). The function $\mathcal{B}[T_{\mathrm{solid,circ}}]$ is defined on $\Gamma := p_{\mathrm{rad}} \cap p$. The set $\partial p_{\mathrm{rad}} \setminus p$ consists of some part lying on the $r = 0$ axis and a phantom closure. For the lower blind hole of the apparatus in Fig. 4.1 on p. 195, this is illustrated in Fig. 3.22. The phantom closure Γ_{ph} (corresponding to Γ_{bottom} or Γ_{top} in Fig. 4.1) is assumed to radiate as a black body at room temperature, setting $\epsilon_{\text{circ}} = 1$ on Γ_{ph}. Thus

$$\bigwedge_{x \in \Gamma_{\text{ph}}} \quad R_{\text{circ}}[x] = \sigma\, T_{\text{room}}^4. \tag{3.7.69}$$

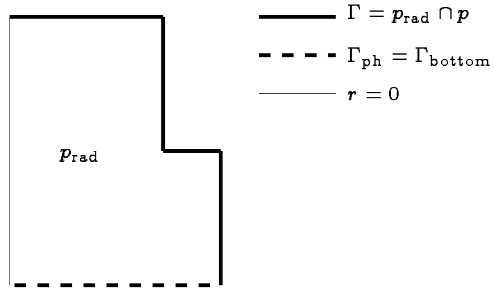


Figure 3.22: Circular projection of the lower blind hole of the configuration of Fig. 4.1 on p. 195.

Now, $\Gamma \cup \Gamma_{\text{ph}}$ is discretized into line segments. To that end, let $\Pi_{\text{rad}} := (\zeta_\kappa)_{\kappa \in I_{\text{rad}}}$ be a partition of $\Gamma \cup \Gamma_{\text{ph}}$ such that each ζ_κ is a line segment. The ζ_κ are called *boundary elements*. With each ζ_κ associate a discretization point $x_\kappa \in \zeta_\kappa$. Moreover, if a constant approximation of radiation is to be reasonable on each ζ_κ, then each ζ_κ should lie within a single solid material. On Γ, Π_{rad} is supposed to be compatible with the partition Π of p in the following sense: For each control volume ω such that $\Gamma \cap \partial_{\text{reg}}\omega \neq \emptyset$, the family $(\zeta_\kappa \cap \omega)_{\kappa \in I_\omega}$ is supposed to form a partition of $\Gamma \cap \partial\omega$, where $I_\omega := \{\kappa \in I_{\text{rad}} : \text{int}[\zeta_\kappa] \cap \partial_{\text{reg}}\omega \neq \emptyset\}$. Furthermore, for the discretization point x_ω of ω, it is presumed that

$$\bigwedge_{\kappa \in I_\omega} \quad x_\omega = x_\kappa. \tag{3.7.70}$$

In particular, I_ω has at most two elements. The situation is illustrated in Fig. 3.23.

So far, for the sake of readability, the fact that $\mathcal{R}_{\text{circ}}$ (and thus $\mathcal{B}$) only depends on $T_{\text{solid,circ}}$ restricted to a fixed time $t \in \tau$, was hidden in the notation. However, this plays a role in the following. Thus, for each $\nu \in \{0, \dots, n\}$, let $T^{(\nu)}_{\text{solid,circ}}$ denote the restriction of $T_{\text{solid,circ}}$ to the time t_ν.

To find $\mathfrak{B}^{(\nu)}_{(k,\mathcal{C})}$ such that the right-hand side of (3.7.67a) approximates the term (3.5.24f), the dependency splitting (cf. Ex. 3.4.12)

$$\mathcal{B}^{\text{ex.-im.}}[(T^{(\nu-1)}_{\text{solid,circ}}, T^{(\nu)}_{\text{solid,circ}})] = \epsilon_{\text{circ}}[(T^{(\nu-1)}_{\text{solid,circ}}, x)] \cdot \mathcal{J}_{\text{circ}}\big[\mathcal{R}_{\text{circ}}[T^{(\nu)}_{\text{solid,circ}}]\big] \tag{3.7.71}$$

is multiplied by r and integrated over ζ_κ for each $\kappa \in I_{\text{rad},\Gamma}$, where $I_{\text{rad},\Gamma} := \{\kappa \in I_{\text{rad}} :$

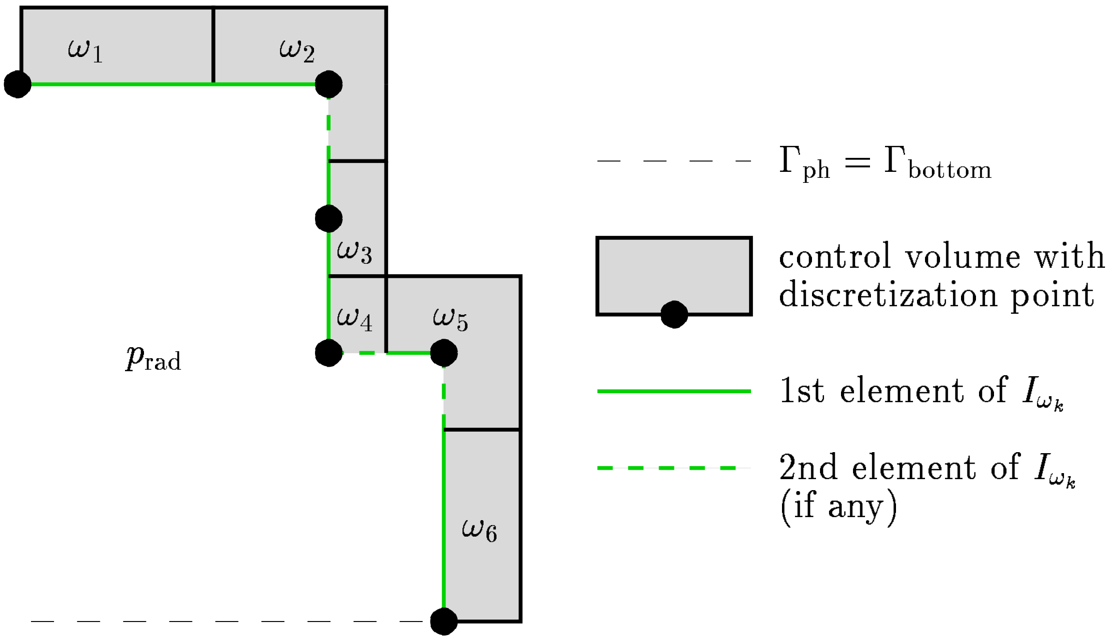


Figure 3.23: Magnification of the radiation region of the lower blind hole that was depicted in Fig. 3.22. Here, to illustrate the assumed compatibility between Π_{rad} and Π, the control volumes adjacent to p_{rad} are also shown.

$\zeta_\kappa \subseteq \Gamma\}$. This yields

$$\bigwedge_{\kappa \in I_{\text{rad},\Gamma}} \int_{\zeta_\kappa} \epsilon_{\text{circ}}\left[\left(T^{(\nu-1)}_{\text{solid,circ}}[(r,z)],(r,z)\right)\right] \cdot \mathcal{J}_{\text{circ}}\left[\mathcal{R}_{\text{circ}}[T^{(\nu)}_{\text{solid,circ}}]\right][(r,z)] \cdot r \,\mathrm{d}(r,z)\,. \tag{3.7.72}$$

Actually, this is the same as integrating $\epsilon[(T^{(\nu-1)}_{\text{solid}}[x],x)] \cdot \mathcal{J}\left[\mathcal{R}[T^{(\nu)}_{\text{solid}}]\right][x]$ over $\pi^{-1}_{\text{circ}}\zeta_\kappa$ and then performing a change of variables analogous to the description in Sec. 3.6.

Now, using that on Γ, with obvious notation, $R^{(\nu)}_{\text{circ}} = \mathcal{R}_{\text{circ}}[T^{(\nu)}_{\text{solid,circ}}]$ according to (2.4.27), (3.7.72) is approximated by evaluating ϵ_{circ}, $T^{(\nu-1)}_{\text{solid,circ}}$, and $R^{(\nu)}_{\text{circ}}$ at the discretization point x_κ, $\kappa \in I_{\text{rad},\Gamma}$. If x_κ lies in the boundary of ζ_κ, then the functions to be evaluated at x_κ might not be continuous at x_κ. However, the functions are continuous on $\text{int}[\zeta_\kappa]$ and can be extended continuously to x_κ. In that case, the following evaluations at x_κ are meant to be those of the continuous extensions.

Thus, the approximation of (3.7.72) yields

$$\bigwedge_{\kappa \in I_{\text{rad},\Gamma}} V_\kappa := \epsilon_{\text{circ}}\left[(T^{(\nu-1)}_{\text{solid,circ}}[x_\kappa],x_\kappa)\right] \int_{\zeta_\kappa} \mathcal{J}_{\text{circ}}[R^{(\nu)}_{\text{circ}}][(r,z)]r\,\mathrm{d}(r,z)\,, \tag{3.7.73}$$

and furthermore, using (2.4.22), one gets

$$\bigwedge_{\kappa\in I_{\mathrm{rad},\Gamma}} \left(\begin{aligned} & \int_{\zeta_\kappa} \mathcal{J}_{\mathrm{circ}}[R^{(\nu)}_{\mathrm{circ}}][(r,z)] r \,\mathrm{d}(r,z) \\ & = \int_{\zeta_\kappa} \int_{\Gamma\cup\Gamma_{\mathrm{ph}}} \Lambda_{\mathrm{circ}}\big[\big((r,z),(\tilde r,\tilde z)\big)\big]\, R^{(\nu)}_{\mathrm{circ}}[(\tilde r,\tilde z)]\, \tilde r \;\mathrm{d}(\tilde r,\tilde z)\, r\,\mathrm{d}(r,z) \\ & = \sum_{\lambda\in I_{\mathrm{rad}}} R^{(\nu)}_{\mathrm{circ}}[x_\lambda] \int_{\zeta_\kappa}\int_{\zeta_\lambda} \Lambda_{\mathrm{circ}}\big[\big((r,z),(\tilde r,\tilde z)\big)\big]\, \tilde r \;\mathrm{d}(\tilde r,\tilde z)\, r\,\mathrm{d}(r,z) \\ & = \sum_{\lambda\in I_{\mathrm{rad}}} R^{(\nu)}_{\mathrm{circ}}[x_\lambda]\, \Lambda_{\kappa,\lambda} \end{aligned} \right), \tag{3.7.74}$$

where

$$\bigwedge_{(\kappa,\lambda)\in I^2_{\mathrm{rad}}} \Lambda_{\kappa,\lambda} := \int_{\zeta_\kappa}\int_{\zeta_\lambda} \Lambda_{\mathrm{circ}}\big[\big((r,z),(\tilde r,\tilde z)\big)\big]\, \tilde r \;\mathrm{d}(\tilde r,\tilde z)\, r\,\mathrm{d}(r,z)\,. \tag{3.7.75}$$

Definitions (2.4.23) and (3.7.75) together with the forms of Λ and ω imply the symmetry condition

$$\bigwedge_{(\kappa,\lambda)\in I^2_{\mathrm{rad}}} \Lambda_{\kappa,\lambda} = \Lambda_{\lambda,\kappa}. \tag{3.7.76}$$

Since $\Gamma\cup\Gamma_{\mathrm{ph}}$ is the circular projection of a closed surface, the conservation of radiation energy (2.4.24) yields

$$\bigwedge_{\kappa\in I_{\mathrm{rad},\Gamma}} \left(\begin{aligned} \sum_{\lambda\in I_{\mathrm{rad}}} \Lambda_{\kappa,\lambda} & = \int_{\zeta_\kappa} \sum_{\lambda\in I_{\mathrm{rad}}} \int_{\zeta_\lambda} \Lambda_{\mathrm{circ}}\big[\big((r,z),(\tilde r,\tilde z)\big)\big]\, \tilde r \;\mathrm{d}(\tilde r,\tilde z)\, r\,\mathrm{d}(r,z) \\ & = \int_{\zeta_\kappa} \int_{\Gamma\cup\Gamma_{\mathrm{ph}}} \Lambda_{\mathrm{circ}}\big[\big((r,z),(\tilde r,\tilde z)\big)\big]\, \tilde r \;\mathrm{d}(\tilde r,\tilde z)\, r\,\mathrm{d}(r,z) \\ & = \int_{\zeta_\kappa} 1\cdot r\,\mathrm{d}(r,z) \;=:\, l_\kappa \end{aligned} \right). \tag{3.7.77}$$

Substituting (3.7.74) in (3.7.73) results in

$$\bigwedge_{\kappa\in I_{\mathrm{rad},\Gamma}} V_\kappa = \epsilon_{\mathrm{circ}}\big[(T^{(\nu-1)}_{\mathrm{solid,circ}}[x_\kappa], x_\kappa)\big] \sum_{\lambda\in I_{\mathrm{rad}}} R^{(\nu)}_{\mathrm{circ}}[x_\lambda]\, \Lambda_{\kappa,\lambda}. \tag{3.7.78}$$

Multiplying (2.4.21) by r, integrating over ζ_κ, $\kappa\in I_{\mathrm{rad},\Gamma}$, and approximating the result by evaluating $R^{(\nu)}_{\mathrm{circ}}$, ϵ_{circ}, $T^{(\nu-1)}_{\mathrm{solid,circ}}$, and $T^{(\nu)}_{\mathrm{solid,circ}}$, at the discretization point x_κ leads to

$$\bigwedge_{\kappa\in I_{\mathrm{rad},\Gamma}} \left(\begin{aligned} & R^{(\nu)}_{\mathrm{circ}}[x_\kappa] l_\kappa - \big(1-\epsilon_{\mathrm{circ}}\big[(T^{(\nu-1)}_{\mathrm{solid,circ}}[x_\kappa], x_\kappa)\big]\big) \int_{\zeta_\kappa} \mathcal{J}_{\mathrm{circ}}[R^{(\nu)}_{\mathrm{circ}}][(r,z)] r\,\mathrm{d}(r,z) \\ & = \sigma\epsilon_{\mathrm{circ}}\big[(T^{(\nu-1)}_{\mathrm{solid,circ}}[x_\kappa], x_\kappa)\big] \big(T^{(\nu)}_{\mathrm{solid,circ}}[x_\kappa]\big)^4 l_\kappa \end{aligned} \right). \tag{3.7.79}$$

The combination of (3.7.79) and (3.7.74) yields

$$\bigwedge_{\kappa \in I_{\mathrm{rad},\Gamma}} \begin{pmatrix} R^{(\nu)}_{\mathrm{circ}}[x_\kappa] l_\kappa - \left(1 - \epsilon_{\mathrm{circ}}\left[(T^{(\nu-1)}_{\mathrm{solid,circ}}[x_\kappa], x_\kappa)\right]\right) \sum_{\lambda \in I_{\mathrm{rad}}} R^{(\nu)}_{\mathrm{circ}}[x_\lambda]\, \Lambda_{\kappa,\lambda} \\ = \sigma \epsilon_{\mathrm{circ}}\left[(T^{(\nu-1)}_{\mathrm{solid,circ}}[x_\kappa], x_\kappa)\right] \left(T^{(\nu)}_{\mathrm{solid,circ}}[x_\kappa]\right)^4 l_\kappa \end{pmatrix}. \tag{3.7.80}$$

If the families of values $\left(T^{(\nu-1)}_{\mathrm{solid,circ}}[x_\kappa]\right)_{\kappa \in I_{\mathrm{rad},\Gamma}}$ and $\left(T^{(\nu)}_{\mathrm{solid,circ}}[x_\kappa]\right)_{\kappa \in I_{\mathrm{rad},\Gamma}}$ are known, then (3.7.80) constitutes a linear system of equations for the determination of the family of values $\left(R^{(\nu)}_{\mathrm{circ}}[x_\kappa]\right)_{\kappa \in I_{\mathrm{rad},\Gamma}}$.

In matrix form, (3.7.80) reads

$$\mathbf{A}\mathbf{X} = \mathbf{Y}, \tag{3.7.81a}$$

with vectors $\mathbf{X} = (X_\kappa)_{\kappa \in I_{\mathrm{rad},\Gamma}} \in \mathbb{R}^{I_{\mathrm{rad},\Gamma}}$, $\mathbf{Y} = (Y_\kappa)_{\kappa \in I_{\mathrm{rad},\Gamma}} \in \mathbb{R}^{I_{\mathrm{rad},\Gamma}}$, and a matrix $\mathbf{A} = (A_{\kappa,\lambda})_{(\kappa,\lambda) \in I^2_{\mathrm{rad},\Gamma}}$,

$$\bigwedge_{\kappa \in I_{\mathrm{rad},\Gamma}} \qquad X_\kappa := R^{(\nu)}_{\mathrm{circ}}[x_\kappa], \tag{3.7.81b}$$

$$\bigwedge_{\kappa \in I_{\mathrm{rad},\Gamma}} \qquad Y_\kappa := \sigma \epsilon_{\mathrm{circ}}\left[\left(T^{(\nu-1)}_{\mathrm{solid,circ}}[x_\kappa], x_\kappa\right)\right] \left(T^{(\nu)}_{\mathrm{solid,circ}}[x_\kappa]\right)^4 l_\kappa. \tag{3.7.81c}$$

The matrix $\mathbf{A}$ has the form

$$\mathbf{A} = \mathbf{D} + \mathbf{L} \tag{3.7.81d}$$

with matrices $\mathbf{D} = (D_{\kappa,\lambda})_{(\kappa,\lambda) \in I^2_{\mathrm{rad},\Gamma}} \in \mathbb{R}^{I^2_{\mathrm{rad},\Gamma}}$ and $\mathbf{L} = (L_{\kappa,\lambda})_{(\kappa,\lambda) \in I^2_{\mathrm{rad},\Gamma}} \in \mathbb{R}^{I^2_{\mathrm{rad},\Gamma}}$, where $\mathbf{D}$ is diagonal,

$$\bigwedge_{(\kappa,\lambda) \in I^2_{\mathrm{rad},\Gamma}} \qquad D_{\kappa,\lambda} := \begin{cases} l_\kappa & \text{for } \kappa = \lambda, \\ 0 & \text{for } \kappa \neq \lambda, \end{cases} \tag{3.7.81e}$$

$$\bigwedge_{(\kappa,\lambda) \in I^2_{\mathrm{rad},\Gamma}} \qquad L_{\kappa,\lambda} := -\left(1 - \epsilon_{\mathrm{circ}}\left[(T^{(\nu-1)}_{\mathrm{solid,circ}}[x_\kappa], x_\kappa)\right]\right) \cdot \Lambda_{\kappa,\lambda}. \tag{3.7.81f}$$

Using Def. C.3.1 and Lem. C.3.2 of App. C.3, the following Lem. 3.7.22 provides some important properties of the matrix $\mathbf{A}$.

Lemma 3.7.22. *If* $1 \geq \epsilon_{\mathrm{circ}} > 0$, *then the following holds:*

(a) $\mathbf{A}$ *is strictly diagonally dominant.*

(b) $\mathbf{A}$ *is an M-matrix. In particular,* $\mathbf{A}$ *is invertible, and* $\mathbf{A}^{-1}$ *is nonnegative.*

Proof. (a): Since r can not vanish identically on ζ_κ, one has

$$\bigwedge_{\kappa \in I_{\mathrm{rad},\Gamma}} \quad l_\kappa > 0 \tag{3.7.82}$$

directly from (3.7.77). In particular, for each $\kappa \in I_{\mathrm{rad},\Gamma}$, there has to be at least one $\lambda \in I_{\mathrm{rad}}$ such that $\Lambda_{\kappa,\lambda} > 0$. If $1 \geq \epsilon_{\mathrm{circ}} > 0$, then (3.7.81f) yields by (3.7.77) and (3.7.82):

$$\bigwedge_{\kappa \in I_{\mathrm{rad},\Gamma}} \quad \sum_{\lambda \in I_{\mathrm{rad},\Gamma}} |L_{\kappa,\lambda}| < \sum_{\lambda \in I_{\mathrm{rad}}} \Lambda_{\kappa,\lambda} = l_\kappa. \tag{3.7.83}$$

Thus

$$\bigwedge_{\kappa \in I_{\mathrm{rad},\Gamma}} \quad \sum_{\lambda \in I_{\mathrm{rad},\Gamma} \setminus \{\kappa\}} |A_{\kappa,\lambda}| < A_{\kappa,\kappa}, \tag{3.7.84}$$

showing that $\mathbf{A}$ is strictly diagonally dominant.

(b): Combining (3.7.81d), (3.7.81e), and (3.7.81f) with (3.7.82) shows that the hypothesis of Lem. C.3.2(b) is satisfied. Then (a) yields that $\mathbf{A}$ is an M-matrix. Thus, $\mathbf{A}$ is invertible, and $\mathbf{A}^{-1}$ is nonnegative according to Def. C.3.1(d) and Lem. C.3.2(a). ∎

Lemma 3.7.22(b) allows to write (3.7.81a) in the form

$$\mathbf{X} = \mathbf{A}^{-1}\,\mathbf{Y}. \tag{3.7.85}$$

Moreover, combining (3.7.85) with Lem. 3.7.22(b), (3.7.81c), and (3.7.81b) yields

$$\bigwedge_{\kappa \in I_{\mathrm{rad},\Gamma}} \quad R^{(\nu)}_{\mathrm{circ}}[x_\kappa] = X_\kappa \geq 0. \tag{3.7.86}$$

Finally, introducing the matrix $\tilde{\mathbf{L}} = (\tilde{L}_{\kappa,\lambda})_{(\kappa,\lambda) \in I^2_{\mathrm{rad},\Gamma}} \in \mathbb{R}^{I^2_{\mathrm{rad},\Gamma}}$,

$$\bigwedge_{(\kappa,\lambda) \in I^2_{\mathrm{rad},\Gamma}} \quad \tilde{L}_{\kappa,\lambda} := \epsilon_{\mathrm{circ}}\big[(T^{(\nu-1)}_{\mathrm{solid,circ}}[x_\kappa], x_\kappa)\big] \cdot \Lambda_{\kappa,\lambda}, \tag{3.7.87}$$

(3.7.85) allows to write (3.7.78) in the form

$$\mathbf{V} = \tilde{\mathbf{L}}\mathbf{A}^{-1}\mathbf{Y}, \tag{3.7.88}$$

where $\mathbf{V} = (V_\kappa)_{\kappa \in I_{\mathrm{rad},\Gamma}}$.

In the present example, the total space domain p can be decomposed into $p = p_{\mathrm{solid}} \cup p_{\mathrm{gas}}$, where p_{solid} and p_{gas} represent the domains of solid materials and gas cavities, respectively. The unknown is the temperature which is called $T_{\mathrm{solid,circ}}$ on p_{solid} and $T_{\mathrm{gas,circ}}$ on p_{gas}. Both $T_{\mathrm{solid,circ}}$ and $T_{\mathrm{gas,circ}}$ are continuous, but the temperature can be discontinuous on $p_{\mathrm{solid}} \cap p_{\mathrm{gas}}$. In particular, for each $k \in I_\Pi$, $\mathcal{G}_{\omega_k}$ has at most two connected components which are referred to by the supscripts "solid" and "gas". Thus, the notation $(k, \mathcal{C}) \in I_{\Pi,\mathfrak{D}}$ is replaced by $(k, \text{solid}) \in \mathrm{I}_{\Pi,\mathfrak{D}}$ and $(k, \text{gas}) \in \mathrm{I}_{\Pi,\mathfrak{D}}$, and

$$\bigwedge_{\nu \in \{0,\dots,n\}} \begin{pmatrix} U^{(\nu)}_{k,\text{solid}} = T^{(\nu)}_{\text{solid,circ}}[x_k] & \text{for } x_k \in p_{\text{solid}}, \\ U^{(\nu)}_{k,\text{gas}} = T^{(\nu)}_{\text{gas,circ}}[x_k] & \text{for } x_k \in p_{\text{gas}} \end{pmatrix}. \tag{3.7.89}$$

Moreover, it follows from the above definitions of $\mathbf{V}$, $\tilde{\mathbf{L}}$, $\mathbf{A}$, and $\mathbf{Y}$, that

$$\mathbf{V} = \mathbf{V}[(U^{(\nu-1)}, U^{(\nu)})] = \mathbf{V}\big[\big((U^{(\nu-1)}_{k,\text{solid}}, U^{(\nu)}_{k,\text{solid}})\big)_{k \in I_\Pi : x_k \in \Gamma}\big]. \tag{3.7.90}$$

One is now in the position to define $\mathfrak{B}^{(\nu)}_{k,\text{solid}}$ such that $-\mathfrak{B}^{(\nu)}_{k,\text{solid}}[(U^{(\nu-1)}, U^{(\nu)})]$ is an approximation of (3.5.24f) by letting

$$\bigwedge_{\substack{\nu \in \{1,\dots,n\}, \\ \Gamma \cap \partial_{\text{reg}}\omega_k \neq \emptyset}} \mathfrak{B}^{(\nu)}_{k,\text{solid}}[(U^{(\nu-1)}, U^{(\nu)})] := \sum_{\kappa \in I_{\omega_k}} V_\kappa[(U^{(\nu-1)}, U^{(\nu)})]. \tag{3.7.91}$$

Here it is used that $\Gamma \cap \partial_{\text{reg}}\omega_k \neq \emptyset$ implies $x_k \in \Gamma \cap \partial\omega_k$ by (dispt-(iii)) and that $x_\kappa = x_k$ for $\kappa \in I_{\omega_k}$ according to (3.7.70).

It was mentioned earlier that the discretization of nonlocal radiation operators on interfaces considered in Ex. 3.1.2(c) can be treated by a procedure analogous to the one presented above. In this case $p_{\text{rad}} \subseteq p$, $\Gamma = \partial p_{\text{rad}} = \Gamma_{\text{con}} \cup \Gamma_{\text{jump}}$, where $\Gamma_{\text{con}} := \Gamma \cap \bigcup_{\gamma \in \mathrm{IF}_{\text{con}}} \gamma$, $\Gamma_{\text{jump}} := \Gamma \cap \bigcup_{\gamma \in \mathrm{IF}_{\text{jump}}} \gamma$, and there is no Γ_{ph}, i.e. $I_{\text{rad},\Gamma} = I_{\text{rad}}$. For each control volume ω such that $I_\omega \neq \emptyset$, let $I_{\omega,\text{con}} := \{\kappa \in I_{\text{rad}} : \Gamma_{\text{con}} \cap \text{int}[\zeta_\kappa] \cap \partial_{\text{reg}}\omega \neq \emptyset\}$, $I_{\omega,\text{jump}} := \{\kappa \in I_{\text{rad}} : \Gamma_{\text{jump}} \cap \text{int}[\zeta_\kappa] \cap \partial_{\text{reg}}\omega \neq \emptyset\}$. Depending on the case of Ex. 3.1.2(c), one has to replace ϵ_{circ} with $\epsilon_{\text{t,circ}}$, $\epsilon_{\text{t,circ}} + \epsilon_{\text{r,circ}}$, or $\epsilon_{\text{r,circ}}$. One is then led to the following definitions of $\mathfrak{A}^{(\nu)}_{\text{con},k,\text{solid}}$ and $\mathfrak{A}^{(\nu)}_{\text{jump},k,\text{solid}}$ such that $-\mathfrak{A}^{(\nu)}_{\text{con},k,\text{solid}}[(U^{(\nu-1)}, U^{(\nu)})]$ and $-\mathfrak{A}^{(\nu)}_{\text{jump},k,\text{solid}}[(U^{(\nu-1)}, U^{(\nu)})]$ are approximations of (3.5.24h) and (3.5.24k), respectively:

$$\bigwedge_{\substack{\nu \in \{1,\dots,n\}, \\ \Gamma_{\text{con}} \cap \partial_{\text{reg}}\omega_k \neq \emptyset}} \mathfrak{A}^{(\nu)}_{\text{con},k,\text{solid}}[(U^{(\nu-1)}, U^{(\nu)})] := \sum_{\kappa \in I_{\omega_k,\text{con}}} V_\kappa[(U^{(\nu-1)}, U^{(\nu)})], \tag{3.7.92}$$

$$\bigwedge_{\substack{\nu \in \{1,\dots,n\}, \\ \Gamma_{\text{jump}} \cap \partial_{\text{reg}}\omega_k \neq \emptyset}} \mathfrak{A}^{(\nu)}_{\text{jump},k,\text{solid}}[(U^{(\nu-1)}, U^{(\nu)})] := \sum_{\kappa \in I_{\omega_k,\text{jump}}} V_\kappa[(U^{(\nu-1)}, U^{(\nu)})]. \tag{3.7.93}$$

It is used that $\Gamma_{\text{con}} \cap \partial_{\text{reg}}\omega_k \neq \emptyset$ implies $x_k \in \Gamma_{\text{con}} \cap \partial\omega_k$ by (3.7.52) and analogously for Γ_{jump}.

The situation of Ex. 3.1.2(c) is depicted in Fig. 3.1 on p. 50. In this case, one has $\Omega_{j_1} \cap \Omega_{j_2} \subseteq \Gamma_{\text{jump}}$, $\Omega_{j_1} \cap \Omega_{j_3} \subseteq \Gamma_{\text{jump}}$, $\Omega_{j_1} \cap \Omega_{j_4} \subseteq \Gamma_{\text{jump}}$, and $\Omega_{j_3} \cap \Omega_{j_4} \subseteq \Gamma_{\text{con}}$.

3.7.9 Upper Bound for Terms on Outer Boundaries

In this section, under suitable hypotheses, upper bounds are proved for the contributions to the operators $\mathfrak{s}^{(\nu)}$ stemming from terms on outer boundaries, i.e. stemming from $\mathfrak{h}^{(\nu)}_{(k,\mathcal{C}),(c)}$, $\mathfrak{h}^{(\nu)}_{(k,\mathcal{C}),(f)}$, and $\mathfrak{h}^{(\nu)}_{(k,\mathcal{C}),(g)}$. Since no universal discretization procedure was given for the nonlocal boundary operators $\mathcal{B}_{j,\iota}$ in Sec. 3.7.7, a general estimate just depending on conditions on the input functions can only be expected if no nonlocal boundary operators are present. Therefore, the strategy in the following is different from the procedure that was used for the corresponding estimates in earlier sections. First, Def. 3.7.23 defines the needed estimate as a property of the discretization operators. If no nonlocal boundary operators are present, Lem. 3.7.25 proves the upper bound, using a sufficient condition on the input functions. Finally, Ex. 3.7.27 proves an upper bound for the case where the nonlocal boundary operator is as in Sec. 3.7.8, i.e. it represents the nonlocal radiation operators arising from Ex. 3.1.3(e).

Definition 3.7.23. The discretizations $\mathfrak{B}^{(\nu)}_{(k,\mathcal{C})}$, $\mathfrak{v}^{(\nu)}_{\mathrm{out},(k,\mathcal{C})}$, and $\mathfrak{a}^{(\nu)}_{\mathrm{out},(k,\mathcal{C})}$, $(k,\mathcal{C}) \in I_{\Pi,\mathfrak{D},\neg\mathrm{Dir}}$, are called *bounded from above* iff they are real-valued and there is $B_{\mathrm{out}}[\mathfrak{C}] \in \mathbb{R}$ such that independently of Π and ν,

$$\sum_{(k,\mathcal{C})\in I_{\Pi,\mathfrak{D},\neg\mathrm{Dir}}} \left(\mathfrak{B}^{(\nu)}_{(k,\mathcal{C})} - \mathfrak{v}^{(\nu)}_{\mathrm{out},(k,\mathcal{C})} - \mathfrak{a}^{(\nu)}_{\mathrm{out},(k,\mathcal{C})}\right) \leq B_{\mathrm{out}}[\mathfrak{C}] \cdot \lambda_{d-1}[\partial p]. \tag{3.7.94}$$

Remark 3.7.24. As a trivial consequence of Def. 3.7.23, if $\mathfrak{B}^{(\nu)}_{(k,\mathcal{C})}$, $\mathfrak{v}^{(\nu)}_{\mathrm{out},(k,\mathcal{C})}$, and $\mathfrak{a}^{(\nu)}_{\mathrm{out},(k,\mathcal{C})}$, $(k,\mathcal{C}) \in I_{\Pi,\mathfrak{D},\neg\mathrm{Dir}}$, are bounded from above, then

$$\bigwedge_{\nu\in\{0,\dots,n\}} \left(\begin{aligned} &-\sum_{(k,\mathcal{C})\in I_{\Pi,\mathfrak{D},\neg\mathrm{Dir}}} \left(\mathfrak{h}^{(\nu)}_{(k,\mathcal{C}),(c)} + \mathfrak{h}^{(\nu)}_{(k,\mathcal{C}),(f)} + \mathfrak{h}^{(\nu)}_{(k,\mathcal{C}),(g)}\right) \\ &= \sum_{(k,\mathcal{C})\in I_{\Pi,\mathfrak{D},\neg\mathrm{Dir}}} \left(\mathfrak{B}^{(\nu)}_{(k,\mathcal{C})} - \mathfrak{v}^{(\nu)}_{\mathrm{out},(k,\mathcal{C})} - \mathfrak{a}^{(\nu)}_{\mathrm{out},(k,\mathcal{C})}\right) \leq B_{\mathrm{out}}[\mathfrak{C}] \cdot \lambda_{d-1}[\partial p] \end{aligned} \right). \tag{3.7.95}$$

Lemma 3.7.25. *Suppose that all nonlocal boundary operators vanish (i.e. $\mathcal{B}_{j,\iota} = \mathfrak{B}^{(\nu)}_{(k,\mathcal{C})} = 0$). Moreover, assume that for each $(j,\iota) \in J \times \big(J_j \setminus \{0\}\big)$, the functions $a^{j,\iota}_{\mathrm{out}}$ are real-valued, and that the function*

$$\begin{aligned} \mathrm{av}^{j,\iota}_{\mathrm{out}} &: \upsilon \times \upsilon \times \tau \times \Gamma_{j,\iota} \longrightarrow \mathbb{R}, \\ \mathrm{av}^{j,\iota}_{\mathrm{out}}[(\tilde{y},y,t,x)] &:= -v_j[(y,t,x)] \bullet n_{p_j}[x] - \left(a^{j,\iota}_{\mathrm{out}}\right)^{\text{ex.-im.}}\big[\big((\tilde{y},y),t,x\big)\big], \end{aligned} \tag{3.7.96}$$

is bounded from above. Then $\mathfrak{B}^{(\nu)}_{(k,\mathcal{C})}$, $\mathfrak{v}^{(\nu)}_{\mathrm{out},(k,\mathcal{C})}$, and $\mathfrak{a}^{(\nu)}_{\mathrm{out},(k,\mathcal{C})}$, $(k,\mathcal{C}) \in I_{\Pi,\mathfrak{D},\neg\mathrm{Dir}}$, are bounded from above with

$$B_{\mathrm{out}}[\mathfrak{C}] := \max\big\{ \sup(\mathrm{av}^{j,\iota}_{\mathrm{out}}) : (j,\iota) \in J \times \big(J_j \setminus \{0\}\big) \big\}. \tag{3.7.97}$$

Proof. The hypothesis implies that each

$$-v^{(\nu)}_{j,\mathrm{sca}}[(y,x_k)]v^{(\nu)}_{j,\mathrm{vec}}[x_k] \bullet n_{\omega_k^{(j)}} - (a^{j,\iota,\nu}_{\mathrm{out}})^{\text{ex.-im.}}\big[\big((\tilde{y},y),x_k\big)\big]$$

is bounded from above by $B_{\mathrm{out}}[\mathfrak{C}]$. Hence, (3.7.94) follows from (3.7.49) and (3.7.51), and since $(\omega_k^{(j)})_{j\in J:k\in I^{(j)}}$ is a partition of ω_k, $k \in I_\Pi$, Π is a partition of p, and $(\Gamma_{j,\iota})_{\iota\in J_j}$ is a partition of $\partial p \cap \partial p_j$. ■

Example 3.7.26. Examples 3.1.3(b),(c),(d), Ex. 3.1.1(b), and the first case of 3.1.1(a) are investigated with respect to the hypothesis of Lem. 3.7.25, i.e. with respect to whether $\mathrm{av}^{j,\iota}_{\mathrm{out}}$ is bounded from above. In each of these cases, it is $\mathcal{B}_{j,\iota} = 0$.

Suppose $\upsilon = [m_\upsilon, \infty[$, as for example if the unknown represents temperature. Moreover, let Γ be a $(d-1)$-dimensional polyhedral subset of ∂p.

It is first assumed that $(a^{j,\iota}_{\mathrm{out}})^{\text{ex.-im.}}\big[\big((\tilde{y},y),t,x\big)\big] = a^{j,\iota}_{\mathrm{out}}[(y,t,x)]$, i.e. there is no dependency splitting.

For the boundary conditions considered in Exs 3.1.3(b),(c),(d), using natural hypotheses, $-a^{j,\iota}_{\mathrm{out}}$ is always bounded from above: Let $a^{j,\iota}_{\mathrm{out}} \in C(\tau \times \Gamma, \mathbb{R})$. Ex. 3.1.3(b): $\sup(-a^{j,\iota}_{\mathrm{out}}) = \max\{-a^{j,\iota}_{\mathrm{out}}[(t,x)] : (t,x) \in \tau \times \Gamma\}$ since $a^{j,\iota}_{\mathrm{out}}$ does not depend on the unknown. Ex. 3.1.3(c): $\sup(-a^{j,\iota}_{\mathrm{out}}) \le \xi\big(\|u_{\mathrm{ext}}\|_{\max} - m_\upsilon\big)$ for $-a^{j,\iota}_{\mathrm{out}}[(y,t,x)] = \xi\big(u_{\mathrm{ext}}[(t,x)] - y\big)$, $\xi \in \mathbb{R}^+$, $u_{\mathrm{ext}} \in C(\tau \times \Gamma, \mathbb{R})$. Ex. 3.1.3(d): $\sup(-a^{j,\iota}_{\mathrm{out}}) \le \sigma T^4_{\mathrm{room}}$ for $m_\upsilon = 0$, $-a^{j,\iota}_{\mathrm{out}}[(y,t,x)] = \sigma\epsilon[(y,t,x)](T^4_{\mathrm{room}} - y^4)$, $\sigma \in \mathbb{R}^+$, $\epsilon \in C\big(\upsilon \times \tau \times \Gamma, [0,1]\big)$, $T_{\mathrm{room}} \in \upsilon$.

Thus, in these cases, $\mathrm{av}^{j,\iota}_{\mathrm{out}}$ is bounded from above if $-v_j\restriction_{\upsilon\times\tau\times\Gamma} \bullet n_{p_j}$ is bounded from above, e.g. if v_j does not depend on the unknown as in the second case of Ex. 3.1.1(b). However, if $-v_j\restriction_{\upsilon\times\tau\times\Gamma} \bullet n_{p_j}$ is not bounded from above, then $\mathrm{av}^{j,\iota}_{\mathrm{out}}$ can only be bounded from above if the two remaining summands of $\mathrm{av}^{j,\iota}_{\mathrm{out}}$ compensate each other. Example 3.1.1(a), first case: One has $-v_j[(y,t,x)] = -y\mathbf{v}_{\mathrm{gas}}[x]$. Letting $\lambda := \max(-\mathbf{v}_{\mathrm{gas}}\restriction_\Gamma \bullet n_{p_j})$, $-v_j\restriction_{\upsilon\times\tau\times\Gamma} \bullet n_{p_j}$ is bounded from above if and only if $\lambda \le 0$. If $\lambda > 0$ and $-a^{j,\iota}_{\mathrm{out}}[(y,t,x)] = \xi\big(u_{\mathrm{ext}}[(t,x)] - y\big)$, $\xi \in \mathbb{R}^+$, then $\mathrm{av}^{j,\iota}_{\mathrm{out}}$ is bounded from above if and only if $\lambda - \xi \le 0$. If $-a^{j,\iota}_{\mathrm{out}}[(y,t,x)] = \sigma\epsilon[(y,t,x)]\big(T^4_{\mathrm{room}} - y^4\big)$, then $\mathrm{av}^{j,\iota}_{\mathrm{out}}$ is bounded from above if ϵ is bounded away from zero. The first case of Ex. 3.1.1(b), where $v_j[(y,t,x)] := \frac{\left(z^{(\mathrm{Ar})}+1\right)R}{M^{(\mathrm{Ar})}}\,\rho_{\mathrm{gas}}\,y\mathbf{v}_{\mathrm{gas}}[x]$, is similar. Example 3.1.1(b), third case: One has $-v_j[(y,t,x)] := -\varepsilon_{\mathrm{gas}}[y]\,\rho_{\mathrm{gas}}[x]\mathbf{v}_{\mathrm{gas}}[x]$, and whether $\mathrm{av}^{j,\iota}_{\mathrm{out}}$ is bounded from above or not depends on the special form of ε.

Finally, consider Ex. 3.1.3(d) with the dependency splitting

$$(a^{j,\iota}_{\mathrm{out}})^{\text{ex.-im.}}\big[\big((\tilde{y},y),t,x\big)\big] = \sigma\epsilon[(\tilde{y},t,x)](y^4 - T^4_{\mathrm{room}}).$$

Since ϵ is $[0,1]$-valued, $-(a^{j,\iota}_{\mathrm{out}})^{\text{ex.-im.}}$ is bounded from above. Moreover, it is still true, that for $-v_j[(y,t,x)] = -y\mathbf{v}_{\mathrm{gas}}[x]$, the function $\mathrm{av}^{j,\iota}_{\mathrm{out}}$ is bounded from above if ϵ is bounded away from zero.

Example 3.7.27. As in Sec. 3.7.8, consider the case where the nonlocal boundary operator $\mathcal{B} := \mathcal{B}_{j,\iota}$ is given by (3.7.68), i.e. it represents the nonlocal radiation operators arising from Ex. 3.1.3(e). Moreover, considering Ex. 3.1.3(e) in axisymmetric form, one has

$$a_{\text{out}}[(T_{\text{solid,circ}}, t, x)] := a_{\text{out}}^{j,\iota}[(T_{\text{solid,circ}}, t, x)] = \epsilon_{\text{circ}}[(T_{\text{solid,circ}}, x)]\, \sigma\, T_{\text{solid,circ}}^4.$$

Thus, using the dependency splitting of Ex. 3.4.12, it is

$$\begin{aligned} &\mathcal{B}^{\text{ex.-im.}}[(T_{\text{solid,circ}}^{(\nu-1)}, T_{\text{solid,circ}}^{(\nu)})][x] - \left(a_{\text{out}}^{(\nu)}\right)^{\text{ex.-im.}}\left[\left((T_{\text{solid,circ}}^{(\nu-1)}, T_{\text{solid,circ}}^{(\nu)}), x\right)\right] \\ &= \epsilon_{\text{circ}}[(T_{\text{solid,circ}}^{(\nu-1)}, x)] \cdot \mathcal{J}_{\text{circ}}\left[\mathcal{R}_{\text{circ}}[T_{\text{solid,circ}}^{(\nu)}]\right] - \epsilon_{\text{circ}}[(T_{\text{solid,circ}}^{(\nu-1)}, x)]\, \sigma \left(T_{\text{solid,circ}}^{(\nu)}\right)^4. \end{aligned} \tag{3.7.98}$$

The considerations of Sec. 3.7.8 led to the definition of $\mathfrak{B}_{(k,\mathcal{C})}^{(\nu)} = \mathfrak{B}_{k,\text{solid}}^{(\nu)}$ in (3.7.91). Together with $\mathfrak{a}_{\text{out},k,\text{solid}}^{(\nu)} = \mathfrak{a}_{\text{out},(k,\mathcal{C})}^{(\nu)}$ defined according to (3.7.51), and recalling (3.7.89), this yields

$$\begin{aligned} &\mathfrak{B}_{k,\text{solid}}^{(\nu)}[(U^{(\nu-1)}, U^{(\nu)})] - \mathfrak{a}_{\text{out},k,\text{solid}}^{(\nu)}[(U_{k,\text{solid}}^{(\nu-1)}, U_{k,\text{solid}}^{(\nu)})] \\ &= \sum_{\kappa \in I_{\omega_k}} \Big(V_\kappa[(U^{(\nu-1)}, U^{(\nu)})] - \epsilon_{\text{circ}}[(U_{k,\text{solid}}^{(\nu-1)}, x_k)]\, \sigma \left(U_{k,\text{solid}}^{(\nu)}\right)^4 l_\kappa\Big). \end{aligned} \tag{3.7.99}$$

Let $I_{\text{rad,ph}} := I_{\text{rad}} \setminus I_{\text{rad},\Gamma}$. The following (3.7.100) is another instance of the conservation of radiation energy. Using that $\Gamma \cup \Gamma_{\text{ph}}$ as defined in Sec. 3.7.8 (s. Fig. 3.22 on p. 123) forms the circular projection of a closed surface, and using (3.7.99), (3.7.89), and (3.7.78), one calculates

$$\begin{aligned} &\sum_{(k,\mathcal{C}) \in I_{\Pi,\mathfrak{D},\neg\text{Dir}}} \left(\mathfrak{B}_{(k,\mathcal{C})}^{(\nu)}[(U^{(\nu-1)}, U^{(\nu)})] - \mathfrak{a}_{\text{out},(k,\mathcal{C})}^{(\nu)}[(U_{(k,\mathcal{C})}^{(\nu-1)}, U_{(k,\mathcal{C})}^{(\nu)})]\right) \\ &= \sum_{\kappa \in I_{\text{rad},\Gamma}} \epsilon_{\text{circ}}\left[(T_{\text{solid,circ}}^{(\nu-1)}[x_\kappa], x_\kappa)\right] \sum_{\lambda \in I_{\text{rad}}} R_{\text{circ}}^{(\nu)}[x_\lambda]\, \Lambda_{\kappa,\lambda} \\ &\qquad - \sum_{\kappa \in I_{\text{rad},\Gamma}} \epsilon_{\text{circ}}\left[(T_{\text{solid,circ}}^{(\nu-1)}[x_\kappa], x_\kappa)\right] \sigma \left(T_{\text{solid,circ}}^{(\nu)}[x_\kappa]\right)^4 l_\kappa \\ &\overset{(3.7.80)}{=} - \sum_{\kappa \in I_{\text{rad},\Gamma}} R_{\text{circ}}^{(\nu)}[x_\kappa] l_\kappa + \sum_{\kappa \in I_{\text{rad},\Gamma}} \sum_{\lambda \in I_{\text{rad}}} R_{\text{circ}}^{(\nu)}[x_\lambda]\, \Lambda_{\kappa,\lambda} \\ &\overset{(3.7.77)}{=} - \sum_{\kappa \in I_{\text{rad},\Gamma}} R_{\text{circ}}^{(\nu)}[x_\kappa] \sum_{\lambda \in I_{\text{rad}}} \Lambda_{\kappa,\lambda} + \sum_{\kappa \in I_{\text{rad},\Gamma}} \sum_{\lambda \in I_{\text{rad}}} R_{\text{circ}}^{(\nu)}[x_\lambda]\, \Lambda_{\kappa,\lambda} \\ &\overset{(3.7.76)}{=} - \sum_{\kappa \in I_{\text{rad},\Gamma}} \sum_{\lambda \in I_{\text{rad}}} R_{\text{circ}}^{(\nu)}[x_\kappa] \Lambda_{\kappa,\lambda} + \sum_{\lambda \in I_{\text{rad},\Gamma}} \sum_{\kappa \in I_{\text{rad}}} R_{\text{circ}}^{(\nu)}[x_\kappa]\, \Lambda_{\kappa,\lambda} \\ &= - \sum_{\kappa \in I_{\text{rad},\Gamma}} \sum_{\lambda \in I_{\text{rad,ph}}} R_{\text{circ}}^{(\nu)}[x_\kappa] \Lambda_{\kappa,\lambda} + \sum_{\lambda \in I_{\text{rad},\Gamma}} \sum_{\kappa \in I_{\text{rad,ph}}} R_{\text{circ}}^{(\nu)}[x_\kappa]\, \Lambda_{\kappa,\lambda} \end{aligned}$$

$$\stackrel{(3.7.86)}{\leq} \sum_{\lambda \in I_{\mathrm{rad},\Gamma}} \sum_{\kappa \in I_{\mathrm{rad,ph}}} R^{(\nu)}_{\mathrm{circ}}[x_\kappa]\, \Lambda_{\kappa,\lambda} \stackrel{(3.7.69)}{\leq} \sigma\, T^4_{\mathrm{room}} \sum_{\lambda \in I_{\mathrm{rad},\Gamma}} \sum_{\kappa \in I_{\mathrm{rad,ph}}} \Lambda_{\kappa,\lambda}$$
$$\stackrel{(3.7.77)}{\leq} \sigma\, T^4_{\mathrm{room}} \sum_{\kappa \in I_{\mathrm{rad,ph}}} l_\kappa \stackrel{(3.7.77)}{\leq} \sigma\, T^4_{\mathrm{room}} \int_{\Gamma_{\mathrm{ph}}} r \,\mathrm{d}(r,z) < \infty. \tag{3.7.100}$$

Thus, for $\mathfrak{v}^{(\nu)}_{\mathrm{out},(k,\mathcal{C})} = 0$, (3.7.100) shows that the operators are bounded from above in the sense of Def. 3.7.23.

It is remarked that it is straightforward to superpose the situation of the present example with the situations considered in Ex. 3.7.26 (discarding the condition $\mathcal{B}_{j,\iota} = 0$ in Ex. 3.7.26).

3.7.10 Upper Bound for Terms on Interfaces

In this section, under suitable hypotheses, upper bounds are proved for the contributions to the operators $\mathfrak{s}^{(\nu)}$ stemming from terms on interfaces, i.e. stemming from $\mathfrak{h}^{(\nu)}_{(k,\mathcal{C}),(d)}$, and $\mathfrak{h}^{(\nu)}_{(k,\mathcal{C}),(h)}, \dots, \mathfrak{h}^{(\nu)}_{(k,\mathcal{C}),(m)}$. The following is organized analogous to the strategy described at the beginning of the previous Sec. 3.7.9.

Definition 3.7.28. The discretizations

$$\begin{gathered}\mathfrak{A}^{(\nu)}_{\mathrm{con},(k,\mathcal{C})}, \mathfrak{v}^{(\nu)}_{\mathrm{con},(k,\mathcal{C})}, \mathfrak{a}^{(\nu)}_{\mathrm{flux,con},(k,\mathcal{C})}, \mathfrak{A}^{(\nu)}_{\mathrm{jump},(k,\mathcal{C})}, \mathfrak{v}^{(\nu)}_{\mathrm{jump},(k,\mathcal{C})},\\ \mathfrak{a}^{(\nu)}_{\mathrm{jump,1,Dir},(k,\mathcal{C})}, \mathfrak{a}^{(\nu)}_{\mathrm{jump,2,Dir},(k,\mathcal{C})}, \mathfrak{a}^{(\nu)}_{\mathrm{flux,jump,2,\neg Dir},(k,\mathcal{C})}, \mathfrak{a}^{(\nu)}_{\mathrm{flux,jump,2,Dir},(k,\mathcal{C})},\end{gathered} \tag{3.7.101}$$

$(k,\mathcal{C}) \in I_{\Pi,\mathfrak{D},\neg\mathrm{Dir}}$, are called *bounded from above* iff they are real-valued and there is $B_{\mathrm{IF}}[\mathfrak{C}] \in \mathbb{R}$ such that independently of Π and ν,

$$\begin{aligned}\sum_{(k,\mathcal{C}) \in I_{\Pi,\mathfrak{D},\neg\mathrm{Dir}}} \Big(&\mathfrak{A}^{(\nu)}_{\mathrm{con},(k,\mathcal{C})} - \mathfrak{v}^{(\nu)}_{\mathrm{con},(k,\mathcal{C})} - \mathfrak{a}^{(\nu)}_{\mathrm{flux,con},(k,\mathcal{C})} + \mathfrak{A}^{(\nu)}_{\mathrm{jump},(k,\mathcal{C})} - \mathfrak{v}^{(\nu)}_{\mathrm{jump},(k,\mathcal{C})} - \mathfrak{a}^{(\nu)}_{\mathrm{jump,1,Dir},(k,\mathcal{C})}\\ &- \mathfrak{a}^{(\nu)}_{\mathrm{jump,2,Dir},(k,\mathcal{C})} - \mathfrak{a}^{(\nu)}_{\mathrm{flux,jump,2,\neg Dir},(k,\mathcal{C})} - \mathfrak{a}^{(\nu)}_{\mathrm{flux,jump,2,Dir},(k,\mathcal{C})}\Big)\\ \leq B_{\mathrm{IF}}[\mathfrak{C}] \cdot \sum_{\gamma \in \mathrm{IF}} \lambda_{d-1}[\gamma].\end{aligned} \tag{3.7.102}$$

—

The following Lem. 3.7.33 is similar to Lems 3.7.4 and 3.7.16.

Lemma 3.7.29. *The following holds:*

$$\bigwedge_{\nu \in \{0,\dots,n\}} \sum_{(k,\mathcal{C}) \in I_{\Pi,\mathfrak{D},\neg\mathrm{Dir}}} \left(\mathfrak{a}^{(\nu)}_{\mathrm{jump,1,\neg Dir},(k,\mathcal{C})} + \mathfrak{a}^{(\nu)}_{\mathrm{jump,2,\neg Dir},(k,\mathcal{C})}\right) = 0. \tag{3.7.103}$$

Proof. Fix $U \in v^{I_{\Pi,\mathfrak{D},\neg\mathrm{Dir}}}$.
Due to (3.7.59), $\mathfrak{a}_1[U] := \sum_{(k,\mathcal{C})\in I_{\Pi,\mathfrak{D},\neg\mathrm{Dir}}} \mathfrak{a}^{(\nu)}_{\mathrm{jump},1,\neg\mathrm{Dir},(k,\mathcal{C})}[U]$ actually involves a sum over the set

$$A := \Big\{ \big((k,\mathcal{C}),\gamma\big) \in I_{\Pi,\mathfrak{D},\neg\mathrm{Dir}} \times G_{\mathrm{jump},1}[\mathcal{C}] : \\ \big(k, \mathcal{C}[(k,i_2[\gamma])]\big) \in I_{\Pi,\mathfrak{D},\neg\mathrm{Dir}},\ \lambda_{d-1}\Big[\gamma \cap \partial\omega_k^{(i_1[\gamma])}\Big] > 0 \Big\}. \tag{3.7.104}$$

Analogously, due to (3.7.65), $\mathfrak{a}_2[U] := \sum_{(k,\mathcal{C})\in I_{\Pi,\mathfrak{D},\neg\mathrm{Dir}}} \mathfrak{a}^{(\nu)}_{\mathrm{jump},2,\neg\mathrm{Dir},(k,\mathcal{C})}[U]$ involves a sum over

$$B := \Big\{ \big((k,\mathcal{C}),\gamma\big) \in I_{\Pi,\mathfrak{D},\neg\mathrm{Dir}} \times G_{\mathrm{jump},2}[\mathcal{C}] : \\ \big(k, \mathcal{C}[(k,i_1[\gamma])]\big) \in I_{\Pi,\mathfrak{D},\neg\mathrm{Dir}},\ \lambda_{d-1}\Big[\gamma \cap \partial\omega_k^{(i_2[\gamma])}\Big] > 0 \Big\}. \tag{3.7.105}$$

Now a bijection $\mathcal{I}: A \longrightarrow B$ is established by letting

$$\mathcal{I}\Big[\big((k,\mathcal{C}),\gamma\big)\Big] := \Big(\big(k,\mathcal{C}[(k,i_2[\gamma])]\big),\gamma\Big). \tag{3.7.106}$$

The proof is completed by observing that for each $\big((k,\mathcal{C}),\gamma\big) \in A$, the summand of $\mathfrak{a}_1[U]$ corresponding to $\big((k,\mathcal{C}),\gamma\big)$ cancels the summand of $\mathfrak{a}_2[U]$ corresponding to $\mathcal{I}\big[\big((k,\mathcal{C}),\gamma\big)\big]$ (cf. Rem. 3.5.7). ■

Remark 3.7.30. As a trivial consequence of Def. 3.7.28 and Lem. 3.7.29, if the discretizations (3.7.101) are bounded from above, then

$$\bigwedge_{\nu\in\{0,\dots,n\}} \left(\begin{aligned} & -\sum_{(k,\mathcal{C})\in I_{\Pi,\mathfrak{D},\neg\mathrm{Dir}}} \Big(\mathfrak{h}^{(\nu)}_{(k,\mathcal{C}),(d)} + \mathfrak{h}^{(\nu)}_{(k,\mathcal{C}),(h)} + \mathfrak{h}^{(\nu)}_{(k,\mathcal{C}),(i)} \\ & \qquad + \mathfrak{h}^{(\nu)}_{(k,\mathcal{C}),(j)} + \mathfrak{h}^{(\nu)}_{(k,\mathcal{C}),(k)} + \mathfrak{h}^{(\nu)}_{(k,\mathcal{C}),(l)} + \mathfrak{h}^{(\nu)}_{(k,\mathcal{C}),(m)} \Big) \\ & = \sum_{(k,\mathcal{C})\in I_{\Pi,\mathfrak{D},\neg\mathrm{Dir}}} \Big(\mathfrak{A}^{(\nu)}_{\mathrm{con},(k,\mathcal{C})} - \mathfrak{v}^{(\nu)}_{\mathrm{con},(k,\mathcal{C})} - \mathfrak{a}^{(\nu)}_{\mathrm{flux,con},(k,\mathcal{C})} \\ & \qquad + \mathfrak{A}^{(\nu)}_{\mathrm{jump},(k,\mathcal{C})} - \mathfrak{v}^{(\nu)}_{\mathrm{jump},(k,\mathcal{C})} - \mathfrak{a}^{(\nu)}_{\mathrm{jump},1,\mathrm{Dir},(k,\mathcal{C})} \\ & \qquad - \mathfrak{a}^{(\nu)}_{\mathrm{jump},2,\mathrm{Dir},(k,\mathcal{C})} - \mathfrak{a}^{(\nu)}_{\mathrm{flux,jump},2,\neg\mathrm{Dir},(k,\mathcal{C})} - \mathfrak{a}^{(\nu)}_{\mathrm{flux,jump},2,\mathrm{Dir},(k,\mathcal{C})} \Big) \\ & \le B_{\mathrm{IF}}[\mathfrak{C}] \cdot \sum_{\gamma\in\mathrm{IF}} \lambda_{d-1}[\gamma] \end{aligned} \right).$$

If there are no nonlocal interface operators, then the operators (3.7.101) are bounded from above, given a sufficient condition on the input function. This is the contents of the following Lems 3.7.31 and 3.7.33, and of Rem. 3.7.35, where Lem. 3.7.31 deals with terms on continuous interfaces, and Lem. 3.7.33 deals with terms on jump interfaces.

Lemma 3.7.31. *If for each $\gamma \in \mathrm{IF}_{\mathrm{con}}$, the functions $a_{\mathrm{flux}}^{\gamma,\alpha}$, $\alpha \in \{1,2\}$, are real-valued, and the function*

$$\begin{aligned} \mathrm{av}_{\mathrm{con}}[\gamma] &: \upsilon \times \upsilon \times \tau \times \gamma \longrightarrow \mathbb{R}, \\ \mathrm{av}_{\mathrm{con}}[\gamma][(\tilde{y},y,t,x)] &:= -\sum_{\alpha\in\{1,2\}} v_{i_\alpha[\gamma]}[(y,t,x)] \bullet n_{p_{i_\alpha[\gamma]}}[x] \\ &\qquad + \left(a_{\mathrm{flux}}^{\gamma,1}\right)^{\text{ex.-im.}}\left[\big((\tilde{y},y),t,x\big)\right] - \left(a_{\mathrm{flux}}^{\gamma,2}\right)^{\text{ex.-im.}}\left[\big((\tilde{y},y),t,x\big)\right] \end{aligned} \tag{3.7.108}$$

is bounded from above, then

$$\bigwedge_{\nu\in\{0,\dots,n\}} \quad \sum_{(k,\mathcal{C})\in I_{\Pi,\mathfrak{D},\neg\mathrm{Dir}}} \left(-\mathfrak{v}_{\mathrm{con},(k,\mathcal{C})}^{(\nu)} - \mathfrak{a}_{\mathrm{flux,con},(k,\mathcal{C})}^{(\nu)}\right) \le B_{\mathrm{con}}[\mathfrak{C}] \cdot \sum_{\gamma\in\mathrm{IF}_{\mathrm{con}}} \lambda_{d-1}[\gamma], \tag{3.7.109}$$

where

$$B_{\mathrm{con}}[\mathfrak{C}] := \max\left\{ \sup(\mathrm{av}_{\mathrm{con}}[\gamma]) : \gamma \in \mathrm{IF}_{\mathrm{con}} \right\}. \tag{3.7.110}$$

Proof. The hypothesis implies that each

$$\begin{aligned} &-\sum_{\alpha\in\{1,2\}} v_{i_\alpha[\gamma],\mathrm{sca}}^{(\nu)}[(y,x_k)]\, v_{i_\alpha[\gamma],\mathrm{vec}}^{(\nu)}[x_k] \bullet n_{\omega_k^{(i_\alpha[\gamma])}} \\ &+\left(a_{\mathrm{flux}}^{\gamma,1,\nu}\right)^{\text{ex.-im.}}\left[\big((\tilde{y},y),x_k\big)\right] - \left(a_{\mathrm{flux}}^{\gamma,2,\nu}\right)^{\text{ex.-im.}}\left[\big((\tilde{y},y),x_k\big)\right] \end{aligned}$$

is bounded from above by $B_{\mathrm{con}}[\mathfrak{C}]$. Hence, (3.7.109) follows from (3.7.54) and (3.7.57), since $(\omega_k^{(j)})_{j\in J:k\in I^{(j)}}$ is a partition of ω_k, $k \in I_\Pi$, Π is a partition of p, and since $\gamma \cap \partial_{\mathrm{reg}}\omega_k^{(j)} \neq \emptyset$ holds if and only if $j \in \{i_1[\gamma], i_2[\gamma]\}$. ∎

Example 3.7.32. Suppose $\gamma \in \mathrm{IF}_{\mathrm{con}}$ is a continuous interface. Let $v_{\alpha,\gamma} := v_{i_\alpha[\gamma]}\restriction_{\upsilon\times\tau\times\gamma}$, $\alpha \in \{1,2\}$. Suppose $\upsilon = [m_\upsilon, \infty[$ and that there is no dependency splitting, i.e. $(a_{\mathrm{flux}}^{\gamma,\alpha})^{\text{ex.-im.}}\left[\big((\tilde{y},y),t,x\big)\right] = a_{\mathrm{flux}}^{\gamma,\alpha}[(y,t,x)]$.

The function $\mathrm{av}_{\mathrm{con}}[\gamma]$ is bounded from above for $a_{\mathrm{flux}}^{\gamma,1} = a_{\mathrm{flux}}^{\gamma,2} = 0$ if both $v_{1,\gamma}$ and $v_{2,\gamma}$ are independent of $y \in \upsilon$ or if $v_{1,\gamma} = v_{2,\gamma}$, i.e. if the convection through γ is continuous.

However, in general, if the convection through the interface γ is discontinuous, then $\mathrm{av}_{\mathrm{con}}[\gamma]$ is only bounded from above for a suitable nonvanishing choice of $a_{\mathrm{flux}}^{\gamma,1}$ and $a_{\mathrm{flux}}^{\gamma,2}$. For example, if $v_{1,\gamma} = 0$ and $v_{2,\gamma}[(y,t,x)] = -y n_{p_{i_2[\gamma]}}$, then $\mathrm{av}_{\mathrm{con}}[\gamma]$ is bounded from above for $a_{\mathrm{flux}}^{\gamma,1} = 0$ and $a_{\mathrm{flux}}^{\gamma,2}[(y,t,x)] = \xi y$, $\xi \in [1,\infty[$.

Lemma 3.7.33. *Assume that for each $\gamma \in \mathrm{IF}_{\mathrm{jump}}$, the functions $a_{\mathrm{flux}}^{\gamma,\alpha}$, and $a_{\mathrm{jump}}^{\gamma,\alpha}$, $\alpha \in \{1,2\}$, are real-valued, and each of the functions*

$$\begin{aligned} &\mathrm{av}_{\mathrm{jump},\alpha}[\gamma] : \upsilon \times \upsilon \times \tau \times \gamma \longrightarrow \mathbb{R}, \quad \alpha \in \{1,2\}, \\ &\mathrm{av}_{\mathrm{jump},1}[\gamma][(\tilde{y},y,t,x)] := -v_{i_1[\gamma]}[(y,t,x)] \bullet n_{p_{i_1[\gamma]}}[x] + \left(a_{\mathrm{flux}}^{\gamma,1}\right)^{\text{ex.-im.}}\left[\big((\tilde{y},y),t,x\big)\right], \\ &\mathrm{av}_{\mathrm{jump},2}[\gamma][(\tilde{y},y,t,x)] := -v_{i_2[\gamma]}[(y,t,x)] \bullet n_{p_{i_2[\gamma]}}[x] - \left(a_{\mathrm{flux}}^{\gamma,2}\right)^{\text{ex.-im.}}\left[\big((\tilde{y},y),t,x\big)\right] \end{aligned} \tag{3.7.111}$$

are bounded from above. For simplicity, also assume that the functions $a^{\gamma,1}_{\text{jump}}$ and $a^{\gamma,2}_{\text{jump}}$ are bounded from below (this assumption can be avoided whenever $\overline{\gamma}$ does not intersect a Dirichlet boundary). Then

$$\bigwedge_{\nu\in\{0,\dots,n\}} \left(\begin{array}{l} \displaystyle\sum_{(k,\mathcal{C})\in I_{\Pi,\mathfrak{D},\neg\mathrm{Dir}}} \Big(-\mathfrak{v}^{(\nu)}_{\text{jump},(k,\mathcal{C})} - \mathfrak{a}^{(\nu)}_{\text{jump},1,\text{Dir},(k,\mathcal{C})} - \mathfrak{a}^{(\nu)}_{\text{jump},2,\text{Dir},(k,\mathcal{C})} \\ \qquad\qquad - \mathfrak{a}^{(\nu)}_{\text{flux},\text{jump},2,\neg\text{Dir},(k,\mathcal{C})} - \mathfrak{a}^{(\nu)}_{\text{flux},\text{jump},2,\text{Dir},(k,\mathcal{C})} \Big) \\ \leq \big(B_{\text{jump}}[\mathfrak{C}] + B_{\text{jump},\text{Dir}}[\mathfrak{C}] \big) \cdot \displaystyle\sum_{\gamma\in\mathrm{IF}_{\text{jump}}} \lambda_{d-1}[\gamma] \end{array} \right), \tag{3.7.112}$$

where

$$\begin{aligned} B_{\text{jump}}[\mathfrak{C}] := & \max\big\{ \sup(\mathrm{av}_{\text{jump},1}[\gamma]) + \sup(\mathrm{av}_{\text{jump},2}[\gamma]) : \gamma\in\mathrm{IF}_{\text{jump}} \big\} \\ & + \max\Big\{ (a^{\gamma,1}_{\text{flux}})^{\text{ex.-im.}} \big[\big((u_{j,\text{Dir}}[(\tilde{t},x)], u_{j,\text{Dir}}[(t,x)]), t, x \big) \big] : \\ & \qquad \gamma\in\mathrm{IF}_{\text{jump}},\ j\in J:\ 0\in J_j,\ (\tilde{t},t,x)\in\tau\times\tau\times\overline{\gamma}\cap\Gamma_{j,\text{Dir}} \Big\}, \end{aligned} \tag{3.7.113}$$

$$\begin{aligned} B_{\text{jump},\text{Dir}}[\mathfrak{C}] := & \max\big\{ \sup(-a^{\gamma,\alpha}_{\text{jump}}) : \gamma\in\mathrm{IF}_{\text{jump}},\ \alpha\in\{1,2\} \big\} \\ & + \max\Big\{ a^{\gamma,\alpha}_{\text{jump}} \big[(u_{j,\text{Dir}}[(t,x)], t, x) \big] : \\ & \qquad \alpha\in\{1,2\},\ \gamma\in\mathrm{IF}_{\text{jump}},\ j\in J:\ 0\in J_j,\ (t,x)\in\tau\times\overline{\gamma}\cap\Gamma_{j,\text{Dir}} \Big\}. \end{aligned} \tag{3.7.114}$$

Proof. The hypothesis implies that each

$$\begin{aligned} & -v^{(\nu)}_{i_1[\gamma],\text{sca}}[(y_1,x_k)]\, v^{(\nu)}_{i_1[\gamma],\text{vec}}[x_k] \bullet n_{\omega_k^{(i_1[\gamma])}} - v^{(\nu)}_{i_2[\gamma],\text{sca}}[(y_2,x_k)]\, v^{(\nu)}_{i_2[\gamma],\text{vec}}[x_k] \bullet n_{\omega_k^{(i_2[\gamma])}} \\ & \quad + (a^{\gamma,1,\nu}_{\text{flux}})^{\text{ex.-im.}} \big[\big((\tilde{y}_1, y_1), x_k \big) \big] - (a^{\gamma,2,\nu}_{\text{flux}})^{\text{ex.-im.}} \big[\big((\tilde{y}_2, y_2), x_k \big) \big] \end{aligned} \tag{3.7.115}$$

is bounded from above by $B_{\text{jump}}[\mathfrak{C}]$ and that this is still the case if summands with index 1 in (3.7.115) are replaced with the Dirichlet term from (3.7.63). Moreover, each summand in (3.7.60) is bounded from below by $-B_{\text{jump},\text{Dir}}[\mathfrak{C}]\lambda_{d-1}\big[\partial\omega_k^{(i_1[\gamma])}\cap\gamma\big]$ and each summand in (3.7.66) is bounded from below by $-B_{\text{jump},\text{Dir}}[\mathfrak{C}]\lambda_{d-1}\big[\partial\omega_k^{(i_2[\gamma])}\cap\gamma\big]$. Hence, (3.7.112) follows from (3.7.55), (3.7.60), (3.7.62), (3.7.63), and (3.7.66), since $(\omega_k^{(j)})_{j\in J: k\in I^{(j)}}$ is a partition of ω_k, $k\in I_\Pi$, Π is a partition of p, and since $\gamma\cap\partial_{\text{reg}}\omega_k^{(j)}\neq\emptyset$ holds if and only if $j\in\{i_1[\gamma], i_2[\gamma]\}$. ■

Example 3.7.34. Suppose $\gamma\in\mathrm{IF}_{\text{jump}}$ is a jump interface.

First, it is remarked that for $a^{\gamma,1}_{\text{jump}}[(y,t,x)] = a^{\gamma,2}_{\text{jump}}[(y,t,x)] = \xi y$, $\xi\in\mathbb{R}^+$, according to Ex. 3.1.2(b), $a^{\gamma,1}_{\text{jump}}$ and $a^{\gamma,2}_{\text{jump}}$ are bounded from below, satisfying the hypothesis of Lem. 3.7.33.

Let $v_{\alpha,\gamma} := v_{i_\alpha[\gamma]}\restriction_{v\times\mathcal{T}\times\gamma}$, $\alpha \in \{1,2\}$. Suppose $v = [m_v, \infty[$ and that there is no dependency splitting, i.e. $(a^{\gamma,\alpha}_{\text{flux}})^{\text{ex.-im.}}\big[\big((\tilde{y},y),t,x\big)\big] = a^{\gamma,\alpha}_{\text{flux}}[(y,t,x)]$.

The situation is similar to Ex. 3.7.32, except that the contributions from the two sides of γ can no longer compensate each other. Still, the $\text{av}_{\text{jump},\alpha}[\gamma]$ are bounded from above for $a^{\gamma,1}_{\text{flux}} = a^{\gamma,2}_{\text{flux}} = 0$, if both v_1 and v_2 are independent of $y \in v$. However, while in Ex. 3.7.32, the hypothesis of Lem. 3.7.25 was satisfied for $v_{1,\gamma} = v_{2,\gamma}$, in the current situation, $v_{1,\gamma} = v_{2,\gamma}$ does not suffice to ensure the hypotheses of Lem. 3.7.33. For example, if $v_{1,\gamma}[(y,t,x)] = v_{2,\gamma}[(y,t,x)] = -y n_{p_{i_2[\gamma]}}$, then $-(v_{1,\gamma} \bullet n_{p_{i_1[\gamma]}})[(y,t,x)] = -y$ is bounded from above, but $-(v_{2,\gamma} \bullet n_{p_{i_2[\gamma]}})[(y,t,x)] = y$ is *not* bounded from above. In particular, $\text{av}_{\text{jump},2}[\gamma]$ is not bounded from above if $a^{\gamma,2}_{\text{flux}} = 0$. However, analogous to Ex. 3.7.32, $\text{av}_{\text{jump},\alpha}[\gamma]$, $\alpha \in \{1,2\}$, are both bounded from above for $a^{\gamma,1}_{\text{flux}} = 0$ and $a^{\gamma,2}_{\text{flux}}[(y,t,x)] = \xi y$, $\xi \in [1,\infty[$.

Remark 3.7.35. The combination of Lems 3.7.31 and 3.7.33 yields that the discretizations (3.7.101) are bounded from above with

$$B_{\text{IF}}[\mathfrak{C}] = \max\big\{B_{\text{con}}[\mathfrak{C}], B_{\text{jump}}[\mathfrak{C}] + B_{\text{jump,Dir}}[\mathfrak{C}]\big\},$$

if all nonlocal interface operators vanish (i.e. $\mathcal{A}_\gamma = \mathfrak{A}^{(\nu)}_{\text{con},(k,\mathcal{C})} = \mathfrak{A}^{(\nu)}_{\text{jump},(k,\mathcal{C})} = 0$) and if the hypotheses of Lems (3.7.31) and (3.7.33) are satisfied.

The following Ex. 3.7.36 is similar to Ex. 3.7.27, showing that under natural hypotheses, the discretizations (3.7.101) are bounded from above if the nonlocal interface operators represent the nonlocal radiation operators that are discretized according to Sec. 3.7.8.

Example 3.7.36. As at the end of Sec. 3.7.8, consider the case where the nonlocal interface operators $\mathcal{A}_\gamma$ represent the nonlocal radiation operators arising from Ex. 3.1.2(c). More precisely, cylindrical symmetry is assumed and only the contributions from the transmittive band are considered (s. Sec. 2.4.4, the contributions from the reflective band can be handled similarly). Thus, using the notation of Fig. 3.1 on p. 50, $\Gamma_{\text{con}} = \Omega_{j_2} \cap \Omega_{j_4}$, $\Gamma_{\text{jump}} = (\Omega_{j_1} \cap \Omega_{j_2}) \cup (\Omega_{j_1} \cap \Omega_{j_3})$ (cf. last paragraph of Sec. 3.7.8), and

$$\begin{aligned}
\mathcal{A}_\gamma[T_{\text{solid,circ}}] &= \epsilon_{\text{t,circ}}[(T_{\text{solid,circ}},x)] \cdot \mathcal{J}_{\text{t,circ}}\big[\mathcal{R}_{\text{t,circ}}[T_{\text{solid,circ}}]\big],\\
a^{\gamma,1}_{\text{flux}}[(T_{\text{solid,circ}},t,x)] &= 0,\\
a^{\gamma,2}_{\text{flux}}[(T_{\text{solid,circ}},t,x)] &= \epsilon_{\text{t,circ}}[(T_{\text{solid,circ}},x)]\,\sigma\,T^4_{\text{solid,circ}}.
\end{aligned}$$

Thus, using the dependency splitting of Ex. 3.4.10, it is

$$\begin{aligned}
&(\mathcal{A}_\gamma)^{\text{ex.-im.}}[(T^{(\nu-1)}_{\text{solid,circ}}, T^{(\nu)}_{\text{solid,circ}})][x] - (a^{\gamma,2,\nu}_{\text{flux}})^{\text{ex.-im.}}\big[\big((T^{(\nu-1)}_{\text{solid,circ}}, T^{(\nu)}_{\text{solid,circ}}),x\big)\big]\\
&= \epsilon_{\text{t,circ}}[(T^{(\nu-1)}_{\text{solid,circ}},x)] \cdot \mathcal{J}_{\text{t,circ}}\big[\mathcal{R}_{\text{t,circ}}[T^{(\nu)}_{\text{solid,circ}}]\big] - \epsilon_{\text{t,circ}}[(T^{(\nu-1)}_{\text{solid,circ}},x)]\,\sigma\,\big(T^{(\nu)}_{\text{solid,circ}}\big)^4.
\end{aligned}$$

Then, if $\mathfrak{A}^{(\nu)}_{\mathrm{con},(k,\mathcal{C})} = \mathfrak{A}^{(\nu)}_{\mathrm{con},k,\mathrm{solid}}$ and $\mathfrak{A}^{(\nu)}_{\mathrm{jump},(k,\mathcal{C})} = \mathfrak{A}^{(\nu)}_{\mathrm{jump},k,\mathrm{solid}}$ are defined by (3.7.92) and (3.7.93), respectively, then together with $\mathfrak{a}^{(\nu)}_{\mathrm{flux,jump},2,\neg\mathrm{Dir},(k,\mathcal{C})} = \mathfrak{a}^{(\nu)}_{\mathrm{flux,jump},2,\neg\mathrm{Dir},k,\mathrm{solid}}$ defined according to (3.7.62), and recalling (3.7.89), this yields

$$\begin{aligned}&\mathfrak{A}^{(\nu)}_{\mathrm{con},k,\mathrm{solid}}[(U^{(\nu-1)},U^{(\nu)})] - \mathfrak{a}^{(\nu)}_{\mathrm{flux,jump},2,\neg\mathrm{Dir},k,\mathrm{solid}}[(U^{(\nu-1)}_{k,\mathrm{solid}},U^{(\nu)}_{k,\mathrm{solid}})]\\ &= \sum_{\kappa\in I_{\omega_k,\mathrm{con}}} \left(V_\kappa[(U^{(\nu-1)},U^{(\nu)})] - \epsilon_{\mathrm{t,circ}}[(U^{(\nu-1)}_{k,\mathrm{solid}},x_k)]\,\sigma\left(U^{(\nu)}_{k,\mathrm{solid}}\right)^4 l_\kappa\right)\end{aligned} \tag{3.7.116}$$

and the analogous equation involving $\mathfrak{A}^{(\nu)}_{\mathrm{jump},k,\mathrm{solid}}$.

Using $\Gamma_{\mathrm{ph}} = \emptyset$, an argument analogous to (3.7.100) shows

$$\begin{aligned}\sum_{(k,\mathcal{C})\in I_{\Pi,\mathfrak{D},\neg\mathrm{Dir}}} &\Big(\mathfrak{A}^{(\nu)}_{\mathrm{con},(k,\mathcal{C})}[(U^{(\nu-1)},U^{(\nu)})] + \mathfrak{A}^{(\nu)}_{\mathrm{jump},(k,\mathcal{C})}[(U^{(\nu-1)},U^{(\nu)})]\\ &\quad - \mathfrak{a}^{(\nu)}_{\mathrm{flux,jump},2,\neg\mathrm{Dir},(k,\mathcal{C})}[(U^{(\nu-1)}_{(k,\mathcal{C})},U^{(\nu)}_{(k,\mathcal{C})})]\Big) = 0.\end{aligned} \tag{3.7.117}$$

Superposing the situation of the present example with the situations considered in Exs 3.7.32 and 3.7.34 shows that under natural hypotheses, the discretizations (3.7.101) are bounded from above.

3.7.11 Source and Sink Terms

(3.5.24n) is discretized by replacing the integrand by its value at x_k, i.e. (3.5.24n) is replaced by

$$\mathfrak{h}^{(\nu)}_{(k,\mathcal{C}),(n)}[U^{(\nu)}] := -\mathfrak{f}^{(\nu)}_{(k,\mathcal{C})}[U^{(\nu)}_{(k,\mathcal{C})}], \tag{3.7.118}$$

where the $\mathfrak{f}^{(\nu)}_{(k,\mathcal{C})} : v \longrightarrow \mathbb{K}$ are defined by:

$$\bigwedge_{\substack{\nu\in\{0,\dots,n\},\\ (k,\mathcal{C})\in I_{\Pi,\mathfrak{D},\neg\mathrm{Dir}}}} \mathfrak{f}^{(\nu)}_{(k,\mathcal{C})}[y] := \sum_{j\in V[\mathcal{C}]} f^{(\nu)}_j[(y,x_k)]\cdot\lambda_d[\omega^{(j)}_k]. \tag{3.7.119}$$

Remark 3.7.37. As mentioned in Sec. 3.3.1, for the mathematical theory, it is often not necessary to assume continuity of the f_j. For example, if one just had square integrability of f_j with respect to x, then one would replace $f^{(\nu)}_j[(y,x_k)]\cdot\lambda_d[\omega^{(j)}_k]$ with $\int_{\omega^{(j)}_k} f^{(\nu)}_j[(y,x)]\,\mathrm{d}x$ in (3.7.119).

As in the previous sections, the contributions to the operators $\mathfrak{s}^{(\nu)}$ are estimated from above:

Lemma 3.7.38. *If each f_j, $j \in J$, is real-valued and bounded from above, then*

$$\bigwedge_{\nu\in\{0,\dots,n\}} \quad -\sum_{(k,\mathcal{C})\in I_{\Pi,\mathfrak{D},\neg\mathrm{Dir}}} \mathfrak{h}^{(\nu)}_{(k,\mathcal{C}),(n)} = \sum_{(k,\mathcal{C})\in I_{\Pi,\mathfrak{D},\neg\mathrm{Dir}}} \mathfrak{f}^{(\nu)}_{(k,\mathcal{C})} \leq B_f[\mathfrak{C}]\cdot\lambda_d[p], \tag{3.7.120}$$

where

$$B_f[\mathfrak{C}] := \max\big\{\sup f_j \,:\, j\in J\big\}. \tag{3.7.121}$$

Proof. By the hypothesis, each $f_j^{(\nu)}[(y,x_k)]$ is bounded from above by $B_f[\mathfrak{C}]$. Hence, (3.7.120) follows from (3.7.119) and since $(\omega_k^{(j)})_{j\in J:\,k\in I^{(j)}}$ is a partition of ω_k, $k\in I_\Pi$, and Π is a partition of p. ■

Example 3.7.39. Example 3.1.1(b) and the first case of Ex. 3.1.1(a) are investigated with respect to the f_j being bounded from above as needed in the hypothesis of Lem. 3.7.38.

The hypothesis of Lem. 3.7.38 is trivially satisfied, where the f_j are independent of the unknown: In the first case of 3.1.1(a), one has $f_j = 0$. In the first case of 3.1.1(b), one has $f_j[(y,t,x)] = \rho_{\mathbf{gas}}[x]\mathbf{g}\bullet\mathbf{v}_{\mathbf{gas}}[x]$.

In the second case of 3.1.1(a), it is $f_j[(y,t,x)] = f^{[\beta_j]}$, where $f^{[\beta_j]}$ is supposed to represent a heat source due to induction heating. Thus, the assumption that the f_j are bounded from above is physically reasonable, since it means that the power density of the heat sources can not become arbitrarily large.

In the third case of 3.1.1(a), $f_j[(y,t,x)] = \varepsilon_{\mathbf{gas}}[y]\,\mathrm{div}\,\big(\rho_{\mathbf{gas}}[x]\mathbf{v}_{\mathbf{gas}}[x]\big) - p_{\mathbf{gas}}[x]\,\mathrm{div}\,\mathbf{v}_{\mathbf{gas}}[x]$. Since the internal energy ε is nonnegative, f_j is bounded from above if and only if ε is bounded from above or $\mathrm{div}(\rho_{\mathbf{gas}}\mathbf{v}_{\mathbf{gas}}) \leq 0$, i.e. there are no gas sources.

3.7.12 Summarizing Definitions

For the sake of easy reference, the ingredients to a finite volume discretization are summarized in the following Defs 3.7.40 and 3.7.41, and the notion of a solution to a finite volume discretization is provided by Def. 3.7.42. Moreover, the estimates proved in Secs 3.7.2 - 3.7.11 are combined into Lem. 3.7.45.

Firstly, Def. 3.7.40 collects the requirements with respect to the polytope discretization Π.

Definition 3.7.40. The partition $\Pi = (\omega_k)_{k\in I_\Pi}$ of p into finitely many d-dimensional polytopes ω_k (*control volumes*) together with a family of *discretization points* $(x_k)_{k\in I_\Pi}$ is called a *space discretization* of the domain complex $\mathfrak{D}$ iff the following conditions (i) – (iv) are satisfied, where according to Sec. 3.5.3, $\Pi^{(j)} := (\omega_k^{(j)})_{k\in I^{(j)}}$, $\omega_k^{(j)} := \overline{\mathrm{int}[\omega_k\cap p_j]}$, $I^{(j)} := \big\{k\in I_\Pi \,:\, \omega_k^{(j)} \neq \emptyset\big\}$.

(i) $\bigwedge_{k \in I_\Pi} \omega_k$ is nontangent to interfaces.

(ii) $\bigwedge_{\{k,l\} \in E_{\mathrm{IF}}[\Pi]} \quad x_k \neq x_l \quad \text{and} \quad \frac{x_l - x_k}{\|x_k - x_l\|_2} = n_{\omega_k} \restriction_{\partial_{\mathrm{reg}}\omega_k \cap \partial_{\mathrm{reg}}\omega_l}.$

(iii) $\bigwedge_{k \in I_\Pi} \bigwedge_{j \in V_{\omega_k}} \quad x_k \in \omega_k^{(j)}.$

(iv) $\bigwedge_{k \in I_\Pi} \bigwedge_{(j,\iota) \in J \times J_j} \quad \Gamma_{j,\iota} \cap \partial_{\mathrm{reg}}\omega_k \neq \emptyset \quad \Rightarrow \quad x_k \in \Gamma_{j,\iota}.$

Conditions (ii) – (iv) are conditions (dispt-(i)) – (dispt-(iii)) from Sec. 3.7.1.

—

Finding discretizations that satisfy Condition 3.7.40(ii) presents no difficulty, as it is fulfilled for every Voronoï discretization as described in App. C.4.3 (s. Rem. C.4.19). A Voronoï discretization yields a discretization of p into d-polytopes that has a prescribed finite point set as discretization points. However, sufficiently many discretization points need to lie on interfaces and boundaries to guarantee Conditions 3.7.40(i),(iii),(iv), and to provide a construction procedure for the general case seems to be difficult.

If $d = 2$, i.e. if p is two-dimensional, then one can discretize the convex hull of p, $\mathrm{conv}[p]$, into triangles satisfying the *constrained Delaunay criterion* (temporarily adding the space domain $p_{\mathrm{conv}} := \overline{\mathrm{conv}[p] \setminus p}$). The constrained Delaunay criterion says that the sum of two opposite angles can be at most 180°, and that angles opposite boundaries or interfaces must be at most 90° (cf. Fig. 3.24). Moreover, each interface and each $\Gamma_{j,\iota}$ must be discretized into triangle edges. A constrained Delaunay triangulation is produced by the grid generator *Triangle* (cf. [She96]), which is used during the numerical simulations of Ch. 4. It is also referred to [She96] for further information and references on Delaunay triangulation. If V is the set of vertices of a constrained Delaunay triangulation of $\mathrm{conv}[p]$, and $(\omega_v)_{v \in V}$ is the induced Voronoï discretization of p, then $(\tilde{\omega}_v)_{v \in V}$ together with the set of discretization points V is a space discretization in the sense of Def. 3.7.40, where $\tilde{\omega}_v := \overline{\omega_v \setminus p_{\mathrm{conv}}}$. Figure 3.25 illustrates that, in general, it does not suffice to use a Delaunay triangulation of just p to guarantee Conditions 3.7.40(iii),(iv).

Definition 3.7.41. A *finite volume discretization* $\mathfrak{F}$ of the evolution equation complex $\mathfrak{C}$ consists of a time discretization $\mathfrak{T}$ of $\mathfrak{C}$, a space discretization $\big(\Pi, (x_k)_{k \in I_\Pi}\big)$ of $\mathfrak{D}$, a family of scalar-vector-splittings $\mathfrak{V}$ for $\mathfrak{C}$, and the family of discretization operators

$$\big(\mathfrak{h}^{(\nu)}_{(k,\mathcal{C})}\big)_{(\nu,(k,\mathcal{C})) \in \{1,\dots,n\} \times I_{\Pi,\mathfrak{D},\neg\mathrm{Dir}}}$$

according to (3.7.7), given by means of the discretization operators defined in Secs 3.7.2 - 3.7.11 (s. (3.7.122) below).

—

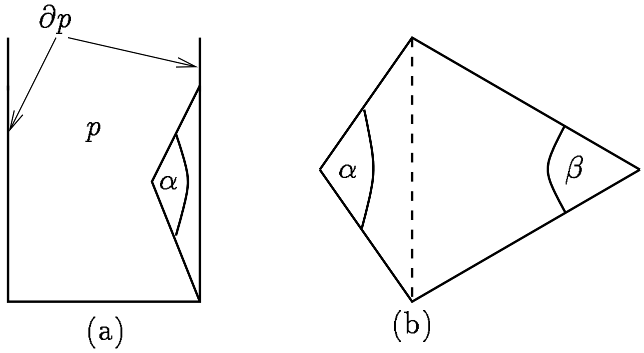
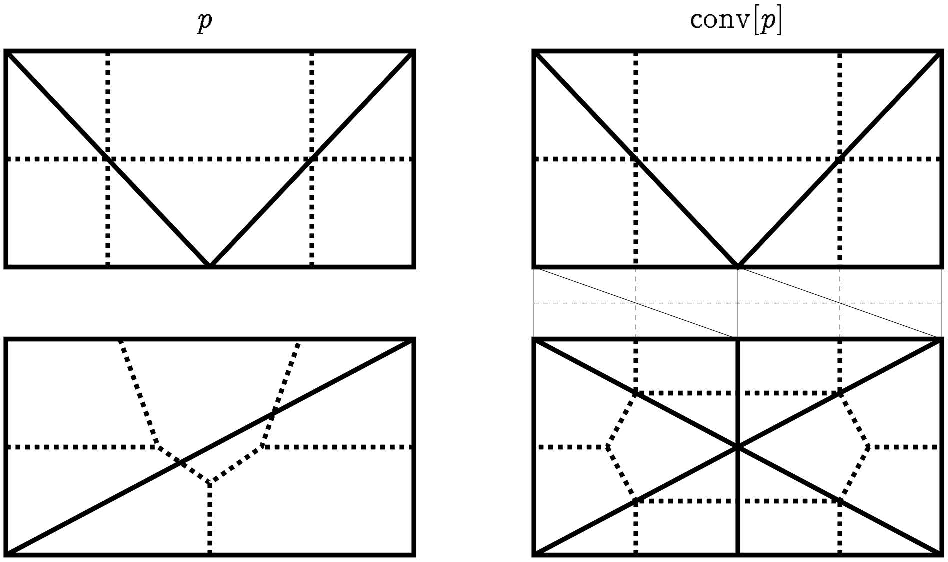


Figure 3.24: The situation in (a) violates the constrained Delaunay criterion, as $\alpha > 90°$. For the situation in (b), $\alpha = 110°$ and $\beta = 60°$, i.e. the constrained Delaunay criterion is violated if and only if the dashed line constitutes an interface between different spatial subdomains p_{j_1} and p_{j_2}.



boundary of Voronoï boxes intersected with p

boundary of Voronoï boxes intersected with $\mathrm{conv}[p] \setminus p$

Figure 3.25: Delaunay triangulations of p and $\mathrm{conv}[p]$ and resulting Voronoï discretizations.

Since the definition of the $\mathfrak{h}^{(\nu)}_{(k,\mathcal{C})}$ is scattered over Secs 3.7.2 - 3.7.11, it can be useful to have the following closed form (3.7.122), even though it is rather lengthy itself: For each $\nu \in \{1, \ldots, n\}$ and for each $(k, \mathcal{C}) \in I_{\Pi,\mathfrak{D},\neg\mathrm{Dir}}$, one has

$$\mathfrak{h}^{(\nu)}_{(k,\mathcal{C})}\big[(U^{(\nu-1)}, U^{(\nu)})\big]$$

$$
\begin{aligned}
&= (t_\nu - t_{\nu-1})^{-1} \left(\mathfrak{b}^{(\nu)}_{(k,\mathcal{C})}[U^{(\nu)}_{(k,\mathcal{C})}] - \mathfrak{b}^{(\nu-1)}_{(k,\mathcal{C})}[U^{(\nu-1)}_{(k,\mathcal{C})}] \right) + \mathfrak{v}^{(\nu)}_{\mathrm{int},\neg\mathrm{Dir},(k,\mathcal{C})}[U^{(\nu)}] + \mathfrak{v}^{(\nu)}_{\mathrm{int},\mathrm{Dir},(k,\mathcal{C})}[U^{(\nu)}_{(k,\mathcal{C})}] \\
&\quad + \mathfrak{v}^{(\nu)}_{\mathrm{out},(k,\mathcal{C})}[U^{(\nu)}_{(k,\mathcal{C})}] + \mathfrak{v}^{(\nu)}_{\mathrm{con},(k,\mathcal{C})}[U^{(\nu)}_{(k,\mathcal{C})}] + \mathfrak{v}^{(\nu)}_{\mathrm{jump},(k,\mathcal{C})}[U^{(\nu)}_{(k,\mathcal{C})}] - \mathfrak{k}^{(\nu)}_{\neg\mathrm{Dir},(k,\mathcal{C})}[U^{(\nu)}] \\
&\quad - \mathfrak{k}^{(\nu)}_{\mathrm{Dir},(k,\mathcal{C})}[U^{(\nu)}_{(k,\mathcal{C})}] - \mathfrak{B}^{(\nu)}_{(k,\mathcal{C})}[(U^{(\nu-1)}, U^{(\nu)})] + \mathfrak{a}^{(\nu)}_{\mathrm{out},(k,\mathcal{C})}[(U^{(\nu-1)}_{(k,\mathcal{C})}, U^{(\nu)}_{(k,\mathcal{C})})] \\
&\quad - \mathfrak{A}^{(\nu)}_{\mathrm{con},(k,\mathcal{C})}[(U^{(\nu-1)}, U^{(\nu)})] + \mathfrak{a}^{(\nu)}_{\mathrm{flux},\mathrm{con},(k,\mathcal{C})}[(U^{(\nu-1)}_{(k,\mathcal{C})}, U^{(\nu)}_{(k,\mathcal{C})})] + \mathfrak{a}^{(\nu)}_{\mathrm{jump},1,\neg\mathrm{Dir},(k,\mathcal{C})}[U^{(\nu)}] \\
&\quad + \mathfrak{a}^{(\nu)}_{\mathrm{jump},1,\mathrm{Dir},(k,\mathcal{C})}[U^{(\nu)}_{(k,\mathcal{C})}] - \mathfrak{A}^{(\nu)}_{\mathrm{jump},(k,\mathcal{C})}[(U^{(\nu-1)}, U^{(\nu)})] + \mathfrak{a}^{(\nu)}_{\mathrm{flux},\mathrm{jump},2,\neg\mathrm{Dir},(k,\mathcal{C})}[(U^{(\nu-1)}, U^{(\nu)})] \\
&\quad + \mathfrak{a}^{(\nu)}_{\mathrm{flux},\mathrm{jump},2,\mathrm{Dir},(k,\mathcal{C})}[(U^{(\nu-1)}_{(k,\mathcal{C})}, U^{(\nu)}_{(k,\mathcal{C})})] + \mathfrak{a}^{(\nu)}_{\mathrm{jump},2,\neg\mathrm{Dir},(k,\mathcal{C})}[U^{(\nu)}] + \mathfrak{a}^{(\nu)}_{\mathrm{jump},2,\mathrm{Dir},(k,\mathcal{C})}[U^{(\nu)}_{(k,\mathcal{C})}] \\
&\quad - \mathfrak{f}^{(\nu)}_{(k,\mathcal{C})}[U^{(\nu)}_{(k,\mathcal{C})}]
\end{aligned}
$$

$$
= (t_\nu - t_{\nu-1})^{-1} \sum_{j \in V[\mathcal{C}]} \left(b^{(\nu)}_j[(U^{(\nu)}_{(k,\mathcal{C})}, x_k)] - b^{(\nu)}_j[(U^{(\nu-1)}_{(k,\mathcal{C})}, x_k)] \right) \cdot \lambda_d[\omega^{(j)}_k] \tag{3.7.122a}
$$

$$
\begin{aligned}
&+ \sum_{\substack{j \in V[\mathcal{C}],\\ l \in \mathrm{nb}_{j,\neg\mathrm{Dir}}[k]}} \left(w^{(\nu)}_j[(k,l)] \cdot v^{(\nu)}_{j,\mathrm{sca}}\left[\left(U^{(\nu)}_{(l,\mathcal{C}[(l,j)])}, x_l\right)\right] \right. \\
&\qquad \left. + \left(1 - w^{(\nu)}_j[(k,l)]\right) \cdot v^{(\nu)}_{j,\mathrm{sol}}[(U^{(\nu)}_{(k,\mathcal{C})}, x_k)] \right) \\
&\qquad \cdot \frac{\left(v^{(\nu)}_{j,\mathrm{vec}}[x_l] + v^{(\nu)}_{j,\mathrm{vec}}[x_k]\right) \bullet (x_l - x_k)}{2\|x_k - x_l\|_2} \cdot \lambda_{d-1}\left[\omega^{(j)}_k \cap \omega^{(j)}_l\right]
\end{aligned} \tag{3.7.122b}
$$

$$
\begin{aligned}
&+ \sum_{\substack{j \in V[\mathcal{C}],\\ l \in \mathrm{nb}_{j,\mathrm{Dir}}[k]}} \left(w^{(\nu)}_j[(k,l)] \cdot v^{(\nu)}_{j,\mathrm{sca}}\left[\left(u_{j_{\mathrm{Dir}}[(l,j)],\mathrm{Dir}}[(t_\nu, x_l)], x_l\right)\right] \right. \\
&\qquad \left. + \left(1 - w^{(\nu)}_j[(k,l)]\right) \cdot v^{(\nu)}_{j,\mathrm{sca}}\left[(U^{(\nu)}_{(k,\mathcal{C})}, x_k)\right] \right) \\
&\qquad \cdot \frac{\left(v^{(\nu)}_{j,\mathrm{vec}}[x_l] + v^{(\nu)}_{j,\mathrm{vec}}[x_k]\right) \bullet (x_l - x_k)}{2\|x_k - x_l\|_2} \cdot \lambda_{d-1}\left[\omega^{(j)}_k \cap \omega^{(j)}_l\right]
\end{aligned} \tag{3.7.122c}
$$

$$
+ \sum_{j \in V[\mathcal{C}]} v^{(\nu)}_{j,\mathrm{sca}}[(U^{(\nu)}_{(k,\mathcal{C})}, x_k)] \int_{\partial\omega^{(j)}_k \cap \partial p} v^{(\nu)}_{j,\mathrm{vec}}[x_k] \bullet n_{\omega^{(j)}_k} \tag{3.7.122d}
$$

$$
+ \sum_{\substack{j \in V[\mathcal{C}],\\ \gamma \in \mathrm{IF}}} v^{(\nu)}_{j,\mathrm{sca}}[(U^{(\nu)}_{(k,\mathcal{C})}, x_k)] \int_{\partial\omega^{(j)}_k \cap \gamma} v^{(\nu)}_{j,\mathrm{vec}}[x_k] \bullet n_{\omega^{(j)}_k} \tag{3.7.122e}
$$

$$
\begin{aligned}
&- \sum_{\substack{j \in V[\mathcal{C}],\\ l \in \mathrm{nb}_{j,\neg\mathrm{Dir}}[k]}} \frac{k^{(\nu)}_j[(U^{(\nu)}_{(k,\mathcal{C})}, x_k)] + k^{(\nu)}_j\left[\left(U^{(\nu)}_{(l,\mathcal{C}[(l,j)])}, x_l\right)\right]}{2} \\
&\qquad \cdot \frac{U^{(\nu)}_{(l,\mathcal{C}[(l,j)])} - U^{(\nu)}_{(k,\mathcal{C})}}{\|x_k - x_l\|_2} \cdot \lambda_{d-1}\left[\omega^{(j)}_k \cap \omega^{(j)}_l\right]
\end{aligned} \tag{3.7.122f}
$$

$$- \sum_{\substack{j\in V[\mathcal{C}],\\ l\in \mathrm{nb}_{j,\mathrm{Dir}}[k]}} \frac{k_j^{(\nu)}\big[\big(U^{(\nu)}_{(k,\mathcal{C})}, x_k\big)\big] + k_j^{(\nu)}\big[\big(u_{j_{\mathrm{Dir}}[(l,j)],\mathrm{Dir}}\big[(t_\nu, x_l)\big], x_l\big)\big]}{2} \cdot \frac{u_{j_{\mathrm{Dir}}[(l,j)],\mathrm{Dir}}\big[(t_\nu, x_l)\big] - U^{(\nu)}_{(k,\mathcal{C})}}{\|x_k - x_l\|_2} \cdot \lambda_{d-1}\big[\omega_k^{(j)} \cap \omega_l^{(j)}\big] \tag{3.7.122g}$$

$$- \mathfrak{B}^{(\nu)}_{(k,\mathcal{C})}\big[\big(U^{(\nu-1)}, U^{(\nu)}\big)\big] \tag{3.7.122h}$$

$$+ \sum_{\substack{(j,\iota)\in V[\mathcal{C}]\times J_j\setminus\{0\}:\\ \lambda_{d-1}[\partial\omega_k^{(j)}\cap\Gamma_{j,\iota}]>0}} \big(a_{\mathrm{out}}^{j,\iota,\nu}\big)^{\text{ex.-im.}}\Big[\Big(\big(U^{(\nu-1)}_{(k,\mathcal{C})}, U^{(\nu)}_{(k,\mathcal{C})}\big), x_k\Big)\Big] \cdot \lambda_{d-1}\big[\partial\omega_k^{(j)} \cap \Gamma_{j,\iota}\big] \tag{3.7.122i}$$

$$- \mathfrak{A}^{(\nu)}_{\mathrm{con},(k,\mathcal{C})}\big[\big(U^{(\nu-1)}, U^{(\nu)}\big)\big] \tag{3.7.122j}$$

$$+ \sum_{\substack{\gamma\in \mathrm{IF}_{\mathrm{con}}:\\ \lambda_{d-1}\left[\gamma\cap\bigcup_{j\in V[\mathcal{C}]}\partial_{\mathrm{reg}}\omega_k^{(j)}\right]>0}} \Big(- \big(a_{\mathrm{flux}}^{\gamma,1,\nu}\big)^{\text{ex.-im.}}\Big[\Big(\big(U^{(\nu-1)}_{(k,\mathcal{C})}, U^{(\nu)}_{(k,\mathcal{C})}\big), x_k\Big)\Big] + \big(a_{\mathrm{flux}}^{\gamma,2,\nu}\big)^{\text{ex.-im.}}\Big[\Big(\big(U^{(\nu-1)}_{(k,\mathcal{C})}, U^{(\nu)}_{(k,\mathcal{C})}\big), x_k\Big)\Big]\Big) \cdot \lambda_{d-1}\left[\gamma \cap \bigcup_{j\in V[\mathcal{C}]} \partial_{\mathrm{reg}}\omega_k^{(j)}\right] \tag{3.7.122k}$$

$$+ \sum_{\substack{\gamma\in G_{\mathrm{jump},1}[\mathcal{C}]:\\ \left(k,\mathcal{C}[(k,i_2[\gamma])]\right)\in I_{\Pi,\mathfrak{D},\neg\mathrm{Dir}},\\ \lambda_{d-1}\left[\partial\omega_k^{(i_1[\gamma])}\cap\gamma\right]>0}} \Big(a_{\mathrm{jump}}^{\gamma,1,\nu}\big[\big(U^{(\nu)}_{(k,\mathcal{C})}, x_k\big)\big] - a_{\mathrm{jump}}^{\gamma,2,\nu}\Big[\Big(U^{(\nu)}_{\left(k,\mathcal{C}[(k,i_2[\gamma])]\right)}, x_k\Big)\Big]\Big) \cdot \lambda_{d-1}\big[\partial\omega_k^{(i_1[\gamma])} \cap \gamma\big] \tag{3.7.122l}$$

$$+ \sum_{\substack{\gamma\in G_{\mathrm{jump},1}[\mathcal{C}]:\\ \left(k,\mathcal{C}[(k,i_2[\gamma])]\right)\in I_{\Pi,\mathfrak{D},\mathrm{Dir}},\\ \lambda_{d-1}\left[\partial\omega_k^{(i_1[\gamma])}\cap\gamma\right]>0}} \Big(a_{\mathrm{jump}}^{\gamma,1,\nu}\big[\big(U^{(\nu)}_{(k,\mathcal{C})}, x_k\big)\big] - a_{\mathrm{jump}}^{\gamma,2,\nu}\big[\big(u_{j_{\mathrm{Dir}}[(k,i_2[\gamma])],\mathrm{Dir}}\big[(t_\nu, x_k)\big], x_k\big)\big]\Big) \cdot \lambda_{d-1}\big[\partial\omega_k^{(i_1[\gamma])} \cap \gamma\big] \tag{3.7.122m}$$

$$- \mathfrak{A}^{(\nu)}_{\mathrm{jump},(k,\mathcal{C})}\big[\big(U^{(\nu-1)}, U^{(\nu)}\big)\big] \tag{3.7.122n}$$

$$+ \sum_{\substack{\gamma\in G_{\mathrm{jump},2}[\mathcal{C}]:\\ \left(k,\mathcal{C}[(k,i_1[\gamma])]\right)\in I_{\Pi,\mathfrak{D},\neg\mathrm{Dir}},\\ \lambda_{d-1}\left[\partial\omega_k^{(i_2[\gamma])}\cap\gamma\right]>0}} \Big(- \big(a_{\mathrm{flux}}^{\gamma,1,\nu}\big)^{\text{ex.-im.}}\Big[\Big(\Big(U^{(\nu-1)}_{\left(k,\mathcal{C}[(k,i_1[\gamma])]\right)}, U^{(\nu)}_{\left(k,\mathcal{C}[(k,i_1[\gamma])]\right)}\Big), x_k\Big)\Big] + \big(a_{\mathrm{flux}}^{\gamma,2,\nu}\big)^{\text{ex.-im.}}\Big[\Big(\big(U^{(\nu-1)}_{(k,\mathcal{C})}, U^{(\nu)}_{(k,\mathcal{C})}\big), x_k\Big)\Big]\Big) \cdot \lambda_{d-1}\big[\partial\omega_k^{(i_2[\gamma])} \cap \gamma\big] \tag{3.7.122o}$$

$$+ \sum_{\substack{\gamma\in G_{\mathrm{jump},2}[\mathcal{C}]:\\ \left(k,\mathcal{C}[(k,i_1[\gamma])]\right)\in I_{\Pi,\mathfrak{D},\mathrm{Dir}},\\ \lambda_{d-1}\left[\partial\omega_k^{(i_2[\gamma])}\cap\gamma\right]>0}} \Big(- \big(a_{\mathrm{flux}}^{\gamma,1,\nu}\big)^{\text{ex.-im.}}\Big[\Big(\big(u_{j_{\mathrm{Dir}}[(k,i_1[\gamma])],\mathrm{Dir}}\big[(t_{\nu-1}, x_k)\big], u_{j_{\mathrm{Dir}}[(k,i_1[\gamma])],\mathrm{Dir}}\big[(t_\nu, x_k)\big]\big), x_k\Big)\Big] + \big(a_{\mathrm{flux}}^{\gamma,2,\nu}\big)^{\text{ex.-im.}}\Big[\Big(\big(U^{(\nu-1)}_{(k,\mathcal{C})}, U^{(\nu)}_{(k,\mathcal{C})}\big), x_k\Big)\Big]\Big) \cdot \lambda_{d-1}\big[\partial\omega_k^{(i_2[\gamma])} \cap \gamma\big] \tag{3.7.122p}$$

$$+ \sum_{\substack{\gamma \in G_{\text{jump},2}[\mathcal{C}]: \\ (k,\mathcal{C}[(k,i_1[\gamma])]) \in I_{\Pi,\mathfrak{D},\neg\text{Dir}}, \\ \lambda_{d-1}\left[\partial\omega_k^{(i_2[\gamma])} \cap \gamma\right] > 0}} \Big(- a_{\text{jump}}^{\gamma,1,\nu}\big[(U^{(\nu)}_{(k,\mathcal{C}[(k,i_1[\gamma])])}, x_k)\big] + a_{\text{jump}}^{\gamma,2,\nu}\big[(U^{(\nu)}_{(k,\mathcal{C})}, x_k)\big] \Big) \cdot \lambda_{d-1}\left[\partial\omega_k^{(i_2[\gamma])} \cap \gamma\right] \tag{3.7.122q}$$

$$+ \sum_{\substack{\gamma \in G_{\text{jump},2}[\mathcal{C}]: \\ (k,\mathcal{C}[(k,i_1[\gamma])]) \in I_{\Pi,\mathfrak{D},\text{Dir}}, \\ \lambda_{d-1}\left[\partial\omega_k^{(i_2[\gamma])} \cap \gamma\right] > 0}} \Big(- a_{\text{jump}}^{\gamma,1,\nu}\big[(u_{j_{\text{Dir}}[(k,i_1[\gamma])],\text{Dir}}[(t_\nu, x_k)], x_k)\big] + a_{\text{jump}}^{\gamma,2,\nu}\big[(U^{(\nu)}_{(k,\mathcal{C})}, x_k)\big] \Big) \cdot \lambda_{d-1}\left[\partial\omega_k^{(i_2[\gamma])} \cap \gamma\right] \tag{3.7.122r}$$

$$- \sum_{j \in V[\mathcal{C}]} f_j^{(\nu)}[(y, x_k)] \cdot \lambda_d[\omega_k^{(j)}]. \tag{3.7.122s}$$

Next, the notion of a solution to a finite volume discretization is defined in Def. 3.7.42. The solution to a finite volume discretization should represent a discrete approximation of a (continuous) solution to an evolution equation complex in the sense of Def. 3.4.7. Thus, as explained in Sec. 3.7.1, for each discrete time t_ν, the solution consists of a vector $U^{(\nu)} = (u^{(\nu)}_{(k,\mathcal{C})})_{(k,\mathcal{C}) \in I_{\Pi,\mathfrak{D}}} \in v^{I_{\Pi,\mathfrak{D}}}$, such that $u^{(\nu)}_{(k,\mathcal{C})}$ should represent the value of a (continuous) solution at the discretization point x_k. If x_k lies in more than one space domain p_j, then the solution can have multiple values at x_k if and only if x_k lies on a jump interface $\gamma \in \text{IF}_{\text{jump}}$. Such multiple values are parametrized by means of the connected components $\mathcal{C}$.

At the initial time t_0, the values of the solution are determined by the initial distribution (Def. 3.7.42(i)), and on Dirichlet boundaries $\Gamma_{j,0}$, the values of the solution are determined by the Dirichlet functions for each t_ν (Def. 3.7.42(ii)). For $t_\nu > t_0$ and x_k not on a Dirichlet boundary, the values of the solution are determined inductively from $t_{\nu-1}$ to t_ν by means of the discretization operators $\mathfrak{h}^{(\nu)}$ (s. (3.7.6), (3.7.122), and Def. 3.7.42(iii)).

Definition 3.7.42. A *solution* to a finite volume discretization $\mathfrak{F}$ of an evolution equation complex $\mathfrak{C}$ is a family of vectors

$$\left(U^{(\nu)}\right)_{\nu \in \{0,\dots,n\}} = (u^{(\nu)}_{(k,\mathcal{C})})_{(\nu,(k,\mathcal{C})) \in \{0,\dots,n\} \times I_{\Pi,\mathfrak{D}}} \in \left(v^{I_{\Pi,\mathfrak{D}}}\right)^{\{0,\dots,n\}}, \tag{3.7.123}$$

satisfying

(i) $\displaystyle\bigwedge_{(k,\mathcal{C}) \in I_{\Pi,\mathfrak{D}}} \bigwedge_{j \in V[\mathcal{C}]} u^{(0)}_{(k,\mathcal{C})} = u_j^{(0)}[x_k].$

(ii) $\displaystyle\bigwedge_{(k,\mathcal{C}) \in I_{\Pi,\mathfrak{D},\text{Dir}}} \bigwedge_{j \in V[\mathcal{C}]} u^{(\nu)}_{(k,\mathcal{C})} = u_{j,\text{Dir}}[(t_\nu, x_k)].$

(iii) $\displaystyle\bigwedge_{\nu \in \{1,\dots,n\}} \mathfrak{h}^{(\nu)}\left[\left(U^{(\nu-1)}\restriction_{I_{\Pi,\mathfrak{D},\neg\text{Dir}}}, U^{(\nu)}\restriction_{I_{\Pi,\mathfrak{D},\neg\text{Dir}}}\right)\right] = 0.$

—

After each definition of the discretization operators in Secs 3.7.3 - 3.7.11, it was proved that the corresponding contributions to the operators $\mathfrak{s}^{(\nu)}$ defined in (3.7.8) are bounded from above. These results are combined into the following Lem. 3.7.45, where Defs 3.7.43 and 3.7.44 collect all the used hypotheses.

Definition 3.7.43. The evolution equation complex $\mathfrak{C}$ is called *bounded from above* iff the following conditions (i) – (iv) hold:

(i) The range of the unknowns u_j has the form $v = [m_v, \infty[$, and each of the functions k_j, $u_{j,\mathrm{Dir}}$, and f_j is real-valued.

(ii) k_j is nonnegative for each $j \in J$.

(iii) There is a scalar-vector-splitting $\mathfrak{V} = \big((v_{j,\mathrm{sca}}, v_{j,\mathrm{vec}})\big)_{j\in J}$ such that each $-v_{j,\mathrm{sca}}$ is bounded from above. Then each such scalar-vector-splitting is called *bnd-admissible.*

(iv) Each f_j is bounded from above, $j \in J$.

Definition 3.7.44. The finite volume discretization $\mathfrak{F}$ of $\mathfrak{C}$ is called *bounded from above* iff the following conditions (i) – (iv) hold:

(i) $\mathfrak{C}$ is bounded from above.

(ii) $\mathfrak{V}$ is bnd-admissible.

(iii) The discretizations $\mathfrak{B}^{(\nu)}_{(k,\mathcal{C})}$, $\mathfrak{v}^{(\nu)}_{\mathrm{out},(k,\mathcal{C})}$, and $\mathfrak{a}^{(\nu)}_{\mathrm{out},(k,\mathcal{C})}$, $(k, \mathcal{C}) \in I_{\Pi,\mathfrak{D},\neg\mathrm{Dir}}$, are bounded from above according to Def. 3.7.23.

(iv) The discretizations (3.7.101) are bounded from above.

Lemma 3.7.45. *If the finite volume discretization $\mathfrak{F}$ of $\mathfrak{C}$ is bounded from above, then the operators $\mathfrak{s}^{(\nu)}$ defined by* (3.7.8) *are real-valued and satisfy*

$$\bigwedge_{\nu\in\{0,\dots,n\}} \sup \mathfrak{s}^{(\nu)} \le B_{\mathfrak{s}}[(\mathfrak{C}, \Pi, \mathfrak{V})], \tag{3.7.124}$$

where

$$\begin{aligned} B_{\mathfrak{s}}[(\mathfrak{C}, \Pi, \mathfrak{V})] :=& B_{k,\mathrm{Dir}}[\mathfrak{C}] \cdot \big(B_{\mathrm{Dir}}[\mathfrak{C}] - m_v\big) \cdot d_{\mathrm{Dir}}[\Pi] \\ &+ \max\big\{B_{v,\mathrm{Dir}}[(\mathfrak{C}, \mathfrak{V})],\ B_{v,\mathrm{sca},\mathrm{Dir}}[(\mathfrak{C}, \mathfrak{V})]\big\} \cdot l_{\mathrm{Dir}}[\Pi] + B_{\mathrm{out}}[\mathfrak{C}] \cdot \lambda_{d-1}[\partial p] \\ &+ B_{\mathrm{IF}}[\mathfrak{C}] \cdot \sum_{\gamma\in\mathrm{IF}} \lambda_{d-1}[\gamma] + B_f[\mathfrak{C}] \cdot \lambda_d[p]. \end{aligned} \tag{3.7.125}$$

Proof. The summation of the conclusions of Lems and Rems 3.7.6, 3.7.18, 3.7.24, 3.7.30, and 3.7.38 yields (3.7.124). ∎

Remark 3.7.46. In the presence of Dirichlet boundaries, $B_{\mathfrak{s}}[(\mathfrak{C},\Pi,,\mathfrak{V})]$ depends on the discretization Π through $d_{\mathrm{Dir}}[\Pi]$ and $l_{\mathrm{Dir}}[\Pi]$. As stated in Rem. 3.7.7, to prove convergence in the presence of Dirichlet boundaries, the dependence on $d_{\mathrm{Dir}}[\Pi]$ needs to be eliminated, since $d_{\mathrm{Dir}}[\Pi]$ does not stay bounded if Π becomes finer. In contrast, the dependence of $l_{\mathrm{Dir}}[\Pi]$ on Π is not serious (s. Rem. 3.7.19).

3.7.13 Discrete L^∞-L^1 A Priori Estimates

Within this section, fix a finite volume discretization $\mathfrak{F}$ of $\mathfrak{C}$ according to Def. 3.7.41. The goal of this section is to prove discrete L^∞-L^1 a priori estimates in Th. 3.7.50.

In the following Def. 3.7.47, the discrete L^1-norms $N^{(\nu)}_{\mathrm{Dir}}$, $N^{(\nu)}_{\neg\mathrm{Dir}}$, and $N^{(\nu)}_{\mathrm{all}}$ are defined, as well as the discrete L^∞-L^1-norms N_{Dir}, $N_{\neg\mathrm{Dir}}$, and N_{all}. For each of these norms, there is a variant just involving Dirichlet indices and a variant just involving non-Dirichlet indices, since different techniques are used to estimate each variant in the sequel. The numbers $N^{(\nu)}_{b,\neg\mathrm{Dir}}$ and $N_{b,\neg\mathrm{Dir}}$ defined in (3.7.126) and (3.7.127), respectively, constitute discrete L^1- and L^∞-L^1-norms, where the vectors are first subject to an application of $b^{(\nu)}_j$. For these norms, the Dirichlet case is omitted, since it is not needed for subsequent use.

Definition 3.7.47. *Discrete L^1-norms composed with $b^{(\nu)}_j$:*

$$\bigwedge_{\nu\in\{0,\dots,n\}} \left(\begin{aligned} &N^{(\nu)}_{b,\neg\mathrm{Dir}} : v^{I_{\Pi,\mathfrak{D},\neg\mathrm{Dir}}} \longrightarrow \mathbb{R}^+_0, \\ &N^{(\nu)}_{b,\neg\mathrm{Dir}}[U] := \sum_{\substack{j\in V[\mathcal{C}],\\ (k,\mathcal{C})\in I_{\Pi,\mathfrak{D},\neg\mathrm{Dir}}}} \left| b^{(\nu)}_j[(U_{(k,\mathcal{C})}, x_k)] \right| \cdot \lambda_d[\omega^{(j)}_k] \end{aligned} \right). \tag{3.7.126}$$

Discrete L^∞-L^1-norms composed with $b^{(\nu)}_j$:

$$\begin{aligned} N_{b,\neg\mathrm{Dir}} &: \left(v^{I_{\Pi,\mathfrak{D},\neg\mathrm{Dir}}}\right)^{\{0,\dots,n\}} \longrightarrow \mathbb{R}^+_0, \\ N_{b,\neg\mathrm{Dir}}\left[(U^{(\nu)})_{\nu\in\{0,\dots,n\}}\right] &:= \max\left\{ N^{(\nu)}_{b,\neg\mathrm{Dir}}[U^{(\nu)}] : \nu\in\{0,\dots,n\}\right\}. \end{aligned} \tag{3.7.127}$$

Discrete L^1-norms:

$$\bigwedge_{\nu\in\{0,\dots,n\}} \left(\begin{aligned} &N^{(\nu)}_{\mathrm{Dir}} : v^{I_{\Pi,\mathfrak{D},\mathrm{Dir}}} \longrightarrow \mathbb{R}^+_0, \\ &N^{(\nu)}_{\mathrm{Dir}}[U] := \sum_{\substack{j\in V[\mathcal{C}],\\ (k,\mathcal{C})\in I_{\Pi,\mathfrak{D},\mathrm{Dir}}}} |U_{(k,\mathcal{C})}| \cdot \lambda_d[\omega^{(j)}_k] \end{aligned} \right), \tag{3.7.128a}$$

$$\bigwedge_{\nu\in\{0,\dots,n\}} \begin{pmatrix} N^{(\nu)}_{\neg\mathrm{Dir}} : \upsilon^{I_{\Pi,\mathfrak{D},\neg\mathrm{Dir}}} \longrightarrow \mathbb{R}^+_0, \\ N^{(\nu)}_{\neg\mathrm{Dir}}[U] := \displaystyle\sum_{\substack{j\in V[\mathcal{C}],\\ (k,\mathcal{C})\in I_{\Pi,\mathfrak{D},\neg\mathrm{Dir}}}} |U_{(k,\mathcal{C})}| \cdot \lambda_d[\omega^{(j)}_k] \end{pmatrix}, \tag{3.7.128b}$$

$$\bigwedge_{\nu\in\{0,\dots,n\}} \begin{pmatrix} N^{(\nu)}_{\mathrm{all}} : \upsilon^{I_{\Pi,\mathfrak{D}}} \longrightarrow \mathbb{R}^+_0, \\ N^{(\nu)}_{\mathrm{all}}[U] := N^{(\nu)}_{\mathrm{Dir}}\left[U\restriction_{I_{\Pi,\mathfrak{D},\mathrm{Dir}}}\right] + N^{(\nu)}_{\neg\mathrm{Dir}}\left[U\restriction_{I_{\Pi,\mathfrak{D},\neg\mathrm{Dir}}}\right] \end{pmatrix}. \tag{3.7.128c}$$

Discrete L^∞-L^1-norms:

$$N_{\mathrm{Dir}} : \left(\upsilon^{I_{\Pi,\mathfrak{D},\mathrm{Dir}}}\right)^{\{0,\dots,n\}} \longrightarrow \mathbb{R}^+_0,$$

$$N_{\mathrm{Dir}}\left[(U^{(\nu)})_{\nu\in\{0,\dots,n\}}\right] := \max\left\{N^{(\nu)}_{\mathrm{Dir}}[U^{(\nu)}] : \nu \in \{0,\dots,n\}\right\}, \tag{3.7.129a}$$

$$N_{\neg\mathrm{Dir}} : \left(\upsilon^{I_{\Pi,\mathfrak{D},\neg\mathrm{Dir}}}\right)^{\{0,\dots,n\}} \longrightarrow \mathbb{R}^+_0,$$

$$N_{\neg\mathrm{Dir}}\left[(U^{(\nu)})_{\nu\in\{0,\dots,n\}}\right] := \max\left\{N^{(\nu)}_{\neg\mathrm{Dir}}[U^{(\nu)}] : \nu \in \{0,\dots,n\}\right\}, \tag{3.7.129b}$$

$$N_{\mathrm{all}} : \left(\upsilon^{I_{\Pi,\mathfrak{D}}}\right)^{\{0,\dots,n\}} \longrightarrow \mathbb{R}^+_0,$$

$$N_{\mathrm{all}}\left[(U^{(\nu)})_{\nu\in\{0,\dots,n\}}\right] := \max\left\{N^{(\nu)}_{\mathrm{all}}[U^{(\nu)}] : \nu \in \{0,\dots,n\}\right\}. \tag{3.7.129c}$$

—

The following Lem. 3.7.48 shows that the discrete norms composed with $b^{(\nu)}_j$ yield an upper bound for the discrete norms themselves, provided that the b_j satisfy a linear growth condition.

Lemma 3.7.48. *If $\upsilon = [m_\upsilon, \infty[$, and for each $j \in J$ and each $(t,x) \in \tau\times p_j$, the function $b_j\restriction_{\upsilon\times\{t\}\times\{x\}}$ is nonnegative, increasing, and inverse $L_{\mathrm{inv},b}$-Lipschitz, $L_{\mathrm{inv},b} \in \mathbb{R}^+$, (s. Def. C.7.10 in App. C), then*

$$\bigwedge_{\nu\in\{0,\dots,n\}} N^{(\nu)}_{\neg\mathrm{Dir}} \le \frac{N^{(\nu)}_{b,\neg\mathrm{Dir}}}{L_{\mathrm{inv},b}} + |m_\upsilon| \cdot \lambda_d[p], \tag{3.7.130a}$$

$$N_{\neg\mathrm{Dir}} \le \frac{N_{b,\neg\mathrm{Dir}}}{L_{\mathrm{inv},b}} + |m_\upsilon| \cdot \lambda_d[p]. \tag{3.7.130b}$$

Analogous formulas hold for the Dirichlet case and for the combined case, but they are not stated, since they are not used in the sequel.

Proof. Using Rem. C.7.12(a) in (3.7.128b), and using $U_{(k,\mathcal{C})} \ge m_\upsilon$, $b_j\restriction_{\upsilon\times\{t\}\times\{x\}} \ge 0$ being increasing, one has for each $(k,\mathcal{C}) \in I_{\Pi,\mathfrak{D},\neg\mathrm{Dir}}$ such that $U_{(k,\mathcal{C})} \ge 0$:

$$|U_{(k,\mathcal{C})}| \le \left|\frac{b^{(\nu)}_j[(U_{(k,\mathcal{C})}, x_k)] - b^{(\nu)}_j[(m_\upsilon, x_k)]}{L_{\mathrm{inv},b}} + m_\upsilon\right| \le \frac{b^{(\nu)}_j[(U_{(k,\mathcal{C})}, x_k)]}{L_{\mathrm{inv},b}} + |m_\upsilon|, \tag{3.7.131a}$$

and for each $(k,\mathcal{C}) \in I_{\Pi,\mathfrak{D},\neg\mathrm{Dir}}$ such that $U_{(k,\mathcal{C})} \leq 0$:

$$|U_{(k,\mathcal{C})}| \leq |m_v| \leq \frac{b_j^{(\nu)}[(U_{(k,\mathcal{C})}, x_k)]}{L_{\mathrm{inv},b}} + |m_v|. \tag{3.7.131b}$$

Combining (3.7.131) with (3.7.126); and taking into account that $(\omega_k^{(j)})_{j\in J:\,k\in I^{(j)}}$ is a partition of ω_k, $k \in I_\Pi$, and that Π is a partition of p, yields for each $U \in v^{I_{\Pi,\mathfrak{D},\neg\mathrm{Dir}}}$:

$$N_{\neg\mathrm{Dir}}^{(\nu)}[U] = \sum_{\substack{j\in V[\mathcal{C}],\\ (k,\mathcal{C})\in I_{\Pi,\mathfrak{D},\neg\mathrm{Dir}}}} |U_{(k,\mathcal{C})}| \cdot \lambda_d[\omega_k^{(j)}] \leq \frac{N_{b,\neg\mathrm{Dir}}^{(\nu)}[U]}{L_{\mathrm{inv},b}} + |m_v| \cdot \lambda_d[p],$$

proving (3.7.130a). Then (3.7.130b) is a direct consequence of (3.7.130a), (3.7.127), and (3.7.129b). ■

Example 3.7.49. It is shown that under natural hypotheses, the functions b_j occurring in Ex. 3.1.1(b) and in the first case of Ex. 3.1.1(a) satisfy the hypotheses of Lem. 3.7.48, i.e. they are nonnegative, increasing, and inverse Lipschitz.

In the first case of Ex. 3.1.1(a), the unknown function represents mass density, i.e. $v = \mathbb{R}_0^+$ is suitable. Then $b_j[(y,t,x)] = y$ is nonnegative, increasing, and inverse 1-Lipschitz.

In Ex. 3.1.1(b), the unknown function represents absolute temperature, i.e. $v = \mathbb{R}_0^+$. In the first case, one has $b_j[(y,t,x)] = \frac{z^{(\mathrm{Ar})}R}{M^{(\mathrm{Ar})}}\rho_{\mathrm{gas}}[x]\cdot y$, i.e. b_j is nonnegative, increasing, and inverse $(\frac{z^{(\mathrm{Ar})}R}{M^{(\mathrm{Ar})}} \operatorname{inv} \rho_{\mathrm{gas}})$-Lipschitz if ρ_{gas} is bounded away from 0. In the second and third case, $b_j[(y,t,x)] = \rho[x]\varepsilon[y]$, which is nonnegative, increasing, and inverse Lipschitz, if ρ is bounded away from 0, and ε is nonnegative, increasing, and inverse Lipschitz.

—

Theorem 3.7.50 combines Lems 3.7.45 and 3.7.48 to establish discrete L^∞-L^1 a priori estimates for each solution to the finite volume discretization $\mathfrak{F}$ according to Def. 3.7.42, provided that $\mathfrak{F}$ is bounded from above and the functions $b_j\restriction_{v\times\{t\}\times\{x\}}$ are nonnegative, increasing, and inverse Lipschitz.

Theorem 3.7.50. *Let*

$$\left(U^{(\nu)}\right)_{\nu\in\{0,\dots,n\}} = \left(u_{(k,\mathcal{C})}^{(\nu)}\right)_{(\nu,(k,\mathcal{C}))\in\{0,\dots,n\}\times I_{\Pi,\mathfrak{D}}} \in \left(v^{I_{\Pi,\mathfrak{D}}}\right)^{\{0,\dots,n\}}$$

be a solution to $\mathfrak{F}$ according to Def. 3.7.42. The initial distribution and the values on Dirichlet boundaries can be estimated without further hypotheses:

$$N_{b,\neg\mathrm{Dir}}^{(0)}\left[U^{(0)}\right] \leq B_{b,0}[\mathfrak{C}] \cdot \lambda_d[p], \tag{3.7.132a}$$

$$N_{\mathrm{Dir}} \leq B_{\mathrm{Dir}}[\mathfrak{C}] \sum_{j\in J:\,0\in J_j} \lambda_d[p_j], \tag{3.7.132b}$$

where $B_{\mathrm{Dir}}[\mathfrak{C}]$ *is defined in* (3.7.27), *and*

$$B_{b,0}[\mathfrak{C}] := \max\left\{ \left| b_j\left[\left(u_j^{(0)}[x], t, x\right)\right]\right| : j \in J,\ (t,x) \in \tau \times p_j \right\}. \tag{3.7.133}$$

Suppose the additional hypotheses (i) *and* (ii) *hold:*

(i) $\mathfrak{F}$ *is bounded from above.*

(ii) *There is* $L_{\mathrm{inv},b}[\mathfrak{C}] \in \mathbb{R}^+$ *such that for each* $j \in J$ *and each* $(t,x) \in \tau \times p_j$, *the function* $b_j\restriction_{v\times\{t\}\times\{x\}}$ *is nonnegative, increasing, and inverse* $L_{\mathrm{inv},b}$*-Lipschitz.*

Then

$$\begin{aligned} N_{b,\neg\mathrm{Dir}} \le & N^{(0)}_{b,\neg\mathrm{Dir}}\left[U^{(0)}\right] + B_{\mathfrak{s}}[(\mathfrak{C},\Pi,\mathfrak{V})]\cdot(t_{\mathrm{f}} - t_0) \\ \le & B_{b,0}[\mathfrak{C}]\cdot\lambda_d[p] + B_{\mathfrak{s}}[(\mathfrak{C},\Pi,\mathfrak{V})]\cdot(t_{\mathrm{f}} - t_0), \end{aligned} \tag{3.7.134a}$$

$$N_{\neg\mathrm{Dir}} \le \left(|m_v| + \frac{B_{b,0}[\mathfrak{C}]}{L_{\mathrm{inv},b}[\mathfrak{C}]}\right)\cdot\lambda_d[p] + \frac{B_{\mathfrak{s}}[(\mathfrak{C},\Pi,\mathfrak{V})]\cdot(t_{\mathrm{f}} - t_0)}{L_{\mathrm{inv},b}[\mathfrak{C}]}, \tag{3.7.134b}$$

$$N_{\mathrm{all}} \le \left(|m_v| + B_{\mathrm{Dir}}[\mathfrak{C}] + \frac{B_{b,0}[\mathfrak{C}]}{L_{\mathrm{inv},b}[\mathfrak{C}]}\right)\cdot\lambda_d[p] + \frac{B_{\mathfrak{s}}[(\mathfrak{C},\Pi,\mathfrak{V})]\cdot(t_{\mathrm{f}} - t_0)}{L_{\mathrm{inv},b}[\mathfrak{C}]}, \tag{3.7.134c}$$

where the number $B_{\mathfrak{s}}[(\mathfrak{C},\Pi,\mathfrak{V})]$ *is defined in* (3.7.125).

It is underscored that the estimates (3.7.132) *and* (3.7.134) *hold idependently of the discretizations* $(t_\nu)_{\nu\in\{0,\dots,n\}}$ *and* Π, *except in the case of the existence of Dirichlet boundaries, where there is a dependence on* Π *via the numbers* $d_{\mathrm{Dir}}[\Pi]$ *and* $l_{\mathrm{Dir}}[\Pi]$ *that occur in the definition of* $B_{\mathfrak{s}}[(\mathfrak{C},\Pi,\mathfrak{V})]$ *in* (3.7.125) *(s. Rems* 3.7.7 *and* 3.7.46*).*

Proof. In each of the estimates (3.7.132) and (3.7.134), it is taken into account that $(\omega_k^{(j)})_{j\in J: k\in I^{(j)}}$ is a partition of ω_k, $k \in I_\Pi$, and that Π is a partition of p.

(3.7.132a) follows from (3.7.126) using Def. 3.7.42(i) and (3.7.133).

(3.7.132b) follows from (3.7.128a) and (3.7.129a), using Def. 3.7.42(ii) and (3.7.27).

To verify (3.7.134a), using that the functions b_j, $j \in J$, are nonnegative, one can compute for each $\nu \in \{1,\dots,n\}$:

$$\begin{aligned} & N^{(\nu)}_{b,\neg\mathrm{Dir}}\left[U^{(\nu)}\restriction_{I_{\Pi,\mathfrak{D},\neg\mathrm{Dir}}}\right] - N^{(\nu-1)}_{b,\neg\mathrm{Dir}}\left[U^{(\nu-1)}\restriction_{I_{\Pi,\mathfrak{D},\neg\mathrm{Dir}}}\right] \\ & \overset{(3.7.126),(3.7.9),(3.7.10)}{=} \sum_{(k,\mathcal{C})\in I_{\Pi,\mathfrak{D},\neg\mathrm{Dir}}} (t_\nu - t_{\nu-1})\cdot\mathfrak{h}^{(\nu)}_{(k,\mathcal{C}),(a)}\left[\left(U^{(\nu-1)}\restriction_{I_{\Pi,\mathfrak{D},\neg\mathrm{Dir}}}, U^{(\nu)}\restriction_{I_{\Pi,\mathfrak{D},\neg\mathrm{Dir}}}\right)\right] \\ & \overset{(3.7.8),\ \mathrm{Def.}\ 3.7.42(\mathrm{iii})}{=} (t_\nu - t_{\nu-1})\cdot\mathfrak{s}^{(\nu)}\left[\left(U^{(\nu-1)}\restriction_{I_{\Pi,\mathfrak{D},\neg\mathrm{Dir}}}, U^{(\nu)}\restriction_{I_{\Pi,\mathfrak{D},\neg\mathrm{Dir}}}\right)\right] \\ & \overset{\mathrm{Lem.}\ 3.7.45}{\le} (t_\nu - t_{\nu-1})\cdot B_{\mathfrak{s}}[(\mathfrak{C},\Pi,\mathfrak{V})]. \end{aligned} \tag{3.7.135}$$

Then (3.7.134a) follows by summing (3.7.135) for $\nu \in \{1, \dots, n\}$, and then using (3.7.132a) in the result.

(3.7.134b) is implied by (3.7.134a) and (3.7.130b).

Combining (3.7.132b) and (3.7.134b) yields (3.7.134c), according to the definition of N_{all} in (3.7.128c) and (3.7.129c). ■

3.8 Existence and Uniqueness of a Discrete Solution

The goal of Sec. 3.8 is to prove the existence and uniqueness of a discrete solution in Th. 3.8.35. More precisely, it is shown in Th. 3.8.35 that for sufficiently large $M \in]m_v, \infty[$, and provided that the time discretization is sufficiently fine, there is a unique family $(u^{(\nu)}_{(k,\mathcal{C})})_{(\nu,(k,\mathcal{C}))\in\{0,\dots,n\}\times I_{\Pi,\mathfrak{D}}} \in \left([m_v, M]^{I_{\Pi,\mathfrak{D}}}\right)^{\{0,\dots,n\}}$ satisfying (i), (ii), and (iii) of Def. 3.7.42.

The proof is based on a fixed point argument, using the Banach Fixed Point Th. 3.8.1. Starting from the initial distribution $u^{(0)}$, the $u^{(\nu)}$, $\nu > 0$, are constructed inductively, assuming $u^{(\nu-1)}$ to be given. In each time step, each operator $\mathfrak{h}^{(\nu)}_{(k,\mathcal{C})}$, $(k, \mathcal{C}) \in I_{\Pi,\mathfrak{D},\neg\mathrm{Dir}}$, acting on $u^{(\nu)}$ is decomposed into a function $h^{(\nu)}_{(k,\mathcal{C})}$, merely depending on the scalar $u^{(\nu)}_{(k,\mathcal{C})}$, and a function $g^{(\nu)}_{(k,\mathcal{C})}$, which can depend on the entire vector $u^{(\nu)}$ (cf. (3.8.51a)). The main auxiliary result is Th. 3.8.4, where it is shown that, if the $h^{(\nu)}_{(k,\mathcal{C})}$ grow sufficiently fast in relation to the growth of the $g^{(\nu)}_{(k,\mathcal{C})}$, then $\mathfrak{h}^{(\nu)}[u] = 0$ has a unique solution in a sufficiently large hypercube $[m, M]^{I_{\Pi,\mathfrak{D},\neg\mathrm{Dir}}}$. The proof of Th. 3.8.35 shows that by choosing the time steps sufficiently fine, one can force the $h^{(\nu)}_{(k,\mathcal{C})}$ to grow sufficiently fast.

As the Banach Fixed Point Theorem does not apply directly to the situation of Th. 3.8.4, it is adapted in the following Sec. 3.8.1 (s. Lems 3.8.2 and 3.8.3).

As the operators $\mathfrak{h}^{(\nu)}_{(k,\mathcal{C})}$ involve a considerable number of terms (s. (3.7.122)), their decomposition into $h^{(\nu)}_{(k,\mathcal{C})}$ and $g^{(\nu)}_{(k,\mathcal{C})}$ as mentioned above, is somewhat tedious. It is carried out term by term in Secs 3.8.3 – 3.8.8. For each term, the part of the decomposition that is to become a summand of $h^{(\nu)}_{(k,\mathcal{C})}$ carries a superscript $\uparrow$ and is occasionally referred to as an $\uparrow$-operator. Correspondingly, the future summands of $g^{(\nu)}_{(k,\mathcal{C})}$ carry a superscript $\downarrow$ and are sometimes called $\downarrow$-operators. Each decomposition is succeeded by a lemma that establishes the properties needed to provide the hypotheses of Lem. 3.8.5 for its application in the proof of Th. 3.8.35.

3.8.1 Existence of Unique Fixed Points

In the current section as well as in the following sections, a number of elementary facts on Lipschitz functions, inverse Lipschitz functions, and contracting functions are used. These facts are provided in App. C.7.2, C.7.3, and C.7.4, respectively.

Banach Fixed Point Theorem 3.8.1. *Suppose C is a closed nonempty subset of a complete metric space, and $f : C \longrightarrow C$ is a contraction. Then there is a unique $x_{\mathrm{fix}} \in C$ such that $f[x_{\mathrm{fix}}] = x_{\mathrm{fix}}$, i.e. f has a unique fixed point in C.*

Proof. See for example [Zei86, p. 17]. ■

The following Lem. 3.8.2 shows that a map f that is sufficiently contracting on a ball, maps the ball into itself, and thus has a unique fixed point if the metric is complete. Here sufficiently contracting means c-contracting, such that c multiplied by the ball's radius is less than the distance of $f[x_0]$ from the ball's complement, x_0 denoting the center of the ball (cf. Fig. 3.26).

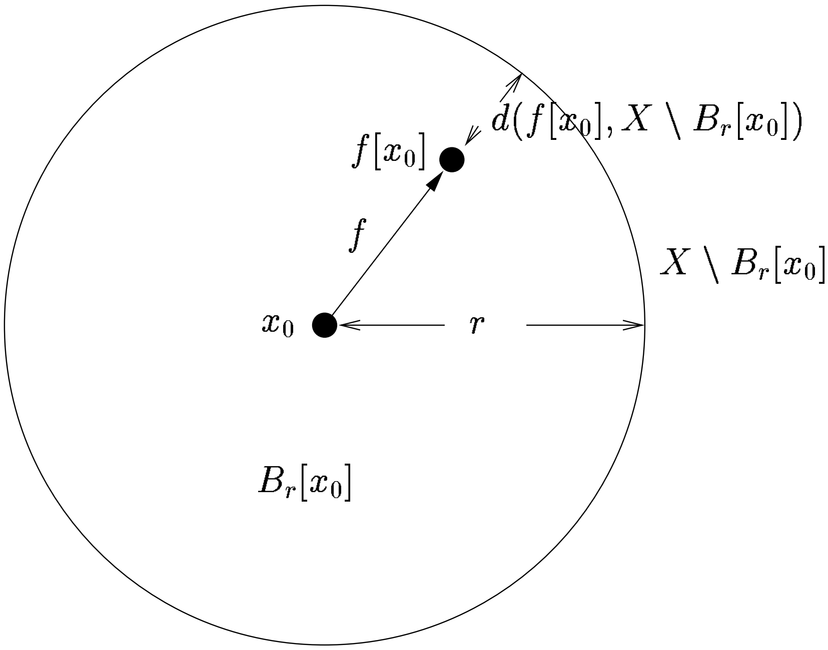


Figure 3.26: Illustration of Lem. 3.8.2: If f is $\frac{d\left(f[x_0], X \setminus B_r[x_0]\right)}{r}$-contracting, then it maps $\overline{B_r[x_0]}$ into itself.

Lemma 3.8.2. *Let (X, d) be a metric space, $x_0 \in X$, $r \in \mathbb{R}^+$, and $f : \overline{B_r[x_0]} \longrightarrow X$. Suppose f is c-contracting for some $c \in [0, 1[$, satisfying*

$$c \leq \frac{d\big(f[x_0], X \setminus B_r[x_0]\big)}{r}. \tag{3.8.1}$$

(a) *It holds that* $f\left[\overline{B_r[x_0]}\right] \subseteq \overline{B_r[x_0]}$.

(b) *If* $(\overline{B_r[x_0]}, d)$ *is a complete metric space, than* f *has a unique fixed point.*

Proof. (a): For each $x \in \overline{B_r[x_0]}$, one calculates

$$d\big[(f[x], f[x_0])\big] \leq c \cdot d\big[(x, x_0)\big] \leq c \cdot r \leq d\big(f[x_0], X \setminus B_r[x_0]\big),$$

i.e. $f[x] \in \overline{B_r[x_0]}$, establishing the case.

(b) is an immediate consequence of (a) and the Banach Fixed Point Th. 3.8.1. ■

The ensuing Lem. 3.8.3 specializes Lem. 3.8.2 to the case $X = ([m, \infty[)^I$ endowed with the max-norm, where I is a finite index set, $x_0 = (m, \dots, m)$ (cf. Fig. 3.27). In the application in Th. 3.8.35, one has $I = I_{\Pi,\mathfrak{D},\neg\mathrm{Dir}}$.

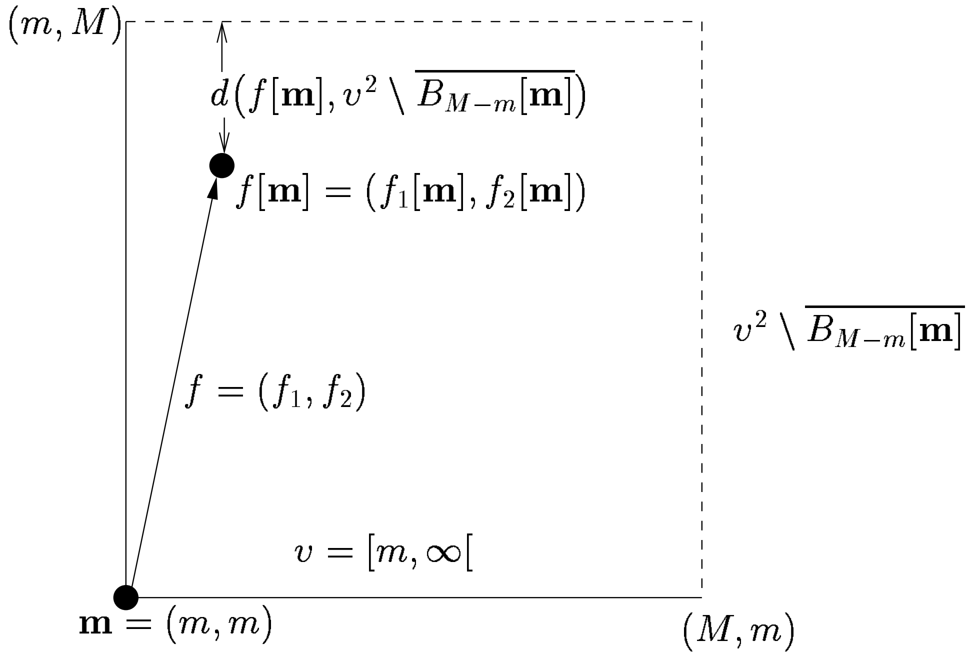


Figure 3.27: Illustration of Lem. 3.8.3: f maps $[m, M]^2$ into itself if f is sufficiently contracting, satisfying (3.8.2b).

Lemma 3.8.3. *Given a finite, nonempty index set* I *and* $m \in \mathbb{R}$, *let* $v := [m, \infty[$. *Let* $M \in]m, \infty[$, *and consider maps* $f_k : [m, M]^I \longrightarrow v$, $k \in I$, *where* $[m, M]^I$ *is endowed with the max-norm. Let* $\mathbf{m} := (m, \dots, m)$. *Suppose*

$$\bigwedge_{k \in I} f_k[\mathbf{m}] \leq M, \tag{3.8.2a}$$

and that there are numbers $c_k \in [0,1[$, $k \in I$, such that

$$c_{\max} := \max\left\{c_k : k \in I\right\} \leq \frac{M - \max\left\{f_k[\mathbf{m}] : k \in I\right\}}{M - m}. \tag{3.8.2b}$$

If each f_k is c_k-contracting, $k \in I$, then the map $f : [m,M]^I \longrightarrow v^I$, $f[x] := \left(f_k[x]\right)_{k \in I}$, maps $[m,M]^I$ into itself and has a unique fixed point.

Proof. By Rem. C.7.14, f is $c_{\max}$-contracting with respect to the max-norm $\| \|_{\max}$ on $\mathbb{R}^I$. Moreover, $[m,M]^I = \overline{B_{M-m}[\mathbf{m}]}$ and

$$\begin{aligned} c_{\max}(M-m) &\leq M - \max\left\{f_k[\mathbf{m}] : k \in I\right\} \\ &= \inf\left\{\|f[\mathbf{m}] - y\|_{\max} : y \in v^I \setminus \overline{B_{M-m}[\mathbf{m}]}\right\}. \end{aligned} \tag{3.8.3}$$

Thus f maps $[m,M]^I$ into itself and has a unique fixed point according to Lem. 3.8.2. ■

3.8.2 A Root Problem

Theorem 3.8.4. *Given a finite, nonempty index set I and $m \in \mathbb{R}$, let $v := [m, \infty[$. Consider an operator*

$$\mathcal{H} : v^I \longrightarrow \mathbb{R}^I, \quad \mathcal{H}[u] = \left(\mathcal{H}_k[u]\right)_{k \in I}. \tag{3.8.4}$$

Assume there are continuous functions $h_k \in C(v, \mathbb{R})$, $g_k \in C(v^I, \mathbb{R})$, $k \in I$, nonnegative real numbers L_g, $L_{\mathrm{inv},h}$, and a real number $M \in]m, \infty[$, such that the following conditions (i) – (vii) *are satisfied. Let $\mathbf{m} := (m, \dots, m)$.*

(i) $\bigwedge_{k \in I} \quad \mathcal{H}_k[u] = h_k[u_k] - g_k[u].$

(ii) *Each h_k is increasing, $k \in I$.*

(iii) $\bigwedge_{k \in I} \bigwedge_{u \in v^I} \quad h_k[m] \leq g_k[u].$

(iv) $L_g < L_{\mathrm{inv},h}.$

(v) $\bigwedge_{k \in I} \quad g_k[\mathbf{m}] < h_k\left[M - (M-m)\frac{L_g}{L_{\mathrm{inv},h}}\right].$

(vi) *Each g_k is L_g-Lipschitz with respect to the max-norm on $[m,M]^I$, $k \in I$.*

(vii) *For each $k \in I$, there is $\lambda_k \in \mathbb{R}$ such that*

$$\bigwedge_{k\in I} \begin{pmatrix} \lambda_k \geq M - (M-m)\dfrac{L_g}{L_{\mathrm{inv},h}}, \\ h_k{\restriction}_{[m,\lambda_k]} \in \mathrm{InLip}_{L_{\mathrm{inv},h}}\Big([m,\lambda_k],\mathbb{R}\Big), \\ h_k[\lambda_k] \geq \max\Big(g_k\left([m,M]^I\right)\Big) \end{pmatrix}. \tag{3.8.5}$$

Then $\mathcal{H}$ has a unique root in $[m,M]^I$, i.e. there is a unique $u_0 \in [m,M]^I$ such that $\mathcal{H}[u_0] = (0,\dots,0)$.

Proof. Before starting the main part of the proof, it is remarked that the right-hand side of (v) is always defined, since by (iv),

$$M > M - (M-m)\frac{L_g}{L_{\mathrm{inv},h}} > M - M + m = m. \tag{3.8.6}$$

To prove the theorem, define

$$f : [m,M]^I \longrightarrow \prod_{k\in I}[m,\lambda_k], \quad \bigwedge_{k\in I} \quad f_k := h_k^{-1} \circ g_k. \tag{3.8.7}$$

It is noted that the h_k^{-1} exist on $\big[h_k[m], h_k[\lambda_k]\big]$ by Rem. C.7.12(b),(c). Moreover, h_k^{-1} can be composed with g_k, since (iii) and (vii) imply that g_k maps $[m,M]^I$ into $\big[h_k[m], h_k[\lambda_k]\big]$.

As (3.8.7) means $g_k = h_k \circ f_k$, Lem. C.7.15 shows that each f_k is $\frac{L_g}{L_{\mathrm{inv},h}}$-contracting, $k \in I$.

Moreover, it follows from (v) that

$$\max\big\{f_k[\mathbf{m}] : k \in I\big\} < M - (M-m)\frac{L_g}{L_{\mathrm{inv},h}}, \tag{3.8.8}$$

implying

$$\frac{L_g}{L_{\mathrm{inv},h}} < \frac{M - \max\big\{f_k[\mathbf{m}] : k \in I\big\}}{M-m}. \tag{3.8.9}$$

Now Lem. 3.8.3 yields that f maps $[m,M]^I$ into itself and has a unique fixed point $u_0 = (u_{0,k})_{k\in I} \in [m,M]^I$. That u_0 is a fixed point of f means

$$\bigwedge_{k\in I} \quad h_k[u_{0,k}] = g_k[u_0]. \tag{3.8.10}$$

According to (i), u_0 is a root of $\mathcal{H}$ if and only if (3.8.10) holds, i.e. the proof is complete. ∎

The following Lem. 3.8.5 gives a criterion for function families (h_k) and (g_k) to satisfy the hypotheses (ii) – (vii) of Th. 3.8.4. It is designed to be directly applicable to the situation arising in the proof of Th. 3.8.35 below.

Lemma 3.8.5. *Given a finite, nonempty index set I and $m \in \mathbb{R}$, let $v := [m, \infty[$. Consider continuous functions $h_k \in C(v, \mathbb{R})$, $g_k \in C(v^I, \mathbb{R})$, $k \in I$.*

Assume there are numbers $\{\delta, L_{\text{inv}}\} \subseteq \mathbb{R}^+$, $P_k \in \mathbb{R}_0^+$, and continuous functions $\tilde{g}_k \in C(v^I, \mathbb{R})$, $b_k \in C(v, \mathbb{R}_0^+)$, $\tilde{h}_k \in C(v, \mathbb{R})$, satisfying the following conditions (i) – (vii). *Let $\mathbf{m} := (m, \dots, m)$.*

(i) $\bigwedge_{k \in I} \quad h_k = \frac{b_k}{\delta} + \tilde{h}_k$.

(ii) $\bigwedge_{k \in I} \quad g_k = \frac{P_k}{\delta} + \tilde{g}_k$.

(iii) *Each b_k and each $\tilde{h}_k$ is increasing, $k \in I$.*

(iv) *Each $\tilde{g}_k$ is minimal at $\mathbf{m}$, $k \in I$.*

(v) $\bigwedge_{k \in I} \quad \frac{b_k[m]}{\delta} + \tilde{h}_k[m] \leq \frac{P_k}{\delta} + \tilde{g}_k[\mathbf{m}]$.

(vi) $\bigwedge_{y \in v} \quad \bigvee_{L_{g,y} \in \mathbb{R}_0^+} \quad \bigwedge_{k \in I}$ *$\tilde{g}_k$ is $L_{g,y}$-Lipschitz on $\overline{B_y[\mathbf{m}]}$ (i.e. $\tilde{g}_k$ is locally Lipschitz).*

(vii) *Each b_k is inverse L_{inv}-Lipschitz, $k \in I$.*

Set

$$S_k := \frac{P_k + \max\{0, \tilde{g}_k[\mathbf{m}]\} - \min\{0, \tilde{h}_k[m]\}}{L_{\text{inv}}} + m, \tag{3.8.11a}$$

$$S := \max\{S_k : \ k \in I\}. \tag{3.8.11b}$$

If

$$M > S, \tag{3.8.12a}$$

$$\delta \cdot L_{g,M-m} < L_{\text{inv}} \cdot \frac{M-S}{M-m}, \tag{3.8.12b}$$

$$\delta \leq 1, \tag{3.8.12c}$$

then g_k, h_k, $k \in I$, and M satisfy conditions (ii) – (vii) *of Th.* 3.8.4 *with $L_g := L_{g,M-m}$ and $L_{\text{inv},h} := \frac{L_{\text{inv}}}{\delta}$.*

Proof. Th. 3.8.4(ii): It follows from (i) and (iii) that h_k is increasing for each $k \in I$.

Th. 3.8.4(iii): It follows from (i), (ii), (iv), and (v) that $h_k[m] \leq g_k[u]$ for each $k \in I$ and each $u \in v^I$.

Th. 3.8.4(iv): If $L_g = 0$, then $L_g < L_{\mathrm{inv},h}$ holds. Assume $L_g > 0$. Using (3.8.12b), one gets $L_{\mathrm{inv},h} = \frac{L_{\mathrm{inv}}}{\delta} > L_{g,M-m} \cdot \frac{M-m}{M-S} \geq L_g$ (it is $S \geq m$ by (3.8.11)).

Th. 3.8.4(v): Using (3.8.12b) and $L_{\mathrm{inv},h} = \frac{L_{\mathrm{inv}}}{\delta}$, one finds

$$\frac{L_g}{L_{\mathrm{inv},h}}(M-m) < M - S, \tag{3.8.13}$$

which implies

$$S < M - (M-m)\,\frac{L_g}{L_{\mathrm{inv},h}}. \tag{3.8.14}$$

Due to (iii), (vii), and (3.8.14), one can apply Rem. C.7.12(a),(b) to conclude

$$\bigwedge_{k\in I} \left(\begin{array}{l} P_k + \max\left\{0, \tilde{g}_k[\mathbf{m}]\right\} - \min\left\{0, \tilde{h}_k[m]\right\} \\ \leq P_k + \max\left\{0, \tilde{g}_k[\mathbf{m}]\right\} - \min\left\{0, \tilde{h}_k[m]\right\} + b_k[m] \\ = L_{\mathrm{inv}} \cdot (S_k - m) + b_k[m] \leq b_k[S] < b_k\left[M - (M-m)\,\dfrac{L_g}{L_{\mathrm{inv},h}}\right] \end{array} \right). \tag{3.8.15}$$

Together with (3.8.12c) and (iii), (3.8.15) implies

$$\bigwedge_{k\in I} \left(\begin{array}{l} P_k + \delta \cdot \tilde{g}_k[\mathbf{m}] < b_k\left[M - (M-m)\,\dfrac{L_g}{L_{\mathrm{inv},h}}\right] + \delta \cdot \tilde{h}_k[m] \\ \leq b_k\left[M - (M-m)\,\dfrac{L_g}{L_{\mathrm{inv},h}}\right] + \delta \cdot \tilde{h}_k\left[M - (M-m)\,\dfrac{L_g}{L_{\mathrm{inv},h}}\right] \end{array} \right). \tag{3.8.16}$$

Dividing (3.8.16) by δ and using (i) and (ii) establishes the case.

Th. 3.8.4(vi): This follows from the definition of L_g and (vi) by observing $[m,M]^I = \overline{B_{M-m}[\mathbf{m}]}$.

Th. 3.8.4(vii): It follows from (i), (iii), (vii), Rem. C.7.12(d),(e), and the definition of $L_{\mathrm{inv},h}$, that h_k is inverse $L_{\mathrm{inv},h}$-Lipschitz on its whole domain v for each $k \in I$. Since the h_k are unbounded from above according to Rem. C.7.12(a), there exist $\lambda_k \in \mathbb{R}$, $k \in I$, such that (3.8.5) holds. ■

3.8.3 Decomposition of Terms Involving Interior Diffusion Flux

Following the strategy outlined at the beginning of Sec. 3.8, Secs 3.8.3 – 3.8.8 provide the decompositions of the summands making up $\mathfrak{h}^{(\nu)}_{(k,\mathcal{C})}$ according to (3.7.122). The summands are decomposed in the same order as they were defined in Secs 3.7.3 – 3.7.11.

The decompositions make use of the concept of the *variation* of a function described in App. C.6.3. It is pointed out that in this work, variation is only used as a technical tool to decompose *locally Lipschitz continuous* functions into increasing locally Lipschitz continuous functions (cf. Rem. C.6.8(h)).

In the present Sec. 3.8.3, the operators $\mathfrak{k}^{(\nu)}_{\neg\mathrm{Dir},(k,\mathcal{C})}$ and $\mathfrak{k}^{(\nu)}_{\mathrm{Dir},(k,\mathcal{C})}$ defined in (3.7.16) and (3.7.17) are decomposed. In preparation, the following Def. 3.8.6 defines the *initial supremum* of a function, and a result concerning its Lipschitz continuity is proved in Lem. 3.8.8. Lemma 3.8.8 is used in the succeeding Lem. 3.8.10. The initial supremum is introduced to be able to establish (3.8.26) in the proof of Lem. 3.8.10.

Definition 3.8.6. Given $m \in \mathbb{R}$, a set A, and a map $k : [m,\infty[\times A \longrightarrow \mathbb{R}$, define the *initial supremum* of k:

$$\mathrm{insup}[k] : [m,\infty[\longrightarrow \mathbb{R}\cup\{\infty\}, \quad y \mapsto \sup\big\{k[(\lambda,x)] : (\lambda,x)\in[m,y]\times A\big\}. \tag{3.8.17}$$

Remark 3.8.7. The initial supremum is always increasing.

Lemma 3.8.8. *Let X be a compact metric space. Consider a continuous map $k : [m,M]\times X \longrightarrow \mathbb{R}$. Suppose $k\restriction_{[m,M]\times\{x\}}$ is Lipschitz for each $x \in X$. If*

$$L := \sup\big\{\|k\restriction_{[m,M]\times\{x\}}\|_{\mathrm{Lip}} : x\in X\big\} < \infty \tag{3.8.18}$$

(cf. Def. C.7.8 of $\|\ \|_{\mathrm{Lip}}$), then $\mathrm{insup}[k]$ is L-Lipschitz.

Proof. First, the special case is considered, where k is independent of $x \in X$:

Claim 1. If $k : [m,M] \longrightarrow \mathbb{R}$ is L-Lipschitz, then $\mathrm{insup}[k]$ is L-Lipschitz.

Proof. Let $\{y_1,y_2\}\subseteq[m,M]$, where $y_1<y_2$. If $\mathrm{insup}[k][y_1]=\mathrm{insup}[k][y_2]$, then there is nothing to show. If $\mathrm{insup}[k][y_1]<\mathrm{insup}[k][y_2]$, then there is $\tilde{y}_2\in]y_1,y_2]$ such that $\mathrm{insup}[k][y_2]=k[\tilde{y}_2]$. By the intermediate value theorem, there is $\tilde{y}_1\in[y_1,\tilde{y}_2[$ such that $\mathrm{insup}[k][y_1]=k[\tilde{y}_1]$. Hence, $|\tilde{y}_2-\tilde{y}_1|\le|y_2-y_1|$, and one calculates

$$\big|\,\mathrm{insup}[k][y_2]-\mathrm{insup}[k][y_1]\big| = \big|k[\tilde{y}_2]-k[\tilde{y}_1]\big| \le L\cdot|\tilde{y}_2-\tilde{y}_1| \le L\cdot|y_2-y_1|,$$

showing that $\mathrm{insup}[k]$ is L-Lipschitz. ▲

Now the general case of Lem. 3.8.8 is treated.

Using Cl. 1, it remains to show that the map $\max_X[k] : [m,M]\longrightarrow\mathbb{R}$, $\max_X[k][y] := \|k\restriction_{\{y\}\times X}\|_{\max}$ is L-Lipschitz. Let $(y_1,y_2)\in[m,M]^2$. By a possible interchange of y_1 and y_2, one can assume $\max_X[k][y_1]\le\max_X[k][y_2]$. There are $(x_1,x_2)\in X^2$ such that $\max_X[k][y_1]=k[(y_1,x_1)]$, $\max_X[k][y_2]=k[(y_2,x_2)]$. One calculates

$$\begin{aligned}\big|\max\nolimits_X[k][y_1]-\max\nolimits_X[k][y_2]\big| &= k[(y_2,x_2)]-k[(y_1,x_1)]\\ &\le k[(y_2,x_2)]-k[(y_1,x_2)] \le L\cdot|y_2-y_1|,\end{aligned}$$

showing that $\max_X[k]$ is L-Lipschitz. ■

However, the following Ex. 3.8.9 shows that, in general, the condition (3.8.18) in Lem. 3.8.8 can not be omitted:

Example 3.8.9. Consider $k : [0,1] \times [0,1] \longrightarrow \mathbb{R}$ defined by

$$k[(y,x)] := \begin{cases} \frac{y}{\sqrt{x}} & \text{for } 0 \le y \le x \le 1, \\ \sqrt{x} & \text{for } 0 \le x \le y \le 1. \end{cases} \tag{3.8.19}$$

Then k is continuous, $k\restriction_{[0,1]\times\{0\}}$ is 0-Lipschitz, and for each $x \in]0,1]$, the function $k\restriction_{[0,1]\times\{x\}}$ is $\frac{1}{\sqrt{x}}$-Lipschitz. However, one has $\operatorname{insup}[k][y] = \sqrt{y}$ for each $y \in [0,1]$, that means $\operatorname{insup}[k]$ is *not* a Lipschitz function.

—

Now, to decompose $\mathfrak{k}^{(\nu)}_{\neg\mathrm{Dir},(k,\mathcal{C})}$ and $\mathfrak{k}^{(\nu)}_{\mathrm{Dir},(k,\mathcal{C})}$, assume $v = [m_v, \infty[$ and that for each $j \in J$, k_j is real-valued and locally Lipschitz in the sense of condition (locLip) of the following Lem. 3.8.10. Let

$$\bigwedge_{(j,\nu,x)\in J\times\{0,\dots,n\}\times p_j} \tilde{k}^{(\nu)}_{j,x} : v \longrightarrow \mathbb{R}, \quad \tilde{k}^{(\nu)}_{j,x}[y] := k^{(\nu)}_j[(y,x)](y - m_v), \tag{3.8.20}$$

$$\bigwedge_{\substack{\nu\in\{0,\dots,n\},\\ (k,\mathcal{C})\in I_{\Pi,\mathfrak{D},\neg\mathrm{Dir}}}} \left(\begin{aligned} &\mathfrak{k}^{\nu,\uparrow}_{\neg\mathrm{Dir},(k,\mathcal{C})} : v \longrightarrow \mathbb{R}, \\ &\mathfrak{k}^{\nu,\uparrow}_{\neg\mathrm{Dir},(k,\mathcal{C})}[y] := \sum_{\substack{j\in V[\mathcal{C}],\\ l\in \mathrm{nb}_{j,\neg\mathrm{Dir}}[k]}} \Bigg(\operatorname{insup}\left[k^{(\nu)}_j\right][y]\cdot(y-m_v) \\ &\qquad\qquad + \operatorname{var}^+\left[\tilde{k}^{(\nu)}_{j,x_k}\right][y]\Bigg) \cdot \frac{\lambda_{d-1}\left[\omega^{(j)}_k \cap \omega^{(j)}_l\right]}{2\cdot\|x_k - x_l\|_2} \end{aligned} \right), \tag{3.8.21a}$$

$$\bigwedge_{\substack{\nu\in\{0,\dots,n\},\\ (k,\mathcal{C})\in I_{\Pi,\mathfrak{D},\neg\mathrm{Dir}}}} \left(\begin{aligned} &\mathfrak{k}^{\nu,\downarrow}_{\neg\mathrm{Dir},(k,\mathcal{C})} : v^{I_{\Pi,\mathfrak{D},\neg\mathrm{Dir}}} \longrightarrow \mathbb{R}, \\ &\mathfrak{k}^{\nu,\downarrow}_{\neg\mathrm{Dir},(k,\mathcal{C})}[U] := \sum_{\substack{j\in V[\mathcal{C}],\\ l\in \mathrm{nb}_{j,\neg\mathrm{Dir}}[k]}} \Bigg(\operatorname{var}^-\left[\tilde{k}^{(\nu)}_{j,x_k}\right][U_{(k,\mathcal{C})}] \\ &\qquad + \left(\operatorname{insup}\left[k^{(\nu)}_j\right][U_{(k,\mathcal{C})}] - k^{(\nu)}_j\left[\left(U_{(l,\mathcal{C}[(l,j)])}, x_l\right)\right]\right) \\ &\qquad\qquad \cdot\left(U_{(k,\mathcal{C})} - m_v\right) \\ &\qquad + \left(k^{(\nu)}_j[(U_{(k,\mathcal{C})}, x_k)] + k^{(\nu)}_j\left[\left(U_{(l,\mathcal{C}[(l,j)])}, x_l\right)\right]\right) \\ &\qquad\qquad \cdot\left(U_{(l,\mathcal{C}[(l,j)])} - m_v\right)\Bigg) \\ &\qquad \cdot \frac{\lambda_{d-1}\left[\omega^{(j)}_k \cap \omega^{(j)}_l\right]}{2\cdot\|x_k - x_l\|_2} \end{aligned} \right) \tag{3.8.21b}$$

$$\bigwedge_{\substack{\nu\in\{0,\dots,n\},\\(k,\mathcal{C})\in I_{\Pi,\mathfrak{D},\neg\mathrm{Dir}}}} \left(\begin{array}{l} \mathfrak{k}^{\nu,\uparrow}_{\mathrm{Dir},(k,\mathcal{C})} : \upsilon \longrightarrow \mathbb{R}, \\ \mathfrak{k}^{\nu,\uparrow}_{\mathrm{Dir},(k,\mathcal{C})}[y] := \displaystyle\sum_{\substack{j\in V[\mathcal{C}],\\ l\in \mathrm{nb}_{j,\mathrm{Dir}}[k]}} \Bigg(\mathrm{var}^{+}\left[\tilde{k}^{(\nu)}_{j,x_k}\right][y] \\ \qquad + \mathrm{var}^{-}\left[k^{(\nu)}_{j}\restriction_{\upsilon\times\{x_k\}}\right][y]\cdot\left(u_{j_{\mathrm{Dir}}[(l,j)],\mathrm{Dir}}[(t_\nu,x_l)] - m_\upsilon\right) \\ \qquad + k^{(\nu)}_{j}\left[\left(u_{j_{\mathrm{Dir}}[(l,j)],\mathrm{Dir}}[(t_\nu,x_l)],x_l\right)\right]\cdot\left(y - u_{j_{\mathrm{Dir}}[(l,j)],\mathrm{Dir}}[(t_\nu,x_l)]\right)\Bigg) \\ \qquad\qquad \cdot \dfrac{\lambda_{d-1}\left[\omega^{(j)}_{k}\cap\omega^{(j)}_{l}\right]}{2\cdot\|x_k - x_l\|_2} \end{array}\right), \tag{3.8.22a}$$

$$\bigwedge_{\substack{\nu\in\{0,\dots,n\},\\(k,\mathcal{C})\in I_{\Pi,\mathfrak{D},\neg\mathrm{Dir}}}} \left(\begin{array}{l} \mathfrak{k}^{\nu,\downarrow}_{\mathrm{Dir},(k,\mathcal{C})} : \upsilon \longrightarrow \mathbb{R}, \\ \mathfrak{k}^{\nu,\downarrow}_{\mathrm{Dir},(k,\mathcal{C})}[y] := \displaystyle\sum_{\substack{j\in V[\mathcal{C}],\\ l\in \mathrm{nb}_{j,\mathrm{Dir}}[k]}} \Bigg(\mathrm{var}^{-}\left[\tilde{k}^{(\nu)}_{j,x_k}\right][y] \\ \qquad + \left(k^{(\nu)}_{j}[(m_\upsilon,x_k)] + \mathrm{var}^{+}\left[k^{(\nu)}_{j}\restriction_{\upsilon\times\{x_k\}}\right][y]\right) \\ \qquad\qquad \cdot\left(u_{j_{\mathrm{Dir}}[(l,j)],\mathrm{Dir}}[(t_\nu,x_l)] - m_\upsilon\right)\Bigg) \\ \qquad\qquad \cdot \dfrac{\lambda_{d-1}\left[\omega^{(j)}_{k}\cap\omega^{(j)}_{l}\right]}{2\cdot\|x_k - x_l\|_2} \end{array}\right). \tag{3.8.22b}$$

Lemma 3.8.10. *Suppose* $\upsilon = [m_\upsilon, \infty[$, *the* k_j *are real-valued, and the conditions* (nn) *and* (locLip) *below both hold:*

(nn) k_j *is nonnegative for each* $j \in J$.

(locLip) $\bigwedge_{r\in\mathbb{R}^+_0} \bigvee_{L_{k,r}[\mathfrak{C}]\in\mathbb{R}^+_0} \bigwedge_{(j,t,x)\in J\times\tau\times p_j} k_j\restriction_{\upsilon\times\{t\}\times\{x\}} \in \mathrm{Lip}_{L_{k,r}[\mathfrak{C}]}\left([m_\upsilon, m_\upsilon + r], \mathbb{R}\right)$, *i.e. each* k_j *is locally Lipschitz with respect to its dependence on* $y \in \upsilon$.

Let $\mathbf{m} := (m_\upsilon, \dots, m_\upsilon)$. *Then the following holds for each* $\nu \in \{0, \dots, n\}$ *and for each* $(k, \mathcal{C}) \in I_{\Pi,\mathfrak{D},\neg\mathrm{Dir}}$:

(a) $-\mathfrak{k}^{(\nu)}_{\neg\mathrm{Dir},(k,\mathcal{C})}[U] = \mathfrak{k}^{\nu,\uparrow}_{\neg\mathrm{Dir},(k,\mathcal{C})}[U_{(k,\mathcal{C})}] - \mathfrak{k}^{\nu,\downarrow}_{\neg\mathrm{Dir},(k,\mathcal{C})}[U]$ *for each* $U \in \upsilon^{I_{\Pi,\mathfrak{D},\neg\mathrm{Dir}}}$.

(b) $\mathfrak{k}^{\nu,\uparrow}_{\neg\mathrm{Dir},(k,\mathcal{C})}$ *is increasing.*

(c) $\mathfrak{k}^{\nu,\downarrow}_{\neg\mathrm{Dir},(k,\mathcal{C})}$ *is minimal at* $\mathbf{m}$.

(d) $\mathfrak{k}^{\nu,\uparrow}_{\neg\mathrm{Dir},(k,\mathcal{C})}[m_\upsilon] \leq \mathfrak{k}^{\nu,\downarrow}_{\neg\mathrm{Dir},(k,\mathcal{C})}[\mathbf{m}]$.

(e) $\max\left\{0, \mathfrak{k}^{\nu,\downarrow}_{\neg\mathrm{Dir},(k,\mathcal{C})}[\mathbf{m}]\right\} = \min\left\{0, \mathfrak{k}^{\nu,\uparrow}_{\neg\mathrm{Dir},(k,\mathcal{C})}[m_v]\right\} = 0.$

(f) $\mathfrak{k}^{\nu,\downarrow}_{\neg\mathrm{Dir},(k,\mathcal{C})}$ *is* $L^{\downarrow}_{k,r}[\mathfrak{C}] \cdot d_{\max}[\Pi]$*-Lipschitz on* $[m_v, m_v + r]^{I_{\Pi,\mathfrak{D},\neg\mathrm{Dir}}}$ *with respect to the max-norm for each* $r \in \mathbb{R}^+$*, where*

$$L^{\downarrow}_{k,r}[\mathfrak{C}] := \frac{5}{2} \cdot \big(2L_{k,r}[\mathfrak{C}] \cdot r + B_{k,m_v}[\mathfrak{C}]\big), \tag{3.8.23}$$

$$B_{k,m_v}[\mathfrak{C}] := \max\left\{\big|k_j[(m_v, t, x)]\big| : (t, x) \in \tau \times p_j,\ j \in J\right\}, \tag{3.8.24}$$

$$d_{\max}[\Pi] := \max\left\{\sum_{j\in J}\ \sum_{l\in \mathrm{nb}_j[k]} \frac{\lambda_{d-1}\big[\omega^{(j)}_k \cap \omega^{(j)}_l\big]}{\|x_k - x_l\|_2} : k \in I_\Pi\right\}. \tag{3.8.25}$$

The number $d_{\max}[\Pi]$ *measures how large the size of interfaces between a control volume and neighboring control volumes can get in relation to the distance between the corresponding discretization points.*

Proof. (a) follows from hypothesis (locLip) and Rem. C.6.8(h).

(b): Each $\mathfrak{k}^{\nu,\uparrow}_{\neg\mathrm{Dir},(k,\mathcal{C})}$ is increasing according to Rems 3.8.7 and C.6.8(c).

(c): It is immediate from (3.8.21b) and Rem. C.6.8(a) that $\mathfrak{k}^{\nu,\downarrow}_{\neg\mathrm{Dir},(k,\mathcal{C})}[\mathbf{m}] = 0$, it suffices to show that $\mathfrak{k}^{\nu,\downarrow}_{\neg\mathrm{Dir},(k,\mathcal{C})}$ is nonnegative. Indeed, each summand in (3.8.21b) is nonnegative: Remark C.6.8(b) yields $\mathrm{var}^-\left[\tilde{k}^{(\nu)}_{j,x}\right] \geq 0$. Moreover, $k^{(\nu)}_j \geq 0$ and $\mathrm{insup}\left[k^{(\nu)}_j\right] \geq 0$ by hypothesis (nn). It remains to show that

$$\bigwedge_{\substack{(\nu,j,(x,z),(\lambda,\mu))\\ \in\{0,\dots,n\}\times J\times p_j^2\times v^2}} \left(\begin{array}{r} k^{\nu,x,z}_{j,\lambda,\mu} := \left(\mathrm{insup}\left[k^{(\nu)}_j\right][\lambda] - k^{(\nu)}_j[(\mu, z)]\right) \cdot (\lambda - m_v) \\ + \left(k^{(\nu)}_j[(\lambda, x)] + k^{(\nu)}_j[(\mu, z)]\right) \cdot (\mu - m_v) \geq 0 \end{array}\right). \tag{3.8.26}$$

If $\lambda \leq \mu$, then $k^{(\nu)}_j[(\mu, z)](\mu - m_v) - k^{(\nu)}_j[(\mu, z)](\lambda - m_v) \geq 0$, since $k^{(\nu)}_j \geq 0$, proving $k^{\nu,x,z}_{j,\lambda,\mu} \geq 0$.

If $\lambda > \mu$, then $\mathrm{insup}\left[k^{(\nu)}_j\right][\lambda] - k^{(\nu)}_j[(\mu, z)] \geq 0$ according to Rem. 3.8.7, again proving $k^{\nu,x,z}_{j,\lambda,\mu} \geq 0$. Thereby (3.8.26) is established and thus (c).

For (d) and (e), it is remarked that $\mathfrak{k}^{\nu,\uparrow}_{\neg\mathrm{Dir},(k,\mathcal{C})}[m_v] = \mathfrak{k}^{\nu,\downarrow}_{\neg\mathrm{Dir},(k,\mathcal{C})}[\mathbf{m}] = 0$, which is a direct consequence of (3.8.21a), (3.8.21b), and Rem. C.6.8(a).

(f): First, the Lipschitz constant of $\tilde{k}^{(\nu)}_{j,x}$ is determined:

Claim 1. For each $r \in \mathbb{R}^+_0$ and for each $(j, \nu, x) \in J \times \{0, \dots, n\} \times p_j$, the map $\tilde{k}^{(\nu)}_{j,x}$ defined in (3.8.20) is L-Lipschitz on $[m_v, m_v + r]$, where $L := 2 \cdot L_{k,r}[\mathfrak{C}] \cdot r + B_{k,m_v}[\mathfrak{C}]$.

Proof. Hypothesis (locLip) and Rem. C.7.7(a),(e) yield the claim. ▲

Thus, by Rem. C.6.8(h), $\operatorname{var}^-\left[\tilde{k}^{(\nu)}_{j,x_k}\right]$ contributes the Lipschitz constant $2L_{k,r}[\mathfrak{C}]\cdot r + B_{k,m_v}[\mathfrak{C}]$. Since $\tau\times p_j$ is compact, and since $\|k_j\restriction_{[m_v,m_v+r]\times\{t\}\times\{x\}}\|_{\mathrm{Lip}} \le L_{k,r}[\mathfrak{C}]$ for each $(r,j,t,x)\in\mathbb{R}^+_0\times J\times\tau\times p_j$ by hypothesis (locLip), Lem. 3.8.8 shows that $\operatorname{insup}\left[k^{(\nu)}_j\right]$ is $L_{k,r}[\mathfrak{C}]$-Lipschitz, and by the same argument as in Cl. 1, $\operatorname{insup}\left[k^{(\nu)}_j\right](U_{(k,\mathcal{C})}-m_v)$ also contributes the Lipschitz constant $2L_{k,r}[\mathfrak{C}]\cdot r + B_{k,m_v}[\mathfrak{C}]$. Remark C.7.7(h) shows that each of the remaining three summands in front of $\frac{\lambda_{d-1}\left[\omega^{(j)}_k\cap\omega^{(j)}_l\right]}{2\cdot\|x_k-x_l\|_2}$ in (3.8.21b) contribute the Lipschitz constant $2L_{k,r}[\mathfrak{C}]\cdot r + B_{k,m_v}[\mathfrak{C}]$. Then, Rem. C.7.7(c),(d) finish the proof of (f). ■

Lemma 3.8.11. *Suppose $v=[m_v,\infty[$, the k_j are real-valued, and the conditions* (nn) *and* (locLip) *of Lem.* 3.8.10 *hold. Then the following holds for each $\nu\in\{0,\dots,n\}$ and for each $(k,\mathcal{C})\in I_{\Pi,\mathfrak{D},\neg\mathrm{Dir}}$:*

(a) $-\mathfrak{k}^{(\nu)}_{\mathrm{Dir},(k,\mathcal{C})} = \mathfrak{k}^{\nu,\uparrow}_{\mathrm{Dir},(k,\mathcal{C})} - \mathfrak{k}^{\nu,\downarrow}_{\mathrm{Dir},(k,\mathcal{C})}$.

(b) $\mathfrak{k}^{\nu,\uparrow}_{\mathrm{Dir},(k,\mathcal{C})}$ *is increasing.*

(c) $\mathfrak{k}^{\nu,\downarrow}_{\mathrm{Dir},(k,\mathcal{C})}$ *is minimal at m_v.*

(d) $\mathfrak{k}^{\nu,\uparrow}_{\mathrm{Dir},(k,\mathcal{C})}[m_v] \le \mathfrak{k}^{\nu,\downarrow}_{\mathrm{Dir},(k,\mathcal{C})}[m_v]$.

(e) $\max\left\{0,\mathfrak{k}^{\nu,\downarrow}_{\mathrm{Dir},(k,\mathcal{C})}[m_v]\right\} - \min\left\{0,\mathfrak{k}^{\nu,\uparrow}_{\mathrm{Dir},(k,\mathcal{C})}[m_v]\right\} \le \frac{1}{2}\left(B^{\downarrow}_{k,\mathrm{Dir}}[\mathfrak{C}] + B^{\uparrow}_{k,\mathrm{Dir}}[\mathfrak{C}]\right)\cdot d_{\max}[\Pi]$, *where*

$$B^{\downarrow}_{k,\mathrm{Dir}}[\mathfrak{C}] := B_{k,m_v}[\mathfrak{C}]\cdot(B_{\mathrm{Dir}}[\mathfrak{C}]-m_v), \tag{3.8.27a}$$
$$B^{\uparrow}_{k,\mathrm{Dir}}[\mathfrak{C}] := B_{k,\mathrm{Dir}}[\mathfrak{C}]\cdot(B_{\mathrm{Dir}}[\mathfrak{C}]-m_v). \tag{3.8.27b}$$

The numbers $B_{\mathrm{Dir}}[\mathfrak{C}]$, $B_{k,\mathrm{Dir}}[\mathfrak{C}]$, $B_{k,m_v}[\mathfrak{C}]$, and $d_{\max}[\Pi]$ were previously defined in (3.7.27), (3.7.28), (3.8.24), *and* (3.8.25), *respectively.*

(f) $\mathfrak{k}^{\nu,\downarrow}_{\mathrm{Dir},(k,\mathcal{C})}$ *is $L_{\mathrm{Dir},k,r}[\mathfrak{C}]\cdot d_{\max}[\Pi]$-Lipschitz on $[m_v,m_v+r]$ for each $r\in\mathbb{R}^+$, where*

$$L_{\mathrm{Dir},k,r}[\mathfrak{C}] := \frac{1}{2}L_{k,r}[\mathfrak{C}]\cdot\big(2r+B_{\mathrm{Dir}}[\mathfrak{C}]-m_v\big) + B_{k,m_v}[\mathfrak{C}]. \tag{3.8.28}$$

Proof. It is noted that the contributions of the Dirichlet terms are constant in $\mathfrak{k}^{\nu,\uparrow}_{\mathrm{Dir},(k,\mathcal{C})}$ and $\mathfrak{k}^{\nu,\downarrow}_{\mathrm{Dir},(k,\mathcal{C})}$.

(a) follows from hypothesis (locLip) and Rem. C.6.8(h).

Both $\mathfrak{k}^{\nu,\uparrow}_{\mathrm{Dir},(k,\mathcal{C})}$ and $\mathfrak{k}^{\nu,\downarrow}_{\mathrm{Dir},(k,\mathcal{C})}$ are increasing due to hypothesis (nn) and Rem. C.6.8(c), proving (b) and (c).

(d) follows from (a), since $\mathfrak{k}^{(\nu)}_{\mathrm{Dir},(k,\mathcal{C})}[m_v] \geq 0$ is immediate from (3.7.17), hypothesis (nn) and $u_{j_{\mathrm{Dir}}[(l,j)],\mathrm{Dir}}[(t_\nu, x_l)] \geq m_v$.

(e): Since the variation terms in (3.8.22a) and (3.8.22b) vanish at m_v (s. Rem. C.6.8(a)), the estimate is immediate from the definitions of $B_{\mathrm{Dir}}[\mathfrak{C}]$, $B_{k,\mathrm{Dir}}[\mathfrak{C}]$, $B_{k,m_v}[\mathfrak{C}]$, and $d_{\max}[\Pi]$.

(f): Since $\mathrm{var}^-\left[\tilde{k}^{(\nu)}_{j,x_k}\right]$ is $(2L_{k,r}[\mathfrak{C}] \cdot r + B_{k,m_v}[\mathfrak{C}])$-Lipschitz by Cl. 1 of Lem. 3.8.10 and Rem. C.6.8(h), and $\mathrm{var}^+\left[k^{(\nu)}_j \restriction_{v \times \{x_k\}}\right]$ is $L_{k,r}[\mathfrak{C}]$-Lipschitz by hypothesis (locLip) and Rem. C.6.8(h), (f) follows the definition of $B_{\mathrm{Dir}}[\mathfrak{C}]$ in (3.7.27) and Rem. C.7.7(3.8.28),(d). ■

3.8.4 Decomposition of Interior Convection Flux Terms

In this section, the operators $\mathfrak{v}^{(\nu)}_{\mathrm{int},\neg\mathrm{Dir},(k,\mathcal{C})}$ defined in (3.7.40) are decomposed. The operators $\mathfrak{v}^{(\nu)}_{\mathrm{int},\mathrm{Dir},(k,\mathcal{C})}$ defined in (3.7.41) are *not* decomposed, as they themselves have all the properties of an $\uparrow$-operator (cf. Lem. 3.8.12,(b),(d),(e) below). Let

$$\bigwedge_{\substack{\nu\in\{0,\dots,n\},\\ (k,\mathcal{C})\in I_{\Pi,\mathfrak{D},\neg\mathrm{Dir}}}} \left(\begin{aligned} &\mathfrak{v}^{\nu,\uparrow}_{\mathrm{int},\neg\mathrm{Dir},(k,\mathcal{C})} : v \longrightarrow \mathbb{R}, \\ &\mathfrak{v}^{\nu,\uparrow}_{\mathrm{int},\neg\mathrm{Dir},(k,\mathcal{C})}[y] := \sum_{\substack{j\in V[\mathcal{C}],\\ l\in \mathrm{nb}_{j,\mathrm{Dir}}[k]}} \left(1 - w^{(\nu)}_j[(k,l)]\right) \cdot v^{(\nu)}_{j,\mathrm{sca}}[(y, x_k)] \\ &\qquad\qquad \cdot \frac{\left(v^{(\nu)}_{j,\mathrm{vec}}[x_l] + v^{(\nu)}_{j,\mathrm{vec}}[x_k]\right) \bullet (x_l - x_k)}{2\|x_k - x_l\|_2} \\ &\qquad\qquad \cdot \lambda_{d-1}\left[\omega^{(j)}_k \cap \omega^{(j)}_l\right] \end{aligned} \right), \tag{3.8.29a}$$

$$\bigwedge_{\substack{\nu\in\{0,\dots,n\},\\ (k,\mathcal{C})\in I_{\Pi,\mathfrak{D},\neg\mathrm{Dir}}}} \left(\begin{aligned} &\mathfrak{v}^{\nu,\downarrow}_{\mathrm{int},\neg\mathrm{Dir},(k,\mathcal{C})} : v^{I_{\Pi,\mathfrak{D},\neg\mathrm{Dir}}} \longrightarrow \mathbb{R}, \\ &\mathfrak{v}^{\nu,\downarrow}_{\mathrm{int},\neg\mathrm{Dir},(k,\mathcal{C})}[U] := -\sum_{\substack{j\in V[\mathcal{C}],\\ l\in \mathrm{nb}_{j,\mathrm{Dir}}[k]}} w^{(\nu)}_j[(k,l)] \cdot v^{(\nu)}_{j,\mathrm{sca}}\left[\left(U_{(l,\mathcal{C}[(l,j)])}, x_l\right)\right] \\ &\qquad\qquad \cdot \frac{\left(v^{(\nu)}_{j,\mathrm{vec}}[x_l] + v^{(\nu)}_{j,\mathrm{vec}}[x_k]\right) \bullet (x_l - x_k)}{2\|x_k - x_l\|_2} \\ &\qquad\qquad \cdot \lambda_{d-1}\left[\omega^{(j)}_k \cap \omega^{(j)}_l\right] \end{aligned} \right). \tag{3.8.29b}$$

Lemma 3.8.12. *Suppose $v = [m_v, \infty[$ and that the conditions* (inc), (np), *and* (locLip) *below all hold:*

(inc) *The family of scalar-vector-splittings $\mathfrak{V} = \left((v_{j,\mathrm{sca}}, v_{j,\mathrm{vec}})\right)_{j\in J}$ is such that the function $v_{j,\mathrm{sca}}\restriction_{v\times\{t\}\times\{x\}}$ is increasing for each $(t,x) \in \tau \times p_j$, $j \in J$.*

(np) *The family of scalar-vector-splittings* $\mathfrak{V}$ *is such that* $v_{j,\mathrm{sca}}[(m_v, t, x)] = 0$ *for each* $(t, x) \in \tau \times p_j$, $j \in J$.

(locLip) *The family of scalar-vector-splittings* $\mathfrak{V}$ *is such that*

$$\bigwedge_{r \in \mathbb{R}_0^+} \bigvee_{L_{v,\mathrm{sca},r}[(\mathfrak{C},\mathfrak{V})] \in \mathbb{R}_0^+} \bigwedge_{(j,t,x) \in J \times \tau \times p_j} v_{j,\mathrm{sca}}\restriction_{v \times \{t\} \times \{x\}} \in \mathrm{Lip}_{L_{v,\mathrm{sca},r}[(\mathfrak{C},\mathfrak{V})]}\big([m_v, m_v + r], \mathbb{R}\big),$$

i.e. each $v_{j,\mathrm{sca}}$ *is locally Lipschitz with respect to its dependence on* $y \in v$.

Let $\mathbf{m} := (m_v, \dots, m_v)$. *Then the following holds for each* $\nu \in \{0, \dots, n\}$ *and for each* $(k, \mathcal{C}) \in I_{\Pi,\mathfrak{D},\neg\mathrm{Dir}}$:

(a) $\mathfrak{v}^{(\nu)}_{\mathrm{int},\neg\mathrm{Dir},(k,\mathcal{C})}[U] = \mathfrak{v}^{\nu,\uparrow}_{\mathrm{int},\neg\mathrm{Dir},(k,\mathcal{C})}[U_{(k,\mathcal{C})}] - \mathfrak{v}^{\nu,\downarrow}_{\mathrm{int},\neg\mathrm{Dir},(k,\mathcal{C})}[U]$ *for each* $U \in v^{I_{\Pi,\mathfrak{D},\neg\mathrm{Dir}}}$.

(b) $\mathfrak{v}^{\nu,\uparrow}_{\mathrm{int},\neg\mathrm{Dir},(k,\mathcal{C})}$ *and* $\mathfrak{v}^{(\nu)}_{\mathrm{int},\mathrm{Dir},(k,\mathcal{C})}$ *are increasing.*

(c) $\mathfrak{v}^{\nu,\downarrow}_{\mathrm{int},\neg\mathrm{Dir},(k,\mathcal{C})}$ *is minimal at* $\mathbf{m}$.

(d) $\mathfrak{v}^{\nu,\uparrow}_{\mathrm{int},\neg\mathrm{Dir},(k,\mathcal{C})}[m_v] = \mathfrak{v}^{\nu,\downarrow}_{\mathrm{int},\neg\mathrm{Dir},(k,\mathcal{C})}[\mathbf{m}] = \mathfrak{v}^{(\nu)}_{\mathrm{int},\mathrm{Dir},(k,\mathcal{C})}[m_v] = 0.$

(e) $\max\big\{0, \mathfrak{v}^{\nu,\downarrow}_{\mathrm{int},\neg\mathrm{Dir},(k,\mathcal{C})}[\mathbf{m}]\big\} = \min\big\{0, \mathfrak{v}^{\nu,\uparrow}_{\mathrm{int},\neg\mathrm{Dir},(k,\mathcal{C})}[m_v]\big\} = \max\big\{0, \mathfrak{v}^{(\nu)}_{\mathrm{int},\mathrm{Dir},(k,\mathcal{C})}[m_v]\big\} = 0.$

(f) $\mathfrak{v}^{\nu,\downarrow}_{\mathrm{int},\neg\mathrm{Dir},(k,\mathcal{C})}$ *is* $\big(L_{v,r}[(\mathfrak{C},\mathfrak{V})] \cdot \lambda_{d-1,\max}[\Pi]\big)$*-Lipschitz on* $[m_v, m_v + r]^{I_{\Pi,\mathfrak{D},\neg\mathrm{Dir}}}$ *with respect to the max-norm for each* $r \in \mathbb{R}^+$, *where*

$$L_{v,r}[(\mathfrak{C},\mathfrak{V})] := L_{v,\mathrm{sca},r}[(\mathfrak{C},\mathfrak{V})] \cdot \max\Big\{\big\|\|v_{j,\mathrm{vec}}\|_2\big\|_{\max} : j \in J\Big\}, \tag{3.8.30}$$

$$\lambda_{d-1,\max}[\Pi] := \max\left\{\sum_{j \in J:\, k \in I^{(j)}} \lambda_{d-1}[\partial\omega_k^{(j)}] \,:\, k \in I_\Pi\right\}. \tag{3.8.31}$$

The number $\lambda_{d-1,\max}[\Pi]$ *measures the maximal size of the combined surfaces of partial control volumes* $\omega_k^{(j)}$ *making up a control volume* ω_k.

Proof. It is noted that in $\mathfrak{v}^{(\nu)}_{\mathrm{int},\mathrm{Dir},(k,\mathcal{C})}$, the summands involving the Dirichlet contributions are constant.

(a) is clear, since (3.8.29a) and (3.8.29b) are merely an algebraic decomposition of (3.7.40).

(b): It follows from (3.7.36) and (3.7.37) that

$$\big(1 - w_j^{(\nu)}[(k,l)]\big) \cdot \big(v^{(\nu)}_{j,\mathrm{vec}}[x_l] + v^{(\nu)}_{j,\mathrm{vec}}[x_k]\big) \bullet (x_l - x_k) \geq 0$$

in the definitions of $\mathfrak{v}^{\nu,\uparrow}_{\text{int},\neg\text{Dir},(k,\mathcal{C})}$ and $\mathfrak{v}^{(\nu)}_{\text{int},\text{Dir},(k,\mathcal{C})}$ in (3.8.29a) and (3.7.41), respectively. This, together with $v^{(\nu)}_{j,\text{sca}}[(y,x_k)]$ being increasing in y by hypothesis (inc) proves (b).

(c): It follows from (3.7.36) and (3.7.37) that

$$-w^{(\nu)}_j[(k,l)] \cdot \left(v^{(\nu)}_{j,\text{vec}}[x_l] + v^{(\nu)}_{j,\text{vec}}[x_k]\right) \bullet (x_l - x_k) \geq 0$$

in the definition of $\mathfrak{v}^{\nu,\downarrow}_{\text{int},\neg\text{Dir},(k,\mathcal{C})}$ in (3.8.29b). This, together with $v^{(\nu)}_{j,\text{sca}}\restriction_{v\times\{x\}}$ being minimal at m_v for each $x \in p_j$ by hypothesis (inc), proves (c).

(d) and (e) are immediate from hypothesis (np).

(f): $\mathfrak{v}^{\nu,\downarrow}_{\text{int},\neg\text{Dir},(k,\mathcal{C})}$ is $\left(L_{v,r}[(\mathfrak{C},\mathfrak{V})] \cdot \lambda_{d-1,\max}[\Pi]\right)$-Lipschitz by hypothesis (locLip), the Cauchy-Schwarz Inequality (Rem. C.2.2), and Rem. C.7.7(c),(g). ■

Remark 3.8.13. If $v = [m_v, \infty[$, then a family $\left((v_{j,\text{sca}}, v_{j,\text{vec}})\right)_{j\in J}$ of scalar-vector-splittings that satisfies condition (inc) of Lem. 3.8.12, also satisfies Def. 3.7.43(iii), since (inc) implies that $v_{j,\text{sca}}$ is bounded from below by $\min\left\{v_{j,\text{sca}}[(m_v,t,x)] : (t,x) \in \tau \times p_j,\ j \in J\right\}$.

Example 3.8.14. It is verified for the cases considered in Ex. 3.7.11 that correspond to Ex. 3.1.1(b) and to the first case of Ex. 3.1.1(a), that under natural hypotheses, $v_{\text{sca}} := v_{j,\text{sca}}$ is increasing in $y \in v$ and vanishes at $y = m_v$, as is required in conditions (np) and (inc) of Lem. 3.8.12. Moreover, v_{sca} is locally Lipschitz in the sense of condition (locLip) of Lem. 3.8.12.

Since in Ex. 3.1.1(b), the unknown represents mass density, and in the first case of Ex. 3.1.1(a), the unknown represents absolute temperature, one has $m_v = 0$.

If $v_{\text{sca}}[(y,t,x)] = y$ or if $v_{\text{sca}}[(y,t,x)] = \frac{\left(z^{(\text{Ar})}+1\right)R}{M^{(\text{Ar})}}\,\rho_{\text{gas}}[x]y$, then $v_{\text{sca}}[(0,t,x)] = 0$, and v_{sca} is an increasing linear function in y, as $\rho_{\text{gas}} \geq 0$. In its y-dependence, v_{sca} is 1-Lipschitz in the first case and $\left(\frac{\left(z^{(\text{Ar})}+1\right)R}{M^{(\text{Ar})}} \cdot \|\rho_{\text{gas}}\|_{\max}\right)$-Lipschitz in the second case.

If $v_{\text{sca}}[(y,t,x)] = \varepsilon_{\text{gas}}[(y,x)]\,\rho_{\text{gas}}[x]$, then v_{sca} vanishes at $y = 0$ and is increasing in y, assuming ε_{gas} vanishes at $y = 0$ and is increasing in y, again using $\rho_{\text{gas}} \geq 0$. Moreover, if ε_{gas} is (locally) Lipschitz in its y-dependence, then so is v_{sca}.

3.8.5 Decomposition of Terms on Outer Boundaries

In this section, the operators $\mathfrak{v}^{(\nu)}_{\text{out},(k,\mathcal{C})}$ and $\mathfrak{a}^{(\nu)}_{\text{out},(k,\mathcal{C})}$ defnined in (3.7.49) and (3.7.51), respectively, are decomposed. The discretized nonlocal operators $\mathfrak{B}^{(\nu)}_{(k,\mathcal{C})}$ are *not* decomposed and are treated in Sec. 3.8.7 below.

The decomposition of the $\mathfrak{v}^{(\nu)}_{\mathrm{out},(k,\mathcal{C})}$ is carried out first. Let

$$\bigwedge_{\substack{\nu\in\{0,\dots,n\},\\ (k,\mathcal{C})\in I_{\Pi,\mathfrak{D},\neg\mathrm{Dir}}}} \left(\begin{aligned} &\mathfrak{v}^{\nu,\uparrow}_{\mathrm{out},(k,\mathcal{C})} : \upsilon \longrightarrow \mathbb{R}, \\ &\mathfrak{v}^{\nu,\uparrow}_{\mathrm{out},(k,\mathcal{C})}[y] := \sum_{j\in V[\mathcal{C}]} v^{(\nu)}_{j,\mathrm{sca}}[(y,x_k)] \cdot \max\left\{0, \int_{\partial\omega_k^{(j)}\cap\partial p} v^{(\nu)}_{j,\mathrm{vec}}[x_k] \bullet n_{\omega_k^{(j)}} \right\} \end{aligned} \right), \tag{3.8.32a}$$

$$\bigwedge_{\substack{\nu\in\{0,\dots,n\},\\ (k,\mathcal{C})\in I_{\Pi,\mathfrak{D},\neg\mathrm{Dir}}}} \left(\begin{aligned} &\mathfrak{v}^{\nu,\downarrow}_{\mathrm{out},(k,\mathcal{C})} : \upsilon \longrightarrow \mathbb{R}, \\ &\mathfrak{v}^{\nu,\downarrow}_{\mathrm{out},(k,\mathcal{C})}[y] := -\sum_{j\in V[\mathcal{C}]} v^{(\nu)}_{j,\mathrm{sca}}[(y,x_k)] \cdot \min\left\{0, \int_{\partial\omega_k^{(j)}\cap\partial p} v^{(\nu)}_{j,\mathrm{vec}}[x_k] \bullet n_{\omega_k^{(j)}} \right\} \end{aligned} \right). \tag{3.8.32b}$$

Lemma 3.8.15. *Suppose $\upsilon = [m_\upsilon, \infty[$, and assume the conditions* (inc)*,* (np)*, and* (locLip) *of Lem.* 3.8.12*. Then the following holds for each $\nu \in \{0,\dots,n\}$ and for each $(k,\mathcal{C}) \in I_{\Pi,\mathfrak{D},\neg\mathrm{Dir}}$:*

(a) $\mathfrak{v}^{(\nu)}_{\mathrm{out},(k,\mathcal{C})} = \mathfrak{v}^{\nu,\uparrow}_{\mathrm{out},(k,\mathcal{C})} - \mathfrak{v}^{\nu,\downarrow}_{\mathrm{out},(k,\mathcal{C})}$.

(b) $\mathfrak{v}^{\nu,\uparrow}_{\mathrm{out},(k,\mathcal{C})}$ *is increasing.*

(c) $\mathfrak{v}^{\nu,\downarrow}_{\mathrm{out},(k,\mathcal{C})}$ *is minimal at m_υ.*

(d) $\mathfrak{v}^{\nu,\uparrow}_{\mathrm{out},(k,\mathcal{C})}[m_\upsilon] = \mathfrak{v}^{\nu,\downarrow}_{\mathrm{out},(k,\mathcal{C})}[m_\upsilon] = 0$.

(e) $\max\left\{0, \mathfrak{v}^{\nu,\downarrow}_{\mathrm{out},(k,\mathcal{C})}[m_\upsilon]\right\} = \min\left\{0, \mathfrak{v}^{\nu,\uparrow}_{\mathrm{out},(k,\mathcal{C})}[m_\upsilon]\right\} = 0$.

(f) $\mathfrak{v}^{\nu,\downarrow}_{\mathrm{out},(k,\mathcal{C})}$ *is $\big(L_{\upsilon,r}[(\mathfrak{C},\mathfrak{V})] \cdot \lambda_{d-1,\max}[\Pi]\big)$-Lipschitz on $[m_\upsilon, m_\upsilon + r]$ for each $r \in \mathbb{R}^+$, where the numbers $L_{\upsilon,r}[(\mathfrak{C},\mathfrak{V})]$ and $\lambda_{d-1,\max}[\Pi]$ are defined in* (3.8.30) *and* (3.8.31)*, respectively.*

Proof. (a) holds, as for each real number λ: $\lambda = \max\{0,\lambda\} + \min\{0,\lambda\}$.

(b) and (c) follow, since $\mathfrak{v}^{\nu,\uparrow}_{\mathrm{out},(k,\mathcal{C})}$ and $\mathfrak{v}^{\nu,\downarrow}_{\mathrm{out},(k,\mathcal{C})}$ are increasing using hypothesis (inc) together with $\max\left\{0, \int_{\partial\omega_k^{(j)}\cap\partial p} v^{(\nu)}_{j,\mathrm{vec}}[x_k] \bullet n_{\omega_k^{(j)}}\right\} \geq 0$ and $-\min\left\{0, \int_{\partial\omega_k^{(j)}\cap\partial p} v^{(\nu)}_{j,\mathrm{vec}}[x_k] \bullet n_{\omega_k^{(j)}}\right\} \geq 0$.

Hypothesis (np) yields (d) and (e).

(f): $\mathfrak{v}^{\nu,\downarrow}_{\mathrm{out},(k,\mathcal{C})}$ is $\big(L_{\upsilon,r}[(\mathfrak{C},\mathfrak{V})] \cdot \lambda_{d-1,\max}[\Pi]\big)$-Lipschitz by hypothesis (locLip), the Cauchy-Schwarz Inequality (Rem. C.2.2), and Rem. C.7.7(c). ∎

Now the operators $\mathfrak{a}^{(\nu)}_{\text{out},(k,\mathcal{C})}$ are decomposed. Assume $\upsilon = [m_\upsilon, \infty[$ as well as condition (locLip) of Lem. 3.8.16 below. Let

$$\bigwedge_{\substack{\nu\in\{0,\dots,n\},\\(k,\mathcal{C})\in I_{\Pi,\mathfrak{D},\neg\mathrm{Dir}}}} \left(\begin{aligned} &\mathfrak{a}^{\nu,\uparrow}_{\text{out},(k,\mathcal{C})} : \upsilon\times\upsilon \longrightarrow \mathbb{K},\\ &\mathfrak{a}^{\nu,\uparrow}_{\text{out},(k,\mathcal{C})}[(\tilde{y},y)] := \sum_{\substack{(j,\iota)\in V[\mathcal{C}]\times J_j\setminus\{0\}:\\ \lambda_{d-1}[\partial\omega^{(j)}_k\cap\Gamma_{j,\iota}]>0}} \Bigg(\left(a^{j,\iota,\nu}_{\text{out}}\right)^{\text{ex.-im.}}\big[\big((\tilde{y},m_\upsilon),x_k\big)\big] \\ &\qquad\qquad + \mathrm{var}^+\left[\left(a^{j,\iota,\nu}_{\text{out}}\right)^{\text{ex.-im.}}\restriction_{\{\tilde{y}\}\times\upsilon\times\{x_k\}}\right][y]\Bigg) \\ &\qquad\qquad \cdot\lambda_{d-1}[\partial\omega^{(j)}_k\cap\Gamma_{j,\iota}] \end{aligned} \right), \tag{3.8.33a}$$

$$\bigwedge_{\substack{\nu\in\{0,\dots,n\},\\(k,\mathcal{C})\in I_{\Pi,\mathfrak{D},\neg\mathrm{Dir}}}} \left(\begin{aligned} &\mathfrak{a}^{\nu,\downarrow}_{\text{out},(k,\mathcal{C})} : \upsilon\times\upsilon \longrightarrow \mathbb{K},\\ &\mathfrak{a}^{\nu,\downarrow}_{\text{out},(k,\mathcal{C})}[(\tilde{y},y)] := \sum_{\substack{(j,\iota)\in V[\mathcal{C}]\times J_j\setminus\{0\}:\\ \lambda_{d-1}[\partial\omega^{(j)}_k\cap\Gamma_{j,\iota}]>0}} \mathrm{var}^-\left[\left(a^{j,\iota,\nu}_{\text{out}}\right)^{\text{ex.-im.}}\restriction_{\{\tilde{y}\}\times\upsilon\times\{x_k\}}\right][y] \\ &\qquad\qquad \cdot\lambda_{d-1}[\partial\omega^{(j)}_k\cap\Gamma_{j,\iota}] \end{aligned} \right). \tag{3.8.33b}$$

Lemma 3.8.16. *Suppose $\upsilon = [m_\upsilon, \infty[$, and let $\mathfrak{S}_{\text{out}} := \left(\left(a^{j,\iota}_{\text{out}}\right)^{\text{ex.-im.}}\right)_{(j,\iota)\in J\times(J_j\setminus\{0\})}$ denote the family of real-valued dependency splittings. Moreover, assume the conditions* (np), (bnd), *and* (locLip) *below:*

(np) $$\bigwedge_{(j,\iota)\in J\times(J_j\setminus\{0\})}\ \bigwedge_{y\in\upsilon}\ \bigwedge_{(t,x)\in\tau\times\Gamma_{j,\iota}} \left(a^{j,\iota}_{\text{out}}\right)^{\text{ex.-im.}}\big[\big((y,m_\upsilon),t,x\big)\big] \le 0.$$

(bnd) $$B_{\text{out},m_\upsilon}[(\mathfrak{C},\mathfrak{S}_{\text{out}})] := -\inf\Big\{\left(a^{j,\iota}_{\text{out}}\right)^{\text{ex.-im.}}\big[\big((y,m_\upsilon),t,x\big)\big] : (y,t,x)\in\upsilon\times\Gamma_{j,\iota},\ (j,\iota)\in J\times(J_j\setminus\{0\})\Big\} < \infty. \tag{3.8.34}$$

(locLip) *Each $\left(a^{j,\iota}_{\text{out}}\right)^{\text{ex.-im.}}$ is locally Lipschitz with respect to its dependence on the second argument, i.e.*

$$\bigwedge_{r\in\mathbb{R}^+_0}\ \bigvee_{L_{\text{out},r}[(\mathfrak{C},\mathfrak{S}_{\text{out}})]\in\mathbb{R}^+_0}\ \bigwedge_{\substack{(j,\iota,y,t,x)\\ \in J\times(J_j\setminus\{0\})\times\upsilon\times\tau\times\Gamma_{j,\iota}}} \left(\begin{aligned} &\left(a^{j,\iota}_{\text{out}}\right)^{\text{ex.-im.}}\restriction_{\{y\}\times\upsilon\times\{t\}\times\{x\}}\\ &\in \mathrm{Lip}_{L_{\text{out},r}[(\mathfrak{C},\mathfrak{S}_{\text{out}})]}\big([m_\upsilon, m_\upsilon+r],\mathbb{R}\big) \end{aligned}\right).$$

Then the following holds for each $y\in\upsilon$, for each $\nu\in\{0,\dots,n\}$, and for each $(k,\mathcal{C})\in I_{\Pi,\mathfrak{D},\neg\mathrm{Dir}}$:

(a) $\mathfrak{a}^{(\nu)}_{\text{out},(k,\mathcal{C})} = \mathfrak{a}^{\nu,\uparrow}_{\text{out},(k,\mathcal{C})} - \mathfrak{a}^{\nu,\downarrow}_{\text{out},(k,\mathcal{C})}$.

(b) *The function* $\mathfrak{a}^{\nu,\uparrow}_{\mathrm{out},(k,\mathcal{C})}\restriction_{\{y\}\times\upsilon}$ *is increasing.*

(c) $\mathfrak{a}^{\nu,\downarrow}_{\mathrm{out},(k,\mathcal{C})}\restriction_{\{y\}\times\upsilon}$ *is minimal at* m_υ.

(d) $\mathfrak{a}^{\nu,\uparrow}_{\mathrm{out},(k,\mathcal{C})}[(y,m_\upsilon)] \le \mathfrak{a}^{\nu,\downarrow}_{\mathrm{out},(k,\mathcal{C})}[(y,m_\upsilon)]$.

(e) *If* $\lambda_{d-1,\max}[\Pi]$ *is the number defined in* (3.8.31), *then*

$$\begin{aligned}&\max\left\{0,\mathfrak{a}^{\nu,\downarrow}_{\mathrm{out},(k,\mathcal{C})}[(y,m_\upsilon)]\right\} - \min\left\{0,\mathfrak{a}^{\nu,\uparrow}_{\mathrm{out},(k,\mathcal{C})}[(y,m_\upsilon)]\right\}\\ &\le \max\left\{0, B_{\mathrm{out},m_\upsilon}[(\mathfrak{C},\mathfrak{S}_{\mathrm{out}})]\right\}\cdot \lambda_{d-1,\max}[\Pi].\end{aligned}$$

(f) *The function* $\mathfrak{a}^{\nu,\downarrow}_{\mathrm{out},(k,\mathcal{C})}\restriction_{\{y\}\times\upsilon}$ *is* $\big(L_{\mathrm{out},r}[(\mathfrak{C},\mathfrak{S}_{\mathrm{out}})]\cdot\lambda_{d-1,\max}[\Pi]\big)$*-Lipschitz on* $[m_\upsilon, m_\upsilon + r]$ *for each* $r\in\mathbb{R}^+$.

Proof. (a) and (f) follow from hypothesis (locLip) and Rem. C.6.8(h). Due to Rem. C.6.8(c), $\mathfrak{a}^{\nu,\uparrow}_{\mathrm{out},(k,\mathcal{C})}\restriction_{\{y\}\times\upsilon}$ and $\mathfrak{a}^{\nu,\downarrow}_{\mathrm{out},(k,\mathcal{C})}\restriction_{\{y\}\times\upsilon}$ are both increasing, proving (b) and (c). Combining (a) with hypothesis (np) yields (d). Finally, (e) follows from Rem. C.6.8(a) together with hypotheses (bnd) and (np). ■

Example 3.8.17. The functions $a^{j,\iota}_{\mathrm{out}}$ arising from Exs 3.1.3(b),(c),(d),(e) are investigated with respect to the hypotheses (np), (bnd), and (locLip) of Lem. 3.8.16.

Suppose $\upsilon = [m_\upsilon,\infty[$, let Γ be a $(d-1)$-dimensional polyhedral subset of ∂p, and let $a^{j,\iota}_{\mathrm{out}} \in C(\tau\times\Gamma,\mathbb{R})$.

It is first assumed that $(a^{j,\iota}_{\mathrm{out}})^{\text{ex.-im.}}\big[\big((\tilde{y},y),t,x\big)\big] = a^{j,\iota}_{\mathrm{out}}[(y,t,x)]$, i.e. there is no dependency splitting. In that case, 3.8.16(bnd) is always satisfied, since τ and Γ are compact.

Ex. 3.1.3(b): 3.8.16(locLip) is trivially satisfied if $a^{j,\iota}_{\mathrm{out}}$ does not depend on $y\in\upsilon$. However, 3.8.16(np) can only be fulfilled if $a^{j,\iota}_{\mathrm{out}}$ is everywhere nonpositive.

Ex. 3.1.3(c): If $a^{j,\iota}_{\mathrm{out}} = \xi(y - u_{\mathrm{ext}}[(t,x)])$, $\xi\in\mathbb{R}^+$, $u_{\mathrm{ext}}\in C(\tau\times\Gamma,\upsilon)$, then 3.8.16(np) holds, as $m_\upsilon - u_{\mathrm{ext}}[(t,x)]\le 0$. 3.8.16(locLip) holds, as $a^{j,\iota}_{\mathrm{out}}\restriction_{\upsilon\times\{t\}\times\{x\}}$ is ξ-Lipschitz.

Ex. 3.1.3(d): In this case, $m_\upsilon = 0$, as the unknown represents absolute temperature. If $a^{j,\iota}_{\mathrm{out}} = \sigma\epsilon[(y,t,x)]\big(y^4 - T^4_{\mathrm{room}}\big)$, $\sigma\in\mathbb{R}^+$, $\epsilon\in C\big(\upsilon\times\tau\times\Gamma,[0,1]\big)$, then 3.8.16(np) holds, as $m_\upsilon\le T_{\mathrm{room}}$. By Rem. C.7.7(h), $a^{j,\iota}_{\mathrm{out}}\restriction_{\upsilon\times\{t\}\times\{x\}}$ is locally Lipschitz and 3.8.16(locLip) holds, if ϵ is locally Lipschitz in its y-dependence, but even for constant $\epsilon\ne 0$, the function $a_{\mathrm{out}}\restriction_{\upsilon\times\{t\}\times\{x\}}$ is not (globally) Lipschitz.

If Ex. 3.1.3(d) is considered with the dependency splitting

$$(a^{j,\iota}_{\mathrm{out}})^{\text{ex.-im.}}\big[\big((\tilde{y},y),t,x\big)\big] = \sigma\epsilon[(\tilde{y},t,x)](y^4 - T^4_{\mathrm{room}}), \tag{3.8.35}$$

then 3.8.16(bnd) and 3.8.16(np) still hold, as ϵ is $[0,1]$-valued. Moreover, 3.8.16(locLip) is now satisfied independently of the Lipschitzness of ϵ, as ϵ is bounded, and ϵ is now independent of y.

With respect to $a_{\text{out}}^{j,\iota}$, 3.1.3(e) is a special case of Ex. 3.1.3(d), letting (in abuse of the notation) $T_{\text{room}} = 0$. Furthermore, the dependency splitting (3.8.35) is analogous to the one used in Ex. 3.4.12.

3.8.6 Decomposition of Terms on Interfaces

In this section, the operators $\mathfrak{v}^{(\nu)}_{\text{con},(k,\mathcal{C})} + \mathfrak{v}^{(\nu)}_{\text{jump},(k,\mathcal{C})}$, $\mathfrak{a}^{(\nu)}_{\text{flux,con},(k,\mathcal{C})}$, $\mathfrak{a}^{(\nu)}_{\text{jump},1,\neg\text{Dir},(k,\mathcal{C})}$, and $\mathfrak{a}^{(\nu)}_{\text{flux,jump},2,\neg\text{Dir},(k,\mathcal{C})} + \mathfrak{a}^{(\nu)}_{\text{jump},2,\neg\text{Dir},(k,\mathcal{C})}$ that were defnined in (3.7.54), (3.7.55), (3.7.57), (3.7.59), (3.7.62), and (3.7.65), respectively, are decomposed. However, the operators $\mathfrak{a}^{(\nu)}_{\text{jump},1,\text{Dir},(k,\mathcal{C})}$ and $\mathfrak{a}^{(\nu)}_{\text{flux,jump},2,\text{Dir},(k,\mathcal{C})} + \mathfrak{a}^{(\nu)}_{\text{jump},2,\text{Dir},(k,\mathcal{C})}$ defined in (3.7.60), (3.7.63), and (3.7.66) are *not* decomposed, as they themselves have all the properties of an $\uparrow$-operator (cf. parts (b), (d), and (e) of Lems 3.8.21 and 3.8.23 below). Moreover, the discretized nonlocal operators $\mathfrak{A}^{(\nu)}_{\text{con},(k,\mathcal{C})}$ and $\mathfrak{A}^{(\nu)}_{\text{jump},(k,\mathcal{C})}$ are *not* decomposed and are treated in Sec. 3.8.7 below.

The decomposition of the $\mathfrak{v}^{(\nu)}_{\text{con},(k,\mathcal{C})} + \mathfrak{v}^{(\nu)}_{\text{jump},(k,\mathcal{C})}$ is carried out first. Let

$$\bigwedge_{\substack{\nu\in\{0,\dots,n\},\\ (k,\mathcal{C})\in I_{\Pi,\mathfrak{D},\neg\text{Dir}}}} \left(\begin{aligned} &\mathfrak{v}^{\nu,\uparrow}_{\text{IF},(k,\mathcal{C})} : v \longrightarrow \mathbb{R}, \\ &\mathfrak{v}^{\nu,\uparrow}_{\text{IF},(k,\mathcal{C})}[y] := \sum_{\substack{j\in V[\mathcal{C}],\\ \gamma\in\text{IF}}} v^{(\nu)}_{j,\text{sca}}[(y,x_k)] \cdot \max\left\{0, \int_{\partial\omega_k^{(j)}\cap\gamma} v^{(\nu)}_{j,\text{vec}}[x_k] \bullet n_{\omega_k^{(j)}}\right\} \end{aligned} \right), \tag{3.8.36a}$$

$$\bigwedge_{\substack{\nu\in\{0,\dots,n\},\\ (k,\mathcal{C})\in I_{\Pi,\mathfrak{D},\neg\text{Dir}}}} \left(\begin{aligned} &\mathfrak{v}^{\nu,\downarrow}_{\text{IF},(k,\mathcal{C})} : v \longrightarrow \mathbb{R}, \\ &\mathfrak{v}^{\nu,\downarrow}_{\text{IF},(k,\mathcal{C})}[y] := -\sum_{\substack{j\in V[\mathcal{C}],\\ \gamma\in\text{IF}}} v^{(\nu)}_{j,\text{sca}}[(y,x_k)] \cdot \min\left\{0, \int_{\partial\omega_k^{(j)}\cap\gamma} v^{(\nu)}_{j,\text{vec}}[x_k] \bullet n_{\omega_k^{(j)}}\right\} \end{aligned} \right). \tag{3.8.36b}$$

Lemma 3.8.18. *Suppose* $v = [m_v, \infty[$, *and assume the conditions* (inc), (np), *and* (locLip) *of Lem.* 3.8.12. *Then the following holds for each* $\nu \in \{0,\dots,n\}$ *and for each* $(k,\mathcal{C}) \in I_{\Pi,\mathfrak{D},\neg\text{Dir}}$*:*

(a) $\mathfrak{v}^{(\nu)}_{\text{con},(k,\mathcal{C})} + \mathfrak{v}^{(\nu)}_{\text{jump},(k,\mathcal{C})} = \mathfrak{v}^{\nu,\uparrow}_{\text{IF},(k,\mathcal{C})} - \mathfrak{v}^{\nu,\downarrow}_{\text{IF},(k,\mathcal{C})}$.

(b) $\mathfrak{v}^{\nu,\uparrow}_{\text{IF},(k,\mathcal{C})}$ *is increasing.*

(c) $\mathfrak{v}^{\nu,\downarrow}_{\text{IF},(k,\mathcal{C})}$ *is minimal at* m_v.

(d) $\mathfrak{v}^{\nu,\uparrow}_{\text{IF},(k,\mathcal{C})}[m_v] = \mathfrak{v}^{\nu,\downarrow}_{\text{IF},(k,\mathcal{C})}[m_v] = 0$.

(e) $\max\left\{0, \mathfrak{v}^{\nu,\downarrow}_{\text{IF},(k,\mathcal{C})}[m_v]\right\} = \min\left\{0, \mathfrak{v}^{\nu,\uparrow}_{\text{IF},(k,\mathcal{C})}[m_v]\right\} = 0$.

(f) $\mathfrak{v}^{\nu,\downarrow}_{\mathrm{IF},(k,\mathcal{C})}$ *is* $\big(L_{v,r}[(\mathfrak{C},\mathfrak{V})]\cdot\lambda_{d-1,\max}[\Pi]\big)$*-Lipschitz on* $[m_v, m_v+r]$ *for each* $r\in\mathbb{R}^+$, *where the numbers* $L_{v,r}[(\mathfrak{C},\mathfrak{V})]$ *and* $\lambda_{d-1,\max}[\Pi]$ *are defined in* (3.8.30) *and* (3.8.31), *respectively.*

Proof. The proof is completely analogous to the proof of Lem. 3.8.15. ∎

Next, the decomposition of the $\mathfrak{a}^{(\nu)}_{\mathrm{flux,con},(k,\mathcal{C})}$ is performed. Let

$$\bigwedge_{\substack{\nu\in\{0,\dots,n\},\\(k,\mathcal{C})\in I_{\Pi,\mathfrak{D},\neg\mathrm{Dir}}}}\left(\begin{aligned}&\mathfrak{a}^{\nu,\uparrow}_{\mathrm{flux,con},(k,\mathcal{C})}: v\times v\longrightarrow\mathbb{K},\\&\mathfrak{a}^{\nu,\uparrow}_{\mathrm{flux,con},(k,\mathcal{C})}[(\tilde y,y)] := \sum_{\substack{\gamma\in\mathrm{IF}_{\mathrm{con}}:\\ \lambda_{d-1}\left[\gamma\cap\bigcup_{j\in V[\mathcal{C}]}\partial_{\mathrm{reg}}\omega_k^{(j)}\right]>0}}(a^{\gamma,2,\nu}_{\mathrm{flux}})^{\text{ex.-im.}}\big[\big((\tilde y,y),x_k\big)\big]\\&\qquad\qquad\cdot\lambda_{d-1}\left[\gamma\cap\bigcup_{j\in V[\mathcal{C}]}\partial_{\mathrm{reg}}\omega_k^{(j)}\right]\end{aligned}\right),\tag{3.8.37a}$$

$$\bigwedge_{\substack{\nu\in\{0,\dots,n\},\\(k,\mathcal{C})\in I_{\Pi,\mathfrak{D},\neg\mathrm{Dir}}}}\left(\begin{aligned}&\mathfrak{a}^{\nu,\downarrow}_{\mathrm{flux,con},(k,\mathcal{C})}: v\times v\longrightarrow\mathbb{K},\\&\mathfrak{a}^{\nu,\downarrow}_{\mathrm{flux,con},(k,\mathcal{C})}[(\tilde y,y)] := \sum_{\substack{\gamma\in\mathrm{IF}_{\mathrm{con}}:\\ \lambda_{d-1}\left[\gamma\cap\bigcup_{j\in V[\mathcal{C}]}\partial_{\mathrm{reg}}\omega_k^{(j)}\right]>0}}(a^{\gamma,1,\nu}_{\mathrm{flux}})^{\text{ex.-im.}}\big[\big((\tilde y,y),x_k\big)\big]\\&\qquad\qquad\cdot\lambda_{d-1}\left[\gamma\cap\bigcup_{j\in V[\mathcal{C}]}\partial_{\mathrm{reg}}\omega_k^{(j)}\right]\end{aligned}\right).\tag{3.8.37b}$$

Lemma 3.8.19. *Suppose* $v=[m_v,\infty[$ *and that the* $a^{\gamma,\alpha}_{\mathrm{flux}}$ *are real-valued,* $\alpha\in\{1,2\}$. *Let* $\mathfrak{S}_{\mathrm{con}} := \big((a^{\gamma,\alpha}_{\mathrm{flux}})^{\text{ex.-im.}}\big)_{(\alpha,\gamma)\in\{1,2\}\times\mathrm{IF}_{\mathrm{con}}}$ *denote the family of real-valued dependency splittings. Moreover, assume the conditions* (np), (bnd), (inc), *and* (locLip) *below:*

(np) $$\bigwedge_{\gamma\in\mathrm{IF}_{\mathrm{con}}}\ \bigwedge_{y\in v}\ \bigwedge_{(t,x)\in\tau\times\gamma}\Big((a^{\gamma,2}_{\mathrm{flux}})^{\text{ex.-im.}}-(a^{\gamma,1}_{\mathrm{flux}})^{\text{ex.-im.}}\Big)\big[\big((y,m_v),t,x\big)\big]\le 0.$$

(bnd) $$B_{\mathrm{con},1,m_v}[(\mathfrak{C},\mathfrak{S}_{\mathrm{con}})] := \sup\Big\{(a^{\gamma,1}_{\mathrm{flux}})^{\text{ex.-im.}}\big[\big((y,m_v),t,x\big)\big]:\ (y,t,x)\in v\times\tau\times\gamma,\ \gamma\in\mathrm{IF}_{\mathrm{con}}\Big\}<\infty,\tag{3.8.38a}$$

$$B_{\mathrm{con},2,m_v}[(\mathfrak{C},\mathfrak{S}_{\mathrm{con}})] := -\inf\Big\{(a^{\gamma,2}_{\mathrm{flux}})^{\text{ex.-im.}}\big[\big((y,m_v),t,x\big)\big]:\ (y,t,x)\in v\times\tau\times\gamma,\ \gamma\in\mathrm{IF}_{\mathrm{con}}\Big\}<\infty.\tag{3.8.38b}$$

(inc) *The functions* $(a^{\gamma,1}_{\mathrm{flux}})^{\text{ex.-im.}}\restriction_{\{y\}\times v\times\{t\}\times\{x\}}$ *and* $(a^{\gamma,2}_{\mathrm{flux}})^{\text{ex.-im.}}\restriction_{\{y\}\times v\times\{t\}\times\{x\}}$ *are increasing for each* $\gamma\in\mathrm{IF}_{\mathrm{con}}$, *for each* $y\in v$, *and for each* $(t,x)\in\tau\times\gamma$.

(locLip) *Each* $(a^{\gamma,1}_{\text{flux}})^{\text{ex.-im.}}$ *is locally Lipschitz with respect to its dependence on the second argument, i.e.*

$$\bigwedge_{r\in\mathbb{R}_0^+}\ \bigvee_{L_{\text{flux},1,r}[(\mathfrak{C},\mathfrak{S}_{\text{con}})]\in\mathbb{R}_0^+}\ \bigwedge_{\substack{(\gamma,y,t,x)\\ \in \mathrm{IF}_{\text{con}}\times\upsilon\times\tau\times\gamma}} \left(\begin{array}{c} (a^{\gamma,1}_{\text{flux}})^{\text{ex.-im.}}\restriction_{\{y\}\times\upsilon\times\{t\}\times\{x\}} \\ \in \mathrm{Lip}_{L_{\text{flux},1,r}[(\mathfrak{C},\mathfrak{S}_{\text{con}})]}\big([m_\upsilon, m_\upsilon + r], \mathbb{R}\big)\end{array}\right).$$

Then the following holds for each $y\in\upsilon$*, for each* $\nu\in\{0,\dots,n\}$*, and for each* $(k,\mathcal{C})\in I_{\Pi,\mathfrak{D},\neg\mathrm{Dir}}$*:*

(a) $\mathfrak{a}^{(\nu)}_{\text{flux,con},(k,\mathcal{C})} = \mathfrak{a}^{\nu,\uparrow}_{\text{flux,con},(k,\mathcal{C})} - \mathfrak{a}^{\nu,\downarrow}_{\text{flux,con},(k,\mathcal{C})}$.

(b) *The function* $\mathfrak{a}^{\nu,\uparrow}_{\text{flux,con},(k,\mathcal{C})}\restriction_{\{y\}\times\upsilon}$ *is increasing.*

(c) $\mathfrak{a}^{\nu,\downarrow}_{\text{flux,con},(k,\mathcal{C})}\restriction_{\{y\}\times\upsilon}$ *is minimal at* m_υ*.*

(d) $\mathfrak{a}^{\nu,\uparrow}_{\text{flux,con},(k,\mathcal{C})}[(y,m_\upsilon)] \le \mathfrak{a}^{\nu,\downarrow}_{\text{flux,con},(k,\mathcal{C})}[(y,m_\upsilon)]$.

(e) *If* $\lambda_{d-1,\max}[\Pi]$ *is the number defined in* (3.8.31)*, then*

$$\begin{aligned}&\max\left\{0, \mathfrak{a}^{\nu,\downarrow}_{\text{flux,con},(k,\mathcal{C})}[(y,m_\upsilon)]\right\} - \min\left\{0, \mathfrak{a}^{\nu,\uparrow}_{\text{flux,con},(k,\mathcal{C})}[(y,m_\upsilon)]\right\}\\ &\le \Big(\max\left\{0, B_{\text{con},1,m_\upsilon}[(\mathfrak{C},\mathfrak{S}_{\text{con}})]\right\} + \max\left\{0, B_{\text{con},2,m_\upsilon}[(\mathfrak{C},\mathfrak{S}_{\text{con}})]\right\}\Big)\cdot\lambda_{d-1,\max}[\Pi].\end{aligned}$$

(f) *The function* $\mathfrak{a}^{\nu,\downarrow}_{\text{flux,con},(k,\mathcal{C})}\restriction_{\{y\}\times\upsilon}$ *is* $\big(L_{\text{flux},1,r}[(\mathfrak{C},\mathfrak{S}_{\text{con}})]\cdot\lambda_{d-1,\max}[\Pi]\big)$*-Lipschitz on* $[m_\upsilon, m_\upsilon + r]$ *for each* $r\in\mathbb{R}^+$*.*

Proof. (a) is clear, since (3.8.37a) and (3.8.37b) are merely an algebraic decomposition of (3.7.57). (b) and (c) are equally clear from hypothesis (inc). Hypothesis (np) yields (d), and hypothesis (bnd) yields (e). Finally, (f) follows from hypothesis (locLip). ∎

Example 3.8.20. Suppose $\gamma\in\mathrm{IF}_{\text{con}}$ is a continuous interface and $\upsilon = [m_\upsilon,\infty[$.

First, assume that there is no dependency splitting, i.e. $(a^{\gamma,\alpha}_{\text{flux}})^{\text{ex.-im.}}\big[\big((\tilde{y},y),t,x\big)\big] = a^{\gamma,\alpha}_{\text{flux}}[(y,t,x)]$. In that case, 3.8.19(bnd) is always satisfied, since τ and γ are compact.

Conditions (np), (inc), and (locLip) of Lem. 3.8.19 are trivially satisfied for $a^{\gamma,1}_{\text{flux}} = a^{\gamma,2}_{\text{flux}} = 0$. In the last case considered in Ex. 3.7.32, where $a^{\gamma,1}_{\text{flux}} = 0$ and $a^{\gamma,2}_{\text{flux}}[(y,t,x)] = \xi y$, $\xi\in[1,\infty[$, condition 3.8.19(np) holds for $m_\upsilon\le 0$, 3.8.19(inc) holds, as both $a^{\gamma,1}_{\text{flux}}$ and $a^{\gamma,2}_{\text{flux}}$ are increasing in y; and 3.8.19(locLip) holds, since $a^{\gamma,1}_{\text{flux}}$ is 0-Lipschitz.

In the first case of Ex. 3.1.2(c), one has $m_\upsilon = 0$, $a^{\gamma,1}_{\text{flux}} = 0$, $a^{\gamma,2}_{\text{flux}}[(y,t,x)] = \sigma\epsilon_{\mathrm{t}}[(y,t,x)]y^4$. Then 3.8.19(np) holds, as $a^{\gamma,1}_{\text{flux}}[(0,t,x)] = a^{\gamma,2}_{\text{flux}}[(0,t,x)] = 0$. 3.8.19(inc) holds trivially for $a^{\gamma,1}_{\text{flux}}$, but $a^{\gamma,2}_{\text{flux}}$ is only increasing in y if ϵ_{t} is sufficiently benign. 3.8.19(locLip) holds, since $a^{\gamma,1}_{\text{flux}}$ is 0-Lipschitz.

Finally, consider the first case of Ex. 3.1.2(c) with the dependency splitting introduced in Ex. 3.8.17, i.e. with $(a_{\text{flux}}^{\gamma,2})^{\text{ex.-im.}}\big[\big((\tilde{y},y),t,x\big)\big] = \sigma\epsilon_t[(\tilde{y},t,x)]y^4$. Then 3.8.19(np) and 3.8.19(locLip) hold as before. Now 3.8.19(inc) holds independently of ϵ_t, as ϵ_t is nonnegative and independent of y. 3.8.19(bnd) also holds, since $(a_{\text{flux}}^{\gamma,2})^{\text{ex.-im.}}\big[\big((\tilde{y},0),t,x\big)\big] = 0$.

—

For the decomposition of the $\mathfrak{a}^{(\nu)}_{\text{jump},1,\neg\text{Dir},(k,\mathcal{C})}$, let

$$\bigwedge_{\substack{\nu\in\{0,\dots,n\},\\(k,\mathcal{C})\in I_{\Pi,\mathfrak{D},\neg\text{Dir}}}}\left(\begin{aligned}&\mathfrak{a}^{\nu,\uparrow}_{\text{jump},1,\neg\text{Dir},(k,\mathcal{C})} : \upsilon \longrightarrow \mathbb{K},\\&\mathfrak{a}^{\nu,\uparrow}_{\text{jump},1,\neg\text{Dir},(k,\mathcal{C})}[y] := \sum_{\substack{\gamma\in G_{\text{jump},1}[\mathcal{C}]:\\ \left(k,\mathcal{C}[(k,i_2[\gamma])]\right)\in I_{\Pi,\mathfrak{D},\neg\text{Dir}},\\ \lambda_{d-1}\left[\partial\omega_k^{(i_1[\gamma])}\cap\gamma\right]>0}} a^{\gamma,1,\nu}_{\text{jump}}[(y,x_k)]\cdot\lambda_{d-1}\left[\partial\omega_k^{(i_1[\gamma])}\cap\gamma\right]\end{aligned}\right), \tag{3.8.39a}$$

$$\bigwedge_{\substack{\nu\in\{0,\dots,n\},\\(k,\mathcal{C})\in I_{\Pi,\mathfrak{D},\neg\text{Dir}}}}\left(\begin{aligned}&\mathfrak{a}^{\nu,\downarrow}_{\text{jump},1,\neg\text{Dir},(k,\mathcal{C})} : \upsilon^{I_{\Pi,\mathfrak{D},\neg\text{Dir}}} \longrightarrow \mathbb{K},\\&\mathfrak{a}^{\nu,\downarrow}_{\text{jump},1,\neg\text{Dir},(k,\mathcal{C})}[U] := \sum_{\substack{\gamma\in G_{\text{jump},1}[\mathcal{C}]:\\ \left(k,\mathcal{C}[(k,i_2[\gamma])]\right)\in I_{\Pi,\mathfrak{D},\neg\text{Dir}},\\ \lambda_{d-1}\left[\partial\omega_k^{(i_1[\gamma])}\cap\gamma\right]>0}} a^{\gamma,2,\nu}_{\text{jump}}\left[\left(U_{\left(k,\mathcal{C}[(k,i_2[\gamma])]\right)},x_k\right)\right]\\&\qquad\qquad\cdot\lambda_{d-1}\left[\partial\omega_k^{(i_1[\gamma])}\cap\gamma\right]\end{aligned}\right). \tag{3.8.39b}$$

Lemma 3.8.21. *Suppose $\upsilon = [m_\upsilon,\infty[$, that the $a^{\gamma,\alpha}_{\text{jump}}$, $\alpha\in\{1,2\}$, are real-valued and that conditions* (np), (inc), *and* (locLip) *below all hold:*

(np) $\left(a^{\gamma,1}_{\text{jump}} - a^{\gamma,2}_{\text{jump}}\right)[(m_\upsilon,t,x)] \le 0$ *for each* $\gamma\in\text{IF}_{\text{jump}}$ *and each* $(t,x)\in\tau\times\gamma$.

(inc) *The functions* $a^{\gamma,\alpha}_{\text{jump}}\restriction_{\upsilon\times\{t\}\times\{x\}}$ *are increasing for each* $\alpha\in\{1,2\}$, *each* $\gamma\in\text{IF}_{\text{jump}}$, *and each* $(t,x)\in\tau\times\gamma$.

(locLip) $\displaystyle\bigwedge_{r\in\mathbb{R}_0^+}\ \bigvee_{L_{\text{jump},2,r}[\mathfrak{C}]\in\mathbb{R}_0^+}\ \bigwedge_{\substack{(\gamma,t,x)\\\in\text{IF}_{\text{jump}}\times\tau\times\gamma}} a^{\gamma,2}_{\text{jump}}\restriction_{\upsilon\times\{t\}\times\{x\}}\in \text{Lip}_{L_{\text{jump},2,r}[\mathfrak{C}]}\big([m_\upsilon,m_\upsilon+r],\mathbb{R}\big)$,

i.e. each $a^{\gamma,2}_{\text{jump}}$ is locally Lipschitz with respect to its y-dependence.

Let $\mathbf{m} := (m_\upsilon,\dots,m_\upsilon)$. Then the following holds for each $\nu\in\{0,\dots,n\}$ and for each $(k,\mathcal{C})\in I_{\Pi,\mathfrak{D},\neg\text{Dir}}$:

(a) $\displaystyle\bigwedge_{U\in\upsilon^{I_{\Pi,\mathfrak{D},\neg\text{Dir}}}} \mathfrak{a}^{(\nu)}_{\text{jump},1,\neg\text{Dir},(k,\mathcal{C})}[U] = \mathfrak{a}^{\nu,\uparrow}_{\text{jump},1,\neg\text{Dir},(k,\mathcal{C})}[U_{(k,\mathcal{C})}] - \mathfrak{a}^{\nu,\downarrow}_{\text{jump},1,\neg\text{Dir},(k,\mathcal{C})}[U]$.

(b) $\mathfrak{a}^{\nu,\uparrow}_{\text{jump},1,\neg\text{Dir},(k,\mathcal{C})}$ *and* $\mathfrak{a}^{(\nu)}_{\text{jump},1,\text{Dir},(k,\mathcal{C})}$ *are increasing.*

(c) $\mathfrak{a}^{\nu,\downarrow}_{\text{jump},1,\neg\text{Dir},(k,\mathcal{C})}$ *is minimal at* $\mathbf{m}$.

(d) $\mathfrak{a}^{\nu,\uparrow}_{\text{jump},1,\neg\text{Dir},(k,\mathcal{C})}[m_v] \leq \mathfrak{a}^{\nu,\downarrow}_{\text{jump},1,\neg\text{Dir},(k,\mathcal{C})}[\mathbf{m}]$ *and* $\mathfrak{a}^{(\nu)}_{\text{jump},1,\text{Dir},(k,\mathcal{C})}[m_v] \leq 0$.

(e) *If* $\lambda_{d-1,\max}[\Pi]$ *is the number defined in* (3.8.31)*, then*

$$\begin{aligned}&\max\left\{0, \mathfrak{a}^{\nu,\downarrow}_{\text{jump},1,\neg\text{Dir},(k,\mathcal{C})}[\mathbf{m}]\right\} - \min\left\{0, \mathfrak{a}^{\nu,\uparrow}_{\text{jump},1,\neg\text{Dir},(k,\mathcal{C})}[m_v]\right\}\\ &\leq B_{\text{jump},m_v}[\mathfrak{C}] \cdot \lambda_{d-1,\max}[\Pi],\end{aligned}$$

and

$$-\min\left\{0, \mathfrak{a}^{(\nu)}_{\text{jump},1,\text{Dir},(k,\mathcal{C})}[m_v]\right\} \leq B_{\text{jump},\text{Dir},m_v}[\mathfrak{C}] \cdot \lambda_{d-1,\max}[\Pi],$$

where

$$\begin{aligned}B_{\text{jump},m_v}[\mathfrak{C}] := &\max\left\{\left|a^{\gamma,1}_{\text{jump}}[(m_v,t,x)]\right| : (t,x) \in \tau \times \gamma,\ \gamma \in \text{IF}_{\text{jump}}\right\}\\ &+ \max\left\{\left|a^{\gamma,2}_{\text{jump}}[(m_v,t,x)]\right| : (t,x) \in \tau \times \gamma,\ \gamma \in \text{IF}_{\text{jump}}\right\},\end{aligned} \tag{3.8.40}$$

$$\begin{aligned}B_{\text{jump},\text{Dir},m_v}[\mathfrak{C}] := &\max\Big\{\left|a^{\gamma,1}_{\text{jump}}[(y,t,x)]\right| :\\ &\qquad (y,t,x) \in [m_v, B_{\text{Dir}}[\mathfrak{C}]] \times \tau \times \gamma,\ \gamma \in \text{IF}_{\text{jump}}\Big\}\\ &+ \max\Big\{\left|a^{\gamma,2}_{\text{jump}}[(y,t,x)]\right| :\\ &\qquad (y,t,x) \in [m_v, B_{\text{Dir}}[\mathfrak{C}]] \times \tau \times \gamma,\ \gamma \in \text{IF}_{\text{jump}}\Big\}.\end{aligned} \tag{3.8.41}$$

Using absolute values in (3.8.40) *and* (3.8.41)*, and using the domain* $[m_v, B_{\text{Dir}}[\mathfrak{C}]]$ *for* y *in both summands of* (3.8.41)*, allows the use of the same bounds* $B_{\text{jump},m_v}[\mathfrak{C}]$ *and* $B_{\text{jump},\text{Dir},m_v}[\mathfrak{C}]$ *in Lem.* 3.8.23(e) *below.*

(f) $\mathfrak{a}^{\nu,\downarrow}_{\text{jump},1,\neg\text{Dir},(k,\mathcal{C})}$ *is* $\big(L_{\text{jump},2,r}[\mathfrak{C}] \cdot \lambda_{d-1,\max}[\Pi]\big)$*-Lipschitz on* $[m_v, m_v + r]^{I_{\Pi,\mathfrak{D},\neg\text{Dir}}}$ *with respect to the max-norm for each* $r \in \mathbb{R}^+$.

Proof. It is noted that in $\mathfrak{a}^{(\nu)}_{\text{jump},1,\text{Dir},(k,\mathcal{C})}$, the summands involving the Dirichlet contributions are constant.

(a) is clear, since (3.8.39a) and (3.8.39b) are merely an algebraic decomposition of (3.7.59). (b) and (c) are immediate consequences of hypothesis (inc).

Hypothesis (np) directly implies the first part of (d). According to (3.7.60), the second part of (d) can also be seen from hypothesis (np), since $m_v \leq u_{j_{\text{Dir}}[(k,i_2[\gamma])],\text{Dir}}[(t_\nu, x_k)]$, and since $a^{\gamma,2,\nu}_{\text{jump}}$ is increasing in y according to hypothesis (inc).

The compactness of γ and τ together with the continuity of $a^{\gamma,1}_{\text{jump}}$ and $a^{\gamma,2}_{\text{jump}}$ implies (e), and hypothesis (locLip) together with Rem. C.7.7(g) yields (f). ■

Example 3.8.22. Suppose $\gamma \in \mathrm{IF}_{\mathrm{jump}}$ is a jump interface, $\upsilon = [m_\upsilon, \infty[$, and consider the case of Ex. 3.1.2(b), i.e. $a^{\gamma,1}_{\mathrm{jump}}[(y,t,x)] = a^{\gamma,2}_{\mathrm{jump}}[(y,t,x)] = \xi y$, $\xi \in \mathbb{R}^+$. Then the hypotheses (np), (inc), and (locLip) of Lem. 3.8.21 are satisfied due to the following obvious facts (a), (b), and (c).

(a) $\left(a^{\gamma,1}_{\mathrm{jump}} - a^{\gamma,2}_{\mathrm{jump}}\right)[(m_\upsilon, t, x)] = 0.$

(b) $a^{\gamma,1}_{\mathrm{jump}}$ and $a^{\gamma,2}_{\mathrm{jump}}$ are increasing.

(c) $a^{\gamma,1}_{\mathrm{jump}}$ and $a^{\gamma,2}_{\mathrm{jump}}$ are both ξ-Lipschitz.

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Finally, $\mathfrak{a}^{(\nu)}_{\mathrm{flux,jump},2,\neg\mathrm{Dir},(k,\mathcal{C})} + \mathfrak{a}^{(\nu)}_{\mathrm{jump},2,\neg\mathrm{Dir},(k,\mathcal{C})}$ is decomposed. Let

$$\bigwedge_{\substack{\nu\in\{0,\dots,n\},\\ (k,\mathcal{C})\in I_{\Pi,\mathfrak{D},\neg\mathrm{Dir}}}} \left(\begin{array}{c} \mathfrak{a}^{\nu,\uparrow}_{\mathrm{jump},2,\neg\mathrm{Dir},(k,\mathcal{C})} : \upsilon \times \upsilon \longrightarrow \mathbb{K}, \\ \mathfrak{a}^{\nu,\uparrow}_{\mathrm{jump},2,\neg\mathrm{Dir},(k,\mathcal{C})}[(\tilde{y}, y)] := \displaystyle\sum_{\substack{\gamma\in G_{\mathrm{jump},2}[\mathcal{C}]:\\ \left(k,\mathcal{C}[(k,i_1[\gamma])]\right)\in I_{\Pi,\mathfrak{D},\neg\mathrm{Dir}},\\ \lambda_{d-1}\left[\partial\omega_k^{(i_2[\gamma])}\cap\gamma\right]>0}} \left((a^{\gamma,2,\nu}_{\mathrm{flux}})^{\mathrm{ex.\text{-}im.}}\left[\left((\tilde{y}, y), x_k\right)\right] + a^{\gamma,2,\nu}_{\mathrm{jump}}[(y, x_k)] \right) \\ \cdot\, \lambda_{d-1}\left[\partial\omega_k^{(i_2[\gamma])} \cap \gamma\right] \end{array} \right), \tag{3.8.42a}$$

$$\bigwedge_{\substack{\nu\in\{0,\dots,n\},\\ (k,\mathcal{C})\in I_{\Pi,\mathfrak{D},\neg\mathrm{Dir}}}} \left(\begin{array}{l} \mathfrak{a}^{\nu,\downarrow}_{\mathrm{jump},2,\neg\mathrm{Dir},(k,\mathcal{C})} : \upsilon^{I_{\Pi,\mathfrak{D},\neg\mathrm{Dir}}} \times \upsilon^{I_{\Pi,\mathfrak{D},\neg\mathrm{Dir}}} \longrightarrow \mathbb{K}, \\ \mathfrak{a}^{\nu,\downarrow}_{\mathrm{jump},2,\neg\mathrm{Dir},(k,\mathcal{C})}[(\tilde{U}, U)] \\ := \displaystyle\sum_{\substack{\gamma\in G_{\mathrm{jump},2}[\mathcal{C}]:\\ \left(k,\mathcal{C}[(k,i_1[\gamma])]\right)\in I_{\Pi,\mathfrak{D},\neg\mathrm{Dir}},\\ \lambda_{d-1}\left[\partial\omega_k^{(i_2[\gamma])}\cap\gamma\right]>0}} \left(\begin{array}{l} (a^{\gamma,1,\nu}_{\mathrm{flux}})^{\mathrm{ex.\text{-}im.}}\left[\left((\tilde{U}_{\left(k,\mathcal{C}[(k,i_1[\gamma])]\right)}, U_{\left(k,\mathcal{C}[(k,i_1[\gamma])]\right)}), x_k\right)\right] \\ \qquad + a^{\gamma,1,\nu}_{\mathrm{jump}}\left[\left(U_{\left(k,\mathcal{C}[(k,i_1[\gamma])]\right)}, x_k\right)\right] \end{array} \right) \\ \qquad\qquad \cdot\, \lambda_{d-1}\left[\partial\omega_k^{(i_2[\gamma])} \cap \gamma\right] \end{array} \right). \tag{3.8.42b}$$

Lemma 3.8.23. *Suppose $\upsilon = [m_\upsilon, \infty[$ and that the $a^{\gamma,1}_{\mathrm{jump}}$ and $a^{\gamma,2}_{\mathrm{jump}}$ are real-valued. Let $\mathfrak{S}_{\mathrm{jump}} := \left((a^{\gamma,\alpha}_{\mathrm{flux}})^{\mathrm{ex.\text{-}im.}}\right)_{(\alpha,\gamma)\in\{1,2\}\times\mathrm{IF}_{\mathrm{jump}}}$ denote the family of real-valued dependency splittings. Moreover, assume the conditions* (np), (inc), (bnd), *and* (locLip) *below:*

(np)
$$\bigwedge_{\gamma\in\mathrm{IF}_{\mathrm{jump}}} \bigwedge_{y\in\upsilon} \bigwedge_{(t,x)\in\tau\times\gamma} \left(\begin{array}{l} \left((a^{\gamma,2}_{\mathrm{flux}})^{\mathrm{ex.\text{-}im.}} - (a^{\gamma,1}_{\mathrm{flux}})^{\mathrm{ex.\text{-}im.}}\right)\left[\left((y, m_\upsilon), t, x\right)\right] \\ + \left(a^{\gamma,2}_{\mathrm{jump}} - a^{\gamma,1}_{\mathrm{jump}}\right)[(m_\upsilon, t, x)] \le 0 \end{array} \right).$$

(bnd)

$$B_{\mathrm{flux,jump},1,m_v}[(\mathfrak{C},\mathfrak{S}_{\mathrm{jump}})] := \sup\Big\{ (a^{\gamma,1}_{\mathrm{flux}})^{\mathrm{ex.\text{-}im.}}\big[((y,m_v),t,x)\big] : \\ (y,t,x)\in v\times\tau\times\gamma,\ \gamma\in \mathrm{IF}_{\mathrm{jump}}\Big\} < \infty, \tag{3.8.43a}$$

$$B_{\mathrm{flux,jump},2,m_v}[(\mathfrak{C},\mathfrak{S}_{\mathrm{jump}})] := -\inf\Big\{ (a^{\gamma,2}_{\mathrm{flux}})^{\mathrm{ex.\text{-}im.}}\big[((y,m_v),t,x)\big] : \\ (y,t,x)\in v\times\tau\times\gamma,\ \gamma\in \mathrm{IF}_{\mathrm{jump}}\Big\} < \infty. \tag{3.8.43b}$$

(inc) *The functions*

$$(a^{\gamma,1}_{\mathrm{flux}})^{\mathrm{ex.\text{-}im.}}\restriction_{\{y\}\times v\times\{t\}\times\{x\}} + a^{\gamma,1}_{\mathrm{jump}}\restriction_{v\times\{t\}\times\{x\}}$$

and

$$(a^{\gamma,2}_{\mathrm{flux}})^{\mathrm{ex.\text{-}im.}}\restriction_{\{y\}\times v\times\{t\}\times\{x\}} + a^{\gamma,2}_{\mathrm{jump}}\restriction_{v\times\{t\}\times\{x\}}$$

are increasing for each $\gamma\in\mathrm{IF}_{\mathrm{jump}}$*, for each* $y\in v$*, and for each* $(t,x)\in\tau\times\gamma$.

(locLip)

$$\bigwedge_{r\in\mathbb{R}^+_0}\ \bigvee_{L_{\mathrm{flux,jump},r}[(\mathfrak{C},\mathfrak{S}_{\mathrm{jump}})]\in\mathbb{R}^+_0}\ \bigwedge_{\substack{(\gamma,y,t,x)\\ \in \mathrm{IF}_{\mathrm{jump}}\times v\times\tau\times\gamma}} \begin{pmatrix} (a^{\gamma,1}_{\mathrm{flux}})^{\mathrm{ex.\text{-}im.}}\restriction_{\{y\}\times v\times\{t\}\times\{x\}} + a^{\gamma,1}_{\mathrm{jump}}\restriction_{v\times\{t\}\times\{x\}} \\ \in \mathrm{Lip}_{L_{\mathrm{flux,jump},r}[(\mathfrak{C},\mathfrak{S}_{\mathrm{jump}})]}\big([m_v, m_v+r],\mathbb{R}\big)\end{pmatrix}.$$

Let $\mathbf{m} := (m_v,\dots,m_v)$*. Then the following holds for each* $y\in v$*, each* $U\in v^{I_{\Pi,\mathfrak{D},\neg\mathrm{Dir}}}$*, each* $\nu\in\{0,\dots,n\}$*, and each* $(k,\mathcal{C})\in I_{\Pi,\mathfrak{D},\neg\mathrm{Dir}}$*:*

(a)
$$\bigwedge_{(\tilde U,U)\in v^{I_{\Pi,\mathfrak{D},\neg\mathrm{Dir}}}\times v^{I_{\Pi,\mathfrak{D},\neg\mathrm{Dir}}}} \begin{pmatrix} \mathfrak{a}^{(\nu)}_{\mathrm{flux,jump},2,\neg\mathrm{Dir},(k,\mathcal{C})}[U] + \mathfrak{a}^{(\nu)}_{\mathrm{jump},2,\neg\mathrm{Dir},(k,\mathcal{C})}[(\tilde U,U)] \\ = \mathfrak{a}^{\nu,\uparrow}_{\mathrm{jump},2,\neg\mathrm{Dir},(k,\mathcal{C})}[(\tilde U_{(k,\mathcal{C})},U_{(k,\mathcal{C})})] - \mathfrak{a}^{\nu,\downarrow}_{\mathrm{jump},2,\neg\mathrm{Dir},(k,\mathcal{C})}[(\tilde U,U)]\end{pmatrix}.$$

(b) *The functions* $\mathfrak{a}^{\nu,\uparrow}_{\mathrm{jump},2,\neg\mathrm{Dir},(k,\mathcal{C})}\restriction_{\{y\}\times v}$ *and* $\mathfrak{a}^{(\nu)}_{\mathrm{flux,jump},2,\mathrm{Dir},(k,\mathcal{C})}\restriction_{\{y\}\times v} + \mathfrak{a}^{(\nu)}_{\mathrm{jump},2,\mathrm{Dir},(k,\mathcal{C})}$ *are increasing.*

(c) $\mathfrak{a}^{\nu,\downarrow}_{\mathrm{jump},2,\neg\mathrm{Dir},(k,\mathcal{C})}\restriction_{\{U\}\times v^{I_{\Pi,\mathfrak{D},\neg\mathrm{Dir}}}}$ *is minimal at* $\mathbf{m}$.

(d)
$$\mathfrak{a}^{\nu,\uparrow}_{\mathrm{jump},2,\neg\mathrm{Dir},(k,\mathcal{C})}[(U_{(k,\mathcal{C})},m_v)] \le \mathfrak{a}^{\nu,\downarrow}_{\mathrm{jump},2,\neg\mathrm{Dir},(k,\mathcal{C})}[(U,\mathbf{m})],$$
$$\mathfrak{a}^{(\nu)}_{\mathrm{flux,jump},2,\mathrm{Dir},(k,\mathcal{C})}[(y,m_v)] + \mathfrak{a}^{(\nu)}_{\mathrm{jump},2,\mathrm{Dir},(k,\mathcal{C})}[m_v] \le 0.$$

(e) *If* $B_{\mathrm{jump},m_v}[\mathfrak{C}]$*,* $B_{\mathrm{jump,Dir},m_v}[\mathfrak{C}]$*, and* $\lambda_{d-1,\max}[\Pi]$ *are the numbers defined in* (3.8.40)*,* (3.8.41)*, and* (3.8.31)*, respectively, then*

$$\max\big\{0,\mathfrak{a}^{\nu,\downarrow}_{\mathrm{jump},2,\neg\mathrm{Dir},(k,\mathcal{C})}[(U,m_v)]\big\} - \min\big\{0,\mathfrak{a}^{\nu,\uparrow}_{\mathrm{jump},2,\neg\mathrm{Dir},(k,\mathcal{C})}[(U_{(k,\mathcal{C})},m_v)]\big\}$$
$$\le \big(\max\big\{0, B_{\mathrm{flux,jump},1,m_v}[(\mathfrak{C},\mathfrak{S}_{\mathrm{jump}})]\big\}$$

$$+ \max\left\{0, B_{\text{flux,jump},2,m_v}[(\mathfrak{C}, \mathfrak{S}_{\text{jump}})]\right\} + B_{\text{jump},m_v}[\mathfrak{C}]\big) \cdot \lambda_{d-1,\max}[\Pi].$$

and

$$\begin{aligned}
&- \min\left\{0, \mathfrak{a}^{(\nu)}_{\text{flux,jump},2,\text{Dir},(k,\mathcal{C})}[(y, m_v)] + \mathfrak{a}^{(\nu)}_{\text{jump},2,\text{Dir},(k,\mathcal{C})}[m_v]\right\} \\
&\leq \big(\max\left\{0, B_{\text{flux,Dir}}[\mathfrak{C}]\right\} \\
&\qquad + \max\left\{0, B_{\text{flux,jump},2,m_v}[(\mathfrak{C}, \mathfrak{S}_{\text{jump}})]\right\} + B_{\text{jump,Dir},m_v}[\mathfrak{C}]\big) \cdot \lambda_{d-1,\max}[\Pi],
\end{aligned}$$

where

$$\begin{aligned}
B_{\text{flux,Dir}}[\mathfrak{C}] := \max\Big\{&\left(a^{\gamma,1}_{\text{flux}}\right)^{\text{ex.-im.}}\left[\big((\tilde{y}, y), t, x\big)\right] : \\
&\big((\tilde{y}, y), t, x\big) \in [m_v, B_{\text{Dir}}[\mathfrak{C}]]^2 \times \tau \times \gamma,\ \gamma \in \mathrm{IF}_{\text{jump}}\Big\}.
\end{aligned} \tag{3.8.44}$$

(f) *The function* $\mathfrak{a}^{\nu,\downarrow}_{\text{jump},2,\neg\text{Dir},(k,\mathcal{C})}\restriction_{\{U\}\times v^{I_{\Pi,\mathfrak{D},\neg\text{Dir}}}}$ *is* $\big(L_{\text{flux,jump},r}[(\mathfrak{C}, \mathfrak{S}_{\text{jump}})] \cdot \lambda_{d-1,\max}[\Pi]\big)$*-Lipschitz on* $[m_v, m_v + r]^{I_{\Pi,\mathfrak{D},\neg\text{Dir}}}$ *with respect to the max-norm for each* $r \in \mathbb{R}^+$.

Proof. It is noted that in $\mathfrak{a}^{(\nu)}_{\text{flux,jump},2,\neg\text{Dir},(k,\mathcal{C})} + \mathfrak{a}^{(\nu)}_{\text{jump},2,\neg\text{Dir},(k,\mathcal{C})}$, the summands involving the Dirichlet contributions are constant.

(a) is clear, since (3.8.42a) and (3.8.42b) are merely an algebraic decomposition of the sum of (3.7.62) and (3.7.65). (b) and (c) are immediate consequences of hypothesis (inc).

Hypothesis (np) directly implies the first inequality in (d). The second inequality in (d) can be seen from (3.7.63), (3.7.66), and hypothesis (np), since

$$m_v \leq u_{j_{\text{Dir}}[(k,i_1[\gamma])],\text{Dir}}[(t_\nu, x_k)],$$

and since each $\left(a^{\gamma,1}_{\text{flux}}\right)^{\text{ex.-im.}}\restriction_{\{y\}\times v\times\{t\}\times\{x\}} + a^{\gamma,1}_{\text{jump}}\restriction_{v\times\{t\}\times\{x\}}$ is increasing according to hypothesis (inc).

Hypothesis (bnd) and the compactness of γ and τ together with the continuity of $a^{\gamma,1}_{\text{jump}}$, $a^{\gamma,2}_{\text{jump}}$, and $u_{j,\text{Dir}}$ imply (e), and hypothesis (locLip) together with Rem. C.7.7(g) yields (f). ∎

Example 3.8.24. As in Ex. 3.8.22, suppose $\gamma \in \mathrm{IF}_{\text{jump}}$ is a jump interface, $v = [m_v, \infty[$, and consider the case of Ex. 3.1.2(b), i.e. $a^{\gamma,1}_{\text{jump}}[(y, t, x)] = a^{\gamma,2}_{\text{jump}}[(y, t, x)] = \xi_{\text{jump}} y$, $\xi_{\text{jump}} \in \mathbb{R}^+$.

In the present example, this situation is combined with a consideration of the cases in Ex. 3.8.20 in the context of a jump interface. The hypotheses of Lem. 3.8.23 are investigated.

First, assume that there is no dependency splitting, i.e. $\left(a^{\gamma,\alpha}_{\text{flux}}\right)^{\text{ex.-im.}}\left[\big((\tilde{y}, y), t, x\big)\right] = a^{\gamma,\alpha}_{\text{flux}}[(y, t, x)]$. Then, analogous to Ex. 3.8.20, 3.8.23(bnd) follows from the compactness of τ and γ.

Conditions (np), (inc), and (locLip) of Lem. 3.8.23 are satisfied according to Ex. 3.8.22 if $a^{\gamma,1}_{\text{flux}} = a^{\gamma,2}_{\text{flux}} = 0$.

In the last case considered in Ex. 3.7.34, where $a^{\gamma,1}_{\text{flux}} = 0$ and $a^{\gamma,2}_{\text{flux}}[(y,t,x)] = \xi_{\text{flux}} y$, $\xi_{\text{flux}} \in [1,\infty[$, condition 3.8.23(np) holds for $m_v \leq 0$, using Ex. 3.8.22(a). 3.8.23(inc) holds, as all the functions $a^{\gamma,1}_{\text{jump}}$, $a^{\gamma,2}_{\text{jump}}$, $a^{\gamma,1}_{\text{flux}}$, and $a^{\gamma,2}_{\text{flux}}$ are increasing in y. Since $a^{\gamma,1}_{\text{flux}} + a^{\gamma,1}_{\text{jump}}$ is ξ_{jump}-Lipschitz and $a^{\gamma,2}_{\text{flux}} + a^{\gamma,2}_{\text{jump}}$ is $(\xi_{\text{jump}} + \xi_{\text{flux}})$-Lipschitz, 3.8.23(locLip) also holds.

In the first case of Ex. 3.1.2(c), one has $m_v = 0$, $a^{\gamma,1}_{\text{flux}} = 0$, $a^{\gamma,2}_{\text{flux}}[(y,t,x)] = \sigma\epsilon_{\text{t}}[(y,t,x)]y^4$. Then 3.8.23(np) holds, combining Ex. 3.8.22(a) with $a^{\gamma,1}_{\text{flux}}[(0,t,x)] = a^{\gamma,2}_{\text{flux}}[(0,t,x)] = 0$. Analogous to Ex. 3.8.20, 3.8.23(inc) always holds for $a^{\gamma,1}_{\text{flux}} + a^{\gamma,1}_{\text{jump}}$, but $a^{\gamma,2}_{\text{flux}} + a^{\gamma,2}_{\text{jump}}$ is only increasing in y if ϵ_{t} is sufficiently benign. 3.8.23(locLip) holds due to Ex. 3.8.22(c).

Finally, as in Ex. 3.8.20, consider the first case of Ex. 3.1.2(c) with the dependency splitting introduced in Ex. 3.8.17, i.e. with $(a^{\gamma,2}_{\text{flux}})^{\text{ex.-im.}}\big[\big((\tilde{y},y),t,x\big)\big] = \sigma\epsilon_{\text{t}}[(\tilde{y},t,x)]y^4$. Then 3.8.23(np) and 3.8.23(locLip) hold as before, but 3.8.23(inc) now holds independently of ϵ_{t}, as ϵ_{t} is nonnegative and independent of y. 3.8.23(bnd) also holds, since $(a^{\gamma,2}_{\text{flux}})^{\text{ex.-im.}}\big[\big((\tilde{y},0),t,x\big)\big] = 0$.

3.8.7 Nonlocal Operators

The discretized nonlocal operators $\mathfrak{B}^{(\nu)}_{(k,\mathcal{C})}$, $\mathfrak{A}^{(\nu)}_{\text{con},(k,\mathcal{C})}$, and $\mathfrak{A}^{(\nu)}_{\text{jump},(k,\mathcal{C})}$ are *not* decomposed, as it is seen in Ex. 3.8.26 below that if the operators arise from nonlocal radiation terms according to (3.7.91), (3.7.92), and (3.7.93) (which is the only concrete case considered in this work), then they themselves have all the properties of a $\downarrow$-operator (s. Def. 3.8.25 below).

Definition 3.8.25. Given the finite volume discretization $\mathfrak{F}$ of $\mathfrak{C}$, it is said that the discretized nonlocal operators $\mathfrak{B}^{(\nu)}_{(k,\mathcal{C})}$, $\mathfrak{A}^{(\nu)}_{\text{con},(k,\mathcal{C})}$, and $\mathfrak{A}^{(\nu)}_{\text{jump},(k,\mathcal{C})}$ have the *$\downarrow$-property* iff they satisfy the following conditions (i) – (iv) for each $u \in \upsilon^{I_{\Pi,\mathfrak{D},\neg\text{Dir}}}$, each $(k,\mathcal{C}) \in I_{\Pi,\mathfrak{D},\neg\text{Dir}}$, and each $\nu \in \{0,\dots,n\}$. Let $\mathbf{m} := (m_v,\dots,m_v)$.

(i) $\mathfrak{B}^{(\nu)}_{(k,\mathcal{C})}\restriction_{\{u\}\times\upsilon^{I_{\Pi,\mathfrak{D},\neg\text{Dir}}}}$, $\mathfrak{A}^{(\nu)}_{\text{con},(k,\mathcal{C})}\restriction_{\{u\}\times\upsilon^{I_{\Pi,\mathfrak{D},\neg\text{Dir}}}}$, and $\mathfrak{A}^{(\nu)}_{\text{jump},(k,\mathcal{C})}\restriction_{\{u\}\times\upsilon^{I_{\Pi,\mathfrak{D},\neg\text{Dir}}}}$ are minimal at $\mathbf{m}$.

(ii) $0 \leq \mathfrak{B}^{(\nu)}_{(k,\mathcal{C})}[(u,\mathbf{m})]$, $0 \leq \mathfrak{A}^{(\nu)}_{\text{con},(k,\mathcal{C})}[(u,\mathbf{m})]$, and $0 \leq \mathfrak{A}^{(\nu)}_{\text{jump},(k,\mathcal{C})}[(u,\mathbf{m})]$.

(iii) There is a number $B_{\text{nonloc}}[\mathfrak{C}] \in \mathbb{R}^+_0$ that is independent of Π and independent of the time discretization and such that $\mathfrak{B}^{(\nu)}_{(k,\mathcal{C})}[(u,\mathbf{m})] \leq B_{\text{nonloc}}[\mathfrak{C}]$, $\mathfrak{A}^{(\nu)}_{\text{con},(k,\mathcal{C})}[(u,\mathbf{m})] \leq B_{\text{nonloc}}[\mathfrak{C}]$, and $\mathfrak{A}^{(\nu)}_{\text{jump},(k,\mathcal{C})}[(u,\mathbf{m})] \leq B_{\text{nonloc}}[\mathfrak{C}]$.

(iv) For each $r \in \mathbb{R}^+$, there is $L_{\text{nonloc},r}[(\mathfrak{C},\Pi)] \in \mathbb{R}^+_0$ that is independent of the time discretization and such that the functions $\mathfrak{B}^{(\nu)}_{(k,\mathcal{C})}\restriction_{\{u\}\times\upsilon^{I_{\Pi,\mathfrak{D},\neg\text{Dir}}}}$, $\mathfrak{A}^{(\nu)}_{\text{con},(k,\mathcal{C})}\restriction_{\{u\}\times\upsilon^{I_{\Pi,\mathfrak{D},\neg\text{Dir}}}}$, and $\mathfrak{A}^{(\nu)}_{\text{jump},(k,\mathcal{C})}\restriction_{\{u\}\times v^{I_{\Pi,\mathfrak{D},\neg\text{Dir}}}}$ are $L_{\text{nonloc},r}[(\mathfrak{C},\Pi)]$-Lipschitz on $[m_v, m_v + r]^{I_{\Pi,\mathfrak{D},\neg\text{Dir}}}$ with respect to the max-norm.

Example 3.8.26. As in Exs 3.7.27 and 3.7.36, the case is considered where $\mathfrak{B}^{(\nu)}_{(k,\mathcal{C})}$, $\mathfrak{A}^{(\nu)}_{\text{con},(k,\mathcal{C})}$, and $\mathfrak{A}^{(\nu)}_{\text{jump},(k,\mathcal{C})}$ are defined by (3.7.91), (3.7.92), and (3.7.93), respectively, that means the nonlocal operators arise as radiation operators according to the axisymmetric cases of Exs 3.1.3(e) and 3.1.2(c).

It is verified that in this case, $\mathfrak{B}^{(\nu)}_{(k,\mathcal{C})}$, $\mathfrak{A}^{(\nu)}_{\text{con},(k,\mathcal{C})}$, and $\mathfrak{A}^{(\nu)}_{\text{jump},(k,\mathcal{C})}$ have the $\downarrow$-property according to Def. 3.8.25.

As the unknown represents absolute temperature, one has $m_v = 0$. It is then immediate from (3.7.81c) and (3.7.88) that $\mathfrak{B}^{(\nu)}_{(k,\mathcal{C})}[(u,\mathbf{m})] = \mathfrak{A}^{(\nu)}_{\text{con},(k,\mathcal{C})}[(u,\mathbf{m})] = \mathfrak{A}^{(\nu)}_{\text{jump},(k,\mathcal{C})}[(u,\mathbf{m})] = 0$, which implies conditions (ii) and (iii) of Def. 3.8.25 with $B_{\text{nonloc}}[\mathfrak{C}] = 0$.

The vector $\mathbf{Y}$ is nonnegative by (3.7.81c), $\mathbf{A}^{-1}$ is nonnegative by Lem. 3.7.22(b), and $\tilde{\mathbf{L}}$ is nonnegative by (3.7.87). Then (3.7.88) shows that $\mathbf{V}$ is also nonnegative and so are $\mathfrak{B}^{(\nu)}_{(k,\mathcal{C})}$, $\mathfrak{A}^{(\nu)}_{\text{con},(k,\mathcal{C})}$, and $\mathfrak{A}^{(\nu)}_{\text{jump},(k,\mathcal{C})}$, proving condition (i) of Def. 3.8.25.

Condition 3.8.25(iv): The function $y \mapsto \lambda \cdot y^4$ is $(4\lambda r^3)$-Lipschitz on $[0,r]$. Thus, according to (3.7.81c), the map $\left(T^{(\nu)}_{\text{solid,circ}}[x_k]\right)_{\kappa\in I_{\text{rad},\Gamma}} \mapsto \mathbf{Y}$ is $(4\sigma \max\{l_\kappa : \kappa \in I_{\text{rad},\Gamma}\} \cdot r^3)$-Lipschitz on $[0,r]^{I_{\text{rad},\Gamma}}$ by Rem. C.7.7(f). Combining this with (3.7.88), Def. and Rem. C.2.3, and Rem. C.7.7(b), shows that the map $\left(T^{(\nu)}_{\text{solid,circ}}[x_k]\right)_{\kappa\in I_{\text{rad},\Gamma}} \mapsto \mathbf{V}$ is $(4\sigma \max\{l_\kappa : \kappa \in I_{\text{rad},\Gamma}\} \cdot \|\tilde{\mathbf{L}}\mathbf{A}^{-1}\| \cdot r^3)$-Lipschitz on $[0,r]^{I_{\text{rad},\Gamma}}$. Then, according to (3.7.91), (3.7.92), and (3.7.93), and using that each I_{ω_k}, $k \in I_\Pi$, can have at most two elements, each of the functions $\mathfrak{B}^{(\nu)}_{(k,\mathcal{C})}\restriction_{\{u\}\times v^{I_{\Pi,\mathfrak{D},\neg\text{Dir}}}}$, $\mathfrak{A}^{(\nu)}_{\text{con},(k,\mathcal{C})}\restriction_{\{u\}\times v^{I_{\Pi,\mathfrak{D},\neg\text{Dir}}}}$, and $\mathfrak{A}^{(\nu)}_{\text{jump},(k,\mathcal{C})}\restriction_{\{u\}\times v^{I_{\Pi,\mathfrak{D},\neg\text{Dir}}}}$ is $L_{\text{nonloc},r}[(\mathfrak{C},\Pi)]$-Lipschitz for each $u \in v^{I_{\Pi,\mathfrak{D},\neg\text{Dir}}}$, where

$$L_{\text{nonloc},r}[(\mathfrak{C},\Pi)] := 8\sigma \max\{l_\kappa : \kappa \in I_{\text{rad},\Gamma}\} \cdot \|\tilde{\mathbf{L}}\mathbf{A}^{-1}\| \cdot r^3. \tag{3.8.45}$$

Since $\epsilon_{\text{circ}}\left[(T^{(\nu-1)}_{\text{solid,circ}}[x_\kappa], x_\kappa)\right]$ is always bounded by 1, $L_{\text{nonloc},r}[(\mathfrak{C},\Pi)]$ does not depend on the time discretization as required in Def. 3.8.25(iv). It does, however, depend on the space discretization Π (a priori, e.g. $I_{\text{rad},\Gamma}$, $\max\{l_\kappa : \kappa \in I_{\text{rad},\Gamma}\}$, and $\|\tilde{\mathbf{L}}\mathbf{A}^{-1}\|$ all depend on Π).

3.8.8 Decomposition of Source and Sink Terms

In this section, the operators $\mathfrak{f}^{(\nu)}_{(k,\mathcal{C})}$ defined in (3.7.119) are decomposed. Assume $v = [m_v, \infty[$ and that for each $j \in J$, f_j is real-valued and locally Lipschitz in the sense of condition (locLip) of Lem. 3.8.27 below. Let

$$\bigwedge_{\substack{\nu\in\{0,\dots,n\},\\ (k,\mathcal{C})\in I_{\Pi,\mathfrak{D},\neg\mathrm{Dir}}}} \left(\begin{aligned} &\mathfrak{f}^{\nu,\uparrow}_{(k,\mathcal{C})} : \upsilon \longrightarrow \mathbb{R},\\ &\mathfrak{f}^{\nu,\uparrow}_{(k,\mathcal{C})}[y] := \sum_{j\in V[\mathcal{C}]} \Big(- f^{(\nu)}_j[(m_\upsilon, x_k)] \\ &\qquad\qquad + \mathrm{var}^+\left[-f^{(\nu)}_j\restriction_{\upsilon\times\{x_k\}}\right][y]\Big)\cdot \lambda_d[\omega^{(j)}_k] \end{aligned} \right), \tag{3.8.46a}$$

$$\bigwedge_{\substack{\nu\in\{0,\dots,n\},\\ (k,\mathcal{C})\in I_{\Pi,\mathfrak{D},\neg\mathrm{Dir}}}} \left(\begin{aligned} &\mathfrak{f}^{\nu,\downarrow}_{(k,\mathcal{C})} : \upsilon \longrightarrow \mathbb{R},\\ &\mathfrak{f}^{\nu,\downarrow}_{(k,\mathcal{C})}[y] := \sum_{j\in V[\mathcal{C}]} \mathrm{var}^-\left[-f^{(\nu)}_j\restriction_{\upsilon\times\{x_k\}}\right][y]\cdot \lambda_d[\omega^{(j)}_k] \end{aligned} \right). \tag{3.8.46b}$$

Lemma 3.8.27. *Suppose $\upsilon = [m_\upsilon, \infty[$, the f_j are real-valued, and the conditions* (np) *and* (locLip) *below both hold:*

(np) $-f_j[(m_\upsilon, t, x)] \leq 0$ *for each* $j \in J$ *and for each* $(t, x) \in \tau \times p_j$.

(locLip) $\bigwedge_{r\in\mathbb{R}^+_0} \bigvee_{L_{f,r}[\mathfrak{C}]\in\mathbb{R}^+_0} \bigwedge_{(j,t,x)\in J\times\tau\times p_j} f_j\restriction_{\upsilon\times\{t\}\times\{x\}} \in \mathrm{Lip}_{L_{f,r}[\mathfrak{C}]}\big([m_\upsilon, m_\upsilon + r], \mathbb{R}\big)$, *i.e. each f_j is locally Lipschitz with respect to its dependence on $y \in \upsilon$.*

Then the following holds for each $\nu \in \{0, \dots, n\}$ and for each $(k, \mathcal{C}) \in I_{\Pi,\mathfrak{D},\neg\mathrm{Dir}}$:

(a) $-\mathfrak{f}^{(\nu)}_{(k,\mathcal{C})} = \mathfrak{f}^{\nu,\uparrow}_{(k,\mathcal{C})} - \mathfrak{f}^{\nu,\downarrow}_{(k,\mathcal{C})}$.

(b) $\mathfrak{f}^{\nu,\uparrow}_{(k,\mathcal{C})}$ *is increasing.*

(c) $\mathfrak{f}^{\nu,\downarrow}_{(k,\mathcal{C})}$ *is minimal at m_υ.*

(d) $\mathfrak{f}^{\nu,\uparrow}_{(k,\mathcal{C})}[m_\upsilon] \leq \mathfrak{f}^{\nu,\downarrow}_{(k,\mathcal{C})}[m_\upsilon]$.

(e) $\max\big\{0, \mathfrak{f}^{\nu,\downarrow}_{(k,\mathcal{C})}[m_\upsilon]\big\} - \min\big\{0, \mathfrak{f}^{\nu,\uparrow}_{(k,\mathcal{C})}[m_\upsilon]\big\} \leq B_{f,m_\upsilon}[\mathfrak{C}] \cdot \lambda_{d,\max}[\Pi]$, *where*

$$B_{f,m_\upsilon}[\mathfrak{C}] := \max\big\{f_j[(m_\upsilon, t, x)] : (t,x) \in \tau \times p_j,\ j \in J\big\}, \tag{3.8.47}$$

$$\lambda_{d,\max}[\Pi] := \max\big\{\lambda_d[\omega_k] : k \in I_\Pi\big\}. \tag{3.8.48}$$

The number $\lambda_{d,\max}[\Pi]$ measures the maximal size of control volumes in terms of Lebesgue measure.

(f) $\mathfrak{f}^{\nu,\downarrow}_{(k,\mathcal{C})}$ *is $L_{f,r}[\mathfrak{C}] \cdot \lambda_{d,\max}[\Pi]$-Lipschitz on $[m_\upsilon, m_\upsilon + r]$ for each $r \in \mathbb{R}^+$.*

Proof. (a) and (f) follow from hypothesis (locLip) and Rem. C.6.8(h). Both $\mathfrak{f}^{\nu,\uparrow}_{(k,\mathcal{C})}$ and $\mathfrak{f}^{\nu,\downarrow}_{(k,\mathcal{C})}$ are increasing due to Rem. C.6.8(c), proving (b) and (c). Combining (a) with hypothesis (np) yields (d). Finally, (e) follows from Rem. C.6.8(a) together with hypothesis (np). ∎

Example 3.8.28. Example 3.1.1(b) and the first case of Ex. 3.1.1(a) are investigated with respect to the hypotheses (np) and (locLip) of Lem. 3.8.27.

Both conditions are trivially satisfied for the first case of Ex. 3.1.1(a) as $f_j = 0$. It remains to consider Ex. 3.1.1(b).

In this example, the unknown represents absolute temperature. Hence $m_v = 0$, and condition 3.8.27(np) is completely natural from the physical point of view, as it states that the system can not be cooled if its absolute temperature is zero. However, the condition can still fail for some concrete model equation, which just means that the model is not valid close to absolute temperature zero.

It is $f_j[(y,t,x)] = \rho_{\mathbf{gas}}[(t,x)]\mathbf{g} \bullet \mathbf{v}_{\mathbf{gas}}[(t,x)]$ in the first case of Ex. 3.1.1(b). Thus, 3.8.27(locLip) holds, as f_j does not depend on $y \in v$, and, assuming $\rho_{\mathbf{gas}} > 0$, 3.8.27(np) holds if and only if $\mathbf{g} \bullet \mathbf{v}_{\mathbf{gas}}[(t,x)] \geq 0$ for each (t,x).

In the second case of Ex. 3.1.1(b), $f_j[(y,t,x)] = f^{[\beta_j]}$, where $f^{[\beta_j]} \geq 0$ is supposed to represent a heat source due to induction heating, i.e. condition 3.8.27(np) is always satisfied. However, investigating the regularity of $f^{[\beta_j]}$ according to the induction heating model is not in the scope of this work.

In the third case of Ex. 3.1.1(b), it is

$$f_j[(y,t,x)] = \varepsilon_{\mathbf{gas}}[(y,t,x)] \operatorname{div}(\rho_{\mathbf{gas}}[(t,x)]\mathbf{v}_{\mathbf{gas}}[(t,x)]) - p_{\mathbf{gas}}[(t,x)] \operatorname{div} \mathbf{v}_{\mathbf{gas}}[(t,x)],$$

i.e., assuming $\varepsilon_{\mathbf{gas}}[(0,t,x)] = 0$, 3.8.27(np) holds if and only if $p_{\mathbf{gas}}[(t,x)] \operatorname{div} \mathbf{v}_{\mathbf{gas}}[(t,x)] \leq 0$ for each (t,x). Moreover, f_j is (locally) Lipschitz in its y-dependence if and only if $\varepsilon_{\mathbf{gas}}$ is.

3.8.9 Statement and Proof of the Theorem

The central part of this section is the statement and the proof of Th. 3.8.35.

The hypotheses of Th. 3.8.35 need to include the hypotheses of Lems 3.8.10 – 3.8.12, 3.8.15, 3.8.16, 3.8.18, 3.8.19, 3.8.21, 3.8.23, and 3.8.27. This collection of lemmas is thus named for the convenience of subsequent reference:

Notation 3.8.29. Lemmas 3.8.10 – 3.8.12, 3.8.15, 3.8.16, 3.8.18, 3.8.19, 3.8.21, 3.8.23, and 3.8.27 are called *Decomposition Lemmas.*

The purpose of the following Defs 3.8.30 – 3.8.33 is the grouping of similar hypotheses of the Decomposition Lemmas. Definition 3.8.30 comprehends the hypotheses of type (inc), where certain functions are required to be increasing. Moreover, Def. 3.8.30(i) provides a growth property of the b_j also needed in the proof of Th. 3.8.35. Definition 3.8.31 comprehends the hypotheses of type (np), where certain functions are required to be nonpositive at $y = m_v$. Definition 3.8.32 comprehends the hypotheses of type (bnd), where dependency splittings are assumed to satisfy a boundedness condition at m_v. Finally, Def. 3.8.33 comprehends the hypotheses of type (locLip), where certain functions are required to be (uniformly) locally Lipschitz in their dependence on $y \in v$.

Definition 3.8.30. The evolution equation complex $\mathfrak{C}$ is called *increasing* iff $v = [m_v, \infty[$, each of the functions b_j, $a^{\gamma,\alpha}_{\text{flux}}$, and $a^{\gamma,\alpha}_{\text{jump}}$, is real-valued, and the following conditions (i) – (v) hold:

(i) There is $L_{\text{inv},b}[\mathfrak{C}] \in \mathbb{R}^+$ such that for each $j \in J$ and each $(t,x) \in \tau \times p_j$, the function $b_j \restriction_{v\times\{t\}\times\{x\}}$ is nonnegative, increasing, and inverse $L_{\text{inv},b}[\mathfrak{C}]$-Lipschitz. Moreover, each $b_j\restriction_{\{m_v\}\times\tau\times\{x\}}$ is decreasing (in $t \in \tau$).

(ii) There exists a family of scalar-vector-splittings $\mathfrak{V} = \big((v_{j,\text{sca}}, v_{j,\text{vec}})\big)_{j\in J}$ such that the function $v_{j,\text{sca}}\restriction_{v\times\{t\}\times\{x\}}$ is increasing for each $(t,x) \in \tau \times p_j$, $j \in J$. Then each such $\mathfrak{V}$ is called *inc-admissible.*

(iii) The functions $a^{\gamma,\alpha}_{\text{flux}}\restriction_{v\times\{t\}\times\{x\}}$ are increasing for each $\alpha \in \{1,2\}$, each $\gamma \in \text{IF}_{\text{con}}$, and each $(t,x) \in \tau \times \gamma$. Then the family of real-valued dependency splittings $\mathfrak{S}_{\text{con}} := \big((a^{\gamma,\alpha}_{\text{flux}})^{\text{ex.-im.}}\big)_{(\alpha,\gamma)\in\{1,2\}\times\text{IF}_{\text{con}}}$ is called *inc-admissible* iff $(a^{\gamma,\alpha}_{\text{flux}})^{\text{ex.-im.}}\restriction_{\{y\}\times v\times\{t\}\times\{x\}}$ are increasing for each $\alpha \in \{1,2\}$, each $\gamma \in \text{IF}_{\text{con}}$, each $y \in v$, and each $(t,x) \in \tau \times \gamma$.

(iv) The functions $a^{\gamma,\alpha}_{\text{jump}}\restriction_{v\times\{t\}\times\{x\}}$ are increasing for each $\alpha \in \{1,2\}$, each $\gamma \in \text{IF}_{\text{jump}}$, and each $(t,x) \in \tau \times \gamma$.

(v) The functions $a^{\gamma,\alpha}_{\text{flux}}\restriction_{v\times\{t\}\times\{x\}} + a^{\gamma,\alpha}_{\text{jump}}\restriction_{v\times\{t\}\times\{x\}}$ are increasing for each $\alpha \in \{1,2\}$, each $\gamma \in \text{IF}_{\text{jump}}$, and each $(t,x) \in \tau\times\gamma$. Then the family of real-valued dependency splittings $\mathfrak{S}_{\text{jump}} := \big((a^{\gamma,\alpha}_{\text{flux}})^{\text{ex.-im.}}\big)_{(\alpha,\gamma)\in\{1,2\}\times\text{IF}_{\text{jump}}}$ is called *inc-admissible* iff the functions $(a^{\gamma,\alpha}_{\text{flux}})^{\text{ex.-im.}}\restriction_{\{y\}\times v\times\{t\}\times\{x\}} + a^{\gamma,\alpha}_{\text{jump}}\restriction_{v\times\{t\}\times\{x\}}$ are increasing for each $\alpha \in \{1,2\}$, each $\gamma \in \text{IF}_{\text{jump}}$, each $y \in v$, and each $(t,x) \in \tau \times \gamma$.

The finite volume discretization $\mathfrak{F}$ of $\mathfrak{C}$ is called *increasing* iff $\mathfrak{C}$ is increasing, $\mathfrak{V}$, $\mathfrak{S}_{\text{con}}$, and $\mathfrak{S}_{\text{jump}}$ are inc-admissible.

Definition 3.8.31. The evolution equation complex $\mathfrak{C}$ is called *nonpositive at* $\mathbf{m} := (m_v, \dots, m_v)$ iff $v = [m_v, \infty[$, each of the functions $a^{j,\iota}_{\text{out}}$, $a^{\gamma,\alpha}_{\text{flux}}$, $a^{\gamma,\alpha}_{\text{jump}}$, and f_j is real-valued, and the following conditions (i) – (vi) hold:

(i) There exists a family of scalar-vector-splittings $\mathfrak{V} = \big((v_{j,\text{sca}}, v_{j,\text{vec}})\big)_{j\in J}$ such that $v_{j,\text{sca}}[(m_v,t,x)] = 0$ for each $(t,x) \in \tau \times p_j$, $j \in J$. Then each such $\mathfrak{V}$ is called *np-admissible.*

(ii) $a^{j,\iota}_{\text{out}}[(m_v, t, x)] \leq 0$ for each $(j, \iota) \in J \times (J_j \setminus \{0\})$ and each $(t, x) \in \tau \times \Gamma_{j,\iota}$. Then the family of real-valued dependency splittings $\mathfrak{S}_{\text{out}} = \left((a^{j,\iota}_{\text{out}})^{\text{ex.-im.}}\right)_{(j,\iota)\in J\times(J_j\setminus\{0\})}$ is called *np-admissible* iff

$$\bigwedge_{(j,\iota)\in J\times(J_j\setminus\{0\})} \ \bigwedge_{y\in v} \ \bigwedge_{(t,x)\in\tau\times\Gamma_{j,\iota}} (a^{j,\iota}_{\text{out}})^{\text{ex.-im.}}\left[\left((y, m_v), t, x\right)\right] \leq 0.$$

(iii) $\left(a^{\gamma,2}_{\text{flux}} - a^{\gamma,1}_{\text{flux}}\right)[(m_v, t, x)] \leq 0$ for each $\gamma \in \mathrm{IF}_{\text{con}}$ and each $(t, x) \in \tau \times \gamma$. Then the family of real-valued dependency splittings $\mathfrak{S}_{\text{con}} := \left((a^{\gamma,\alpha}_{\text{flux}})^{\text{ex.-im.}}\right)_{(\alpha,\gamma)\in\{1,2\}\times\mathrm{IF}_{\text{con}}}$ is called *np-admissible* iff

$$\bigwedge_{\gamma\in\mathrm{IF}_{\text{con}}} \ \bigwedge_{y\in v} \ \bigwedge_{(t,x)\in\tau\times\gamma} \left((a^{\gamma,2}_{\text{flux}})^{\text{ex.-im.}} - (a^{\gamma,1}_{\text{flux}})^{\text{ex.-im.}}\right)\left[\left((y, m_v), t, x\right)\right] \leq 0.$$

(iv) $\left(a^{\gamma,1}_{\text{jump}} - a^{\gamma,2}_{\text{jump}}\right)[(m_v, t, x)] \leq 0$ for each $\gamma \in \mathrm{IF}_{\text{jump}}$ and each $(t, x) \in \tau \times \gamma$.

(v) $\left(a^{\gamma,2}_{\text{flux}} - a^{\gamma,1}_{\text{flux}}\right)[(m_v, t, x)] + \left(a^{\gamma,2}_{\text{jump}} - a^{\gamma,1}_{\text{jump}}\right)[(m_v, t, x)] \leq 0$ for each $\gamma \in \mathrm{IF}_{\text{jump}}$ and each $(t, x) \in \tau \times \gamma$. Then the family of real-valued dependency splittings $\mathfrak{S}_{\text{jump}} := \left((a^{\gamma,\alpha}_{\text{flux}})^{\text{ex.-im.}}\right)_{(\alpha,\gamma)\in\{1,2\}\times\mathrm{IF}_{\text{jump}}}$ is called *np-admissible* iff

$$\bigwedge_{\gamma\in\mathrm{IF}_{\text{jump}}} \ \bigwedge_{y\in v} \ \bigwedge_{(t,x)\in\tau\times\gamma} \begin{pmatrix} \left((a^{\gamma,2}_{\text{flux}})^{\text{ex.-im.}} - (a^{\gamma,1}_{\text{flux}})^{\text{ex.-im.}}\right)\left[\left((y, m_v), t, x\right)\right] \\ + \left(a^{\gamma,2}_{\text{jump}} - a^{\gamma,1}_{\text{jump}}\right)[(m_v, t, x)] \leq 0 \end{pmatrix}.$$

(vi) $-f_j[(m_v, t, x)] \leq 0$ for each $j \in J$ and for each $(t, x) \in \tau \times p_j$.

The finite volume discretization $\mathfrak{F}$ of $\mathfrak{C}$ is called *nonpositive at* $\mathbf{m}$ iff $\mathfrak{C}$ is nonpositive at $\mathbf{m}$, and $\mathfrak{V}$, $\mathfrak{S}_{\text{out}}$, $\mathfrak{S}_{\text{con}}$, and $\mathfrak{S}_{\text{jump}}$ are np-admissible.

Definition 3.8.32. Supposed $v = [m_v, \infty[$. Consider the families of real-valued dependency splittings $\mathfrak{S}_{\text{out}} = \left((a^{j,\iota}_{\text{out}})^{\text{ex.-im.}}\right)_{(j,\iota)\in J\times(J_j\setminus\{0\})}$, $\mathfrak{S}_{\text{con}} := \left((a^{\gamma,\alpha}_{\text{flux}})^{\text{ex.-im.}}\right)_{(\alpha,\gamma)\in\{1,2\}\times\mathrm{IF}_{\text{con}}}$, and $\mathfrak{S}_{\text{jump}} := \left((a^{\gamma,\alpha}_{\text{flux}})^{\text{ex.-im.}}\right)_{(\alpha,\gamma)\in\{1,2\}\times\mathrm{IF}_{\text{jump}}}$.

(a) $\mathfrak{S}_{\text{out}}$ is called *bounded at* m_v iff $B_{\text{out},m_v}[(\mathfrak{C}, \mathfrak{S}_{\text{out}})] < \infty$, where $B_{\text{out},m_v}[(\mathfrak{C}, \mathfrak{S}_{\text{out}})]$ is the number defined in (3.8.34).

(b) $\mathfrak{S}_{\text{con}}$ is called *bounded at* m_v iff $B_{\text{con},1,m_v}[(\mathfrak{C}, \mathfrak{S}_{\text{con}})] < \infty$ and $B_{\text{con},2,m_v}[(\mathfrak{C}, \mathfrak{S}_{\text{con}})] < \infty$, where $B_{\text{con},1,m_v}[(\mathfrak{C}, \mathfrak{S}_{\text{con}})]$ and $B_{\text{con},2,m_v}[(\mathfrak{C}, \mathfrak{S}_{\text{con}})]$ are the numbers defined in (3.8.38).

(c) $\mathfrak{S}_{\text{jump}}$ is called *bounded at* m_v iff $B_{\text{flux,jump},1,m_v}[(\mathfrak{C}, \mathfrak{S}_{\text{jump}})] < \infty$ and

$$B_{\text{flux,jump},2,m_v}[(\mathfrak{C}, \mathfrak{S}_{\text{jump}})] < \infty,$$

where $B_{\text{flux,jump},1,m_v}[(\mathfrak{C}, \mathfrak{S}_{\text{jump}})]$ and $B_{\text{flux,jump},2,m_v}[(\mathfrak{C}, \mathfrak{S}_{\text{jump}})]$ are the numbers defined in (3.8.43).

Definition 3.8.33. The evolution equation complex $\mathfrak{C}$ is called *locally Lipschitz* iff $\upsilon = [m_\upsilon, \infty[$, each of the functions k_j, $a^{j,\iota}_{\text{out}}$, $a^{j,\iota}_{\text{out}}$, $a^{\gamma,1}_{\text{flux}}$, $a^{\gamma,2}_{\text{jump}}$, and f_j is real-valued, and the following conditions (i) – (vii) hold:

(i) There exists a family of scalar-vector-splittings $\mathfrak{V} = \big((v_{j,\text{sca}}, v_{j,\text{vec}})\big)_{j\in J}$ such that

$$\bigwedge_{r\in\mathbb{R}^+_0} \; \bigvee_{L_{\upsilon,\text{sca},r}[(\mathfrak{C},\mathfrak{V})]\in\mathbb{R}^+_0} \; \bigwedge_{(j,t,x)\in J\times\tau\times p_j} v_{j,\text{sca}}\restriction_{\upsilon\times\{t\}\times\{x\}} \in \operatorname{Lip}_{L_{\upsilon,\text{sca},r}[(\mathfrak{C},\mathfrak{V})]}\big([m_\upsilon, m_\upsilon + r], \mathbb{R}\big),$$

i.e. each $v_{j,\text{sca}}$ is locally Lipschitz with respect to its dependence on $y \in \upsilon$. Then each such $\mathfrak{V}$ is called *locLip-admissible.*

(ii) $\bigwedge_{r\in\mathbb{R}^+_0} \bigvee_{L_{k,r}[\mathfrak{C}]\in\mathbb{R}^+_0} \bigwedge_{(j,t,x)\in J\times\tau\times p_j} k_j\restriction_{\upsilon\times\{t\}\times\{x\}} \in \operatorname{Lip}_{L_{k,r}[\mathfrak{C}]}\big([m_\upsilon, m_\upsilon + r], \mathbb{R}\big)$, i.e. each k_j is locally Lipschitz with respect to its dependence on $y \in \upsilon$.

(iii) Each $a^{j,\iota}_{\text{out}}$ is locally Lipschitz with respect to its y-dependence, i.e.

$$\bigwedge_{r\in\mathbb{R}^+_0} \; \bigvee_{L_{\text{out},r}[\mathfrak{C}]\in\mathbb{R}^+_0} \; \bigwedge_{\substack{(j,\iota,t,x)\\ \in J\times(J_j\setminus\{0\})\times\tau\times\Gamma_{j,\iota}}} a^{j,\iota}_{\text{out}}\restriction_{\upsilon\times\{t\}\times\{x\}} \in \operatorname{Lip}_{L_{\text{out},r}[\mathfrak{C}]}\big([m_\upsilon, m_\upsilon + r], \mathbb{R}\big).$$

Then the family of real-valued dependency splittings

$$\mathfrak{S}_{\text{out}} = \Big(\big(a^{j,\iota}_{\text{out}}\big)^{\text{ex.-im.}}\Big)_{(j,\iota)\in J\times(J_j\setminus\{0\})}$$

is called *locLip-admissible* iff each $\big(a^{j,\iota}_{\text{out}}\big)^{\text{ex.-im.}}$ is locally Lipschitz with respect to its dependence on the second argument, i.e.

$$\bigwedge_{r\in\mathbb{R}^+_0} \; \bigvee_{L_{\text{out},r}[(\mathfrak{C},\mathfrak{S}_{\text{out}})]\in\mathbb{R}^+_0} \; \bigwedge_{\substack{(j,\iota,y,t,x)\\ \in J\times(J_j\setminus\{0\})\times\upsilon\times\tau\times\Gamma_{j,\iota}}} \begin{pmatrix} \big(a^{j,\iota}_{\text{out}}\big)^{\text{ex.-im.}}\restriction_{\{y\}\times\upsilon\times\{t\}\times\{x\}} \\ \in \operatorname{Lip}_{L_{\text{out},r}[(\mathfrak{C},\mathfrak{S}_{\text{out}})]}\big([m_\upsilon, m_\upsilon + r], \mathbb{R}\big) \end{pmatrix}.$$

(iv) Each $a^{\gamma,1}_{\text{flux}}$ is locally Lipschitz with respect to its y-dependence, i.e.

$$\bigwedge_{r\in\mathbb{R}^+_0} \; \bigvee_{L_{\text{flux},1,r}[\mathfrak{C}]\in\mathbb{R}^+_0} \; \bigwedge_{\substack{(\gamma,t,x)\\ \in\mathrm{IF}_{\text{con}}\times\tau\times\gamma}} \begin{pmatrix} a^{\gamma,1}_{\text{flux}}\restriction_{\upsilon\times\{t\}\times\{x\}} \\ \in \operatorname{Lip}_{L_{\text{flux},1,r}[\mathfrak{C}]}\big([m_\upsilon, m_\upsilon + r], \mathbb{R}\big) \end{pmatrix}.$$

Then the family of real-valued dependency splittings

$$\mathfrak{S}_{\text{con}} := \Big(\big(a^{\gamma,\alpha}_{\text{flux}}\big)^{\text{ex.-im.}}\Big)_{(\alpha,\gamma)\in\{1,2\}\times\mathrm{IF}_{\text{con}}}$$

is called *locLip-admissible* iff each $\big(a^{\gamma,1}_{\text{flux}}\big)^{\text{ex.-im.}}$ is locally Lipschitz with respect to its dependence on the second argument, i.e.

$$\bigwedge_{r\in\mathbb{R}^+_0} \; \bigvee_{L_{\text{flux},1,r}[(\mathfrak{C},\mathfrak{S}_{\text{con}})]\in\mathbb{R}^+_0} \; \bigwedge_{\substack{(\gamma,y,t,x)\\ \in\mathrm{IF}_{\text{con}}\times\upsilon\times\tau\times\gamma}} \begin{pmatrix} \big(a^{\gamma,1}_{\text{flux}}\big)^{\text{ex.-im.}}\restriction_{\{y\}\times\upsilon\times\{t\}\times\{x\}} \\ \in \operatorname{Lip}_{L_{\text{flux},1,r}[(\mathfrak{C},\mathfrak{S}_{\text{con}})]}\big([m_\upsilon, m_\upsilon + r], \mathbb{R}\big) \end{pmatrix}.$$

(v) $\bigwedge_{r\in\mathbb{R}_0^+} \bigvee_{L_{\text{jump},2,r}[\mathfrak{C}]\in\mathbb{R}_0^+} \bigwedge_{\substack{(\gamma,t,x)\\ \in\text{IF}_{\text{jump}}\times\tau\times\gamma}} a_{\text{jump}}^{\gamma,2}\restriction_{v\times\{t\}\times\{x\}}\in \operatorname{Lip}_{L_{\text{jump},2,r}[\mathfrak{C}]}\big([m_v, m_v + r],\mathbb{R}\big)$, i.e. each $a_{\text{jump}}^{\gamma,2}$ is locally Lipschitz with respect to its y-dependence.

(vi) Each $a_{\text{flux}}^{\gamma,1}\restriction_{v\times\{t\}\times\{x\}} + a_{\text{jump}}^{\gamma,1}\restriction_{v\times\{t\}\times\{x\}}$ is locally Lipschitz with respect to its y-dependence, i.e.

$$\bigwedge_{r\in\mathbb{R}_0^+} \bigvee_{L_{\text{flux,jump},r}[\mathfrak{C}]\in\mathbb{R}_0^+} \bigwedge_{\substack{(\gamma,t,x)\\ \in\text{IF}_{\text{jump}}\times\tau\times\gamma}} \begin{pmatrix} \big(a_{\text{flux}}^{\gamma,1} + a_{\text{jump}}^{\gamma,1}\big)\restriction_{v\times\{t\}\times\{x\}} \\ \in \operatorname{Lip}_{L_{\text{flux,jump},r}[\mathfrak{C}]}\big([m_v, m_v + r],\mathbb{R}\big)\end{pmatrix}.$$

Then the family of real-valued dependency splittings

$$\mathfrak{S}_{\text{jump}} := \Big(\big(a_{\text{flux}}^{\gamma,\alpha}\big)^{\text{ex.-im.}}\Big)_{(\alpha,\gamma)\in\{1,2\}\times\text{IF}_{\text{jump}}}$$

is called *locLip-admissible* iff

$$\bigwedge_{r\in\mathbb{R}_0^+} \bigvee_{L_{\text{flux,jump},r}[(\mathfrak{C},\mathfrak{S}_{\text{jump}})]\in\mathbb{R}_0^+} \bigwedge_{\substack{(\gamma,y,t,x)\\ \in\text{IF}_{\text{jump}}\times v\times\tau\times\gamma}} \begin{pmatrix} \big(a_{\text{flux}}^{\gamma,1}\big)^{\text{ex.-im.}}\restriction_{\{y\}\times v\times\{t\}\times\{x\}} + a_{\text{jump}}^{\gamma,1}\restriction_{v\times\{t\}\times\{x\}} \\ \in \operatorname{Lip}_{L_{\text{flux,jump},r}[(\mathfrak{C},\mathfrak{S}_{\text{jump}})]}\big([m_v, m_v + r],\mathbb{R}\big)\end{pmatrix}.$$

(vii) $\bigwedge_{r\in\mathbb{R}_0^+} \bigvee_{L_{f,r}[\mathfrak{C}]\in\mathbb{R}_0^+} \bigwedge_{(j,t,x)\in J\times\tau\times p_j} f_j\restriction_{v\times\{t\}\times\{x\}}\in \operatorname{Lip}_{L_{f,r}[\mathfrak{C}]}\big([m_v, m_v + r],\mathbb{R}\big)$, i.e. each f_j is locally Lipschitz with respect to its dependence on $y \in v$.

The finite volume discretization $\mathfrak{F}$ of $\mathfrak{C}$ is called *locally Lipschitz* iff $\mathfrak{C}$ is locally Lipschitz and $\mathfrak{V}$, $\mathfrak{S}_{\text{out}}$, $\mathfrak{S}_{\text{con}}$, and $\mathfrak{S}_{\text{jump}}$ are locLip-admissible.

Remark 3.8.34. If $\mathfrak{F}$ is increasing, nonpositive at $\mathbf{m}$, and locally Lipschitz; and if $\mathfrak{S}_{\text{out}}$, $\mathfrak{S}_{\text{con}}$, and $\mathfrak{S}_{\text{jump}}$ are bounded at m_v, then all the hypotheses of the Decomposition Lemmas are satisfied with the possible exception of Lem. 3.8.10(nn). However, Lem. 3.8.10(nn) is also satisfied if $\mathfrak{F}$ is bounded from above (s. Def. 3.7.43(ii)).

—

If the hypotheses (i) – (iv) of the following Th. 3.8.35 are satisfied, then for each sufficiently large $M \in]m_v,\infty[$, the finite volume discretization $\mathfrak{F}$ has a unique solution in $\big([m_v, M]^{I_{\Pi,\mathfrak{D}}}\big)^{\{0,\dots,n\}}$ (cf. Def. 3.7.42), provided that the fineness Δ of the time discretization is sufficiently small, where, in general, Δ needs to be chosen smaller if M is chosen larger. The precise statement reads as follows:

Theorem 3.8.35. *Let $\mathfrak{F}$ be a finite volume discretization of the evolution equation complex $\mathfrak{C}$ according to Def.* 3.7.41, *$v = [m_v,\infty[$, $\mathbf{m} := (m_v,\dots,m_v)$.*

Assume conditions (i) – (iv) *below. Let* $B^{\downarrow,\uparrow}[(\mathfrak{C},\Pi,\mathfrak{V},\mathfrak{S}_{\text{out}},\mathfrak{S}_{\text{con}},\mathfrak{S}_{\text{jump}})]$, $L_{\text{inv},b}[\mathfrak{C}]$, $\lambda_{d,\min}[\Pi]$, *and* $B_{\text{Dir}}[\mathfrak{C}]$ *be the values defined in* (3.8.58), *Def.* 3.8.30(i), (3.8.55), *and* (3.7.27), *respectively. Then for each* $M \in]m_v,\infty[$ *satisfying*

$$M > S := \frac{B^{\downarrow,\uparrow}[(\mathfrak{C},\Pi,\mathfrak{V},\mathfrak{S}_{\text{out}},\mathfrak{S}_{\text{con}},\mathfrak{S}_{\text{jump}})]}{L_{\text{inv},b}[\mathfrak{C}]\cdot\lambda_{d,\min}[\Pi]} + m_v, \tag{3.8.49a}$$

$$M \geq \max\Big\{B_{\text{Dir}}[\mathfrak{C}],\, \max\big\{\|u_j^{(0)}\|_{\max} :\, j\in J\big\}\Big\}, \tag{3.8.49b}$$

$\mathfrak{F}$ *has a unique solution*

$$\big(U^{(\nu)}\big)_{\nu\in\{0,\dots,n\}} = (u^{(\nu)}_{(k,\mathcal{C})})_{(\nu,(k,\mathcal{C}))\in\{0,\dots,n\}\times I_{\Pi,\mathfrak{D}}} \in \big([m_v,M]^{I_{\Pi,\mathfrak{D}}}\big)^{\{0,\dots,n\}},$$

provided that

$$\Delta\cdot L_{M-m_v}[(\mathfrak{C},\Pi,\mathfrak{V},\mathfrak{S}_{\text{out}},\mathfrak{S}_{\text{con}},\mathfrak{S}_{\text{jump}})] < \big(L_{\text{inv},b}[\mathfrak{C}]\cdot\lambda_{d,\min}[\Pi]\big)\cdot\frac{M-S}{M-m_v}, \tag{3.8.49c}$$

$$\Delta \leq 1, \tag{3.8.49d}$$

where the number $L_{M-m_v}[(\mathfrak{C},\Pi,\mathfrak{V},\mathfrak{S}_{\text{out}},\mathfrak{S}_{\text{con}},\mathfrak{S}_{\text{jump}})]$ *is according to the definition in* (3.8.54) *below.*

(i) $\mathfrak{F}$ *is bounded from above.*

(ii) $\mathfrak{F}$ *is increasing, nonpositive at* $\mathbf{m}$, *and locally Lipschitz.*

(iii) *The families of dependency splittings* $\mathfrak{S}_{\text{out}}$, $\mathfrak{S}_{\text{con}}$, *and* $\mathfrak{S}_{\text{jump}}$ *are bounded at* m_v.

(iv) $\mathfrak{F}$ *is such that the discretized nonlocal operators* $\mathfrak{B}^{(\nu)}_{(k,\mathcal{C})}$, $\mathfrak{A}^{(\nu)}_{\text{con},(k,\mathcal{C})}$, *and* $\mathfrak{A}^{(\nu)}_{\text{jump},(k,\mathcal{C})}$ *have the* $\downarrow$*-property.*

Proof. If $(k,\mathcal{C})\in I_{\Pi,\mathfrak{D},\text{Dir}}$, then for each $\nu\in\{0,\dots,n\}$, $u^{(\nu)}_{(k,\mathcal{C})}$ is uniquely defined by Def. 3.7.42(ii), where $u^{(\nu)}_{(k,\mathcal{C})}$ is well-defined, since it is required in Def. 3.4.6(ii) that different Dirichlet functions must agree on common continuous interfaces.

For non-Dirichlet indices, the solution $(u^{(\nu)})_{\nu\in\{0,\dots,n\}}\in(v^{I_{\Pi\mathfrak{D},\neg\text{Dir}}})^{\{0,\dots,n\}}$ is constructed by induction on ν.

For $\nu=0$, the solution is uniquely defined by Def. 3.7.42(i), i.e. $u^{(0)}_{(k,\mathcal{C})} := u^{(0)}_j[x_k]$, picking any $j\in V[\mathcal{C}]$. This is well-defined by Def. 3.4.6(i),(iii).

Now assume $\nu>0$. By induction, there is a unique

$$(u^{(\tilde\nu)})_{\tilde\nu\in\{0,\dots,\nu-1\}}\in\big([m_v,M]^{I_{\Pi,\mathfrak{D},\neg\text{Dir}}}\big)^{\{0,\dots,\nu-1\}},$$

satisfying Def. 3.7.42(iii) for each $\tilde\nu\in\{1,\dots,\nu-1\}$. One needs to show that there is a unique $u^{(\nu)}\in[m_v,M]^{I_{\Pi,\mathfrak{D},\neg\text{Dir}}}$ such that Def. 3.7.42(iii) holds for ν.

Define

$$\bigwedge_{(k,\mathcal{C})\in I_{\Pi,\mathfrak{D},\neg\mathrm{Dir}}} \mathcal{H}^{(\nu)}_{(k,\mathcal{C})} : v^{I_{\Pi,\mathfrak{D},\neg\mathrm{Dir}}} \longrightarrow \mathbb{R}, \quad \mathcal{H}^{(\nu)}_{(k,\mathcal{C})}[u] := \mathfrak{h}^{(\nu)}_{(k,\mathcal{C})}\left[\left(u^{(\nu-1)}, u\right)\right]. \tag{3.8.50}$$

Theorem 3.8.4 is applied to prove the existence and uniqueness of $u^{(\nu)} \in [m_v, M]^{I_{\Pi,\mathfrak{D},\neg\mathrm{Dir}}}$ satisfying Def. 3.7.42(iii). The strategy is to find continuous functions $h^{(\nu)}_{(k,\mathcal{C})}$, $g^{(\nu)}_{(k,\mathcal{C})}$, $\tilde{g}^{(\nu)}_{(k,\mathcal{C})}$, $b^{(\nu)}_{(k,\mathcal{C})}$, $\tilde{h}^{(\nu)}_{(k,\mathcal{C})}$, and numbers $P^{(\nu)}_{(k,\mathcal{C})}$ and Δ_ν such that for each $(k,\mathcal{C}) \in I_{\Pi,\mathfrak{D},\neg\mathrm{Dir}}$:

$$\bigwedge_{u\in v^{I_{\Pi,\mathfrak{D},\neg\mathrm{Dir}}}} \mathcal{H}^{(\nu)}_{(k,\mathcal{C})}[u] = h^{(\nu)}_{(k,\mathcal{C})}[u_{(k,\mathcal{C})}] - g^{(\nu)}_{(k,\mathcal{C})}[u], \tag{3.8.51a}$$

$$g^{(\nu)}_{(k,\mathcal{C})} = \frac{P^{(\nu)}_{(k,\mathcal{C})}}{\Delta_\nu} + \tilde{g}^{(\nu)}_{(k,\mathcal{C})}, \tag{3.8.51b}$$

$$h^{(\nu)}_{(k,\mathcal{C})} = \frac{b^{(\nu)}_{(k,\mathcal{C})}}{\Delta_\nu} + \tilde{h}^{(\nu)}_{(k,\mathcal{C})}, \tag{3.8.51c}$$

and such that the hypotheses of Lem. 3.8.5 are satisfied. To that end, the decompositions of the discretization operators provided in Secs 3.8.3 – 3.8.8 are used to define for each $(k,\mathcal{C}) \in I_{\Pi,\mathfrak{D},\neg\mathrm{Dir}}$:

$$\begin{aligned}
&\tilde{h}^{(\nu)}_{(k,\mathcal{C})} : v \longrightarrow \mathbb{R},\\
&\tilde{h}^{(\nu)}_{(k,\mathcal{C})} := \mathfrak{v}^{\nu,\uparrow}_{\mathrm{int},\neg\mathrm{Dir},(k,\mathcal{C})} + \mathfrak{v}^{(\nu)}_{\mathrm{int},\mathrm{Dir},(k,\mathcal{C})} + \mathfrak{v}^{\nu,\uparrow}_{\mathrm{out},(k,\mathcal{C})} + \mathfrak{v}^{\nu,\uparrow}_{\mathrm{IF},(k,\mathcal{C})} + \mathfrak{k}^{\nu,\uparrow}_{\neg\mathrm{Dir},(k,\mathcal{C})} + \mathfrak{k}^{\nu,\uparrow}_{\mathrm{Dir},(k,\mathcal{C})}\\
&\qquad + \mathfrak{a}^{\nu,\uparrow}_{\mathrm{out},(k,\mathcal{C})}{\restriction}_{\{u^{(\nu-1)}_{(k,\mathcal{C})}\}\times v} + \mathfrak{a}^{\nu,\uparrow}_{\mathrm{flux,con},(k,\mathcal{C})}{\restriction}_{\{u^{(\nu-1)}_{(k,\mathcal{C})}\}\times v} + \mathfrak{a}^{\nu,\uparrow}_{\mathrm{jump},1,\neg\mathrm{Dir},(k,\mathcal{C})} + \mathfrak{a}^{(\nu)}_{\mathrm{jump},1,\mathrm{Dir},(k,\mathcal{C})}\\
&\qquad + \mathfrak{a}^{\nu,\uparrow}_{\mathrm{jump},2,\neg\mathrm{Dir},(k,\mathcal{C})}{\restriction}_{\{u^{(\nu-1)}_{(k,\mathcal{C})}\}\times v} + \mathfrak{a}^{(\nu)}_{\mathrm{jump},2,\mathrm{Dir},(k,\mathcal{C})}{\restriction}_{\{u^{(\nu-1)}_{(k,\mathcal{C})}\}\times v} + \mathfrak{f}^{\nu,\uparrow}_{(k,\mathcal{C})},
\end{aligned} \tag{3.8.52a}$$

$$\begin{aligned}
&\tilde{g}^{(\nu)}_{(k,\mathcal{C})} : v^{I_{\Pi,\mathfrak{D},\neg\mathrm{Dir}}} \longrightarrow \mathbb{R},\\
&\tilde{g}^{(\nu)}_{(k,\mathcal{C})}[u] := \mathfrak{v}^{\nu,\downarrow}_{\mathrm{int},\neg\mathrm{Dir},(k,\mathcal{C})}[u] + \mathfrak{v}^{\nu,\downarrow}_{\mathrm{out},(k,\mathcal{C})}[u_{(k,\mathcal{C})}] + \mathfrak{v}^{\nu,\downarrow}_{\mathrm{IF},(k,\mathcal{C})}[u_{(k,\mathcal{C})}] + \mathfrak{k}^{\nu,\downarrow}_{\neg\mathrm{Dir},(k,\mathcal{C})}[u] + \mathfrak{k}^{\nu,\downarrow}_{\mathrm{Dir},(k,\mathcal{C})}[u]\\
&\qquad + \mathfrak{B}^{(\nu)}_{(k,\mathcal{C})}[(u^{(\nu-1)}, u)] + \mathfrak{a}^{\nu,\downarrow}_{\mathrm{out},(k,\mathcal{C})}[(u^{(\nu-1)}_{(k,\mathcal{C})}, u_{(k,\mathcal{C})})] + \mathfrak{A}^{(\nu)}_{\mathrm{con},(k,\mathcal{C})}[(u^{(\nu-1)}, u)]\\
&\qquad + \mathfrak{a}^{\nu,\downarrow}_{\mathrm{flux,con},(k,\mathcal{C})}[(u^{(\nu-1)}_{(k,\mathcal{C})}, u_{(k,\mathcal{C})})] + \mathfrak{a}^{\nu,\downarrow}_{\mathrm{jump},1,\neg\mathrm{Dir},(k,\mathcal{C})}[u] + \mathfrak{A}^{(\nu)}_{\mathrm{jump},(k,\mathcal{C})}[(u^{(\nu-1)}, u)]\\
&\qquad + \mathfrak{a}^{\nu,\downarrow}_{\mathrm{jump},2,\neg\mathrm{Dir},(k,\mathcal{C})}[(u^{(\nu-1)}, u)] + \mathfrak{f}^{\nu,\downarrow}_{(k,\mathcal{C})}[u_{(k,\mathcal{C})}].
\end{aligned} \tag{3.8.52b}$$

Moreover, let

$$P^{(\nu)}_{(k,\mathcal{C})} := \mathfrak{b}^{(\nu-1)}_{(k,\mathcal{C})}\left[u^{(\nu-1)}_{(k,\mathcal{C})}\right], \tag{3.8.52c}$$

$$\Delta_\nu := t_\nu - t_{\nu-1}, \tag{3.8.52d}$$

$$b^{(\nu)}_{(k,\mathcal{C})} : \upsilon \longrightarrow \mathbb{R}^+_0, \qquad b^{(\nu)}_{(k,\mathcal{C})} := \mathfrak{b}^{(\nu)}_{(k,\mathcal{C})}, \tag{3.8.52e}$$

$$h^{(\nu)}_{(k,\mathcal{C})} : \upsilon \longrightarrow \mathbb{R}, \qquad h^{(\nu)}_{(k,\mathcal{C})}[y] := \frac{b^{(\nu)}_{(k,\mathcal{C})}[y]}{\Delta_\nu} + \tilde{h}^{(\nu)}_{(k,\mathcal{C})}[y], \tag{3.8.52f}$$

$$g^{(\nu)}_{(k,\mathcal{C})} : \upsilon^{I_{\Pi,\mathfrak{D},\neg\mathrm{Dir}}} \longrightarrow \mathbb{R}, \qquad g^{(\nu)}_{(k,\mathcal{C})}[u] := \frac{P^{(\nu)}_{(k,\mathcal{C})}}{\Delta_\nu} + \tilde{g}^{(\nu)}_{(k,\mathcal{C})}[u]. \tag{3.8.52g}$$

It remains to verify (3.8.51a) and the hypotheses of Lem. 3.8.5, which is done in the following. The conclusions of the Decomposition Lemmas (s. Def. 3.8.29) are used below, where hypotheses (i), (ii), and (iii) of Th. 3.8.35 ensure that the hypotheses of the Decomposition Lemmas are satisfied (s. Rem. 3.8.34).

(3.8.51a): To show $\mathfrak{h}^{(\nu)}_{(k,\mathcal{C})}\left[\left(u^{(\nu-1)}, u\right)\right] = h^{(\nu)}_{(k,\mathcal{C})}[u_{(k,\mathcal{C})}] - g^{(\nu)}_{(k,\mathcal{C})}[u]$, observe

$$\frac{b^{(\nu)}_{(k,\mathcal{C})}[u_{(k,\mathcal{C})}] - P^{(\nu)}_{(k,\mathcal{C})}}{\Delta_\nu} = \mathfrak{h}^{(\nu)}_{(k,\mathcal{C}),(a)}\left[\left(u^{(\nu-1)}, u\right)\right]$$

by (3.7.9), and

$$\tilde{h}^{(\nu)}_{(k,\mathcal{C})}[u_{(k,\mathcal{C})}] - \tilde{g}^{(\nu)}_{(k,\mathcal{C})}[u] = \mathfrak{h}^{(\nu)}_{(k,\mathcal{C}),(b)}\left[\left(u^{(\nu-1)}, u\right)\right] + \cdots + \mathfrak{h}^{(\nu)}_{(k,\mathcal{C}),(n)}[u], \tag{3.8.53}$$

where (3.8.53) is precisely what was proved in parts (a) of the Decomposition Lemmas (s. Def. 3.8.29).

It is $\Delta_\nu \in \mathbb{R}^+$, since the sequence $(t_\nu)_{\nu\in\{0,\dots,n\}}$ is strictly increasing. The definition of $\mathfrak{b}^{(\nu)}_{(k,\mathcal{C})}$ in (3.7.10) shows that $P^{(\nu)}_{(k,\mathcal{C})} \in \mathbb{R}^+_0$ and that $b^{(\nu)}_{(k,\mathcal{C})}$ is nonnegative, since the b_j are nonnegative by hypothesis (ii).

That the $h^{(\nu)}_{(k,\mathcal{C})}$ and $g^{(\nu)}_{(k,\mathcal{C})}$ have the forms required in Lem. 3.8.5(i),(ii) is ensured by the definitions in (3.8.52f) and (3.8.52g), respectively.

Lem. 3.8.5(iii): The $b^{(\nu)}_{(k,\mathcal{C})}$ are increasing using (3.7.10) and that the maps $b_j\restriction_{\upsilon\times\{t\}\times\{x\}}$, $(t,x) \in \tau \times p_j$, are increasing by hypothesis (ii). The $\tilde{h}^{(\nu)}_{(k,\mathcal{C})}$ are increasing, since all its summands according to (3.8.52a) are increasing, as was proved in parts (b) of the Decomposition Lemmas (s. Def. 3.8.29).

Lem. 3.8.5(iv): The $\tilde{g}^{(\nu)}_{(k,\mathcal{C})}$ are minimal at $\mathbf{m}$, since all its summands according to (3.8.52b) are minimal at $\mathbf{m}$, as is granted by hypothesis (iv) for $\mathfrak{B}^{(\nu)}_{(k,\mathcal{C})}$, $\mathfrak{A}^{(\nu)}_{\mathrm{con},(k,\mathcal{C})}$, and $\mathfrak{A}^{(\nu)}_{\mathrm{jump},(k,\mathcal{C})}$ (cf. Def. 3.8.25(i)), and was proved in parts (c) of the Decomposition Lemmas (s. Def. 3.8.29) for all other summands.

Lem. 3.8.5(v): It suffices to show $b^{(\nu)}_{(k,\mathcal{C})}[m_\upsilon] \le P^{(\nu)}_{(k,\mathcal{C})}$ and $\tilde{h}^{(\nu)}_{(k,\mathcal{C})}[m_\upsilon] \le \tilde{g}^{(\nu)}_{(k,\mathcal{C})}[\mathbf{m}]$. It is

$$b^{(\nu)}_{(k,\mathcal{C})}[m_\upsilon] = \mathfrak{b}^{(\nu)}_{(k,\mathcal{C})}[m_\upsilon] \le \mathfrak{b}^{(\nu-1)}_{(k,\mathcal{C})}[m_\upsilon] \le \mathfrak{b}^{(\nu-1)}_{(k,\mathcal{C})}\left[u^{(\nu-1)}_{(k,\mathcal{C})}\right] = P^{(\nu)}_{(k,\mathcal{C})},$$

since the $b_j \restriction_{\{m_v\}\times\tau\times\{x\}}$, $x \in p_j$, are decreasing by hypothesis (ii), $m_v \le u^{(\nu-1)}_{(k,\mathcal{C})}$, and the $b_j \restriction_{v\times\{t\}\times\{x\}}$, $(t,x) \in \tau \times p_j$, are increasing by hypothesis (ii). The remaining estimate $\tilde{h}^{(\nu)}_{(k,\mathcal{C})}[m_v] \le \tilde{g}^{(\nu)}_{(k,\mathcal{C})}[\mathbf{m}]$ follows by summing the statements in parts (d) of the Decomposition Lemmas (s. Def. 3.8.29) and combining the result with Def. 3.8.25(ii).

Lem. 3.8.5(vi): Each $\tilde{g}^{(\nu)}_{(k,\mathcal{C})}$ is $L_r[(\mathfrak{C}, \Pi, \mathfrak{V}, \mathfrak{S}_{\text{out}}, \mathfrak{S}_{\text{con}}, \mathfrak{S}_{\text{jump}})]$-Lipschitz on $[m_v, m_v + r]^{I_{\Pi,\mathfrak{D},\neg\text{Dir}}}$ for each $r \in \mathbb{R}^+$ and independently of $(k,\mathcal{C}) \in I_{\Pi,\mathfrak{D},\neg\text{Dir}}$ and $\nu \in \{0,\dots,n\}$, where

$$\begin{aligned}
&L_r[(\mathfrak{C}, \Pi, \mathfrak{V}, \mathfrak{S}_{\text{out}}, \mathfrak{S}_{\text{con}}, \mathfrak{S}_{\text{jump}})] \\
&:= 3 \cdot L_{\text{nonloc},r}[(\mathfrak{C},\Pi)] + \left(L^{\downarrow}_{k,r}[\mathfrak{C}] + L_{\text{Dir},k,r}[\mathfrak{C}]\right) \cdot d_{\max}[\Pi] + L_{f,r}[\mathfrak{C}] \cdot \lambda_{d,\max}[\Pi] \\
&\quad + \Big(3 \cdot L_{v,r}[(\mathfrak{C},\mathfrak{V})] + L_{\text{out},r}[(\mathfrak{C},\mathfrak{S}_{\text{out}})] + L_{\text{flux},1,r}[(\mathfrak{C},\mathfrak{S}_{\text{con}})] \\
&\qquad + L_{\text{jump},2,r}[\mathfrak{C}] + L_{\text{flux,jump},r}[(\mathfrak{C},\mathfrak{S}_{\text{jump}})]\Big) \cdot \lambda_{d-1,\max}[\Pi] : \qquad (3.8.54)
\end{aligned}$$

The Lipschitz constants for the summands of $\tilde{g}^{(\nu)}_{(k,\mathcal{C})}$ according to (3.8.52b) are given by Def. 3.8.25(iv) for $\mathfrak{B}^{(\nu)}_{(k,\mathcal{C})}$, $\mathfrak{A}^{(\nu)}_{\text{con},(k,\mathcal{C})}$, and $\mathfrak{A}^{(\nu)}_{\text{jump},(k,\mathcal{C})}$, and were already proved in parts (f) of the Decomposition Lemmas (s. Def. 3.8.29) for the remaining summands. Then the Lipschitz constant of $\tilde{g}^{(\nu)}_{(k,\mathcal{C})}$ is given by the sum of the Lipschitz constants of its summands (s. Rem. C.7.7(d)).

Lem. 3.8.5(vii): It follows from (3.7.10), hypothesis (ii), and 3.8.30(i) that each $b^{(\nu)}_{(k,\mathcal{C})}$, $(k,\mathcal{C}) \in I_{\Pi,\mathfrak{D},\neg\text{Dir}}$, is inverse $(L_{\text{inv},b}[\mathfrak{C}] \cdot \lambda_{d,\min}[\Pi])$-Lipschitz, where

$$\lambda_{d,\min}[\Pi] := \min\left\{\lambda_d[\omega^{(j)}_k] : (k,j) \in I_\Pi \times J\right\}. \qquad (3.8.55)$$

It is noted that $\lambda_{d,\min}[\Pi] > 0$, since each $\omega^{(j)}_k$ is a d-polytope (s. Sec. 3.5.3).

Corresponding to (3.8.11), let

$$S^{(\nu)}_{(k,\mathcal{C})} := \frac{P^{(\nu)}_{(k,\mathcal{C})} + \max\left\{0, \tilde{g}^{(\nu)}_{(k,\mathcal{C})}[\mathbf{m}]\right\} - \min\left\{0, \tilde{h}^{(\nu)}_{(k,\mathcal{C})}[m]\right\}}{L_{\text{inv},b}[\mathfrak{C}] \cdot \lambda_{d,\min}[\Pi]} + m_v, \qquad (3.8.56a)$$

$$S^{(\nu)} := \max\left\{S^{(\nu)}_{(k,\mathcal{C})} : (k,\mathcal{C}) \in I_{\Pi,\mathfrak{D},\neg\text{Dir}}\right\}. \qquad (3.8.56b)$$

The following Cl. 1 shows that the numbers $S^{(\nu)}$ can be bounded independently of $\nu \in \{0,\dots,n\}$, i.e. independently of the time discretization.

Claim 1. It holds true that

$$S^{(\nu)} \le S = \frac{B^{\downarrow,\uparrow}[(\mathfrak{C}, \Pi, \mathfrak{V}, \mathfrak{S}_{\text{out}}, \mathfrak{S}_{\text{con}}, \mathfrak{S}_{\text{jump}})]}{L_{\text{inv},b}[\mathfrak{C}] \cdot \lambda_{d,\min}[\Pi]} + m_v, \qquad (3.8.57)$$

where

$B^{\downarrow,\uparrow}[(\mathfrak{C}, \Pi, \mathfrak{V}, \mathfrak{S}_{\text{out}}, \mathfrak{S}_{\text{con}}, \mathfrak{S}_{\text{jump}})]$

$$
\begin{aligned}
:= {} & B_{b,0}[\mathfrak{C}] \cdot \lambda_d[p] + B_{\mathfrak{s}}[(\mathfrak{C},\Pi,\mathfrak{V})] \cdot (t_{\mathrm{f}} - t_0) + \frac{1}{2}\big(B^{\downarrow}_{k,\mathrm{Dir}}[\mathfrak{C}] + B^{\uparrow}_{k,\mathrm{Dir}}[\mathfrak{C}]\big) \cdot d_{\max}[\Pi] \\
& + \Big(\max\big\{0, B_{\mathrm{out},m_v}[(\mathfrak{C},\mathfrak{S}_{\mathrm{out}})]\big\} + \max\big\{0, B_{\mathrm{con},1,m_v}[(\mathfrak{C},\mathfrak{S}_{\mathrm{con}})]\big\} \\
& \quad + \max\big\{0, B_{\mathrm{con},2,m_v}[(\mathfrak{C},\mathfrak{S}_{\mathrm{con}})]\big\} + 2 \cdot B_{\mathrm{jump},m_v}[\mathfrak{C}] + 2 \cdot B_{\mathrm{jump,Dir},m_v}[\mathfrak{C}] \\
& \quad + \max\big\{0, B_{\mathrm{flux,jump},1,m_v}[(\mathfrak{C},\mathfrak{S}_{\mathrm{jump}})]\big\} + 2 \cdot \max\big\{0, B_{\mathrm{flux,jump},2,m_v}[(\mathfrak{C},\mathfrak{S}_{\mathrm{jump}})]\big\} \\
& \quad + \max\big\{0, B_{\mathrm{flux,Dir}}[\mathfrak{C}]\big\}\Big) \cdot \lambda_{d-1,\max}[\Pi] \\
& + B_{f,m_v}[\mathfrak{C}] \cdot \lambda_{d,\max}[\Pi].
\end{aligned} \tag{3.8.58}
$$

Proof. Hypotheses (i) and (ii) grant the hypotheses (i) and (ii) of Th. 3.7.50. Thus, using (3.7.134a):

$$0 \leq P^{(\nu)}_{(k,\mathcal{C})} \leq N_{b,\neg\mathrm{Dir}} \leq B_{b,0}[\mathfrak{C}] \cdot \lambda_d[p] + B_{\mathfrak{s}}[(\mathfrak{C},\Pi,\mathfrak{V})] \cdot (t_{\mathrm{f}} - t_0). \tag{3.8.59}$$

The proof of (3.8.58) is concluded by remarking that the summands according to (3.8.52a) and (3.8.52b) are bounded by Def. 3.8.25(iii) together with the estimates proved in parts (e) of the Decomposition Lemmas (s. Def. 3.8.29). ▲

The only hypotheses of Lem. 3.8.5 that remain to be verified are (3.8.12), where (3.8.12a) and (3.8.12c) are just hypotheses (3.8.49a) and (3.8.49d), respectively, taking into account $\Delta_\nu \leq \Delta$. Finally, by hypothesis (3.8.49c):

$$
\begin{aligned}
\Delta_\nu \cdot L_{M-m_v}[(\mathfrak{C},\Pi,\mathfrak{V},\mathfrak{S}_{\mathrm{out}},\mathfrak{S}_{\mathrm{con}},\mathfrak{S}_{\mathrm{jump}})] &\leq \Delta \cdot L_{M-m_v}[(\mathfrak{C},\Pi,\mathfrak{V},\mathfrak{S}_{\mathrm{out}},\mathfrak{S}_{\mathrm{con}},\mathfrak{S}_{\mathrm{jump}})] \\
&< \big(L_{\mathrm{inv},b}[\mathfrak{C}] \cdot \lambda_{d,\min}[\Pi]\big) \cdot \frac{M-S}{M-m_v},
\end{aligned}
$$

which yields (3.8.12b).

Now, due to the conclusion of Lem. 3.8.5, all hypotheses of Th. 3.8.4 are satisfied, and the conclusion of Th. 3.8.4 provides a unique vector $(u^{(\nu)}_{(k,\mathcal{C})})_{(k,\mathcal{C})\in I_{\Pi,\mathfrak{D},\neg\mathrm{Dir}}} \in [m_v, M]^{I_{\Pi,\mathfrak{D},\neg\mathrm{Dir}}}$ satisfying Def. 3.7.42(iii). ■

Remark 3.8.36. It is noted that

$$\lim_{M\to\infty} \frac{M-S}{M-m_v} = 1. \tag{3.8.60}$$

Thus, given $1 > \delta > 0$, one can impose the additional condition, to choose M sufficiently large such that $\frac{M-S}{M-m_v} > \delta$, which is assumed within the current remark.

If the number $L_{M-m_v}[(\mathfrak{C},\Pi,\mathfrak{V},\mathfrak{S}_{\mathrm{out}},\mathfrak{S}_{\mathrm{con}},\mathfrak{S}_{\mathrm{jump}})]$, occurring in (3.8.49c) in Th. 3.8.35, is independent of M (i.e. if $L_r[(\mathfrak{C},\Pi,\mathfrak{V},\mathfrak{S}_{\mathrm{out}},\mathfrak{S}_{\mathrm{con}},\mathfrak{S}_{\mathrm{jump}})]$ defined in (3.8.54) is independent of r), then Δ just needs to satisfy (3.8.49d) and

$$\Delta \cdot L_{M-m_v}[(\mathfrak{C},\Pi,\mathfrak{V},\mathfrak{S}_{\mathrm{out}},\mathfrak{S}_{\mathrm{con}},\mathfrak{S}_{\mathrm{jump}})] < \big(L_{\mathrm{inv},b}[\mathfrak{C}] \cdot \lambda_{d,\min}[\Pi]\big) \cdot \delta, \tag{3.8.61}$$

i.e. Δ can be chosen independently of M.

3.8.10 Example: Coupled Transient Heat Equations

In the general situation of Th. 3.8.35, the dependence of the fineness Δ of the discretization of the time domain τ on the fineness h of the space discretization (cf. (3.5.2)) can be very complicated. In general, $\lambda_{d,\min}$, L_{M-m_v}, and also the number M itself all depend on the space discretization Π. Therefore, the purpose of the present section is to consider situations, where the dependence of Δ on h is computed explicitly. The chosen setting is the situation of coupled transient heat equations, where one equation is considered on a gas domain and another equation is considered on a solid domain (s. Ex. 3.1.1(b)).

Domains

As usual, let $\tau = [t_0, t_f]$ denote the time domain. Let p_1 denote the domain of the gas phase, and let p_2 denote the domain of the solid material β_j. For simplicity, it is further assumed that the shape of the domains is such that they can be discretized into cubes of equal size (s. Fig. 3.28). Thus, the polytope discretization $\Pi = (\omega_k)_{k \in I_\Pi}$ of $p = p_1 \cup p_2$ is supposed to be such that each ω_k is a cube, each side having length h, where the discretization points are chosen such that $\|x_k - x_l\|_2 \geq h$ whenever $\partial_{\text{reg}}\omega_k \cap \partial_{\text{reg}}\omega_l \neq \emptyset$. In consequence, $\lambda_3[\omega_k] = h^3$ and $\lambda_2[\partial\omega_k] = 6h^2$ for each $k \in I_\Pi$, $\lambda_{d,\max}[\Pi] = h^3$, $d_{\max}[\Pi] \leq \frac{\lambda_2[\partial\omega_k]}{h} = 6h$. Furthermore, it is assumed that the $\omega_k^{(j)}$ are such that $\lambda_3[\omega_k^{(j)}] \geq \frac{h^3}{8}$ (i.e. $\lambda_{d,\min}[\Pi] \geq \frac{h^3}{8}$), $\lambda_{d-1,\max}[\Pi] \leq 2 \cdot \lambda_2[\partial\omega_k] = 12h^2$.

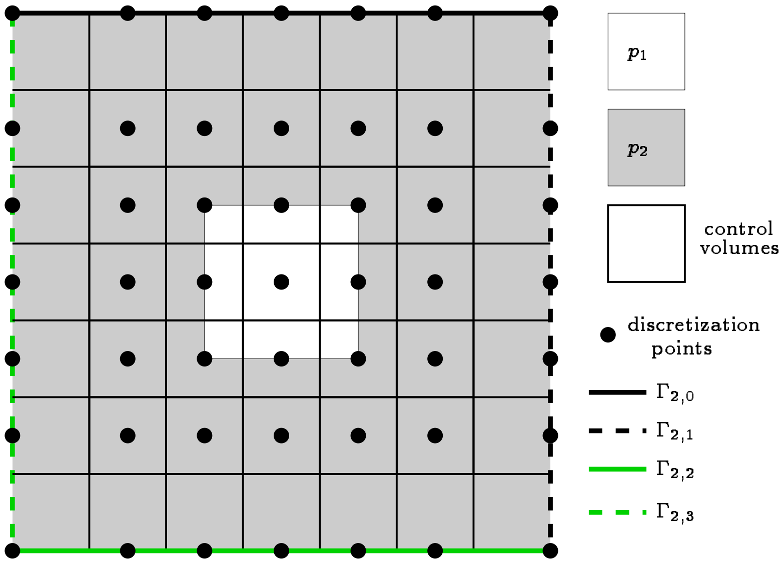


Figure 3.28: Section through the discretized cubic domain $p = p_1 \cup p_2$.

As the unknowns u_1 and u_2 are supposed to represent absolute temperature, their range is $\upsilon = [m_\upsilon, \infty[$ with $m_\upsilon = 0$.

Input Functions of the Heat Equations

The situation of Ex. 3.1.1(b) is considered with $c_{\mathrm{sp}}^{[\beta_j]}$, and $f^{[\beta_j]}$ being independent of the unknown. For simplicity, let $\mathbf{v}_{\mathrm{gas}} = 0$. Thus, letting $u_1 := T_{\mathrm{gas}}$ and $u_2 := T^{[\beta_j]}$, one has $b_1[(u_1, t, x)] = \frac{z^{(\mathrm{Ar})} R}{M^{(\mathrm{Ar})}} \rho_{\mathrm{gas}}[x]\, u_1$, $k_1[(u_1, t, x)] = \kappa^{(\mathrm{Ar})}[(u_1, t, x)]$, $v_1[(u_1, t, x)] = 0$, and $f_1[(u_1, t, x)] = 0$, and $b_2[(u_2, t, x)] := \rho^{[\beta_j]}[x]\, c_{\mathrm{sp}}^{[\beta_j]}[x]\, u_2$, $k_2[(u_2, t, x)] := \kappa^{[\beta_j]}[(u_2, t, x)]$, $v_2[(u_2, t, x)] := 0$, and $f_2[(u_2, t, x)] := f^{[\beta_j]}[(t, x)]$.

The only reasonable choice for $\mathfrak{V}$ then is $\mathfrak{V} = \big((0,0)\big)_{j \in \{1,2\}}$.

It is assumed that ρ_{gas}, $\rho^{[\beta_j]}$, and $c_{\mathrm{sp}}^{[\beta_j]}$ are bounded away from zero, i.e. there is $\delta_{\min} \in \mathbb{R}^+$ such that $\rho_{\mathrm{gas}} > \delta_{\min}$, $\rho^{[\beta_j]} > \delta_{\min}$, and $c_{\mathrm{sp}}^{[\beta_j]} > \delta_{\min}$. It is convenient for subsequent use, to choose $\delta_{\min}$ sufficiently small, such that $\frac{z^{(\mathrm{Ar})} R}{M^{(\mathrm{Ar})}} \geq \delta_{\min}$.

Interface Conditions

It is presumed that $\gamma := \partial_{\mathrm{reg}} p_1 \cap \partial_{\mathrm{reg}} p_2$ is a jump interface, where, as in Ex. 3.1.2(b), $a_{\mathrm{jump}}^{\gamma,1}[(u_1, t, x)] := \xi_{\mathrm{jump}} u_1$, $a_{\mathrm{jump}}^{\gamma,2}[(u_2, t, x)] := \xi_{\mathrm{jump}} u_2$, $\xi_{\mathrm{jump}} \in \mathbb{R}^+$. In particular, $\mathrm{IF}_{\mathrm{con}} = \emptyset$. The flux interface condition is supposed to have its most simple form, i.e. $a_{\mathrm{flux}}^{\gamma,1} = a_{\mathrm{flux}}^{\gamma,2} = \mathcal{A}_\gamma = 0$, and also $\big(a_{\mathrm{flux}}^{\gamma,1}\big)^{\text{ex.-im.}} = \big(a_{\mathrm{flux}}^{\gamma,2}\big)^{\text{ex.-im.}} = \big(\mathcal{A}_\gamma\big)^{\text{ex.-im.}} = 0$.

Boundary Conditions

The boundary conditions of Ex. 3.1.3(a),(b),(c) are allowed in the current example, where the boundary conditions of Ex. 3.1.3(d) is later added in Ex. 3.8.38 below. As in Fig. 3.28, the case is considered where only p_2 has outer boudaries. To permit the prescription of the different boundary conditions on $\partial p = \partial p_2 \cap \partial p$, there is a partition $(\Gamma_{2,\iota})_{\iota \in \{0,1,2,3\}}$ of ∂p (s. Fig. 3.28), such that $u_{2,\mathrm{Dir}} = 0$ on $\Gamma_{2,0}$, $a_{\mathrm{out}}^{2,1}$ is independent of u_2 on $\Gamma_{2,1}$, $a_{\mathrm{out}}^{2,2}[(u_2, t, x)] = \xi_{\mathrm{out}} \big(u_2 - u_{\mathrm{ext}}[(t, x)]\big)$, $\xi_{\mathrm{out}} \in \mathbb{R}^+$, on $\Gamma_{2,2}$, and $\mathcal{B}_{2,\iota} = 0$ for each $\iota \in \{1, 2, 3\}$. The function $a_{\mathrm{out}}^{2,3}$ on $\Gamma_{2,3}$ is specified in Exs 3.8.37 and 3.8.38, respectively. No dependency splitting is considered, i.e. $\big(a_{\mathrm{out}}^{j,\iota}\big)^{\text{ex.-im.}}\big[\big((\tilde{y}, y), t, x\big)\big] = a_{\mathrm{out}}^{j,\iota}[(y, t, x)]$ and $\big(\mathcal{B}_{2,\iota}\big)^{\text{ex.-im.}} = 0$ for each $\iota \in \{1, 2, 3\}$.

Linear, Coupled Transient Heat Equations

Example 3.8.37. It is assumed that $\kappa^{(\mathrm{Ar})}$ and $\kappa^{[\beta_j]}$ are independent of the unknown, i.e. $k_1[(u_1, t, x)] = \kappa^{(\mathrm{Ar})}[(t, x)]$ and $k_2[(u_2, t, x)] := \kappa^{[\beta_j]}[(t, x)]$. Moreover, let $a_{\mathrm{out}}^{2,3} = 0$.

Calculation of $B_{\mathfrak{s}}[(\mathfrak{C},\Pi,\mathfrak{V})]$: One has $B_{\mathrm{Dir}}[\mathfrak{C}]=0$, $B_{v,\mathrm{Dir}}[(\mathfrak{C},\mathfrak{V})]=0$, $B_{v,\mathrm{sca,Dir}}[(\mathfrak{C},\mathfrak{V})]=0$. In the current situation, Lem. 3.7.25 applies with $\mathrm{av}_{\mathrm{out}}^{2,\iota}[(\tilde{y},y,t,x)]=-a_{\mathrm{out}}^{2,\iota}[(y,t,x)]$, i.e. with $B_{\mathrm{out}}[\mathfrak{C}]=\max\big\{\sup(-a_{\mathrm{out}}^{2,\iota}):\ \iota\in\{1,2,3\}\big\}$. Moreover, $B_{\mathrm{con}}[\mathfrak{C}]=0$ as $\mathrm{IF}_{\mathrm{con}}=\emptyset$, and Lem. 3.7.33 applies with $\mathrm{av}_{\mathrm{jump},\alpha}[\gamma]=0$, $\alpha\in\{1,2\}$, $B_{\mathrm{jump}}[\mathfrak{C}]=0$, and $B_{\mathrm{jump,Dir}}[\mathfrak{C}]=0$, since for $\alpha\in\{1,2\}$, $\sup(-a_{\mathrm{jump}}^{\gamma,\alpha})=0$ as well as $a_{\mathrm{jump}}^{\gamma,\alpha}[(0,t,x)]=0$. Then, $B_{\mathrm{IF}}[\mathfrak{C}]=0$ according to Rem. 3.7.35. Thus,

$$B_{\mathfrak{s}}[(\mathfrak{C},\Pi,\mathfrak{V})]=B_{\mathrm{out}}[\mathfrak{C}]\cdot\lambda_{d-1}[\partial p]+B_f[\mathfrak{C}]\cdot\lambda_d[p]. \tag{3.8.62}$$

Calculation of $B^{\downarrow,\uparrow}[(\mathfrak{C},\Pi,\mathfrak{V},\mathfrak{S}_{\mathrm{out}},\mathfrak{S}_{\mathrm{con}},\mathfrak{S}_{\mathrm{jump}})]$: Since $B_{\mathrm{Dir}}[\mathfrak{C}]=0$, one has $B_{k,\mathrm{Dir}}^{\uparrow}[\mathfrak{C}]=B_{k,\mathrm{Dir}}^{\downarrow}[\mathfrak{C}]=0$. Lemma 3.8.16 applies with $B_{\mathrm{out},m_v}[(\mathfrak{C},\mathfrak{S}_{\mathrm{out}})]=B_{\mathrm{out}}[\mathfrak{C}]$ (see above). From $\mathrm{IF}_{\mathrm{con}}=\emptyset$, one gets $B_{\mathrm{con},1,m_v}[(\mathfrak{C},\mathfrak{S}_{\mathrm{con}})]=B_{\mathrm{con},2,m_v}[(\mathfrak{C},\mathfrak{S}_{\mathrm{con}})]=0$, and since $B_{\mathrm{Dir}}[\mathfrak{C}]=0$ as well as $a_{\mathrm{jump}}^{\gamma,\alpha}[(0,t,x)]=0$, $\alpha\in\{1,2\}$, Lem. 3.8.21 applies with $B_{\mathrm{jump},m_v}[\mathfrak{C}]=B_{\mathrm{jump,Dir},m_v}[\mathfrak{C}]=0$. Lemma 3.8.23 applies with $B_{\mathrm{flux,jump},1,m_v}[(\mathfrak{C},\mathfrak{S}_{\mathrm{jump}})]=B_{\mathrm{flux,jump},2,m_v}[(\mathfrak{C},\mathfrak{S}_{\mathrm{jump}})]=B_{\mathrm{flux,Dir}}[\mathfrak{C}]=0$. The u_j-independence of the f_j yields $B_{f,m_v}[\mathfrak{C}]=B_f[\mathfrak{C}]$. Thus,

$$\begin{aligned}&B^{\downarrow,\uparrow}[(\mathfrak{C},\Pi,\mathfrak{V},\mathfrak{S}_{\mathrm{out}},\mathfrak{S}_{\mathrm{con}},\mathfrak{S}_{\mathrm{jump}})]\\&\le B_{b,0}[\mathfrak{C}]\cdot\lambda_d[p]+\big(B_{\mathrm{out}}[\mathfrak{C}]\cdot\lambda_{d-1}[\partial p]+B_f[\mathfrak{C}]\cdot\lambda_d[p]\big)\cdot(t_{\mathrm{f}}-t_0)\\&\quad+12B_{\mathrm{out}}[\mathfrak{C}]h^2+B_f[\mathfrak{C}]h^3.\end{aligned} \tag{3.8.63}$$

Next, one can choose $L_{\mathrm{inv},b}[\mathfrak{C}]=\delta_{\mathrm{min}}^2$.

Then, according to (3.8.49a),

$$S\le\frac{8\cdot B^{\downarrow,\uparrow}[(\mathfrak{C},\Pi,\mathfrak{V},\mathfrak{S}_{\mathrm{out}},\mathfrak{S}_{\mathrm{con}},\mathfrak{S}_{\mathrm{jump}})]}{\delta_{\mathrm{min}}^2h^3}. \tag{3.8.64}$$

According to (3.8.49), one has to choose

$$M>\max\Big\{S,\ \max\big\{\|u_j^{(0)}\|_{\max}:\ j\in\{1,2\}\big\}\Big\}. \tag{3.8.65}$$

Calculation of $L_r[(\mathfrak{C},\Pi,\mathfrak{V},\mathfrak{S}_{\mathrm{out}},\mathfrak{S}_{\mathrm{con}},\mathfrak{S}_{\mathrm{jump}})]$, $r\in\mathbb{R}^+$: Since all nonlocal operators vanish, $L_{\mathrm{nonloc},r}[(\mathfrak{C},\Pi)]=0$. Also, $L_{v,r}[\mathfrak{C}]=0$ by the above definition of $\mathfrak{V}$, and $L_{\mathrm{flux},1,r}[(\mathfrak{C},\mathfrak{S}_{\mathrm{con}})]=0$ since $\mathrm{IF}_{\mathrm{con}}=\emptyset$. Since the k_j and f_j are independent of the solution, one can choose $L_{k,r}[\mathfrak{C}]=L_{f,r}[\mathfrak{C}]=0$. In consequence, $L_{k,r}^{\downarrow}[\mathfrak{C}]=\frac{5}{2}\cdot B_{k,m_v}[\mathfrak{C}]$, $L_{\mathrm{Dir},k,r}[\mathfrak{C}]=B_{k,m_v}[\mathfrak{C}]$. As each $a_{\mathrm{out}}^{2,\iota}$ is either 0-Lipschitz or ξ_{out}-Lipschitz, one can choose $L_{\mathrm{out},r}[(\mathfrak{C},\mathfrak{S}_{\mathrm{out}})]=\xi_{\mathrm{out}}$. As $a_{\mathrm{jump}}^{\gamma,2}$ is ξ_{jump}-Lipschitz, one can choose $L_{\mathrm{jump},2,r}[\mathfrak{C}]=\xi_{\mathrm{jump}}$. As $(a_{\mathrm{flux}}^{\gamma,1})^{\text{ex.-im.}}=0$ and $a_{\mathrm{jump}}^{\gamma,1}$ is ξ_{jump}-Lipschitz, one can choose $L_{\mathrm{flux,jump},r}[(\mathfrak{C},\mathfrak{S}_{\mathrm{jump}})]=\xi_{\mathrm{jump}}$. Thus,

$$L_r[(\mathfrak{C},\Pi,\mathfrak{V},\mathfrak{S}_{\mathrm{out}},\mathfrak{S}_{\mathrm{con}},\mathfrak{S}_{\mathrm{jump}})]\le\frac{7}{2}\cdot B_{k,m_v}[\mathfrak{C}]\cdot 6h+\big(\xi_{\mathrm{out}}+2\xi_{\mathrm{jump}}\big)\cdot 12h^2. \tag{3.8.66}$$

In particular, $L_r[(\mathfrak{C}, \Pi, \mathfrak{V}, \mathfrak{S}_{\mathrm{out}}, \mathfrak{S}_{\mathrm{con}}, \mathfrak{S}_{\mathrm{jump}})]$ is independent of r (cf. Rem. 3.8.36).

Now, according to (3.8.49), Δ can be chosen

$$\Delta < \min\left\{1,\ \frac{\delta_{\min}^2 h^3}{21 \cdot B_{k,m_v}[\mathfrak{C}] \cdot h + \left(\xi_{\mathrm{out}} + 2\xi_{\mathrm{jump}}\right) \cdot 12h^2} \cdot \left(1 - \frac{S}{M}\right)\right\}, \tag{3.8.67}$$

showing that the fineness of the time discretization depends quadratically on the fineness of the space discretization for $h \to 0$.

Nonlinear, Coupled Transient Heat Equations

Example 3.8.38. The only difference between this example and Ex. 3.8.37 is the consideration of nonlinearities in the k_j and in the boundary conditions on $\Gamma_{2,3}$.

One might want to choose k_1 according to (A.2.2). However, the function in (A.2.2) is *not* locally Lipschitz at $T = 0$, and thus not admissable.[1] Therefore, it is set $k_1[(u_1, t, x)] := u_1$, and a proper nonlinearity is only considered in k_2, where

$$k_2[(u_2, t, x)] := a_k e^{b_k u_2} \tag{3.8.68}$$

with positive real numbers a_k and b_k. Then k_2 has the form (A.3.5c). It is continuously differentiable with respect to u_2, and the derivative is

$$k_2'[(u_2, t, x)] := a_k b_k e^{b_k u_2}. \tag{3.8.69}$$

Furthermore, let

$$a_{\mathrm{out}}^{2,3}[(u_2, t, x)] = \sigma\, \epsilon\big(u_2^4 - T_{\mathrm{room}}^4\big), \tag{3.8.70}$$

$\epsilon \in]0, 1]$. Then $a_{\mathrm{out}}^{2,3}$ is continuously differentiable with respect to u_2, and the derivative is

$$(a_{\mathrm{out}}^{2,3})'[(u_2, t, x)] = 4\sigma\, \epsilon\, u_2^3. \tag{3.8.71}$$

Calculation of $B_{\mathfrak{s}}[(\mathfrak{C}, \Pi, \mathfrak{V})]$ and $B^{\downarrow,\uparrow}[(\mathfrak{C}, \Pi, \mathfrak{V}, \mathfrak{S}_{\mathrm{out}}, \mathfrak{S}_{\mathrm{con}}, \mathfrak{S}_{\mathrm{jump}})]$: There is basically no change in comparison with the calculations in Ex. 3.8.37, and, in particular, (3.8.62) and (3.8.63) still hold: Since $B_{\mathrm{Dir}} = 0$, the k_j do not contribute to $B_{\mathfrak{s}}[(\mathfrak{C}, \Pi, \mathfrak{V})]$. The only change can occur in the value of $B_{\mathrm{out}}[\mathfrak{C}]$, as $\sup(-a_{\mathrm{out}}^{2,3}) = 0$ in Ex. 3.8.37, and $0 < \sup(-a_{\mathrm{out}}^{2,3}) \le \sigma T_{\mathrm{room}}^4$ in the present example.

One can still choose $L_{\mathrm{inv},b}[\mathfrak{C}] = \delta_{\min}^2$, and (3.8.64) remains valid as well as (3.8.65).

[1] As (A.2.2) was fitted according to data for $T \ge 290\,\mathrm{K}$ anyway, one could consider a Lipschitz continuous cutoff for small T. However, this was not done here, as, in practice, it was not necessary for the simulations. Analogous remarks also apply with respect to some of the other material functions in App. A.

The main difference between Exs 3.8.37 and 3.8.38 lies in the calculation of the number $L_r[(\mathfrak{C}, \Pi, \mathfrak{V}, \mathfrak{S}_{\text{out}}, \mathfrak{S}_{\text{con}}, \mathfrak{S}_{\text{jump}})]$, $r \in \mathbb{R}^+$. Even so, one still has

$$L_{\text{nonloc},r}[(\mathfrak{C}, \Pi)] = L_{v,r}[\mathfrak{C}] = L_{\text{flux},1,r}[(\mathfrak{C}, \mathfrak{S}_{\text{con}})] = L_{f,r}[\mathfrak{C}] = 0,$$

$$L_{\text{jump},2,r}[\mathfrak{C}] = L_{\text{flux,jump},r}[(\mathfrak{C}, \mathfrak{S}_{\text{jump}})] = \xi_{\text{jump}}.$$

According to Rem. C.7.7(i), $k_2 \restriction_{\upsilon\times\{t\}\times\{x\}}$ is $(a_k b_k e^{b_k r})$-Lipschitz on $[0, r]$, since k_2' is increasing in u_2. As $k_1 \restriction_{\upsilon\times\{t\}\times\{x\}}$ is 1-Lipschitz, one can choose $L_{k,r}[\mathfrak{C}] = \max\{1,\ a_k b_k e^{b_k r}\}$. Moreover, $B_{k,m_v}[\mathfrak{C}] = a_k$, such that $L^{\downarrow}_{k,r}[\mathfrak{C}] = 5r \max\{1,\ a_k b_k e^{b_k r}\} + \frac{5}{2} a_k$, $L_{\text{Dir,k,r}}[\mathfrak{C}] := r \max\{1,\ a_k b_k e^{b_k r}\} + a_k$. To choose $L_{\text{out},r}[(\mathfrak{C}, \mathfrak{S}_{\text{out}})]$, it is observed that $a^{2,1}_{\text{out}} \restriction_{\upsilon\times\{t\}\times\{x\}}$ is 0-Lipschitz, $a^{2,2}_{\text{out}} \restriction_{\upsilon\times\{t\}\times\{x\}}$ is ξ_{out}-Lipschitz, and $a^{2,3}_{\text{out}} \restriction_{\upsilon\times\{t\}\times\{x\}}$ is $(4\sigma\,\epsilon\, r^3)$-Lipschitz on $[0, r]$ by Rem. C.7.7(i), since $(a^{2,3}_{\text{out}})'$ is increasing in u_2. Hence, one can choose $L_{\text{out},r}[(\mathfrak{C}, \mathfrak{S}_{\text{out}})] = \max\{\xi_{\text{out}}, 4\sigma\,\epsilon\, r^3\}$. Thus,

$$\begin{aligned} L_r[(\mathfrak{C}, \Pi, \mathfrak{V}, \mathfrak{S}_{\text{out}}, \mathfrak{S}_{\text{con}}, \mathfrak{S}_{\text{jump}})] \leq & \big(36 \cdot r \max\{1,\ a_k b_k e^{b_k r}\} + 21 \cdot a_k\big)\, h \\ & + \big(\max\{\xi_{\text{out}}, 4\sigma\,\epsilon\, r^3\} + 2\xi_{\text{jump}}\big) \cdot 12h^2. \end{aligned} \tag{3.8.72}$$

Now M is chosen sufficiently large, such that $1 - \frac{S}{M} \geq \frac{1}{2}$, $\max\{1,\ a_k b_k e^{b_k M}\} = a_k b_k e^{b_k M}$, and $\max\{\xi_{\text{out}}, 4\sigma\,\epsilon\, M^3\} = 4\sigma\,\epsilon\, M^3$. Then Δ can be chosen

$$\Delta < \min\left\{1,\ \frac{\delta^2_{\min} h^3}{\big(72 \cdot M\, a_k b_k e^{b_k M} + 42 \cdot a_k\big)\, h + \big(4\sigma\,\epsilon\, M^3 + 2\xi_{\text{jump}}\big) \cdot 24h^2}\right\}, \tag{3.8.73}$$

showing that for fixed M, the fineness of the time discretization still depends quadratically on the fineness of the space discretization for $h \to 0$. However, in the present case, the exponential function in k_2 yields an exponential dependence of Δ on M.

3.9 Perspectives on Convergence

Given a number $h \in \mathbb{R}^+$, call a finite volume discretization $\mathfrak{F}$ of $\mathfrak{C}$ *h-admissible* iff its space discretization Π has fineness less than h (cf. (3.5.2)) and $\mathfrak{F}$ satisfies the hypotheses of Th. 3.8.35. In particular, the fineness Δ of the time discretization of $\mathfrak{F}$ has to be sufficiently fine. Let $\mathcal{S}_h$ denote the set of all h-admissible finite volume discretizations of $\mathfrak{C}$, and let $\mathcal{S} := \bigcup_{h\in\mathbb{R}^+} \mathcal{S}_h$.

Given $\mathfrak{F} \in \mathcal{S}$, Th. 3.8.35 provides a solution $\mathfrak{U}_{\mathfrak{F}}$ to $\mathfrak{F}$:

$$\mathfrak{U}_{\mathfrak{F}} = \big(u^{\nu,\mathfrak{F}}_{(k,\mathcal{C})}\big)_{(\nu,(k,\mathcal{C}))\in\{0,\dots,n_{\mathfrak{F}}\}\times I_{\Pi_{\mathfrak{F}},\mathfrak{D}}}.$$

According to Th. 3.7.50, one has a discrete L^∞-L^1 a priori bound $N_{\text{all}}[\mathfrak{U}_{\mathfrak{F}}] \leq B[(\mathfrak{C}, \mathcal{V})]$, where $B[(\mathfrak{C}, \mathcal{V})]$ is independent of $\Pi_{\mathfrak{F}}$, assuming that there are no Dirichlet boundaries.

A suitable interpolation of $\mathfrak{U}_{\mathfrak{F}}$ should yield an approximation $u_{\mathfrak{F}}$ of a solution to $\mathfrak{C}$. For example, one can use constant interpolation in space and linear interpolation in time: Given $j \in J$ and $x \in p_j$, there is a unique $(k, \mathcal{C}) \in I_{\Pi_{\mathfrak{F}}, \mathfrak{D}}$ such that $x \in \omega^{(j)}_{k,\mathfrak{F}}$ and $j \in V[\mathcal{C}]$, $\mathcal{C} \in \operatorname{CoCmp}[\mathcal{G}_{\omega_{k,\mathfrak{F}}}]$. For $t \in [t^{(\mathfrak{F})}_{\nu+1}, t^{(\mathfrak{F})}_{\nu}]$, let

$$u_{j,\mathfrak{F}}[(t,x)] := \frac{u^{\nu+1,\mathfrak{F}}_{(k,\mathcal{C})} - u^{\nu,\mathfrak{F}}_{(k,\mathcal{C})}}{t^{(\mathfrak{F})}_{\nu+1} - t^{(\mathfrak{F})}_{\nu}} \cdot (t - t^{(\mathfrak{F})}_{\nu}) + u^{\nu,\mathfrak{F}}_{(k,\mathcal{C})}. \tag{3.9.1}$$

Then $u_{\mathfrak{F}}$ defined by $u_{\mathfrak{F}} \restriction_{\tau \times p_j} := u_{j,\mathfrak{F}}$ is an element of the evolution space $L^\infty(\tau, L^1[p])$, where

$$\begin{aligned} \|u_{\mathfrak{F}}\|_{L^\infty(\tau, L^1[p])} &= \max\left\{ \sum_{\substack{j \in V[\mathcal{C}], \\ (k,\mathcal{C}) \in I_{\Pi_{\mathfrak{F}}, \mathfrak{D}}}} |u^{\nu,\mathfrak{F}}_{(k,\mathcal{C})}| \cdot \lambda_d[\omega^{(j)}_{k,\mathfrak{F}}] : \nu \in \{0, \dots, n_{\mathfrak{F}}\} \right\} \\ &= N_{\text{all}}[\mathfrak{U}_{\mathfrak{F}}] \le B[(\mathfrak{C}, \mathcal{V})]. \end{aligned} \tag{3.9.2}$$

Since τ is a compact interval, one also has $u_{\mathfrak{F}} \in L^a(\tau, L^1[p])$ for each $a \in [1, \infty[$. Thus, for each $a \in [1, \infty[$, there is a closed ball B_a in $L^a(\tau, L^1[p])$ such that $\{u_{\mathfrak{F}} : \mathfrak{F} \in \mathcal{S}\} \subseteq B_a$.

Given a sequence $h_i \to 0$, and finite volume discretizations $\mathfrak{F}_{h_i} \in \mathcal{S}_{h_i}$ with corresponding solutions $u_{\mathfrak{F}_{h_i}}$, one would like to establish the existence of some u such that a subsequence of $(u_{\mathfrak{F}_{h_i}})_{i \in \mathbb{N}}$ converges to u in a suitable space. To use standard compactness techniques, a suitable space is the dual of some (separable, reflexive) function space, and $L^a(\tau, L^1[p])$ is not suitable in that respect. Thus, a canonical next step is to improve (3.9.2) into an analogous result in, e.g., $L^\infty(\tau, L^2[p])$ (using additional hypotheses where appropriate). Usually, one also needs further estimates for discrete gradients and for time and space translates (see below). Finally, one needs to show that the limit u is a solution to $\mathfrak{C}$, at least in a certain weak sense and, ideally, in the (strong) sense of Def. 3.4.7.

In [MR01], the method outlined above is used to establish the convergence of a semi-implicit finite volume scheme for the nonlinear evolution equation

$$\partial_t u - \operatorname{div}\big(k\big[|\nabla G * u|\big] \nabla u\big) = f[u], \tag{3.9.3}$$

where G is a C^∞-function with compact support, and "$*$" denotes convolution: A discrete L^∞-L^2 estimate ([MR01, Lem. 3.1(i)]), estimates for the discrete gradients in space ([MR01, Lem. 3.1(ii)]) and time ([MR01, Lem. 3.1(iii)]), and estimates for space and time translates ([MR01, Lems 3.2 and 3.3]) are used to prove the existence of a limit u for $(h, \Delta) \to (0,0)$ by applying the Fréchet-Kolmogorov Theorem [Bré83, Th. IV.25] ([MR01, Lem. 3.5]). Subsequently, it is shown that the limit u constitutes a weak solution ([MR01, Sec. 3.3]).

Chapter 4

Numerical Results

4.1 General Setting and Methods

Throughout this chapter, it is assumed that all components of the growth system are cylindrically symmetric, and that all relevant physical quantities are cylindrically symmetric as well.

All numerical simulations presented in the following were performed for the growth system displayed in Fig. 4.1, consisting of a container placed inside of 5 hollow rectangular-shaped copper induction rings. The geometric proportions of the system are provided in Sec. 4.2.2 and Fig. 4.2.

During each specific physical growth run, the SiC source powder graphitizes and sinters, and chemical reactions inside the solid parts of the graphite crucible lead to changes in its porosity and can cause nonsealing joints. Moreover, accumulation of Si in the insulation felt is observed. It is not feasible to account for these changes at the current stage of numerical simulations. Hence, all simulations presented in this chapter are performed for an idealized growth apparatus, treating all solid materials as homogeneous and pure. Typical material data are used where available. The material data that have been used during the following numerical experiments are collected in App. A.

As described in Sec. 2.1.4, for simulations of the temperature distribution evolution, it is reasonable to assume that the gas phase is made up solely of argon.

Making the aforementioned assumptions, neglecting any mechanical or chemical interactions inside both solid and gas as well as radiative and convective contributions inside the gas phase (cf. [KPSW01] for numerical simulations including convection), according to (2.1.34c) and (2.2.1), heat transport in the growth apparatus is described by

$$\frac{z^{(\mathrm{Ar})}R}{M^{(\mathrm{Ar})}}\frac{\partial}{\partial t}\left(\rho_{\mathrm{gas}}T\right) - \operatorname{div}\left(\kappa^{(\mathrm{Ar})}\nabla T\right) = 0 \qquad \text{(gas phase)}, \tag{4.1.1a}$$

$$\rho^{[\beta_j]}c_{\mathrm{sp}}^{[\beta_j]}\frac{\partial T}{\partial t} - \operatorname{div}\left(\kappa^{[\beta_j]}\nabla T\right) = f^{[\beta_j]} \qquad \text{(solid component } \beta_j\text{)}. \tag{4.1.1b}$$

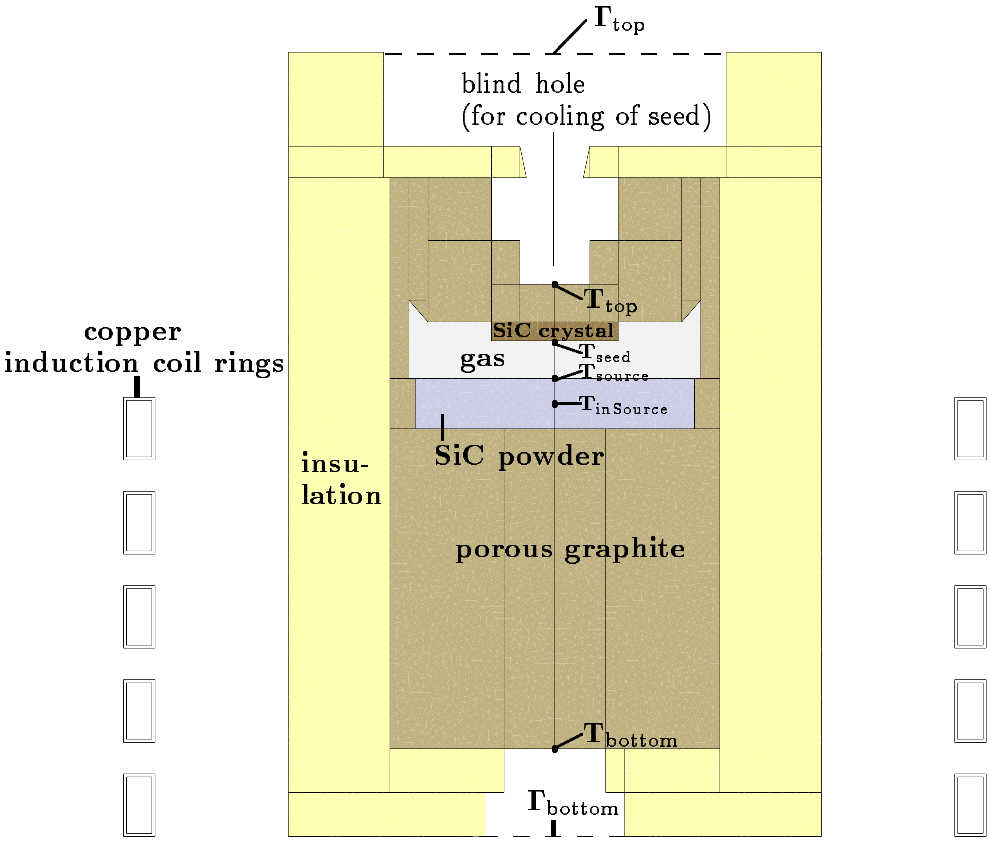


Figure 4.1: Setup of growth apparatus according to [PAC+99, Fig. 2] indicating locations of temperatures monitored in the simulations, and also indicating the phantom closures $\mathbf{\Gamma}_{bottom}$ and $\mathbf{\Gamma}_{top}$.

In (4.1.1), the temperatures T_{gas} and $T^{[\beta_j]}$ have been replaced by a single temperature T, as in absence of data on transition coefficients ξ_j (cf. (2.3.2b′)), for the simulations of this chapter, the temperature is presumed to be continuous throughout the whole apparatus.

It is noted that the relaxation times of the pressure and of the temperature in the gas phase always lie orders of magnitude below the corresponding relaxation times in the solid components. Since the gas does not have a significant influence on the temperature of the solid parts, each temporal snapshot of a transient simulation furnishes the quasi-stationary temperature distribution in the gas phase determined by the temperature distribution on the adjacent solid surfaces. In particular, for a given constant pressure $p^{(\mathrm{Ar})}$, the time derivative in (4.1.1a) vanishes identically as can be seen from (2.1.33d). Thus, the quasi-stationary temperature distribution in the gas phase does not depend on the gas pressure. The same result was stated in [KP01, p. 10]; however the reasoning therein is not completely correct as it is based on [KP01, (3.2)] that contains an error in its time derivative. The time derivative in [KP01, (3.2)] should simply read $\frac{3}{2}\partial_t p^{(\mathrm{Ar})}$

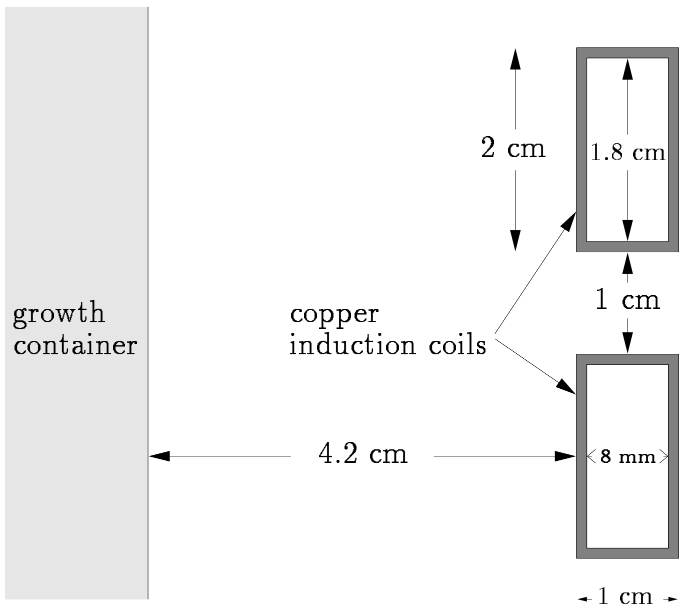


Figure 4.2: Geometric proportions of induction coil rings.

as follows from (2.1.33d) and (4.1.1a).

The argument of the preceding paragraph suggests that (4.1.1b) could be coupled with the stationary version of (4.1.1a), i.e. with

$$\operatorname{div}\left(\kappa^{(\mathrm{Ar})}\,\nabla T\right) = 0. \tag{4.1.2}$$

However, for the regularity of the problem, it is advantageous to keep the time derivative in the gas equation, which is also helpful within the present code implementation. Hence, for the following simulations, (4.1.1a) is used with the constant density $\rho_{\mathrm{gas}} = \rho^{(\mathrm{Ar})} = 3.73 \cdot 10^{-3}\ \mathrm{kg/m^3}$ corresponding to $T = 2575$ K and $p^{(\mathrm{Ar})} = 2 \cdot 10^3$ Pa in an ideal gas.

Apart from the continuity interface conditions (2.3.2a) and (2.3.2b) for the temperature, interface conditions (2.3.1) are used for the heat flux. On interfaces adjacent to cavities or adjacent to the semi-transparent SiC single crystal, the flux interface conditions include radiative contributions according to the modeling in Sec. 2.4 (s. (2.4.38) and (2.4.39)).

The nonlocal outer boundary condition (2.4.17) is used on outer boundaries bordering the outer and lower blind hole, where black body phantom closures such as Γ_{top} and Γ_{bottom} in Fig. 4.1 are used as described at the end of Sec. 2.3. On all remaining outer boundaries, the Stefan-Boltzmann emission condition (2.3.3) is used.

Induction heating is modeled according to Sec. 2.5, in particular using cylindrical symmetry and the model assumptions of Sec. 2.5.1 as well as sinusoidal time dependence according to Sec. 2.5.6. The average total power $\overline{P_{\mathrm{total}}}$ is prescribed according to the method in Sec. 2.5.7. The power is increased linearly during each simulation (s. Sec. 4.2.2). It was found in [KP01, Sec. 3.2] that a domain of radius 1.2 m and height 1.8 m having the configuration Fig. 4.1 (radius: 8.4 cm without coil, height: 25 cm) in its center, is sufficiently large for accurate computations of heat sources.

A finite volume method as described in Ch. 3 is used for the discretizations arising in the stationary computation of the magnetic scalar potential and in the transient temperature simulations. An implicit Euler scheme provides the time discretization; only emissivity terms are evaluated explicitly, i.e. using the temperature at the previous time step. The nonlinear systems arising from the finite volume discretization of the nonlinear heat transport problem are solved by Newton's method.

The space domains are discretized into unstructured grids of triangles satisfying the constrained Delaunay criterion. The triangles are used to construct control volumes as Voronoi boxes (cf. the paragraphs after Def. 3.7.40 and App. C.4.3). A grid of 7247 triangles is used to discretize the growth apparatus without coil rings for the transient temperature computations, and a grid of some 100000 triangles is used to discretize the larger domain, where the magnetic scalar potential is computed. Even though the grid is chosen extremely fine in the coil rings and rather coarse far from the rings, it is my impression that the discretization could still be optimized to get the same accuracy with considerably less triangles. However, for the time being, grid optimzation was not pursued for the benefit of other tasks.

The standard time step control algorithm implemented in the program package *pdelib* (see below) is employed. It tries to predict the maximal size of the solution change during time step number $\nu + 1$, linearly interpolating the maximal size of the solution change that occurred during the ν-th time step. The size of the time step is chosen such that the predicted maximal size of the solution change equals a prescribed value. The time step is discarded and repeated with a smaller step size, if the actual solution change is considerably larger than the predicted one.

The finite volume discretization of the nonlocal radiation terms according to Secs 3.7.7 and 3.7.8 involves the calculation of visibility and view factors according to (3.7.75) and (2.4.23). Even for an axisymmetric configuration, in general, this is a complicated task. The method used is based on [DNR$^+$90] and described in [KPSW01, Sec. 4].

The software resulting from the implementation of the discrete scheme has been named *WIAS-HiTNIHS*[1]. It is based on the program package *pdelib* being developed at the *Weierstrass Institute of Applied Analysis and Stochastics (WIAS)*, Berlin (cf. [FKL01]), and it uses the grid generator *Triangle* (cf. [She96]), the interpreted extension language

[1]High Temperature Numerical Induction Heating Simulator; pronounciation: ~nice.

Lua (cf. [IFF96]), the graphics software *OpenGL* (cf. [Shr99]), together with its *X-Windows* based emulation *Mesa*, and the sparse matrix solver *PARDISO* (cf. [SGFS00]).

4.2 Compilation of Equations and Parameter Values Used in Simulations

4.2.1 Equations Used in Simulations

All equations are considered in an axisymmetric setting, i.e. in two space dimensions using cylindrical coordinates. During the computation of the evolution of the unknown temperature T, one has to take into account the heat sources due to induction heating. The heat sources are computed via (4.2.1c), where the complex magnetic scalar potential $\phi_{A,0}^{\text{complex}}$ is determined using the method described in Sec. 2.5.7 for a prescribed average total power $\overline{P_{\text{total}}}[t]$. The $\phi_{A,0}^{\text{complex}}$ are redetermined in each time step of the transient problem for T, to account for temperature dependence of the electrical conductivity and for changing coil positions.

The transient problem for T consists of the following system (4.2.1), where (2.1.34c) yields (4.2.1a), (2.2.1) yields (4.2.1b), (2.5.31) and (2.5.33b) yield (4.2.1c), (2.3.2a) and (2.3.2b) yield (4.2.1d), (2.3.1a) yields (4.2.1e), (2.4.39a) yields (4.2.1f), (2.4.39b) yields (4.2.1g), (2.4.39c) yields (4.2.1h), (2.4.17) yields (4.2.1i), and (2.3.3) yields (4.2.1j).

Gas Domain

$$\frac{z^{(\text{Ar})} R}{M^{(\text{Ar})}} \frac{\partial}{\partial t}\left(\rho^{(\text{Ar})} T\right) - \operatorname{div}\left(\kappa^{(\text{Ar})} \nabla T\right) = 0 \qquad \text{in gas,} \tag{4.2.1a}$$

Solid Domains

$$\rho^{[\beta_j]} c_{\text{sp}}^{[\beta_j]} \frac{\partial T}{\partial t} - \operatorname{div}\left(\kappa^{[\beta_j]} \nabla T\right) = f^{[\beta_j]} \qquad \text{in each solid } \beta_j, \tag{4.2.1b}$$

$$f^{[\beta_j]} = \frac{\sigma_c^{[\beta_j]} \omega^2 \phi_{A,0}^{\text{complex}} \overline{\phi_{A,0}^{\text{complex}}}}{2} \quad \text{in each solid } \beta_j, \tag{4.2.1c}$$

Interface Conditions

$$T \text{ is continuous on each interface,} \tag{4.2.1d}$$

$$\begin{pmatrix} \left(\kappa^{[\beta_{j_1}]} \nabla T^{[\beta_{j_1}]}\right) \bullet \mathbf{n}^{[\beta_{j_1}]} = \left(\kappa^{[\beta_{j_2}]} \nabla T^{[\beta_{j_2}]}\right) \bullet \mathbf{n}^{[\beta_{j_1}]} \\ \text{on each interface between solids } \beta_{j_1},\, \beta_{j_2} \text{ if } \ \text{SiC-Crystal} \notin \{\beta_{j_1}, \beta_{j_2}\} \end{pmatrix}, \tag{4.2.1e}$$

$$\begin{pmatrix} \mathbf{q}^{[\text{SiC-Crystal}]} \bullet \mathbf{n}^{[\text{SiC-Crystal}]} + \epsilon_{\mathrm{t}} \cdot \left(\mathcal{J}_{\mathrm{t}}\left[\mathcal{R}_{\mathrm{t}}[T]\right] - \sigma T^4\right) = \mathbf{q}^{[\beta_j]} \bullet \mathbf{n}^{[\text{SiC-Crystal}]} \\ \text{on each interface between SiC-Crystal and solid } \beta_j \end{pmatrix}, \tag{4.2.1f}$$

$$\begin{pmatrix} \mathbf{q}_{\text{gas}} \bullet \mathbf{n}_{\text{gas}} + \epsilon_{\mathrm{r}} \cdot \left(\mathcal{J}_{\mathrm{r}}\left[\mathcal{R}_{\mathrm{r}}[T]\right] - \sigma T^4\right) \\ \qquad + \epsilon_{\mathrm{t}} \cdot \left(\mathcal{J}_{\mathrm{t}}\left[\mathcal{R}_{\mathrm{t}}[T]\right] - \sigma T^4\right) = \mathbf{q}^{[\beta_j]} \bullet \mathbf{n}_{\text{gas}} \\ \text{on each interface between solid } \beta_j \text{ and gas} \end{pmatrix}, \tag{4.2.1g}$$

$$\begin{pmatrix} \mathbf{q}_{\text{gas}} \bullet \mathbf{n}_{\text{gas}} + \epsilon_{\mathrm{r}} \cdot \left(\mathcal{J}_{\mathrm{r}}\left[\mathcal{R}_{\mathrm{r}}[T]\right] - \sigma T^4\right) = \mathbf{q}^{[\text{SiC-Crystal}]} \bullet \mathbf{n}_{\text{gas}} \\ \text{on each interface between SiC-Crystal and gas} \end{pmatrix}. \tag{4.2.1h}$$

Outer Boundary Conditions

$$\begin{pmatrix} \mathbf{q}^{[\beta_j]} \bullet \mathbf{n}^{[\beta_j]} + \epsilon^{[\beta_j]} \cdot \left(\mathcal{J}\left[\mathcal{R}[T]\right] - \sigma T^4\right) = 0 \\ \text{on each outer boundary of solid } \beta_j \text{ inside the blind holes} \end{pmatrix}, \tag{4.2.1i}$$

$$\begin{pmatrix} -\left(\kappa^{[\beta_j]} \nabla T\right) \bullet \mathbf{n}^{[\beta_j]} = \sigma \epsilon^{[\beta_j]} \left(T^4 - T_{\text{room}}^4\right) \\ \text{on each outer boundary of solid } \beta_j \text{ outside the blind holes} \end{pmatrix}. \tag{4.2.1j}$$

4.2.2 Parameters Used in Simulations

Material data and physical constants are *not* collected in this section, but in App. A.

The configuration in Fig. 4.1 is used in the simulations, assuming a radius of 8.4 cm and a height of 25 cm for the apparatus without coil rings. The precise geometric proportions of the coil rings are depicted in Fig. 4.2. While the horizontal gap between container and coil is fixed at 4.2 cm in all the numerical experiments, the vertical coil position is varied during the simulations in Sec. 4.3.

The angular frequency ω used for induction heating is calculated according to $\omega = 2\pi f$, where $f = 10$ kHz. The average total power $\overline{P_{\text{total}}}$ is prescribed according to the method in Sec. 2.5.7. A so-called ramp is used to prescribe $\overline{P_{\text{total}}}[t]$, increasing the power linearly from 0 to $P_{\max}$, letting

$$\overline{P_{\text{total}}}[t] := \begin{cases} \frac{P_{\max}}{t_{\text{ramp}}} \cdot t & \text{for } 0 \le t \le t_{\text{ramp}}, \\ P_{\max} & \text{for } t \ge t_{\text{ramp}}, \end{cases} \tag{4.2.2}$$

where $t_{\text{ramp}} = 2$ h and $P_{\max}$ is varied as a control parameter.

Each simulation starts at $T_{\text{room}} = 293$ K.

4.3 Transient Numerical Investigation of Control Parameters Affecting the Temperature Evolution

4.3.1 Description of Numerical Experiments

In Sec. 4.3, results of numerical computations are presented and discussed, simulating the temperature distribution evolution during the heating process of SiC growth by PVT. The general setting is described in Sec. 4.1, the governing equations and the fixed parameters are collected in Sec. 4.2, and the used material parameters can be found in App. A.

The system is heated, starting at room temperature, using a ramp for the heating power according to (4.2.2). The temperature distribution evolution is studied, varying P_{max} and the coil position. The investigation is similar to the one in [KP01, Sec. 3.3], except that in [KP01] the heating voltage was prescribed and no ramp was used. Moreover, some aspects are discussed that were not considered in [KP01], namely the relation between the temperature differences $T_{\mathrm{source}} - T_{\mathrm{seed}}$ and $T_{\mathrm{bottom}} - T_{\mathrm{top}}$ (s. Fig. 4.6), and the time lag between the heating of the body of the apparatus and the heating of the source powder (s. Fig. 4.7).

Three series of numerical experiments are considered, referred to as C_0^{14}, C_2^{16}, and C_4^{18}, respectively, each series using a different vertical coil position. For C_0^{14}, the coil is positioned between $z = 0$ and $z = 14$ cm, i.e. the lower rim of the bottom coil ring is at $z = 0$, and the upper rim of the top coil ring is at $z = 14$ cm. The meaning of C_2^{16} and C_4^{18} is analogous. There are five experiments in each series, using different values for P_{max}, namely $P_{\mathrm{max}} = 4.0$ kW, 5.5 kW, 7.0 kW, 8.5 kW, and 10.0 kW. Subsequently, a fourth series $\mathrm{C}_{4\to 0}^{18\to 14}$ is considered, using a moving induction coil.

Results for the time evolution and the final values of the temperature evolution at four points of particular importance are depicted in Figs 4.3, 4.4, and 4.5, respectively. The monitored points are located at the blind holes at the top and at the bottom of the growth apparatus, and at the surface of the crystal seed and of the source powder, respectively (labeled T_{top}, T_{bottom}, T_{seed}, and T_{source} in Fig. 4.1). The significance of T_{top} and T_{bottom} lies in the blind holes being the principal locations for temperature measurements; T_{seed} and T_{source} are of interest, since their difference is a key control factor for the crystal's growth rate and quality (cf. e.g. [Kon95], [SBP98]). Figure 4.6 compares $T_{\mathrm{source}} - T_{\mathrm{seed}}$ to the measurable quantity $T_{\mathrm{bottom}} - T_{\mathrm{top}}$. In Fig. 4.7, the evolution of the temperature inside the source (i.e. at the point labeled T_{inSource} in Fig. 4.1) is compared to the evolution of T_{source} and T_{top}. Results of the time evolution of the *global* temperature field and the heat sources are shown in Fig. 4.8, and results of the quasi-stationary temperature distributions at the crystal and its immediate surroundings are depicted in Fig. 4.9. The results are discussed in detail in the following Secs

4.3.2, 4.3.3, and 4.3.4 .

4.3.2 Temperature Evolution at Points of Interest

The numerical results for the time evolution and the final values of T_{top}, T_{bottom}, T_{seed}, and T_{source} are considered.

In [KP01], it was found that for each time t, the temperatures T_{top}, T_{bottom}, T_{seed}, and T_{source} depend nearly linearly on the prescribed effective voltage V_{eff}. It can be seen in Figs 4.3 and 4.4 that for fixed t, the dependence of T_{top}, T_{bottom}, and T_{seed} on $P_{\max}$ is *not* nearly linear, since the distance between the 4 kW and the 5.5 kW curves is considerably bigger than the distance between the 7.5 kW and the 10 kW curves.

The exact relation between the prescribed power P and the resulting temperature T at a given location in the growth apparatus is actually quite complicated. If the electrical conductivity σ_{c} is constant, then it can be seen from (2.5.32) and (2.5.65) that the relation between $\sqrt{P}$ and the magnetic scalar potential $\phi_{A,0}^{\text{complex}}$ is linear. However, here σ_{c} depends nonlinearly on T (s. (A.3.2b)), and $\phi_{A,0}^{\text{complex}}$ depends nonlinearly on σ_{c} by (2.5.32c). Moreover, the coupling between $\phi_{A,0}^{\text{complex}}$ and T through (4.2.1c) and (4.2.1b) is quite intricate e.g. due to the nonlinear functions of thermal conductivity (s. e.g. (A.3.2c) and (A.3.5c)) and the nonlinear boundary condition (4.2.1j). As a deeper analysis of these relations is not the subject of this work, it is merely observed that for the quasi-stationary state at $t = 30\ 000$ s, T_{top}, T_{bottom}, and T_{seed}, as well as $T_{\text{source}} - T_{\text{seed}}$ depend on $P_{\max}$ approximately according to the power law $T \propto \sqrt[4]{P_{\max}}$ (s. Fig. 4.5).

Figures 4.3, 4.4, and 4.5 show furthermore that T_{top} and T_{seed} increase significantly between C_0^{14} (low coil position) and C_4^{18} (high coil position), whereas T_{bottom} decreases slightly. This can be explained by the heat sources being shifted upwards and the source powder's insulating property which, though less prominent, is still effective even at high temperatures (cf. Fig. 4.8(a) and (A.3.5c)), thereby hindering heat generated below the source powder from reaching regions above the source powder and vice versa.

The shape of the curves in row (4) of Figs 4.3 and 4.4 depicting $T_{\text{source}} - T_{\text{seed}}$ is also due to the insulating characteristic of the source powder and the gas phase, initially keeping the powder's surface below the temperature of the seed which the heat reaches via conduction through the graphite. This causes the negative peak in the corresponding graphs. At higher temperatures, radiative heat transfer becomes more effective both in the gas phase and the porous source, resulting in the source growing warmer than the seed, as is required for crystal growth. Moreover, it is seen in Fig. 4.5(4) that at the quasi-stationary state, a lower coil position or a higher heating power result in $T_{\text{source}} - T_{\text{seed}}$ being increased (in [KP01], it was stated incorrectly that a higher coil position increases $T_{\text{source}} - T_{\text{seed}}$). If the heat is generated below the source powder, then it passes through the powder and then through the gas phase to reach the seed (s. Figs

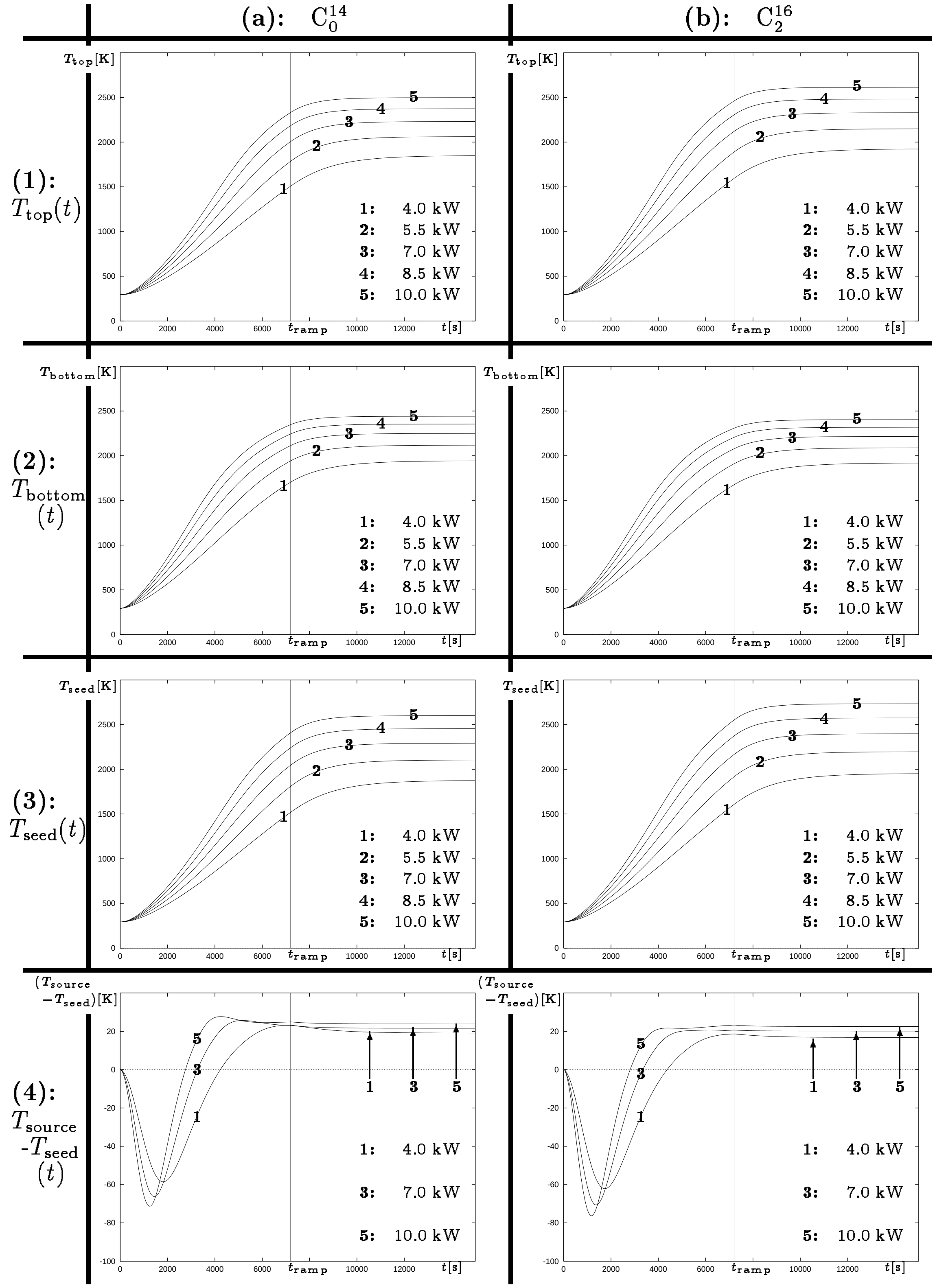


Figure 4.3: Time evolution of T_{top} (row (1)), T_{bottom} (row (2)), T_{seed} (row (3)), and $T_{source} - T_{seed}$ (row (4)) for the simulation series C_0^{14} (column (a)) and C_2^{16} (column (b)).

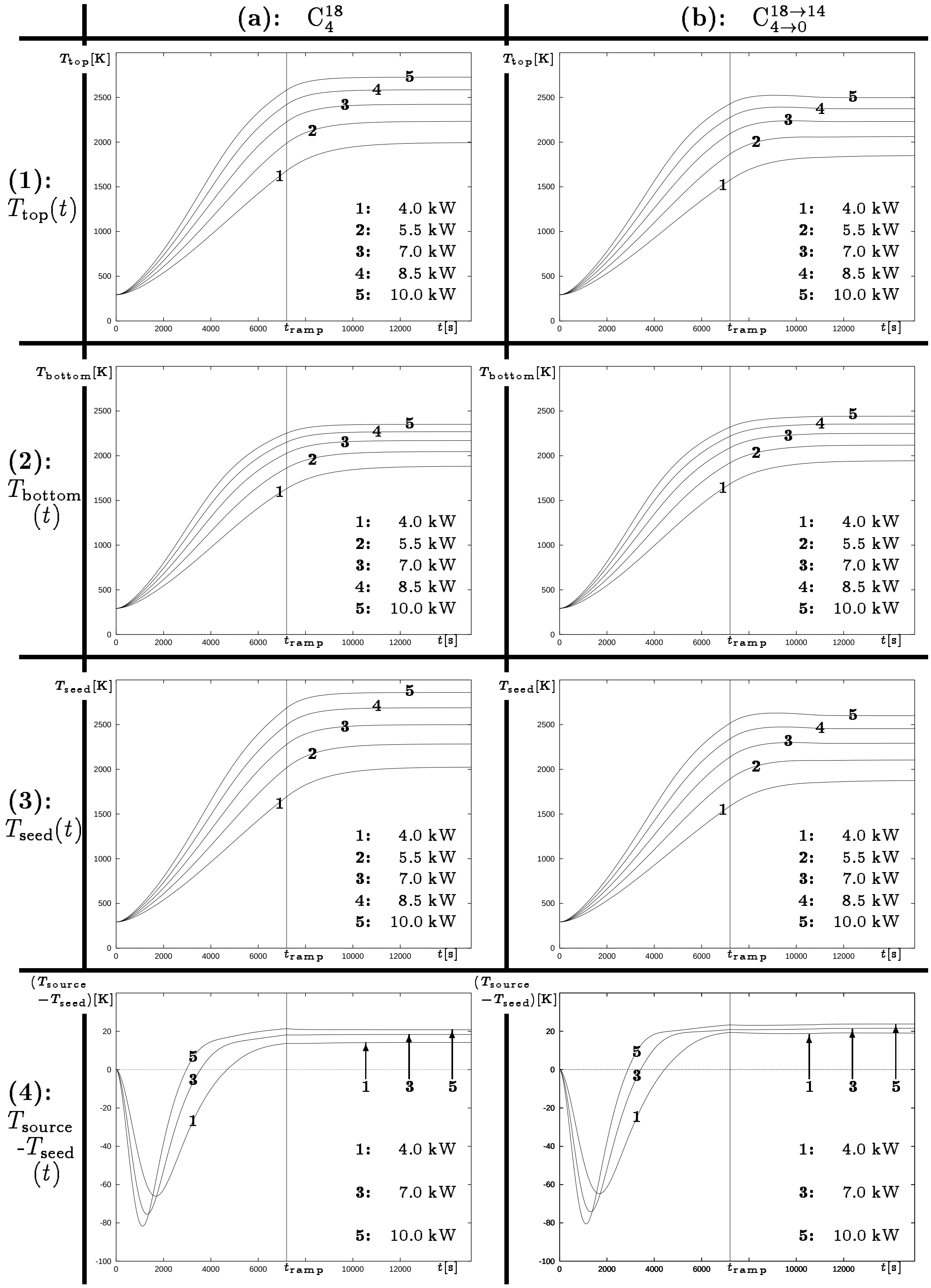


Figure 4.4: Time evolution of T_{top} (row (1)), T_{bottom} (row (2)), T_{seed} (row (3)), and $T_{source} - T_{seed}$ (row (4)) for simulation series C_4^{18} (column (a)) and $C_{4\to0}^{18\to14}$ (column (b)).

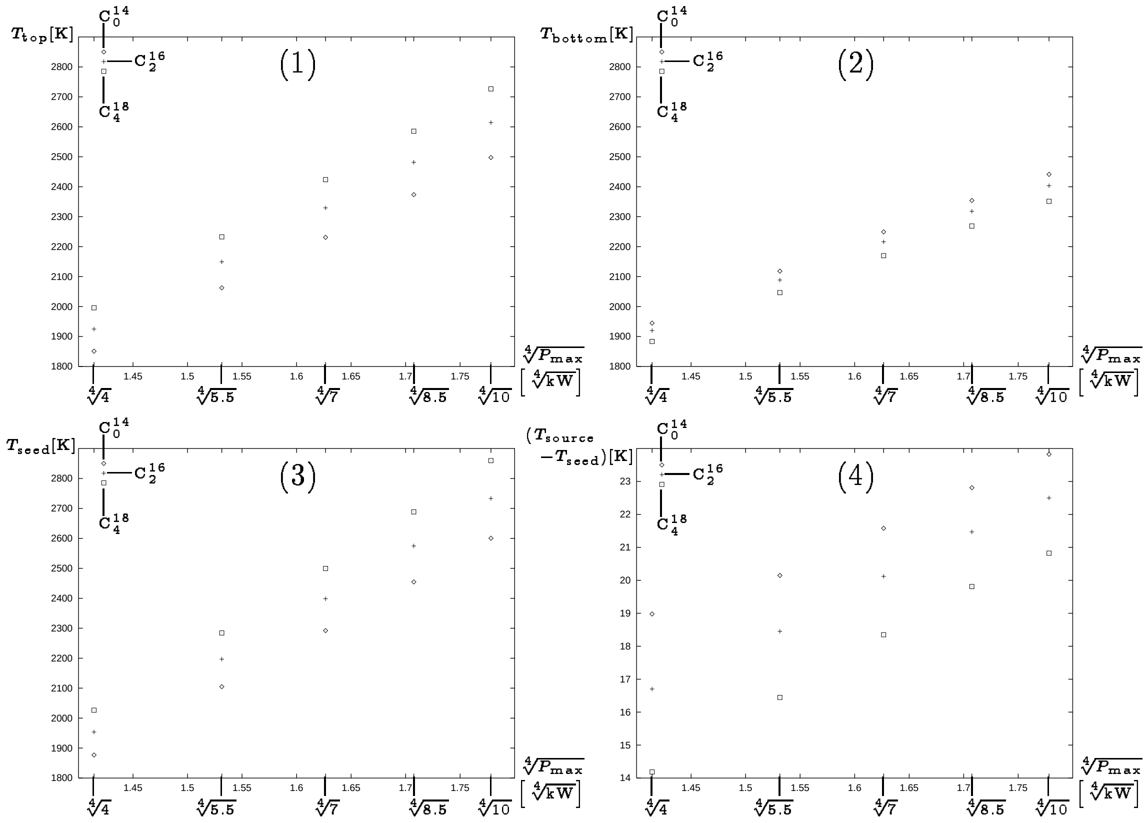


Figure 4.5: Temperatures T_{top} (in (1)), T_{bottom} (in (2)), T_{seed} (in (3)), and $T_{\text{source}} - T_{\text{seed}}$ (in (4)) for the quasi-stationary state at $t = 30\ 000$ s for the simulation series C_0^{14}, C_2^{16}, and C_4^{18} depending on the 4-th root of the maximal heating power P_{max}.

4.8(a) and 4.9). A higher power leading to a higher difference $T_{\text{source}} - T_{\text{seed}}$ thus means that a higher temperature below the powder enhances the powder's ability to transport heat even more effectively than it enhances the corresponding ability of the gas phase. For a higher coil position, more heat is generated in upper parts of the apparatus, where it can reach the seed without passing through the powder, thus explaining $T_{\text{source}} - T_{\text{seed}}$ being bigger for lower coil positions. Figure 4.5(4) indicates that $T_{\text{source}} - T_{\text{seed}}$ can be tuned effectively by controling the heating power and the vertical coil position.

Now, the series of numerical experiments $C_{4\to0}^{18\to14}$ is discussed, where the coil starts at the position used for C_4^{18}, moves downwards at the rate 1.33 cm/h, and stops at the position used for C_0^{14}. During these simulations, the grid for the heat source computations is newly generated in each time step. The objective of the series $C_{4\to0}^{18\to14}$ is to study how a moving coil affects the temperature field evolution during the heating process. In this work, there is no investigation of coil movements that follow the growing crystal in the quasi-stationary temperature field, which are often used in growth experiments to compensate the influence of the growing crystal on the temperature distribution. The rate of such coil movements is usually in the order of 1 mm/h, and the movement starts after the apparatus is fully heated, i.e. after the simulations considered here have reached their respective quasi-stationary final states.

As expected, the curves for the moving coil (Fig. 4.4(b)) initially coincide with the corresponding curves of C_4^{18} (Fig. 4.4(a)) and coincide with the corresponding curves of C_0^{14} (Fig. 4.3(a)) after the coil's lowest position is reached at $t = 3$ h.

4.3.3 Phenomena Inaccessible to Direct Measurements

In this section, simulation results are discussed which give some insight into phenomena that are inaccessible to direct measurements, but can be of considerable importance with respect to the quality of the growth process and the resulting single crystals.

In physical growth experiments, the measured temperature difference $T_{\mathrm{bt}} := T_{\mathrm{bottom}} - T_{\mathrm{top}}$ is often used as an indicator for $T_{\mathrm{ss}} := T_{\mathrm{source}} - T_{\mathrm{seed}}$ which is not accessible to direct measurements. The simulation results depicted in Fig. 4.6 show that one has to use care when using this method, as it is not admissible in general. According to Fig. 4.6, T_{bt} is a good indicator for T_{ss} only for the lowest coil position C_0^{14} and only in the quasi-stationary state (right side of Figs 4.6(1) and 4.6(4)). For the higher coil positions C_2^{16} and C_4^{18}, not even the signs of T_{bt} and T_{ss} agree in the quasi-stationary state. Thus, in practice, the validity of using T_{bt} as an indicator for T_{ss} should be verified by some other method (e.g. numerical simulation).

As described in Sec. 1.1, the growth system is usually kept at some 1200 K for a certain time, to bake out contaminants from the source powder. It is seen in each situation dipicted in Fig. 4.7 that in the initial heating phase, there is a time lack of up to 20 minutes between the temperature T_{inSource} inside the source (s. Fig. 4.1), and both T_{source} and T_{top}. Thus, depending on the configuration of the growth system, it can be of paramount importance to take into account this time lack, in order to allow sufficient time for the contaminant bake-out phase.

4.3.4 Evolution of Global Distribution of Temperature and of Heat Sources

For the experiment $C_{4\to 0}^{18\to 14}$-7 kW, results concerning the time evolution of the global temperature distribution and the heat sources are discussed. It can be seen in column (a) of Fig. 4.8 that the minimal temperature T_{min} is always established at the outside of the outer insulation material, where the isotherms become very dense at higher temperatures, producing the dark outer regions in Fig. 4.8 (2)(a) and (3)(a). The maximal temperature T_{max} is found in the graphite strip between source and insulation in Fig. 4.8 (1)(a) and inside the labeled isotherms below the source in Fig. 4.8 (2)(a)

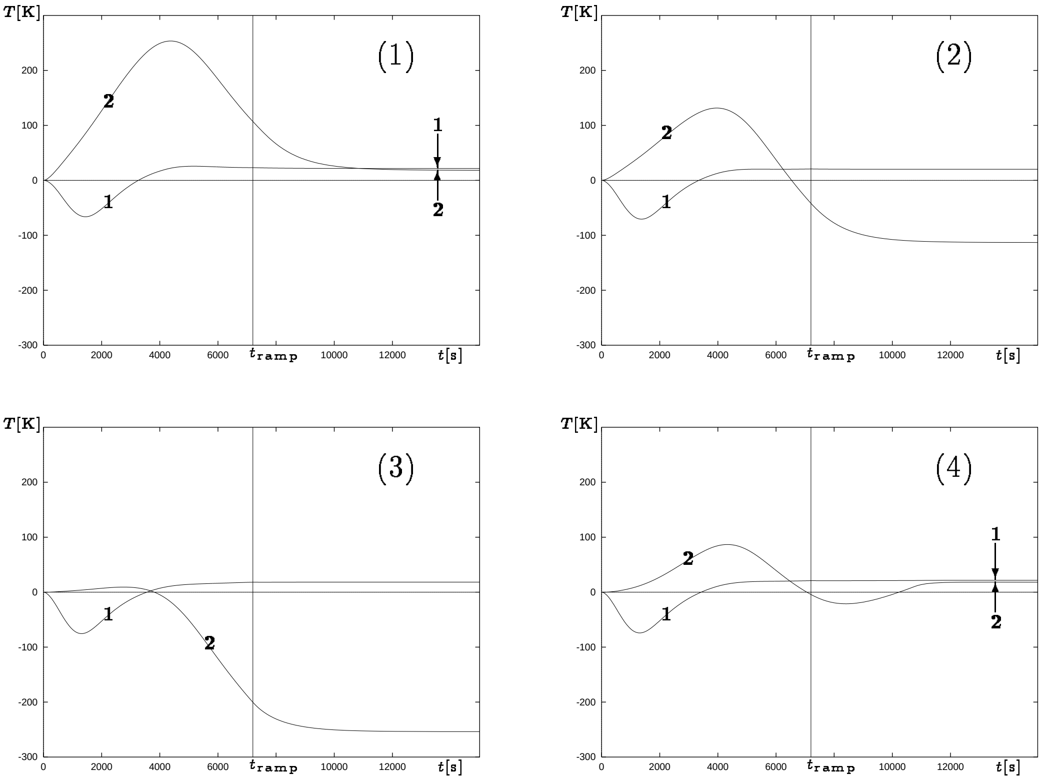


Figure 4.6: For the numerical experiments C_0^{14} (in (1)), C_2^{16} (in (2)), C_4^{18} (in (3)), and $C_{4\to0}^{18\to14}$ (in (4)) ($P_{\max} = 7$ kW in all four cases), the graphs labeled by "1" show the evolution of $T_{\text{source}} - T_{\text{seed}}$, whereas the graphs labeled by "2" show the evolution of $T_{\text{bottom}} - T_{\text{top}}$.

and (3)(a). The change of the location of $T_{\max}$ corresponds to the heat sources moving downwards together with the induction coil according to Fig. 4.8(b).

Figure 4.8(a) also demonstrates how the insulating property of the gas phase and the source powder changes with time, causing a large temperature gradient in the gas phase in 4.8(1)(a) as well as a local minimum in the source. Due to radiative heat transfer through the gas phase and through the pores of the source, the temperature in the growth chamber is more homogeneous in 4.8(2)(a) and 4.8(3)(a), where the local minimum in the source has vanished, even though some of the source's insulating quality persists.

Finally, Fig. 4.9 displays close-ups of the final temperature distributions in the crystal's immediate surroundings for $P_{\max} = 7$ kW and the three coil positions C_0^{14}, C_2^{16}, and C_4^{18}. The picture in Fig. 4.9 (a) also constitutes a close-up of Fig. 4.8(3)(a), since the stationary states are identical for the simulations C_0^{14}-7 kW and $C_{4\to0}^{18\to14}$-7 kW. The

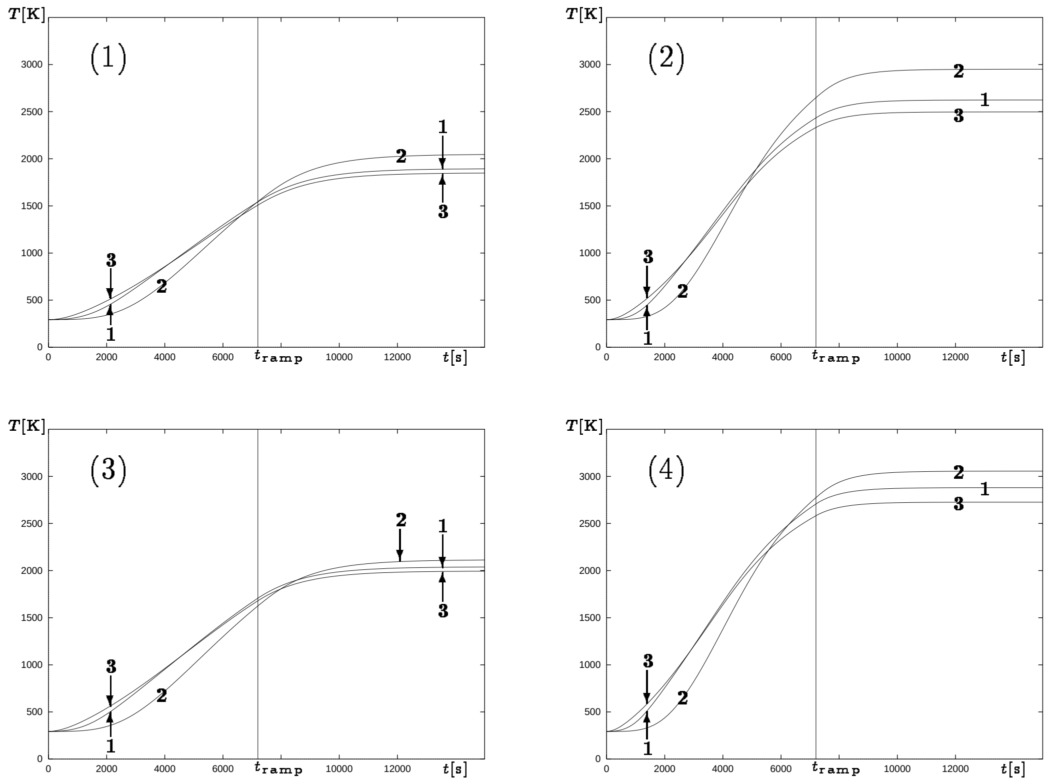


Figure 4.7: For the numerical experiments C_0^{14}, $P_{\text{max}} = 4$ kW (in (1)), C_0^{14}, $P_{\text{max}} = 10$ kW (in (2)), C_4^{18}, $P_{\text{max}} = 4$ kW (in (3)), and C_4^{18}, $P_{\text{max}} = 10$ kW (in (4)), the graphs labeled by "1", "2", and "3" show the evolution of T_{source}, T_{inSource}, and T_{top}, respectively.

lower temperatures found for C_0^{14} in Fig. 4.9(a), are once more explained by the powder source forming a barrier for heat generated in the lower part of the apparatus. Moreover,

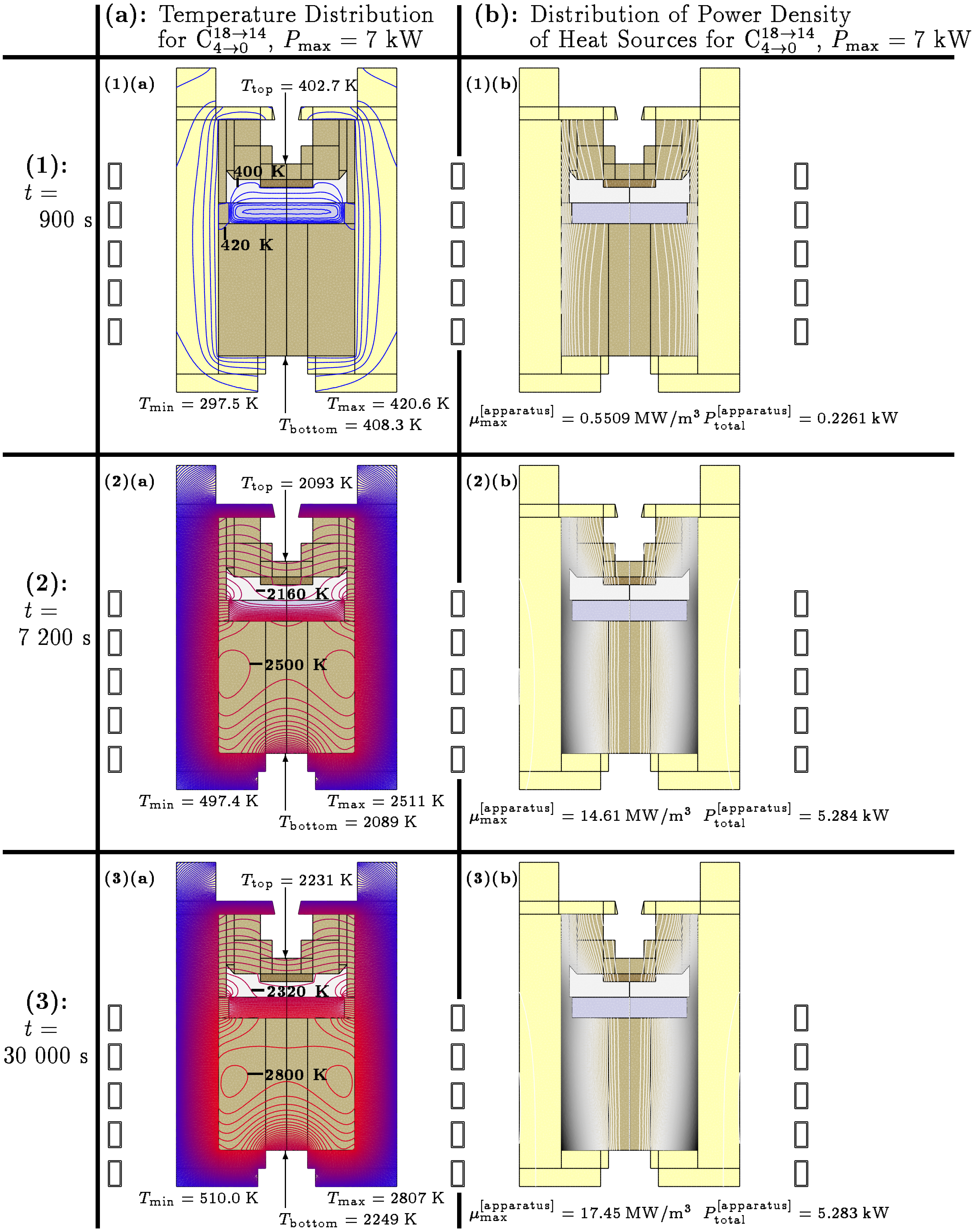


Figure 4.8: Time evolution of heating process for numerical experiment $C^{18\to14}_{4\to0}$, $P_{\max} = 7$ kW (coil moving at -1.33 cm/h). Column (a): temperature evolution, difference between neighboring isotherms is 20 K. Column (b): heat source evolution, difference between isolevels is 10 kW/m^3, darker regions indicate larger heat sources.

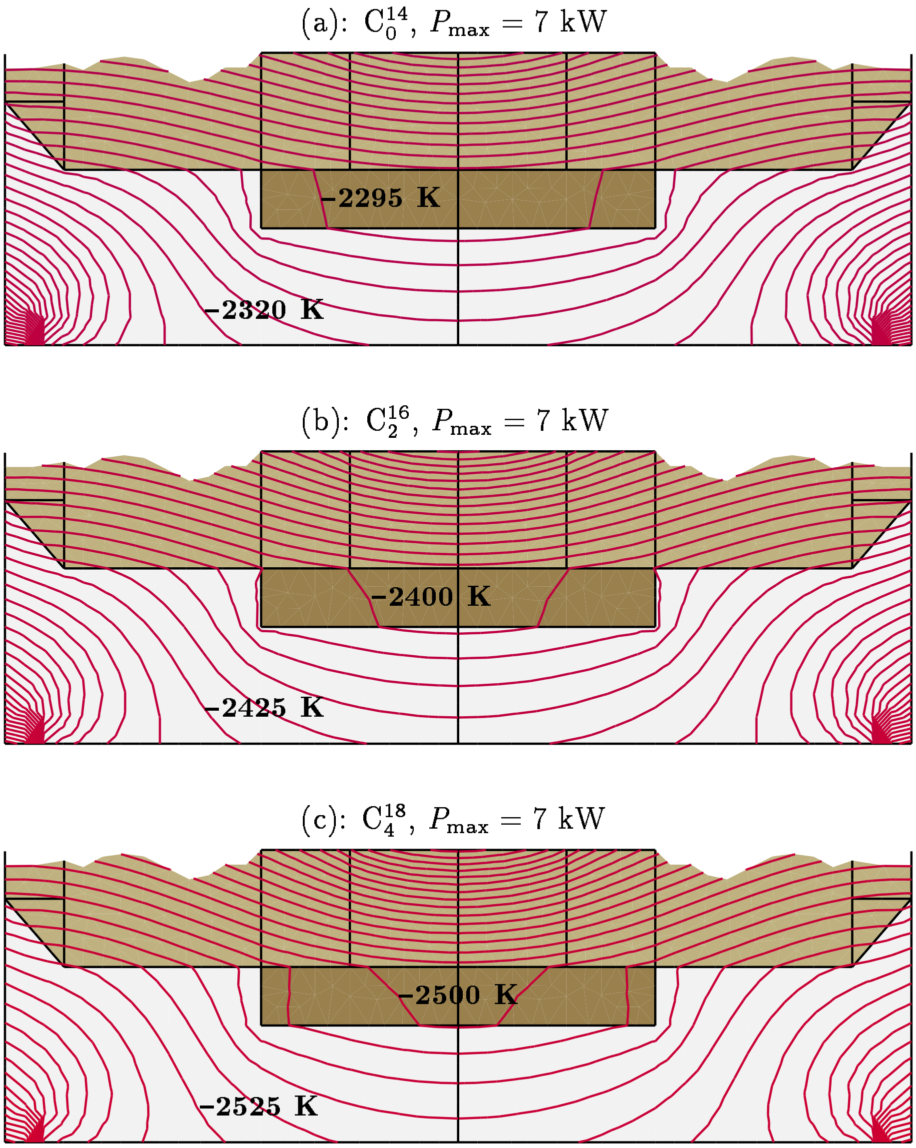


Figure 4.9: Close-ups of the temperature distribution in the crystal, the gas phase, and the crucible directly above the crystal for the quasi-stationary states at $t = 30\,000$ s of the numerical experiments C_0^{14} (in (a)), C_2^{16} (in (b)), and C_4^{18} (in (c)), where $P_{\text{max}} = 7$ kW in all three cases. Temperature difference between neighboring isotherms is 5 K.

Fig. 4.9 shows that the final temperature gradient between source and seed is nearly independent of the coil position and approximately constant along the $r = 0$ axis with a slight increase at the seed.

Appendix A

Material Data

In order to guarantee the satisfactory performance of the numerical algorithms used in the simulations , it was necessary to fit the individual segments of piecewise defined functions together smoothly. For this reason, some of the following coefficients had to be considered with a high accuracy which does not reflect the accuracy of the physical values. Figure A.1 demonstrates that e.g. restricting to six relevant digits in (A.2.2b) would result in discontinuities at $T = 500$ K and $T = 600$ K. Such discontinuities would lead to a failure of Newton's method which is used to solve the nonlinear systems of equations arising during the numerical simulations.

A.1 General Physical Constants

Boltzmann Radiation Constant: $\sigma = 5.6696 \cdot 10^{-8} \frac{\mathrm{W}}{\mathrm{m^2 K^4}}$.

Universal Gas Constant: $R = 8.31441 \frac{\mathrm{J}}{\mathrm{mol\ K}}$.

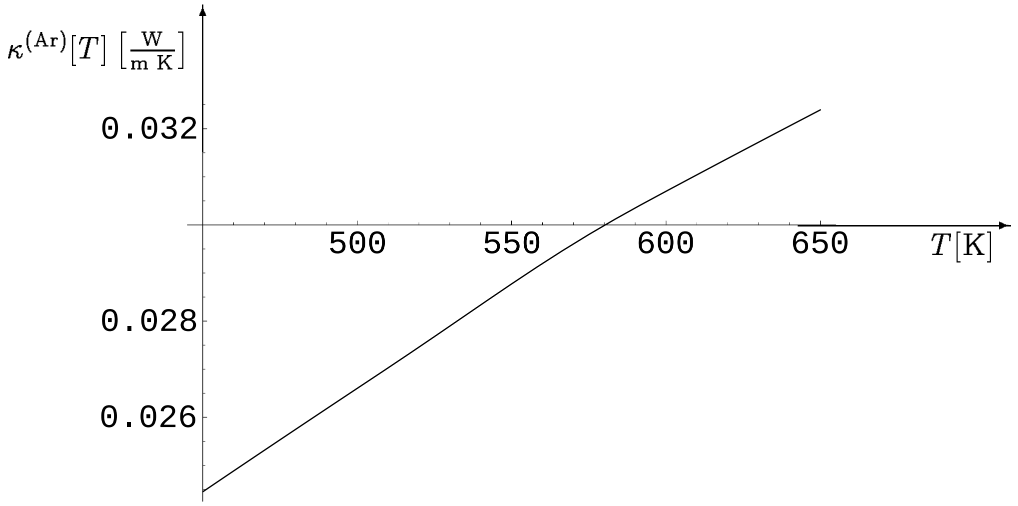
A.1.1 Molecular Masses

$M^{(\mathrm{Ar})} = 39.948 \cdot 10^{-3}\ \frac{\mathrm{kg}}{\mathrm{mol}}$, $M^{(\mathrm{C})} = 12.011 \cdot 10^{-3}\ \frac{\mathrm{kg}}{\mathrm{mol}}$, $M^{(\mathrm{H})} = 1.0078 \cdot 10^{-3}\ \frac{\mathrm{kg}}{\mathrm{mol}}$, $M^{(\mathrm{Si})} = 28.086 \cdot 10^{-3}\ \frac{\mathrm{kg}}{\mathrm{mol}}$, $M^{(\mathrm{Si_2C})} = 68.183 \cdot 10^{-3}\ \frac{\mathrm{kg}}{\mathrm{mol}}$, $M^{(\mathrm{SiC_2})} = 52.108 \cdot 10^{-3}\ \frac{\mathrm{kg}}{\mathrm{mol}}$.

A.2 Gas Phase

A.2.1 Argon

Since Ar is single-atomic, $z^{(\mathrm{Ar})} = 1.5$.



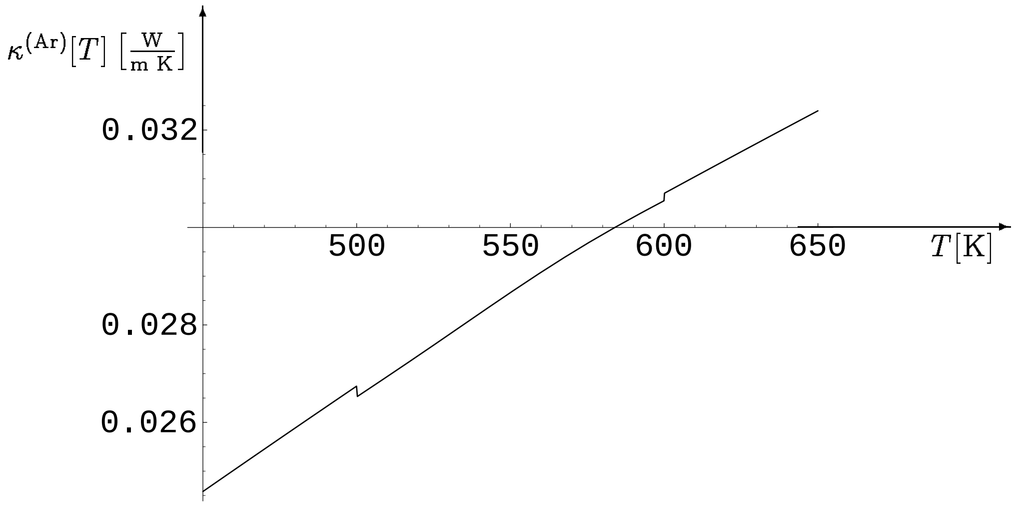


Figure A.1: Plots of $\kappa^{(\mathrm{Ar})}[T]$ over T according to (A.2.2), where in the upper plot the accuracy of the coefficients is as in (A.2.2b), and in the lower plot the accuracy of the coefficients is restricted to six relevant digits.

According to (2.1.4c) and the ideal gas law (2.1.31a), one has

$$\rho^{(\mathrm{Ar})}[(T,p)] = \frac{M^{(\mathrm{Ar})}}{R} \cdot \frac{p}{T} = 4.8047 \cdot 10^{-3}\, \frac{\mathrm{K\ s}^2}{\mathrm{m}^2} \cdot \frac{p}{T}. \tag{A.2.1}$$

In the simulations the density at $T = 2575$ K and $p^{(\mathrm{Ar})} = 2 \cdot 10^3$ Pa is used, i.e. $\rho^{(\mathrm{Ar})} = 3.73 \cdot 10^{-3}$ kg/m^3.

It remains to provide the thermal conductivity $\kappa^{(\mathrm{Ar})}$. According to [Lid95, S. 6-251], the thermal conductivity of gases changes less than one percent if the pressure is varied below normal pressure, i.e. below 10^5 Pa. Hence for the purpose of this work the thermal conductivity is considered to be independent of the pressure. For the reader's convenience, Tab. A.2.1 for $\kappa^{(\mathrm{Ar})}$ is reproduced from [Var75, p. 561].

T[K]	$\kappa\left[10^{-2}\frac{\mathrm{W}}{\mathrm{m\cdot K}}\right]$	T[K]	$\kappa\left[10^{-2}\frac{\mathrm{W}}{\mathrm{m\cdot K}}\right]$	T[K]	$\kappa\left[10^{-2}\frac{\mathrm{W}}{\mathrm{m\cdot K}}\right]$
290	1.72	520	2.75	1150	4.76
300	1.77	540	2.83	1200	4.89
310	1.82	560	2.91	1250	5.02
320	1.86	580	2.99	1300	5.14
330	1.92	600	3.07	1350	5.26
340	1.96	650	3.24	1400	5.37
350	2.00	700	3.41	1500	5.60
360	2.05	750	3.58	1600	5.83
380	2.13	800	3.74	1700	6.05
400	2.22	850	3.91	1800	6.26
420	2.30	900	4.06	1900	6.47
440	2.39	950	4.22	2000	6.67
460	2.48	1000	4.36	2500	8.00
480	2.57	1050	4.50	3000	9.10
500	2.66	1100	4.63	3500	10.20

Table A.2.1: Thermal conductivity of Ar at 10^5 Pa according to [Var75, p. 561].

The values of Tab. A.2.1 have been used to fit $\kappa^{(\mathrm{Ar})}$ as written in (A.2.2) below. Figure A.2 shows the agreement between the fitted function in (A.2.2) and the values from Tab. A.2.1.

$$\kappa^{(\mathrm{Ar})}[T] = \begin{cases} 1.83914\cdot 10^{-4}\frac{\mathrm{W}}{\mathrm{m\,K}}\left(\frac{T}{\mathrm{K}}\right)^{0.800404} & \text{for } T \le 500\ \mathrm{K}, \\ f_\kappa^{(\mathrm{Ar})}\frac{\mathrm{W}}{\mathrm{m\,K}}\left(\frac{T}{100\,\mathrm{K}}\right)^5 + e_\kappa^{(\mathrm{Ar})}\frac{\mathrm{W}}{\mathrm{m\,K}}\left(\frac{T}{100\,\mathrm{K}}\right)^4 + d_\kappa^{(\mathrm{Ar})}\frac{\mathrm{W}}{\mathrm{m\,K}}\left(\frac{T}{100\,\mathrm{K}}\right)^3 & \\ \qquad + c_\kappa^{(\mathrm{Ar})}\frac{\mathrm{W}}{\mathrm{m\,K}}\left(\frac{T}{100\,\mathrm{K}}\right)^2 + b_\kappa^{(\mathrm{Ar})}\frac{\mathrm{W}}{\mathrm{m\,K}}\left(\frac{T}{100\,\mathrm{K}}\right) & \\ \qquad + a_\kappa^{(\mathrm{Ar})}\frac{\mathrm{W}}{\mathrm{m\,K}} & \text{for } 500\ \mathrm{K} \le T \le 600\ \mathrm{K}, \\ 4.19440\cdot 10^{-4}\frac{\mathrm{W}}{\mathrm{m\,K}}\left(\frac{T}{\mathrm{K}}\right)^{0.671118} & \text{for } T \ge 600\ \mathrm{K} \end{cases} \tag{A.2.2a}$$

where

$$\begin{aligned} a_\kappa^{(\mathrm{Ar})} &= -7.1287382681160803, & b_\kappa^{(\mathrm{Ar})} &= 6.610288591812101, \\ c_\kappa^{(\mathrm{Ar})} &= -2.4408398303081513 25, & d_\kappa^{(\mathrm{Ar})} &= 0.4497633940115560911, \\ e_\kappa^{(\mathrm{Ar})} &= -0.0413251721439221090, & f_\kappa^{(\mathrm{Ar})} &= 0.001514463800685296. \end{aligned} \tag{A.2.2b}$$

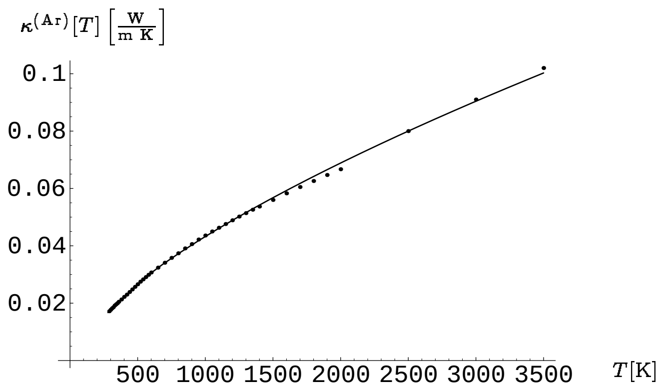


Figure A.2: Comparison of $\kappa^{(\mathrm{Ar})}[T]$ according to Tab. A.2.1 and according to (A.2.2).

A.2.2 General Estimates

The purpose of this section is to justify the following estimates (A.2.3) and (A.2.4) inside the gas mixture.

Estimates Involving Diffusion Velocities:

$$\bigwedge_{\iota \in \{1,\dots,A\}} \max\left\{\rho^{(\alpha_\iota)} \left|\left(\mathbf{u}^{(\alpha_\iota)} \otimes \mathbf{u}^{(\alpha_\iota)}\right)_{i,j}\right| : (i,j) \in \{1,2,3\}^2\right\} \ll p^{(\alpha_\iota)}, \tag{A.2.3a}$$

$$\bigwedge_{\iota \in \{1,\dots,A\}} \frac{1}{2}\left(\mathbf{u}^{(\alpha_\iota)}\right)^2 \ll \varepsilon^{(\alpha_\iota)}. \tag{A.2.3b}$$

Estimates Involving the Local Mean Velocity of the Gas Phase:

$$\max\left\{\rho_{\mathbf{gas}} \left|\left(\mathbf{v}_{\mathbf{gas}} \otimes \mathbf{v}_{\mathbf{gas}}\right)_{i,j}\right| : (i,j) \in \{1,2,3\}^2\right\} \ll p_{\mathbf{gas}}, \tag{A.2.4a}$$

$$\frac{1}{2}\left(\mathbf{v}_{\mathbf{gas}}\right)^2 \ll \varepsilon_{\mathbf{gas}}. \tag{A.2.4b}$$

Using (B.1.1), (B.1.3), the ideal gas laws (2.1.31), and (2.1.4c), it suffices to show for (A.2.3) that

$$\bigwedge_{\iota \in \{1,\dots,A\}} \ \bigwedge_{(i,j) \in \{1,2,3\}^2} \left|u_i^{(\alpha_\iota)} u_j^{(\alpha_\iota)}\right| \ll \frac{R}{M^{(\alpha_\iota)}} T_{\mathbf{gas}}. \tag{A.2.5a}$$

Using (B.1.1), (B.1.3), the ideal gas laws (2.1.32a) and (2.1.32b), and (2.1.5), it suffices to show for (A.2.4) that

$$\bigwedge_{(i,j) \in \{1,2,3\}^2} \left|\left(\mathbf{v}_{\mathbf{gas}}\right)_i \left(\mathbf{v}_{\mathbf{gas}}\right)_j\right| \ll \min\left\{\frac{R}{M^{(\alpha_\iota)}} T_{\mathbf{gas}} : \iota \in \{1,\dots,A\}\right\}. \tag{A.2.5b}$$

At the current stage of research the range of velocities occurring in PVT growth systems is still the subject of debate. In [EGG+98, Sec. 3] gas speeds of a "few meters per second" are mentioned. In [RMD+99, Fig. 2] simulated velocity fields are depicted showing speeds well below a few meters per second. In any case, the following estimates should be rather conservative:

$$\bigwedge_{\iota\in\{1,\dots,A\}} \bigwedge_{(i,j)\in\{1,2,3\}^2} \left|u_i^{(\alpha_\iota)} u_j^{(\alpha_\iota)}\right| \leq 10\frac{\mathrm{m}^2}{\mathrm{s}^2}, \tag{A.2.6a}$$

$$\bigwedge_{(i,j)\in\{1,2,3\}^2} \left|(\mathbf{v}_{\mathrm{gas}})_i\,(\mathbf{v}_{\mathrm{gas}})_j\right| \leq 10\frac{\mathrm{m}^2}{\mathrm{s}^2}. \tag{A.2.6b}$$

As Ar, Si, Si_2C, and SiC_2 are the predominant gas species, let $\alpha_1 := \mathrm{Ar}$, $\alpha_2 := \mathrm{Si}$, $\alpha_3 := \mathrm{Si_2C}$, and $\alpha_4 := \mathrm{SiC_2}$, $I_{\mathrm{gas}} := \{1,2,3,4\}$.

Then $M^{(\alpha_\iota)} < 0.1\,\frac{\mathrm{kg}}{\mathrm{mol}}$ for each $\iota \in I_{\mathrm{gas}}$ according to App. A.1.1. Combining this with an assumed temperature range of $290\,\mathrm{K} \leq T_{\mathrm{gas}} \leq 3000\,\mathrm{K}$ yields

$$\bigwedge_{\iota\in\{1,\dots,A\}} 20\,000\,\frac{\mathrm{m}^2}{\mathrm{s}^2} < \frac{R}{M^{(\alpha_\iota)}} T_{\mathrm{gas}}. \tag{A.2.7}$$

Now (A.2.6) and (A.2.7) show that (A.2.5) (and hence also (A.2.3) and (A.2.4)) hold.

A.3 Solid Materials

The growth apparatus used to conduct the numerical experiments presented in Ch. 4 employs the following solid components: A porous graphite crucible referred to as "Crucible", graphite soft felt sheets for thermal insulation referred to as "Insulation", silicon carbide source powder referred to as "SiC-Powder", and the silicon carbide single crystal referred to as "SiC-Crystal" (see Fig. 4.1). Moreover, the copper (Cu) induction coil is needed in the heat source computations, but is outside the domain where the temperature field is simulated.

Each solid material β of the apparatus is specified by the following potentially temperature dependent functions: mass density $\rho^{[\beta]}[T]$, thermal conductivity $\kappa^{[\beta]}[T]$, specific heat $c_{\mathrm{sp}}^{[\beta]}[T]$, emissivity $\varepsilon^{[\beta]}[T]$, and electrical conductivity $\sigma_{\mathrm{c}}^{[\beta]}[T]$.

To compute the magnetic scalar potential in the Cu induction coil, the only material parameters needed are $\rho^{[\mathrm{Cu}]}$ and $\sigma_{\mathrm{c}}^{[\mathrm{Cu}]}$. No temperature dependence needs to be considered, as the induction coil is virtually kept at room temperature by an effective water cooling system.

A.3.1 Copper

The material parameters for Cu at room temperature used for the induction coil are

$$\rho^{[\mathrm{Cu}]} = 8930 \frac{\mathrm{kg}}{\mathrm{m}^3}, \tag{A.3.1a}$$

$$\sigma_{\mathrm{c}}^{[\mathrm{Cu}]} = (1.7 \cdot 10^{-8}\ \Omega\mathrm{m})^{-1} = 5.9 \cdot 10^7 \frac{1}{\Omega\mathrm{m}}. \tag{A.3.1b}$$

The values for $\rho^{[\mathrm{Cu}]}$ and $\sigma_{\mathrm{c}}^{[\mathrm{Cu}]}$ are according to [Ben90].

A.3.2 Graphite Crucible

The material parameters for graphite used for the graphite crucible are

$$\rho^{[\mathrm{Crucible}]}[T] = 1750 \frac{\mathrm{kg}}{\mathrm{m}^3}, \tag{A.3.2a}$$

$$\sigma_{\mathrm{c}}^{[\mathrm{Crucible}]}[T] = \left(28.9 - 18.8 \cdot \exp\left[-\left(\frac{\ln\left[\frac{T}{1023\,\mathrm{K}}\right]}{2.37}\right)^2\right]\right)^{-1} \frac{10^6}{\Omega\mathrm{m}}, \tag{A.3.2b}$$

$$\kappa^{[\mathrm{Crucible}]}[T] = 37.7158 \frac{\mathrm{W}}{\mathrm{m\ K}} e^{-1.96095 \cdot 10^{-4} \frac{T}{\mathrm{K}}}, \tag{A.3.2c}$$

$$c_{\mathrm{sp}}^{[\mathrm{Crucible}]}[T] = \frac{\frac{\mathrm{J}}{\mathrm{kg\ K}}}{441.12 \left[\frac{T}{\mathrm{K}}\right]^{-2.30676} + 7.97093 \cdot 10^{-4} \left[\frac{T}{\mathrm{K}}\right]^{-6.65256 \cdot 10^{-2}}}, \tag{A.3.2d}$$

$$\varepsilon^{[\mathrm{Crucible}]}[T] = \begin{cases} 0.67 & \text{for } T \le 1200\ \mathrm{K}, \\ e_\varepsilon^{[\mathrm{Crucible}]} \left[\frac{T}{\mathrm{K}}\right]^4 + d_\varepsilon^{[\mathrm{Crucible}]} \left[\frac{T}{\mathrm{K}}\right]^3 + c_\varepsilon^{[\mathrm{Crucible}]} \left[\frac{T}{\mathrm{K}}\right]^2 & \\ \qquad + b_\varepsilon^{[\mathrm{Crucible}]} \left[\frac{T}{\mathrm{K}}\right] + a_\varepsilon^{[\mathrm{Crucible}]} & \text{for } 1200\ \mathrm{K} \le T \le 2200\ \mathrm{K}, \\ 0.79 & \text{for } T \ge 2200\ \mathrm{K} \end{cases} \tag{A.3.2e}$$

where $a_\varepsilon^{[\mathrm{Crucible}]} = \frac{46901}{125} \cdot 10^{-2}$, $b_\varepsilon^{[\mathrm{Crucible}]} = -\frac{1859}{25} \cdot 10^{-4}$, $c_\varepsilon^{[\mathrm{Crucible}]} = \frac{19249}{3} \cdot 10^{-9}$, $d_\varepsilon^{[\mathrm{Crucible}]} = -\frac{701}{3} \cdot 10^{-11}$, $e_\varepsilon^{[\mathrm{Crucible}]} = \frac{37}{12} \cdot 10^{-13}$.

The references for $\rho^{[\mathrm{Crucible}]}$ and $\sigma_{\mathrm{c}}^{[\mathrm{Crucible}]}$ are [MSS99a] and [Hus84], respectively. The functions for $\kappa^{[\mathrm{Crucible}]}$ and $\varepsilon^{[\mathrm{Crucible}]}$ have been fitted using Tables A.1 and A.2, respectively, which contain data as given by [MSS99a]. Since [Lid95, p. 10-297] states that the range of emissivity of graphite is between 0.7 and 0.8 if $0 \le T \le 3600$ K, it seems reasonable to extrapolate Tab. A.2 by a constant function for low and high temperatures. Figure A.3 relates the values of Tab. A.1 to (A.3.2c), and Fig. A.4 does likewise for Tab. A.2 and (A.3.2e). The function for $c_{\mathrm{sp}}^{[\mathrm{Crucible}]}$ has been fitted according to the data in [BK73, p. 209], reproduced in Tab. A.3.2. Figure A.5 depicts the fitted function (A.3.2d) together with the data of Tab. A.3.2.

T[K]	1000	1200	1400	1600	1800	2000	2200
$\kappa^{[\text{Crucible}]}\left[\frac{\text{W}}{\text{m K}}\right]$	31.0	29.5	28.5	27.0	26.5	25.5	24.5

Table A.1: Thermal conductivity of graphite crucible according to [MSS99a].

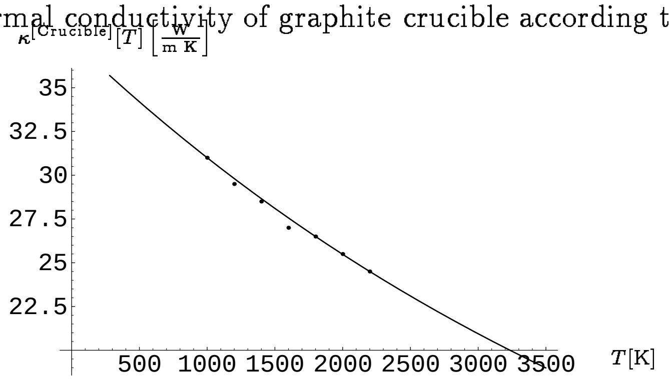


Figure A.3: Comparison between $\kappa^{[\text{Crucible}]}[T]$ according to Tab. A.1 and according to (A.3.2c).

T[K]	1200	1400	1600	1800	2000	2200
ε	0.67	0.69	0.73	0.76	0.77	0.79

Table A.2: Emissivity of graphite crucible according to [MSS99a].

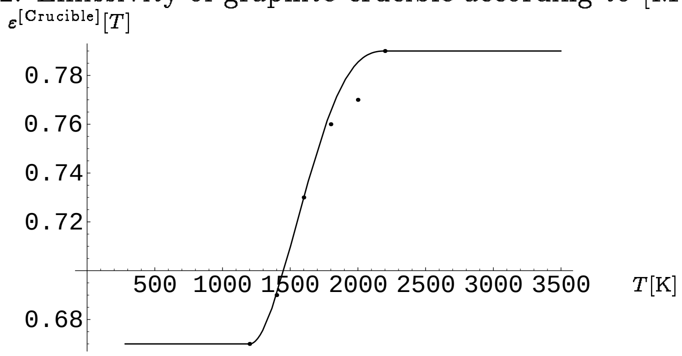


Figure A.4: Comparison between $\varepsilon^{[\text{Crucible}]}[T]$ according to Tab. A.1 and according to (A.3.2e).

A.3.3 Graphite Felt Insulation

The material parameters for graphite felt used as thermal insulation are

$$\rho^{[\text{Insulation}]}[T] = 170\frac{\text{kg}}{\text{m}^3}, \tag{A.3.3a}$$

T[K]	c_{sp} $\left[\frac{J}{kg\,K}\right]$	T[K]	c_{sp} $\left[\frac{J}{kg\,K}\right]$	T[K]	c_{sp} $\left[\frac{J}{kg\,K}\right]$
298.15	709.3	1400.00	1954.4	2600.00	2089.3
300.00	716.2	1500.00	1977.1	2700.00	2095.2
400.00	993.9	1600.00	1995.5	2800.00	2100.9
500.00	1219.4	1700.00	2010.6	2900.00	2106.5
600.00	1407.0	1800.00	2023.2	3000.00	2112.0
700.00	1549.2	1900.00	2034.2	3100.00	2117.4
800.00	1652.3	2000.00	2044.4	3200.00	2122.8
900.00	1732.7	2100.00	2054.0	3300.00	2128.1
1000.00	1797.2	2200.00	2062.1	3400.00	2133.4
1100.00	1849.3	2300.00	2069.6	3500.00	2138.8
1200.00	1891.8	2400.00	2076.6	3600.00	2144.2
1300.00	1926.4	2500.00	2083.1	3700.00	2149.6

Table A.3.2: Specific heat of graphite according to [BK73, p. 209].

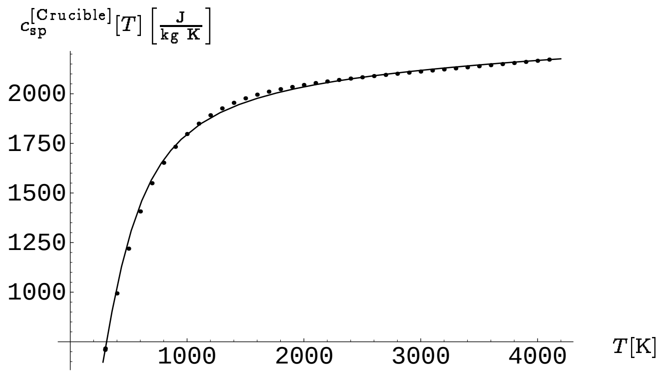


Figure A.5: Comparison between $c_{sp}^{[\text{Crucible}]}[T]$ according to Tab. A.3.2 and according to (A.3.2d).

$$\sigma_c^{[\text{Insulation}]}[T] = \frac{245.7}{1+\frac{T}{2500\,\text{K}}}\,\frac{1}{\Omega\text{m}}, \tag{A.3.3b}$$

$$\kappa^{[\text{Insulation}]}[T] = \begin{cases} \left(8.1759\cdot 10^{-2} + 2.48571\cdot 10^{-4}\frac{T}{\text{K}}\right)\frac{\text{W}}{\text{m K}} & \text{for } T \le 1473\text{ K}, \\ f_\kappa^{[\text{Insulation}]}\frac{\text{W}}{\text{m K}}\left(\frac{T}{\text{K}}\right)^5 + e_\kappa^{[\text{Insulation}]}\frac{\text{W}}{\text{m K}}\left(\frac{T}{\text{K}}\right)^4 & \\ \quad + d_\kappa^{[\text{Insulation}]}\frac{\text{W}}{\text{m K}}\left(\frac{T}{\text{K}}\right)^3 + c_\kappa^{[\text{Insulation}]}\frac{\text{W}}{\text{m K}}\left(\frac{T}{\text{K}}\right)^2 & \\ \quad + b_\kappa^{[\text{Insulation}]}\frac{\text{W}}{\text{m K}}\cdot\frac{T}{\text{K}} & \\ \quad + a_\kappa^{[\text{Insulation}]}\frac{\text{W}}{\text{m K}} & \text{for } 1473\text{ K} \le T \le 1873\text{ K}, \\ \left(-0.74475 + 7.5\cdot 10^{-4}\frac{T}{\text{K}}\right)\frac{\text{W}}{\text{m K}} & \text{for } T \ge 1873\text{ K}, \end{cases} \tag{A.3.3c}$$

$$c_{\text{sp}}^{[\text{Insulation}]}[T] = 2100 \frac{\text{J}}{\text{kg K}}, \tag{A.3.3d}$$
$$\varepsilon^{[\text{Insulation}]}[T] = 0.53 \tag{A.3.3e}$$

where

$$a_{\kappa}^{[\text{Insulation}]} = -\frac{6093962923083737740835\,43}{512} \cdot 10^{-19}, \tag{A.3.4a}$$
$$b_{\kappa}^{[\text{Insulation}]} = \frac{3551631314827782041\,91}{1024} \cdot 10^{-18}, \tag{A.3.4b}$$
$$c_{\kappa}^{[\text{Insulation}]} = -\frac{204652204018369767}{512} \cdot 10^{-18}, \tag{A.3.4c}$$
$$d_{\kappa}^{[\text{Insulation}]} = \frac{116893623135279}{512} \cdot 10^{-18}, \tag{A.3.4d}$$
$$e_{\kappa}^{[\text{Insulation}]} = -\frac{66155269623}{1024} \cdot 10^{-18}, \tag{A.3.4e}$$
$$f_{\kappa}^{[\text{Insulation}]} = \frac{37145151}{512} \cdot 10^{-19}. \tag{A.3.4f}$$

The quantities $\rho^{[\text{Insulation}]}$ and $\kappa^{[\text{Insulation}]}$ are provided by [MSS99a], where the function for $\kappa^{[\text{Insulation}]}$ was fitted using the data in Tab. A.3. Figure A.6 displays (A.3.3c) in comparison with Tab. A.3. The quantities $\sigma_{\text{c}}^{[\text{Insulation}]}$ and $c_{\text{sp}}^{[\text{Insulation}]}$ are according to [Råb96] and [MSS99b], respectively. Since no data for the emissivity of graphite felt were available, the value given for carbon filament in [Lid95, p. 10-297] was used.

T[K]	673	873	1073	1273	1473	1673	1873	2073	2273
$\kappa\ \left[\frac{\text{W}}{\text{m K}}\right]$	0.25	0.3	0.35	0.39	0.45	0.5	0.67	0.82	0.95

Table A.3: Thermal conductivity of graphite felt according to [MSS99a].

A.3.4 SiC Source Powder

The material parameters for SiC source powder are

$$\rho^{[\text{SiC-Powder}]}[T] = 1700 \frac{\text{kg}}{\text{m}^3}, \tag{A.3.5a}$$
$$\sigma_{\text{c}}^{[\text{SiC-Powder}]}[T] = 100\ \frac{1}{\Omega\text{m}}, \tag{A.3.5b}$$

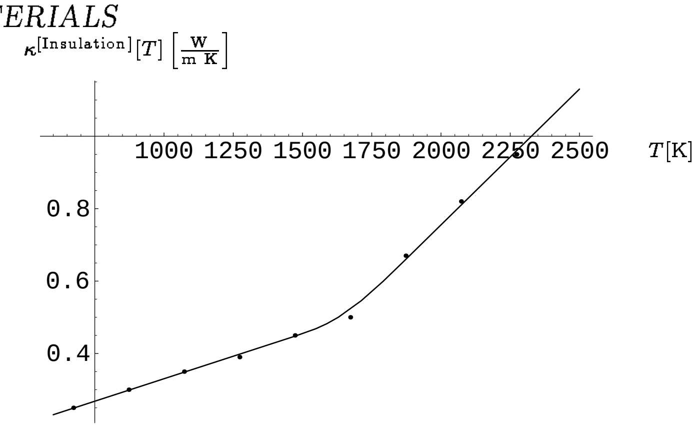


Figure A.6: Comparison between $\kappa^{[\text{Insulation}]}[T]$ according to Tab. A.3 and according to (A.3.3c).

$$\kappa^{[\text{SiC-Powder}]}[T] = 6.83991 \cdot 10^{-3}\, e^{\frac{1.07296\cdot 10^{-3}\, T}{\text{K}}}\, \frac{\text{W}}{\text{m K}}, \tag{A.3.5c}$$

$$c_{\text{sp}}^{[\text{SiC-Powder}]}[T] = 1000 \frac{\text{J}}{\text{kg K}}, \tag{A.3.5d}$$

$$\varepsilon^{[\text{SiC-Powder}]}[T] = 0.85. \tag{A.3.5e}$$

The values in (A.3.5a) and (A.3.5d) are according to [MSS99b], whereas $\sigma_{\text{c}}^{[\text{SiC-Powder}]}$ is according to [Råb96]. The data for $\varepsilon^{[\text{SiC-Powder}]}$ provided by [TdW72, p. 793] vary between 0.3 and 0.9, most data points displayed in the range between 0.8 and 0.9. Thus (A.3.5e) seems to be a reasonable assumption. The dependence of the thermal conductivity of SiC powder on its porosity, its particle sizes, its transmissivity and the ambient gas pressure is described in [KRRS98]. The common features of the presented results are that the range of the thermal conductivity lies between $5 \cdot 10^{-3} \frac{\text{W}}{\text{m K}}$ and $5 \cdot 10^{-1} \frac{\text{W}}{\text{m K}}$ and that the thermal conductivity usually increases with temperature. In absence of precise data for the porosity and particle size of SiC powder used in actual growth experiments, the simple approximation given in (A.3.5c) is used. It is noted that the source graphitizes and sinters during a growth run, resulting in considerable changes of emissivity, porosity and thermal conductivity, which are not reflected in the data (A.3.5) and which were not accounted for in the simulations of Ch. 4.

A.3.5 SiC Single Crystal

The material parameters for the SiC single crystal are

$$\rho^{[\text{SiC-Crystal}]}[T] = 3140 \frac{\text{kg}}{\text{m}^3}, \tag{A.3.6a}$$

$$\sigma_{\text{c}}^{[\text{SiC-Crystal}]}[T] = 10^5\, \frac{1}{\Omega\text{m}}, \tag{A.3.6b}$$

$$\kappa^{[\text{SiC-Crystal}]}[T] = \frac{61100}{\frac{T}{\text{K}} - 115}\, \frac{\text{W}}{\text{m K}}, \tag{A.3.6c}$$

$$c_{\mathrm{sp}}^{[\text{SiC-Crystal}]}[T] = \frac{\frac{\mathrm{J}}{\mathrm{kg\,K}}}{39161\left(\frac{T}{\mathrm{K}}\right)^{-3.17377} + 1.83598\cdot 10^{-3}\left(\frac{T}{\mathrm{K}}\right)^{-0.117995}}, \tag{A.3.6d}$$

$$\varepsilon^{[\text{SiC-Crystal}]}[(T,\lambda)] = 0.85 \quad \text{on} \quad I_{\mathrm{r}}. \tag{A.3.6e}$$

The quantities $\rho^{[\text{SiC-Crystal}]}$ and $\kappa^{[\text{SiC-Crystal}]}$ are according to [NMH+97], while $\sigma_{\mathrm{c}}^{[\text{SiC}-\text{Crystal}]}$ is according to [Råb96]. The function for $c_{\mathrm{sp}}^{[\text{SiC}-\text{Crystal}]}$ has been fitted using the data in Tab. A.3.5 which are reproduced from [BK73, p. 1342]. The fit (A.3.6d) and the data from Tab. A.3.5 are related in Fig. A.7. In absence of other data the constant value from (A.3.5e) for the emissivity $\varepsilon^{[\text{SiC-Crystal}]}(T,\lambda)$ in the reflective band I_{r} is used. As mentioned in [BK90, p. 2833], the energy gap for the 6H polytype shifts from 3 eV (corresponding to $I_{\mathrm{r}} = [0, 413\ \mathrm{nm}]$) at 300 K to some 2.5 eV (corresponding to $I_{\mathrm{r}} = [0, 495\ \mathrm{nm}]$) at 2400 K, indicating that the energy-band model of semi-transparency is not completely accurate if the range of temperatures is large. In the simulations of Ch. 4 it is assumed that the band of wavelengths interacting with the crystal is $I_{\mathrm{r}} = [1\,\mathrm{nm}, 500\,\mathrm{nm}]$.

T[K]	$c_{\mathrm{sp}}\left[\frac{\mathrm{J}}{\mathrm{kg\,K}}\right]$	T[K]	$c_{\mathrm{sp}}\left[\frac{\mathrm{J}}{\mathrm{kg\,K}}\right]$	T[K]	$c_{\mathrm{sp}}\left[\frac{\mathrm{J}}{\mathrm{kg\,K}}\right]$
298.15	672.8	1300.00	1266.6	2400.00	1363.6
300.00	675.7	1400.00	1279.6	2500.00	1369.9
400.00	838.9	1500.00	1291.1	2600.00	1376.1
500.00	963.8	1600.00	1301.5	2700.00	1382.2
600.00	1049.7	1700.00	1311.1	2800.00	1388.1
700.00	1109.9	1800.00	1319.8	2900.00	1393.9
800.00	1153.8	1900.00	1328.1	3000.00	1399.7
900.00	1187.0	2000.00	1335.8	3100.00	1405.3
1000.00	1213.0	2100.00	1343.2	3200.00	1410.9
1100.00	1234.1	2200.00	1350.2	3245.00	1413.4
1200.00	1251.7	2300.00	1357.0		

Table A.3.5: Specific heat of SiC crystal according to [BK73, p. 1342].

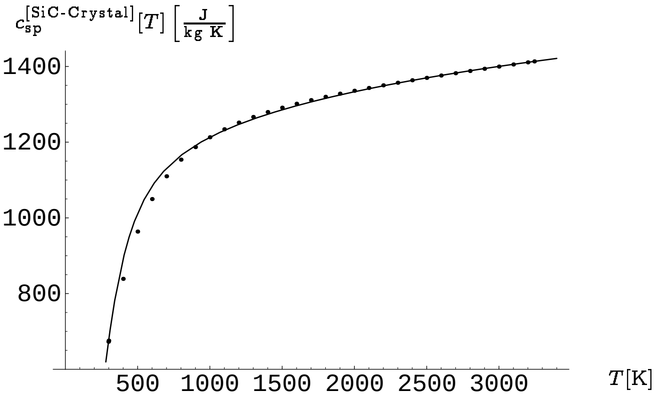


Figure A.7: Comparison between $c_{sp}^{[\mathrm{SiC\text{-}Crystal}]}[T]$ according to Tab. A.3.5 and according to (A.3.6d).

Appendix B

Formulas and Computations

B.1 Vectors, Tensors, and Differential Operators

The setting of this section is a finite dimensional real vector space $\mathcal{V} = \mathbb{R}^I$, where I is a finite index set. In the physical applications in Ch. 2, $\mathbb{R}^I$ consists of the three-dimensional domain of physical space coordinates.

In the present section vectors are elements of $\mathcal{V}$, and tensors are elements of $\mathbb{R}^{I\times I} \cong \mathrm{Lin}(\mathcal{V},\mathcal{V})$. Vectors are denoted by $\mathbf{u} = (u_i)_{i\in I}$, $\mathbf{v} = (v_i)_{i\in I}$, and tensors are denoted by $\mathbf{A} = (a_{i,j})_{(i,j)\in I\times I}$, $\mathbf{B} = (b_{i,j})_{(i,j)\in I\times I}$. The notation $\mathbf{Av}$ means that $\mathbf{A}$ is applied to $\mathbf{v}$ in the sense of matrix multiplication, where $\mathbf{v}$ is considered as a column vector.

For the purposes of this work it is convenient to define the scalar product for three situations, namely for two vectors, for two tensors, and for a vector and a tensor (see Def. B.1.1). In the first two cases the result is a scalar, whereas in abuse of its name it is a vector in the third case.

Definition B.1.1. Let $\mathbf{u}$, $\mathbf{v}$ be vectors, and let $\mathbf{A}$, $\mathbf{B}$ be tensors. The *scalar product* is defined by

$$\mathbf{u}\bullet\mathbf{v} := \sum_{i\in I} a_i b_i, \quad \mathbf{A}\bullet\mathbf{B} := \sum_{(i,j)\in I\times I} a_{i,j} b_{i,j}, \quad \mathbf{u}\bullet\mathbf{A} := \mathbf{A}\bullet\mathbf{u} := \left(\sum_{j\in I} v_j a_{j,i}\right)_{i\in I}. \tag{B.1.1}$$

The abbreviation $\mathbf{u}^2$ is used for $\mathbf{u}\bullet\mathbf{u}$.

Remark B.1.2. The scalar product has the following elementary properties:

(a) Commutativity: $\mathbf{u}\bullet\mathbf{v} = \mathbf{v}\bullet\mathbf{u}$, $\quad \mathbf{A}\bullet\mathbf{B} = \mathbf{B}\bullet\mathbf{A}$, $\quad \mathbf{u}\bullet\mathbf{A} = \mathbf{A}\bullet\mathbf{u}$.

(b) Bilinearity: For scalars λ, μ, one has

$$(\lambda\mathbf{u}^{(1)} + \mu\mathbf{u}^{(2)})\bullet\mathbf{v} = \lambda(\mathbf{u}^{(1)}\bullet\mathbf{v}) + \mu(\mathbf{u}^{(2)}\bullet\mathbf{v}), \tag{B.1.2a}$$

$$\mathbf{u} \bullet (\lambda \mathbf{v}^{(1)} + \mu \mathbf{v}^{(2)}) = \lambda(\mathbf{u} \bullet \mathbf{v}^{(1)}) + \mu(\mathbf{u} \bullet \mathbf{v}^{(2)}), \tag{B.1.2b}$$

and analogously for the scalar product of two vectors and for the scalar product of one vector and one tensor.

Definition B.1.3. The *tensor product* of two vectors $\mathbf{u}$, $\mathbf{v}$ is defined by

$$\mathbf{u} \otimes \mathbf{v} := (u_i v_j)_{(i,j) \in I \times I}. \tag{B.1.3}$$

Remark B.1.4. The tensor product is bilinear, i.e. for scalars λ, μ, one has

$$(\lambda \mathbf{u}^{(1)} + \mu \mathbf{u}^{(2)}) \otimes \mathbf{v} = \lambda(\mathbf{u}^{(1)} \otimes \mathbf{v}) + \mu(\mathbf{u}^{(2)} \otimes \mathbf{v}), \tag{B.1.4a}$$

$$\mathbf{u} \otimes (\lambda \mathbf{v}^{(1)} + \mu \mathbf{v}^{(2)}) = \lambda(\mathbf{u} \otimes \mathbf{v}^{(1)}) + \mu(\mathbf{u} \otimes \mathbf{v}^{(2)}). \tag{B.1.4b}$$

Remark B.1.5. For vectors $\mathbf{u}$, $\mathbf{v}$ it holds that

$$(\mathbf{u} \otimes \mathbf{u})\mathbf{v} = (\mathbf{u} \bullet \mathbf{v})\mathbf{u}. \tag{B.1.5}$$

In Def. B.1.6 the differential operators ∇ and div are defined. The gradient of a scalar is a vector, the gradient of a vector is a tensor, the divergence of a vector is a scalar, and the divergence of a tensor is a vector.

Definition B.1.6. The *gradient* ∇ and the divergence div are defined as follows:

$$\nabla : C^1[\mathcal{V}] \longrightarrow C(\mathcal{V}, \mathcal{V}), \qquad \nabla f := (\partial_i f)_{i \in I}, \tag{B.1.6a}$$

$$\nabla : C^1(\mathcal{V}, \mathcal{V}) \longrightarrow C\big(\mathcal{V}, \mathrm{Lin}(\mathcal{V}, \mathcal{V})\big), \qquad \nabla \mathbf{u} := (\partial_i u_j)_{(i,j) \in I \times I}, \tag{B.1.6b}$$

$$\mathrm{div} : C^1(\mathcal{V}, \mathcal{V}) \longrightarrow C[\mathcal{V}], \qquad \mathrm{div}\, \mathbf{u} := \sum_{i \in I} \partial_i v_i, \tag{B.1.6c}$$

$$\mathrm{div} : C^1\big(\mathcal{V}, \mathrm{Lin}(\mathcal{V}, \mathcal{V})\big) \longrightarrow C(\mathcal{V}, \mathcal{V}), \qquad \mathrm{div}\, \mathbf{A} := \left(\sum_{j \in I} \partial_j a_{i,j}\right)_{i \in I}. \tag{B.1.6d}$$

Remark B.1.7. The gradient and the divergence are linear operators.

Remark B.1.8. Product rules for the gradient: If $(f, g) \in (C^1[\mathcal{V}])^2$, $\mathbf{u} \in C^1(\mathcal{V}, \mathcal{V})$, and $\mathbf{v} \in \mathcal{F}(\mathcal{V}, \mathcal{V})$ then

$$\nabla(fg) = f \nabla g + g \nabla f, \tag{B.1.7a}$$

$$\mathbf{v} \bullet \nabla(f\mathbf{u}) = f\mathbf{v} \bullet \nabla \mathbf{u} + (\mathbf{v} \bullet \nabla f)\mathbf{u}, \tag{B.1.7b}$$

$$\mathbf{v} \bullet \nabla(f\mathbf{u}^2) = \mathbf{u}^2(\mathbf{v} \bullet \nabla f) + 2\mathbf{u} \bullet (f\mathbf{v} \bullet \nabla \mathbf{u}). \tag{B.1.7c}$$

Remark B.1.9. Product rules for the divergence: If $f \in C^1[\mathcal{V}]$ and $\mathbf{u} \in C^1(\mathcal{V}, \mathcal{V})$, then

$$\mathrm{div}(f\mathbf{u}) = \mathbf{u} \bullet \nabla f + f\, \mathrm{div}\, \mathbf{u}. \tag{B.1.8a}$$

If $\mathbf{u} \in C^1(\mathcal{V},\mathcal{V})$ and $\mathbf{A} \in C^1\big(\mathcal{V}, \mathrm{Lin}(\mathcal{V},\mathcal{V})\big)$ such that $\mathbf{A}[\mathbf{v}]$ is symmetric for each $\mathbf{v} \in \mathcal{V}$, then

$$\operatorname{div}(\mathbf{A}\mathbf{u}) = \mathbf{u} \bullet \operatorname{div} \mathbf{A} + \mathbf{A} \bullet \nabla \mathbf{u}. \tag{B.1.8b}$$

If $\mathbf{u} \in C^1(\mathcal{V},\mathcal{V})$, $\mathbf{v} \in C^1(\mathcal{V},\mathcal{V})$, and $\mathbf{w} \in \mathcal{F}(\mathcal{V},\mathcal{V})$, then

$$\operatorname{div}\left(\mathbf{v}^2\mathbf{u}\right) = \mathbf{v}^2 \operatorname{div} \mathbf{u} + 2\cdot(\mathbf{u}\otimes\mathbf{v}) \bullet \nabla \mathbf{v}, \tag{B.1.8c}$$

$$\operatorname{div}(\mathbf{u}\otimes\mathbf{v}) = (\operatorname{div}\mathbf{v})\mathbf{u} + \mathbf{v} \bullet \nabla \mathbf{u}, \tag{B.1.8d}$$

$$\mathbf{w} \bullet \operatorname{div}(\mathbf{v}\otimes\mathbf{u}) = (\mathbf{v}\bullet\mathbf{w}) \operatorname{div}\mathbf{u} + (\mathbf{u}\otimes\mathbf{w}) \bullet \nabla \mathbf{v}. \tag{B.1.8e}$$

B.2 Balance and Field Equations

B.2.1 Some Identities

Lemma B.2.1. *If* (2.1.4) *and* (2.1.6) *are satisfied, then the following identities hold true:*

$$\sum_{\iota=1}^{A} \rho^{(\alpha_\iota)}\mathbf{u}^{(\alpha_\iota)} = \sum_{\iota=1}^{A} \rho^{(\alpha_\iota)}\left(\mathbf{v}^{(\alpha_\iota)} - \mathbf{v}_{\mathbf{gas}}\right) = 0, \tag{B.2.1}$$

$$\sum_{\iota=1}^{A} \rho^{(\alpha_\iota)}\left(\mathbf{b}^{(\alpha_\iota)} \bullet \mathbf{v}^{(\alpha_\iota)} + r^{(\alpha_\iota)}\right) = \rho_{\mathbf{gas}}\mathbf{b}_{\mathbf{gas}} \bullet \mathbf{v}_{\mathbf{gas}} + \rho_{\mathbf{gas}} r_{\mathbf{gas}}, \tag{B.2.2}$$

$$\bigwedge_{\iota\in\{1,\dots,A\}} \left(\mathbf{u}^{(\alpha_\iota)}\right)^2 = \left(\mathbf{v}^{(\alpha_\iota)}\right)^2 - 2\cdot\mathbf{v}^{(\alpha_\iota)} \bullet \mathbf{v}_{\mathbf{gas}} + \left(\mathbf{v}_{\mathbf{gas}}\right)^2, \tag{B.2.3}$$

$$\bigwedge_{\iota\in\{1,\dots,A\}} \begin{pmatrix} \mathbf{u}^{(\alpha_\iota)} \otimes \mathbf{u}^{(\alpha_\iota)} \\ = \mathbf{v}^{(\alpha_\iota)} \otimes \mathbf{v}^{(\alpha_\iota)} - \mathbf{v}^{(\alpha_\iota)} \otimes \mathbf{v}_{\mathbf{gas}} - \mathbf{v}_{\mathbf{gas}} \otimes \mathbf{v}^{(\alpha_\iota)} + \mathbf{v}_{\mathbf{gas}} \otimes \mathbf{v}_{\mathbf{gas}} \end{pmatrix}, \tag{B.2.4}$$

$$\sum_{\iota=1}^{A} \rho^{(\alpha_\iota)}\left(\mathbf{u}^{(\alpha_\iota)}\right)^2\mathbf{u}^{(\alpha_\iota)} = \sum_{\iota=1}^{A} \rho^{(\alpha_\iota)}\left(\mathbf{v}^{(\alpha_\iota)}\right)^2\mathbf{u}^{(\alpha_\iota)} - 2\cdot\sum_{\iota=1}^{A} \rho^{(\alpha_\iota)}\left(\mathbf{v}^{(\alpha_\iota)} \bullet \mathbf{v}_{\mathbf{gas}}\right)\mathbf{u}^{(\alpha_\iota)}, \tag{B.2.5}$$

$$\sum_{\iota=1}^{A} \rho^{(\alpha_\iota)}\left(\left(\mathbf{v}^{(\alpha_\iota)}\right)^2 - \left(\mathbf{u}^{(\alpha_\iota)}\right)^2\right) = \rho_{\mathbf{gas}}\left(\mathbf{v}_{\mathbf{gas}}\right)^2, \tag{B.2.6}$$

$$\sum_{\iota=1}^{A} \rho^{(\alpha_\iota)}\left(\mathbf{v}^{(\alpha_\iota)} \otimes \mathbf{v}^{(\alpha_\iota)} - \mathbf{u}^{(\alpha_\iota)} \otimes \mathbf{u}^{(\alpha_\iota)}\right) = \rho_{\mathbf{gas}}\mathbf{v}_{\mathbf{gas}} \otimes \mathbf{v}_{\mathbf{gas}}, \tag{B.2.7}$$

$$\sum_{\iota=1}^{A} \rho^{(\alpha_\iota)}\left(\varepsilon^{(\alpha_\iota)} + \frac{1}{2}\left(\mathbf{v}^{(\alpha_\iota)}\right)^2\right) = \rho_{\mathbf{gas}}\left(\varepsilon_{\mathbf{gas}} + \frac{1}{2}\left(\mathbf{v}_{\mathbf{gas}}\right)^2\right), \tag{B.2.8}$$

$$\begin{aligned}&\sum_{\iota=1}^{A}\left(\rho^{(\alpha_\iota)}\left(\varepsilon^{(\alpha_\iota)}+\frac{1}{2}\left(\mathbf{v}^{(\alpha_\iota)}\right)^2\right)\mathbf{v}^{(\alpha_\iota)}+\mathbf{q}^{(\alpha_\iota)}-\mathbf{T}^{(\alpha_\iota)}\mathbf{v}^{(\alpha_\iota)}\right)\\&=\rho_{\mathrm{gas}}\left(\varepsilon_{\mathrm{gas}}+\frac{1}{2}\left(\mathbf{v}_{\mathrm{gas}}\right)^2\right)\mathbf{v}_{\mathrm{gas}}+\mathbf{q}_{\mathrm{gas}}-\mathbf{T}_{\mathrm{gas}}\mathbf{v}_{\mathrm{gas}},\end{aligned}\tag{B.2.9}$$

$$\bigwedge_{\iota\in\{1,\ldots,A\}}\rho_{\mathrm{gas}}\frac{\partial c^{(\alpha_\iota)}}{\partial t}+c^{(\alpha_\iota)}\frac{\partial\rho_{\mathrm{gas}}}{\partial t}=\frac{\partial\rho^{(\alpha_\iota)}}{\partial t},\tag{B.2.10}$$

$$\bigwedge_{\iota\in\{1,\ldots,A\}}\rho_{\mathrm{gas}}\mathbf{v}_{\mathrm{gas}}\bullet\nabla c^{(\alpha_\iota)}+c^{(\alpha_\iota)}\mathbf{v}_{\mathrm{gas}}\bullet\nabla\rho_{\mathrm{gas}}=\mathbf{v}_{\mathrm{gas}}\bullet\nabla\rho^{(\alpha_\iota)}.\tag{B.2.11}$$

Proof. (B.2.1): Use (2.1.4d) and (2.1.4b).

(B.2.2): Use (2.1.4d), Rem. B.1.2(b), (2.1.6b), and (2.1.6d).

(B.2.3): Use (2.1.4d) and Rem. B.1.2 (a), (b).

(B.2.4): Use (2.1.4d) and Rem. B.1.4.

(B.2.5): Multiply (B.2.3) by $\rho^{(\alpha_\iota)}\mathbf{u}^{(\alpha_\iota)}$, sum over ι, and use (B.2.1).

(B.2.6): Use (B.2.3), (B.2.1), Rem. B.1.2(b), and (2.1.4b).

(B.2.7): Use (B.2.4), (B.2.1), Rem. B.1.4, and (2.1.4b).

(B.2.8): Use (2.1.6c) and (B.2.6).

(B.2.9): Use (2.1.4d), (B.2.8), (2.1.6e), Rem. B.1.5, (B.2.5), (2.1.6a), and (B.2.1).

(B.2.10): Use (2.1.4c) and the product rule for ∂_t.

(B.2.11): Use (2.1.4c) and (B.1.7c). ■

B.2.2 The Balance Equations Imply the Field Equations

In preparation some identities are proved.

Lemma B.2.2. *If the balance equations* (2.1.3) *and the global conservation laws* (2.1.7) *hold, then the following identities are satisfied, where equations depending on ι hold for each $\iota\in\{1,\ldots,A\}$:*

$$\frac{\partial(\rho_{\mathrm{gas}}\mathbf{v}_{\mathrm{gas}})}{\partial t}+\operatorname{div}\left(\rho_{\mathrm{gas}}\mathbf{v}_{\mathrm{gas}}\otimes\mathbf{v}_{\mathrm{gas}}\right)=\rho_{\mathrm{gas}}\frac{\partial\mathbf{v}_{\mathrm{gas}}}{\partial t}+\rho_{\mathrm{gas}}\mathbf{v}_{\mathrm{gas}}\bullet\nabla\mathbf{v}_{\mathrm{gas}}.\tag{B.2.12}$$

$$\begin{aligned}&-\rho^{*(\alpha_\iota)}\mathbf{v}^{(\alpha_\iota)}+\mathbf{p}^{*(\alpha_\iota)}+\rho^{(\alpha_\iota)}\mathbf{b}^{(\alpha_\iota)}+\operatorname{div}\mathbf{T}^{(\alpha_\iota)}-c^{(\alpha_\iota)}\operatorname{div}\mathbf{T}_{\mathrm{gas}}-\rho^{(\alpha_\iota)}\mathbf{b}_{\mathrm{gas}}\\&=-\mathbf{v}^{(\alpha_\iota)}\operatorname{div}\left(\rho^{(\alpha_\iota)}\mathbf{v}^{(\alpha_\iota)}\right)+\rho^{(\alpha_\iota)}\frac{\partial\mathbf{v}^{(\alpha_\iota)}}{\partial t}+\operatorname{div}\left(\rho^{(\alpha_\iota)}\mathbf{v}^{(\alpha_\iota)}\otimes\mathbf{v}^{(\alpha_\iota)}\right)\\&\quad+c^{(\alpha_\iota)}\mathbf{v}_{\mathrm{gas}}\operatorname{div}\left(\rho_{\mathrm{gas}}\mathbf{v}_{\mathrm{gas}}\right)-\rho^{(\alpha_\iota)}\frac{\partial\mathbf{v}_{\mathrm{gas}}}{\partial t}-c^{(\alpha_\iota)}\operatorname{div}\left(\rho_{\mathrm{gas}}\mathbf{v}_{\mathrm{gas}}\otimes\mathbf{v}_{\mathrm{gas}}\right).\end{aligned}\tag{B.2.13}$$

$$\frac{\partial}{\partial t}\left(\frac{1}{2}\rho_{\mathbf{gas}}\left(\mathbf{v}_{\mathbf{gas}}\right)^{2}\right)-\frac{\partial(\rho_{\mathbf{gas}}\mathbf{v}_{\mathbf{gas}})}{\partial t}\bullet\mathbf{v}_{\mathbf{gas}}=\frac{1}{2}\left(\mathbf{v}_{\mathbf{gas}}\right)^{2}\operatorname{div}(\rho_{\mathbf{gas}}\mathbf{v}_{\mathbf{gas}}). \tag{B.2.14}$$

$$\operatorname{div}\left(\frac{1}{2}\rho_{\mathbf{gas}}\left(\mathbf{v}_{\mathbf{gas}}\right)^{2}\mathbf{v}_{\mathbf{gas}}\right)-\mathbf{v}_{\mathbf{gas}}\bullet\operatorname{div}\left(\rho_{\mathbf{gas}}\mathbf{v}_{\mathbf{gas}}\otimes\mathbf{v}_{\mathbf{gas}}\right)=-\frac{1}{2}\left(\mathbf{v}_{\mathbf{gas}}\right)^{2}\operatorname{div}(\rho_{\mathbf{gas}}\mathbf{v}_{\mathbf{gas}}). \tag{B.2.15}$$

$$\begin{aligned}\rho_{\mathbf{gas}}r_{\mathbf{gas}}=&\rho_{\mathbf{gas}}\frac{\partial\varepsilon_{\mathbf{gas}}}{\partial t}+\rho_{\mathbf{gas}}\mathbf{v}_{\mathbf{gas}}\bullet\nabla\,\varepsilon_{\mathbf{gas}}+\operatorname{div}\mathbf{q}_{\mathbf{gas}}\\&-\operatorname{div}(\mathbf{T}_{\mathbf{gas}}\mathbf{v}_{\mathbf{gas}})+\mathbf{v}_{\mathbf{gas}}\bullet\operatorname{div}\mathbf{T}_{\mathbf{gas}}\\&+\frac{\partial}{\partial t}\left(\frac{1}{2}\rho_{\mathbf{gas}}\left(\mathbf{v}_{\mathbf{gas}}\right)^{2}\right)+\operatorname{div}\left(\frac{1}{2}\rho_{\mathbf{gas}}\left(\mathbf{v}_{\mathbf{gas}}\right)^{2}\mathbf{v}_{\mathbf{gas}}\right)\\&-\frac{\partial(\rho_{\mathbf{gas}}\mathbf{v}_{\mathbf{gas}})}{\partial t}\bullet\mathbf{v}_{\mathbf{gas}}-\mathbf{v}_{\mathbf{gas}}\bullet\operatorname{div}\left(\rho_{\mathbf{gas}}\mathbf{v}_{\mathbf{gas}}\otimes\mathbf{v}_{\mathbf{gas}}\right).\end{aligned} \tag{B.2.16}$$

$$\begin{aligned}\operatorname{div}\left(\rho_{\mathbf{gas}}c^{(\alpha_\iota)}\mathbf{u}^{(\alpha_\iota)}\right)=&\mathbf{v}^{(\alpha_\iota)}\bullet\nabla\,\rho^{(\alpha_\iota)}+\rho^{(\alpha_\iota)}\operatorname{div}\left(\mathbf{v}^{(\alpha_\iota)}-\mathbf{v}_{\mathbf{gas}}\right)\\&-\mathbf{v}_{\mathbf{gas}}\bullet\left(c^{(\alpha_\iota)}\,\nabla\,\rho_{\mathbf{gas}}+\rho_{\mathbf{gas}}\,\nabla\,c^{(\alpha_\iota)}\right).\end{aligned} \tag{B.2.17}$$

$$\begin{aligned}\rho^{*(\alpha_\iota)}=&\rho_{\mathbf{gas}}\frac{\partial c^{(\alpha_\iota)}}{\partial t}-c^{(\alpha_\iota)}\mathbf{v}_{\mathbf{gas}}\bullet\nabla\,\rho_{\mathbf{gas}}-\rho^{(\alpha_\iota)}\operatorname{div}\mathbf{v}_{\mathbf{gas}}\\&+\mathbf{v}^{(\alpha_\iota)}\bullet\nabla\,\rho^{(\alpha_\iota)}+\rho^{(\alpha_\iota)}\operatorname{div}\mathbf{v}^{(\alpha_\iota)}.\end{aligned} \tag{B.2.18}$$

Proof. As shown in Lem. 2.1.1, (2.1.3) and (2.1.7) imply (2.1.11), which are used below.

(B.2.12): Use the product rule for ∂_t, (2.1.11a), and (B.1.8d) with $\mathbf{u} = \mathbf{v}_{\mathbf{gas}}$ and $\mathbf{v} = \rho_{\mathbf{gas}}\mathbf{v}_{\mathbf{gas}}$.

(B.2.13): Use (2.1.3a), (2.1.3b), the product rule for ∂_t, the linearity of ∂_t and div, (2.1.11b), (2.1.4c), and (2.1.11a).

(B.2.14): Use the product rule for ∂_t and (2.1.11a).

(B.2.15): Follows from (B.1.8c) and (B.1.8e) by letting $\mathbf{u} := \rho_{\mathbf{gas}}\mathbf{v}_{\mathbf{gas}}$ and $\mathbf{w} := \mathbf{v} := \mathbf{v}_{\mathbf{gas}}$.

(B.2.16): Use (2.1.3c), (2.1.11b), the linearity of ∂_t and div, the product rule for ∂_t, (B.1.8a), and (2.1.11a).

(B.2.17): Use (2.1.4c), (2.1.4d), (B.1.8a), and (B.1.7c).

(B.2.18): Follows from (2.1.3a), (2.1.4c), the product rule for ∂_t, (B.1.8a), and (2.1.11a). ∎

Lemma B.2.3. *The balance equations* (2.1.3) *together with the global conservation laws* (2.1.7) *imply the field equations* (2.1.14).

Proof. (2.1.14a): Use Rem. B.1.7, Lem. 2.1.1, (2.1.11b), and (B.2.12).

(2.1.14b): Use (B.2.13), (2.1.4c), (2.1.4d), the linearity of ∂_t and ∇, and (B.1.8d) once with $\mathbf{u} = \mathbf{v}^{(\alpha_\iota)}$, $\mathbf{v} = \rho^{(\alpha_\iota)}\mathbf{v}^{(\alpha_\iota)}$ and once with $\mathbf{u} = \mathbf{v}_{\mathbf{gas}}$, $\mathbf{v} = \rho_{\mathbf{gas}}\mathbf{v}_{\mathbf{gas}}$.

(2.1.14c): Use (B.2.16), (B.1.8c), (B.2.14), and (B.2.15).

(2.1.14d): Use Lem. 2.1.1, (2.1.11a) and (B.1.8a).

(2.1.14e): Use (B.2.17) and (B.2.18). ■

B.2.3 The Field Equations Imply the Balance Equations

Lemma B.2.4. *The field equations* (2.1.14) *together with* (2.1.5) *imply the balance equations* (2.1.3) *and the global conservation laws* (2.1.7).

Proof. (2.1.7a): Sum (2.1.14e) over ι and use (2.1.5).

(2.1.3a): Use (2.1.14e), (B.2.10), (B.2.11), (2.1.4d), (B.1.8a), and (2.1.14d).

(2.1.3b): Use (2.1.14b), (2.1.4c), (2.1.4d), the linearity of ∂_t and ∇, (2.1.14a), and (2.1.3a) to get

$$\begin{aligned}\mathbf{p}^{*\,(\alpha_\iota)} + \rho^{(\alpha_\iota)}\mathbf{b}^{(\alpha_\iota)} =& \rho^{(\alpha_\iota)}\frac{\partial \mathbf{v}^{(\alpha_\iota)}}{\partial t} + \rho^{(\alpha_\iota)}\mathbf{v}^{(\alpha_\iota)} \bullet \nabla\, \mathbf{v}^{(\alpha_\iota)} - \operatorname{div} \mathbf{T}^{(\alpha_\iota)} \\ &+ \mathbf{v}^{(\alpha_\iota)}\frac{\partial \rho^{(\alpha_\iota)}}{\partial t} + \mathbf{v}^{(\alpha_\iota)} \operatorname{div}\left(\rho^{(\alpha_\iota)}\mathbf{v}^{(\alpha_\iota)}\right).\end{aligned} \tag{B.2.19}$$

Now (2.1.3b) follows from (B.2.19), the product fule for ∂_t, the linearity of div, and (B.1.8d) with $\mathbf{u} = \mathbf{v}^{(\alpha_\iota)}$ and $\mathbf{v} = \rho^{(\alpha_\iota)}\mathbf{v}^{(\alpha_\iota)}$.

(2.1.7b): Use (2.1.3b), the linearity of div and ∂_t, (2.1.6a), (2.1.6b), (2.1.14a), (2.1.4b), the product rule for ∂_t, and (B.2.7) to get

$$\sum_{\iota=1}^{A} \mathbf{p}^{*\,(\alpha_\iota)} = \mathbf{v}_{\mathbf{gas}}\frac{\partial \rho_{\mathbf{gas}}}{\partial t} + \operatorname{div}(\rho_{\mathbf{gas}}\mathbf{v}_{\mathbf{gas}} \otimes \mathbf{v}_{\mathbf{gas}}) - \rho_{\mathbf{gas}}\mathbf{v}_{\mathbf{gas}} \bullet \nabla\, \mathbf{v}_{\mathbf{gas}}. \tag{B.2.20}$$

Now (2.1.7b) follows from (B.2.20), (2.1.14d), (B.1.7b) with $f = \rho_{\mathbf{gas}}$ and $\mathbf{u} = \mathbf{v} = \mathbf{v}_{\mathbf{gas}}$, and (B.1.8d) with $\mathbf{u} = \rho_{\mathbf{gas}}\mathbf{v}_{\mathbf{gas}}$ and $\mathbf{v} = \mathbf{v}_{\mathbf{gas}}$.

(2.1.3c): Using the product rule for ∂_t, (2.1.14d), (B.1.8a) with $f = \rho_{\mathbf{gas}}\mathbf{v}_{\mathbf{gas}}^2$ and $\mathbf{u} = \mathbf{v}_{\mathbf{gas}}$, and (B.1.7c) with $f = \rho_{\mathbf{gas}}$ and $\mathbf{u} = \mathbf{v} = \mathbf{v}_{\mathbf{gas}}$ yields

$$\begin{aligned}&\frac{1}{2}\frac{\partial\left(\rho_{\mathbf{gas}}\mathbf{v}_{\mathbf{gas}}^2\right)}{\partial t} + \frac{1}{2}\operatorname{div}\left(\rho_{\mathbf{gas}}\mathbf{v}_{\mathbf{gas}}^2\mathbf{v}_{\mathbf{gas}}\right) \\ &= \mathbf{v}_{\mathbf{gas}} \bullet \left(\rho_{\mathbf{gas}}\frac{\partial \mathbf{v}_{\mathbf{gas}}}{\partial t}\right) + \mathbf{v}_{\mathbf{gas}} \bullet \left(\rho_{\mathbf{gas}}\mathbf{v}_{\mathbf{gas}} \bullet \nabla\, \mathbf{v}_{\mathbf{gas}}\right).\end{aligned} \tag{B.2.21}$$

Using (2.1.14c), the product rule for ∂_t, (2.1.14d), (B.1.7a) with $f = \varepsilon_{\mathbf{gas}}$ and $g = \rho_{\mathbf{gas}}$, (B.1.8a) with $f = \rho_{\mathbf{gas}}\varepsilon_{\mathbf{gas}}$ and $\mathbf{u} = \mathbf{v}_{\mathbf{gas}}$, (B.1.8b) with $\mathbf{A} = \mathbf{T}_{\mathbf{gas}}$ and $\mathbf{u} = \mathbf{v}_{\mathbf{gas}}$, and (2.1.14a) yields

$$\begin{aligned}\rho_{\mathbf{gas}} r_{\mathbf{gas}} =& \frac{\partial(\rho_{\mathbf{gas}}\varepsilon_{\mathbf{gas}})}{\partial t} + \operatorname{div}(\rho_{\mathbf{gas}}\varepsilon_{\mathbf{gas}}\mathbf{v}_{\mathbf{gas}}) + \operatorname{div}\mathbf{q}_{\mathbf{gas}} \\ & + \mathbf{v}_{\mathbf{gas}} \bullet \left(\rho_{\mathbf{gas}}\frac{\partial \mathbf{v}_{\mathbf{gas}}}{\partial t}\right) + \mathbf{v}_{\mathbf{gas}} \bullet (\rho_{\mathbf{gas}}\mathbf{v}_{\mathbf{gas}} \bullet \nabla \mathbf{v}_{\mathbf{gas}}) \\ & - \rho_{\mathbf{gas}}\mathbf{b}_{\mathbf{gas}} \bullet \mathbf{v}_{\mathbf{gas}} - \operatorname{div}(\mathbf{T}_{\mathbf{gas}}\mathbf{v}_{\mathbf{gas}}).\end{aligned} \tag{B.2.22}$$

Now (2.1.3c) is implied by (B.2.22), the linearity of ∂_t and div, together with (B.2.21). ■

B.2.4 Equations (2.1.11a), (2.1.11b), (2.1.3c) Are Equivalent to Equations (2.1.14a), (2.1.14c), (2.1.14d)

Equations (2.1.11a) and (2.1.14d) are equivalent, which is immediate from (B.1.8a), letting $f = \rho_{\mathbf{gas}}$ and $\mathbf{u} = \mathbf{v}_{\mathbf{gas}}$.

It was shown in App. B.2.2 that (2.1.11a) and (2.1.11b) imply (2.1.14a). It was also shown in App. B.2.2 that (2.1.11a), (2.1.11b), and (2.1.3c) imply (2.1.14c).

That (2.1.14a) and (2.1.11a) imply (2.1.11b) is seen by using the product rule for ∂_t, and (B.1.8d) with $\mathbf{u} = \mathbf{v}_{\mathbf{gas}}$ and $\mathbf{v} = \rho_{\mathbf{gas}}\mathbf{v}_{\mathbf{gas}}$.

Finally, it was shown in App. B.2.3 that (2.1.14a), (2.1.14c), and (2.1.14d) imply (2.1.3c).

B.2.5 Simplifications

Lemma B.2.5. *The simplifications of Sec. 2.1.2 applied to the quantities* (2.1.6) *yield* (2.1.27).

Proof. (2.1.27a) and (2.1.27b) are identical to (2.1.19) and (2.1.24), respectively.

(2.1.27c) follows from (2.1.6c), (2.1.4c), and (2.1.26a).

(2.1.27d) is implied by (2.1.6d), (2.1.4c), (2.1.24), and (2.1.5).

(2.1.27e) follows using (2.1.6e), (2.1.4c), (2.1.26a), (2.1.17), and replacing the remaining $\mathbf{u}^{(\alpha_i)}$ by means of (2.1.15). ■

Lemma B.2.6. *The simplifications of Sec.* 2.1.2 *applied to the field equations* (2.1.14) *(with* (2.1.14a), (2.1.14c), *and* (2.1.14d) *replaced by the equivalent equations* (2.1.11a), (2.1.11b), *and* (2.1.3c), *cf. App.* B.2.4*) yield* (2.1.28).

Proof. (2.1.28a) is the same as (2.1.11a).

(2.1.28b) is inferred from (2.1.11b), (2.1.24), and (2.1.26c).

(2.1.28c) follows from (2.1.3c), (2.1.19), (2.1.24), and (2.1.26b).

(2.1.28d) results from replacing $\mathbf{u}^{(\alpha_\iota)}$ in (2.1.14e) using (2.1.15). ∎

B.3 Cylindrical Coordinates

B.3.1 Definition and Elementary Properties

Definition B.3.1. Let $\Omega := \mathbb{R}_0^+ \times [0, 2\pi] \times \mathbb{R}$, and consider the following coordinate transformation T_{cyl}:

$$T_{\text{cyl}} : \Omega \longrightarrow \mathbb{R}^3, \quad T_{\text{cyl}}[(r, \vartheta, z)] := (r\cos[\vartheta], r\sin[\vartheta], z). \tag{B.3.1}$$

If $\mathbf{x} \in \mathbb{R}^3$ and $\mathbf{x} = T_{\text{cyl}}[(r, \vartheta, z)]$, then (r, ϑ, z) are called *cylindrical coordinates* of $\mathbf{x}$. Moreover, one defines the coordinate-dependent standard basis $\{\mathbf{e}_r, \mathbf{e}_\vartheta, \mathbf{e}_z\}$ by

$$\mathbf{e}_r[(r, \vartheta, z)] := (\cos[\vartheta], \sin[\vartheta], 0), \tag{B.3.2a}$$
$$\mathbf{e}_\vartheta[(r, \vartheta, z)] := (-\sin[\vartheta], \cos[\vartheta], 0), \tag{B.3.2b}$$
$$\mathbf{e}_z[(r, \vartheta, z)] := (0, 0, 1). \tag{B.3.2c}$$

—

Some important elementary properties of cylindrical coordinates are collected in Rem. B.3.2.

Remark B.3.2. (a) T_{cyl} is onto.

(b) T_{cyl} is one-to-one on $\text{int}[\Omega]$, i.e. cylindrical coordinates are unique if $r \neq 0$ and $\vartheta \notin \{0, 2\pi\}$.

(c) $T_{\text{cyl}}\restriction_{\text{int}[\Omega]}$ is a diffeomorphism, i.e. both $T_{\text{cyl}}\restriction_{\text{int}[\Omega]}$ and $(T_{\text{cyl}}\restriction_{\text{int}[\Omega]})^{-1}$ are differentiable. For $(r, \vartheta, z) \in \text{int}[\Omega]$ it is

$$T'_{\text{cyl}}[(r, \vartheta, z)] := \begin{pmatrix} \cos[\vartheta] & -r\sin[\vartheta] & 0 \\ \sin[\vartheta] & r\cos[\vartheta] & 0 \\ 0 & 0 & 1 \end{pmatrix}, \tag{B.3.3a}$$

$$(T'_{\text{cyl}})^{-1}[(r, \vartheta, z)] := \begin{pmatrix} \cos[\vartheta] & \sin[\vartheta] & 0 \\ \frac{-\sin[\vartheta]}{r} & \frac{\cos[\vartheta]}{r} & 0 \\ 0 & 0 & 1 \end{pmatrix}. \tag{B.3.3b}$$

The Jacobian is

$$J_{T_{\mathrm{cyl}}}[(r,\vartheta,z)] = \det\left[T'_{\mathrm{cyl}}[(r,\vartheta,z)]\right] = r. \tag{B.3.4}$$

Remark B.3.3. Let O be an open subset of $\mathbb{R}^3$ and let $f : O \longrightarrow \mathbb{K}$ be differentiable. Then by the chain rule it holds for each $\mathbf{r} := (r,\vartheta,z) \in \operatorname{int}[\Omega]$ that

$$\begin{aligned}
\big((\nabla f)\circ T_{\mathrm{cyl}}\big)[\mathbf{r}] &= \big(\nabla(f\circ T_{\mathrm{cyl}})\big)[\mathbf{r}]\cdot (T'_{\mathrm{cyl}})^{-1}[\mathbf{r}] \\
&= \left(\frac{\partial(f\circ T_{\mathrm{cyl}})}{\partial r}[\mathbf{r}], \frac{\partial(f\circ T_{\mathrm{cyl}})}{\partial\vartheta}[\mathbf{r}], \frac{\partial(f\circ T_{\mathrm{cyl}})}{\partial z}[\mathbf{r}]\right)\cdot\begin{pmatrix}\cos[\vartheta] & \sin[\vartheta] & 0\\ \frac{-\sin[\vartheta]}{r} & \frac{\cos[\vartheta]}{r} & 0\\ 0 & 0 & 1\end{pmatrix} \\
&= \frac{\partial(f\circ T_{\mathrm{cyl}})}{\partial r}[\mathbf{r}]\cdot\mathbf{e}_r[\mathbf{r}] + \frac{1}{r}\frac{\partial(f\circ T_{\mathrm{cyl}})}{\partial\vartheta}[\mathbf{r}]\cdot\mathbf{e}_\vartheta[\mathbf{r}] + \frac{\partial(f\circ T_{\mathrm{cyl}})}{\partial z}[\mathbf{r}]\cdot\mathbf{e}_z[\mathbf{r}].
\end{aligned} \tag{B.3.5}$$

—

Remark B.3.3 is the precise justification for (B.3.6), where the composition with T_{cyl} is supressed in the notation, as is usually done. Similar reasoning can be used to prove (B.3.7) and (B.3.8).

B.3.2 Grad, Div, Curl in Cylindrical Coordinates

The gradient of a function $f(r,\vartheta,z)$ is given by

$$\nabla f = \frac{\partial f}{\partial r}\mathbf{e}_r + \frac{1}{r}\frac{\partial f}{\partial\vartheta}\mathbf{e}_\vartheta + \frac{\partial f}{\partial z}\mathbf{e}_z. \tag{B.3.6}$$

The divergence and the curl of a vector field $\mathbf{A} = A_r\mathbf{e}_r + A_\vartheta\mathbf{e}_\vartheta + A_z\mathbf{e}_z$ read

$$\operatorname{div}\mathbf{A} = \frac{1}{r}\frac{\partial(rA_r)}{\partial r} + \frac{1}{r}\frac{\partial A_\vartheta}{\partial\vartheta} + \frac{\partial A_z}{\partial z}, \tag{B.3.7}$$

$$\operatorname{curl}\mathbf{A} = \left(\frac{1}{r}\frac{\partial A_z}{\partial\vartheta} - \frac{\partial A_\vartheta}{\partial z}\right)\mathbf{e}_r + \left(\frac{\partial A_r}{\partial z} - \frac{\partial A_z}{\partial r}\right)\mathbf{e}_\vartheta + \frac{1}{r}\left(\frac{\partial(rA_\vartheta)}{\partial r} - \frac{\partial A_r}{\partial\vartheta}\right)\mathbf{e}_z. \tag{B.3.8}$$

B.4 Existence of a Magnetic Scalar Potential

If (2.5.7) holds and B_r and B_z are continuously differentiable, then there is a function ϕ_A satisfying (2.5.9). This is the contents of the following Th. B.4.1, where B_1 and B_2 is written instead of B_r and B_z, respectively, to avoid confusion with the variables r and z. Since the vector potential $\mathbf{A}$ does not occur in Th. B.4.1, the notation ϕ_A is simplified to ϕ.

Theorem B.4.1. *Given functions $B_i \in C^1(\mathbb{R}_0^+ \times \mathbb{R}, \mathbb{R})$, $i \in \{1,2\}$, satisfying*

$$\bigwedge_{(r,z)\in\mathbb{R}_0^+\times\mathbb{R}} \left(\partial_1(rB_1)\right)[(r,z)] + (r\partial_2 B_2)[(r,z)] = 0, \tag{B.4.1}$$

there is a function $\phi \in C^2(\mathbb{R}_0^+ \times \mathbb{R}, \mathbb{R})$ such that (B.4.2a) *and* (B.4.2b) *both hold:*

$$B_1 = -\partial_2\phi, \tag{B.4.2a}$$

$$rB_2 = \partial_1(r\phi). \tag{B.4.2b}$$

Proof. Integrating (B.4.1) with respect to r yields

$$\bigwedge_{(r,z)\in\mathbb{R}_0^+\times\mathbb{R}} rB_1[(r,z)] + \int_0^r \tilde{r}\,(\partial_2 B_2)[(\tilde{r},z)]\,\mathrm{d}\tilde{r} = 0. \tag{B.4.3}$$

Integrating (B.4.3) with respect to z yields

$$\bigwedge_{(r,z)\in\mathbb{R}_0^+\times\mathbb{R}} \int_0^z rB_1[(r,\tilde{z})]\,\mathrm{d}\tilde{z} + \int_0^r \tilde{r}B_2[(\tilde{r},z)]\,\mathrm{d}\tilde{r} - \int_0^r \tilde{r}B_2[(\tilde{r},0)]\,\mathrm{d}\tilde{r} = 0. \tag{B.4.4}$$

The hypothesis $B_2 \in C^1(\mathbb{R}_0^+ \times \mathbb{R}, \mathbb{R})$ implies

$$\lim_{r\downarrow 0} \frac{1}{r}\int_0^r \tilde{r}B_2[(\tilde{r},0)]\,\mathrm{d}\tilde{r} = 0. \tag{B.4.5}$$

If one now defines

$$\bigwedge_{(r,z)\in\mathbb{R}_0^+\times\mathbb{R}} \phi[(r,z)] := \begin{cases} -\int_0^z B_1[(r,\tilde{z})]\,\mathrm{d}\tilde{z} + \frac{1}{r}\int_0^r \tilde{r}B_2[(\tilde{r},0)]\,\mathrm{d}\tilde{r} & \text{if } r > 0, \\ -\int_0^z B_1[(0,\tilde{z})]\,\mathrm{d}\tilde{z} & \text{if } r = 0, \end{cases} \tag{B.4.6}$$

then (B.4.4) implies

$$\bigwedge_{(r,z)\in\mathbb{R}_0^+\times\mathbb{R}} r\phi[(r,z)] = \int_0^r \tilde{r}B_2[(\tilde{r},z)]\,\mathrm{d}\tilde{r}\,. \tag{B.4.7}$$

Finally, differentiating (B.4.6) with respect to z gives (B.4.2a), and differentiating (B.4.7) with respect to r gives (B.4.2b). ∎

Appendix C

Mathematical Background Material

C.1 Topology

C.1.1 Elementary Notions

Definition C.1.1. If X is a topological space, $\mathcal{O}$ being its topology, and $A \subseteq X$, then $\mathcal{O}_A := \{A \cap O : O \in \mathcal{O}\}$ is called the *relative topology* on A with respect to $\mathcal{O}$.

Definition C.1.2. If X is a topological space, $\mathcal{O}$ being its topology, and $A \subseteq X$, then the *closure* of A (denoted $\mathrm{cl}_{\mathcal{O}}[A]$) is the intersection of all closed sets containing A. The *interior* of $A \subseteq X$ (denoted $\mathrm{int}_{\mathcal{O}}[A]$) is the union of all open sets contained in A. The *(topological) boundary* $\partial_{\mathcal{O}} A$ of A is the set of all points $x \in X$ such that each open set containing x has a nonempty intersection with both A and $X \setminus A$. Often the topology is understood and the subscript $\mathcal{O}$ is dropped. In that case $\overline{A}$ is used instead of $\mathrm{cl}[A]$.

Definition C.1.3. Let X be a topological space, and let $\mathcal{F} := (X_i)_{i \in I}$ be a family of subsets of X.

(a) $\mathcal{F}$ is called an *open cover* of X iff each X_i is open and $X = \bigcup_{i \in I} X_i$.

(b) $\mathcal{F}$ is called a *partition* of $A \subseteq X$ iff $A = \bigcup_{i \in I} \overline{X_i}$ and $\mathrm{int}[X_i] \cap \mathrm{int}[X_{i'}] = \emptyset$ for each $i \neq i'$.

Definition C.1.4. A map $f : X \longrightarrow Y$ between topological spaces X and Y is called *continuous* iff $f^{-1}O$ is open in X for each open set $O \subseteq Y$. Moreover, f is called *piecewise continuous* iff there is a partition $(X_i)_{i \in I}$ of X and a family of continuous maps $f_i : \overline{X_i} \longrightarrow Y$, $i \in I$, such that $f_i \restriction_{X_i} = f \restriction_{X_i}$ for each $i \in I$. The set of all continuous (respectively piecewise continuous) maps from X into Y is denoted by $C(X, Y)$ (respectively $C_{\mathrm{pw}}(X, Y)$).

Definition C.1.5. A topological space X is called *compact* iff each open cover of X has a finite open subcover.

Remark and Definition C.1.6. Let f be a continuous real-valued map on a compact topological space C. Then f assumes its maximum and its minimum. Define the *max-norm*

$$\|f\|_{\max} := \max\left\{\left|f[x]\right| : x \in C\right\}. \tag{C.1.1}$$

Remark C.1.7. If X is a metric space, then X is compact if and only if each sequence in X has a subsequence that converges in X.

Remark and Definition C.1.8. If $\mathcal{V}$ is a normed vector space, then the norm on $\mathcal{V}$ gives rise to a topology on $\mathcal{V}$. If $\mathcal{V}$ is finite-dimensional, then all norms on $\mathcal{V}$ are equivalent, i.e. all norms on $\mathcal{V}$ define the same topology on $\mathcal{V}$, called the *norm topology*.

Remark C.1.9. A subset $A \subseteq \mathcal{V}$ of a finite-dimensional normed vector space, endowed with the norm topology $\mathcal{O}$, is compact with respect to $\mathcal{O}_A$ if and only if A is bounded and $\mathcal{O}$-closed.

C.1.2 Domain Invariance

Definition C.1.10. A bijective map between topological spaces is called a *homeomorphism* iff both the map and its inverse map are continuous.

—

The Domain Invariance Th. C.1.11 is a classical result of algebraic topology.

Domain Invariance Theorem C.1.11. *Let A and B be subsets of $\mathbb{R}^d$, $d \in \mathbb{N}$, and let $f : A \longrightarrow B$ be a homeomorphism.*

(a) *If A is open, then B is open.*

(b) $f(\mathrm{int}[A]) = \mathrm{int}[B]$.

(c) $f(A \cap \partial A) = B \cap \partial B$.

Proof. (a): See for example [Oss92, Th. 5.6.15].

(b) and (c) are immediate consequences of (a) and the bijectiveness of f. ∎

C.2 Norms

Definition C.2.1. Let $d \in \mathbb{N}$ and $p \in [0, \infty[$. The maps

$$N_p : \mathbb{R}^d \longrightarrow \mathbb{R}_0^+, \quad N_p\left[(x_i)_{i\in\{1,\dots,d\}}\right] = \left(\sum_{i\in\{1,\dots,d\}} |x_i|^p\right)^{\frac{1}{p}}, \tag{C.2.1a}$$

$$N_\infty : \mathbb{R}^d \longrightarrow \mathbb{R}_0^+, \quad N_\infty\left[(x_i)_{i\in\{1,\dots,d\}}\right] = \max\left\{|x_i| : i \in \{1,\dots,d\}\right\} \tag{C.2.1b}$$

are called the *l_p-norm* on $\mathbb{R}^d$ and the *l_∞-norm* or *max-norm* on $\mathbb{R}^d$. The notation $\|x\|_p$ is used instead of $N_p[x]$, and $\|x\|_{\max}$ is used instead of $N_\infty[x]$.

Remark C.2.2. *Cauchy-Schwarz Inequality*: For each $\{x_1, x_2\} \subseteq \mathbb{R}^d$, $d \in \mathbb{N}$, it holds that $|x_1 \bullet x_2| \leq \|x_1\|_2 \cdot \|x_2\|_2$.

Definition and Remark C.2.3. Let $d \in \mathbb{N}$, and let $\|\ \|$ be a norm on $\mathbb{R}^d$. Given a linear map $A : \mathbb{R}^d \longrightarrow \mathbb{R}^d$, define the *operator norm* $\|A\|$ of A by

$$\|A\| := \sup\left\{\big\|A[x]\big\| : x \in \mathbb{R}^d,\ \|x\| = 1\right\}. \tag{C.2.2}$$

As a direct consequence of (C.2.2), one has

$$\bigwedge_{(x,y)\in\mathbb{R}^d\times\mathbb{R}^d} \big\|A[y] - A[x]\big\| \leq \|A\| \cdot \|y - x\|, \tag{C.2.3}$$

i.e. A is $\|A\|$-Lipschitz (cf. App. C.7.2).

C.3 Matrix Theory

Definition C.3.1. Let I be a finite index set, and let $\mathbf{A} := (a_{i,j})_{(i,j)\in I\times I}$ be a real square matrix.

(a) $\mathbf{A}$ is called *nonnegative* iff $a_{i,j} \geq 0$ for each $(i, j) \in I \times I$.

(b) $\mathbf{A}$ is called *diagonally dominant* iff

$$\bigwedge_{i\in I} \sum_{j\in I\setminus\{i\}} |a_{i,j}| \leq a_{i,i}. \tag{C.3.1}$$

$\mathbf{A}$ is called *strictly diagonally dominant* iff the inequality in (C.3.1) is strict.

(c) $\mathbf{A}$ is called *monotone* iff given $\mathbf{x} \in \mathbb{R}^I$, $\mathbf{A}\mathbf{x} \geq 0$ implies $\mathbf{x} \geq 0$.

(d) $\mathbf{A}$ is called an *M-matrix* iff $\mathbf{A}$ is monotone and $a_{i,j} \le 0$ for each $\{(i,j) \in I \times I : i \ne j\}$.

Lemma C.3.2. *Let I be a finite index set, and let $\mathbf{A} := (a_{i,j})_{(i,j)\in I\times I}$ be a real square matrix.*

(a) *$\mathbf{A}$ is monotone if and only if $\mathbf{A}$ is invertible and $\mathbf{A}^{-1}$ is nonnegative.*

(b) *Suppose*

$$\bigwedge_{(i,j)\in I^2} \quad a_{i,j} \le 0 \text{ for } i \ne j, \qquad a_{i,j} > 0 \text{ for } i = j. \tag{C.3.2}$$

If $\mathbf{A}$ is strictly diagonally dominant, then $\mathbf{A}$ is an M-matrix.

Proof. (a): See [Axe94, Lem. 6.1]. (b): See [Axe94, Lem. 6.2]. ■

C.4 Affine Geometry

C.4.1 Affine Subspaces

Definition C.4.1. A subset $\mathcal{A}$ of $\mathbb{R}^d$, $d \in \mathbb{N}$, is called an *affine subspace* of $\mathbb{R}^d$ iff there is a linear subspace $\mathcal{V}$ of $\mathbb{R}^d$ and $a_0 \in \mathbb{R}^d$ such that $\mathcal{A} = \mathcal{V} + a_0$. Moreover, define the dimension $\dim \mathcal{A} := \dim \mathcal{V}$.

Definition C.4.2. Given finitely many vectors $(v_i)_{i\in I}$, $\#I < \infty$, in a real vector space and real numbers $(\lambda_i)_{i\in I}$, such that $\sum_{i\in I} \lambda_i = 1$, the vector $\sum_{i\in I} \lambda_i v_i$ is called an *affine combination* of the vectors v_i, $i \in I$. The vectors v_i, $i \in I$, are called *affinely independent* iff for each pair of families of real numbers $((\lambda_i)_{i\in I}, (\mu_i)_{i\in I})$, it holds that $\sum_{i\in I} \lambda_i v_i = \sum_{i\in I} \mu_i v_i$ and $\sum_{i\in I} \lambda_i = \sum_{i\in I} \mu_i = 1$ imply $\lambda_i = \mu_i$ for each $i \in I$, i.e. iff the coefficients of affine combinations of the vectors v_i, $i \in I$, are unique.

Definition C.4.3. Let $A \subseteq \mathbb{R}^d$, $d \in \mathbb{N}$. The set $\operatorname{aff}[A]$ is defined as the set of all affine combinations of finitely many elements of A, i.e.

$$\operatorname{aff}[A] := \left\{ \sum_{i\in I} \lambda_i v_i : \#I < \infty,\ v_i \in A,\ \lambda_i \in \mathbb{R},\ \sum_{i\in I} \lambda_i = 1 \right\}. \tag{C.4.1}$$

The set $\operatorname{aff}[A]$ is called the *affine hull* of A.

Remark C.4.4. $\mathcal{A} \subseteq \mathbb{R}^d$ is an affine subspace if and only if there is a nonempty finite set of points V such that $\mathcal{A} = \operatorname{aff}[V]$.

C.4.2 Polyhedral Sets

Following [Grü67] and [Zie98], polyhedral sets can be unbounded. Bounded polyhedral sets are called polytopes.

Definition C.4.5. A subset A of a real vector space is called *convex* iff for each $(v_0, v_1) \in A^2$ and for each $\lambda \in [0, 1]$, it holds that $\lambda v_0 + (1 - \lambda)v_1 \in A$.

—

Intersections of convex sets are convex, giving rise to the following definition.

Definition C.4.6. If A is a subset of a real vector space, then $\mathrm{conv}[A]$ is the intersection of all convex sets containing A and is called the *convex hull* of A.

Definition C.4.7. Given affinely independent vectors $v_0, \ldots, v_d$, $d \in \mathbb{N}_0$, in a real vector space $\mathcal{V}$, the set $\sigma := \mathrm{conv}[\{v_0, \ldots, v_d\}]$ is called a *d-simplex* in $\mathcal{V}$. The elements of $V[\sigma] := \{v_0, \ldots, v_d\}$ are called the *vertices* of σ. Let $\mathrm{sim}_d[\mathcal{V}]$ denote the set of all d-simplices in $\mathcal{V}$. Each d-simplex, $d \in \mathbb{N}_0$, is called a *simplex* and the set of all simplices in $\mathcal{V}$ is denoted by $\mathrm{sim}[\mathcal{V}]$.

—

So a d-simplex is the convex hull of $d + 1$ affinely independent points.

Definition C.4.8. Given a real vector space $\mathcal{V}$ and $\sigma \in \mathrm{sim}[\mathcal{V}]$, the *boundary* of σ is the set

$$\partial\sigma := \bigcup_{v \in V[\sigma]} \mathrm{conv}\left[V[\sigma] \setminus \{v\}\right]. \tag{C.4.2}$$

The set $\mathrm{int}[\sigma] := \sigma \setminus \partial\sigma$ is called the *interior* of σ.

—

For example in $\mathbb{R}^2$, that means in the plane, there are 0-simplices (points), 1-simplices (line segments), and 2-simplices (triangles) as depicted in Fig. C.1. Figure C.1 also displays the corresponding boundaries, where $\partial\sigma_0 = \emptyset$.

Polytopes are finite unions of simplices. For the purposes of this work, it suffices to consider polytopes that are made up of simplices of the same dimension. This leads to the following Def. C.4.9.

Definition C.4.9. A subset p of a real vector space $\mathcal{V}$ is called a *d-polytope*, $d \in \mathbb{N}_0$, iff there are finitely many d-simplices in $\mathcal{V}$, denoted by σ_i, $i \in I$, $\#I < \infty$, such that $p = \bigcup_{i \in I} \sigma_i$. The set of d-polytopes in $\mathcal{V}$ is denoted by $\mathrm{pt}_d[\mathcal{V}]$. A *polytope* is a set p that is a d-polytope for some $d \in \mathbb{N}_0$. The set of all polytopes in $\mathcal{V}$ is denoted by $\mathrm{pt}[\mathcal{V}]$.

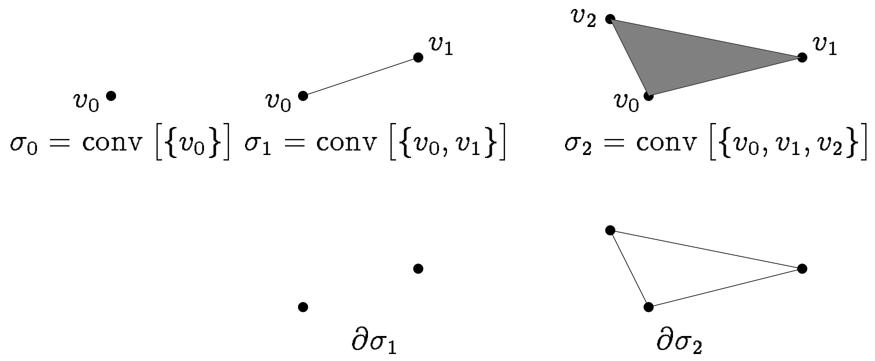


Figure C.1: Simplices in $\mathbb{R}^2$ and corresponding boundaries.

Remark C.4.10. Let p_1 and p_2 be d-polytopes in a finite-dimensional real vector space $\mathcal{V}$, $\dim[\mathcal{V}] = d$, $d \in \mathbb{N}$. Let $\mathcal{O}$ denote the norm topology on $\mathcal{V}$. If $\operatorname{int}_{\mathcal{O}}[p_1 \cap p_2] \neq \emptyset$, then $\operatorname{int}_{\mathcal{O}}[p_1 \cap p_2]$ is a d-polytope.

—

Here, with the exception of boundaries of simplices, only boundaries of polytopes in finite-dimensional real vector spaces $\mathcal{V}$, $\dim[\mathcal{V}] = d$, $d \in \mathbb{N}$, are considered, that have the same dimension d as the ambient space. Restricting to this case allows the following simple definition of polytope boundaries.

Definition C.4.11. The *boundary* of a d-polytope $p \subseteq \mathcal{V}$ in a finite-dimensional real vector space $\mathcal{V}$, $\dim[\mathcal{V}] = d$, $d \in \mathbb{N}$, is its topological boundary, where $\mathcal{V}$ is endowed with the norm topology. It is denoted by ∂p. A point $v \in \partial p$ is called *regular* iff there is a $(d-1)$-simplex $\sigma \subseteq \partial p$ such that $v \in \operatorname{int}[\sigma]$. Points in ∂p that are not regular are called *singular*. Let $\partial_{\mathrm{reg}} p$ be the set of regular points in ∂p, and let $\partial_{\mathrm{sin}} p$ be the set of singular points in ∂p.

Remark C.4.12. Definition C.4.11 is consistent in the sense that, if one considers d-simplices, $d \in \mathbb{N}$, as polytopes according to Def. C.4.9, then the two boundary notions given by Defs C.4.8 and C.4.11 coincide.

—

Figure C.2 shows six examples of polytopes in $\mathbb{R}^2$. Polytopes can be multiply connected as p_2 and p_4, simply connected as p_1 or not connected as p_3, p_5, and p_6. The sets p_1, p_2, and p_3 are 2-polytopes, the sets p_4 and p_5 are 1-polytopes, and the set p_6 is a 0-polytope.

Remark C.4.13. Let $\mathcal{V}$ be a d-dimensional real vector space and $p \in \operatorname{pt}_d[\mathcal{V}]$, $d \in \mathbb{N}$. Suppose J is a finite index set, $p_j \in \operatorname{pt}_d[\mathcal{V}]$ for each $j \in J$, and $(p_j)_{j \in J}$ is a partition of p

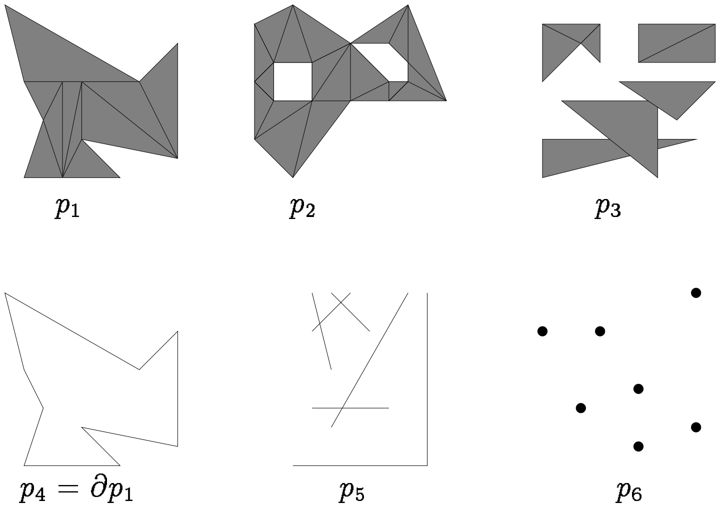


Figure C.2: Polytopes in $\mathbb{R}^2$.

with respect to the norm topology. Let $(j_1, j_2) \in J^2$, $j_1 \neq j_2$, and $\gamma := \partial_{\text{reg}} p_{j_1} \cap \partial_{\text{reg}} p_{j_2} \neq \emptyset$. If $j \in J$ and $\partial_{\text{reg}} p_j \cap \gamma \neq \emptyset$, then $j \in \{j_1, j_2\}$. That means there are precisely two polytopes adjacent to the interface γ.

Definition C.4.14. Let $\mathcal{A}$ be an affine subspace of $\mathbb{R}^d$, $d \in \mathbb{N}$, and let $x \in \mathbb{R}^d$. Then, x is called *perpendicular* to $\mathcal{A}$ iff $x \bullet (a_1 - a_2) = 0$ for each $(a_1, a_2) \in \mathcal{A}^2$.

Notation C.4.15. Given two distinct points v and w in $\mathbb{R}^d$, $d \in \mathbb{N}$, let $\mathcal{A}^\perp[(v, w)] := \{x \in \mathbb{R}^d : \|v - x\|_2 = \|w - x\|_2\}$.

Remark and Definition C.4.16. Given two distinct points v and w in $\mathbb{R}^d$, $d \in \mathbb{N}$, $\mathcal{A}^\perp[(v, w)]$ is an affine subspace and $v - w$ is perpendicular to $\mathcal{A}^\perp[(v, w)]$.

Remark and Definition C.4.17. Let p be a d-polytope in $\mathbb{R}^d$, $d \in \mathbb{N}$, and let $x \in \partial_{\text{reg}} p$. Then there exists a unique vector $n_p[x] \in \mathbb{R}^d$ with the following properties (i) – (iii):

(i) $\|n_p[x]\|_2 = 1$.

(ii) If $\sigma \subseteq \partial p$ is a $(d-1)$-simplex such that $x \in \text{int}[\sigma]$, then $n_p[x]$ is perpendicular to $\text{aff}[\sigma]$.

(iii) There is $\epsilon_0 \in \mathbb{R}^+$ such that $\{x + \epsilon n_p[x] : \epsilon \in]0, \epsilon_0[\} \cap p = \emptyset$ and $\{x - \epsilon n_p[x] : \epsilon \in]0, \epsilon_0[\} \subseteq p$.

The map $n_p : \partial_{\text{reg}} p \longrightarrow \mathbb{R}^d$ (the vector $n_p[x]$) is called the *outer unit normal vector* of p (at x). The map n_p is continuous, since it is only defined on the (usually disconnected) set $\partial_{\text{reg}} p$.

Figure C.3 illustrates Defs C.4.11 and C.4.17.

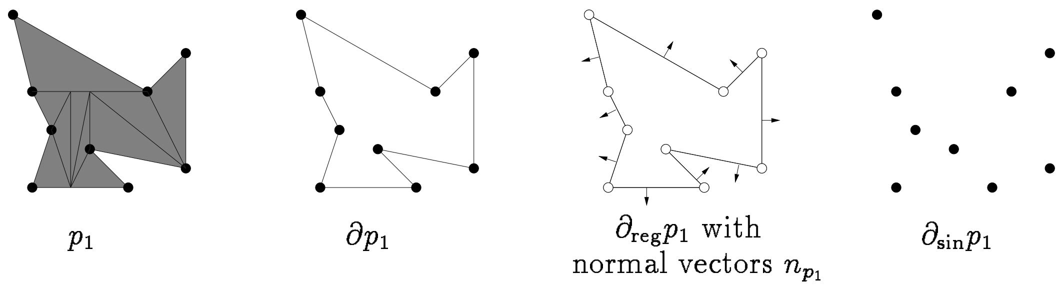


Figure C.3: Regular and singular boundary of the 2-polytope p_1.

C.4.3 Voronoï Discretization

Definition C.4.18. Let p be a d-polytope in $\mathbb{R}^d$, $d \in \mathbb{N}$, and let V be a nonempty finite subset of p. Then the induced *Voronoï discretization* of p, denoted by $\Pi[V] = (\omega_v)_{v \in V}$, consists of the so-called *Voronoï boxes* ω_v, where

$$\bigwedge_{v \in V} \quad \omega_v := \overline{\left\{x \in p : \|x - v\|_2 < \|x - w\|_2 \text{ for each } w \in V \setminus \{v\}\right\}}. \tag{C.4.3}$$

The $v \in V$ are called the *discretization points* of the Voronoï discretization (cf. Def. 3.7.40).

Remark C.4.19. Let p be a d-polytope in $\mathbb{R}^d$, $d \in \mathbb{N}$, let V be a nonempty finite subset of p, and let $\Pi[V] = (\omega_v)_{v \in V}$ be the induced Voronoï discretization of p. Then, $\Pi[V]$ is a partition of p into d-polytopes such that $v \in \omega_v$ for each $v \in V$. Moreover, for each $(v, w) \in V^2$, $v \neq w$, one has that $\partial\omega_v \cap \partial\omega_w \subseteq \mathcal{A}^\perp[(v, w)]$, and, in particular, $\frac{w-v}{\|w-v\|_2} = n_{\omega_v}\restriction_{\partial_{\text{reg}}\omega_v \cap \partial_{\text{reg}}\omega_w}$.

Example C.4.20. Figure C.4 displays the Voronoï discretization induced by the set $V := \{v_1, \dots, v_9\}$. It illustrates that one can not replace "$<$" in (C.4.3) by "$\leq$" without losing the property that the Voronoï boxes are always d-polytopes: If "$\leq$" were used in (C.4.3), then the isolated point x would be an element of ω_{x_8}, assuming $\|v_8 - x\|_2 = \|v_9 - x\|_2$.

C.5 Graph Theory

Definition C.5.1. A *graph* is a pair $\mathcal{G} = (V, E)$ consisting of a set of *vertices* $V = V[\mathcal{G}]$ and a set of *edges* $E = E[\mathcal{G}] \subseteq \binom{V}{2}$, where $\binom{V}{2}$ denotes the set of all subsets of V that have precisely two elements. For each $V_0 \subseteq V$, the set $\mathcal{G}\restriction_{V_0} := (V_0, E \cap \binom{V_0}{2})$ is called the *induced subgraph* of $\mathcal{G}$ on V_0.

Definition C.5.2. Consider a graph $\mathcal{G} = (V, E)$. A one-to-one map $\mathfrak{p} : \{0, \dots, n\} \longrightarrow V$, $n \in \mathbb{N}_0$, such that either $n = 0$ or $\{\mathfrak{p}[\nu], \mathfrak{p}[\nu + 1]\} \in E$ for each $\nu \in \{0, \dots, n - 1\}$, is called a *path* in $\mathcal{G}$. If $v = \mathfrak{p}[0]$ and $v' = \mathfrak{p}[n]$, then $\mathfrak{p}$ is also called a *vv'-path* in $\mathcal{G}$.

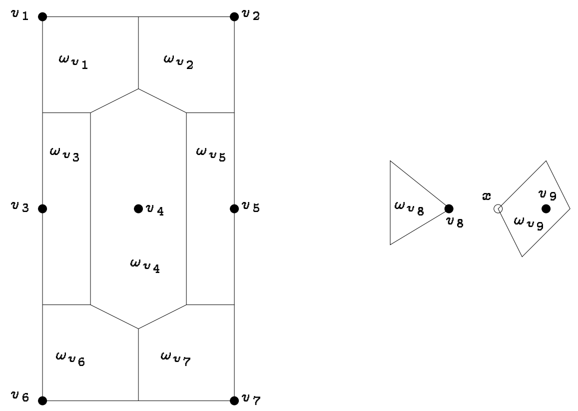


Figure C.4: Voronoï discretization, s. Ex. C.4.20.

Definition C.5.3. Let $\mathcal{G} = (V, E)$ be a graph. The *connected component* in $\mathcal{G}$ of a vertex $v \in V$ is the set of all vertices $v' \in V$ such that there is a *vv'-path* in $\mathcal{G}$. The connected component in $\mathcal{G}$ of $v \in V$ is denoted by $\mathrm{CoCmp}_{\mathcal{G}}[v]$ or by $\mathrm{CoCmp}[v]$ if the graph $\mathcal{G}$ is understood.

Remark C.5.4. For each graph $\mathcal{G} = (V, E)$,

$$v \sim v' \quad \Leftrightarrow \quad v' \in \mathrm{CoCmp}[v] \tag{C.5.1}$$

defines an equivalence relation on V.

Definition C.5.5. Let $\mathcal{G} = (V, E)$ be a graph. The induced subgraphs $\mathcal{G}\restriction_C$ on the equivalence classes $C \subseteq V$ of the equivalence relation defined in (C.5.1) are called the *connected components* of $\mathcal{G}$. The set of all connected components of $\mathcal{G}$ is denoted by $\mathrm{CoCmp}[\mathcal{G}]$.

C.6 Regularity Notions of Functions

C.6.1 Continuous Differentiability

In this work only real differentiability plays a role, even for functions between complex spaces, i.e. the derivatives are not required to be $\mathbb{C}$-linear, just $\mathbb{R}$-linear. Hence, in the current section only real subsets of real spaces are treated. The considerations apply to complex spaces by identifying $\mathbb{C}^d$ with $\mathbb{R}^{2d}$.

Notation C.6.1. If $(d, d') \in \mathbb{N}^2$, $k \in \mathbb{N}_0$, $O \subseteq \mathbb{R}^d$, $B \subseteq \mathbb{R}^{d'}$, and O is open, then the set of all functions $f : O \longrightarrow B$ having continuous partial derivatives up to k-th order, is called $C^k(O, B)$. Moreover, $C^\infty(O, B) := \bigcap_{k \in \mathbb{N}} C^k(O, B)$. If $A = \overline{\mathrm{int}[A]}$ is an arbitrary subset of $\mathbb{R}^d$ that is the closure of its interior, then $C^k(A, B)$, $k \in \mathbb{N}_0 \cup \{\infty\}$, denotes the set of all functions $f: A \longrightarrow B$ such that the restriction $f\restriction_{\mathrm{int}[A]}$ is in $C^k(\mathrm{int}[A], B)$, and all its partial derivatives extend to A continuously. The extensions are then called partial derivatives of f, denoted by ∂_i, $i \in \{1\dots,d\}$. Let $C^k[A] := C^k(A,\mathbb{R})$, $C(A,B) := C^0(A,B)$, and $C[A] := C(A,\mathbb{R})$.

—

Requiring $A = \overline{\mathrm{int}[A]}$ in Not. C.6.1 guarantees that partial derivatives are always unique.

Notation C.6.2. For $d \in \mathbb{N}$ and $A = \overline{\mathrm{int}[A]} \subseteq \mathbb{R}^d$, let

$$\begin{aligned} &\nabla: C^1[A] \longrightarrow C\left(A,\mathbb{R}^d\right), \quad \nabla f := (\partial_i f)_{i\in\{1\dots,d\}}, \\ &\mathrm{div}: C^1\left(A,\mathbb{R}^d\right) \longrightarrow C[A], \quad \mathrm{div}(f_i)_{i\in\{1\dots,d\}} := \sum_{i\in\{1\dots,d\}} \partial_i f_i. \end{aligned} \tag{C.6.1}$$

Next, some notation for differentiating functions defined on time-space domains is provided. In this case, the gradient and the divergence act on the space variables only:

Notation C.6.3. Let $Q = [t_0, t_f] \times \Omega$, $\Omega \subseteq \mathbb{R}^d$, be a time-space domain (cf. (3.1.2)). For real-valued functions defined on Q, the symbol ∂_t denotes the partial derivative with respect to the time variable $t \in [t_0, t_f]$, and ∂_{x_i}, $i \in \{1\dots,d\}$, denotes the partial derivative with respect to the i-th space variable x_i, $(x_i)_{i\in\{1\dots,d\}} \in \Omega$. Furthermore, for functions f, f_i, $i \in \{1\dots,d\}$, defined on Q and having partial space derivatives, let

$$\nabla f := (\partial_{x_i} f)_{i\in\{1\dots,d\}}, \quad \mathrm{div}(f_i)_{i\in\{1\dots,d\}} := \sum_{i\in\{1\dots,d\}} \partial_{x_i} f_i. \tag{C.6.2}$$

C.6.2 Monotonicity

Definition C.6.4. Let $A \subseteq \mathbb{R}$ and $f: A \longrightarrow \mathbb{R}$. Then f is called *increasing* iff

$$\bigwedge_{(a,b)\in A^2} \quad a < b \quad \Rightarrow \quad f[a] \le f[b], \tag{C.6.3}$$

and f is called *strictly increasing* iff the inequality in the conclusion of (C.6.3) is strict.

C.6.3 Variation

The topic of this section is the variation of real-valued functions on bounded and unbounded intervals.

Notation C.6.5. For each $a \in \mathbb{R}$, let

$$\mathcal{I}_a := \big\{[a,b]: b \in [a,\infty[\big\} \cup \big\{[a,b[: b \in [a,\infty[\big\} \cup \big\{[a,\infty[\big\} \tag{C.6.4}$$

be the set of all intervals with minimum a.

Definition C.6.6. Given a real interval $I := [a, b]$, a *discretization* of I is a finite, strictly increasing sequence $(t_\nu)_{\nu \in \{0,\dots,n\}}$, $n \in \mathbb{N}$, satisfying

$$t_0 = a \quad \text{and} \quad t_n = b. \tag{C.6.5}$$

Definition C.6.7. Let $a \in \mathbb{R}$ and $I \in \mathcal{I}_a$. For each function $f : I \longrightarrow \mathbb{R}$, define the functions

$$\begin{gathered}
\operatorname{var}[f] : I \longrightarrow [0, \infty], \\
\operatorname{var}[f][a] := 0, \\
\bigwedge_{\lambda \in I \setminus \{a\}} \left(\operatorname{var}[f][\lambda] := \sup \left\{ \sum_{\nu \in \{1,\dots,n\}} \left| f[t_\nu] - f[t_{\nu-1}] \right| : \right.\right. \\
\left.\left. (t_\nu)_{\nu \in \{0,\dots,n\}} \text{ is a discretization of } [a, \lambda] \right\} \right),
\end{gathered} \tag{C.6.6a}$$

$$\begin{gathered}
\operatorname{var}^+[f] : I \longrightarrow [0, \infty], \\
\operatorname{var}^+[f][a] := 0, \\
\bigwedge_{\lambda \in I \setminus \{a\}} \left(\operatorname{var}^+[f][\lambda] := \sup \left\{ \sum_{\nu \in \{1,\dots,n\}} \max \left\{ 0, f[t_\nu] - f[t_{\nu-1}] \right\} : \right.\right. \\
\left.\left. (t_\nu)_{\nu \in \{0,\dots,n\}} \text{ is a discretization of } [a, \lambda] \right\} \right),
\end{gathered} \tag{C.6.6b}$$

$$\begin{gathered}
\operatorname{var}^-[f] : I \longrightarrow [0, \infty], \\
\operatorname{var}^-[f][a] := 0, \\
\bigwedge_{\lambda \in I \setminus \{a\}} \left(\operatorname{var}^-[f][\lambda] := \sup \left\{ - \sum_{\nu \in \{1,\dots,n\}} \min \left\{ 0, f[t_\nu] - f[t_{\nu-1}] \right\} : \right.\right. \\
\left.\left. (t_\nu)_{\nu \in \{0,\dots,n\}} \text{ is a discretization of } [a, \lambda] \right\} \right).
\end{gathered} \tag{C.6.6c}$$

The function $\operatorname{var}[f]$ is called the *total variation function* of f. Analogously, $\operatorname{var}^+[f]$ is called the *positive variation function* of f, and $\operatorname{var}^+[f]$ is called the *negative variation function* of f. The function f is called *of bounded variation* iff the total variation function of f remains finite, i.e. $\sup\big(\operatorname{var}[f]\big) < \infty$.

—

The following Rem. C.6.8 states some useful elementary properties of variation.

Remark C.6.8. Let $a \in \mathbb{R}$ and $I \in \mathcal{I}_a$. For each function $f : I \longrightarrow \mathbb{R}$, the following holds:

(a) $\operatorname{var}[f][a] = \operatorname{var}^+[f][a] = \operatorname{var}^-[f][a] = 0$.

(b) Each of the functions $\operatorname{var}[f]$, $\operatorname{var}^+[f]$, and $\operatorname{var}^-[f]$ is nonnegative.

(c) Each of the functions $\operatorname{var}[f]$, $\operatorname{var}^+[f]$, and $\operatorname{var}^-[f]$ is increasing.

(d) $\operatorname{var}[f] = \operatorname{var}^+[f] + \operatorname{var}^-[f]$.

(e) If $b \in I$ and $\operatorname{var}[f][b] < \infty$, then $f = f[a] + \operatorname{var}^+[f] - \operatorname{var}^-[f]$ on $[a, b]$.

(f) For each $(\lambda, \mu) \in I^2$ with $\lambda < \mu$, it holds that

$$\operatorname{var}[f][\mu] = \operatorname{var}[f][\lambda] + \operatorname{var}\left[f\restriction_{I\cap[\lambda,\infty[}\right][\mu], \tag{C.6.7a}$$

$$\operatorname{var}^+[f][\mu] = \operatorname{var}^+[f][\lambda] + \operatorname{var}^+\left[f\restriction_{I\cap[\lambda,\infty[}\right][\mu], \tag{C.6.7b}$$

$$\operatorname{var}^-[f][\mu] = \operatorname{var}^-[f][\lambda] + \operatorname{var}^-\left[f\restriction_{I\cap[\lambda,\infty[}\right][\mu]. \tag{C.6.7c}$$

(g) If $L \in \mathbb{R}_0^+$ and f is L-Lipschitz (cf. Def. C.7.4), then each of the functions $\operatorname{var}^+[f]$, $\operatorname{var}^-[f]$, and $\operatorname{var}[f]$ is L-Lipschitz. In particular, the functions all are of bounded variation on each compact interval contained in I, and $f = f[a]+\operatorname{var}^+[f]-\operatorname{var}^-[f]$.

(h) If f is locally Lipschitz (cf. Def. C.7.5), then each of the functions $\operatorname{var}^+[f]$, $\operatorname{var}^-[f]$, and $\operatorname{var}[f]$ is locally Lipschitz. In particular, the functions all are of bounded variation on each compact interval contained in I, and $f = f[a]+\operatorname{var}^+[f]-\operatorname{var}^-[f]$.

C.7 Some Subjects in Metric Spaces

C.7.1 Elementary Notation

Definition C.7.1. Given a finite index set I and metric spaces (X_k, d_{X_k}), $k \in I$, set $X := \prod_{k\in I} X_k$. The function

$$d:\ X^2 \longrightarrow \mathbb{R}_0^+, \quad d[(x,y)] := \max\left\{d_{X_k}[(x_k, y_k)] :\ k \in I\right\} \tag{C.7.1}$$

is called the *max-metric* on X.

Notation C.7.2. Let (X, d) be a metric space, $x \in X$, and $A \subseteq X$. Define $d(x, A) := \inf\left\{d[(x,a)] :\ a \in A\right\}$.

Definition C.7.3. If (X, d) is a metric space, $x_0 \in X$, and $r \in \mathbb{R}^+$, then

$$B_{d,r}[x_0] := \left\{x \in X :\ d[(x_0, x)] < r\right\} \tag{C.7.2}$$

is called the (open) *r-ball* with *center* x_0 and with respect to d. One also writes $B_r[x_0]$ if d is understood.

C.7.2 Lipschitz Functions

Definition C.7.4. Let (X, d_X) and (Y, d_Y) be metric spaces, $L \in \mathbb{R}_0^+$. A map $f : X \longrightarrow Y$ is called *L-Lipschitz continuous* or just *L-Lipschitz* iff

$$\bigwedge_{(x_1,x_2)\in X^2} d_Y\big[(f[x_1], f[x_2])\big] \leq L \cdot d_X\big[(x_1, x_2)\big]. \tag{C.7.3}$$

Moreover, f is called *Lipschitz continuous* or *Lipschitz* iff f is L-Lipschitz for some $L \in \mathbb{R}_0^+$. The set of all L-Lipschitz functions from X into Y is denoted by $\mathrm{Lip}_L(X, Y)$, while $\mathrm{Lip}(X, Y)$ is the set of all Lipschitz functions from X into Y.

Definition C.7.5. Let (X, d_X) and (Y, d_Y) be metric spaces. A map $f : X \longrightarrow Y$ is called *locally Lipschitz* iff for each $x \in X$, there is an $r \in \mathbb{R}^+$ such that f is Lipschitz in $B_r[x]$.

Remark C.7.6. Let $(d, d') \in \mathbb{N}^2$, $X \subseteq \mathbb{R}^d$, $Y \subseteq \mathbb{R}^{d'}$. A map $f : X \longrightarrow Y$ is locally Lipschitz if and only if f is Lipschitz on each compact subset of X.

—

The following Rem. C.7.7 collects some elementary properties of Lipschitz functions, that are used in this work.

Remark C.7.7. (a) Let $f : [m, M] \longrightarrow \mathbb{R}$ be L-Lipschitz, $L \in \mathbb{R}_0^+$. Then $f[M] \leq f[m] + L \cdot (M - m)$.

(b) Compositions of Lipschitz functions are Lipschitz functions: If (X, d_X), (Y, d_Y), (Z, d_Z) are metric spaces, $f \in \mathrm{Lip}_{L_f}(X, Y)$, $g \in \mathrm{Lip}_{L_g}(Y, Z)$, $\{L_f, L_g\} \subseteq \mathbb{R}_0^+$, then $g \circ f \in \mathrm{Lip}_{L_f \cdot L_g}(X, Z)$.

(c) Scaled (locally) Lipschitz functions are (locally) Lipschitz functions: Let (X, d_X) be a metric space, and let $(Y, \|\ \|)$ be a normed vector space. If $f \in \mathrm{Lip}_L(X, Y)$, $L \in \mathbb{R}_0^+$, $\lambda \in \mathbb{R}$, then $\lambda \cdot f \in \mathrm{Lip}_{|\lambda| \cdot L}(X, Y)$.

(d) Sums of (locally) Lipschitz functions are (locally) Lipschitz functions: Let (X, d_X) be a metric space, and let $(Y, \|\ \|)$ be a normed vector space. If $f_k \in \mathrm{Lip}_{L_k}(X, Y)$, $L_k \in \mathbb{R}_0^+$, $k \in I$, $\#I < \infty$, then $\sum_{k\in I} f_k \in \mathrm{Lip}_L(X, Y)$, where $L := \sum_{k\in I} L_k$.

(e) The product of two real-valued bounded Lipschitz functions is a Lipschitz function: Let (X, d_X) be a metric space, $f \in \mathrm{Lip}_{L_f}(X, \mathbb{R})$, $g \in \mathrm{Lip}_{L_g}(X, \mathbb{R})$, and $\max\big\{\|f\|_{\sup}, \|g\|_{\sup}\big\} < \infty$, then $f \cdot g \in \mathrm{Lip}_L(X, \mathbb{R})$, where $L = \|f\|_{\sup} L_g + \|g\|_{\sup} L_f$.

In particular, if X is compact, then $f \cdot g$ is Lipschitz. Also, if f and g are locally Lipschitz, then $f \cdot g$ is locally Lipschitz.

(f) The cartesian product of (locally) Lipschitz maps is (locally) Lipschitz with respect to the max-metric: Given a finite index set I and metric spaces (X, d_X), (Y, d_Y), let X^I and Y^I be endowed with the respective max-metrics, denoted by $d_{X,\max}$ and $d_{Y,\max}$, respectively. If $f_k \in \mathrm{Lip}_L(X, Y)$, $L \in \mathbb{R}_0^+$, $k \in I$, then the map $f := (f_k)_{k\in I} : X^I \longrightarrow Y^I$, is L-Lipschitz.

(g) The sum of (locally) Lipschitz maps depending on different variables is (locally) Lipschitz with respect to the max-metric: Given a finite index set I, a metric space (X, d_X), and a normed vector space $(Y, \|\ \|)$, let X^I be endowed with the max-metric, denoted by $d_{X,\max}$. If $f_k \in \mathrm{Lip}_{L_k}(X, Y)$, $L_k \in \mathbb{R}_0^+$, $k \in I$, then the map $f : X^I \longrightarrow Y$, $f[x] := \sum_{k\in I} f_k[x_k]$ is L-Lipschitz, where $L := \sum_{k\in I} L_k$.

(h) The product of two real-valued bounded Lipschitz maps depending on different variables is Lipschitz with respect to the max-metric: Given a finite index set I and a metric space (X, d_X), let X^I be endowed with the max-metric, denoted by $d_{X,\max}$. If $f \in \mathrm{Lip}_{L_f}(X, \mathbb{R})$, $g \in \mathrm{Lip}_{L_g}(X, \mathbb{R})$, and $\max\{\|f\|_{\sup}, \|g\|_{\sup}\} < \infty$, then for each $(k, l) \in I^2$, the map $fg : X^I \longrightarrow Y$, $(fg)[x] := f[x_k] \cdot g[x_l]$ is L-Lipschitz, where $L := \|f\|_{\sup} L_g + \|g\|_{\sup} L_f$.

In particular, if X is compact, then fg is Lipschitz. Also, if f and g are locally Lipschitz, then fg is locally Lipschitz.

(i) Suppose C is a convex subset of $\mathbb{R}^d$, $d \in \mathbb{N}$, and $f \in C(C, \mathbb{R})$ is diffenrentiable on $\mathrm{int}[C]$ such that all partial derivatives of f are bounded, i.e. such that there is $M \in \mathbb{R}_0^+$ satisfying $|\partial_i f[x]| \le M$ for each $i \in \{1, \dots, d\}$ and for each $x \in \mathrm{int}[C]$.

Then for any $(x, y) \in (\mathrm{int}[C])^2$, one can use the mean value theorem to get $\xi \in \mathrm{conv}[\{x, y\}] \subseteq C$ such that

$$f[y] - f[x] = \nabla f[\xi] \bullet (y - x), \tag{C.7.4}$$

and hence

$$|f[y] - f[x]| \le d\,M \|x - y\|_{\max}. \tag{C.7.5}$$

If C contains boundary points, then (C.7.5) extends to these points by the continuity of f. Hence f is dM-Lipschitz continuous with respect to the max-norm.

In particular, if f is continuously differentiable, then f is locally Lipschitz with respect to the max-norm.

Definition C.7.8. Let (X, d_X) and (Y, d_Y) be metric spaces. For each map $f : X \longrightarrow Y$, let

$$\|f\|_{\mathrm{Lip}} := \sup\left\{ \frac{d_Y\left[\left(f[x_1], f[x_2]\right)\right]}{d_X[(x_1, x_2)]} : (x_1, x_2) \in X^2,\ x_1 \neq x_2 \right\}. \tag{C.7.6}$$

Remark C.7.9. A map $f : X \longrightarrow Y$ between two metric spaces is Lipschitz if and only if $\|f\|_{\mathrm{Lip}} < \infty$. Moreover, for each $f \in \mathrm{Lip}(X, Y)$, it holds that

$$\|f\|_{\mathrm{Lip}} = \min\left\{L \in \mathbb{R}_0^+ : f \in \mathrm{Lip}_L(X, Y)\right\}. \tag{C.7.7}$$

C.7.3 Inverse Lipschitz Functions

Definition C.7.10. Let (X, d_X) and (Y, d_Y) be metric spaces, $L_{\mathrm{inv}} \in \mathbb{R}^+$. A map $f : X \longrightarrow Y$ is called *inverse L_{inv}-Lipschitz* iff

$$\bigwedge_{(x_1,x_2)\in X^2} d_Y\big[(f[x_1], f[x_2])\big] \geq L_{\mathrm{inv}} \cdot d_X\big[(x_1, x_2)\big]. \tag{C.7.8}$$

Moreover, f is called *inverse Lipschitz* iff it is inverse L_{inv}-Lipschitz for some $L_{\mathrm{inv}} \in \mathbb{R}^+$. The set of all inverse L_{inv}-Lipschitz functions from X into Y is denoted by $\mathrm{InLip}_{L_{\mathrm{inv}}}(X, Y)$. Analogously, the set of all inverse Lipschitz functions from X into Y is denoted by $\mathrm{InLip}(X, Y)$.

Remark C.7.11. The name *inverse Lipschitz* is justified: Let (X, d_X) and (Y, d_Y) be metric spaces. If the bijective map $f : X \longrightarrow Y$ is inverse L_{inv}-Lipschitz for some $L_{\mathrm{inv}} \in \mathbb{R}^+$, then its inverse map f^{-1} is L_{inv}^{-1}-Lipschitz.

—

As a caveat it is pointed out that in contrast to Lipschitz functions which are always continuous, functions that are inverse Lipschitz can be discontinuous.

The following Rem. C.7.12 collects some elementary properties of increasing inverse Lipschitz functions, that are used in this work.

Remark C.7.12. Let I be an interval, $I \subseteq \mathbb{R}$, and let $f : I \longrightarrow \mathbb{R}$ be inverse L_{inv}-Lipschitz for some $L_{\mathrm{inv}} \in \mathbb{R}^+$. Moreover, suppose that f is increasing.

(a) $\bigwedge_{(a,b)\in I^2 : a<b} f[b] \geq L_{\mathrm{inv}}(b-a) + f[a] > f[a]$. In particular, if $\sup I = \infty$, then f is unbounded from above.

(b) f is one-to-one, hence f is strictly increasing, and thus f^{-1} exists on $f[I]$.

(c) f is continuous if and only if the range of f is an interval.

(d) $\bigwedge_{\lambda\in\mathbb{R}^+} \lambda f$ is inverse λL_{inv}-Lipschitz.

(e) If $g : I \longrightarrow \mathbb{R}$ is increasing, then $f + g$ is inverse L_{inv}-Lipschitz.

C.7.4 Contracting Maps

Definition C.7.13. Let (X, d_X) and (Y, d_Y) be metric spaces. A map $f : X \longrightarrow Y$ is called *c-contracting* or a *c-contraction* for $c \in [0, 1[$ iff f is c-Lipschitz, i.e.

$$\bigwedge_{(x_1,x_2)\in X^2} d_Y\big[(f[x_1], f[x_2])\big] \leq c \cdot d_X\big[(x_1, x_2)\big]. \tag{C.7.9}$$

If (C.7.9) holds for some $c \in [0, 1[$, then f is called *contracting* or a *contraction.*

Remark C.7.14. A map into a product space endowed with the max-metric is contracting if all its component maps are contracting. More precisely, given a finite index set I and metric spaces (X, d_X), (Y_k, d_{Y_k}), $k \in I$, set $Y := \prod_{k \in I} Y_k$, and let d_Y be the max-metric on Y. If there are numbers $c_k \in [0,1[$ such that each f_k is c_k-contracting, $k \in I$, then the map $f : X \longrightarrow Y$, $x \mapsto \big(f_k[x]\big)_{k \in I}$, is $\max\{c_k : k \in I\}$-contracting.

Lemma C.7.15. *Let (X, d_X), (Y, d_Y), and (Z, d_Z) be metric spaces, and $f : X \longrightarrow Y$. Suppose there are $g \in \mathrm{Lip}_L(X, Z)$, $L \in \mathbb{R}_0^+$, $h \in \mathrm{InLip}_{L_{\mathrm{inv}}}(Y, Z)$, $L_{\mathrm{inv}} \in \mathbb{R}^+$, such that $g = h \circ f$. If $L_{\mathrm{inv}} > L$, then f is $\frac{L}{L_{\mathrm{inv}}}$-Lipschitz, i.e. f is $\frac{L}{L_{\mathrm{inv}}}$-contracting.*

Proof. One calculates

$$\bigwedge_{(x_1,x_2) \in X^2} \left(\begin{aligned} L_{\mathrm{inv}} \cdot d_Y\big[(f[x_1], f[x_2])\big] &\le d_Z\big[(h[f[x_1]], h[f[x_2]])\big] \\ &= d_Z\big[(g[x_1], g[x_2])\big] \le L \cdot d_X\big[(x_1, x_2)\big] \end{aligned} \right). \tag{C.7.10}$$

Dividing (C.7.10) by L_{inv} establishes the case. ∎

C.8 Integration

C.8.1 Notation for Lebesgue Measure

Notation C.8.1. Let λ_d denote d-dimensional Lebesgue measure, $d \in \mathbb{N}$. For singleton sets $\{x\}$, also define $\lambda_0\{x\} := 1$.

C.8.2 Integration Theorems

In Th. C.8.2 the Gauss-Green Integration Theorem is stated in a form that is suitable for the needs of this work. Since the general notion of a manifold is not required elsewhere in this text, a rigorous definition is omitted. Intuitively, the hypothesis made on the boundary of the integration region in Th. C.8.2 says that the boundary can have corners and (hyper)-edges of finite angles, and that, locally, small translations either shift the boundary totally inside or totally outside of the integration region. For details, it is referred to [Zei86, Sec. 6.2] and [Zei90, Sec. 18.2].

For the applications in Ch. 3, the closure of the set O in C.8.2 is acually always a polytope.

Gauss-Green Integration Theorem C.8.2. *If O is a bounded open connected nonempty subset of $\mathbb{R}^d$, $d \in \mathbb{N}$, such that ∂O is an $(d-1)$-dimensional Lipschitz manifold and such that O lies locally on one side of ∂O, and if $f \in C^1(\overline{O}, \mathbb{R}^{d'})$, $d' \in \mathbb{N}$, then*

$$\int_O \operatorname{div} f = \int_{\partial O} \operatorname{tr}_{\partial O} f \bullet n_O, \tag{C.8.1}$$

where n_O is the outward unit normal that is defined almost everywhere on ∂O. Extensions: Equation (C.8.1) *still holds if* (a) $\overline{O} \in \mathrm{pt}_d[\mathbb{R}^d]$, $d \in \mathbb{N}$, *or* (b) $\operatorname{div} f$ *only exists in a weak sense, e.g. for* $f \in H(\operatorname{div}, O)$, *where* $H(\operatorname{div}, O)$ *is the space defined in* [Bey98, *Def.* 1.1.36], *or* (c) f *has values in* $\mathbb{C}^{d'}$.

Proof. Confer e.g. [Neč67, p. 121]. Extension (a): Let $(\sigma_i)_{i \in I}$, $\#I < \infty$, be a finite partition of $p := \overline{O}$ into d-simplices. Since C.8.2 applies to each σ_i, $i \in I$, and since $f \bullet n_{\sigma_i} = -f \bullet n_{\sigma_j}$ on $\partial_{\mathrm{reg}} n_{\sigma_i} \cap \partial_{\mathrm{reg}} n_{\sigma_j}$ whenever $(i,j) \in I^2$, $i \neq j$, a finite summation establishes the case. Extension (b) for $f \in H(\operatorname{div}, O)$ follows from the continuously differentiable case, as $C^\infty(\overline{O}, \mathbb{R}^{d'})$ is dense in $H(\operatorname{div}, O)$ (cf. [Bey98, Lem. 1.1.37]). Extension (c) follows by applying the real theorem to the real and imaginary parts of f. ∎

Change of Variables Theorem C.8.3. *Let O be an open subset of $\mathbb{R}^d$, $d \in \mathbb{N}$, and let $T : O \longrightarrow \mathbb{R}^d$ a one-to-one map that is differentiable (in the classical sense). Let $T' : O \longrightarrow \mathrm{Lin}(\mathbb{R}^d, \mathbb{R}^d)$ denote the derivative of T, and let $J_T : O \longrightarrow \mathbb{R}$, $x \mapsto \det[T']$, denote its Jacobian. If $f : \mathbb{R}^d \longrightarrow \mathbb{K}$ is measurable, then $(f \circ T) \cdot |J_T|$ is measurable, and*

$$\int_O (f \circ T) \cdot |J_T| = \int_{TO} f. \tag{C.8.2}$$

Proof. See [Rud87, Th. 7.26]. The complex case follows by applying the real theorem to the real and imaginary parts of f. ∎

Fubini Theorem C.8.4. *Let $A \subseteq \mathbb{R}^d$, $B \subseteq \mathbb{R}^{d'}$, $(d, d') \in \mathbb{N}^2$, be measurable sets. Suppose $f \in L^1(A \times B, \mathbb{K})$. Then $f\restriction_{\{a\}\times B} \in L^1(B, \mathbb{K})$ for almost all $a \in A$, $f\restriction_{A\times\{b\}} \in L^1(A, \mathbb{K})$ for almost all $b \in B$. Moreover, an element of $L^1(A, \mathbb{K})$ is defined by $a \mapsto \int_B f\restriction_{\{a\}\times B}$ almost everywhere, an element of $L^1(B, \mathbb{K})$ is defined by $b \mapsto \int_A f\restriction_{A\times\{b\}}$ almost everywhere, and it holds that*

$$\int_A \left(\int_B f\restriction_{\{a\}\times B} \right) = \int_{A \times B} f = \int_B \left(\int_A f\restriction_{A\times\{b\}} \right). \tag{C.8.3}$$

Proof. See [Rud87, Th. 8.8(c)]. ∎

Bibliography

[ABEP98] J. Aubreton, E. Blanquet, M.F. Elchinger, and M. Pons. *Les Différentes Voies de Modélisation Macroscopique du Procédé de Dépôt de SiC par Voie Gazeuse*. Ann. Chim. Sci. Mat. **23** (1998), 753–789 (French).

[Axe94] O. Axelsson. *Iterative Solution Methods*. Cambridge University Press, Cambridge, UK, 1994.

[Ben90] G. Benkowsky. *Induktionserwärmung. Härten, Glühen, Schmelzen, Löten, Schweißen*, 5th ed. Verlag Technik GmbH, Berlin, 1990 (German).

[Bey98] J. Bey. *Finite-Volumen- und Mehrgitter-Verfahren für elliptische Randwertprobleme*. Advances in Numerical Mathematics, B.G.Teubner, Stuttgart, Germany, 1998 (German).

[BK73] I. Barin and O. Knacke. *Thermodynamical Properties of Inorganic Substances*. Springer-Verlag, Berlin, 1973.

[BK90] D.P. Birnie and W.D. Kingery. *The limit of non-stoiciometry in silicon carbide*. J. Mater. Sci. **25** (1990), 2827–2834.

[BKP+99] N. Bubner, O. Klein, P. Philip, J. Sprekels, and K. Wilmański. *A transient model for the sublimation growth of silicon carbide single crystals*. J. Crystal Growth **205** (1999), 294–304.

[BMH+93] D.L. Barrett, J.P. McHugh, H.M. Hobgood, R.H. Hopkins, P.G. McMullin, R.C. Clarke, and W.J. Choyke. *Growth of large SiC single crystals*. J. Crystal Growth **128** (1993), 358–362.

[Bré83] H. Brézis. *Analyse fonctionnelle*. Masson, Paris, 1983 (French).

[BSG+91] D.L. Barrett, R.G. Seidensticker, W. Gaida, R.H. Hopkins, and W.J. Choyke. *SiC boule growth by sublimation vapor transport*. J. Crystal Growth **109** (1991), 17–23.

[CAB+99] K. Chourou, M. Anikin, J.M. Bluet, J.M. Dedulle, R. Madar, M. Pons, E. Blanquet, C. Bernard, P. Grosse, C. Faure, G. Basset, and Y. Grange. *Modelling of SiC sublimation growth process: analyses of macrodefects formation*. Mater. Sci. Eng. B **61-62** (1999), 82–85.

[CH98] T. Cazenave and A. Haraux. *An Introduction to Semilinear Evolution Equations.* Oxford Lecture Series in Mathematics and its Applications, vol. 13, Oxford University Press, Oxford, UK, 1998.

[CL00] P.G. Ciarlet and J.L. Lions (eds.). *Handbook of Numerical Analysis.* vol. 7, North-Holland/ Elsevier, Amsterdam, The Netherlands, 2000.

[CRS94] S. Clain, J. Rappaz, and M. Swierkosz. *Coupling between nonlinear Maxwell and heat equations for an induction heating problem: Modeling and numerical methods*, in [Kri94], pp. 163–171.

[CTG+99] C.H. Carter, Jr., V.F. Tsvetkov, R.C. Glass, D. Henshall, M. Brady, St.G. Müller, O. Kordina, K. Irvine, J.A. Edmond, H.-S. Kong, R. Singh, S.T. Allen, and J.W Palmour. *Progress in SiC: from material growth to commercial device development.* Mater. Sci. Eng. B **61-62** (1999), 1–8.

[CZP+99] Q.-S. Chen, H. Zhang, V. Prasad, C.M. Balkas, and N.K. Yushin. *A System Model for Silicon Carbide Crystal Growth by Physical Vapor Transport Method.* 1999 National Heat Transfer Conference, NHTC99-222. ASME, 1999, pp. 1–8.

[DMI58] P. Drowart, G. De Maria, and M.G. Inghram. *Thermodynamic Study of SiC Utilizing a Mass Spectrometer.* J. Chem. Phys. **29** (1958), no. 5, 1015–1021.

[DNR+90] F. Dupret, P. Nicodéme, Y. Ryckmans, P. Wouters, and M.J. Crochet. *Global modelling of heat transfer in crystal growth furnaces.* Intern. J. Heat Mass Transfer **33** (1990), no. 9, 1849–1871.

[EGG+98] Yu.E. Egorov, A.O. Galyukov, S.G. Gurevich, Yu.N. Makarov, E.N. Mokhov, M.G. Ramm, M.S. Ramm, A.D. Roenkov, A.S. Segal, Yu.A. Vodakov, A.N. Vorob'ev, and A.I. Zhmakin. *Modeling analysis of temperature field and species transport, inside the system for sublimation growth of SiC in Tantalum Container.* Mat. Sci. Forum **264-268** (1998), 61–64.

[EGH00] R. Eymard, T. Gallouët, and R. Herbin. *Finite Volume Methods*, pp. 713–1020 in Ciarlet and Lions [CL00], 2000.

[EKI+98] A. Ellison, T. Kimoto, I.G. Ivanov, Q. Wahab, A. Henry, O. Kordina, J. Zhang, C.G. Hemmingsson, C.-Yu Gu, M.R. Leys, and E. Janzén. *Growth and characterization of SiC of thick SiC epilayers by high temperature CVD.* Materials Science Forum **264–268** (1998), 103–106.

[FKL01] J. Fuhrmann, Th. Koprucki, and H. Langmach. *pdelib: An open modular tool box for the numerical solution of partial differential equations. Design patterns*, in [pro01].

[FL01] J. Fuhrmann and H. Langmach. *Stability and existence of solutions of time-implicit finite volume schemes for viscous nonlinear conservation laws.* Applied Numerical Mathematics **37** (2001), 201–230.

[GGZ74] H. Gajewski, K. Gröger, and K. Zacharias. *Nichtlineare Operatorgleichungen und Operatordifferentialgleichungen.* Akademie-Verlag, Berlin, 1974 (German).

[GHTC97] R.C. Glass, D. Henshall, V.F. Tsvektov, and C.H. Carter, Jr. *SiC Seeded Crystal Growth.* Phys. Stat. Sol. (b) **202** (1997), 149–162.

[GKO95] B. Gustafsson, H.-O. Kreiss, and J. Oliger. *Time Dependent Problems and Difference Methods.* Pure and Applied Mathematics, John Wiley & Sons, Inc., New York, USA, 1995.

[GO92] G.H. Golub and J.M. Ortega. *Scientific Computing and Differential Equations. An Introduction to Numerical Methods. Revised Edition.* Academic Press, Inc, Boston, USA, 1992.

[Grü67] B. Grünbaum. *Convex Polytopes.* Pure and Applied Mathematics, vol. XVI, Interscience Publishers, London, 1967.

[Gri99] J.A. Griepentrog. *Zur Regularität linearer elliptischer und parabolischer Randwertprobleme mit nichtglatten Daten.* Ph.D. thesis, Humboldt-Universität Berlin, Germany, 1999 (German).

[Har95] G.L. Harris (ed.). *Properties of Silicon Carbide.* EMIS Datareview Series, no. 13, Institution of Electrical Engineers, INSPEC, London, UK, 1995.

[Hei87] B. Heinrich. *Finite Difference Methods on Irregular Networks.* International Series of Numerical Mathematics, vol. 82, Birkhäuser Verlag, Basel, Switzerland, 1987.

[Hei88] B. Heinrich. *Coercive and inverse-isotone discretization of diffusion-convection problems.* Preprint P-MATH-19/88, Akademie der Wissenschaften der DDR, Karl Weierstraß-Institut für Mathematik, 1988.

[HHW+95] D. Hofmann, M. Heinze, A. Winnacker, F. Durst, L. Kadinski, P. Kaufmann, Y. Makarov, and M. Schäfer. *On the sublimation growth of SiC bulk crystals: development of a numerical process model.* J. Crystal Growth **146** (1995), 214–219.

[HMW98] D. Hofmann, M. Müller, and A. Winnacker. *Prospects in the use of liquid phase techniques for the growth of bulk silicon carbide crystals.* Abstracts of the 2nd European Conference on Silicon Carbide and Related Materials. 1998.

[Hof01] K.-H. Hoffmann (ed.). *Smart Materials.* Berlin, Germany, Springer-Verlag, 2001, Proceedings of the 1st caesarium, Bonn, November 17-19, 1999.

[Hus84] J.G. Hust (ed.). *Standard Reference Materials: Fine-grained, isotropic graphite for use as NBS thermophysical property RM's from 5 to 2500 K*, Tech. Report NBS/SP-260/89, National Bureau of Standards, September 1984.

[IFF96] R. IERUSALIMSCHY, L.H. DE FIGUEIREDO, and W.C. FILHO. *Lua–an extensible extension language*. Software: Practice & Experience **26** (1996), no. 6, 635–652.

[Jär96] J. JÄRVINEN. *Mathematical Modeling and Numerical Simulation of Czochralski Silicon Crystal Growth*. Ph.D. thesis, University of Jyväskylä, Finland, 1996.

[Kel96] A. KELLER. *The fast Calculation of Form Factors using Low Discrepancy Point Sequences*, in [pro96d], pp. 195 – 204.

[KKZ+00] S.YU. KARPOV, A.V. KULIK, I.A. ZHMAKIN, YU.N. MAKAROV, E.N. MOKHOV, M.G. RAMM, M.S. RAMM, A.D. ROENKOV, and YU.A. VODAKOV. *Analysis of sublimation growth of bulk SiC crystals in tantalum container*. J. Crystal Growth **211** (2000), 347–351.

[KMR97] S.YU. KARPOV, YU.N. MAKAROV, and M.G. RAMM. *Simulation of Sublimation Growth of SiC Single crystals*. Phys. Stat. Sol. (b) **202** (1997), 201–220.

[Kon95] A.O. KONSTANTINOV. *Sublimation growth of SiC*, in [Har95], pp. 170–203.

[KP99] O. KLEIN and P. PHILIP. *Transient Numerical Simulation of Sublimation Growth of SiC Single Crystals*, in [Hof01], Proceedings of the 1st caesarium, Bonn, November 17-19, 1999.

[KP01] O. KLEIN and P. PHILIP. *Transient numerical investigation of induction heating during sublimation growth of silicon carbide single crystals*. Preprint No. 659, Weierstraß-Institut für Angewandte Analysis und Stochastik, Berlin, 2001, [KP03] is a revised version of this paper.

[KP02] O. KLEIN and P. PHILIP. *Correct voltage distribution for axisymmetric sinusoidal modeling of induction heating with prescribed current, voltage, or power*. IEEE Trans. Mag. **38** (2002), no. 3, 1519–1523.

[KP03] O. KLEIN and P. PHILIP. *Transient numerical investigation of induction heating during sublimation growth of silicon carbide single crystals*. J. Crystal Growth **247** (2003), no. 1–2, 219–235.

[KPSW01] O. KLEIN, P. PHILIP, J. SPREKELS, and K. WILMAŃSKI. *Radiation- and convection-driven transient heat transfer during sublimation growth of silicon carbide single crystals*. J. Crystal Growth **222** (2001), 832–851.

[Krö97] D. KRÖNER. *Numerical Schemes for Conservation Laws*. Advances in Numerical Mathematics, Wiley Teubner, Chichester, UK, Stuttgart, Germany, 1997.

[Kri94] M. KRIZEK et al. (ed.). *Finite element methods. 50 years of the Courant element*. Lect. Notes Pure Appl. Math., vol. 164, New York, NY, Marcel Dekker, Inc., 1994.

[KRRS98] E.L. KITANIN, M.S. RAMM, V.V. RIS, and A.A. SCHMIDT. *Heat transfer through source powder in sublimation growth of SiC crystal*. Mater. Sci. Eng. B **55** (1998), 174–183.

[Lel55] J.A. Lely. *Darstellung von Einkristallen von Siliciumcarbid und Beherrschung von Art und Menge der eingebauten Verunreingungen.* Ber. Deut. Keram. Ges. **32** (1955), 229–231 (German).

[Lid95] D.R. Lide. *CRC Handbook of Chemistry and Physics.* CRC Press, Boca Raton, USA, 1995.

[LT00] M. Laitinen and T. Tiihonen. *Conductive-Radiative Heat Transfer in Grey Materials.* Reports of the Department of Mathematical Information Technology Series B. Scientific Computing. No. B 6/2000. University of Jyväskylä, Finland, 2000.

[Mac53] R. H. MacNeal. *An asymmetrical finite difference network.* Quaterly of Applied Math **11** (1953), no. 3, 295–310.

[MGH+00] St.G. Müller, R.C. Glass, H.M. Hobgood, V.F. Tsvetkov, M. Brady, D. Henshall, J.R. Jenny, D. Malta, and C.H. Carter Jr. *The status of SiC bulk growth from an industial point of view.* J. Crystal Growth **211** (2000), 325–332.

[Mod93] M.F. Modest. *Radiative Heat Transfer.* McGraw-Hill Series in Mechanical Engineering, McGraw-Hill, Inc., New York, USA, 1993.

[MR01] K. Mikula and N. Ramarosy. *Semi-implicit finite volume scheme for solving nonlinear diffusion equations in image processing.* Numer. Math. **89** (2001), 561–590.

[MRRV97] E.N. Mokhov, M.G. Ramm, A.D. Roenkov, and Yu.A. Vodakov. *Growth of silicon carbide bulk crystals by the sublimation sandwich method.* Mater. Sci. Eng. B **46** (1997), 317–323.

[MSS99a] T. Müller, D. Schulz, and D. Siche. 1999, material vendor's data, communicated by the Institut für Kristallzüchtung, Berlin.

[MSS99b] T. Müller, D. Schulz, and D. Siche. Institut für Kristallzüchtung, Berlin, 1999, unpublished experimental data.

[Mül85] I. Müller. *Thermodynamics.* Interaction of Mechanics and Mathematics, Pitman Publishing Limited, London, 1985.

[Neč67] J. Nečas. *Les méthodes directes en théorie des equations elliptiques.* Academia, Prague, 1967 (French).

[Nis95a] S. Nishino. *Bulk growth of SiC,* in [Har95], pp. 163–169.

[Nis95b] S. Nishino. *Chemical vapour deposition of SiC,* in [Har95], pp. 204–213.

[NMH+97] O. Nilsson, H. Mehling, R. Horn, J. Fricke, R. Hofmann, S.G. Müller, R. Eckstein, and D. Hofmann. *Determination of the thermal diffusivity and conductivity of monocrystalline silicon carbide (300-2300 K).* High Temp. – High Press. **29** (1997), no. 1, 73–80.

[Ohl01] M. Ohlberger. *A posteriori error estimates and adaptive methods for convection dominated transport processes.* Ph.D. thesis, Albert-Ludwigs-Universität Freiburg, Germany, 2001.

[Oss92] E. Ossa. *Topologie.* vieweg studium, vol. 42, Vieweg, Braunschweig, Germany, 1992 (German).

[PAC+99] M. Pons, M. Anikin, K. Chourou, J.M. Dedulle, R. Madar, E. Blanquet, A. Pisch, C. Bernard, P. Grosse, C. Faure, G. Basset, and Y. Grange. *State of the art in the modelling of SiC sublimation growth.* Mater. Sci. Eng. B **61-62** (1999), 18–28.

[PBD+96] M. Pons, E. Blanquet, J.M. Dedulle, I. Garcon, R. Madar, and C. Bernard. *Thermodynamic Heat Transfer and Mass Transport Modelling of the Sublimation Growth of Silicon Carbide Crystals.* J. Electrochem. Soc. **143** (1996), no. 11, 3727–3735.

[pro96a] *Modelling and optimization of distributed parameter systems (Warsaw, 1995).* New York, Chapman & Hall, 1996.

[pro96b] *Proc. European Material Research Society.* 1996.

[pro96c] *First Workshop on Applied Computational Geometry (Philadelphia, Pennsylvania).* ACM, May 1996.

[pro96d] *Proceedings of the 12th Spring Conference on Computer Graphics.* Bratislava, 1996.

[pro01] *Proceedings of the 14th GAMM Seminar on Concepts of Numerical Software, Kiel, January 23–25, 1998.* Kiel, Germany, 2001.

[PTVF96] W.H. Press, S.A. Teukolsky, W.T. Vetterling, and B.P. Flannery. *Numerical Recipes in C. The Art of Scientific Computing*, 2nd ed. Cambridge University Press, New York, USA, 1996.

[Råb96] P. Råback. *Modeling of the Sublimation Growth of Silicon Carbide Crystals.* Ph.D. thesis, Helsinki University of Technology, 1996.

[RCB96] P. Rocabois, C. Chiatillon, and C. Bernard. *Thermodynamics of the Si – C system: I. Mass spectrometric studies of the condensed phases at high temperature.* High Temp. – High Press. **27/28** (1995/1996), 3–23.

[Ric31] L.A. Richards. *Capillary conduction of liquids through porous mediums.* Phys. **1** (1931), 318–333.

[RMD+99] M.S. Ramm, E.N. Mokhov, S.E. Demina, M.G. Ramm, A.D. Roenkov, Yu.A. Vodakov, A.S. Segal, A.N. Vorob'ev, S.Yu. Karpov, A.V. Kulik, and Yu.N. Makarov. *Optimization of sublimation growth of SiC bulk crystals using modeling.* Mater. Sci. Eng. B **61-62** (1999), 107–112.

[RR96] M. RENARDY and R.C. ROGERS. *An Introduction to Partial Differential Equations.* Texts in Applied Mathematics, vol. 13, Springer-Verlag, New York, 1996, corrected 2nd printing.

[RS96] J. RAPPAZ and M. SWIERKOSZ. *Modelling in numerical simulation of electromagnetic heating*, in [pro96a], pp. 313–320.

[RSD+99] H.-J. ROST, D. SICHE, J. DOLLE, W. EISERBECK, T. MÜLLER, D. SCHULZ, G. WAGNER, and J. WOLLWEBER. *Influence of different growth parameters and related conditions on 6H-SiC crystals grown by the modified Lely method.* Mater. Sci. Eng. B **61-62** (1999), 68–72.

[Rud87] W. RUDIN. *Real and Complex Analysis*, 3rd ed. McGraw-Hill Book Company, New York, 1987.

[SBP98] N. SCHULZE, D.L. BARRETT, and G. PENSL. *Near-equilibrium growth of mircopipe-free 6H-SiC single crystals by physical vapor transport.* Appl. Phys. Lett. **72** (1998), no. 13, 1632–1634.

[SC78] E.M. SPARROW and R.D. CESS. *Radiation Heat Transfer.* Hemisphere Publishing Corporation, Washington, D.C., USA, 1978.

[SGFS00] OLAF SCHENK, K. GÄRTNER, W. FICHTNER, and A. STRICKER. *PARDISO: A high-performance serial and parallel sparse linear solver in semiconductor device simulation.* Journal of Future Generation Computer Systems **789** (2000), 1–9.

[SH93] P. SCHRÖDER and P. HANRAHAN. *A Closed Form Expression for the Form Factor between Two Polygons*, Tech. Report TR-404-93, Computer Science Department at Princeton University, Princeton, USA, January 1993.

[She96] J.R. SHEWCHUK. *Triangle: Engineering a 2D Quality Mesh Generator and Delaunay Triangulator*, in [pro96c], pp. 124–133.

[Shr99] D. SHREINER (ed.). *OpenGL Reference Manual: The Official Reference Document to OpenGL, Version 1.2*, 3rd ed. Addison-Wesley, Reading, USA, 1999.

[SKM+00] M. SELDER, L. KADINSKI, YU. MAKAROV, F. DURST, P. WELLMANN, T. STRAUBINGER, D. HOFFMANN, S. KARPOV, and M. RAMM. *Global numerical simulation of heat and mass transfer for SiC bulk crystal growth by PVT.* J. Crystal Growth **211** (2000), 333–338.

[SVK+00] A.S. SEGAL, A.N. VOROB'EV, S.YU. KARPOV, E.N. MOKHOV, M.G. RAMM, M.S. RAMM, A.D. ROENKOV, YU.A. VODAKOV, and YU.N. MAKAROV. *Growth of silicon carbide by sublimation sandwich method in the atmosphere of inert gas.* J. Crystal Growth **208** (2000), 431–441.

[TdW72] Y.S. TOULOUKIAN and D.P. DE WITT. *Thermal Radiative Properties - Nonmetallic Solids.* Thermophysical Properties of Matter: The TPRC Data Series, vol. 8, IFI/Plenum, New York, USA, 1972.

[Tii97] T. TIIHONEN. *A nonlocal problem arising from heat radiation on non-convex surfaces.* Eur. J. App. Math. **8** (1997), 403–416.

[TT78] YU.M. TAIROV and V.F. TSVETKOV. *Investigation of Growth Processes of Ingots of Silicon Carbide Single Crystals.* J. Crystal Growth **43** (1978), 209–212.

[TT81] YU.M. TAIROV and V.F. TSVETKOV. *General Principles of Growing Large-Size Single Crystals of Various Silicon Carbide Polytypes.* J. Crystal Growth **52** (1981), 146–150.

[Var75] N.B. VARGAFTIK. *Tables on the Thermophysical Properties of Liquids and Gases.* Hemisphere, Washington, D.C., USA, 1975.

[VMRR79] YU.A. VODAKOV, E.N. MOKHOV, M.G. RAMM, and A.D. ROENKOV. *Epitaxial Growth of Silicon Carbide Layers by Sublimation „Sandwich Method"(I): Growth Kinetics in Vacuum.* Kristall und Technik **14** (1979), no. 6, 729–740.

[VRR+97] YU.A. VODAKOV, A.D. ROENKOV, M.G. RAMM, E.N. MOKHOV, and YU.N. MAKAROV. *Use of Ta-Container for Sublimation Growth and Doping of SiC Bulk Crystals and Epitaxial Layers.* Phys. Stat. Sol. (b) **202** (1997), 177–200.

[Wil98] K. WILMAŃSKI. *Thermomechanics of Continua.* Springer-Verlag, Berlin, New York, 1998.

[Wlo82] J. WLOKA. *Partielle Differentialgleichungen.* B.G. Teubner, Stuttgart, Germany, 1982 (German).

[Zei86] E. ZEIDLER. *Nonlinear Functional Analysis and its Applications.* vol. I, Springer-Verlag, New York, 1986.

[Zei90] E. ZEIDLER. *Nonlinear Functional Analysis and its Applications.* vol. II/A, Springer-Verlag, New York, 1990.

[Zie98] G.M. ZIEGLER. *Lectures on Polytopes*, revised 1st ed. Graduate Texts in Mathematics, vol. 152, Springer, New York, 1998.

List of Symbols

Apparently, it is practically unavoidable that occasionally a symbol occurs with different meanings in different contexts. In the following list, each symbol is listed with all its meanings occurring in the text. In case the symbol is defined in the text, the list provides a reference to the page or to the formula with the respective definition.

Symbols that are not based on a letter are listed first, followed by letter-based symbols in alphabetical order. For each letter, stylized letters are listed first, followed by Greek letters, followed by Roman letters, where upper case letters are listed before lower case letters, e.g. ∂, Δ, δ, D, d. Moreover, the following order is used for fonts: blackboard bold, Fraktur, calligraphic, bold, roman, e.g. $\mathbb{D}$, $\mathfrak{D}$, $\mathcal{D}$, $\mathbf{D}$, D.

See $f\ldots$ for some function-related symbols.

Symbol	Meaning	Ref.
$[\ldots]$	function argument	p. x
$(\ldots)$	grouped terms	p. x
$\vert\ \vert$	absolute value	
$\Vert\ \Vert$	abstract norm	
$\Vert\ \Vert_{\mathrm{Lip}}$	Lipschitz norm	(C.7.6)
$\Vert\ \Vert_{\max}$	max-norm	(C.1.1)
$\Vert\ \Vert_p$	l_p-norm	Def. C.2.1
$\Vert\ \Vert_{\sup}$	$\Vert f\Vert_{\sup} := \sup\left\{f[a] : a \text{ in domain of } f\right\}$	
$:=$	equals by definition	
$\cong$	isomorphic	
$\approx$	approximately equal	
$\ll$	much less	
$\bigwedge\limits_x \phi[x]$	formula ϕ holds for each x	p. x
$\bigvee\limits_x \phi[x]$	there exists x such that formula ϕ holds for x	p. x
$\emptyset$	empty set	
$\setminus$	set-theoretic difference	
$\cap$	set-theoretic intersection	
$\cup$	set-theoretic union	
$\bigcup_{j\in J} A_j$	union of sets A_j	
$\dot\cup$	disjoint set-theoretic union	

Symbol	Meaning	Ref.
$\times$	cartesian product	
$\prod_{j\in J} A_j$	cartesian product of sets A_j	
$\circ$	composition of functions	
$\bullet$	scalar product	(B.1.1)
$\otimes$	tensor product	(B.1.3)
∇	gradient	(B.1.6)
$\int_A$	integral over A	
$\mathbf{1}$	identity matrix	
α	absorptivity	p. 25
α	variable with domain $\{1, 2\}$	
α_ι	variable for gas phase constituents	p. 10
$\mathfrak{A}^{(\nu)}_{\mathrm{con},(k,\mathcal{C})}$	discretized nonlocal interface operator	p. 121
$\mathfrak{A}^{(\nu)}_{\mathrm{con},k,\mathrm{solid}}$	. . . .	(3.7.92)
$\mathfrak{A}^{(\nu)}_{\mathrm{jump},(k,\mathcal{C})}$	discretized nonlocal interface operator	p. 121
$\mathfrak{A}^{(\nu)}_{\mathrm{jump},k,\mathrm{solid}}$	. . . .	(3.7.93)
$\mathcal{A}$	variable for affine subspaces	p. 235
$\mathcal{A}^\perp[(v,w)]$	$\mathcal{A}^\perp[(v,w)] := \{x \in \mathbb{R}^d : \Vert v-x\Vert_2 = \Vert w-x\Vert_2\}$	Not. C.4.15
$\mathcal{A}_\gamma$	nonlocal interface operator	(3.4.10)
$\underline{\mathcal{A}_\gamma}$	. . . .	p. 88
$(\mathcal{A}_\gamma)^{\text{ex.-im.}}$	dependency splitting of $\mathcal{A}_\gamma$	(3.4.22)
$(\underline{\mathcal{A}_\gamma})^{\text{ex.-im.}}$	. . . .	p. 89
$\mathbf{A}$	variable for tensors and matrices	p. 222
$\mathbf{A}$	matrix arising during radiation discretization	p. 126
$\mathbf{A}$	magnetic vector potential	(2.5.8)
$\mathbf{A}^\top$	transpose of matrix $\mathbf{A}$	
A	number of gas phase constituents	p. 10
A	variable for a set	
$\overline{A}$	closure of the set A	p. 232
$\#A$	number of elements of the set A, cardinality of A	
A^I	set of functions from I into A, identical to the cartesian product of $\#I$ copies of A	
$\mathfrak{a}^{(\nu)}_{\mathrm{flux},\mathrm{con},(k,\mathcal{C})}$	. . . .	(3.7.57)
$\mathfrak{a}^{\nu,\uparrow}_{\mathrm{flux},\mathrm{con},(k,\mathcal{C})}$	. . . .	(3.8.37a)
$\mathfrak{a}^{\nu,\downarrow}_{\mathrm{flux},\mathrm{con},(k,\mathcal{C})}$	. . . .	(3.8.37b)
$\mathfrak{a}^{(\nu)}_{\mathrm{flux},\mathrm{jump},2,\mathrm{Dir},(k,\mathcal{C})}$	. . . .	(3.7.63)
$\mathfrak{a}^{(\nu)}_{\mathrm{flux},\mathrm{jump},2,\neg\mathrm{Dir},(k,\mathcal{C})}$	. . . .	(3.7.62)
$\mathfrak{a}^{(\nu)}_{\mathrm{jump},1,\mathrm{Dir},(k,\mathcal{C})}$	. . . .	(3.7.60)
$\mathfrak{a}^{(\nu)}_{\mathrm{jump},1,\neg\mathrm{Dir},(k,\mathcal{C})}$	. . . .	(3.7.59)

Symbol	Meaning	Ref.
$\mathfrak{a}^{\nu,\uparrow}_{\text{jump},1,\neg\text{Dir},(k,\mathcal{C})}$	. . . .	(3.8.39a)
$\mathfrak{a}^{\nu,\downarrow}_{\text{jump},1,\neg\text{Dir},(k,\mathcal{C})}$	. . . .	(3.8.39b)
$\mathfrak{a}^{(\nu)}_{\text{jump},2,\text{Dir},(k,\mathcal{C})}$	. . . .	(3.7.66)
$\mathfrak{a}^{(\nu)}_{\text{jump},2,\neg\text{Dir},(k,\mathcal{C})}$	. . . .	(3.7.65)
$\mathfrak{a}^{\nu,\uparrow}_{\text{jump},2,\neg\text{Dir},(k,\mathcal{C})}$	. . . .	(3.8.42a)
$\mathfrak{a}^{\nu,\downarrow}_{\text{jump},2,\neg\text{Dir},(k,\mathcal{C})}$	. . . .	(3.8.42b)
$\mathfrak{a}^{(\nu)}_{\text{out},(k,\mathcal{C})}$	. . . .	(3.7.51)
$\mathfrak{a}^{\nu,\uparrow}_{\text{out},(k,\mathcal{C})}$	. . . .	(3.8.33a)
$\mathfrak{a}^{\nu,\downarrow}_{\text{out},(k,\mathcal{C})}$	. . . .	(3.8.33b)
a	variable for set elements	
$a^{\gamma,1}_{\text{flux}}$	first given function in flux interface condition	(3.4.9b)
$a^{\gamma,2}_{\text{flux}}$	second given function in flux interface condition	(3.4.9b)
$\underline{a}^{\gamma,\alpha}_{\text{flux}}$	. . . .	p. 88
$(a^{\gamma,\alpha}_{\text{flux}})^{\text{ex.-im.}}$	dependency splitting of $a^{\gamma,\alpha}_{\text{flux}}$	(3.4.23)
$(\underline{a}^{\gamma,\alpha}_{\text{flux}})^{\text{ex.-im.}}$	. . . .	p. 89
$(a^{\gamma,\alpha,\nu}_{\text{flux}})^{\text{ex.-im.}}$	time-discrete dependency splitting of $a^{\gamma,\alpha}_{\text{flux}}$	(3.4.25)
$(\underline{a}^{\gamma,\alpha,\nu}_{\text{flux}})^{\text{ex.-im.}}$	. . . .	p. 89
$a_{i,j}$	components of the tensor $\mathbf{A}$	p. 222
$a^{\gamma,1}_{\text{jump}}$	first given function in jump interface condition	(3.4.9a)
$a^{\gamma,2}_{\text{jump}}$	second given function in jump interface condition	(3.4.9a)
$\underline{a}^{\gamma,\alpha}_{\text{jump}}$	. . . .	p. 88
$a^{\gamma,\alpha,\nu}_{\text{jump}}$	time-discrete given functions in jump interface condition	(3.4.21)
$\underline{a}^{\gamma,\alpha,\nu}_{\text{jump}}$	. . . .	p. 89
$a^{j,\iota}_{\text{out}}$	. . . .	(3.4.12b)
$\underline{a}^{j,\iota}_{\text{out}}$	. . . .	p. 88
$(a^{j,\iota}_{\text{out}})^{\text{ex.-im.}}$	dependency splitting of $a^{j,\iota}_{\text{out}}$	(3.4.30)
$(\underline{a}^{j,\iota}_{\text{out}})^{\text{ex.-im.}}$	. . . .	p. 89
$(a^{j,\iota,\nu}_{\text{out}})^{\text{ex.-im.}}$	time-discrete dependency splitting of $a^{j,\iota}_{\text{out}}$	(3.4.32)
$(\underline{a}^{j,\iota,\nu}_{\text{out}})^{\text{ex.-im.}}$	. . . .	p. 89
$\text{aff}[A]$	affine hull of A	(C.4.1)
$\text{av}_{\text{con}}[\gamma]$	. . . .	(3.7.108)
$\text{av}_{\text{jump},\alpha}[\gamma]$	. . . .	(3.7.111)
$\text{av}^{j,\iota}_{\text{out}}$	. . . .	(3.7.96)
β	variable for solid materials	

Symbol	Meaning	Ref.
β'	variable for solid materials	
β_j	variable for solid materials	p. 20
$\mathfrak{B}^{(\nu)}_{(k,\mathcal{C})}$	discretized nonlocal boundary operator	p. 121
$\mathfrak{B}^{(\nu)}_{k,\mathrm{solid}}$		(3.7.91)
$\mathcal{B}$		p. 122
$\mathcal{B}_{j,\iota}$	nonlocal boundary operator	(3.4.13)
$\underline{\mathcal{B}}_{j,\iota}$		p. 88
$(\mathcal{B}_{j,\iota})^{\text{ex.-im.}}$	dependency splitting of $\mathcal{B}_{j,\iota}$	(3.4.29)
$(\underline{\mathcal{B}}_{j,\iota})^{\text{ex.-im.}}$		p. 89
$\mathbf{B}$	variable for tensors	p. 222
$\mathbf{B}$	magnectic induction	p. 32
B	variable for a set	
$B^{\downarrow,\uparrow}[(\dots)]$		(3.8.58)
$B_{b,0}[\mathfrak{C}]$		(3.7.133)
$B_{\mathrm{con}}[\mathfrak{C}]$		(3.7.110)
$B_{\mathrm{con},1,m_v}[(\mathfrak{C},\mathfrak{S}_{\mathrm{con}})]$		(3.8.38a)
$B_{\mathrm{con},2,m_v}[(\mathfrak{C},\mathfrak{S}_{\mathrm{con}})]$		(3.8.38b)
$B_{\mathrm{Dir}}[\mathfrak{C}]$		(3.7.27)
$B_{d,r}[x_0]$	open r-ball with center x_0 and with respect to metric d	(C.7.2)
$B_f[\mathfrak{C}]$		(3.7.121)
$B_{f,m_v}[\mathfrak{C}]$		(3.8.47)
$B_{\mathrm{flux,Dir}}[\mathfrak{C}]$		(3.8.44)
$B_{\mathrm{flux,jump},1,m_v}[(\mathfrak{C},\mathfrak{S}_{\mathrm{jump}})]$		(3.8.43a)
$B_{\mathrm{flux,jump},2,m_v}[(\mathfrak{C},\mathfrak{S}_{\mathrm{jump}})]$		(3.8.43b)
$B_{\mathrm{IF}}[\mathfrak{C}]$		Def. 3.7.28
$B_{\mathrm{jump}}[\mathfrak{C}]$		(3.7.113)
$B_{\mathrm{jump,Dir}}[\mathfrak{C}]$		(3.7.114)
$B_{\mathrm{jump,Dir},m_v}[\mathfrak{C}]$		(3.8.41)
$B_{\mathrm{jump},m_v}[\mathfrak{C}]$		(3.8.40)
$B_{k,\mathrm{Dir}}[\mathfrak{C}]$		(3.7.28)
$B^{\uparrow}_{k,\mathrm{Dir}}[\mathfrak{C}]$		(3.8.27b)
$B^{\downarrow}_{k,\mathrm{Dir}}[\mathfrak{C}]$		(3.8.27a)
$B_{k,m_v}[\mathfrak{C}]$		(3.8.24)
$B_{\mathrm{nonloc}}[\mathfrak{C}]$		Def. 3.8.25
$B_{\mathrm{out}}[\mathfrak{C}]$		p. 129
$B_{\mathrm{out},m_v}[(\mathfrak{C},\mathfrak{S}_{\mathrm{out}})]$		(3.8.34)
$B_r[x_0]$	open r-ball with center x_0	Def. C.7.3
$B_{\mathfrak{s}}[(\mathfrak{C},\Pi,\mathfrak{V})]$		(3.7.125)
$B_{v,\mathrm{Dir}}[(\mathfrak{C},\mathfrak{V})]$		(3.7.45)
$B_{v,\mathrm{sca,Dir}}[(\mathfrak{C},\mathfrak{V})]$		(3.7.46)

Symbol	Meaning	Ref.
$\mathfrak{b}^{(\nu)}_{(k,\mathcal{C})}$	. . . .	(3.7.10)
$\mathbf{b}^{(\alpha_\iota)}$	partial force density of constituent α_ι	p. 11
$\mathbf{b}_{\mathbf{gas}}$	total force density of the gas mixture	(2.1.6b)
b	variable for set elements	
b	variable for function under the time derivative	(3.3.2a)
b_j	function under the time derivative in the j-th material	(3.1.1)
$\underline{b}_j$	. . . .	p. 88
$b_{i,j}$	components of the tensor $\mathbf{B}$	p. 222
$b^{(\nu)}$	function b at discrete time t_ν	(3.3.9a)
$b^{(\nu)}_{(k,\mathcal{C})}$	$b^{(\nu)}_{(k,\mathcal{C})} := \mathfrak{b}^{(\nu)}_{(k,\mathcal{C})}$	(3.8.52e)
$\mathbb{C}$	the set of complex numbers	
$\mathfrak{C}$	evolution equation complex	Def. 3.4.6
$\underline{\mathfrak{C}}$	. . . .	p. 88
$\mathcal{C}$	variable for connected components of $\mathcal{G}_{\omega_k}$	
$\mathcal{C}[(l,j)]$	$\mathcal{C}[(l,j)] = \mathrm{CoCmp}_{\mathcal{G}_{\omega_l}}[j]$	(3.7.13)
$C[X]$	set of continuous functions from X into $\mathbb{R}$	Not. C.6.1
$C(X,Y)$	set of continuous functions from X into Y	p. 232
$C^k[A]$	set of functions from A into $\mathbb{R}$ having continuous partial derivatives up to order k	Not. C.6.1
$C^k(A,B)$	set of functions from A into B having continuous partial derivatives up to order k	Not. C.6.1
$C^k(A,B)$	set of functions from A into B having continuous partial derivatives of all orders	Not. C.6.1
$C_{\mathrm{pw}}(X,Y)$	set of piecewise continuous functions from X into Y	p. 232
$c^{(\alpha_\iota)}$	concentration of constituent α_ι	(2.1.4c)
$c_{\mathrm{sp}}^{[\beta_j]}$	specific heat of solid material β_j	p. 21
c^{complex}	variable for complex numbers	
$\overline{c^{\mathrm{complex}}}$	complex conjugate of c^{complex}	
$\mathrm{cl}_{\mathcal{O}}[A]$	closure of A with respect to topology $\mathcal{O}$	p. 232
$\mathrm{CoCmp}[\mathcal{G}]$	connected components of graph $\mathcal{G}$	Def. C.5.5
$\mathrm{CoCmp}_{\mathcal{G}}[v]$	connected component in graph $\mathcal{G}$ of vertex v	Def. C.5.3
$\mathrm{conv}[A]$	convex hull of set A	Def. C.4.6
$\partial_{\dots}$	partial derivative	Not. C.6.3
∂A	boundary of set A	p. 232
$\partial\sigma$	boundary of simplex σ	(C.4.8)
$\partial_{\mathrm{reg}}p$	regular boundary of polytope p	Def. C.4.11
$\partial_{\mathrm{sin}}p$	singular boundary of polytope p	Def. C.4.11
$\frac{d}{dt}$	material derivative	(2.1.13)
Δ	fineness of time discretization	(3.3.7)

Symbol	Meaning	Ref.
	$\Delta_\nu := t_\nu - t_{\nu-1}$	(3.8.52d)
$\mathfrak{D}$	domain complex	Def. 3.4.5
$\underline{\mathfrak{D}}$	. . . .	p. 88
$\mathbf{D}$	matrix arising during radiation discretization	p. 126
$D^{(\alpha_\iota)}$	diffusion coefficient of constituent α_ι	(2.1.21)
$D_{\kappa,\lambda}$	components of matrix $\mathbf{D}$	(3.7.81e)
$\mathrm{d}m[x]$	integration with respect to measure m and variable x	
d	dimension of space domain	p. 46
d	variable for finite dimensions	
d	variable for metrics	p. 243
$d(x, A)$	distance of x from set A in metric d	Not. C.7.2
d'	dimension of q	Def. 3.6.1
d'	variable for finite dimensions	
$d_{\mathrm{Dir}}[\Pi]$	. . . .	(3.7.29)
$d_{\max}[\Pi]$	. . . .	(3.8.25)
det	determinant	
diam A	diameter of set A	(3.5.1)
dim	dimension	
div	divergence	(B.1.6)
$\epsilon[(T[\mathrm{x}], \mathrm{x})]$	emissivity	(2.4.2)
$\epsilon[(T[\mathrm{x}], \mathrm{x}, \lambda)]$	monochromatic emissivity	p. 30
$\epsilon^{[\beta]}$	emissivity of solid β	p. 22
ϵ_{circ}	. . . .	p. 27
ϵ_{r}	emissivity of reflective band	(2.4.31a)
ϵ_{t}	emissivity of transmittive band	(2.4.31b)
$\varepsilon^{(\alpha_\iota)}$	partial internal energy of constituent α_ι	p. 11
$\varepsilon^{*(\alpha_\iota)}$	partial energy source of constituent α_ι	(2.1.9)
$\varepsilon_{\mathrm{gas}}$	total internal energy of the gas mixture	(2.1.6c)
$\mathcal{E}$	radiation operator	(2.4.13b)
$\mathcal{E}_{\mathrm{circ}}$	radiation operator	(2.4.26b)
$\mathbf{E}$	electric field	p. 32
E	emitted radiation	(2.4.3)
$E[\mathcal{G}]$	set of edges of graph $\mathcal{G}$	Def. C.5.1
E_{con}	$E_{\mathrm{con}} := \{e[\gamma] : \gamma \in \mathrm{IF}_{\mathrm{con}}\}$	p. 60
E_{IF}	. . . .	(3.4.4)
$E_{\mathrm{IF}}[\Pi]$	. . . .	(3.7.11)
E_{jump}	$E_{\mathrm{jump}} := \{e[\gamma] : \gamma \in \mathrm{IF}_{\mathrm{jump}}\}$	p. 60
E_{r}	reflective emitted radiation	p. 29
E_{t}	transmittive emitted radiation	p. 29
$\mathbf{e}_r$	radial cylindrical basis vector	(B.3.2a)
$\mathbf{e}_\vartheta$	angular cylindrical basis vector	(B.3.2b)

Symbol	Meaning	Ref.
$\mathbf{e}_z$	vertical cylindrical basis vector	(B.3.2c)
e	2.718...	
e	map, assigning the set of indices $\{j_1, j_2\}$ to each interface $\partial_{\mathrm{reg}} p_{j_1} \cap \partial_{\mathrm{reg}} p_{j_2}$	p. 60
ϕ_A	magnetic scalar potential	p. 34
$\phi_{A,0}$	amplitude of sinusoidal magnetic scalar potential	(2.5.25c)
$\phi_A^{\mathrm{complex}}$	complex magnetic scalar potential	(2.5.26c)
$\phi_{A,0}^{\mathrm{complex}}$	. . . .	(2.5.28c)
$\phi_{A,l,0}^{\mathrm{complex}}$	solution to (PDE$_l$: $\phi_{A,0}^{\mathrm{complex}}$)	p. 43
φ	variable for real numbers	
$\mathfrak{F}$	finite volume discretization	Def. 3.7.41
$\mathcal{F}(A, B)$	set of functions from A into B	
F	variable for a function	
F_j	flux $k_j[(u_j, t, x)]\,\nabla u_j$	p. 48
$F_{j,\partial\omega}$	flux through the boundary of $\omega \subseteq p_j$	(3.4.1)
$F_{j,\partial\omega}^{(\nu)}$	flux through the boundary of $\omega \subseteq p_j$ at time t_ν	(3.4.18)
$\mathfrak{f}_{(k,\mathcal{C})}^{(\nu)}$	. . . .	(3.7.119)
$\mathfrak{f}_{(k,\mathcal{C})}^{\nu,\uparrow}$	. . . .	(3.8.46a)
$\mathfrak{f}_{(k,\mathcal{C})}^{\nu,\downarrow}$	. . . .	(3.8.46b)
f	variable for a function	
f	variable for a source or sink function	(3.3.2d)
fA	$fA := \{f[a] : a \in A\}$	
f'	derivative of f	
f^{-1}	inverse function of f	
$f^{-1}B$	$f^{-1}B := \{a : f[a] \in B\}$	
$f\restriction_A$	f restricted to set A	
$f^{[\beta_j]}$	power density per volume in solid material β_j	p. 21
f_{circ}	$f_{\mathrm{circ}} := f\restriction_{\pi_{\mathrm{circ}} A}$	p. 27
f_j	source or sink function in the j-th material	(3.1.1)
$\underline{f}_j$	. . . .	p. 88
$f^{(\nu)}$	function f at discrete time t_ν	(3.3.9d)
$f^{[\mathrm{ring}]}$	power density per volume in coil rings	(2.5.34a)
Γ	path	p. 36
Γ	solid surface	p. 24
Γ	$\Gamma := p_{\mathrm{rad}} \cap p$	p. 122
Γ_{bottom}	lower phantom closure	p. 195
Γ_{con}	$\Gamma_{\mathrm{con}} := \Gamma \cap \bigcup_{\gamma \in \mathrm{IF}_{\mathrm{con}}} \gamma$	p. 128
$\Gamma_{j,\iota}$	non-Dirichlet boundary of type ι of j-th space domain	p. 50

Symbol	Meaning	Ref.
$\Gamma_{j,0}$	Dirichlet boundary of j-th space domain	p. 63
$\Gamma_{j,\mathrm{Dir}}$	Dirichlet boundary of j-th space domain	p. 50
Γ_{jump}	$\Gamma_{\mathrm{jump}} := \Gamma \cap \bigcup_{\gamma \in \mathrm{IF}_{\mathrm{jump}}} \gamma$	p. 128
Γ_{ph}	black body phantom closure	p. 122
Γ_{sin}	singular part of surface Γ	p. 24
Γ_{reg}	regular part of surface Γ	p. 24
Γ_{t}	boundary of transmittive radiation region	p. 29
$\Gamma_{\mathrm{t,reg}}$	regular part of Γ_{t}	p. 29
Γ_{top}	upper phantom closure	p. 195
γ	variable for interfaces	p. 48
$\underline{\gamma}$	variable for elements of $\underline{\mathrm{IF}}$	p. 88
$\gamma_a^{(\alpha_\iota)}$	stoichiometric coefficients of constituent α_ι	p. 19
$\gamma_{\beta,\beta'}$	solid-solid interface	p. 22
$\gamma_{\beta',\mathrm{gas}}$	solid-gas interface	p. 22
$\gamma_{\gamma_1,\gamma_2}$	interface between materials γ_1 and γ_2	p. 37
γ_j	index for both solid materials and gas	p. 37
γ_{j_1,j_2}	interface between materials j_1 and j_2	p. 48
$\mathcal{G}$	radiation operator	(2.4.13a)
$\mathcal{G}$	variable for graphs	Def. C.5.1
$\mathcal{G}\restriction_{V_0}$	induced subgraph of $\mathcal{G}$ on vertex set $V_0\restriction_{V_0}$	Def. C.5.1
$\mathcal{G}_{\mathrm{circ}}$	radiation operator	(2.4.26a)
$\mathcal{G}_k$	$\mathcal{G}_k := \mathcal{G}_{\omega_k}$	p. 83
$\mathcal{G}_\omega$	associated graph of ω	Def. 3.5.3
$G_{\mathrm{jump},\alpha}$	. . . .	(3.5.20)
$\mathbf{g}$	gravimetric acceleration	p. 17
g	variable for a function	
g_i	components of the vector $\mathbf{g}$	
$g^{(\nu)}_{(k,\mathcal{C})}$	. . . .	(3.8.52g)
$\tilde{g}^{(\nu)}_{(k,\mathcal{C})}$	. . . .	(3.8.52b)
$\mathcal{H}^{(\nu)}_{(k,\mathcal{C})}$	. . . .	(3.8.50)
$\mathbf{H}$	magnectic field	p. 32
$H_{b,v,k,f}$	evolution operator	(3.3.3)
H_{b_j,v_j,k_j,f_j}	evolution operator on j-th space domain	p. 58
$H_{\underline{b}_j,\underline{v}_j,\underline{k}_j,\underline{f}_j}$	. . . .	p. 88
$H^{(\nu)}_{b,v,k,f}$	time-discrete evolution operator	(3.3.8)
$H^{(\nu)}_{\underline{b}_j,\underline{v}_j,\underline{k}_j,\underline{f}_j}$	. . . .	p. 89
$\mathfrak{h}^{(\nu)}$	. . . .	(3.7.6)
$\mathfrak{h}^{(\nu)}_{(k,\mathcal{C})}$	. . . .	(3.7.122)
$\mathfrak{h}^{(\nu)}_{(k,\mathcal{C}),(a)}$	. . . .	(3.7.9)

Symbol	Meaning	Ref.
$\mathfrak{h}^{(\nu)}_{(k,\mathcal{C}),(b)}$	. . . .	(3.7.39)
$\mathfrak{h}^{(\nu)}_{(k,\mathcal{C}),(c)}$	. . . .	(3.7.48)
$\mathfrak{h}^{(\nu)}_{(k,\mathcal{C}),(d)}$	. . . .	(3.7.53)
$\mathfrak{h}^{(\nu)}_{(k,\mathcal{C}),(e)}$	. . . .	(3.7.15)
$\mathfrak{h}^{(\nu)}_{(k,\mathcal{C}),(f)}$	. . . .	(3.7.67a)
$\mathfrak{h}^{(\nu)}_{(k,\mathcal{C}),(g)}$	. . . .	(3.7.50)
$\mathfrak{h}^{(\nu)}_{(k,\mathcal{C}),(h)}$	. . . .	(3.7.67b)
$\mathfrak{h}^{(\nu)}_{(k,\mathcal{C}),(i)}$	. . . .	(3.7.56)
$\mathfrak{h}^{(\nu)}_{(k,\mathcal{C}),(j)}$	. . . .	(3.7.58)
$\mathfrak{h}^{(\nu)}_{(k,\mathcal{C}),(k)}$	. . . .	(3.7.67c)
$\mathfrak{h}^{(\nu)}_{(k,\mathcal{C}),(l)}$	. . . .	(3.7.61)
$\mathfrak{h}^{(\nu)}_{(k,\mathcal{C}),(m)}$	. . . .	(3.7.64)
$\mathfrak{h}^{(\nu)}_{(k,\mathcal{C}),(n)}$	. . . .	(3.7.118)
$h^{(\nu)}_{(k,\mathcal{C})}$	. . . .	(3.8.52f)
$\tilde{h}^{(\nu)}_{(k,\mathcal{C})}$	. . . .	(3.8.52a)
$h^{(j)}$	fineness of the partition $\Pi^{(j)}$	(3.5.2)
ι	index for gas phase constituents	p. 10
ι	index for non-Dirichlet boundaries	p. 50
$\mathcal{I}_a$	set of intervals with min a	(C.6.4)
I	index set	
I	variable for intervals	
$I^{(j)}$	finite index set for partition $\Pi^{(j)}$	(3.5.15)
$I_{\mathrm{b},\lambda}$	Planck function	(2.4.32)
I_{gas}	finite index set for gas constituents	p. 214
I_r	reflective band of wavelengths	p. 28
I_{rad}	finite index set for partition Π_{rad}	p. 123
$I_{\mathrm{rad},\Gamma}$	$I_{\mathrm{rad},\Gamma} := \{\kappa \in I_{\mathrm{rad}} : \zeta_\kappa \subseteq \Gamma\}$	p. 124
$I_{\mathrm{rad,ph}}$	$I_{\mathrm{rad,ph}} := I_{\mathrm{rad}} \setminus I_{\mathrm{rad},\Gamma}$	p. 131
I_Π	finite index set for partition Π	p. 78
$I_{\Pi,\mathfrak{D}}$	. . . .	(3.7.2)
$I_{\Pi,\mathfrak{D},\mathrm{Dir}}$	. . . .	(3.7.4a)
$I_{\Pi,\mathfrak{D},\neg\mathrm{Dir}}$	. . . .	(3.7.4a)
I_t	reflective band of wavelengths	p. 29
I_ω	$I_\omega := \{\kappa \in I_{\mathrm{rad}} : \mathrm{int}[\zeta_\kappa] \cap \partial_{\mathrm{reg}}\omega \neq \emptyset\}$	p. 123
$I_{\omega,\mathrm{con}}$	$I_{\omega,\mathrm{con}} := \{\kappa \in I_{\mathrm{rad}} : \Gamma_{\mathrm{con}} \cap \mathrm{int}[\zeta_\kappa] \cap \partial_{\mathrm{reg}}\omega \neq \emptyset\}$	p. 128
$I_{\omega,\mathrm{jump}}$	$I_{\omega,\mathrm{jump}} := \{\kappa \in I_{\mathrm{rad}} : \Gamma_{\mathrm{jump}} \cap \mathrm{int}[\zeta_\kappa] \cap \partial_{\mathrm{reg}}\omega \neq \emptyset\}$	p. 128
IF	set of all interfaces	(3.4.3)
$\underline{\mathrm{IF}}$	. . . .	p. 88

Symbol	Meaning	Ref.
$\mathrm{IF}_{\mathrm{con}}$	set of continuous interfaces	p. 60
$\mathrm{IF}_{\mathrm{jump}}$	set of jump interfaces	p. 60
$\underline{\mathrm{IF}}_{\mathrm{jump}}$	. . . .	p. 88
$\mathrm{Im}[c^{\mathrm{complex}}]$	imaginary part of c^{complex}	
$\mathrm{InLip}(X,Y)$	set of all inverse Lipschitz functions from X into Y	Def. C.7.10
$\mathrm{InLip}_{L_{\mathrm{inv}}}(X,Y)$	set of all inverse L_{inv}-Lipschitz functions from X into Y	Def. C.7.10
i	abstract indices or indices referring to space coordinates	
i	imaginary unit	Sec. 2.5.6
$i_1[\gamma]$	index of first subdomain at γ	p. 61
$i_2[\gamma]$	index of second subdomain at γ	p. 61
$\inf F$	infimum of function F	Def. 3.7.17
$\mathrm{insup}[k]$	initial supremum of function k	(3.8.17)
$\mathrm{int}[A]$	interior of set A	p. 232
$\mathrm{int}[\sigma]$	interior of simplex σ	p. 236
$\mathcal{J}$	integral irradiation operator	(2.4.7)
$\mathcal{J}_r$	reflective irradiation operator	(2.4.35a)
$\mathcal{J}_t$	transmittive irradiation operator	(2.4.35b)
$\mathcal{J}_{\mathrm{circ}}$	. . . .	(2.4.22)
J	irradiation	(2.4.7)
J	set of indices for abstract materials	p. 46
J_f	Jacobian of f: $J_f := \det[f']$	
J_{given}	given total current	(2.5.39)
$J_{\mathrm{given},0}$	amplitude of given total current	(2.5.39)
J_j	finite index set for non-Dirichlet boundaries	p. 50
J_j	. . . .	p. 88
$J_{j,0}$	. . . .	(3.6.2)
$\underline{J}_j$	. . . .	p. 88
J_k	total current in k-th coil ring	(2.5.35)
$J_{k,0}^{\mathrm{complex}}$	. . . .	(2.5.37)
$J_{l,k,\mathrm{ref}}$	. . . .	(2.5.56)
$J_{l,k,\mathrm{ref},0}^{\mathrm{complex}}$	. . . .	(2.5.57)
J_r	reflective irradiation	p. 29
$J_{T,p}$	. . . .	(3.6.20)
$J_{T,q}$	. . . .	(3.6.20)
J_t	transmittive irradiation	p. 29
J_{ref}	reflected radiation	(2.4.4)
$J_{\mathrm{ref,r}}$	reflective reflected radiation	p. 29
$J_{\mathrm{ref,t}}$	transmittive reflected radiation	p. 29
J_{total}	total current	(2.5.38a)

Symbol	Meaning	Ref.
$J_{\mathrm{total},0}^{\mathrm{complex}}$	. . . .	(2.5.38b)
$\mathbf{j}$	current density vector	p. 32
j	current density	p. 32
j	abstract indices or indices referring to space coordinates, solid materials or abstract materials	
j^{complex}	complex current density	(2.5.26b)
j_0^{complex}	. . . .	(2.5.28b)
j_0	amplitude of sinusoidal current density	(2.5.25b)
$j_{\mathrm{Dir}}[(l,j)]$	. . . .	Not. 3.7.3
κ	index for boundary elements	p. 123
$\kappa^{(\mathrm{Ar})}$	thermal conductivity of Ar	(A.2.2)
$\kappa^{[\beta_j]}$	thermal conductivity of solid material β_j	p. 21
κ_{gas}	thermal conductivity of the gas mixture	p. 19
$\mathbb{K}$	$\mathbb{K} = \mathbb{R}$ or $\mathbb{C}$	
K	permeability	p. 48
$\mathfrak{k}_{\neg\mathrm{Dir},(k,\mathcal{C})}^{(\nu)}$	. . . .	(3.7.16)
$\mathfrak{k}_{\neg\mathrm{Dir},(k,\mathcal{C})}^{\nu,\uparrow}$	. . . .	(3.8.21a)
$\mathfrak{k}_{\neg\mathrm{Dir},(k,\mathcal{C})}^{\nu,\downarrow}$	. . . .	(3.8.21b)
$\mathfrak{k}_{\mathrm{Dir},(k,\mathcal{C})}^{(\nu)}$	. . . .	(3.7.17)
$\mathfrak{k}_{\mathrm{Dir},(k,\mathcal{C})}^{\nu,\uparrow}$	. . . .	(3.8.22a)
$\mathfrak{k}_{\mathrm{Dir},(k,\mathcal{C})}^{\nu,\downarrow}$	. . . .	(3.8.22b)
k	index for induction coil rings	p. 36
k	index for control volumes	p. 73
k	abstract index	
k	variable for diffusion function	(3.3.2c)
k_j	diffusion function in the j-th material	(3.1.1)
$\underline{k}_j$	. . . .	p. 88
$k^{(\nu)}$	function k at discrete time t_ν	(3.3.9c)
$\tilde{k}_{j,x}^{(\nu)}$	. . . .	(3.8.20)
Λ	visibility factor	(2.4.8)
Λ_a	rates of chemical reactions or phase transitions	p. 19
Λ_{circ}	. . . .	(2.4.23)
$\Lambda_{\kappa,\lambda}$	. . . .	(3.7.75)
λ	variable for real numbers	
λ	wavelength	p. 30
$\lambda_{d-1,\max}[\Pi]$	. . . .	(3.8.31)
λ_d	d-dimensional Lebesgue measure	Not. C.8.1
$\lambda_{d,\max}[\Pi]$	. . . .	(3.8.48)

Symbol	Meaning	Ref.
$\lambda_{d,\min}[\Pi]$	. . . .	(3.8.55)
$\mathbf{L}$	matrix arising during radiation discretization	p. 126
$\tilde{\mathbf{L}}$	matrix arising during radiation discretization	p. 127
L	variable for Lipschitz constants	p. 244
$L_{\mathrm{Dir},k,r}[\mathfrak{C}]$	. . . .	(3.8.28)
$L_{f,r}[\mathfrak{C}]$	. . . .	Lem. 3.8.27
$L_{\mathrm{flux},1,r}[(\mathfrak{C},\mathfrak{S}_{\mathrm{con}})]$	. . . .	Lem. 3.8.19
$L_{\mathrm{flux},\mathrm{jump},r}[(\mathfrak{C},\mathfrak{S}_{\mathrm{jump}})]$	. . . .	Lem. 3.8.23
L_{inv}	. . . .	Def. C.7.10
$L_{\mathrm{inv},b}[\mathfrak{C}]$	. . . .	Def. 3.8.30
$L_{\kappa,\lambda}$	components of matrix $\mathbf{L}$	(3.7.81f)
$\tilde{L}_{\kappa,\lambda}$	components of matrix $\tilde{\mathbf{L}}$	(3.7.87)
$L_{k,r}[\mathfrak{C}]$	. . . .	Lem. 3.8.10
$L^{\downarrow}_{k,r}[\mathfrak{C}]$	. . . .	(3.8.23)
$L_{M-m_v}[(\dots)]$	. . . .	(3.8.54)
$L_{\mathrm{nonloc},r}[(\mathfrak{C},\Pi)]$	. . . .	Def. 3.8.25
$L_{\mathrm{out},r}[(\mathfrak{C},\mathfrak{S}_{\mathrm{out}})]$	. . . .	Lem. 3.8.16
$L_r[(\dots)]$	. . . .	(3.8.54)
$L_{v,r}[\mathfrak{C}]$	. . . .	(3.8.30)
$\mathrm{Lin}(\mathcal{V},\mathcal{V})$	set of linear maps from $\mathcal{V}$ into $\mathcal{V}$	
$\mathrm{Lip}(X,Y)$	set of all Lipschitz functions from X into Y	Def. C.7.4
$\mathrm{Lip}_L(X,Y)$	set of all L-Lipschitz functions from X into Y	Def. C.7.4
l	index for induction coil rings	p. 43
$l_{\mathrm{Dir}}[\Pi]$	. . . .	(3.7.47)
l_κ	. . . .	(3.7.77)
μ	variable for real numbers	
μ	magnetic permeability	p. 32
M	variable for maxima of intervals	
$M^{(\alpha_\iota)}$	molecular mass of constituent α_ι	p. 210
$\mathbf{m}$	$\mathbf{m} = (m_v, \dots, m_v)$	
m	variable for minima of intervals	
m_v	minimum of $v = [m_v, \infty[$	
ν	magnetic reluctivity	p. 33
ν	index for discrete time instances	p. 56
ν_γ	magnetic reluctivity in material γ	p. 37
n	number of time steps	p. 56
$\mathbb{N}$	set of natural numbers $1, 2, \dots$	
$\mathbb{N}_0$	$\mathbb{N}_0 = \{0, 1, 2, \dots\}$	
N	number of solid materials	Sec. 2.2
N	number of induction coil rings	p. 36
N_{all}	discrete L^1-norm	(3.7.129c)
$N^{(\nu)}_{\mathrm{all}}$	discrete L^1-norm	(3.7.128c)

Symbol	Meaning	Ref.
$N_{b,\neg\mathrm{Dir}}$	discrete L^∞-L^1-norm composed with $b_j^{(\nu)}$	(3.7.127)
$N_{b,\neg\mathrm{Dir}}^{(\nu)}$	discrete L^1-norm composed with $b_j^{(\nu)}$	(3.7.126)
N_{Dir}	discrete L^∞-L^1-norm	(3.7.129a)
$N_{\mathrm{Dir}}^{(\nu)}$	discrete L^1-norm	(3.7.128a)
$N_{\neg\mathrm{Dir}}$	discrete L^∞-L^1-norm	(3.7.129b)
$N_{\neg\mathrm{Dir}}^{(\nu)}$	discrete L^1-norm	(3.7.128b)
n_A	outer unit normal vector to set A	
n_p	outer unit normal vector to polytope p	Def. C.4.17
$\mathbf{n}^{[\beta]}$	outer unit normal vector to solid β	p. 22
$\mathbf{n}_\gamma$	outer unit normal vector to material γ	p. 37
$\mathbf{n}_{\mathrm{gas}}$	outer unit normal vector to gas phase	p. 22
$\mathrm{nb}_j[k]$	set of indices of j-neighbors of ω_k	(3.7.12)
$\mathrm{nb}_{j,\mathrm{Dir}}[k]$	set of indices of Dirichlet j-neighbors of ω_k	(3.7.14)
$\mathrm{nb}_{j,\neg\mathrm{Dir}}[k]$	set of indices of non-Dirichlet j-neighbors of ω_k	(3.7.14)
$\mathcal{O}$	variable for topologies	
$\mathcal{O}_A$	relative topology on A with respect to $\mathcal{O}$	p. 232
O	variable for open sets	
Π	$\Pi = (\omega_k)_{k\in I_\Pi}$	p. 73
$\Pi[V]$	Voronoï discretization induced by point set V	Def. C.4.18
$\Pi^{(j)}$	$\Pi^{(j)} = (\omega_k^{(j)})_{k\in I^{(j)}}$	p. 73
Π_{rad}	$\Pi_{\mathrm{rad}} := (\zeta_\kappa)_{\kappa\in I_{\mathrm{rad}}}$	p. 123
π	$\pi = 3.14\ldots$	
π_{circ}	circular projection	(2.4.20)
$\mathcal{P}[A]$	power set of A	
P_k	electrical power in k-th coil ring	(2.5.46)
$\overline{P_k}$	average electrical power in k-th coil ring	(2.5.47)
$P_{(k,\mathcal{C})}^{(\nu)}$	$P_{(k,\mathcal{C})}^{(\nu)} := \mathfrak{b}_{(k,\mathcal{C})}^{(\nu-1)}\left[u_{(k,\mathcal{C})}^{(\nu-1)}\right]$	(3.8.52c)
P_{total}	total electrical power	(2.5.48)
$\overline{P_{\mathrm{total}}}$	total electrical power	(2.5.49)
$P_{\mathrm{total},\lambda}$	. . . .	(2.5.52)
$\overline{P_{\mathrm{total},\lambda}}$	. . . .	(2.5.53)
(PDE: ϕ_A)	system for ϕ_A	p. 39
(PDE: $\phi_{A,0}^{\mathrm{complex}}$)	system for $\phi_{A,0}^{\mathrm{complex}}$	p. 39
(PDE$_l$: $\phi_{A,0}^{\mathrm{complex}}$)	. . . .	p. 43
$\mathbf{p}^{*(\alpha_\iota)}$	partial momentum source of constituent α_ι	p. 11
p	pressure	
p	polyhedral total space domain	p. 58
p	variable for nonnegative real numbers	
$p^{(\alpha_\iota)}$	partial pressure of constituent α_ι	p. 16
$p^{(\mathrm{Ar})}$	pressure of Ar	211

Symbol	Meaning	Ref.
p_{gas}	pressure of the gas mixture	(2.1.16)
p_{gas}	domain of gas phase	p. 127
p_j	polyhedral space domain of the j-th material	p. 46
p_{rad}	circular projection of radiation region	p. 122
p_{solid}	domain of solid materials	p. 127
$\mathrm{pt}[\mathcal{V}]$	set of all polytopes in $\mathcal{V}$	Def. C.4.9
$\mathrm{pt}_d[\mathcal{V}]$	set of d-polytopes in $\mathcal{V}$	Def. C.4.9
$\mathbf{q}^{(\alpha_\iota)}$	partial heat flux of constituent α_ι	p. 11
$\mathbf{q}_{\mathrm{gas}}$	total heat flux of the gas mixture	(2.1.6e)
$\mathbf{q}^{[\beta_j]}$	heat flux of solid material β_j	p. 21
q	$q = \prod_{i\in\{1,\dots,d'\}}[\lambda_i, \mu_i]$	Def. 3.6.2
$\rho^{(\alpha_\iota)}$	partial mass density of constituent α_ι	p. 11
$\rho^{(\mathrm{Ar})}$	mass density of Ar	(A.2.1)
$\rho^{*(\alpha_\iota)}$	partial mass source of constituent α_ι	p. 11
ρ_{gas}	mass density of the gas mixture	(2.1.4a)
$\rho^{[\beta_j]}$	mass density of solid material β_j	p. 21
ϱ	reflectivity	p. 24
ϱ_{r}	reflective reflectivity	(2.4.34a)
ϱ_{t}	transmittive reflectivity	(2.4.34b)
$\mathbb{R}$	the set of real numbers	
$\mathbb{R}_0^+$	the set of nonnegative real numbers	
$\mathcal{R}$	radiation operator	(2.4.13c)
$\mathcal{R}_{\mathrm{circ}}$	radiation operator	(2.4.26c)
$\mathcal{R}_{\mathrm{circ}}^{(\nu)}$	. . . .	p. 124
$\mathcal{R}_{\mathrm{r}}$	reflective radiation operator	p. 31
$\mathcal{R}_{\mathrm{t}}$	transmittive radiation operator	p. 31
R	radiosity	(2.4.1)
R	universal gas constant	p. 210
R_{circ}	. . . .	p. 27
R_{r}	reflective radiosity	p. 29
R_{t}	transmittive radiosity	p. 29
$\mathrm{Re}[c^{\mathrm{complex}}]$	real part of c^{complex}	
$\mathbf{r}$	vector in cylindrical coordinates	p. 230
r	radial cylindrical coordinate	p. 229
$r^{(\alpha_\iota)}$	partial radiation of constituent α_ι	p. 11
r_{gas}	total radiation of the gas mixture	(2.1.6d)
σ	Boltzmann radiation constant	p. 210
σ	variable for simplices	p. 236
$\sigma_{\mathrm{c}}^{[\beta]}$	electrical conductivity of solid material β	p. 32
$\sigma_{\mathrm{c}}^{[\mathrm{ring}]}$	electrical conductivity of coil ring	
$\sigma_{\mathrm{c},k}$	. . . .	(2.5.36)

Symbol	Meaning	Ref.
$\mathfrak{S}_{\text{con}}$	family of dependency splittings	Lem. 3.8.19
$\mathfrak{S}_{\text{jump}}$	family of dependency splittings	Lem. 3.8.23
$\mathfrak{S}_{\text{out}}$	family of dependency splittings	Lem. 3.8.16
S	. . . .	(3.8.49a)
$S^{(\nu)}$	. . . .	(3.8.56b)
$S^{(\nu)}_{(k,\mathcal{C})}$	. . . .	(3.8.56a)
S_{solid}	variable for absolute temperature of solid material	
$\mathfrak{s}^{(\nu)}$	. . . .	(3.7.8)
$\text{sim}[\mathcal{V}]$	set of all simplices in $\mathcal{V}$	Def. C.4.7
$\text{sim}_d[\mathcal{V}]$	set of all d-simplices in $\mathcal{V}$	Def. C.4.7
$\sup F$	supremum of function F	Def. 3.7.17
τ	time domain	(3.1.2)
θ	saturation	p. 48
ϑ	angular cylindrical coordinate	p. 229
$\mathfrak{T}$	time discretization of evolution equation complex	(3.4.33)
$\underline{\mathfrak{T}}$	. . . .	p. 89
$\mathbf{T}^{(\alpha_\iota)}$	partial stress tensor of constituent α_ι	p. 11
$\mathbf{T}_{\text{gas}}$	total stress tensor of the gas mixture	(2.1.6a)
T	absolute temperature	
T	coordinate transformation	Def. 3.6.1
$\bar{T}$	$\bar{T}[A \times q] = \overline{T((A \cap O) \times \text{int}[q])}$	(3.6.1)
$\tilde{T}$	matrix occurring in symmetry condition, related to the derivative of coordinate transformation T	(3.6.18a)
$T^{[\beta_j]}$	absolute temperature of solid material β_j	p. 21
T_{cyl}	coordinate transformation for cylindrical coordinates	(B.3.1)
T_{gas}	absolute temperature of the gas mixture	p. 13
$T_{\text{gas,circ}}$	absolute temperature on domain p_{gas}	p. 127
T_{room}	room temperature	p. 23
T_{solid}	absolute temperature of solid material	p. 24
$T_{\text{solid,circ}}$	. . . .	p. 27
$T^{(\nu)}_{\text{solid,circ}}$	. . . .	p. 123
t	time	p. 11
t_0	initial time	(3.1.2)
t_{f}	final time	(3.1.2)
$t_{\phi_A,0}$	time for phase shift	(2.5.25c)
$\tilde{t}_{i,i'}$	components of matrix $\tilde{T}$	(3.6.18a)
$t^{(\alpha_\iota)}_{i,j}$	components of the partial stress tensor of constituent α_ι	p. 11

Symbol	Meaning	Ref.
$t_{j,0}$	time for phase shift	(2.5.25b)
t_ν	discrete time instant	p. 56
$t_{V,k,0}$	time for phase shift	(2.5.25a)
$\mathrm{tr}_A\, f$	trace of the equivalence class of functions f on the set A	
$\mathcal{U}$	domain of evolution operator	p. 55
$\mathcal{U}_j$	domain of evolution operator on j-th space domain	p. 55
$\mathcal{U}^{(\nu)}$	reservoir set of time-discrete solutions at t_ν	p. 57
$\mathcal{U}_j^{(\nu)}$	reservoir set of time-discrete solutions at t_ν on j-th space domain	p. 71
$\underline{\mathcal{U}}_j^{(\nu)}$	. . . .	p. 89
$U^{(\nu)}$	discrete solution vector at time t_ν	p. 103
$U_{k,\mathrm{gas}}^{(\nu)}$	. . . .	(3.7.89)
$U_{k,\mathrm{solid}}^{(\nu)}$	. . . .	(3.7.89)
u	$\mathrm{u} = (u_j)_{j\in J}$	p. 62
$\mathrm{u}\restriction_{\{t\}}$	$\mathrm{u}\restriction_{\{t\}} = \left(u_j\restriction_{\{t\}\times p_j}\right)_{j\in J}$	p. 62
$\mathrm{u}^{(\nu)}$	$\mathrm{u}^{(\nu)} = (u_j^{(\nu)})_{j\in J}$	(3.4.34)
$\underline{\mathrm{u}}^{(\nu)}$	. . . .	p. 89
$\mathbf{u}$	variable for vectors	p. 222
$\mathbf{u}^{(\alpha_\iota)}$	diffusion velocity of constituent α_ι	(2.1.4d)
$\mathbf{u}^2$	$\mathbf{u}^2 := \mathbf{u} \bullet \mathbf{u}$	p. 222
u	variable for unknown function	
u	capillary pressure	p. 48
u_i	components of the vector $\mathbf{u}$	p. 222
u_j	unknown function in the j-th material	(3.1.1)
$u_j^{(0)}$	initial distribution in the j-th material	(3.1.10)
$\underline{u}_j^{(0)}$	. . . .	p. 88
u_j	time-discrete unknown function in the j-th material	(3.4.34)
$\underline{u}_j^{(\nu)}$	. . . .	p. 89
$u_{j,\mathrm{Dir}}$	Dirichlet function	(3.4.12a)
$\underline{u}_{j,\mathrm{Dir}}$	. . . .	p. 88
$u_{j,\mathrm{Dir}}^{(\nu)}$	time-discrete Dirichlet function	(3.4.28)
$\underline{u}_{j,\mathrm{Dir}}^{(\nu)}$	. . . .	p. 89
$u^{(\nu)}$	unknown at discrete time t_ν	p. 56
$u_{(k,j)}^{(\nu)}$	. . . .	p. 102
$u_{(k,\mathcal{C})}^{(\nu)}$	$(k,\mathcal{C})$-component of discrete solution vector at time t_ν	p. 103

Symbol	Meaning	Ref.
$(u_1, u_2)^{\text{sp.}}$	. . . .	(3.6.4)
$u^{\text{sp.}}$	. . . .	(3.3.13)
$u^{\text{t.-sp.}}$	. . . .	(3.3.6)
$\mathfrak{V}$	variable for families of scalar-vector-splittings	(3.7.31)
$\mathcal{V}$	variable for vector spaces	
$\mathbf{V}$	vector arising during radiation discretization	(3.7.88)
V	finite set of points	p. 235
$V[\mathcal{C}]$	vertex set of connected component $\mathcal{C}$	p. 81
$V[\sigma]$	set of simplex vertices	p. 236
$V^{[\beta]}$	voltage in material β	p. 36
V_κ	components of vector $\mathbf{V}$	(3.7.73)
$V_k^{[\text{ring}]}$	voltage in k-th coil ring	p. 36
$V_{k,0}^{[\text{ring}]}$	amplitude of sinusoidal voltage in k-th coil ring	(2.5.25a)
$V_k^{[\text{ring}],\text{complex}}$	complex voltage in k-th coil ring	(2.5.26a)
$V[\mathcal{G}]$	set of vertices of graph $\mathcal{G}$	Def. C.5.1
$V_{k,0}^{[\text{ring}],\text{complex}}$	. . . .	(2.5.28a)
V_{ref}	reference voltage	p. 43
V_{total}	given total voltage	(2.5.41)
$V_{\text{total},0}$	amplitude of given total voltage	(2.5.41)
$V_{\text{total}}^{\text{complex}}$	. . . .	(2.5.44)
V_{ω_k}	$V_{\omega_k} := \{j \in J : \text{int}\,[\omega_k \cap p_j] \neq \emptyset\}$	(3.5.17)
$\mathfrak{v}^{(\nu)}_{\text{con},(k,\mathcal{C})}$	. . . .	(3.7.54)
$\mathfrak{v}^{\nu,\uparrow}_{\text{IF},(k,\mathcal{C})}$	. . . .	(3.8.36a)
$\mathfrak{v}^{\nu,\downarrow}_{\text{IF},(k,\mathcal{C})}$	. . . .	(3.8.36b)
$\mathfrak{v}^{(\nu)}_{\text{int},\text{Dir},(k,\mathcal{C})}$	. . . .	(3.7.41)
$\mathfrak{v}^{(\nu)}_{\text{int},\neg\text{Dir},(k,\mathcal{C})}$	. . . .	(3.7.40)
$\mathfrak{v}^{\nu,\uparrow}_{\text{int},\neg\text{Dir},(k,\mathcal{C})}$	. . . .	(3.8.29a)
$\mathfrak{v}^{\nu,\downarrow}_{\text{int},\neg\text{Dir},(k,\mathcal{C})}$	. . . .	(3.8.29b)
$\mathfrak{v}^{(\nu)}_{\text{jump},(k,\mathcal{C})}$	. . . .	(3.7.55)
$\mathfrak{v}^{(\nu)}_{\text{out},(k,\mathcal{C})}$	. . . .	(3.7.49)
$\mathfrak{v}^{\nu,\uparrow}_{\text{out},(k,\mathcal{C})}$	. . . .	(3.8.32a)
$\mathfrak{v}^{\nu,\downarrow}_{\text{out},(k,\mathcal{C})}$	. . . .	(3.8.32b)
$\mathbf{v}$	variable for vectors	p. 222
$\mathbf{v}^{(\alpha_\iota)}$	partial local mean velocity of particles of constituent α_ι	p. 11
$\mathbf{v}_{\text{gas}}$	local mean velocity of all gas particles	(2.1.4b)
v	variable for convective function	(3.3.2b)

Symbol	Meaning	Ref.
v	variable for elements of abstract vector spaces	
v	variable for vertices	
v_i	components of the vector $\mathbf{v}$	p. 222
v_j	convective function in the j-th material	(3.1.1)
$\underline{v}_j$	. . . .	p. 88
$v^{(\nu)}$	function v at discrete time t_ν	(3.3.9b)
v_{sca}	. . . .	Def. 3.7.30
$v_{j,\mathrm{sca}}^{(\nu)}$	. . . .	(3.7.33a)
v_{vec}	. . . .	Def. 3.7.30
$v_{j,\mathrm{vec}}^{(\nu)}$	. . . .	(3.7.33b)
$\mathrm{var}[f]$	total variation function of f	(C.6.6a)
$\mathrm{var}[f]^+$	positive variation function of f	(C.6.6b)
$\mathrm{var}[f]^-$	negative variation function of f	(C.6.6c)
$\mathbf{w}$	variable for vectors	
w	variable for elements of abstract vector spaces	
$w_j^{(\nu)}$	upwind function for $\Pi^{(j)}$ and $v_{j,\mathrm{vec}}^{(\nu)}$	p. 114
ξ_β	factor in interface conditions	(2.3.2b′)
$\mathbf{X}$	vector arising during radiation discretization	p. 126
X	variable for topological spaces or metric spaces	
X_κ	components of vector $\mathbf{X}$	(3.7.81b)
$\mathbf{x}$	(physical) vector of space coordinates	
x	(abstract) vector of space coordinates	
x_κ	discretization point of boundary element ζ_κ	p. 123
x_k	discretization point of control volume ω_k	(3.7.1)
x_p	variable for elements of p	(3.6.18a)
x_q	variable for elements of q	(3.6.18a)
υ	range of the unknown	p. 53
$\mathbf{Y}$	vector arising during radiation discretization	p. 126
Y	variable for topological spaces or metric spaces	
Y_κ	components of vector $\mathbf{Y}$	(3.7.81c)
$\mathbf{y}$	physical vector of space coordinates	
y	variable for elements of υ	
$\tilde{y}$	variable for elements of υ	
ζ_κ	boundary element	p. 123
Z	variable for metric spaces	
z	vertical cylindrical coordinate	p. 229
$z^{(\mathrm{Ar})}$	configuration number of Ar	p. 210
Ω	space domain	
Ω	$\Omega := O \times \mathrm{int}[q]$	Def. 3.6.2
$\Omega^{[\beta]}$	domain of material β	p. 35
$\Omega_{\mathrm{appCon}}^{[\beta]}$	domain of conducting material β in	

Symbol	Meaning	Ref.
	growth apparatus	p. 36
Ω_j	space domain of the j-th material	(3.1.2)
$\Omega_k^{[\mathrm{ring}]}$	domain of k-th coil ring	p. 36
ω	angular frequency	p. 37
ω	view factor	(2.4.9)
ω_k	control volume	p. 78
$\omega_k^{(j)}$	control volume in domain p_j	(3.5.14)
ω_v	Voronoï box	(C.4.3)

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