Spatial and Physical Splittings of Semilinear Parabolic Problems

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Abstract

Splitting methods are widely used temporal approximation schemes for parabolic partial differential equations (PDEs). These schemes may be very efficient when a problem can be naturally decomposed into multiple parts.

In this thesis, splitting methods are analysed when applied to spatial splittings (partitions of the computational domain) and physical splittings (separations of physical processes) of semilinear parabolic problems. The thesis is organized into three major themes: optimal convergence order analysis, spatial splittings and a physical splitting application.

In view of the first theme, temporal semi-discretizations based on splitting methods are considered. An analysis is performed which yields convergence without order under weak regularity assumptions on the solution, and convergence orders ranging up to classical for progressively more regular solutions. The analysis is performed in the framework of maximal dissipative operators, which includes a large number of parabolic problems. The temporal results are also combined with convergence studies of spatial discretizations to prove simultaneous space–time convergence orders for full discretizations.

For the second theme, two spatial splitting formulations are considered. For dimension splittings each part of the formulation represents the evolution in one spatial dimension only. Thereby, multidimensional problems can be reduced to families of one-dimensional problems. For domain decomposition splittings each part represents a problem on only a smaller subdomain of the full domain of the PDE. The results of the first theme are applied to prove optimal convergence orders for splitting schemes used in conjunction with these two splitting formulations.

The last theme concerns the evaluation of a physical splitting procedure in an interdisciplinary application. A model for axonal growth out of nerve cells is considered. This model features several challenges to be addressed by a successful numerical method. It consists of a linear PDE coupled to nonlinear ordinary differential equations via a moving boundary, which is part of the solution. The biological model parameters imply a wide range of scales, both in time and space. Based on a physical splitting, a tailored scheme for this model is constructed. Its robustness and efficiency are then verified by numerical experiments.

Populärvetenskaplig sammanfattning

För att skapa matematiska beskrivningar av fysiska fenomen inom bland annat naturvetenskap, teknik och medicin används ofta *partiella differentialekvationer*. Listan med tillämpningar kan göras hur lång som helst: sådana ekvationer kan beskriva hur en snöflinga bildas, hur strukturer deformeras när de utsätts för mekaniska krafter, hur partiklar interagerar på kvantnivå, hur blodet flödar i hjärnans kapillärer, hur axontillväxten ser ut i nervceller och så vidare. Den sistnämnda tillämpningen återkommer vi till. Genom att använda partiella differentialekvationer för att skapa matematiska modeller av fysiska fenomen kan vi nå en djupare förståelse av komplexa processer. Dessutom är skapandet och analysen av en matematisk modell i allmänhet betydligt billigare än fysiska experiment.

Såsom antyds av listan med tillämpningar används partiella differentialekvationer ofta för att modellera processer som varierar i både tid och rum. Dessa ekvationer kan nästan aldrig lösas exakt. Istället används i praktiken numeriska metoder för att hitta approximativa (ungefärliga) lösningar med hjälp av datorer. Givetvis är det av största vikt att metoderna som används är både snabba och noggranna. Att säkerställa detta är centralt i den forskning som genomförs inom numerisk analys.

I många fall kan partiella differentialekvationer vara så komplicerade att det inte är tänkbart att hitta en approximativ lösning till hela ekvationen på en gång. Istället kan man dela upp ekvationen i delar som var och en är betydligt enklare att approximera. Sådana uppdelningar kallas för *splittingformuleringar* och numeriska metoder som använder sig av dessa kallas för *splittingmetoder*. Givetvis införs ett approximationsfel när delarna hanteras separat. Vi måste väga förenklade beräkningar mot ett ökat fel. För att kunna göra detta måste vi förstå oss på hur felet ser ut.

Vi kräver alltså att våra numeriska metoder är både snabba och noggranna. Det sistnämnda innebär att metoderna genererar små approximationsfel. Genom att uppskatta dessa fels storlek kan man avgöra hur noggrann en approximation är. Av speciellt intresse är feluppskattningar som skildrar hur mycket felet minskar om man ökar mängden datorkraft som används i beräkningarna. I denna avhandling härleder vi feluppskattningar för

ett antal splittingmetoder. Vilken noggrannhet vi får beror på vilken splittingmetod som analyseras och på egenskaper hos lösningen till den approximerade differentialekvationen.

Vår analys gäller för splittingmetoder när de appliceras på så kallade *semilinjära* partiella differentialekvationer. Viss konvergensordningsanalys för sådana ekvationer finns sedan tidigare i litteraturen men då under begränsande antaganden som utesluter många intressanta fall. Våra resultat, å andra sidan, kan appliceras på många olika klasser av semilinjära ekvationer.

Vi lägger extra fokus på att använda våra konvergensresultat för att analysera två olika splittingformuleringar: fysikaliska och rumsberoende. För ett klassiskt exempel på den förstnämnda föreställer vi oss luftföroreningar i atmosfären. Med en fysikalisk splitting kan föroreningarnas rörelser (diffusion) hanteras separat från deras kemiska reaktioner med varandra. För ännu effektivare beräkningar kan vi dessutom införa en rumsberoende splitting. Till exempel kan vi alternera mellan olika riktningar i atmosfären och beräkna föroreningarnas diffusion i en riktning åt gången. Alternativt kan vi hantera diffusionen i olika delar av atmosfären var för sig. En numerisk metod baserad på dessa splittingformuleringar lämpar sig väl för parallella beräkningar, till exempel på ett kluster av datorer.

Utöver de generella analyser som vi diskuterat hittills genomför vi också en djupare studie av en semilinjär partiell differentialekvation hämtad från en tillämpning inom teoretisk biologi. Från varje nervcell växer en lång, tubformad nervtråd ut från cellkroppen. Utväxten kallas axon och byggs upp av proteinet tubulin. Detta protein produceras i cellkroppen och transporteras sedan längs med axonet för att slutligen monteras i andra änden av denna nervtråd. För att simulera dessa processer skapar vi en matematisk modell som bland annat består av en partiell differentialekvation. Sedan approximerar vi modellen via en fysikalisk splitting som låter oss hantera tubulinets förflyttning längs axonet separat från uppbyggnadsprocessen i axonets ände. Våra experiment visar att en numerisk metod baserad på denna splittingformulering ger snabba beräkningar och noggranna resultat.

List of Papers

This thesis is based on the following papers, which will be referred to in the text by their Roman numerals. The papers are appended at the end of the work.

I. E. Hansen and E. Henningsson,
A convergence analysis of the Peaceman–Rachford scheme for semilinear evolution equations,
SIAM Journal on Numerical Analysis, 51(4):1900–1910, 2013.

II. E. Hansen and E. Henningsson,
A full space–time convergence order analysis of operator splittings for linear dissipative evolution equations,
Communications in Computational Physics, 19(5):1302–1316, 2016.

III. E. Hansen and E. Henningsson,
Additive domain decomposition operator splittings—convergence analyses in a dissipative framework,
accepted for publication in IMA Journal of Numerical Analysis, 2016.

IV. S. Diehl, E. Henningsson, A. Heyden and S. Perna,
A one-dimensional moving-boundary model for tubulin-driven axonal growth,
Journal of Theoretical Biology, 7(358):194–207, 2014.

V. S. Diehl, E. Henningsson and A. Heyden,
Efficient simulations of tubulin-driven axonal growth,
Journal of Computational Neuroscience, 41(1):45–63, 2016.

Moreover, the thesis also contains previously unpublished research. Parts of Chapter 3 is based on these new results.

Author's contribution

My contribution to the papers is listed below.

I. I participated in the analysis and I designed, implemented, and performed the numerical experiments.

II. I designed the abstract setting to be used and in it I performed the convergence analysis. I performed most of the analysis concerning the application to dimension splittings. I designed, implemented, and performed the numerical experiments. I am the corresponding author and wrote all of the paper.

III. I conceived of the project idea. I and the co-author designed the variational setting and analysed it. I carried out the convergence analysis and interpreted the results. I designed, implemented, and performed the numerical experiments. I am the corresponding author and wrote all of the paper.

IV. I designed, implemented, and performed the stability experiments and wrote Section 6.

V. I chose the numerical scheme and performed the analysis of it. I designed, implemented, performed and analysed all numerical experiments. I am the corresponding author and wrote most of the paper.

All the work on the previously unpublished results is due to me.

Acknowledgments

As this thesis marks the end of my journey as a Ph.D. student I would like to thank those people that have supported and assisted me along the way. Without you, of course, this thesis could not have been written.

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A special thanks to my fellow Ph.D. students, present and past: Tony, Dara, Christian, Azahar, Fatemeh and Peter, a truly diverse set of interesting and fun personalities. Thank you for your support and all the helpful discussions, regarding math and other fascinating subjects. In particular I thank Tony Stillfjord; you are a better friend than you think. I do not know how I managed to survive over a year without being able to just walk over to your office whenever a stupid question pops up.

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My most heartfelt gratitudes I direct to my family for all your support and all the great times we have. I am very grateful for how well we work together.

Last but not least, thank you Ylva Johansson for being who you are. All my love to you for putting up with me when work brings me down. Your support in all parts of my life is incomparable.

Erik Henningsson, Lund, 2016

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Contents

Chapter 1

Introduction

Modelling with partial differential equations (PDEs) constitutes one of the most powerful tools for constructing mathematical representations of physical phenomena. In the vast list of examples we find models of ice crystal formation, planetary motion, air pollution, wave propagation, pattern formation on animals and axonal growth in nerve cells, to just mention a few.

In this thesis we study temporal discretization schemes for semilinear parabolic PDEs. As a prototypical example of such a PDE we consider the FitzHugh–Nagumo diffusion–reaction equations

$$\begin{cases} \dot{u}_1 = D_1 \Delta u_1 + u_1 - u_1^3/3 - u_2, \\ \dot{u}_2 = D_2 \Delta u_2 + a u_1 - b u_2, \end{cases} \tag{1.1}$$

which can be used to model the propagation of an electrical potential u_1 in, e.g., nerve cells, cf. [27, 56]. The reaction part describes an activator–inhibitor system with a positive feedback $u_1 - u_1^3/3$ (the inequality $|u_1| \leq \sqrt{3}$ mostly applies) and a negative feedback given by the recovery voltage u_2. Here Δ denotes the Laplace operator and D_1, D_2, a and b are positive parameters. We say that (1.1) is semilinear since its vector field can be split into the sum of a linear term A (diffusion) and a nonlinear term F (reaction):

$$Au = \begin{pmatrix} D_1 \Delta u_1 \\ D_2 \Delta u_2 \end{pmatrix} \quad \text{and} \quad Fu = \begin{pmatrix} u_1 - u_1^3/3 - u_2 \\ a u_1 - b u_2 \end{pmatrix}, \tag{1.2}$$

where $u = (u_1, u_2)^{\mathrm{T}}$. Note that the different physical processes have here been separated from each other. We refer to formulations given by such separations as physical splittings. See Figure 1.1 for a simulation illustrating the characteristic oscillatory behaviour of solutions to the two-dimensional FitzHugh–Nagumo equations.

The stiffness of the diffusion, present in the FitzHugh–Nagumo equations, calls for an implicit time discretization method. However, such a method requires the solution of

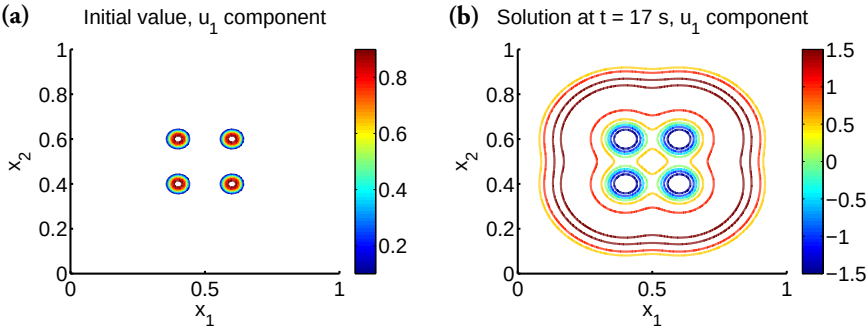


Figure 1.1: The propagation of four initial "hump" potentials in the unit square. The "humps" oscillate and a wave travels out from the centre. Here the parameter values $D_1 = 1 \cdot 10^{-4}$, $D_2 = 8 \cdot 10^{-6}$, $a = 0.08$ *and* $b = 0.064$ *have been used. The* u_1 *component initial data is given as the sum of four translated "humps",* $g_{y,\epsilon}(x) := \exp(1 - \epsilon^2/(\epsilon^2 - |x-y|^2))$ *if* $|x-y| < \epsilon$, 0 *otherwise, with centres at* $y = (0.4, 0.4), (0.4, 0.6), (0.6, 0.4), (0.6, 0.6)$ *and all with radius* $\epsilon = 0.05$. *The initial data of the second component is given by scaling that of the first component by a factor* 0.1.

nonlinear equations coupled over space and the potentials, and is therefore costly to use. The splitting idea, on the other hand, consists of iterating between the equations in the splitting formulation,

$$\dot{u} = Au, \tag{1.3a}$$
$$\dot{u} = Fu, \tag{1.3b}$$

and solving the equations (exactly or numerically) separately. Then the results are combined to construct an approximation of the solution to the full problem. The first equation can be handled by a solver for stiff linear problems; no nonlinear solver is needed. Since the second equation does not involve any of the Laplace operators, it decouples over space. That is, after a space discretization is applied to (1.3b) the solution at each point in space may be updated independently of the others. A procedure that additionally is easy to parallelize. Exactly how to iterate between (1.3a) and (1.3b) is dictated by a splitting method. We introduce an equidistant grid in time and consider, as an example, the Peaceman–Rachford scheme

$$S_h = \big(I - \tfrac{h}{2}F\big)^{-1}\big(I + \tfrac{h}{2}A\big)\big(I - \tfrac{h}{2}A\big)^{-1}\big(I + \tfrac{h}{2}F\big),$$

where I is the identity operator and S_h denotes the operator that takes one time step of size $h > 0$. To clarify the notation, consider e.g. the resolvent $(I - h/2\,F)^{-1}$ of F: applying it to the function u amounts here to solving for v in the nonlinear system of

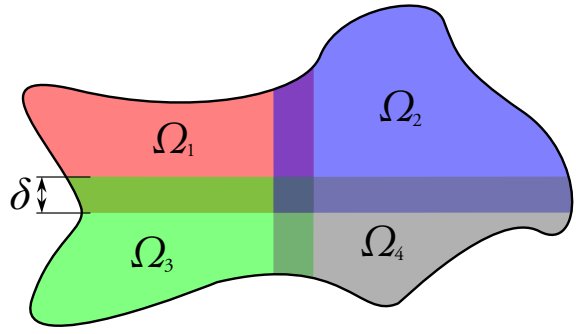


Figure 1.2: An example of an overlapping domain decomposition of $\Omega = \cup_{k=1}^{4}\Omega_k$. The characteristic overlap length is denoted by δ. Large values on this parameter typically result in more accurate approximations at the expense of more computations.

equations

$$v = \left(I - \tfrac{h}{2}F\right)^{-1}u \quad \Longleftrightarrow \quad \left(I - \tfrac{h}{2}F\right)v = u \quad \Longleftrightarrow$$
$$\begin{pmatrix} v_1 \\ v_2 \end{pmatrix} - \frac{h}{2}\begin{pmatrix} v_1 - v_1^3/3 - v_2 \\ av_1 - bv_2 \end{pmatrix} = \begin{pmatrix} u_1 \\ u_2 \end{pmatrix}.$$

That is, evaluating the action of the resolvent $(I - h/2\,F)^{-1}$ is equivalent to taking an implicit Euler step of size $h/2$ when the continuous equation is given by (1.3b). Thus, taking one step with the Peaceman–Rachford scheme involves first taking one explicit Euler step with (1.3b), then using the result as an input for an implicit Euler step with (1.3a) and so on. Note that a discretization of the whole vector field $A + F$ at the same time is never used. An overview of splitting methods will be given in Chapter 2. See in particular Section 2.3 where, among others, the specific benefits of using the Peaceman–Rachford scheme and other alternating direction implicit (ADI) methods will be discussed.

We noted above that, when considering the FitzHugh–Nagumo equations (1.1), the subproblem (1.3b) can easily be approximated using parallel computations. On the other hand, due to the Laplace operators, a space discretization of (1.3a) results in a coupled linear system. It is thus not as straight-forward to parallelize the solution procedure of this subproblem. For large-scale computations a commonly used technique to resolve the issue is to do a domain decomposition. Assume that the PDE (1.1) is defined on the domain Ω and consider a family of overlapping subdomains $\{\Omega_k\}_{k=1}^{q}$, cf. Figure 1.2. Then, split the Laplace operator as

$$\Delta = \sum_{k=1}^{q} \Delta_k,$$

where Δ_k represents Δ on the subdomain Ω_k (only). This formulation is an example of a spatial splitting as the operators Δ_k are defined from a separation of the domain Ω. Note

that, in contrast to formulations given by physical splittings like (1.2), all the operators Δ_k here represent the same physical process.

A splitting method well suited to handle the combined physical and spatial splitting of the FitzHugh–Nagumo equations is the additive splitting scheme

$$S_h = (I - hF)^{-1}\Big(\frac{1}{q}\sum_{k=1}^{q}(I - hqA_k)^{-1}\Big),$$

where

$$A_k = \begin{pmatrix} D_1\Delta_k & 0 \\ 0 & D_2\Delta_k \end{pmatrix}.$$

Due to the relatively small size of Ω_k compared to Ω the actions of the resolvents $(I - hqA_k)^{-1}$ may be computed at a considerably lower cost than required for the action of the full resolvent $(I - hA)^{-1}$. Furthermore, note that they can be computed separately. The additive splitting scheme is thus ideal for parallel implementation. We discuss spatial splittings in Chapter 4.

After this motivation of splitting schemes using (1.1) as an example problem we are ready to formulate the goal of the research presented in this thesis. To this end, we now step back from the FitzHugh–Nagumo equations and consider general semilinear parabolic PDEs. The main goal of this thesis can be summarized as follows:

> *Analyse convergence of additive and ADI splitting methods applied to physical and/or spatial splittings of a broad range of semilinear parabolic PDEs, and utilize the advantages of these methods for efficient simulation of interdisciplinary applications.*

In the following sections, this goal is broken down to three major themes: optimal convergence order analysis, spatial splittings and a physical splitting application: axonal growth.

1.1 Theme 1: Optimal convergence order analysis

In view of the first theme of the thesis, consider a semilinear parabolic PDE which has been split e.g. by a physical and/or a spatial splitting. Further, consider the temporal discretization given by applying a splitting method to this formulation. Denote by $u^n := S_h^n u(0)$ the numerical approximation of the exact solution $u(nh)$ at the fixed time $t = nh$. A central goal of the presented research is to prove convergence orders in time. This can be achieved by showing error bounds of the type

$$\|u(nh) - u^n\| \leq Ch^p,$$

where the integer p is the order and C is a positive constant. As we have left the spatial part of the PDE non-discretized, these temporal results are independent of any subsequent

space discretization. They may therefore be used as building blocks for the analysis of full space–time discretizations.

As we aim to perform temporal convergence analyses that apply to a wide range of semilinear parabolic PDEs, we want a broad abstract framework to carry out our studies in. The framework of maximal dissipative operators is the candidate of choice for this thesis, since it encapsulates crucial properties of many parabolic PDEs. Furthermore, not only parabolic PDEs can be described as dissipative evolution equations; other applications may be found, e.g., among hyperbolic PDEs and Schrödinger-type equations, see e.g. [6, Chapter 5] and [79, Chapter 19]. Neither are we limited to spatial and physical splittings; our abstract analyses will apply to general semilinear splitting formulations. The framework of maximal dissipative operators is properly defined and discussed in Section 3.2.

Proving convergence with an order for numerical methods applied to PDEs often requires regularity assumptions on the solution u. Many parabolic problems, like linear diffusion–reaction equations, do have smooth solutions. However, when such regularity is not present we may still have convergence. We thus strive to perform an optimal convergence order analysis with orders ranging from classical down to convergence without order ($o(1)$-convergence), depending on the regularity of the solution. Convergence without order is defined by

$$\lim_{n\to\infty} \left\| u(t) - S_{t/n}^n u(0) \right\| = 0,$$

and with classical order we mean the order exhibited by the method when applied to bounded linear operators (matrices), cf. Section 3.1.

The second goal for the optimal convergence order analysis in this thesis is to show how the temporal results can be used in a full space–time analysis. In particular, we will demonstrate a proof technique that can be used to combine the temporal convergence theorems with spatial error analyses to prove simultaneous space–time orders

$$\|u(nh) - u_{\Delta x}^n\| \leq C(h^p + (\Delta x)^s).$$

Here $u_{\Delta x}^n$ denotes the approximate solution given by applying both a temporal and a spatial discretization to the parabolic PDE. Further, Δx represents how fine the space discretization is, typically given by a mesh width. The positive number s denotes the order of this discretization.

Also here we aim to produce results that apply widely. Therefore, the strategy is to not specify a particular spatial discretization, but rather to list certain requirements on it, most prominently that it converges with an order. We are thus ready to state the first aim of the thesis:

Aim 1. *Prove optimal convergence orders, ranging from $o(1)$ to classical ones depending on the smoothness of the solution, for additive and ADI splitting schemes when applied to semilinear parabolic PDEs. Moreover, use these results in conjunction with analyses of spatial discretizations to form full space–time convergence order analyses.*

Temporal semi-discretizations are analysed in Papers I and III. Previous studies within this area either consider linear PDEs, Lipschitz continuous nonlinear terms, specific equations or only prove convergence without order. Note that the linearity and Lipschitz assumptions are rather restrictive, e.g. each excludes the FitzHugh–Nagumo equations (1.1). Full discretizations are considered in Paper II, where optimal convergence orders, simultaneously in time and space are proven, for dissipative problems. Previous studies in this context either consider splittings where some of the operators are bounded (which, e.g., excludes spatial splittings) or only prove convergence without order. A literature overview is given in Chapter 2 and the convergence results are summarized and unified in Chapter 3.

Throughout the thesis we provide several examples of physical splittings that fit into the dissipative framework and further examples can be found in the literature. However, spatial splittings have not previously been as well explored. Thus, for these we perform a deeper investigation which merits its own theme.

1.2 Theme 2: Spatial splittings

For the second theme of the thesis we analyse spatial splittings and prove that these indeed fit into the abstract framework of Aim 1. We consider two such splitting formulations: dimension splittings and domain decomposition splittings. These techniques are based on a separation of the spatial domain of the parabolic PDE. From this separation a formulation is constructed that consists of a set of smaller problems, which are easier to solve and can be handled in parallel. Then a temporal discretization is given by applying a splitting scheme to this formulation.

Domain decomposition splittings were already introduced above, when splitting the FitzHugh–Nagumo equations (1.1). The idea is to split the spatial derivative into several parts where each represents the PDE only on a smaller subset of the full domain, cf. Figure 1.2. A different approach is used by dimension splittings. These instead split the derivative with respect to the spatial dimensions. That is, each part of the splitting only represents a family of 1D problems. Both techniques are properly introduced in Section 2.6.

The aim of the second theme is to perform an optimal convergence order analysis for splitting schemes applied to these spatial splitting formulations. Our strategy is to decompose linear and semilinear parabolic model problems by using spatial splittings and then formulate the procedure in the framework of maximal dissipative operators. After that, we can interpret the results of Aim 1 to conclude convergence, in time or simultaneously in time and space, and possibly with orders. We aim to perform an analysis that asserts convergence under non-restrictive assumptions on the model problems. Furthermore, for convergence with order for linear problems, we aim to use the tools provided in this setting to derive the required regularity of the solution only from assumptions on the initial data. We summarize this in the second aim of the research presented in this thesis:

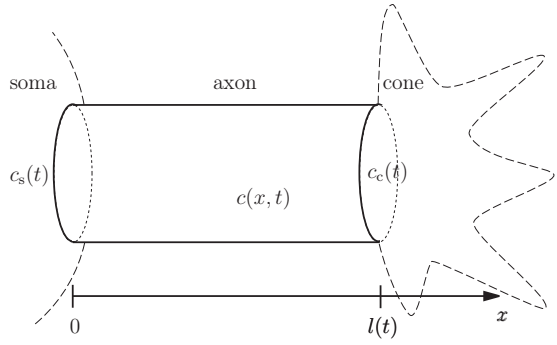


Figure 1.3: Schematic illustration of axon outgrowth from a nerve cell. The soma produces tubulin which is transported along the axon to the growth cone. There, the tubulin is used to expand the axon. The tubulin concentration is denoted by c_s in the soma, by c in the axon and by c_c in the cone. The length of the axon is denoted by l.

Aim 2. *Perform optimal convergence order analyses of temporal discretization methods based on spatial splittings of linear and semilinear parabolic PDEs.*

The analyses are performed in Papers II–III and are summarized in Chapter 4. Domain decomposition splittings have previously not been formulated and properly analysed in the framework of dissipative operators. Furthermore, all results presented in this thesis regarding full discretizations of spatial splittings are new. An overview of the literature is given in Section 2.6.

1.3 Theme 3: A physical splitting application: axonal growth

The third theme of the thesis concerns the evaluation of splitting methods when used in interdisciplinary applications. Such applications may take us outside the framework of our convergence studies, but may instead demonstrate the flexibility and usefulness of the discussed splitting schemes.

The particular application of interest is given by a model for axonal growth in nerve cells (neurons). Axons are long, thin outgrowths from the cell body, the soma. They fill the purpose of transmitting electrical signals to other neurons. The concentration of the protein tubulin in the tip of the axon, the growth cone, is of fundamental importance for the growth rate of the axon. However, tubulin is produced in the soma and then transported along the axon to the growth cone, cf. Figure 1.3. We consider a 1D linear parabolic PDE describing the tubulin concentration in the axon, coupled with nonlinear

ordinary differential equations (ODEs) which model the processes governing the axon elongation in the cone.

Any steady-state solution can be obtained explicitly, however, to describe the dynamical behaviour numerical approximations are required. In this setting the axon model features several challenges that must be addressed by a numerical method. The most important ones are the varying size of the domain of the PDE, the coupling to the nonlinear ODEs through a boundary condition and a solution that exhibits transient phenomena on largely different time scales. The axonal growth model constitutes a good application for a splitting technique as a physical splitting, separating the PDE from the ODEs, enables us to take advantage of the linearity of the PDE. We summarize in the third aim of the thesis:

Aim 3. *Develop an efficient and robust numerical discretization based on a physical splitting of the axonal growth model, perform numerical experiments to illustrate convergence orders of the discretization and further evaluate it by how well it deals with the specific challenges offered by the model.*

The model and the numerical scheme are analysed in Papers IV and V, respectively. A summary is given in Chapter 5.

Chapter 2

Splitting methods

Consider the abstract semilinear evolution equation

$$\dot{u} = Au + Fu \tag{2.1a}$$

$$= \sum_{k=1}^{q} A_k u + Fu, \quad u(0) = \eta, \tag{2.1b}$$

where the operator F is (possibly) nonlinear, the operator A is linear and may be further split into q operators A_k. The first splitting formulation (2.1a) typically represents a physical splitting, e.g. involving a diffusion A and a reaction F. The additional splitting of A in (2.1b) is typically given by a spatial splitting. Thus, the evolution equation will mainly represent semilinear parabolic PDEs. In this case, the boundary conditions of the problems are handled by the domains of the operators in (2.1).

We will also frequently consider linear problems on the form

$$\dot{u} = Au = \sum_{k=1}^{q} A_k u, \quad u(0) = \eta, \tag{2.2}$$

which typically represent spatial splittings.

For many problems it is considerably cheaper and/or easier to find solutions, exact or numerical, to the subproblems

$$\dot{u} = Au, \quad \dot{u} = Fu \quad \text{and} \quad \dot{u} = A_k u, \quad k = 1, \ldots, q, \tag{2.3}$$

than to the full problem (2.1). This is the main motivation for using splitting methods. These time-stepping schemes, in each step, iterate between solving the subproblems to construct an approximation of the solution to the full problem. Questions of existence and uniqueness of solutions to the full problems and the subproblems will be properly

discussed in the next chapter. Until then, the reader may regard the presented methods as formal.

In the current chapter we introduce the methods that will be analysed in upcoming chapters. The presentation is accompanied by a literature overview. The first four sections discuss splitting schemes. Of particular interest for this thesis are the additive and alternating direction implicit (ADI) schemes which are given their own sections. For introductory surveys on splitting methods see e.g. [32, 43, 51, 54], which offer more details on the schemes discussed in this chapter and also include several other methods. The chapter is concluded by discussing full space–time discretizations, dimension splittings and domain decomposition splittings.

As the evolution equation (2.1) usually represents a PDE the involved operators are typically unbounded and defined on infinite-dimensional spaces. (We here use the word unbounded in a general sense to exclude e.g. Lipschitz continuity and similar concepts.) Our literature overview focuses on previous convergence studies in this context. Just as we will do in the next chapter, many of the cited studies use the framework of maximal dissipative operators. The reader is reminded that dissipative equations encapsulate crucial properties of parabolic problems and thus represents many of these PDEs. We give several example applications in Papers I–III, see also [6, Chapter 5] and [79, Chapter 19].

2.1 Exponential splitting schemes

As a first example we consider the two-operator formulation of the exponential Lie–Trotter splitting method. Given the approximation u^n of the solution u at time $t = t^n := nh$, we get the approximation u^{n+1} at the next time step by, in sequence, solving the two equations

$$\dot{v} = Av \quad \text{for} \quad t^n < t \leq t^{n+1} \quad \text{with} \quad v(t^n) = u^n, \tag{2.4a}$$

$$\dot{w} = Fw \quad \text{for} \quad t^n < t \leq t^{n+1} \quad \text{with} \quad w(t^n) = v(t^{n+1}), \tag{2.4b}$$

and then letting $u^{n+1} := w(t^{n+1})$. By using flow notation the Lie–Trotter time step S_h can be more compactly written as

$$u^{n+1} = S_h u^n = \mathrm{e}^{hF}\mathrm{e}^{hA}u^n. \tag{2.5}$$

Here, e^{hA} denotes the flow of the first subproblem, i.e. $\mathrm{e}^{hA}u^n := v(t^{n+1})$, the exact solution of (2.4a). The same applies for e^{hF} in relation to (2.4b). See [73] from 1951 for an early reference to the Lie–Trotter scheme in the context of unbounded operators. However, the scheme, when applied to matrices, was known in the literature long before that.

More generally, we may construct higher-order exponential splitting schemes on the form

$$S_h = \prod_{i=1}^{r} \mathrm{e}^{\alpha_i hF}\mathrm{e}^{\beta_i hA} \tag{2.6}$$

by specific choices of the (complex-valued) coefficients α_i and β_i. For example, the first-order Lie–Trotter scheme is given by choosing $r = 1$ and $\alpha_1 = \beta_1 = 1$. By combining the subproblems in another way we get the second-order Strang splitting scheme [69]

$$S_h = \mathrm{e}^{\frac{1}{2}hA}\mathrm{e}^{hF}\mathrm{e}^{\frac{1}{2}hA}.$$

For higher-order exponential splitting schemes see e.g. [10, 35, 78], [32, Section II.4] and [64, Section 13.1]. Generalizations to splittings involving more operators are naturally constructed by inserting the flows of further subproblems in the product (2.6).

We give a brief account of contemporary convergence studies for exponential splitting schemes for abstract evolution equations. When A and F are linear, A unbounded but F bounded relative to A, it is proven in [45] that classical orders of the Lie–Trotter and Strang splitting methods are preserved. When also F is unbounded convergence of exponential splitting schemes of arbitrary order is proven in [34] under certain regularity assumptions on u. For a range of different schemes these results are generalized in [26] to inhomogeneous equations and in [37] to semilinear equations with Fréchet differentiable nonlinearities F. See also [19] for further convergence studies of the Strang splitting scheme applied to linear systems. Convergence without order for the Lie–Trotter scheme is proven for fully nonlinear problems in [8].

For studies of exponential splitting methods applied to specific problems classes we mention, e.g. [41] for conservation laws and [25, 50] for Shrödinger-type equations.

2.2 Full Lie- and IMEX-type schemes

For exponential splitting schemes the exact solutions of the subproblems (2.3) are used. However, in the applications we are interested in these exact solutions are generally not easy to compute. This may be due to the parabolic problems studied, e.g. they may feature space-dependent diffusion coefficients, nonlinear reactions or they may be defined on domains Ω with complex boundaries. Alternatively, or additionally, the difficulty to find exact solutions may come from the way we construct the split equation (2.1). This is e.g. true for domain decomposition splittings where space-dependent weight functions are introduced. In these cases, the exact flows of the subproblems may be approximated by (other) numerical methods, as long as their errors are small compared to that of the splitting scheme. The analysis of these schemes requires then that the splitting method is considered in combination with the approximations of the subproblems, see e.g. [7].

Alternatively, we may directly construct splitting methods S_h from low-order approximations of the subproblems. These methods, referred to as full splitting schemes (not to be confused with full discretization with which we mean a problem discretized both in time and space), can then be directly used and analysed without having to consider possible further approximations. In the introduction we already saw two examples of full splitting methods: the Peaceman–Rachford scheme and an additive splitting scheme,

which both are constructed from Euler approximations of the subproblems (2.3). These schemes will be further discussed and motivated in the upcoming sections. Before that we give a short introduction to two other commonly used full splitting schemes: the full Lie splitting method and the IMEX (implicit–explicit) Euler method,

$$S_h = (I - hF)^{-1}(I - hA)^{-1} \quad \text{and} \tag{2.7}$$

$$S_h = (I - hA)^{-1}(I + hF), \tag{2.8}$$

respectively. Both methods are first order and also only use Euler discretizations of the subproblems (2.3). The IMEX method is a suitable choice when the explicit Euler step $(I+hF)$ does not result in a significant time-step restriction, e.g. it may be a good choice when F is Lipschitz continuous. Then it may be more efficient than the full Lie method where a nonlinear equation must be solved to compute the action of $(I - hF)^{-1}$.

Higher-order versions of the above full splitting schemes may also be constructed, see e.g. [43, Sections IV.2 and IV.4]. For the full Lie splitting method (2.7) first-order convergence is proven in [33] when A and F are linear and dissipative. When these operators are nonlinear convergence without order is proven in [8, 36]. First-order convergence of IMEX Euler (2.8) and classical orders of many other methods are proven in [57] for a linear F that is bounded relative to A. For a nonlinear F that fulfils a Lipschitz-type assumption classical orders are proven in [2] for several different IMEX methods. In the same setting simultaneous space–time convergence orders are proven in [48, 71]. For fully nonlinear dissipative problems convergence with order at least $p = 1/2$ is proven in [39, 68] for various splitting methods similar to full Lie and IMEX Euler. In the context of viscosity solutions convergence with order is proven in [46] for an IMEX-type scheme applied to strongly degenerate parabolic problems.

2.3 ADI splitting schemes

In this section we introduce the two alternating direction implicit (ADI) methods that we will analyse in the upcoming chapters: the Peaceman–Rachford scheme

$$S_h = \big(I - \tfrac{h}{2}F\big)^{-1}\big(I + \tfrac{h}{2}A\big)\big(I - \tfrac{h}{2}A\big)^{-1}\big(I + \tfrac{h}{2}F\big), \tag{2.9}$$

of classical order two, and the Douglas–Rachford scheme

$$S_h = (I - hF)^{-1}(I - hA)^{-1}(I + h^2AF), \tag{2.10}$$

of classical order one. There seems to be no clear definition of which methods are classified as ADI methods. Thus, in this thesis, we use ADI to refer to exactly these two methods. We will consider them both in the semilinear setting as above, discretizing (2.1a), and in the fully linear setting, discretizing (2.2) with $q = 2$:

$$S_h = \big(I - \tfrac{h}{2}A_2\big)^{-1}\big(I + \tfrac{h}{2}A_1\big)\big(I - \tfrac{h}{2}A_1\big)^{-1}\big(I + \tfrac{h}{2}A_2\big), \tag{2.11}$$

$$S_h = (I - hA_2)^{-1}(I - hA_1)^{-1}(I + h^2A_1A_2). \tag{2.12}$$

The ADI schemes were first introduced in [20, 59] during the 1950s to perform dimension splittings of the heat equation. This application also named the method class; recall that using dimension splittings involves alternating between different dimensions (directions). However, the name is rather confusing in the current context since not only ADI methods may be used in conjunction with dimension splittings and, more importantly, ADI methods may be used for other applications than this, as can be seen in the examples presented in this thesis. However, the name is well-established so we will continue to use it.

The Douglas–Rachford scheme may be regarded as a modified Lie splitting scheme (2.7). Despite the extra operator $(I+h^2AF)$ it has excellent stability properties; it is well-known in the classical analysis that both schemes (2.9) and (2.10) are unconditionally stable when applied to stiff equations, see e.g. [22, 43]. However, a fair question is: what is gained by including the extra operator $(I + h^2AF)$? The answer is twofold: when this factor is included the method exhibits a more favourable local error structure and its internal stages are consistent. These two properties are both shared by the Peaceman–Rachford scheme and are explained in the following paragraphs.

As seen in the introduction splitting methods have superior efficiency in many applications. The price for this is the splitting error. For example, in the dissipative setting, assuming that the solution u is smooth enough, the local errors of full Lie, respectively, Douglas–Rachford contain the terms

$$\ddot{u},\ A\dot{u},\ A^2u, \quad \text{respectively,} \quad \ddot{u},\ A\dot{u}. \tag{2.13}$$

See Paper I and Section 3.3 for a derivation and [38] for a similar discussion in a linear setting. The term $\ddot{u}$ would show up also in an error analysis of implicit Euler, whereas the terms $A\dot{u}$ and A^2u are introduced by the splitting scheme. These are more difficult to bound since they are not naturally related to the temporal regularity of the evolution equation (2.1a). As we will see in the upcoming chapters, the lack of the term A^2u in the local error of Douglas–Rachford is essential for many of the positive results presented in this thesis. Similarly, we will use that the Peaceman–Rachford scheme has a more favourable local error structure than other second-order splitting methods.

The Peaceman–Rachford scheme (2.9) has one consistent internal stage

$$u^{n+\frac{1}{2}} = \big(I - \tfrac{h}{2}A\big)^{-1}\big(I + \tfrac{h}{2}F\big)u^n,$$

approximating $u(t^{n+1/2})$. Similarly, the Douglas–Rachford scheme (2.10) has two internal stages which are consistent approximations of $u(t^{n+1})$, however to reveal these the method has to be written on another form, cf. [43, Section IV.3.2]. In the same reference and in [42] it is shown that the consistent internal stages make these methods good choices for inhomogeneous PDEs. Another consequence is that fixed points $\bar{u}$ of the exact flow are preserved by the splitting method, i.e. if $\mathrm{e}^{hG}\bar{u} = \bar{u}$ then $S_h\bar{u} = \bar{u}$ [49]. This in turn means that the ADI schemes can be used when studying convergence to steady

states, a property of utmost importance for the axonal growth application of Papers IV–V and Chapter 5. Note that splitting methods in general do not have consistent internal stages. Many IMEX methods have this property, but e.g. exponential splitting methods and the full Lie scheme lack it.

We also note that, in contrast to what one might believe at first glance, taking a step with Peaceman–Rachford or Douglas–Rachford costs as little as a step with full Lie (2.7). This can be seen by introducing the change of variables $u^n = (I - h/2\,F)^{-1}v^n$ to rewrite the scheme (2.9) as

$$v^{n+1} = \Big(2\big(I - \tfrac{h}{2}A\big)^{-1} - I\Big)\Big(2\big(I - \tfrac{h}{2}F\big)^{-1} - I\Big)v^n.$$

Similarly, with $u^n = (I - hF)^{-1}v^n$ the scheme (2.10) can be rewritten as

$$v^{n+1} = \big((I - hA)^{-1}(2(I - hF)^{-1} - I) + I - (I - hF)^{-1}\big)v^n.$$

Other splitting schemes commonly classified as ADI methods are usually constructed as generalizations of the Douglas–Rachford scheme. Prominent examples include formulations for splittings involving more than two operators [21] and versions with classical order two [9]. However, such generalizations usually suffer from either worsened local error structure or worsened stability properties, see e.g. [22, 52].

For dissipative evolution equations on Hilbert spaces, when both operators are linear and unbounded, preservation of classical orders were proven in [33] for the Peaceman–Rachford scheme and in [38] for the Douglas–Rachford scheme. In the latter the evolution equation may be inhomogeneous, for more on this see also [66]. Further details on the stability of the Peaceman–Rachford scheme in the linear setting are given in [65]. Previous studies of this method in the semilinear setting include [18] where second-order convergence is proven for a diffusion–reaction system with F Lipschitz continuous and seven times differentiable. A partial convergence study is carried out in [42] on finite-dimensional spaces. For nonlinear and multivalued dissipative evolution equations convergence without orders are proven in [49] for both schemes.

2.4 Additive splitting schemes

In this section we will mainly discuss the first-order additive splitting scheme

$$S_h = \frac{1}{q}\sum_{k=1}^{q}(I - hqA_k)^{-1}, \tag{2.14}$$

employed as a temporal discretization of the linear evolution equation (2.2), and two generalizations of it to semilinear problems. Recall that the Douglas–Rachford scheme can be constructed as a modification of the full Lie splitting method (2.7) e.g. to improve

the local error structure. Likewise, the scheme (2.14) can be regarded as an additive version of the full Lie scheme. The principal motivation is to enable implementation on parallel hardware.

Much like the history of ADI schemes we find additive schemes employed in conjunction with dimension splittings in many of the early references, see e.g. [29, 77]. In [70] a second order scheme was introduced

$$\begin{aligned} S_h = {} & \tfrac{1}{2}\big(I - \tfrac{h}{2}A_q\big)^{-1}\big(I + \tfrac{h}{2}A_q\big)\cdots\big(I - \tfrac{h}{2}A_1\big)^{-1}\big(I + \tfrac{h}{2}A_1\big) \\ & + \tfrac{1}{2}\big(I - \tfrac{h}{2}A_1\big)^{-1}\big(I + \tfrac{h}{2}A_1\big)\cdots\big(I - \tfrac{h}{2}A_q\big)^{-1}\big(I + \tfrac{h}{2}A_q\big), \end{aligned} \tag{2.15}$$

which can be regarded as a combination of a Lie-type scheme and an additive scheme.

Similarly to the full Lie scheme (2.7) the additive schemes (2.14) and (2.15) are unconditionally stable when applied to parabolic equations (2.1b), independently of the number of operators q making up the vector field. In the dissipative setting, assuming that the solution u is smooth enough, the local error of the first-order scheme (2.14) contains the terms

$$\ddot{u},\ A_k^2 u, \quad k = 1, \dots, q,$$ [1]

see Paper III. As expected, for two-operator splittings, the error structure is not as good as for ADI schemes. The advantage here, however, is that it does not deteriorate with a growing number of operators.

In Paper III and Section 3.3 we analyse two extensions of (2.14) to semilinear evolution equations (2.1b). For unbounded nonlinear operators F the already introduced additive scheme

$$S_h = (I - hF)^{-1}\Big(\frac{1}{q}\sum_{k=1}^{q}(I - hqA_k)^{-1}\Big), \tag{2.16}$$

is a good choice. If F is Lipschitz continuous we may instead consider

$$S_h = \Big(\frac{1}{q}\sum_{k=1}^{q}(I - hqA_k)^{-1}\Big)(I + hF), \tag{2.17}$$

for simpler computations.

Additive splitting schemes in the setting of dissipative and unbounded operators have not previously been analysed in the literature to the same extent as other splitting methods. However, in the early article [13] convergence without order was proven for (2.14) when $q = 2$ and when applied to a nonlinear conservation law. This result was generalized to nonlinear dissipative operators in [36]. High-order additive exponential schemes for two operators are studied in [17] under the assumption that one is linear and the other is sufficiently many times Fréchet differentiable, depending on the order of the method.

[1] In the linear setting we have $A\dot{u} = \ddot{u}$ which is why the term $A\dot{u}$ in (2.13) is not found here.

2.5 Abstract full space–time discretizations

When considering full space–time discretizations we limit our attention to linear PDEs on the form (2.2). As mentioned in the introduction we do not specify a particular space discretization. We instead require that it fulfils certain assumptions, e.g. that it converges with an order. Thus, consider the abstract semi-discretization, represented by the finite-dimensional evolution equation

$$\dot{u}_{\Delta x} = A_{\Delta x} u_{\Delta x} = \sum_{k=1}^{q} A_{k,\Delta x} u_{\Delta x}, \quad u_{\Delta x}(0) = \eta_{\Delta x},$$

where $\eta_{\Delta x}$ is a finite-dimensional approximation of η. The operators $A_{1,\Delta x}, \dots, A_{q,\Delta x}$ and $A_{\Delta x}$ are discrete representatives of their counterparts in (2.2). A full discretization is given by also applying a time discretization method, e.g. using the additive scheme (2.14) gives

$$S_{h,\Delta x} = \frac{1}{q} \sum_{k=1}^{q} (I - hqA_{k,\Delta x})^{-1}.$$

As indicated above we discretize first in space, then in time. This is also how our analysis will be performed; we will thus apply our temporal results to the spatial semi-discretization. This idea follows in the spirit of [14, 71] where simultaneous space–time convergence orders are proven when the temporal discretization is given by the implicit Euler or the Crank–Nicholson scheme.

We give a short account of previous full space–time analyses involving splitting methods and general space discretizations. In [2] simultaneous orders are given for IMEX methods discretizing a semilinear problem where the nonlinearity fulfils a Lipschitz-type condition. Convergence without orders are proven in [7] when exponential splitting methods are used for the temporal discretization. For the Peaceman–Rachford scheme partial results with orders in time can be found in [42].

2.6 Spatial splitting formulations

We here discuss dimension splittings and domain decomposition splittings. The latter are also commonly referred to as domain decomposition operator splittings. This gives the abbreviation DDOSs that we will frequently use. To introduce the spatial splittings we consider a model problem given by the linear diffusion–advection–reaction equation

$$\dot{u} = Au = \nabla \cdot (\lambda \nabla u) - \rho \cdot \nabla u - \sigma u, \quad u(0) = \eta, \tag{2.18}$$

defined on a bounded domain $\Omega \subset \mathbb{R}^d$, where $d \geq 1$ is an integer. The space-dependent equation coefficients are given by the $d \times d$ matrix λ, the d vector ρ and the scalar function σ. With the exception of certain semilinear extensions we will, throughout the

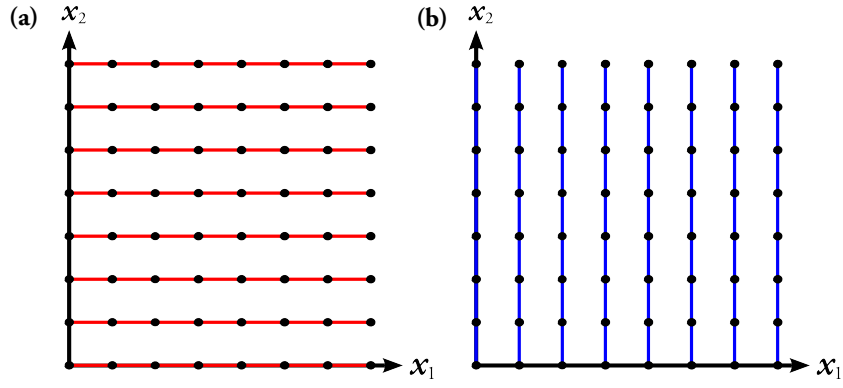


Figure 2.1: A schematic drawing of a 2D dimension splitting (2.19)*. The dots in the figures represent a uniform mesh used for discretizing this splitting formulation in space, e.g. with a finite difference method. Computing the action of the resolvent* $(I - hA_{1,\Delta x})^{-1}$ *then amounts to solving a family of 1D problems. In (a) each red line represents one of those problems. The solution of each of them only requires solving a linear system involving the nodes connected in the corresponding line. Similarly, computing the action of the resolvent* $(I - hA_{2,\Delta x})^{-1}$ *amounts to solving 1D problems coupled in the* x_2*-direction, marked by the blue lines in (b). Thus, a splitting scheme applied to the dimension splitting* (2.19) *alternates between the directions, solving the PDE one dimension at time.*

thesis, only consider (2.18) when discussing spatial splittings. However, we note that these techniques can be applied more generally where the most important prerequisite is that A contains spatial derivatives, more examples are given in Paper III.

As the dimension splitting procedure is the oldest of the two discussed techniques we introduce it first. Consider (2.18) with $d = 2$, ρ and σ identically zero and λ diagonal with $\lambda_{1,1}(x) = \lambda_{2,2}(x) = a(x_1)b(x_2)$ for some one-dimensional functions a and b. This gives the operators

$$A_1 u = \frac{\partial}{\partial x_1}\Big(\lambda_{1,1}\frac{\partial}{\partial x_1}u\Big) \quad \text{and} \quad A_2 u = \frac{\partial}{\partial x_2}\Big(\lambda_{2,2}\frac{\partial}{\partial x_2}u\Big), \tag{2.19}$$

defining a dimension splitting of the two-dimensional diffusion equation. Each operator A_k represents the diffusion in one space dimension only. If a splitting method is subsequently applied to this formulation we get a scheme that alternates between updating in the x_1-direction and the x_2-direction.

To describe how we may gain in efficiency by performing dimension splittings it is easier to first discretize in a space, cf. Figure 2.1. Let Ω be the unit square $(0, 1)^2$ and introduce on it a structured mesh consisting of squares of the same size and aligned with the axes. Then let the space discretization of (2.19) be given by either a finite difference method or a finite element method (with mass lumping). An implicit Euler

step $(I - hA_{\Delta x})^{-1}$, e.g., would require the solution of a large, irreducible linear equation system. On the other hand, due to the structure of the diffusion coefficients, $A_{1,\Delta x}$ and $A_{2,\Delta x}$ decouple into block diagonal matrices where each block corresponds to a 1D problem. Thus, computing the action of the resolvent $(I - hA_{1,\Delta x})^{-1}$, as part of a splitting scheme, requires only the solution of a family of independent 1D problems. The action can therefore be computed in parallel, furthermore, the linear equation systems to solve are far smaller than the full one.

Domain decomposition splittings were first introduced as alternatives to dimension splittings. Instead of splitting the derivatives by dimension these techniques split based on a decomposition of the domain $\Omega = \bigcup_{k=1}^{q} \Omega_k$, where any pair of subdomains may overlap, cf. Figure 1.2. As such the DDOS procedure constitutes a particular type of domain decomposition method, specifically designed to solve parabolic problems in conjunction with splitting schemes.

However, traditionally domain decomposition methods are iterative schemes used to solve stationary problems like the elliptic equation

$$Au = f,$$

with A as in (2.18) and where f is a given function. Each iteration involves a solution step and a communication step. The solution step consists of (exactly or numerically) solving the stationary problem on each subdomain Ω_k. This can, on each Ω_k, be done independently from all other subdomains and the systems to solve are thus smaller and the computations can easily be parallelized. The results in the overlaps are then communicated between affected neighbouring subdomains (only). These results are then used for the solution step in the next iteration. A key observation here is the lack of global communication.

There are several ways to generalize the domain decomposition procedure to parabolic problems like (2.18). The classical way is to first apply a standard implicit time discretization method, like implicit Euler. This defines a sequence of stationary problems (the time steps) which are then, each in turn, treated as above. Traditional domain decomposition methods are also often used as preconditioners for other iterative solvers. See e.g. [61, 72] for general surveys.

As mentioned above, DDOSs constitute an alternative approach for generalizing the domain decomposition procedure to parabolic problems. A DDOS is based on a partition of unity given by a family of continuous weight functions $\{\chi_k\}_{k=1}^{q}$. Each such function vanishes except on its corresponding subdomain Ω_k, cf. Figure 2.2. Using these we define the operators

$$A_k u = \nabla \cdot (\chi_k \lambda \nabla u) - \chi_k \rho \cdot \nabla u - \chi_k \sigma u, \tag{2.20}$$

which each maps to zero outside the corresponding subdomain Ω_k. Note how each subdomain Ω_k corresponds to one weight function χ_k and one operator A_k. Applying e.g. the additive splitting scheme (2.14) to the DDOS formulation means that, in each time

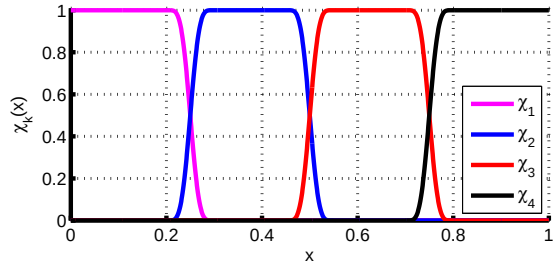


Figure 2.2: An example partition of unity $\{\chi_k\}_{k=1}^4$*, subordinate to the overlapping domain decomposition:* $\Omega_1 = (0, 0.3)$*,* $\Omega_2 = (0.2, 0.55)$*,* $\Omega_3 = (0.45, 0.8)$*,* $\Omega_4 = (0.7, 1)$ *of* $\Omega = (0, 1)$*. Note that each weight function* χ_k *is zero outside its corresponding subdomain* Ω_k*.*

step, the action of the resolvents $(I - hqA_k)^{-1}$ must be evaluated. This only entails independent computations on each domain and local communication of the results, just as for the classical domain decomposition techniques. However, we note that a fundamental difference is that the DDOS-based schemes are non-iterative. That is, the action of each resolvent is, in each time step, only computed a fixed number of times, e.g. only once when using the additive scheme (2.14). This lack of iterations may result in more efficient schemes. Further, note that the lack of global communication is an important benefit of DDOSs over dimension splittings.

The details on how to construct the subdomains and the weight functions are postponed to Section 4.1. There we also discuss how useful domain decompositions may be formed even when only two operators are allowed as for the ADI schemes.

We conclude the chapter by a short literature overview. In this thesis we only consider two-dimensional problems when analysing dimension splittings. However, the procedure can easily be generalized to more dimensions by including more operators or by bundling several dimensions into each, cf. [33]. Although mixed derivatives, like

$$\frac{\partial}{\partial x_1}\lambda_{1,2}\frac{\partial}{\partial x_2} \quad \text{and} \quad \frac{\partial}{\partial x_2}\lambda_{2,1}\frac{\partial}{\partial x_1},$$

are troublesome for dimension splittings, efforts have been made to also include them, see [44, 53]. Different nonlinear settings are considered in [36, 42].

Both spatial splitting techniques discussed here have a strong historic and modern connection to the splitting methods considered in this thesis. See, e.g. [13, 20, 29, 59, 77] for early references of both ADI and additive schemes employed to perform dimension splittings. DDOSs were introduced in [52, 74] and were there discretized by ADI schemes. Contemporary studies of dimension splittings of parabolic problems include [33, 36, 42, 44]. For recent studies of ADI and additive schemes applied in conjunction with DDOSs on finite-dimensional spaces we refer to [5, 60, 63, 75, 76].

Chapter 3

Optimal convergence order analysis

In the current chapter we summarize the optimal convergence studies of splitting schemes called for by Aim 1. That is, for the temporal analysis, we will prove orders, ranging from $o(1)$ to classical, depending on the smoothness of the solution. To clarify what we mean by classical order we begin by giving an example convergence analysis for linear ODEs in Section 3.1. Then, to obtain the tools needed to treat semilinear parabolic PDEs, we introduce the framework of maximal dissipative operators in Section 3.2. With this framework in place we can discuss existence and uniqueness of solutions to the full problem

$$\dot{u} = Au + Fu \tag{3.1a}$$

$$= \sum_{k=1}^{q} A_k u + Fu, \quad u(0) = \eta, \tag{3.1b}$$

and the subproblems

$$\dot{u} = Au, \quad \dot{u} = Fu \quad \text{and} \quad \dot{u} = A_k u, \quad k = 1, \dots, q.$$

Furthermore, we can make sense of the notation $\mathrm{e}^{h(A+F)}\eta$ even for unbounded operators on infinite-dimensional spaces. The optimal convergence order studies in this setting are summarized in Section 3.3.

The chapter is concluded in Section 3.4 where the temporal results are used in the analysis of full space–time discretizations. We demonstrate a proof technique for combining the temporal convergence theorems with spatial error analyses to prove simultaneous space–time orders. Finally, we apply this technique to the considered splitting schemes combined with converging space discretizations.

3.1 Classical orders

Consider first the finite-dimensional linear setting, i.e. assume that

$$\dot{u} = A_1 u + A_2 u, \quad u(0) = \eta$$

is an ODE and that the operators A_1 and A_2 are matrices. The local error of the additive scheme

$$S_h = \tfrac{1}{2}\big((I - 2hA_1)^{-1} + (I - 2hA_2)^{-1}\big)$$

can then easily be found by using a Taylor expansion. We get

$$\begin{aligned}
\mathrm{e}^{h(A_1+A_2)} - S_h &= \mathrm{e}^{h(A_1+A_2)} - \tfrac{1}{2}\big((I - 2hA_1)^{-1} + (I - 2hA_2)^{-1}\big) \\
&= I + h(A_1 + A_2) + \tfrac{h^2}{2}(A_1^2 + A_1A_2 + A_2A_1 + A_2^2) + \mathcal{O}(h^3) \\
&\quad - \tfrac{1}{2}(I + 2hA_1 + 4h^2A_1^2 + \mathcal{O}(h^3)) \\
&\quad - \tfrac{1}{2}(I + 2hA_2 + 4h^2A_2^2 + \mathcal{O}(h^3)) \\
&= \tfrac{h^2}{2}(-3A_1^2 + A_1A_2 + A_2A_1 - 3A_2^2) + \mathcal{O}(h^3).
\end{aligned}$$

The expansion holds for h sufficiently small as A_1 and A_2 are bounded. Let $|\cdot|$ denote the Euclidean matrix norm. Stability follows from the bound

$$\begin{aligned}
|S_h| &= \tfrac{1}{2}\big(|(I - 2hA_1)^{-1}| + |(I - 2hA_2)^{-1}|\big) \\
&\leq \tfrac{1}{2}\Big(\frac{1}{1 - 2h|A_1|} + \frac{1}{1 - 2h|A_2|}\Big) \\
&\leq \tfrac{1}{2}\big(\mathrm{e}^{4h|A_1|} + \mathrm{e}^{4h|A_2|}\big) \leq \mathrm{e}^{4h(|A_1|+|A_2|)},
\end{aligned}$$

which holds for h sufficiently small and where the first inequality can be proven e.g. using a singular value decomposition. Thus we can conclude that the additive scheme converges with order $p = 1$. Similarly, Taylor expansions can be used to prove order of consistency when the vector field of the ODE is nonlinear but has bounded derivatives of sufficient orders, see e.g. [32, 43]. We refer to the convergence orders given in the finite-dimensional, i.e. bounded, setting as classical orders.

For PDEs, which are analysed in infinite-dimensional spaces, the vector fields are often defined by unbounded operators. Then, Taylor expansions can not be used as they depend on the norm of these operators. However, the framework of maximal dissipative operators provides tools well suited for convergence studies in the unbounded setting.

3.2 Maximal dissipative operators

Let $\mathcal{H}$ be a real Hilbert space equipped with the inner product $(\cdot, \cdot)$ and induced norm $\|\cdot\|$. Let I denote the identity operator on $\mathcal{H}$ and consider the (possibly) nonlinear operator $E : \mathcal{D}(E) \subset \mathcal{H} \to \mathcal{H}$ with domain $\mathcal{D}(E)$. We say that E is Lipschitz continuous

if its Lipschitz constant $L[E]$ is finite, where $L[E]$ is the smallest possible number such that

$$\|Eu - Ev\| \leq L[E] \|u - v\|, \quad \text{for all } u, v \in \mathcal{D}(E).$$

The operators of (3.1), i.e. $A_1, \ldots, A_q$, A, F and $A + F$, are typically not Lipschitz continuous, however, we will assume that they are maximal dissipative.

Definition 1. The operator $E : \mathcal{D}(E) \subset \mathcal{H} \to \mathcal{H}$ is maximal dissipative on $\mathcal{H}$ if and only if there is a constant $M[E] \geq 0$ such that E satisfies the dissipativity condition

$$(Eu - Ev, u - v) \leq M[E] \|u - v\|^2 \quad \text{for all } u, v \in \mathcal{D}(E), \tag{3.2}$$

and the maximality condition

$$\mathcal{R}(I - hE) = \mathcal{H} \quad \text{for all } h > 0 \text{ with } hM[E] < 1, \tag{3.3}$$

where $\mathcal{R}(I - hE)$ denotes the range of $I - hE$.

Example 1. The classical example of a linear maximal dissipative operator is the Laplacian. With $E = A + F = \Delta + 0$ the evolution equation (3.1) becomes the heat equation. Let it be equipped with homogeneous Dirichlet boundary conditions on a bounded domain $\Omega \subset \mathbb{R}^d$, $d \geq 1$. If Ω has a sufficiently regular boundary the Laplacian $\Delta : \mathcal{D}(\Delta) \subset L^2(\Omega) \to L^2(\Omega)$ can be proven to fulfil the conditions of Definition 1 with $M[\Delta] = 0$ and

$$\mathcal{D}(\Delta) = H^2(\Omega) \cap H_0^1(\Omega),$$

cf. [14, Section 1], [31, Section 9.1] and [58, Section 7.2]. Similar results can be proven under homogeneous Neumann or periodic boundary conditions.

Example 2. Consider the FitzHugh–Nagumo equations (1.1) equipped with homogeneous Dirichlet boundary conditions on a bounded domain $\Omega \subset \mathbb{R}^d$, $d = 1, 2$ or 3. The vector field is then given by the nonlinear operator

$$(A + F)u = \begin{pmatrix} D_1 \Delta u_1 \\ D_2 \Delta u_2 \end{pmatrix} + \begin{pmatrix} u_1 - u_1^3/3 - u_2 \\ a u_1 - b u_2 \end{pmatrix}.$$

Let $\mathcal{H} = (L^2(\Omega))^2$ with inner product $(u, v) = (u_1, v_1)_{L^2(\Omega)} + (u_2, v_2)_{L^2(\Omega)}$. If Ω has a smooth enough boundary, then $A + F$ is maximal dissipative on $\mathcal{H}$ with $M[A + F] \leq 1 + |1 - a|/2$ and

$$\mathcal{D}(A + F) = \left(H^2(\Omega) \cap H_0^1(\Omega)\right)^2.$$

This can be proven following along the lines of the proof for phase field models in [6, Section 5.4] and Paper I, Section 6. Similar results hold under Neumann or periodic boundary conditions.

Assume that E is maximal dissipative, then, according to [6, Proposition 3.4], it is closed. Furthermore, its resolvent

$$(I - hE)^{-1} : \mathcal{H} \to \mathcal{D}(E) \subset \mathcal{H}$$

is well defined for all $h > 0$ such that $hM[E] < 1$. Additionally, from [6, Propositions 3.2] we get that, for these h, the resolvent is Lipschitz continuous

$$L\big[(I - hE)^{-1}\big] \leq \frac{1}{1 - hM[E]}. \tag{3.4}$$

We now connect the concept of maximal dissipativity to the evolution equation of interest (3.1) by stating the central assumption of the presented research.

Assumption 1. *The operator $A+F\colon \mathcal{D}(A+F)\subset\mathcal{H}\to\mathcal{H}$ of* (3.1) *is maximal dissipative on $\mathcal{H}$.*

With this assumption in place we can finally guarantee the existence of a unique solution to the evolution equation (3.1). However, this solution is not necessarily classical, i.e., we can not assure that u is differentiable. Instead, we need to consider a more general type of solution, referred to as a mild solution. This is defined through the implicit Euler discretization of (3.1). More precisely, by the limit

$$\mathrm{e}^{t(A+F)}\eta := \lim_{n\to\infty} \big(I - \tfrac{t}{n}(A+F)\big)^{-n}\eta,$$

which exists for all $t \geq 0$ and $\eta \in \mathcal{D} := \overline{\mathcal{D}(A+F)}$, the closure of $\mathcal{D}(A+F)$, see [6, Theorem 4.3 and Proposition 4.2]. On this closure the flow forms a continuous semigroup of contractions $\{\mathrm{e}^{t(A+F)}\}_{t\geq 0}$. That is, the nonlinear operators $\mathrm{e}^{t(A+F)} : \mathcal{D} \to \mathcal{D}$ of the semigroup fulfil the properties:

- $\mathrm{e}^{(t+s)(A+F)}\eta = \mathrm{e}^{t(A+F)}\mathrm{e}^{s(A+F)}\eta$ for all $t, s \geq 0$ and $\eta \in \mathcal{D}$.
- $\mathrm{e}^{t(A+F)}\eta = \eta$ for all $\eta \in \mathcal{D}$ when $t = 0$.
- For every $\eta \in \mathcal{D}$ the function $t \mapsto \mathrm{e}^{t(A+F)}\eta$ is continuous on $[0, \infty)$.
- For every $t \geq 0$ the following Lipschitz bound holds:

$$\left\|\mathrm{e}^{t(A+F)}\eta - \mathrm{e}^{t(A+F)}\zeta\right\| \leq \mathrm{e}^{tM[A+F]}\left\|\eta - \zeta\right\|, \tag{3.5}$$

  for all $\eta, \zeta \in \mathcal{D}$.

This semigroup defines the unique mild solution

$$u(t) := \mathrm{e}^{t(A+F)}\eta, \tag{3.6}$$

of the evolution equation (3.1). Every classical solution is also a mild solution. However, generally, the mild solution u is continuous, but not necessarily differentiable. We refer to [6, Sections 3.1 and 4.1] for more on nonlinear maximal dissipative operators, the solution of (3.1), and semigroups in more general Banach settings.

Linear maximal dissipative operators A yield semigroups $\{e^{tA}\}_{t\geq 0}$ with further properties. In this setting, for any $\eta \in \mathcal{D}(A)$, the mild solution $u(t) = \mathrm{e}^{tA}\eta$ is a classical solution, i.e. u is continuously differentiable with respect to $\mathcal{H}$ and $u(t) \in \mathcal{D}(A)$ for all $t \geq 0$. The derivative is given by

$$\dot{u}(t) = \frac{\mathrm{d}}{\mathrm{d}t}\mathrm{e}^{tA}\eta = A\mathrm{e}^{tA}\eta. \tag{3.7}$$

Furthermore, the operator A commutes with its resolvent $(I - hA)^{-1}$ and its flow e^{tA}. Finally, we mention also that a linear maximal dissipative operator has a domain $\mathcal{D}(A)$ that is dense in $\mathcal{H}$. See [24, 58, 62] for more details on the linear setting.

3.3 Temporal convergence order analysis

In this section we summarize the temporal convergence results called for by Aim 1. That is, we present optimal-order theorems for the ADI schemes and additive schemes of Chapter 2, with orders depending on the regularity of the solution u. To illustrate the proof technique we begin by showing first-order convergence for the Douglas–Rachford scheme

$$S_h = (I - hF)^{-1}(I - hA)^{-1}(I + h^2AF), \tag{3.8}$$

discretizing the semilinear problem (3.1a). Order one for this scheme has not been proven in the semilinear setting in any of the appended or cited papers; the following proof is a new result which has not previously been published. The rest of the convergence theorems presented in this section were first proven in Papers I and III (except for the $o(1)$-convergence of the ADI schemes).

In Assumption 1 we assumed that $A + F$ is maximal dissipative which guarantees the existence of a unique solution to (3.1a). However, to ensure stability of the numerical scheme we must assume that also the operators A and F are maximal dissipative. We formalize this in the following assumption where we also include the operators $A_1, \ldots, A_q$ for future reference.

Assumption 2. *The operators* $A_1 : \mathcal{D}(A_1) \subset \mathcal{H} \to \mathcal{H}$, $\ldots$, $A_q : \mathcal{D}(A_q) \subset \mathcal{H} \to \mathcal{H}$, $A : \mathcal{D}(A) \subset \mathcal{H} \to \mathcal{H}$ *and* $F : \mathcal{D}(F) \subset \mathcal{H} \to \mathcal{H}$ *are maximal dissipative on* $\mathcal{H}$. *Further, the domains fulfil the relationships* $\mathcal{D}(A) = \bigcap_{k=1}^{q} \mathcal{D}(A_k)$ *and* $\mathcal{D}(A + F) = \mathcal{D}(A) \cap \mathcal{D}(F)$.

Remark 1. When verifying the domain relationships in Assumption 2 it is actually enough to show that $\mathcal{D}(A) \subset \bigcap_{k=1}^{q} \mathcal{D}(A_k)$ and $\mathcal{D}(A + F) \subset \mathcal{D}(A) \cap \mathcal{D}(F)$. The equality of the domains then follows from the maximality of the involved operators.

To simplify the notation in the proof we introduce the abbreviations

$$a = hA, \quad \alpha = (I - a)^{-1}, \quad f = hF \quad \text{and} \quad \varphi = (I - f)^{-1}.$$

We will also frequently use the identities

$$I = \alpha - a\alpha \quad \text{and} \quad I = \varphi - f\varphi. \tag{3.9}$$

Due to the boundedness of α the first identity implies that also $a\alpha$ is a bounded operator on $\mathcal{H}$. Then, since $\mathcal{D}(A)$ is dense in $\mathcal{H}$ the operator αa can be extended to a bounded operator on all of $\mathcal{H}$ using the relationship $\alpha a = a\alpha$.

With the assumptions and notation in place the first part of the proof technique is to separate the question of convergence into a question of stability and consistency. As discussed in the introduction, proving convergence with an order requires certain regularity assumptions on the solution u. We begin by assuming that u is a classical solution. This implies that $u(t) \in \mathcal{D}(A + F) = \mathcal{D}(A) \cap \mathcal{D}(F)$ for all $t \in [0, T]$, where $T > 0$ is a finite end time. Let $t^j := jh$ and $nh \leq T$, then expand the global error using the telescopic sum

$$\begin{aligned} \|u(nh) - S_h^n \eta\| &= \Big\| \sum_{j=1}^{n} S_h^{n-j} u(t^j) - S_h^{n-j+1} u(t^{j-1}) \Big\| \\ &\leq \sum_{j=1}^{n} L[S_h^{n-j}\varphi] \left\| (I - f)u(t^j) - (I - f)S_h u(t^{j-1}) \right\|. \end{aligned} \tag{3.10}$$

To prove stability of the Douglas–Rachford scheme we first note that

$$\begin{aligned} S_h^{n-j}\varphi &= \big(\varphi\alpha(I + af)\big)^{n-j}\varphi \\ &= \varphi\big(\alpha(I + af)\varphi\big)^{n-j} \\ &= \varphi\big(\tfrac{1}{2}(I + a)\alpha(I + f)\varphi + \tfrac{1}{2}(\alpha - a\alpha)(\varphi - f\varphi)\big)^{n-j} \\ &= \varphi\big(\tfrac{1}{2}(I + a)\alpha(I + f)\varphi + \tfrac{1}{2}I\big)^{n-j}. \end{aligned} \tag{3.11}$$

Then, to bound $(I + f)\varphi$, we will use the inequality

$$\begin{aligned} \|(I + f)u - (I + f)v\|^2 &= \|u - v\|^2 + 2(fu - fv, u - v) + \|fu - fv\|^2 \\ &\leq (1 + 2hM[F]) \|u - v\|^2 + \|fu - fv\|^2 \\ &\leq (1 + 4hM[F]) \|u - v\|^2 - 2(fu - fv, u - v) + \|fu - fv\|^2 \\ &= 4hM[F] \|u - v\|^2 + \|(I - f)u - (I - f)v\|^2, \end{aligned}$$

which follows from the dissipativity of F for any $u, v \in \mathcal{D}(F)$. By replacing u and v by φz and φw, where $z, w \in \mathcal{H}$, we get

$$\begin{aligned} \|(I + f)\varphi z - (I + f)\varphi w\| &\leq (4hM[F]L[\varphi]^2 + 1)^{1/2} \|z - w\| \\ &\leq (1 + hM[F])/(1 - hM[F]) \|z - w\|, \end{aligned}$$

where we have also used the Lipschitz continuity of the resolvent (3.4). Thus, we have

$$L[(I+f)\varphi] \le (1+hM[F])/(1-hM[F]) \le \mathrm{e}^{3hM[F]},$$

where the last inequality is valid for $hM[F] \le 1/2$. The same type of Lipschitz continuity also holds for $(I+a)\alpha$. Finally, the stability of the Douglas–Rachford scheme follows by applying the derived Lipschitz constants to the identity (3.11), i.e.,

$$\begin{aligned} L[S_h^{n-j}\varphi] &\le L[\varphi]L[\tfrac{1}{2}(I+a)\alpha(I+f)\varphi + \tfrac{1}{2}I]^{n-j} \\ &\le L[\varphi]\big(\tfrac{1}{2}L[(I+a)\alpha]L[(I+f)\varphi] + \tfrac{1}{2}\big)^{n-j} \\ &\le \mathrm{e}^{hM[F]}\,\big(\tfrac{1}{2}\mathrm{e}^{3h(M[A]+M[F])} + \tfrac{1}{2}\big)^{n-j} \\ &\le \mathrm{e}^{hM[F]}\,\mathrm{e}^{3h(n-j)(M[A]+M[F])} \le \mathrm{e}^{3T(M[A]+M[F])}. \end{aligned} \tag{3.12}$$

To prove consistency we expand the local error by twice using the first of the identities (3.9), i.e.,

$$\begin{aligned} (I-f)u(t^j) - (I-f)S_h u(t^{j-1}) &= (\alpha - a\alpha - (\alpha - a\alpha)f)u(t^j) \\ &\quad - \alpha(I+af)u(t^{j-1}) \\ &= \alpha\big(u(t^j) - u(t^{j-1}) - (a+f)u(t^j)\big) \\ &\quad + a\alpha\big(fu(t^j) - fu(t^{j-1})\big). \end{aligned}$$

Then, for sufficiently regular u the quadrature error can be rewritten as

$$\alpha\big(u(t^j) - u(t^{j-1}) - (a+f)u(t^j)\big) = -h\alpha\int_{t^{j-1}}^{t^j} \frac{s-t^{j-1}}{h}\ddot{u}(s)\,\mathrm{d}s,$$

and the splitting error as

$$\begin{aligned} a\alpha\big(fu(t^j) - fu(t^{j-1})\big) &= a\alpha\big(h[\dot{u}(t^j) - \dot{u}(t^{j-1})] - a[u(t^j) - u(t^{j-1})]\big) \\ &= ha\alpha\Big(\int_{t^{j-1}}^{t^j}\ddot{u}(s)\,\mathrm{d}s - \int_{t^{j-1}}^{t^j} A\dot{u}(s)\,\mathrm{d}s\Big). \end{aligned}$$

Here the operator A has been interchanged with integrations which is possible since A is closed as a consequence of being maximal dissipative. Now, also observing that $L[\alpha] \le 2$ and $L[a\alpha] \le L[\alpha] + L[I] \le 3$ when $hM[A] \le 1/2$, we arrive at the following local error bound

$$\big\|(I-f)u(t^j) - (I-f)S_h u(t^{j-1})\big\| \le 5h\int_{t^{j-1}}^{t^j}\sum_{i=0}^{1}\big\|A^{1-i}u^{(i+1)}(s)\big\|\,\mathrm{d}s,$$

where $u^{(i+1)}$ denotes the time derivative of order $i+1$ of the solution u. Combining with the stability estimate (3.12) in the telescopic sum (3.10) gives the following convergence theorem where we have also included the Peaceman–Rachford scheme

$$S_h = \big(I - \tfrac{h}{2}F\big)^{-1}\big(I + \tfrac{h}{2}A\big)\big(I - \tfrac{h}{2}A\big)^{-1}\big(I + \tfrac{h}{2}F\big). \tag{3.13}$$

Theorem 1. *Consider the approximate solution $S_h^n\eta$ given by the Douglas–Rachford* (3.8) *or the Peaceman–Rachford* (3.13) *discretization of the evolution equation* (3.1a)*. If the operators A, F and $A+F$ fulfil Assumptions 1 and 2, $h\max\{M[A], M[F]\} < 1/2$ and u is a classical solution which is regular enough, then the global error can be bounded as*

$$\|u(nh) - S_h^n\eta\| \le 5h^p \mathrm{e}^{3T(M[A]+M[F])} \sum_{i=0}^{p} \big\|A^{p-i}u^{(i+1)}\big\|_{L^1(0,T;\mathcal{H})}, \quad nh \le T,$$

with first-order convergence, $p=1$, for both schemes or second-order convergence, $p=2$, for the Peaceman–Rachford scheme, depending on the regularity of the solution.

As can be seen from the above Douglas–Rachford proof the regularity assumption on u exactly translates to the possibility of bounding the terms in the global error estimate. For example, to get first order in the theorem we require that $A\dot{u}, \ddot{u} \in L^1(0,T;\mathcal{H})$. The first- and second-order convergence of the Peaceman–Rachford scheme is provided by Theorem 2 of Paper I.

Consider now the semilinear evolution equation (3.1b) where A has been further split into the operators A_k. Moreover, recall the two additive splitting schemes defined in Section 2.4:

$$S_h = (I - hF)^{-1}\Big(\frac{1}{q}\sum_{k=1}^{q}(I - hqA_k)^{-1}\Big) \quad \text{and} \tag{3.14}$$

$$S_h = \Big(\frac{1}{q}\sum_{k=1}^{q}(I - hqA_k)^{-1}\Big)(I + hF). \tag{3.15}$$

We here reproduce Theorem 3.9 of Paper III providing first-order convergence for these schemes. To this end, let $M := \max\{M[A_1], \dots, M[A_q]\}$.

Theorem 2. *Consider the approximate solution $S_h^n\eta$ given by applying one of the additive splitting schemes* (3.14) *or* (3.15) *to the evolution equation* (3.1b)*. Assume that Assumptions 1 and 2 are valid, that $hqM < 1/2$ and that u is a classical solution which is regular enough. Then, if $hM[F] \le 1/2$, the scheme* (3.14) *is first-order convergent with global error bounded as*

$$\|u(nh) - S_h^n\eta\| \le$$
$$2h\mathrm{e}^{2T(qM+M[F])}\Big(\sum_{i=0}^{1}\big\|A^{1-i}u^{(i+1)}\big\|_{L^1(0,T;\mathcal{H})} + 2qT\sum_{k=1}^{q}\big\|A_k^2 u\big\|_{C([0,T];\mathcal{H})}\Big),$$

where $nh \leq T$. *If* F *is Lipschitz continuous, the scheme* (3.15) *is first-order convergent with global error bounded as*

$$\|u(nh) - S_h^n \eta\| \leq$$
$$h \mathrm{e}^{T(2qM+L[F])} \Big(\big\|\ddot{u}\big\|_{L^1(0,T;\mathcal{H})} + 2T \sum_{k=1}^{q} \big\|A_k F u + q A_k^2 u\big\|_{C([0,T];\mathcal{H})} \Big),$$

where $nh \leq T$.

By comparing the above theorems we observe the favourable error structure of the ADI schemes. For first-order convergence the structures are similar comparing Theorem 1 with Theorem 2 except that the latter also includes the terms $A_k^2 u$. Furthermore, in the theorems it is clear how the order of convergence is affected by the regularity of the solution u. In particular, note how it determines if we get first or second order for the Peaceman–Rachford scheme. Recall that performing such a convergence study is part of the first theme of the thesis. To complete the temporal analysis called for by Aim 1 it remains to prove $o(1)$-convergence to the mild solution (3.6), i.e., in the absence of the regularity required above.

For the ADI schemes $o(1)$-convergence was already proven in [49, Theorem 2] for nonlinear operators with $M[A] = M[F] = 0$. However, our proof in the semilinear setting is significantly shorter. The following theorem extends Theorem 3 of Paper I to include also the Douglas–Rachford scheme.

Theorem 3. *Consider the approximate solution* $S_{t/n}^n \eta$ *given by the Douglas–Rachford* (3.8) *or the Peaceman–Rachford* (3.13) *discretization of the evolution equation* (3.1a). *If the operators* A, F *and* $A + F$ *fulfil Assumptions 1 and 2 and* $\mathcal{D}(A) \cap \mathcal{D}(F)$ *is dense in* $\mathcal{H}$, *then both schemes are convergent, i.e.,*

$$\lim_{n\to\infty} \big\|u(t) - S_{t/n}^n \eta\big\| = 0,$$

for every $\eta \in \mathcal{D}(F)$ *and* $t \geq 0$.

Only details differ in the proof for the Douglas–Rachford scheme.[1] Note that we need $\eta \in \mathcal{D}(F)$ for the ADI schemes, the additive scheme (3.14), on the other hand, does not need such a regularity requirement on the initial data to converge.

Theorem 4. *Consider the approximate solution* $S_{t/n}^n \eta$ *given by applying one of the additive schemes* (3.14) *or* (3.15) *to the evolution equation* (3.1b). *Assume that Assumptions 1 and 2 are valid. Then, if* $\mathcal{D}(A) \cap \mathcal{D}(F)$ *is dense in* $\mathcal{H}$ *the scheme* (3.14) *is convergent, i.e.,*

$$\lim_{n\to\infty} \big\|u(t) - S_{t/n}^n \eta\big\| = 0,$$

[1] The operator R found in the proof of Theorem 3 in Paper I is for the Douglas–Rachford scheme given by

$$R = I + a\alpha + f\varphi + 2(\alpha - I)(f\varphi - f) + 2(\alpha - I)f.$$

for every $\eta \in \mathcal{H}$ *and* $t \geq 0$. *Furthermore, if* F *is also Lipschitz continuous and* $\mathcal{D}(F) = \mathcal{H}$, *the scheme* (3.15) *is convergent.*

Remark 2. Note that convergence, with order one or without order, for the full Lie scheme

$$S_h = (I - hF)^{-1}(I - hA)^{-1} \tag{3.16}$$

and the IMEX Euler scheme (2.8) follows from Theorems 2 and 4 by letting $q = 1$ (which implies $A = A_1$). For a convergence analysis of the additive scheme (2.15) we refer to Theorem 3.12 of Paper III. There, second-order convergence is proven when the scheme is applied to linear equations (2.2) with a vector field consisting of arbitrarily many operators.

Example 3. Consider the FitzHugh–Nagumo equations (1.1) defined on a bounded domain $\Omega \subset \mathbb{R}^d$, $d = 1, 2$ or 3. In Example 2 we saw that Assumption 1 is fulfilled for regular domains Ω and homogeneous Dirichlet boundary conditions. Following the same proofs as cited in that example we get that also the operators A and F defined by the physical splitting (1.2) are maximal dissipative on $\mathcal{H} = (L^2(\Omega))^2$ with $M[A] = 0$, $M[F] \leq 1 + |1 - a|/2$,

$$\mathcal{D}(A) = \left(H^2(\Omega) \cap H_0^1(\Omega)\right)^2 \quad \text{and} \quad \mathcal{D}(F) = L^6(\Omega) \times L^2(\Omega).$$

Due to the Sobolev imbedding theorem [1, Theorem 4.12.1.A] the inclusion $\mathcal{D}(A) \subset \mathcal{D}(F)$ holds and therefore $\mathcal{D}(A) \cap \mathcal{D}(F) = \mathcal{D}(A) = \mathcal{D}(A + F)$. Thus, the operators A and F fulfil Assumption 2.

Furthermore, $\mathcal{D}(A) = \mathcal{D}(A) \cap \mathcal{D}(F)$ is dense in $\mathcal{H}$ as a consequence of A being linear and maximal dissipative. Thus, when discretizing the FitzHugh–Nagumo equations, the ADI schemes (3.8) and (3.13) converge for any $\eta \in \mathcal{D}(F)$ and the full Lie splitting scheme (3.16) even for $\eta \in \mathcal{H}$. Similar conclusions can be drawn under Neumann or periodic boundary conditions. Regularity results for the solution of FitzHugh–Nagumo-type equations can be found in e.g. [40].

Remark 3. The theorems in this section clearly hold also in the linear setting of (2.2). For the additive scheme (2.14) we note that Theorems 2 and 4 can be directly used after just letting $F = 0$. However, to use Theorems 1 and 3 in the linear setting, i.e. for the ADI schemes on the forms (2.11) and (2.12), we must substitute A by A_1 and F by A_2 in these theorems and in Assumptions 1 and 2.

3.3.1 Numerical experiments – temporal convergence orders

We verify the above theorems by performing numerical convergence experiments. To this end we return to our prototypical semilinear parabolic problem, the FitzHugh–Nagumo equations. As usual we split (1.1) into two components according to (1.2). To this physical splitting we apply the Douglas–Rachford (3.8), Peaceman–Rachford (3.13) and

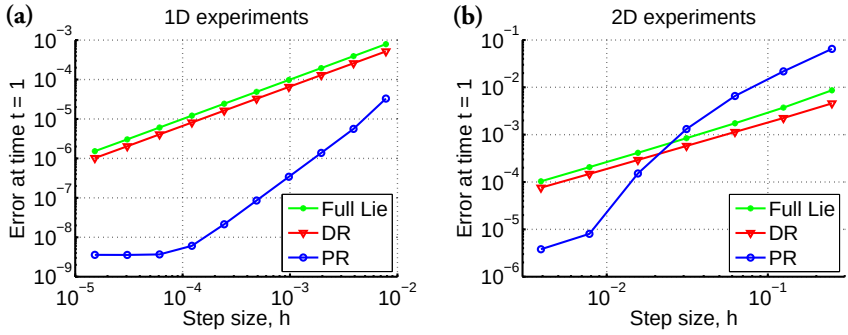


Figure 3.1: Temporal convergence order experiments verifying the theorems of Section 3.3. The FitzHugh–Nagumo equations (1.1), (1.2) *are integrated by the Douglas–Rachford* (3.8), *Peaceman–Rachford* (3.13) *and full Lie* (3.16) *schemes. The predicted convergence orders can be observed both in the 1D experiments (a) and in the 2D experiments (b). For the Peaceman–Rachford scheme the spatial error dominates for the smallest time steps.*

full Lie (3.16) schemes. Note that since we here only consider the physical splitting (3.1a) given by (1.2) the full Lie scheme is the same as the additive scheme (3.14) and thus we can expect first-order convergence due to Theorem 2, see also Remark 2.

We perform the convergence-order experiments in one and two space dimensions. The diffusion coefficients $D_1 = 0.02$ and $D_2 = 0.0016$ are chosen large to facilitate computations in the stiff regime. The same values as for Figure 1.1 are used for the remaining parameters $a = 0.08$ and $b = 0.064$. Similarly, in 2D, the same four "humps" are used as initial data η_1 on $\Omega = (0,1)^2$, however, here with $\eta_2 := \eta_1$. In 1D, we let η_1 and η_2 be given as the sum of two "humps" on $\Omega = (0,1)$ with radius $\epsilon = 0.05$ and centres at $y = 0.4$ and $y = 0.6$.

For the spatial discretization in 1D we use a uniform mesh with a fine grid size $\Delta x = 2^{-15}$. On this mesh standard continuous, piecewise linear finite elements are defined and the trapezoidal quadrature rule is used for the construction of the mass and stiffness matrices. (For the mass matrix this is equivalent to mass lumping.) Similarly, in 2D piecewise bilinear elements are used on a square mesh with element width $\Delta x = 2^{-9}$. Reference solutions are found by using the Peaceman–Rachford scheme and the same spatial discretizations with finer parameters: $\Delta x = 2^{-16}$ and $h = 2^{-20}$ in 1D and $\Delta x = h = 2^{-10}$ in 2D.

In Figure 3.1 the errors in $(L^2(\Omega))^2$-norm are plotted at time $t = 1$ for different time step sizes. The convergence orders predicted by Examples 2 and 3 and Theorems 1 and 2 can be observed. In 1D the slope of the Peaceman–Rachford curve is two almost throughout the entire range of step sizes. However, in 2D we see a steeper slope which reflects a property of the scheme often observed. Commonly, we see large errors for

the Peaceman–Rachford method when large time steps are used. When decreasing the step size, these errors quickly vanish, explaining the steep slope in Figure 3.1b. Then the second-order convergence can usually be observed. Here, however, the spatial error dominates before that. It is not possible to compute a reference solution with a finer Δx in 2D within reasonable time on a standard desktop computer. Instead we refer to the previously discussed 1D experiments for the correct slope in the stiff regime and before the spatial error dominates.

3.4 Full space–time convergence order analysis

We now limit our attention to the linear evolution equation

$$\dot{u} = Au = \sum_{k=1}^{q} A_k u, \quad u(0) = \eta, \tag{3.17}$$

which is assumed to represent a PDE. In this setting we demonstrate a proof technique for showing simultaneous space–time convergence orders. The idea is to use temporal convergence theorems of the type found in the previous section in conjunction with spatial convergence results.

For the demonstration of the proof technique we will employ the additive splitting scheme (2.14) as an example of a temporal discretization. Simultaneous space–time convergence orders is a new result for this scheme which can not be found in the appended papers. For the ADI schemes simultaneous orders were first proven in Paper II. The analysis is performed on finite-dimensional spaces given by the spatial semi-discretization. Therefore, no dissipativity assumptions are needed from the operators $A_1, \ldots, A_q$, instead we assume these properties from the corresponding discrete operators. The only assumption we will require from the continuous problem (3.17) is that A is maximal dissipative.

Thus, the first step is to apply a space discretization to (3.17). We do not specify a particular discretization, instead we will assume certain properties of it. In contrast to the previous section we do not list these in assumptions. To simplify the presentation we instead focus on the central concepts of the proof technique and mention the requirements when needed. For the details we refer to Paper II.

Let $\{\mathcal{H}_{\Delta x}\}_{0<\Delta x\leq\Delta x_{\max}}$ be a family of finite-dimensional spaces of increasing dimension as Δx tends to zero. Equip each of them with an inner product $(\cdot,\cdot)_{\Delta x}$ depending on the parameter Δx, which typically denotes a mesh width. Additionally, define the discrete operators $A_{1,\Delta x} : \mathcal{H}_{\Delta x} \to \mathcal{H}_{\Delta x}, \ldots, A_{q,\Delta x} : \mathcal{H}_{\Delta x} \to \mathcal{H}_{\Delta x}$ and $A_{\Delta x} : \mathcal{H}_{\Delta x} \to \mathcal{H}_{\Delta x}$. The spatial semi-discretization is then given by the finite-dimensional evolution equation

$$\dot{u}_{\Delta x} = A_{\Delta x} u_{\Delta x} = \sum_{k=1}^{q} A_{k,\Delta x} u_{\Delta x}, \quad u_{\Delta x}(0) = \eta_{\Delta x}, \tag{3.18}$$

where $\eta_{\Delta x} \in \mathcal{H}_{\Delta x}$ is an approximation of η.

To get a full discretization we apply a temporal method, e.g. a splitting scheme, to (3.18). Denote the numerical flow by $S_{h,\Delta x}$, i.e., this operator defines the time step of the full discretization. The central idea of the proof technique is to split the global error into three parts:

$$\begin{aligned}\left\|\mathrm{e}^{nhA}\eta - S_{h,\Delta x}^n \eta_h\right\| \leq{}& \left\|\mathrm{e}^{nhA}\eta - \mathrm{e}^{nhA_{\Delta x}} Z_{\Delta x}\eta\right\| && \text{(spatial error)}\\ &+ \left\|\mathrm{e}^{nhA_{\Delta x}} Z_{\Delta x}\eta - S_{h,\Delta x}^n Z_{\Delta x}\eta\right\| && \text{(temporal error)}\\ &+ \left\|S_{h,\Delta x}^n (Z_{\Delta x}\eta - \eta_{\Delta x})\right\|. && \text{(initial value error)}\end{aligned} \tag{3.19}$$

Recall that $u(nh) = \mathrm{e}^{nhA}\eta$ denotes the exact solution of (3.17). Similarly $\mathrm{e}^{nhA_{\Delta x}} Z_{\Delta x}\eta$ denotes the exact solution of (3.18) with initial condition $u_{\Delta x}(0) = Z_{\Delta x}\eta$, cf. Section 3.2. The operator

$$Z_{\Delta x} = A_{\Delta x}^{-(p+1)} P_{\Delta x} A^{p+1} : \mathcal{D}(A^{p+r+1}) \subset \mathcal{H} \to \mathcal{H}_{\Delta x}$$

introduced here enables interpretation of the regularity of η in the discrete setting. The integer p is the order of the temporal method and the operator $P_{\Delta x} : \mathcal{D}(A^r) \subset \mathcal{H} \to \mathcal{H}_{\Delta x}$ is similar to a projection from $\mathcal{H}$ to $\mathcal{H}_{\Delta x}$. If $P_{\Delta x}$ is indeed the orthogonal projection of $\mathcal{H}$ onto $\mathcal{H}_{\Delta x}$ we have $r = 0$. However, for greater flexibility in the choice of $P_{\Delta x}$ we allow r to be a positive integer.

To bound the spatial error of (3.19) we assume that the spatial method converges with order $s > 0$ when discretizing the stationary problem $Au = f$. That is, assume that

$$\left\|A^{-1}f - A_{\Delta x}^{-1} P_{\Delta x} f\right\| \leq C(\Delta x)^s \sum_{i=0}^{r} \left\|A^i f\right\|, \quad \text{for all } f \in \mathcal{D}(A^r). \tag{3.20}$$

In this section we use C as a generic constant taking different values at different occurrences, however it is always independent of Δx, h and n. Under the assumption that A and $A_{\Delta x}$ are maximal dissipative the above bound can then be transferred to the dynamical setting of (3.19) by using the linear semigroup theory. From Lemma 2.1 of Paper II we get

$$\left\|\mathrm{e}^{nhA}\eta - \mathrm{e}^{nhA_{\Delta x}} Z_{\Delta x}\eta\right\| \leq C\Big(\left\|Z_{\Delta x}\eta - \eta\right\| + (\Delta x)^s \sum_{i=1}^{r+2} \left\|A^i \eta\right\|\Big). \tag{3.21}$$

A bound with order s for the first term will be given further down.

Remark 4. It is implicitly assumed in (3.20) that A and $A_{\Delta x}$ are invertible. For the latter we will also need that it has a uniformly bounded inverse. These assumptions are made for the sake of simplicity. However, the theory holds also when A and $A_{\Delta x}$ are not invertible by introducing minor modifications which use the maximal dissipativity of the operators.

Example 4. Consider a conforming finite element discretization of an elliptic equation $Au = f$ on $\mathcal{H} = L^2(\Omega)$. Let the classical assumptions about the regularity of the domain, the mesh and the elliptic problem be valid, see [11, Chapter 3]. Further, assume that the basis functions are piecewise linear. Then, Δx denotes the mesh size and we have $(\cdot,\cdot)_{\Delta x} = (\cdot,\cdot)_{L^2(\Omega)}$. The operator $P_{\Delta x}$ is the orthogonal projection onto the finite element space and thus $r = 0$. The bound (3.20) is then the Aubin–Nitsche estimate [11, Theorem 3.2.5] of the finite element error which holds with $s = 2$.

Consider the second part of the error separation (3.19), which represents the temporal error given when applying a time discretization to the finite-dimensional evolution equation (3.18) equipped with the initial condition $u_{\Delta x}(0) = Z_{\Delta x}\eta$. To bound the temporal error we need a convergence theorem of the type given in the previous section. To exemplify how such a theorem is used in the presented proof technique we now assume that (3.18) is discretized by the additive scheme (2.14). This gives $p = 1$ and the full discretization

$$S_{h,\Delta x} = \frac{1}{q}\sum_{k=1}^{q}(I - hqA_{k,\Delta x})^{-1}. \tag{3.22}$$

Since the temporal discretization is only considered on the finite-dimensional spaces $\mathcal{H}_{\Delta x}$ Assumptions 1 and 2 must be fulfilled by the discrete operators (only). That is, to be able to use Theorem 2 we assume that the operators $A_{1,\Delta x},\dots,A_{q,\Delta x}$ are dissipative (for simplicity with $M[A_{1,\Delta x}] = \cdots = M[A_{q,\Delta x}] = 0$). As $\mathcal{H}_{\Delta x}$ is finite dimensional it follows from the dissipativity of the considered operators that they are also maximal. Actually, the already assumed maximal dissipativity of $A_{\Delta x}$ also follows.

With Assumptions 1 and 2 in place it remains to show that the solution fulfils the regularity requirements in Theorem 2. In the current linear, finite-dimensional setting all of the involved operators are bounded. Thus, as we shall see below, the required regularity follows from the smoothness of the initial data. However, to not lose order we must show bounds which are uniform in Δx.

We begin by noting that $\mathrm{e}^{tA_{\Delta x}}Z_{\Delta x}\eta$, where $t = nh$, is a classical solution, as $A_{\Delta x}$ is linear and $Z_{\Delta x}\eta \in \mathcal{H}_{\Delta x} = \mathcal{D}(A_{\Delta x})$, cf. Section 3.2. In the current fully discrete setting the error expansion in Theorem 2 (with $F = 0$ and $M = 0$) reads as

$$\begin{aligned}\big\|\mathrm{e}^{tA_{\Delta x}}Z_{\Delta x}\eta - S_{h,\Delta x}^n Z_{\Delta x}\eta\big\| &\le C\big\|\mathrm{e}^{tA_{\Delta x}}Z_{\Delta x}\eta - S_{h,\Delta x}^n Z_{\Delta x}\eta\big\|_{\Delta x}\\ &\le Ch\Big(\big\|\frac{\mathrm{d}^2}{\mathrm{d}t^2}\mathrm{e}^{tA_{\Delta x}}Z_{\Delta x}\eta\big\|_{L^1(0,T;\mathcal{H}_{\Delta x})}\\ &\quad + 2qT\sum_{k=1}^{q}\big\|A_{k,\Delta x}^2\mathrm{e}^{tA_{\Delta x}}Z_{\Delta x}\eta\big\|_{C([0,T];\mathcal{H}_{\Delta x})}\Big),\end{aligned} \tag{3.23}$$

where we, for the first inequality, have assumed that the norms $\|\cdot\|$ and $\|\cdot\|_{\Delta x}$ are uniformly equivalent on $\mathcal{H}_{\Delta x}$. Consider, e.g., one of the terms in the above sum. By using

that the semigroup is non-expansive (3.5) and that the operators $A_{\Delta x}$ and $\mathrm{e}^{tA_{\Delta x}}$ commute, we get the bound

$$\begin{aligned}\left\|A_{k,\Delta x}^2 \mathrm{e}^{tA_{\Delta x}} Z_{\Delta x}\eta\right\|_{C([0,T];\mathcal{H}_{\Delta x})} &= \sup_{t\in[0,T]} \left\|A_{k,\Delta x}^2 \mathrm{e}^{tA_{\Delta x}} Z_{\Delta x}\eta\right\|_{\Delta x} \\ &\leq \left\|A_{k,\Delta x}^2 A_{\Delta x}^{-2}\right\|_{\Delta x} \sup_{t\in[0,T]} \left\|\mathrm{e}^{tA_{\Delta x}}\right\|_{\Delta x} \left\|A_{\Delta x}^2 Z_{\Delta x}\eta\right\|_{\Delta x} \\ &\leq \left\|A_{k,\Delta x}^2 A_{\Delta x}^{-2}\right\|_{\Delta x} \left\|A_{\Delta x}^2 Z_{\Delta x}\eta\right\|_{\Delta x}.\end{aligned}$$

Since all involved operators are finite dimensional the norms in the right-hand side are bounded and the required regularity follows from that of the initial data. We may reach the same conclusion for the first term of the right-hand side in (3.23) by also using the derivative characterisation (3.7). It remains, however, to show that the norms are bounded uniformly in Δx.

To summarize, for the additive scheme (3.22) the temporal error in (3.19) can now be bounded as

$$\left\|\mathrm{e}^{tA_{\Delta x}} Z_{\Delta x}\eta - S_{h,\Delta x}^n Z_{\Delta x}\eta\right\| \leq Ch \sum_{k=1}^{q} \left\|A_{k,\Delta x}^2 A_{\Delta x}^{-2}\right\|_{\Delta x} \left\|A_{\Delta x}^2 Z_{\Delta x}\eta\right\|_{\Delta x}.$$

The uniform bound, in Δx, of $\|A_{k,\Delta x}^2 A_{\Delta x}^{-2}\|_{\Delta x}$ needs to be stated as an assumption. However, for $\|A_{\Delta x}^2 Z_{\Delta x}\eta\|_{\Delta x}$ such a bound is given by the regularity of the initial data according to

$$\left\|A_{\Delta x}^2 Z_{\Delta x}\eta\right\|_{\Delta x} = \left\|P_{\Delta x} A^2 \eta\right\|_{\Delta x} \leq C\left\|P_{\Delta x} A^2 \eta\right\| \leq C \sum_{i=0}^{r} \left\|A^{2+i}\eta\right\|.$$

The last inequality follows from an assumed (uniform) approximation property of the operator $P_{\Delta x}$. For example, if $P_{\Delta x}$ is the orthogonal projection, as in Example 4, the inequality follows directly with $r = 0$.

Finally, we consider the initial value error in (3.19). By using the stability of the temporal scheme and the equivalence of the norms we get

$$\left\|S_{h,\Delta x}^n (Z_{\Delta x}\eta - \eta_{\Delta x})\right\| \leq C\left\|Z_{\Delta x}\eta - \eta_{\Delta x}\right\| \leq C\big(\left\|Z_{\Delta x}\eta - \eta\right\| + \left\|\eta - \eta_{\Delta x}\right\|\big),$$

where the latter term can be bounded with order s for appropriately chosen approximations $\eta_{\Delta x}$ of the initial data η. The first term, also found in (3.21), can be bounded

according to

$$\begin{aligned}\|Z_{\Delta x}\eta - \eta\| &\leq \|A_{\Delta x}^{-2}P_{\Delta x}A^2\eta - A_{\Delta x}^{-1}P_{\Delta x}A\eta\| + \|A_{\Delta x}^{-1}P_{\Delta x}A\eta - \eta\| \\ &\leq C\|A_{\Delta x}^{-1}P_{\Delta x}A^2\eta - P_{\Delta x}A\eta\| + \|A_{\Delta x}^{-1}P_{\Delta x}A\eta - \eta\| \\ &\leq C\Big(\|(A_{\Delta x}^{-1}P_{\Delta x} - A^{-1})A^2\eta\| + \|A\eta - P_{\Delta x}A\eta\|\Big) \\ &+ \|(A_{\Delta x}^{-1}P_{\Delta x} - A^{-1})A\eta\| \\ &\leq C(\Delta x)^s \sum_{i=0}^{r+1} \|A^{i+1}\eta\|,\end{aligned}$$

where we have used the uniform bound of $A_{\Delta x}^{-1}$, the spatial convergence (3.20) and the uniform approximation property of $P_{\Delta x}$. With all the parts in the error (3.19) bounded with an order the proof is complete.

Simultaneous space–time convergence orders for the ADI schemes follow in exactly the same way as for the additive scheme. Therefore, we also include these schemes in the following theorem, the proof was derived in Paper II. To this end, consider the spatial semi-discretization (3.18) with $q = 2$. Then, to get a full discretization apply to this either the Peaceman–Rachford scheme

$$S_{h,\Delta x} = \big(I - \tfrac{h}{2}A_{2,\Delta x}\big)^{-1}\big(I + \tfrac{h}{2}A_{1,\Delta x}\big)\big(I - \tfrac{h}{2}A_{1,\Delta x}\big)^{-1}\big(I + \tfrac{h}{2}A_{2,\Delta x}\big), \quad (3.24)$$

or the Douglas–Rachford scheme

$$S_{h,\Delta x} = (I - hA_{2,\Delta x})^{-1}(I - hA_{1,\Delta x})^{-1}(I + h^2A_{1,\Delta x}A_{2,\Delta x}). \quad (3.25)$$

Theorem 5. *Let the numerical flow $S_{h,\Delta x}$ be defined by either the additive scheme* (3.22)*, the Peaceman–Rachford scheme* (3.24) *or the Douglas–Rachford scheme* (3.25)*. Assume that A is maximal dissipative and invertible. Then, if the spatial semi-discretization* (3.18) *fulfils Assumptions 2 and 3 of Paper II*[2] *and $\eta \in \mathcal{D}(A^{p+r+1})$, we have the simultaneous space–time global error bound*

$$\|u(nh) - S_{h,\Delta x}^n\eta_{\Delta x}\| \leq C\big((\Delta x)^s + h^p\big) \sum_{i=1}^{p+r+1} \|A^i\eta\|,$$

with first-order convergence in time, $p = 1$, for all schemes or second-order convergence, $p = 2$, for the Peaceman–Rachford scheme. The approximate initial data $\eta_{\Delta x}$ is assumed to be the Ritz projection $\eta_{\Delta x} = A_{\Delta x}^{-1}P_{\Delta x}A\eta$ of η. The constant C can be chosen uniformly on bounded time intervals and, in particular, independently of Δx, h and n.

[2]For the additive scheme Assumption 2.3 of Paper II needs to hold for all operators $A_{k,\Delta x}$. Further, for this scheme, Assumption 3 requires uniform bounds in $\|\cdot\|_{\Delta x}$-norm on all operators $A_{k,\Delta x}^2A_{\Delta x}^{-2}$.

Chapter 4

Spatial splittings

We will here apply the convergence results of the previous chapter to the spatial splittings introduced in Section 2.6. Thus, again consider the linear diffusion–advection–reaction model problem

$$\dot{u} = Au = \nabla \cdot (\lambda \nabla u) - \rho \cdot \nabla u - \sigma u, \quad u(0) = \eta, \tag{4.1}$$

on a bounded domain $\Omega \subset \mathbb{R}^d$. In this chapter we will summarize results showing that when splitting this problem by dimension splittings or domain decomposition splittings (DDOSs) we get dissipative evolution equations on the form

$$\dot{u} = Au = \sum_{k=1}^{q} A_k u, \quad u(0) = \eta. \tag{4.2}$$

That is, the operators A and A_k fulfil Assumptions 1 and 2 of Chapter 3. Thus, we will conclude from the theorems of Section 3.3 that when either of the Peaceman–Rachford

$$S_h = \big(I - \tfrac{h}{2}A_2\big)^{-1}\big(I + \tfrac{h}{2}A_1\big)\big(I - \tfrac{h}{2}A_1\big)^{-1}\big(I + \tfrac{h}{2}A_2\big), \tag{4.3}$$

the Douglas–Rachford

$$S_h = (I - hA_2)^{-1}(I - hA_1)^{-1}(I + h^2 A_1 A_2), \tag{4.4}$$

or the additive scheme

$$S_h = \frac{1}{q}\sum_{k=1}^{q}(I - hqA_k)^{-1}, \tag{4.5}$$

integrates spatial splittings it converges, possibly with an order.

Details of what is assumed of the domain Ω, the boundary condition and the equation coefficients λ, ρ and σ are given in the upcoming sections. In Section 4.1 the domain

decomposition splittings are considered. We exemplify how the weight functions χ_k can be constructed and specify which requirements they must fulfil. When interpreting the temporal convergence theorems of Section 3.3 we use the theory of linear semigroups to simplify the regularity requirements on u. We also analyse combined domain decomposition and physical splittings using the semilinear FitzHugh–Nagumo equations as an example problem. Dimension splittings are finally considered in Section 4.2 where we focus on simultaneous space–time analysis by applying the results of Section 3.4.

4.1 Domain decomposition splittings (DDOSs)

In contrast to what have previously been done in the literature we here formulate DDOSs and analyse splitting schemes applied to them without first introducing a space discretization.

4.1.1 Constructing DDOSs

To explain the DDOS technique we consider the prototypical parabolic problem (4.1) where the bounded and open Lipschitz domain $\Omega \subset \mathbb{R}^d$ is either convex or has a boundary in C^2. The positive integer d denotes an arbitrary dimension. The elements of the $d \times d$ diffusion matrix λ are assumed to be differentiable, $\lambda_{i,j} \in C^1(\overline{\Omega})$ for $i, j = 1, \ldots, d$, and to fulfil the uniform ellipticity condition

$$\sum_{i,j=1}^{d} \lambda_{i,j}(x)\xi_i\xi_j \geq \lambda_0|\xi|^2, \quad \text{for all } x \in \Omega \text{ and } \xi \in \mathbb{R}^d,$$

where $|\cdot|$ denotes the Euclidean norm in $\mathbb{R}^d$ and λ_0 is a positive constant. Further assume that the advection and reaction coefficients are (essentially) bounded, $\rho_i, \sigma \in L^\infty(\Omega)$ for $i = 1, \ldots, d$. Finally, equip the problem with homogeneous Dirichlet or Neumann boundary conditions.

The formulation of a DDOS involves three steps to be performed in sequence:

1. Construct an overlapping domain decomposition of open subdomains Ω_k such that $\Omega = \bigcup_{k=1}^{d} \Omega_k$.
2. Define the weight functions χ_k subordinate to the decomposition.
3. Insert the weight functions in the parabolic problem (4.1) to get the operators

$$A_k u = \nabla \cdot (\chi_k \lambda \nabla u) - \chi_k \rho \cdot \nabla u - \chi_k \sigma u. \tag{4.6}$$

Then a splitting scheme, (4.3), (4.4) or (4.5), is applied to achieve the temporal semi-discretization based on domain decompositions.

An overlapping domain decomposition may for example be constructed by starting with a non-overlapping decomposition and expanding each subdomain as is done in [5, Section 3.2] and [52, Section 4.1]. An example is given in Figure 1.2 where a decomposition into four subdomains is depicted. Coupled with each subdomain Ω_k we define a continuous weight function χ_k. Each such function is an indicator of its corresponding subdomain in the sense that it vanishes outside of it. To be precise we assume that $\{\chi_k\}_{k=1}^q$ is a partition of unity that fulfils

$$\chi_k \in W^{1,\infty}(\Omega), \quad 0 \leq \chi_k \leq 1, \quad \sum_{k=1}^{q} \chi_k = 1 \quad \text{and} \quad \operatorname{supp}(\chi_k) \subset \overline{\Omega}_k, \tag{4.7}$$

for $k = 1, \ldots, q$. See Figure 2.2 for an example partition of unity fulfilling the above requirements.

In the upcoming corollaries we will simply assume that the requirements (4.7) are fulfilled. However, a simple procedure for constructing piecewise smooth weight functions is given in [52, Section 4.1]. If the decomposition $\{\Omega_k\}_{k=1}^q$ is reasonable the procedure results in functions fulfilling the assumptions in (4.7). The construction involves two steps: for each $k = 1, \ldots, q$ define

$$\tilde{\chi}_k(x) = \begin{cases} \inf\limits_{y \in \partial\Omega_k} |x - y|, & x \in \Omega_k, \\ 0, & x \in \Omega \setminus \Omega_k, \end{cases}$$

and then normalize

$$\chi_k(x) = \begin{cases} \dfrac{\tilde{\chi}_k(x)}{\sum_{\ell=1}^q \tilde{\chi}_\ell(x)}, & x \in \Omega_k, \\ 0, & x \in \Omega \setminus \Omega_k. \end{cases}$$

It is clear that the first-order weak partial derivatives of χ_k are of size $\mathcal{O}(1/\delta)$, where δ is the characteristic overlap length. See also [52, Proposition 4.1] asserting the existence of partitions of unity of arbitrary regularity where the rth order derivatives of each χ_k is of size $\mathcal{O}(1/\delta^r)$.

With the partition of unity $\{\chi_k\}_{k=1}^q$ in place we can define the operators A_k of the DDOS. Formally, they are given by (4.6). Note how each subdomain Ω_k corresponds to one weight function χ_k and one operator A_k. To properly define the operators their domains $\mathcal{D}(A_k)$ must be specified. In Section 2 of Paper III we do this using weighted Sobolev spaces. As this is rather technical we do not give the definition here but instead refer the reader to the appended paper.

Before stating the corollaries to the theorems in Section 3.3 we make one more comment on the construction of domain decompositions $\{\Omega_k\}_{k=1}^q$. Recall that when an ADI scheme is used we only allow for two-operator splittings which is rather prohibitive

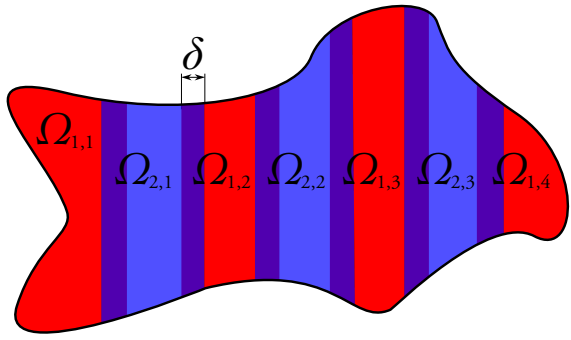


Figure 4.1: An example of an overlapping domain decomposition of $\Omega = \Omega_1 \cup \Omega_2$ *where each subdomain is the union of a family of disjoint subsubdomains,* $\Omega_k = \bigcup_l \Omega_{k,l}$*. The characteristic overlap length is denoted by* δ*.*

in the current setting since it implies only two subdomains. However, we may circumvent the problem by choosing each subdomain as the union of a family of disjoint sets $\Omega_k = \bigcup_\ell \Omega_{k,l}$, cf. Figure 4.1. Then, also the computation of the action of the resolvent $(I - hA_k)^{-1}$ may be parallelized as each subsubdomain $\Omega_{k,l}$ may be considered separately. Thus, not only the additive scheme (4.5), but also the Peaceman–Rachford (4.3) and Douglas–Rachford (4.4), schemes can be used for parallel computations. Note, however, that more subdomains (and thereby operators) grants a greater flexibility, see e.g. the widely used decomposition of rectangles in Figure 4.2.

4.1.2 Convergence of splitting schemes applied to DDOSs

With the above assumptions on the diffusion–advection–reaction equation (4.1) and the weight functions χ_k in place we can finally apply the theorems of Section 3.3. To this end, let $\mathcal{H} = L^2(\Omega)$ and let the domains $\mathcal{D}(A_k)$ and $\mathcal{D}(A)$ be defined as in Section 2 of Paper III. Then, under the assumptions above on $\Omega, \lambda, \rho, \sigma$, the weight functions χ_k and the boundary conditions, it is proven in Lemmas 2.3 and 2.4 of Paper III that the operators $A_1, \ldots, A_q$ and A fulfil Assumptions 1 and 2 of Chapter 3 (see also Remarks 1 and 3). The dissipativity constants are given by

$$M[A_1] = \cdots = M[A_q] = M[A] = \max\{0, P^2/(2\lambda_0) - \sigma_0\},$$

where

$$P^2 := \sum_{i=1}^{d} \|\rho_i\|^2_{L^\infty(\Omega)} \quad \text{and} \quad \sigma_0 := \operatorname*{ess\,inf}_{x\in\Omega} \sigma(x).$$

Thus, we may state the following corollaries of Theorems 1 and 3 and Theorems 2 and 4.

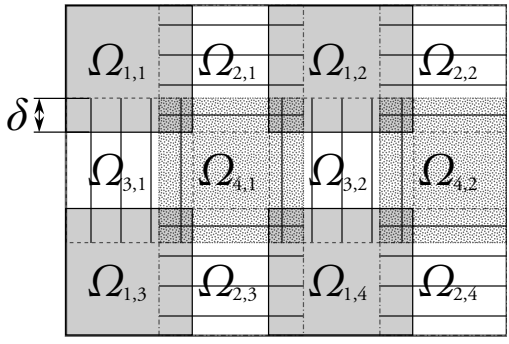


Figure 4.2: A widely used overlapping domain decomposition for rectangular domains $\Omega = \bigcup_{k=1}^{4} \Omega_k$ where each subdomain is the union of a family of disjoint subsubdomains, $\Omega_k = \bigcup_l \Omega_{k,l}$. The characteristic overlap length is denoted by δ.

Corollary 6. *Consider the Peaceman–Rachford* (4.3) *or Douglas–Rachford* (4.4) *discretization of the domain decomposition splitting* (4.6) *of the linear parabolic problem* (4.1). *Under the above assumptions on the domain Ω, the equation coefficients, the weight functions, the boundary conditions and with $\mathcal{D}(A_1), \mathcal{D}(A_2)$ and $\mathcal{D}(A)$ defined as in Section 2 of Paper III we have:*

- *Both schemes converge if $\eta \in \mathcal{D}(A_2)$.*
- *Both schemes converge with at least order one if $\eta \in \mathcal{D}(A^2)$.*
- *The Peaceman–Rachford scheme converges with order two if the solution u is regular enough for the global error bound in Theorem 1 to be valid.*

Corollary 7. *Consider the additive scheme* (4.5) *applied to the domain decomposition splitting* (4.6) *of the linear parabolic problem* (4.1). *Under the above assumptions on the domain Ω, the equation coefficients, the weight functions, the boundary conditions and with $\mathcal{D}(A_1), \ldots, \mathcal{D}(A_q)$ and $\mathcal{D}(A)$ defined as in Section 2 of Paper III we have:*

- *The additive scheme converges for any $\eta \in \mathcal{H}$.*
- *The additive scheme converges with order one if the solution u is regular enough for the global error bound in Theorem 2 to be valid.*

We note that the statements are stronger in the above corollaries compared to those made in the corresponding theorems. The reason is that we here also have used the extra structure available in the linear setting, cf. Section 3.2. Since $\mathcal{D}(A)$ is dense in $L^2(\Omega)$ as a direct consequence of being linear and maximal dissipative we do not need to assume this in the current context. Thus, we can conclude that the considered splitting

methods discretizing a DDOS of the parabolic problem (4.1) converges without needing any regularity requirements on the solution; only a weak assumption on the initial data is needed, and only for the ADI schemes. The most remarkable result, however, is that the ADI schemes converge with at least order one under just the extra assumption of $\eta \in \mathcal{D}(A^2)$. This is a consequence of the favourable error structures of these schemes and can be proven using linear semigroup theory.

We finally turn our attention to semilinear PDEs. More precisely, consider evolution equations on the form

$$\dot{u} = Au + Fu = \sum_{k=1}^{q} A_k u + Fu, \quad u(0) = \eta.$$

Let $A_1, \dots A_q$ and A be as above and assume that also $A + F$ is maximal dissipative. Then, we get from Theorems 2 and 4 that the additive scheme

$$S_h = (I - hF)^{-1}\Big(\frac{1}{q}\sum_{k=1}^{q}(I - hqA_k)^{-1}\Big), \tag{4.8}$$

converges if F is maximal dissipative and $\overline{\mathcal{D}(A) \cap \mathcal{D}(F)} = \mathcal{H}$, and the scheme

$$S_h = \Big(\frac{1}{q}\sum_{k=1}^{q}(I - hqA_k)^{-1}\Big)(I + hF),$$

converges if F is Lipschitz continuous and $\mathcal{D}(F) = \mathcal{H}$. Further, for solutions u regular enough we have convergence with order one. If F does not contain any derivatives, but rather represents a nonlinear reaction, the additive schemes can be easily implemented for efficient parallel computations as is discussed in the introduction.

To come full circle we return to the prototypical semilinear parabolic problem of the introduction, the FitzHugh–Nagumo equations (1.1). Already in Examples 2 and 3 we saw that the operators A, F and $A + F$ fulfil Assumptions 1 and 2 when chosen as in (1.2). If we further perform the domain decomposition splitting

$$Au = \begin{pmatrix} D_1\Delta u_1 \\ D_2\Delta u_2 \end{pmatrix} = \sum_{k=1}^{q} A_k u = \sum_{k=1}^{q} \begin{pmatrix} D_1\nabla\cdot(\chi_k\nabla u_1) \\ D_2\nabla\cdot(\chi_k\nabla u_2) \end{pmatrix}, \tag{4.9}$$

with weight functions as above, we obtain operators A_k that also fulfil the assumptions. Finally, according to Example 3 we have $\mathcal{D}(A) \cap \mathcal{D}(F) = \mathcal{D}(A)$ and therefore $\mathcal{D}(A) \cap \mathcal{D}(F)$ is dense in $\mathcal{H}$. Thus, the additive scheme (4.8) converges when applied to the combined physical and spatial splitting of the FitzHugh–Nagumo equations. We formalize in the following corollary.

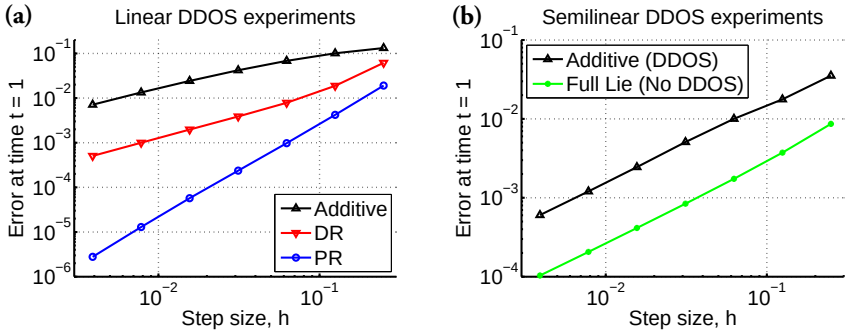


Figure 4.3: Temporal convergence order experiments verifying the corollaries of Section 4.1.2. In (a) the linear diffusion–advection–reaction equation (4.1) *is integrated by the Peaceman–Rachford* (4.3)*, Douglas–Rachford* (4.4) *and additive* (4.5) *schemes with operators given by a DDOS. In (b) the FitzHugh–Nagumo equations* (1.1) *are integrated by the additive scheme* (4.8) *in the presence of both the physical* (1.2) *splitting and the same domain decomposition splitting as in (a). The green curve represents the same errors as it does in Figure 3.1. We can thus see the extra errors introduced by the DDOS. All predicted convergence orders are observed in both plots.*

Corollary 8. *Consider the additive splitting scheme* (4.8) *applied to the physical* (1.2) *and domain decomposition* (4.9) *splitting of the FitzHugh–Nagumo equations* (1.1)*. Let*

$$\mathcal{D}(A) \cap \mathcal{D}(F) = \mathcal{D}(A) = (H^2(\Omega) \cap H_0^1(\Omega))^2, \quad \mathcal{D}(F) = L^6(\Omega) \times L^2(\Omega),$$

and let $\mathcal{D}(A_1), \ldots, \mathcal{D}(A_q)$ *be defined as in Section 2 of Paper III. Then, under the above assumptions on the domain* Ω*, the weight functions and the boundary conditions, we have:*

- *The additive scheme* (4.8) *converges for any* $\eta \in \mathcal{H}$*.*
- *The additive scheme* (4.8) *converges with order one if the solution* u *is regular enough for the global error bound in Theorem 2 to be valid.*

For further semilinear DDOS applications see Examples 3.7 and 3.8 of Paper III.

4.1.3 Numerical experiments – temporal convergence orders

We verify the above corollaries by numerical experiments in two space dimensions, both in the linear and the semilinear settings. Consider the linear diffusion–advection–reaction equation (4.1), for simplicity defined on the unit square $\Omega = (0, 1)^2$. In Figure 4.3a we see the results of experiments where a domain decomposition splitting is applied to this PDE. These results are reproduced from the convergence experiments performed for Section 4.2 of Paper III. We refer to that section for details, in particular for definitions of

the anisotropic equation coefficients λ, ρ and σ. The subdomains are given by four vertical stripes with an overlap length $\delta = 1/10$, cf. Figure 4.1. This implies four operators $A_1, \ldots, A_4$ for the additive scheme (4.5) whereas the subdomains need to be properly merged to create a two-operator formulation for the ADI schemes (4.3) and (4.4). The expected orders are observed verifying Corollaries 6 and 7.

Finally, we consider again the FitzHugh–Nagumo equations (1.1). For the additive scheme (4.8) we perform the same experiments as presented in Figure 3.1b, but here we also further split the A operator with the same four-operator-DDOS as above. First-order convergence is observed as predicted by Corollary 8.

4.2 Dimension splittings

Temporal convergence orders for splitting schemes discretizing dimension splittings were proven already in [33]. We here take the analysis a step further by providing simultaneous space–time convergence orders for full discretizations.

Recall the dimension splitting

$$A_1 u = \frac{\partial}{\partial x_1}\Big(\lambda_{1,1}\frac{\partial}{\partial x_1}u\Big) \quad \text{and} \quad A_2 u = \frac{\partial}{\partial x_2}\Big(\lambda_{2,2}\frac{\partial}{\partial x_2}u\Big), \tag{4.10}$$

of the two-dimensional diffusion equation discussed in Section 2.6. There we assumed that Ω is the open square $(0,1)^2$ in $\mathbb{R}^2$ and that $\lambda_{1,1}(x) = \lambda_{2,2}(x) = a(x_1)b(x_2)$ for some one-dimensional functions a and b. Now, further assume that $a, b \in C^2([0,1])$ and that $\lambda_{1,1}(x), \lambda_{2,2}(x) \geq \lambda_0 > 0$, for all $x \in \Omega$ where λ_0 is a constant. Moreover, let $\mathcal{H} = L^2(\Omega)$ and equip the equation with homogeneous Dirichlet boundary conditions.

In the above settings it is proven in [33, Section 5] that the operators A_1, A_2 and A fulfil the assumptions of Theorems 1 and 2. These theorems then imply that the temporal semi-discretizations given by the Peaceman–Rachford scheme (4.3), the Douglas–Rachford scheme (4.4) and the additive splitting scheme (4.5) converge with classical orders when applied to (4.10).

In Section 4 of Paper II the above dimension splitting is analysed in a full discretization setting, where a quadrature finite element method is used in space and the Douglas–Rachford scheme

$$S_{h,\Delta x} = (I - hA_{2,\Delta x})^{-1}(I - hA_{1,\Delta x})^{-1}(I + h^2 A_{1,\Delta x}A_{2,\Delta x}) \tag{4.11}$$

in time. We here summarize the setting and the central convergence result, for the details see the appended paper. Recall the notation of Section 3.4 and define on Ω a uniform quadrilateral mesh $\{(x_{1,i}, x_{2,j}) = (ih, jh)\}_{i,j=0}^{N}$. Here, N is a positive integer and the element width is denoted by $\Delta x = 1/N$. Further, introduce on this mesh continuous, piecewise bilinear basis functions and let $\mathcal{H}_{\Delta x}$ denote the finite element space given by the span of these functions.

The operators $A_{1,\Delta x}$, $A_{2,\Delta x}$ and $A_{\Delta x}$ are defined through variational formulations related to (4.10). To construct the mass and stiffness matrices, which represent these operators, the inner products of the variational formulations must be computed or approximated. We here do the latter by using the trapezoidal quadrature rule

$$(u,v)_{\Delta x} = \frac{(\Delta x)^2}{4} \sum_{i,j=0}^{N-1} \sum_{i',j'=0}^{1} (uv)(x_{1,i+i'}, x_{2,j+j'}), \tag{4.12}$$

which is defined for $u, v \in C(\overline{\Omega})$. The purpose of doing this approximation is to get mass and stiffness matrices that are suitable for splitting schemes. For example note that, for the mass matrix, using this quadrature rule is equivalent to mass lumping, which gives a diagonal matrix. The full discretization (4.11) then defines an efficient scheme where only families of 1D problems must be solved in each time step, possibly in parallel, as described in Section 2.6.

We prove in Paper II that the assumptions of Theorem 5 are valid in the above setting and we thus get the following corollary:

Corollary 9. *Consider the dimension splitting* (4.10) *discretized in space by a quadrature finite element method as described above (see Section 4 of Paper II for details). Then, if the time discretization is given by the Douglas–Rachford scheme* (4.11) *and* $\eta \in \mathcal{D}(A^3)$*, where* $\mathcal{D}(A) = H^2(\Omega) \cap H_0^1(\Omega)$*, we get the simultaneous space–time global error bound*

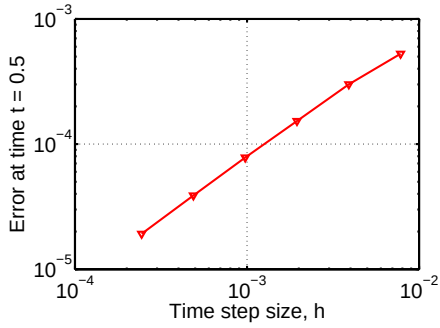
$$\left\| u(nh) - S_{h,\Delta x}^n \eta_{\Delta x} \right\| \leq C\big((\Delta x)^2 + h\big) \sum_{i=1}^{3} \left\| A^i \eta \right\|,$$

where the approximate initial data is given by $\eta_{\Delta x} = A_{\Delta x}^{-1} P_{\Delta x} A \eta$ *and the constant* C *can be chosen uniformly on bounded time intervals and, in particular, independently of* Δx*,* h *and* n*.*

Proving the spatial convergence of the stationary problem (3.20) requires elliptic regularity results [30, 31] and convergence results for quadrature finite element methods applied to elliptic problems [11, Chapter 4] and [12]. The dissipativity of $A_{1,\Delta x}$ and $A_{2,\Delta x}$ follows from the ellipticity of $-A_1$ and $-A_2$. Finally, from an analysis of the stiffness matrices we get the uniform spatial stability bound

$$\left\| A_{1,\Delta x} A_{\Delta x}^{-1} \right\|_{\Delta x} \leq C,$$

required for first-order convergence of the Douglas–Rachford scheme, cf. Assumption 3 of Paper II. Here C is a constant independent of Δx. However, we have not verified the corresponding uniform bounds on the operators $A_{1,\Delta x}^2 A_{\Delta x}^{-2}$ and $A_{2,\Delta x}^2 A_{\Delta x}^{-2}$ required by the additive scheme (3.22) and we can therefore not include this scheme in the corollary. The same applies to the Peaceman–Rachford scheme (3.24).



h	Δx	Error
1/128	1/16	5.3E-4
1/256	1/23	3.0E-4
1/512	1/32	1.5E-4
1/1024	1/45	7.8E-5
1/2048	1/64	3.9E-5
1/4096	1/91	1.9E-5

Figure 4.4: Simultaneous space–time convergence orders for the Douglas–Rachford scheme (4.11) *applied to the dimension splitting* (4.10)*. The values of h are chosen proportional to $(\Delta x)^2$ to verify that the temporal and spatial errors indeed vary according to Corollary 9.*

Remark 5. That the trapezoidal quadrature rule (4.12) is not defined on all of $L^2(\Omega)$ is the reason why we must allow for positive values on r in the abstract analysis of Section 3.4. For example, to get a spatial convergence bound of the type (3.20) we need to define the operator $P_{\Delta x}$ as the projection onto $\mathcal{H}_{\Delta x}$ orthogonal with respect to $(\cdot,\cdot)_{\Delta x}$. Then, since (4.12) is not defined on all of $L^2(\Omega)$, neither is $P_{\Delta x}$. Instead we define $P_{\Delta x}$ on the subspace $\mathcal{D}(A) = H^2(\Omega) \cap H_0^1(\Omega) \subset C(\overline{\Omega})$, i.e., we here require that $r = 1$. Finally, we remark that, when the bilinear form (4.12) is restricted to $\mathcal{H}_{\Delta x}$, it is an inner product, uniformly equivalent to $(\cdot,\cdot)_{L^2(\Omega)}$.

The predictions of Corollary 9 are illustrated by numerical experiments with a non-stiff toy problem. For details on equation coefficients, the initial data and the reference solution see Section 5 of Paper II. The results are presented in Figure 4.4. For this experiment, we have found values of h and Δx such that the temporal and spatial errors are of approximately the same size. Then, these parameters are varied such that h is proportional to $(\Delta x)^2$.

Chapter 5

A physical splitting application: axonal growth

In this chapter, we discuss the third theme of the thesis: evaluation of splitting schemes when applied to an interdisciplinary application. The application of choice, the axonal growth model, was described already in the introduction. The model consists of a 1D linear PDE coupled to nonlinear ODEs. By and large this is a semilinear parabolic problem on the form

$$\dot{u} = Au + Fu, \quad u(0) = \eta, \tag{5.1}$$

where A represents the PDE and F represents the ODEs. However, the model has not been formulated as a dissipative equation and we therefore now leave the framework used in the previous chapters. Instead we consider a tailored numerical scheme based on a physical splitting strategy. We evaluate it using numerical experiments and the known steady-state solutions. The objective is, above all, to investigate how well the scheme deals with the particular challenges offered by the axonal growth model.

The model and the numerical scheme were developed and analysed in Papers IV and V, respectively. Here we introduce the model equations in Section 5.1. We further discuss the particular challenges exhibited by the model and how to choose a numerical method that addresses these challenges. In Section 5.2 we present numerical experiments illustrating the dynamical behaviour of the model and the expected temporal convergence order of the numerical scheme.

5.1 Model description and choice of numerical scheme

The axonal growth model of Papers IV and V is a one-dimensional moving-boundary problem consisting of a linear diffusion–advection–reaction PDE coupled to two ODEs

through a boundary condition. Consider the schematic illustration of an idealized growing axon in Figure 1.3. Let l denote the time-dependent length of the axon. Furthermore, let $c(x,t)$ denote the tubulin concentration at time $t \geq 0$ and at the point $x \in (0, l(t))$ in the axon. The growth cone concentration is denoted by c_{c}, which is an unknown together with l and c. The function c_{s} defines a time-dependent boundary condition at $x = 0$. Additionally, let c_x^- denote the left derivative of the concentration c at the right hand boundary, $x = l(t)$, of the domain. The model is then given by

$$
\begin{cases}
\dot{c} = D\dfrac{\partial^2 c}{\partial x^2} - a\dfrac{\partial c}{\partial x} - gc, & 0 < x < l(t), t > 0, \\
\dot{c}_{\mathrm{c}} = \dfrac{(a - gl_{\mathrm{c}})c_{\mathrm{c}} - Dc_x^- - (r_{\mathrm{g}}c_{\mathrm{c}} + \tilde{r}_{\mathrm{g}}l_{\mathrm{c}})(c_{\mathrm{c}} - c_\infty)}{l_{\mathrm{c}}}, & t > 0, \\
\dot{l} = r_{\mathrm{g}}(c_{\mathrm{c}} - c_\infty), & t > 0, \\
c(0,t) = c_{\mathrm{s}}(t), & t \geq 0, \\
c(l(t),t) = c_{\mathrm{c}}(t), & t > 0, \\
c(x,0) = c_0(x), & 0 \leq x \leq l(0), \\
c_{\mathrm{c}}(0) = c_0(l_0), & \\
l(0) = l_0, &
\end{cases}
\tag{5.2}
$$

where c_0 is the initial tubulin concentration along the axon with initial length l_0 and the positive constants D, a, g, l_{c} r_{g}, $\tilde{r}_{\mathrm{g}}$, and c_∞ are physical and biological parameters. See Sections 1–3 of Paper IV for relevant references and for a detailed derivation of the model and the values of its parameters.

Of particular interest is the study of the dynamic outgrowth of tiny axons to their steady-state lengths, which may be several magnitudes larger. This range of length scales presents a challenge for a numerical scheme discretizing (5.2). Furthermore, the model also exhibits transient phenomena on largely different time scales: the cone concentration c_{c} tends very fast to its steady-state value (hours) whereas the axon length l tends slowly to its (years), cf. Figures 2 and 3 of Paper V.

We summarize the challenges raised by the axonal growth model (5.2) in the following list. A successful numerical method should handle:

1. The moving boundary of the domain $\Omega = (0, l(t))$ of the PDE.

2. Dynamics on largely different length and time scales.

3. The coupling of the PDE to the nonlinear ODEs at the moving boundary.

4. The stiffness of the problem.

5. Marching towards steady states, i.e. the method should preserve fixed points.

The expanding (and contracting) domain was considered already in [55] and Paper IV where a spatial scaling was proposed. To alleviate the problem of dynamics on different scales we also introduced a solution-dependent time transformation in Paper V. Assume that $l(t) > 0$ at all times and define the new space and time variables

$$\begin{cases} y := \dfrac{x}{l(t)}, \\ \\ \tau := \Gamma(t) := a \displaystyle\int_0^t \frac{1}{l(s)} \mathrm{d}s, \end{cases} \qquad 0 \le x \le l(t),\, t \ge 0.$$

The inverse transform is given by

$$\begin{cases} x = y\bar{l}(\tau), \\ t = \Gamma^{-1}(\tau), \end{cases} \qquad 0 \le y \le 1,\, \tau \ge 0,$$

where $\bar{l}(\tau) := l(\Gamma^{-1}(\tau)) = l(t)$. Hence we can expand the dynamical system (5.2) with the ODE

$$\frac{\mathrm{d}t}{\mathrm{d}\tau} = \frac{\mathrm{d}}{\mathrm{d}\tau}\Gamma^{-1} = \frac{1}{a}\bar{l},$$

for updating the time t. Furthermore, if we let $\bar{c}(y,\tau) := c(x,t)$ and $\bar{c}_{\mathrm{c}}(\tau) := c_{\mathrm{c}}(t)$, then the model (5.2) can be transformed and expanded into

$$\begin{cases} \dfrac{\partial \bar{c}}{\partial \tau} = \dfrac{D}{a}\dfrac{1}{\bar{l}}\dfrac{\partial^2 \bar{c}}{\partial y^2} - (1 - \dfrac{r_{\mathrm{g}}}{a} y(\bar{c}_{\mathrm{c}} - c_\infty))\dfrac{\partial \bar{c}}{\partial y} - \dfrac{g}{a}\bar{l}\bar{c}, & 0 < y < 1, \tau > 0, \\ \dfrac{\mathrm{d}\bar{c}_{\mathrm{c}}}{\mathrm{d}\tau} = \dfrac{(a - g l_{\mathrm{c}})\bar{l}\bar{c}_{\mathrm{c}} - D\bar{c}_y^- - \bar{l}(r_{\mathrm{g}}\bar{c}_{\mathrm{c}} + \tilde{r}_{\mathrm{g}} l_{\mathrm{c}})(\bar{c}_{\mathrm{c}} - c_\infty)}{a l_{\mathrm{c}}}, & \tau > 0, \\ \dfrac{\mathrm{d}\bar{l}}{\mathrm{d}\tau} = \dfrac{r_{\mathrm{g}}}{a}\bar{l}(\bar{c}_{\mathrm{c}} - c_\infty), & \tau > 0, \\ \dfrac{\mathrm{d}t}{\mathrm{d}\tau} = \dfrac{1}{a}\bar{l}, & \tau > 0, \\ \bar{c}(0,\tau) = c_{\mathrm{s}}(t(\tau)), & \tau \ge 0, \\ \bar{c}(1,\tau) = \bar{c}_{\mathrm{c}}(\tau), & \tau > 0, \\ \bar{c}(y,0) = c_0(y l_0), & 0 \le y \le 1, \\ \bar{c}_{\mathrm{c}}(0) = c_0(l_0), \\ \bar{l}(0) = l_0, \\ t(0) = 0. \end{cases} \tag{5.3}$$

See Sections 3.2 and 5.4 of Paper V where also a more aggressive time scaling is discussed.

The time and space scalings address the first two items on the list of challenges. The remaining three items are treated by carefully choosing which numerical method to apply

to (5.3). Note that the PDE is linear in $\bar{c}$ but has coefficients and boundary conditions that depend on $\bar{c}_{\mathrm{c}}$, $\bar{l}$, and t. To take advantage of this linearity, we formally split the equation according to (5.1) with

$$
\begin{aligned}
u &= \begin{pmatrix} \bar{c} & \bar{c}_{\mathrm{c}} & \bar{l} & t \end{pmatrix}^{\mathrm{T}}, \\
Au &= \begin{pmatrix} \frac{D}{a}\frac{1}{\bar{l}}\frac{\partial^2 \bar{c}}{\partial y^2} - (1 - \frac{r_{\mathrm{g}}}{a} y(\bar{c}_{\mathrm{c}} - c_\infty))\frac{\partial \bar{c}}{\partial y} - \frac{g}{a}\bar{l}\bar{c} \\ 0 \\ 0 \\ 0 \end{pmatrix}, \\
Fu &= \begin{pmatrix} 0 \\ \frac{(a - g l_{\mathrm{c}})\bar{l}\bar{c}_{\mathrm{c}} - D\bar{c}_y^- - \bar{l}(r_{\mathrm{g}}\bar{c}_{\mathrm{c}} + \tilde{r}_{\mathrm{g}} l_{\mathrm{c}})(\bar{c}_{\mathrm{c}} - c_\infty)}{a l_{\mathrm{c}}} \\ \frac{r_{\mathrm{g}}}{a}\bar{l}(\bar{c}_{\mathrm{c}} - c_\infty) \\ \frac{1}{a}\bar{l} \end{pmatrix},
\end{aligned}
\tag{5.4}
$$

where the domain of A consists of functions fulfilling the boundary conditions of (5.3). With this physical splitting the PDE fully decouples from the ODEs and item number three on the list of challenges is thus addressed. To determine which splitting method to use for the integration of (5.4), we consider the last two items on the list. Since exact solutions to the ODEs are not straight forward to find, full splitting schemes are preferred. Furthermore, due to the stiffness of the equations an implicit method, at least in A, is required. Finally, since the convergence to steady state is of interest, a fixed-point preserving scheme is a necessity. Recall the discussion in Section 2.3, the ADI schemes fulfil all the requirements. Thus, in Paper V we apply the Peaceman–Rachford scheme

$$
S_h = \big(I - \tfrac{h}{2}F\big)^{-1}\big(I + \tfrac{h}{2}A\big)\big(I - \tfrac{h}{2}A\big)^{-1}\big(I + \tfrac{h}{2}F\big), \tag{5.5}
$$

to the splitting (5.4) of the scaled model (5.3).

We do not provide an analytic framework in which the transformed equations (5.3) with the splitting (5.4) fulfil Assumptions 1 and 2. Thus, the theorems of Section 3.3 do not apply. The term $\bar{c}_y^-$ constitutes the main difficulty when trying to find a framework in which (5.3) is dissipative; we have not been able to bound an inner-product as required by (3.2). Instead, to make sense out of the splitting, we first apply a standard second-order finite difference space discretization and consider the finite-dimensional semi-discretization, see Section 4 of Paper V. In Lemma 1 of that paper we provide conditions under which the action of the resolvent $(I - h/2\, A)^{-1}$ is well-defined. However, we have not proven convergence for the full numerical scheme.

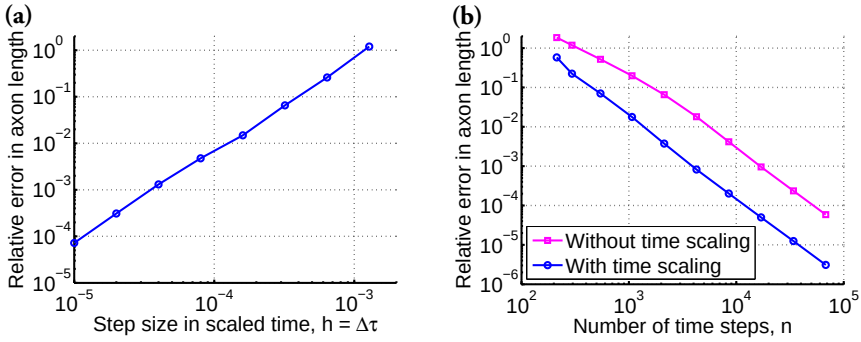


Figure 5.1: Temporal convergence order experiments for the Peaceman–Rachford scheme discretizing the axonal growth model. In (a) errors are plotted for different values of $h = \Delta\tau$ when the fully scaled model (5.3) *is discretized. The simulations are run until end time $T = 86\,400\,\mathrm{s} = 1$ day giving a final axon length of approximately* 1.2 mm. *We observe the expected second-order convergence. In (b) similar experiments are performed but with $T = 60\,\mathrm{s}$ during which the axon grows to approximately* 11 µm. *Very small time steps are used to be able to observe second-order convergence also when time scaling is not used. The results are plotted over the number of time steps for easy comparison.*

5.2 Numerical experiments

In the current section we will use numerical experiments to illustrate that the Peaceman–Rachford scheme applied to the scaled model (5.3) indeed can handle the list of challenges presented in the previous section. We will pay extra attention to the need for time scaling and also provide experiments showing the expected second-order convergence in time.

To this end consider again the spatial semi-discretization of (5.3) on an equidistant grid with mesh width Δy, cf. Section 4.1 of Paper V. We note that the application of an explicit temporal discretization method to the semi-discretization comes with a CFL condition of the type $h < C(\Delta y)^2$ due to the parabolic nature of the problem. However, a traditional implicit method must, in each time step, solve a big, non-linear system of equations. The splitting (5.4) resolves the latter issue and, as our experiments will show, employing an implicit splitting method, like the Peaceman–Rachford scheme, resolves the former.

5.2.1 Convergence of the Peaceman–Rachford scheme

In Figure 5.1a, we see the results from a numerical experiment indicating that we have second-order convergence for the Peaceman–Rachford scheme (5.5) when it is applied to the axonal growth model. This experiment is performed with nominal values on the physical and biological parameters, see Table 1 of Paper IV. For the left boundary condition we use the constant soma concentration $c_s(t) = 2c_\infty = 23.80\,\mathrm{mmol/m^3}$. The initial length

is chosen small $l_0 = 1\,\mu\text{m}$ and the initial tubulin concentration in the axon is chosen constant $c_0(x) = 2c_\infty$. The axonal growth is terminated after one day, $T = 86\,400\,\text{s}$. After retrieving a semi-discretization on a fine spatial grid, $\Delta y = 10^{-4}$, we discretize in time using the Peaceman–Rachford scheme. In Figure 5.1a, the supremum over time of the relative error in axon length is plotted for different values of $h = \Delta\tau$. The reference solution is found by using the same discretization method on a very fine grid, $\Delta y = 10^{-5}$ and $h = \Delta\tau = 10^{-6}$.

Our experiments show that the stiffness of the model is successfully handled by the Peaceman–Rachford scheme. In Figure 5.1a, we see the errors of stable numerical computations that indeed indicate the absence of a CFL condition for values of $D/(a\bar{l}) \cdot h/(\Delta y)^2$ far bigger than allowed by, e.g., the explicit Euler scheme; in the above experiment we have $D/(a\bar{l}(0)) \cdot h/(\Delta y)^2 \approx 10^8$ on the coarsest temporal mesh.

5.2.2 The need for time scaling

Consider now the system (5.2) after transforming it only with the spatial scaling $y = x/l(t)$. Further, discretize this partially transformed model with finite differences and Peaceman–Rachford using the same physical, biological and numerical parameter values as used for the discretization of the fully transformed system (5.3) above. Performing these computations, which lack the time scaling, gives no reasonable results due to the large time steps taken during the first parts of the simulations. This shows the strength of using time scaling to allocate more steps where it is needed. If we use very small time steps throughout the entire simulation we can get reasonable results also without time scaling, however, at the cost of impractically large CPU times. This is explored in Figure 5.1b which shows results from an experiment similar to the one presented in Figure 5.1a. However, here the end time is chosen very small, $T = 60\,\text{s}$, to enable fast computations with tiny time steps. The reference solution is found in the same way as above, but here with $h = \Delta\tau = 10^{-7}$. As we have $h = \Delta\tau$ when using time scaling and $h = \Delta t$ when not we here instead plot the errors over the number of time steps n for easy comparison. To this end, for each value of h $(= \Delta\tau)$, we store the number of time steps used when integrating the fully scaled model. Then a simulation without scaling is performed with the same number of time steps. Second-order convergence can be observed both when using time scaling and when not.

5.2.3 Dynamical behaviour and convergence to steady states

In Figure 5.2, we see the dynamical behaviour of the axon length l and the tubulin concentration along the axon c. Both variables tend to their steady states, which are explicitly obtained in Section 4 of Paper IV. The parameter values are chosen as before except for the time step $h = \Delta\tau = 5 \cdot 10^{-4}$, a much larger end time $T = 6 \cdot 10^8\,\text{s}$ and a time-

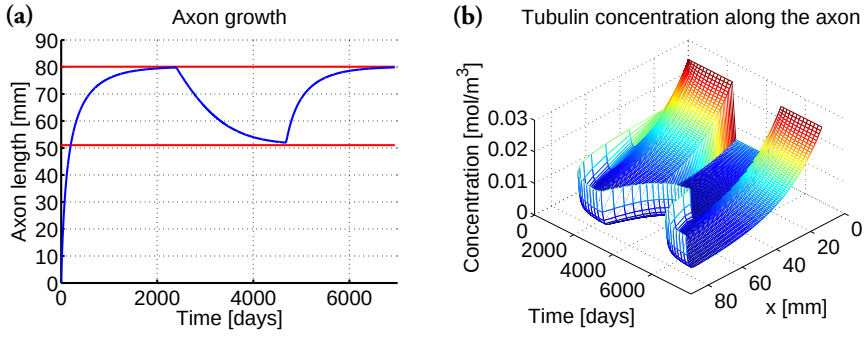


Figure 5.2: Numerical solution of the axonal growth problem discretized in time by the Peaceman–Rachford scheme. In (a) we see the axon length l increasing and decreasing as an effect of the varying tubulin concentration in the soma (5.6)*. The red lines represents the steady-state lengths related to the two different values of this concentration. In (b) the tubulin concentration c in the axon is plotted as a function of time and space. Note the characteristic concentration profile which was studied in Section 4 of Paper IV.*

dependent soma concentration

$$c_s(t) = \begin{cases} 2c_\infty = 23.80\,\text{mmol/m}^3, & 0 \le t < 2 \cdot 10^8\,\text{s}, \\ \dfrac{c_\infty}{2} = 5.95\,\text{mmol/m}^3, & 2 \cdot 10^8\,\text{s} \le t < 4 \cdot 10^8\,\text{s}, \\ 2c_\infty = 23.80\,\text{mmol/m}^3, & 4 \cdot 10^8\,\text{s} \le t. \end{cases} \tag{5.6}$$

Note how the variation in soma concentration triggers both expansion and contraction of the axon. The results indicate that the Peaceman–Rachford scheme indeed may be used when marching towards known steady states. Also note the characteristic spatial profile of the tubulin concentration c with a very steep increase near the growth cone, compare with the figures in Section 4 of Paper IV.

To conclude the chapter we refer to the parameter studies performed in Section 5.5 of Paper V which, in addition to having biological relevance, also demonstrate the flexibility and robustness of the developed numerical scheme. For the sake of brevity we do not reproduce these experiments here.

Chapter 6

Conclusions and future work

In this thesis we have presented analyses and applications of splitting schemes when used as temporal discretizations of semilinear parabolic problems. We here conclude and present ideas for future research considering the three themes of the thesis.

6.1 Conclusions

During the work with the first theme of the thesis we have proven optimal temporal convergence orders for ADI and additive splitting schemes when applied to semilinear parabolic problems with unbounded vector fields. Depending on the regularity of the solution, we get convergence of either second order, first order or without order. This fills a gap in the literature as earlier studies have considered either fully linear problems, Lipschitz continuous nonlinear terms, specific equations or only proven convergence without order.

The convergence analysis has been performed in the abstract framework of dissipative operators. As a consequence our results apply, not only to parabolic PDEs, but to a wide range of problems, as exemplified by the physical splitting applications given in the thesis. An additional benefit is that our theorems are independent of any subsequent space discretization and may be used as a building block for the analysis of full discretizations. We have also demonstrated how this can be done in the linear setting. All theoretical results have been verified by numerical experiments.

In view of the second theme, we have demonstrated how our temporal convergence results can be used to analyse spatial splittings. In particular, we have constructed a variational framework for non-iterative domain decomposition procedures based on splitting schemes. In this setting, the decomposed linear or semilinear parabolic problems can be interpreted as dissipative evolution equations. Thus, convergence with optimal orders for the domain decomposition splittings (DDOSs) follows from our abstract analysis. Fur-

thermore, for dimension splittings we have proven simultaneous space–time orders. The accompanying numerical experiments verify the convergence theorems.

The third theme of the thesis concerns the semilinear model of axonal growth in nerve cells developed in Paper IV. The model consists of two ODEs coupled to a parabolic PDE defined on an expanding (and contracting) domain. We have seen that an efficient numerical scheme can be constructed by using space and time scalings, splitting the ODEs from the PDE, and then employing an implicit splitting scheme like the Peaceman–Rachford method. Although no convergence proof has been obtained, all dynamical simulations have converged to the known steady-state solutions. Further numerical experiments have shown that the expected second-order convergence is achieved. Finally, the flexibility, robustness and efficiency of the scheme have been demonstrated by performing parameter studies.

6.2 Future work

During the thesis work several ideas for future research have emerged which we summarize here.

Parabolic problems typically have smooth solutions, even when the initial data is irregular. In the general framework of dissipative operators and strongly continuous semigroups we have not been able to take advantage of this smoothing property. By instead employing the (less general) framework of analytic semigroups, the parabolic smoothing may be used to weaken the regularity assumptions in Theorems 1 and 2, the central results of the first theme of the thesis. See e.g. [6, Section 4.1] and [58, Section 2.5] for introductions to analytic semigroups and their nonlinear generalizations. See also [71, Chapters 3 and 14] where nonsmooth data error estimates are given for the IMEX Euler method discretizing parabolic problems.

When considering analytic semigroups, further questions arise that call for deeper investigation. For example, can we, in this framework, prove stability for ADI schemes in more general Banach spaces? Compare with [15] where the Crank–Nicholson method discretizing linear equations was considered. Moreover, an analysis of ADI schemes with more than two operators would be of interest, especially for the spatial splitting applications. The eigenvalue analysis in [43, Section VI.3.2] indicates that the structure granted by the framework of analytic semigroups may enable us to prove stability also in this case.

A natural extension for domain decomposition splittings is to apply the same technique with weight functions, as used in the linear setting, also to nonlinear differential operators, like the p-Laplacian. We may also direct our attention to the development and analysis of non-iterative methods constructed from non-overlapping decompositions combined with splitting schemes. Such an analysis should probably be based on a reformulation of the PDE as a transmission problem, see e.g. [67]. Furthermore, a full space–time convergence order analysis for DDOSs would also be of interest. For this, we may use the abstract results of Section 3.4 as we already did for dimension splittings in

Section 4.2.

To complement the convergence theorems of Section 4.1, it would be interesting to carry out efficiency experiments for DDOSs; in particular to compare these non-iterative methods with traditional, iterative, domain decomposition techniques. We have already started the work on this project; a Python implementation for parallel and distributed computations for 2D and 3D problems is under development. The goal is to perform the efficiency experiments using large-scale interdisciplinary applications, e.g. air pollution models, discretized in space on unstructured meshes. Preliminary results from this work show great potential for DDOSs. For several test cases the error is only slightly larger when using splitting schemes based on domain decompositions compared to solving the full problem with implicit Euler or Crank–Nicolson.

Temporarily leaving the parabolic problems aside, we note that the Douglas–Rachford scheme is commonly used as a fixed point iteration for finding approximate solutions to stationary problems $(A_1 + A_2)v = f$, see e.g. [16, 23, 28]. Now, let $A_1 + A_2$ be a differential operator and split it using a domain decomposition as in Section 4.1. Then, the Douglas–Rachford fixed point iteration can be seen as a modification of a classical overlapping domain decomposition method: the multiplicative Schwarz algorithm. It would be of great interest to investigate whether this modification results in faster convergence. Compare with the more favourable error structure the extra factor $(I + h^2 A_1 A_2)$ grants in the evolutionary case, see (2.13) and Figure 3.1.

The axonal growth model (5.3) is by and large a parabolic problem. However, we have not yet been able to fit the model into the setting of dissipative evolution equations. To achieve this, we need to further investigate the special boundary condition coupling and how to treat the left derivative $\bar{c}_y^-$. This could be an interesting line of research in future work. An additional idea is to study a more realistic axonal growth model given by extending the current one to include a varying axon cross-section area.

Finally, we mention also co-simulation of coupled differential algebraic equations. This technique is closely related to splitting methods; also here the idea is to decouple the equations to enable independent computations with tailored methods for each subsystem, cf. [3, 4, 47]. It would be interesting to investigate these connections and how the special benefits of the splitting schemes considered in this thesis might manifest in the co-simulation context.

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