Analyses and Applications of the Peaceman--Rachford and Douglas--Rachford Splitting Schemes

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Abstract

Splitting methods are widely used as temporal discretizations of evolution equations. Such methods usually constitute competitive choices whenever a vector field can be split into a sum of two or more parts that each generates a flow easier to compute or approximate than the flow of the sum. In the research presented in this Licentiate thesis we consider dissipative evolution equations with vector fields given by unbounded operators. Dynamical systems that fit into this framework can for example be found among Hamiltonian systems and parabolic and hyperbolic partial differential equations (PDEs).

The goal of the presented research is to perform convergence analyses for the *alternating direction implicit* (ADI) methods in the setting of dissipative operators. In this context these methods are known to possess excellent stability properties. Additionally, they generate easily computable numerical flows and are ideal choices for studying convergence to stationary solutions, a property related to their favorable local error structure. In this thesis we consider the Peaceman–Rachford and Douglas–Rachford schemes, which were the first ADI methods to be constructed and to this day are the most representative members of the ADI method class.

We perform convergence studies for the Peaceman–Rachford and Douglas–Rachford schemes when applied to semilinear, dissipative evolution equations, that is, when the vector fields are given by the sum of a linear and a nonlinear dissipative operator. Optimal convergence orders are proven when the solution is sufficiently regular. With less regularity present we are still able to prove convergence, however of suboptimal order or without order. In contrast to previous convergence order analyses we do not assume Lipschitz continuity of the nonlinear operator.

In the context of linear, dissipative evolution equations we consider full space-time discretizations. We assume that the full discretization is given by combining one of the two aforementioned ADI methods with a general, converging spatial discretization method. In this setting we prove optimal, simultaneous space-time convergence orders.

Advection-diffusion-reaction models, encountered in physics, chemistry, and biology are important examples of dissipative evolution equations. In this thesis we present such a model describing the growth of axons in nerve cells. The model consists of a parabolic PDE, which has a non-trivial coupling to nonlinear ordinary differential equations via a

moving boundary, which is part of the solution. Since additionally the biological model parameters imply a wide range of scales, both in time and space, the application of a numerical method is involved. We make an argument for a discretization consisting of a splitting which is integrated by the Peaceman–Rachford scheme. The choice is motivate by the results of some numerical experiments.

Populärvetenskaplig sammanfattning

Partiella differentialekvationerna är kraftfulla verktyg som kan användas för att beskriva fysikaliska fenomen inom bland annat naturvetenskap, teknik, ekonomi och medicin. Listan med tillämpningar kan göras hur lång som helst: Partiella differentialekvationer kan beskriva hur en snöflinga bildas, hur strukturer deformeras när de utsätts för mekaniska krafter, 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 fysikaliska 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 dynamiska system definierade över ett område i rummet. Modeller av komplicerade processer där många fysikaliska fenomen samverkar leder ofta till stora ekvationssystem där varje obekant varierar med tid och rum. Sådana system av partiella differentialekvationer kan nästan aldrig lösas exakt. Istället används i praktiken numeriska metoder för att hitta approximativa lösningar med hjälp av datorernas enorma beräkningskapacitet. Givetvis är det av största vikt att metoderna som används är både effektiva och pålitliga. Att säkerställa detta är centralt i den forskning som genomförs inom numerisk analys.

I många fall kan system av partiella differentialekvationer vara så komplicerade att det inte är tänkbart att hitta en approximativ lösning till hela systemet på en gång. Istället delar man upp systemet i mindre problem och approximerar dem var för sig. Metoder som tillämpar denna idé kallas *splittingmetoder*. Givetvis införs ett approximationsfel när en sådan splitting genomförs. Vi måste alltså väga förenklade beräkningar mot ett ökat fel. För att kunna göra detta måste vi förstå oss på hur felet ser ut.

Många analyser av splittingfel har tidigare genomförts för olika sorters splittingapproximationer applicerade på olika familjer av partiella differentialekvationer. I forskningen som presenteras i denna uppsats analyserar vi de splittingmetoder som går under

namnet *alternative direction implicit methods* (ADI-metoder). Dessa användes för första gången i början av 50-talet för att lösa värmeledningsproblem i flera dimensioner. Modellen gavs även där av en partiell differentialekvation och lösningstekniken var att alternera mellan de olika rumsdimensionerna och lösa ekvationen en dimension åt gången.

I vår forskning utvidgar vi felanalysen för ADI-metoder till nya familjer av partiella differentialekvationer. Vår analys täcker till exempel in modeller för skapandet av snöflingor och modeller för mönsterbildning i naturen. För dessa modeller och för många, många fler har vi nu en god förståelse för hur stort approximationsfel som skapas när en splitting genomförs.

Som nämndes tidigare modellerar partiella differentialekvationer ofta fysikaliska system som varierar både i tid och rum. ADI-metoderna approximerar lösningarnas variation med tiden. Men, för att kunna göra beräkningar på en dator måste dessa metoder kombineras med en metod som approximerar variationen i rummet. I vår forskning har vi därför dessutom analyserat sådana metodkombinationer. Analysen täcker till exempel in det ovan nämnda splittingförfarande för värmeledningsekvationen.

Vi har också genomfört en djupare analys av den tidigare nämnda tillämpningen angående axontillväxt i nervceller. I en sådan cell växer en lång, tubformad nervtråd ut från cellkroppen. Utväxten kallas axon och byggs upp av proteinet tubulin. Detta protein produceras i cellkroppen och färdas sedan längs med axonet för att slutligen monteras i andra änden av denna nervtråd. För att beskriva dessa processer skapar vi en matematiska modell som bland annat består av en partiell differentialekvation. Vi applicerar en ADI-metod för att hantera tubulinets förflyttning längs axonet separat från uppbyggnadsprocessen i axonets ände. Våra experiment visar att denna splittingmetod ger effektiva och pålitliga numeriska resultat.

List of Papers

This Licentiate 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 and I describe my contribution to each of them on the next page.

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

II. E. Hansen and E. Henningsson.
A full space-time convergence order analysis of operator splitting for linear dissipative evolution equations.
Preprint, 2014, Lund University, www.maths.lth.se/na/staff/erik/, accessed 2014-10-20.

III. S. Diehl, E. Henningsson, A. Heyden, and S. Perna.
A one-dimensional moving-boundary model for tubulin-driven axonal growth.
J. Theor. Biol., 7(358):194–207, 2014.

In this thesis I also present some new research results which cannot be found in any of the three listed papers. Parts of Section 2.2 and most of Chapter 3 are based on these results.

Author's contribution

Since all the appended papers where co-authored I here describe my contribution to each.

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 splitting. I designed, implemented, and performed the numerical experiments.

III. I designed, implemented, and performed the stability experiments.

The aforementioned new research results, which are not part of any of the three listed papers, are my own contribution with the exception of the time scaling idea presented in Section 3.1.

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Erik Henningsson
Lund, October, 2014

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Contents

Chapter 1

Introduction

The research presented in this Licentiate thesis is concerned with splitting methods as numerical time integration schemes for dynamical systems. First and foremost we analyze convergence and prove optimal orders. Additionally, we present some preliminary results in an application to axonal growth in neurons. In Section 1.1 we give a brief motivation of the competitiveness of splitting methods with examples of situations where they constitute ideal choices. We also overview some important classes of splitting methods, particularly the *alternating direction implicit* (ADI) methods which are of principal interest in the presented work. The aim of the research is presented in Section 1.2 in relation to the current state of the art in the research of ADI methods.

1.1 Overview of splitting methods

1.1.1 Motivation

Evolution equations are frequently used to model time dependent processes with applications found first and foremost in the natural and applied sciences. These equations may, for example, be used to describe advection-diffusion-reaction processes, wave propagations, fluid flows, and mechanical motions. We consider evolution equations on the form

$$\dot{u} = Fu, \quad u(0) = \eta. \tag{1.1}$$

where u is a time dependent solution and the dot denotes the time derivative. Here η denotes the initial value and F denotes a possibly nonlinear operator, also referred to as the vector field. Both ordinary differential equations (ODEs) and partial differential equations (PDEs) may be represented by Equation (1.1). In the former case the solutions $u(t)$ at a time t are elements of finite-dimensional state spaces. In the latter, these state spaces are infinite-dimensional function spaces. Therefore an analysis of numerical

time discretization schemes applied to Equation (1.1) can all at once cover a big variety of evolution systems. This equation is therefore commonly referred to as an *abstract* evolution equation. For PDEs there is also the added advantage that analysis results are independent of potential space discretizations. Not only does this give a general theory, but it also means that convergence order analyses automatically give orders independent of space discretization parameters.

In the research presented in this thesis we analyze splitting methods employed as temporal discretizations of Equation (1.1). After introducing a grid in time, the idea is to split the operator F,

$$F = F_1 + F_2, \tag{1.2}$$

and then in each time step iterate between the *subproblems*

$$\dot{\varphi} = F_1\varphi \quad \text{and} \quad \dot{\psi} = F_2\psi, \tag{1.3}$$

finding exact or approximate solutions to them, one at a time. Splitting into more terms is of course also possible, but for now we confine the study to splittings with two terms. Additionally, note that at this stage we are not concerned with the existence or uniqueness of solutions. In Section 2.1 we will introduce the framework of dissipative operators in which the existence of unique solutions is guaranteed, until then, the reader may consider the presented methods as formal.

As a first example we consider the simple *Lie–Trotter* splitting method taking n time steps of size k to find the approximation u_n of the exact solution u at time $t = nk$. One step of the method is given by, in sequence, solving the two evolution equations

$$\dot{\varphi} = F_1\varphi \quad \text{for} \quad nk < t \leq (n+1)k \quad \text{with} \quad \varphi(nk) = u_n, \tag{1.4}$$

$$\dot{\psi} = F_2\psi \quad \text{for} \quad nk < t \leq (n+1)k \quad \text{with} \quad \psi(nk) = \varphi((n+1)k), \tag{1.5}$$

and then taking $u_{n+1} = \psi((n+1)k)$. Let e^{tF} denote the exact flow of the evolution equation (1.1), that is

$$u(t) = \mathrm{e}^{tF}\eta. \tag{1.6}$$

We use similar notation for the flows of the subproblems, referred to as *partial flows*. Thus, one step S_k of the Lie–Trotter method can be written as

$$u_{n+1} = S_k u_n = \mathrm{e}^{kF_2}\mathrm{e}^{kF_1}u_n. \tag{1.7}$$

The scheme appeared already in the late 19th century as Lie's product formula for matrices and the analysis was extended to certain unbounded linear operators in [51].

Before we introduce more advanced splitting methods we linger a while longer with the Lie–Trotter scheme to illustrate the advantages of splitting methods. These advantages can be seen in many applications where the error introduced by the splitting is a small price to pay compared to what can be gained from the separation of the flows.

Therefore, the splitting methods are in general employed when the subproblems (1.3) are considerably easier to solve than the full problem (1.1). A good illustration is given by the following example which is taken from the study of Hamiltonian ODEs:

Example 1. Let $u_1(t) \in \mathbb{R}^{3d}$ denote the momenta and $u_2(t) \in \mathbb{R}^{3d}$ denote the positions of d particles moving in a potential $U : \mathbb{R}^{3d} \to \mathbb{R}$ in a three-dimensional domain. Their movements are governed by the Hamiltonian system

$$\begin{cases} \dot{u}_1 = -(\dfrac{\partial}{\partial u_2} U)(u_2), \\ \dot{u}_2 = M^{-1} u_1, \end{cases}$$

where M is a diagonal matrix containing the masses of the particles. The flow of the coupled system is in general difficult to characterize whereas the splitting

$$F_1 : \begin{pmatrix} v_1 \\ v_2 \end{pmatrix} \mapsto \begin{pmatrix} 0 \\ M^{-1} v_1 \end{pmatrix}, \quad F_2 : \begin{pmatrix} v_1 \\ v_2 \end{pmatrix} \mapsto \begin{pmatrix} -(\frac{\partial}{\partial v_2} U)(v_2) \\ 0 \end{pmatrix},$$

gives the simple partial flows

$$\mathrm{e}^{kF_1} : \begin{pmatrix} v_1 \\ v_2 \end{pmatrix} \mapsto \begin{pmatrix} v_1 \\ v_2 + kM^{-1} v_1 \end{pmatrix}, \quad \mathrm{e}^{kF_2} : \begin{pmatrix} v_1 \\ v_2 \end{pmatrix} \mapsto \begin{pmatrix} v_1 - k(\frac{\partial}{\partial v_2} U)(v_2) \\ v_2 \end{pmatrix},$$

where $v = (v_1 \ v_2)^{\mathrm{T}}$ denotes any vector in $\mathbb{R}^{6d}$. Furthermore, with this splitting the Lie–Trotter scheme is built from exact solutions of Hamiltonian systems and is therefore a symplectic integrator. See [15, 20, 37, 44] for more on splitting methods for Hamiltonian systems and in particular [20, Section II.5] for details on the current example.

It is not always as easy to find the partial flows as in Example 1. However, splitting methods can still be motivated when the flows of the operators F_1 and F_2 are easier to approximate than the full flow. This may for example happen when F_1 and F_2 exhibit different characteristics as illustrated by the following Gray–Scott pattern formation model:

Example 2. Let $u_1(x,t)$ and $u_2(x,t)$ denote the concentrations of two chemical compounds where the spatial variable x is given in a rectangular domain in $\mathbb{R}^2$. The Gray–Scott equations then read

$$\begin{cases} \dot{u}_1 = C_1 \Delta u_1 - u_1 u_2^2 + C_2(1 - u_1), \\ \dot{u}_2 = C_3 \Delta u_2 + u_1 u_2^2 - C_4 u_2, \end{cases}$$

for some positive parameters C_i. The stiffness induced by the Laplace operator calls for an implicit time integration method. However, the application of an implicit solver to the

whole system requires the solution of nonlinear equations coupled over the compounds and over space. On the other hand, for $v = (v_1\ v_2)^{\mathrm{T}} = (v_1(x)\ v_2(x))^{\mathrm{T}}$ consider the splitting

$$F_1 : \begin{pmatrix} v_1 \\ v_2 \end{pmatrix} \mapsto \begin{pmatrix} C_1 \Delta v_1 \\ C_3 \Delta v_2 \end{pmatrix}, \quad F_2 : \begin{pmatrix} v_1 \\ v_2 \end{pmatrix} \mapsto \begin{pmatrix} -v_1 v_2^2 + C_2(1 - v_1) \\ v_1 v_2^2 - C_4 v_2 \end{pmatrix}.$$

With this splitting Equation (1.4) is a linear, constant-coefficient diffusion equation, thus an approximate solution can easily be found, for example by using a spectral method. Moreover, Equation (1.5) is nonstiff and an approximate solution can therefore be found by an explicit Runge–Kutta method, for example. This may be done by taking a number of substeps in the interval $(nk, (n+1)k]$ of size smaller than k. For more on splitting methods for advection-diffusion-reaction systems see [30, 36] and, particularly, for details on the current example see [30, Section I.1.4] and Example 6 of Paper I.

In what follows we will overview some important classes of splitting methods. Convergence of these methods for ODEs, when the operators F_1 and F_2 are smooth, is well understood and treated in detail for all presented classes in [20, 30, 36, 37, 44]. In this setting, consistency orders can be found by comparing Taylor expansions of the exact flow e^{kF} and the numerical flow S_k. We refer to convergence orders found in this setting as *classical orders*. In the infinite-dimensional case, when for example splitting PDEs, the operators are commonly unbounded, consider for example the Laplace operator in Example 2. In this setting Taylor expansion is not an option in convergence considerations. In the following subsections we refer to convergence studies that are relevant to the specific classes of splitting methods in the infinite-dimensional setting.

1.1.2 Exponential splitting methods

In this section we overview *exponential* splitting methods. These methods can be written as products of the partial flows

$$S_k = \prod_{i=1}^{r} \mathrm{e}^{\alpha_i k F_1} \mathrm{e}^{\beta_i k F_2}$$

for some complex coefficients α_i and β_i. We assume here that the subproblems defined by the partial flows are either solved exactly or that approximations are given with errors small compared to the splitting error.

The most characteristic exponential splitting method is the Lie–Trotter scheme (1.7), which has classical order one. The other prominent member of this class is the second order *Strang splitting*

$$S_k = \mathrm{e}^{\frac{1}{2} k F_2} \mathrm{e}^{k F_1} \mathrm{e}^{\frac{1}{2} k F_2},$$

which was introduced in 1968 in [48]. This method is symmetric, meaning that $S_{-k} S_k$ is the identity operator. One way to construct methods of higher classical orders is to use

Yoshida's triple jump composition, introduced in [52]. Assume that S_k is an arbitrary numerical method of order p, then the composite method

$$u_{n+1} = S_{\gamma_1 k} S_{\gamma_2 k} S_{\gamma_1 k} u_n \tag{1.8}$$

with

$$\gamma_1 = (2 - 2^{1/(p+1)})^{-1}, \quad \gamma_2 = -2^{1/(p+1)} \cdot (2 - 2^{1/(p+1)})^{-1}$$

is of order $p + 2$ if S_k is symmetric and of order $p + 1$ otherwise. Thus, the triple jump composition with S_k as in the Strang splitting results in a fourth order symmetric splitting method. More details and more general compositions are presented in [20, Section II.4] and [44, Section 13.1].

For convergence studies of exponential splitting methods in the presence of unbounded operators we refer to [11, 21, 22, 24] for parabolic, [28] for hyperbolic, and [15, 35] for Schrödinger type problems, see also references therein. As an example we mention here the results of [24], where it is shown that classical convergence orders of exponential splittings are retained for linear, dissipative evolution equations.

Since the coefficients γ_1 and γ_2 in the composition (1.8) have different signs, negative flows are present. This can be problematic, especially for parabolic PDEs, such as the heat equation, which may be ill-posed for negative time progressions. In fact, all exponential splitting methods of order higher than two with real coefficients must evaluate negative flows of both operators, see [17, 47]. However, higher order splitting methods can still be used for parabolic PDEs if one allows for complex coefficients, confer [6, 25].

We conclude this overview of exponential splitting methods by noting that they can also be constructed for operators F split into more than two components, for example, for m operators the Lie–Trotter splitting has the form

$$S_k = \mathrm{e}^{kF_m} \cdots \mathrm{e}^{kF_2} \mathrm{e}^{kF_1}.$$

Additional generalizations are given by considering linear combinations of exponential splittings. For more on these generalizations see [30, Sections IV.1.1–IV.1.3]. See also [16] for a study of exponential splitting methods in the setting of inhomogeneous evolution equations.

1.1.3 ADI and IMEX methods

In general the subproblems (1.3) cannot be solved exactly. In Example 2 we saw how this can be resolved by choosing suitable numerical methods for each subproblem depending on their characteristics. Another approach is to directly construct the method S_k from low order approximations of the partial flows. Since there are several splitting methods that are based on this idea, we discuss here only those that are most relevant to the current presentation. These can be separated into two classes, the alternating direction implicit (ADI) methods and the *implicit-explicit* (IMEX) methods (also referred to

as semi-implicit methods). We refer to [30, Chapter IV] and [36] for more details on the presented method classes and others that are left out here.

The ADI methods where introduced in the 1950s to perform dimension splitting of the heat equation

$$F_1 + F_2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}.$$

The name of the class also comes from this application since the integration of a dimension splitting means alternating between the spatial directions. The first ADI method, the *Peaceman–Rachford* (PR) scheme, which has classical order two, was introduced in 1955 in [12, 41]. The scheme is constructed from low order approximations given by explicit and implicit Euler steps. More precisely, let I denote the identity operator, then the scheme can be written as

$$S_k = (I - \frac{k}{2}F_2)^{-1}(I + \frac{k}{2}F_1)(I - \frac{k}{2}F_1)^{-1}(I + \frac{k}{2}F_2). \tag{1.9}$$

The year after, the first order *Douglas–Rachford* (DR) scheme,

$$S_k = (I - kF_2)^{-1}[(I - kF_1)^{-1}(I + kF_2) - kF_2], \tag{1.10}$$

was introduced in [13] with the argument that it can be easily extended to the case where the operator F is split into more than two terms—this is not true for the PR scheme.

The DR scheme can be derived as a modification of the simple, first order *Lie* splitting

$$S_k = (I - kF_2)^{-1}(I - kF_1)^{-1}. \tag{1.11}$$

which is a *locally one-dimensional* (LOD) method. See [30, Section IV.2] and [36, Chapter II] for overviews of these methods. In [26, 46] it is shown that the modification that constructs the DR scheme also makes it a suitable method when considering inhomogeneous problems or problems with inhomogeneous boundary conditions. See also [29] for a study of the PR scheme applied to an inhomogeneous problem and [30, Section IV.3] for more on both methods in this setting.

In Paper I and [26] it is shown that the PR and DR schemes both have advantageous local error structures. We will discuss this in further detail in Section 2.2. A direct consequence of their favorable error structure is that both schemes preserve fixed points of the exact flow, that is, if $\mathrm{e}^{kF}\bar{u} = \bar{u}$ then $S_k\bar{u} = \bar{u}$. This means that they are suitable for marching towards solutions of the stationary problem, $F\bar{u} = 0$, confer [30, Section IV.3] and [34]. In general, splitting methods do not preserve fixed points, for example the Lie splitting (1.11) does not exhibit this property.

Additionally, the PR and DR schemes are known to possess excellent stability properties. See [10, 23, 26, 29, 34, 45] and [30, Section IV.3] for stability considerations in various settings. In this thesis we will advance the state of the art in convergence studies for the PR and DR schemes. We will thus discuss the mentioned literature in greater

detail in Section 1.2 when stating the aims and goals of the research presented in this thesis.

Furthermore, in contrast to what one might believe at first glance, taking a step with PR or DR costs as little as a step with Lie (1.11). This can be seen by using the change of variables $u_n = (I - k/2 \cdot F_2)^{-1} w_n$ to rewrite the scheme (1.9) as

$$w_{n+1} = [2(I - \frac{k}{2}F_1)^{-1} - I][2(I - \frac{k}{2}F_2)^{-1} - I]w_n.$$

Similarly, with $u_n = (I - kF_2)^{-1} w_n$ the scheme (1.10) can be rewritten as

$$w_{n+1} = [(I - kF_1)^{-1}(2(I - kF_2)^{-1} - I) + I - (I - kF_2)^{-1}]w_n.$$

In addition to the PR and DR schemes there are commonly used generalizations of the DR scheme which are usually classified as ADI methods, confer [30, Section IV.3.2]. However, there seems to be no well-recognized definition of what constitutes an ADI method. In our experience, when used in the literature, ADI seems to refer to the PR and DR schemes and possible generalizations of them where the key aspects are fixed point preservation and implicitness in both operators F_1 and F_2.

The IMEX methods constitute another class of methods that approximate the partial flows. They are applicable to situations where the operator F_2 is nonstiff, as in Example 2. The representative method is the first order *IMEX Euler* scheme

$$S_k = (I - kF_1)^{-1}(I + kF_2),$$

which is constructed from the conventional Euler methods. However, IMEX methods may be constructed by other combinations of implicit and explicit methods, see [30, Section IV.4] for constructions involving multistep and Runge–Kutta methods. Convergence orders for IMEX Euler applied to semilinear parabolic PDEs are proven in [32, 50]. Convergence and stability considerations for IMEX methods applied to semilinear evolution equations are carried out in [2, 39]. For convergence studies in the fully nonlinear setting see [27, 31].

1.2 Research goals and thesis overview

The overall goal of the research presented in this Licentiate thesis is:

> *Perform convergence studies for the PR and DR schemes for linear and semilinear, dissipative evolution equations and verify the results on relevant applications within science and technology.*

Since we want to cover a big variety of evolution equations we are interested in the general, infinite-dimensional setting of unbounded vector fields. The most typical examples of evolution systems that fit into the framework of dissipative operators are found

among the parabolic PDEs. However, applications may also be found among hyperbolic PDEs and Schrödinger type equations, confer for example [53, Chapter 19].

Under the assumption that both operators F_1 and F_2 are linear and dissipative optimal convergence orders were proven in [23] for the the PR scheme (1.9) and in [26] for the DR scheme (1.10). By optimal orders we mean that the classical orders (which apply in the ODE context) are preserved in the more general setting, in this case, for unbounded operators. This leads to the first of the three topics that define the aim of the research:

Research topic 1. *Prove optimal convergence orders for the PR and DR schemes in the unbounded, dissipative, semilinear setting, that is F_1 linear and F_2 (possibly) nonlinear, both unbounded and dissipative.*

This is discussed in Section 2.2 which is mainly based on Paper I. Previous studies for the PR scheme in the semilinear setting include [10] where second order convergence is proven when F_2 is bounded and seven times continuously differentiable. Convergence without orders are proven for nonlinear evolution equations in [34]. Partial convergence studies are carried out in [29, 45].

For PDEs the time discretization needs to be combined with a space discretization. For instance, when finding an approximate solution to the parabolic PDE in Example 2 we may employ a finite difference or finite element method to discretize the spatial derivatives. When both a temporal and a spatial discretization has been used to approximate Equation (1.1) we refer to it as being *fully discretized*. We consider general spatial discretization which are convergent for the stationary problem: $Fv = f$ for a given f. We formulate the second research topic:

Research topic 2. *Prove optimal, simultaneous space-time convergence orders for full discretizations of evolution equations when the PR or DR scheme is used as temporal discretization and when the only assumptions on the operator F are that it is linear and dissipative.*

The analysis is presented in Paper II and summarized in Section 2.3. Simultaneous space-time convergence orders when the explicit Euler or the Crank–Nicholson scheme is used as temporal discretization have been proven in [9, 50] under similar assumptions as ours. In [2, 32, 50] full space-time convergence orders are given when IMEX methods are applied to various semilinear problems. Convergence without orders are proven in [4] when exponential splittings are used for the temporal discretization. For the PR scheme partial results with orders in time can be found in [29].

We move on from the general, abstract convergence studies and arrive at a biological model for which the choice and application of a numerical method is non-trivial. We find this problem in the modeling of axon growth in neurons (nerve cells). Axons are long, thin outgrowths from the cell body, the soma, with the purpose of transmitting electrical signals to other neurons. The concentration of the globular 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. In [38] a one-dimensional advection-diffusion-reaction model is constructed for the tubulin concentration along the axon. In Paper III we propose a modification and extension of this model to include the processes governing tubulin concentration in the growth cone. Mathematically we arrive at a parabolic PDE coupled with nonlinear ODEs through a boundary condition at a moving boundary. This system of differential equations is then used in a thorough study of steady-states. In the current research we focus on efficient and accurate numerical simulations. To this end we state the third research topic:

Research topic 3. *The wide range of axon length scales, the moving boundary, the boundary condition coupling with nonlinear ODEs, and the stiffness of the diffusion makes the application of a numerical method to the axon growth problem non-trivial. We aim to construct an efficient numerical scheme based on the the operator splitting and excellent stability properties of the PR method. We will evaluate the scheme on how well it deals with the aforementioned difficulties of the model and how useful it is in the study of steady-states.*

The model is presented in detail in Paper III. We discuss it in Section 3.1 and give some preliminary numerical experiments in Section 3.2.

Chapter 2

Convergence Studies

In the current chapter we summarize the convergence studies called for by the first two research topics. In Section 2.1 we overview the theory of semigroups and maximal dissipative operators that is needed for the analyses. Convergence orders for the PR scheme applied to semilinear evolution equations are proven in Paper I. The results are summarized in Section 2.2, where also convergence orders for the DR scheme are given. The full discretizations are analyzed in Paper II and a summary is given in Section 2.3. In Section 2.4 we give an example of a linear, parabolic PDE that fits into the framework of maximal dissipative operators.

2.1 Maximal dissipative operators

In the classical convergence analysis Taylor expansions are used to characterize the errors caused by numerical methods. However, these expansions rely on the boundedness of the operators F_1 and F_2 of Equation (1.2). Since we do not want to limit the attention to bounded operators the classical analysis cannot be applied. In this section we summarize some properties of maximal dissipative operators that give us the tools needed to perform convergence studies in the setting of unbounded operators.

Denote the state space by $\mathcal{H}$ and assume that it is a real Hilbert space equipped with the scalar product $(\cdot,\cdot)$ and related norm $\|\cdot\|$. The latter notation is also used for the induced operator norm. Consider the operator $G : \mathcal{D}(G) \subset \mathcal{H} \to \mathcal{H}$ with domain $\mathcal{D}(G)$ and let I denote the identity operator on $\mathcal{H}$. The operator G is maximal dissipative if and only if there is a constant $M[G] \geq 0$ such that G satisfies the range condition

$$\mathcal{R}(I - kG) = \mathcal{H} \quad \text{for all } k > 0 \text{ with } kM[G] < 1 \tag{2.1}$$

and the dissipativity condition

$$(Gv_1 - Gv_2, v_1 - v_2) \leq M[G]\|v_1 - v_2\|^2 \quad \text{for all } v_1, v_2 \in \mathcal{D}(G). \tag{2.2}$$

For maximal dissipative operators the resolvent

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

related to G is well defined for all $k > 0$ such that $kM[G] < 1$. Additionally, the resolvent is Lipschitz continuous:

$$\|(I - kG)^{-1}v_1 - (I - kG)^{-1}v_2\| \leq \frac{1}{1 - kM[G]}\|v_1 - v_2\|, \tag{2.3}$$

for all v_1, v_2 in $\mathcal{H}$, confer [3, Proposition 3.2].

We are now ready to state the central assumption of the presented research:

ASSUMPTION 1. *The operator $F : \mathcal{D}(F) \subset \mathcal{H} \to \mathcal{H}$ of Equation* (1.1) *is maximal dissipative on $\mathcal{H}$.*

For the stability analysis, we will also use that the operators F_1 and F_2 exhibit this property since this enables us to use bounds of the type (2.3) to prove stability of the PR and DR schemes. However, since the details of the splittings differ between the studies we will assume properties for the partial vector fields at first in the upcoming sections.

In Equation (1.6) we introduced the flow e^{tF} of Equation (1.1). Under Assumption 1 the flow can be characterized by the limit

$$u(t) = \mathrm{e}^{tF}\eta = \lim_{n\to\infty}(I - \frac{t}{n}F)^{-n}\eta. \tag{2.4}$$

For η in the closure of $\mathcal{D}(F)$ the maximal dissipativity ensures that the limit exists and that it is the unique mild solution of Equation (1.1). On this closure the flows form a strongly continuous semigroup $\{e^{tF}\}_{t\geq 0}$ of nonlinear operators. Furthermore, they fulfill the bound

$$\|\mathrm{e}^{tF}\eta_1 - \mathrm{e}^{tF}\eta_2\| \leq \mathrm{e}^{tM[F]}\|\eta_1 - \eta_2\|, \tag{2.5}$$

for all $t \geq 0$ and η_1, η_2 in the closure of $\mathcal{D}(F)$. This Lipschitz continuity serves as a potent tool in the stability analysis of exponential splitting methods and in Paper II we use it to transfer bounds of the solution $\mathrm{e}^{tF}\eta$ to bounds on the initial data η. We refer to [3, Sections 3.1 and 4.1] for more on nonlinear dissipative operators, the solution of Equation (1.1), and semigroups in more general Banach settings.

Linear operators $F = L$ fulfilling Assumption 1 have a domain $\mathcal{D}(L)$ that is dense in $\mathcal{H}$. As a direct consequence the semigroup $\{e^{tL}\}_{t\geq 0}$ is defined on the whole space $\mathcal{H}$. Furthermore, for any $\eta \in \mathcal{D}(L)$ the mild solution $\mathrm{e}^{t\bar{L}}\eta$ is a classical solution in the sense that it is an element of $\mathscr{C}^1([0,T];\mathcal{H})$. The derivative is given by

$$\dot{u}(t) = \frac{\mathrm{d}}{\mathrm{d}t}e^{tL}\eta = Le^{tL}\eta.$$

Additionally, the operator L commutes with its resolvent $(I - kL)^{-1}$ and its flow e^{tL}. Confer [14, 40] for more on the linear setting.

2.2 Semilinear evolution equations

In this section we summarize the results of Paper I where convergence orders are proven for the PR scheme when applied to semilinear, dissipative evolution equations. The optimal second order convergence is achieved for regular enough solutions u. However, with less regularity we may still get first order convergence or convergence without order. With the proof techniques used for the PR scheme in Paper I the same analysis can be performed for the DR scheme with just slight modifications of the details. Thus, we are here able to give the full spectrum of convergence orders for both the PR and the DR schemes depending on the regularity of the solution u. To this end we interpret the splitting (1.2) of the semilinear evolution equation (1.1) in the framework set up in the previous section.

ASSUMPTION 2. *The operator $F_1 = A$ is linear.*

ASSUMPTION 3. *The operators $A : \mathcal{D}(A) \subset \mathcal{H} \to \mathcal{H}$ and $F_2 : \mathcal{D}(F_2) \subset \mathcal{H} \to \mathcal{H}$ are maximal dissipative on $\mathcal{H}$.*

Let the evolution equation (1.1) be defined for times $t \in [0, T]$ where $T > 0$ is a finite end time. To derive convergence with orders we need the following regularity assumption:

ASSUMPTION 4. *Equation* (1.1) *has a classical solution $u \in \mathscr{C}^1([0, T]; \mathcal{H})$ that satisfies one of the following two regularity statements:*

1. *$u \in W^{2,1}(0, T; \mathcal{H})$ and $A\dot{u} \in L^1(0, T; \mathcal{H})$,*
2. *$u \in W^{3,1}(0, T; \mathcal{H})$, $A\ddot{u} \in L^1(0, T; \mathcal{H})$, and $A^2\dot{u} \in L^1(0, T; \mathcal{H})$.*

Furthermore, the domains fulfill the equality $\mathcal{D}(F) = \mathcal{D}(A) \cap \mathcal{D}(F_2)$.

Remark 1. According to [43, Lemma 7.1] the space $W^{2,1}(0, T; \mathcal{H})$ is continuously imbedded in $\mathscr{C}^1([0, T]; \mathcal{H})$. See also Sections 1.5 and 7.1 in this reference for more on Sobolev–Bochner spaces.

We can now state the convergence order theorem which is an extension of Theorem 2 in Paper I, the main result of that article.

Theorem 1. *Consider the approximate solution $S_k^n\eta$ given by the PR* (1.9) *or DR* (1.10) *discretization of the evolution equation* (1.1)*. If Assumptions 1, 2, and 3, are valid and $k \max\{M[A], M[F_2]\} < 1/(2C)$, then the global error can be bounded as*

$$\|u(nk) - S_k^n\eta\| \leq 5Ck^p \mathrm{e}^{3CT(M[A]+M[F_2])} \sum_{i=0}^{p} \|A^{p-i}u^{(i+1)}\|_{L^1(0,T;\mathcal{H})}, \quad nk < T,$$

with first order convergence, $p = 1$, for both schemes under Assumption 4.1 or second order convergence, $p = 2$, for the PR scheme under Assumption 4.2. The constant C is $1/2$ for

the PR scheme and 1 *for the DR scheme. Here,* $u^{(i)}$ *denotes time derivative number* i *of the solution* u*.*

The full proof for the PR scheme can be found in Paper I. Stability is proven solely using Assumption 3 whereas the consistency proof also relies on the other assumptions. The convergence orders for the DR scheme can be proven with the same techniques. See also Lemma 2 in Paper II where convergence of the DR scheme in a linear finite-dimensional setting is considered.

Even if the solution u does not exhibit the regularity dictated by Assumption 4 convergence without order can still be proven. This is not a new result since $o(1)$-convergence for the PR and DR schemes are given already by [34, Theorem 2] for $M[A] = M[F_2] = 0$. However, our proof in the semilinear setting is significantly shorter. The following theorem extends Theorem 3 of Paper I to include also the DR scheme.

Theorem 2. *Consider the approximate solution* $S^n_{t/n}\eta$ *given by the PR* (1.9) *or DR* (1.10) *discretization of the evolution equation* (1.1)*. If Assumptions 1, 2, and 3 are valid and* $\mathcal{D}(F) = \mathcal{D}(A) \cap \mathcal{D}(F_2)$ *is dense in* $\mathcal{H}$*, then*

$$\lim_{n\to\infty} S^n_{t/n}\eta = u(t),$$

for every $\eta \in \mathcal{D}(F_2)$ *and* $t \geq 0$*.*

Note that in the absence of Assumption 4 we generally do not have a classical solution of Equation (1.1), instead convergence happens to the mild solution (2.4). Only details differ in the proof for the DR scheme.[1]

In Paper I we also prove first order convergence for the Lie splitting (1.11). We present the results here to illustrate the advantageous error structure of the PR and DR schemes. For Lie the regularity assumption 4.1 is replaced by the following more restrictive assumption:

ASSUMPTION 5. *Equation* (1.1) *has a classical solution* $u \in \mathscr{C}^1([0,T];\mathcal{H})$ *such that* $u \in W^{2,1}(0,T;\mathcal{H})$ *and* $A\dot{u}, A^2u \in \mathscr{C}([0,T],\mathcal{H})$*. Furthermore, the domains fulfill the equality* $\mathcal{D}(F) = \mathcal{D}(A) \cap \mathcal{D}(F_2)$*.*

Theorem 3. *Consider the approximate solution* $S^n_k\eta$ *given by the Lie discretization* (1.11) *of the evolution equation* (1.1)*. If* $k\max\{M[A], M[F_2]\} \leq 1/2$ *and Assumptions 1, 2, 3, and 5 are valid, then the global error can be bounded as*

$$\|u(nk) - S^n_k\eta\| \leq 2k\mathrm{e}^{2T(M[A]+M[F_2])}(\|\ddot{u}\|_{L^1(0,T;\mathcal{H})} + T\|A\dot{u} - A^2u\|_{\mathscr{C}([0,T];\mathcal{H})}),$$

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

$$\begin{aligned} R &= I + kA(I-kA)^{-1} + kF_2(I-kF_2)^{-1} \\ &\quad + 2k[(I-kA)^{-1} - I][F_2(I-kF_2)^{-1} - F_2] + 2k[(I-kA)^{-1} - I]F_2. \end{aligned}$$

for $nk < T$.

Remark 2. Assumption 5 is an erratum of Assumption 3 in Paper I. Instead of prescribing $A\dot{u}, A^2u \in \mathscr{C}([0,T],\mathcal{H})$ the latter prescribes $A\dot{u}(t), A^2u(t) \in \mathcal{H}$ for every $t \in [0,T]$ which is not enough since the proof of Theorem 3 (also Theorem 4 of Paper I) requires that the supremum of $\|A\dot{u}(t) - A^2u(t)\|$ in the time interval $[0,T]$ is finite.

Note that the term A^2u found in Assumption 5 is not present in Assumption 4.1. That is, to obtain first order convergence, the PR and DR schemes require less regularity than the Lie splitting. An example where this advantage proves useful is in the analysis of full discretization as we will see in the next section.

2.3 Full space-time discretizations

In Paper II we consider simultaneous space-time convergence. That is, we assume that the evolution equation (1.1) is discretized both in time and space and look for a global error representation on the form

$$\mathcal{O}(h^s + k^p),$$

for some positive numbers s and p and where h measures the accuracy of the space discretization. In this section we supplement the presentation of Paper II by expanding on the connection to Paper I and Section 2.2. We limit the attention to fully linear problems:

ASSUMPTION 6. *The operators* $F_1 = A$ *and* $F_2 = B$ *(and therefore also* $F = L$*) are linear.*

Let $\{\mathcal{H}_h\}_{0<h\leq h_{\max}}$ be a family of finite-dimensional spaces of increasing dimension as h tends to zero. Equip each of them with an inner product $(\cdot,\cdot)_h$ which may depend on the parameter h. Additionally, define the discrete operators $A_h : \mathcal{H}_h \to \mathcal{H}_h$, $B_h : \mathcal{H}_h \to \mathcal{H}_h$, and $L_h = A_h + B_h$. The spatial semi-discretization is then given by the ODE

$$\dot{u}_h = L_h u_h = (A_h + B_h)u_h, \quad u_h(0) = \eta_h, \tag{2.6}$$

for an approximation $\eta_h \in \mathcal{H}_h$ of η. We consider general space discretizations that are convergent for the stationary problem $Lv = f$, that is

$$\|L^{-1}f - L_h^{-1}P_h f\| \leq Ch^s \sum_{i=0}^{q} \|L^i f\|, \quad \text{for every } f \in \mathcal{D}(L^q), \tag{2.7}$$

where $q = 0$ or 1, and the operator $P_h : \mathcal{D}(L^q) \subset \mathcal{H} \to \mathcal{H}_h$ is similar to a projection from $\mathcal{H}$ to $\mathcal{H}_h$. The details are given in Assumption 2 of Paper II. In this section we use C as a generic constant taking different values at different occurrences, however always independent of h, k and n. Note that it is implicitly assumed here that L and L_h are

invertible, this assumption is made for the sake of simplicity, the theory holds even for noninvertible operators by making some small changes.

Our convergence analysis only consider the temporal discretizations on the spaces $\mathcal{H}_h$ and therefore no maximal dissipativity assumptions are needed for A and B. Instead we assume these properties from the discrete operators A_h and B_h (and L_h) for which they are generally easier to prove. Only Assumptions 1 and 6 are required from the infinite-dimensional operators. The former assumption is needed to ensure the existence of a unique solution to Equation (1.1) and to enable us to use the semigroup theory of Section 2.1. The analysis also relies on the linearity prescribed by the latter assumption. With this in place we get solutions that are differentiable in time and vector fields that commute with their corresponding flows.

Assumption 2 of Paper II prescribes convergence of the stationary problem and dissipativity of the discrete operators (with $M[A_h] = M[B_h] = M[L_h] = 0$ for the sake of simplicity). Additionally, it lists some technical assumptions that we do not recapitulate here. We also note that in the linear, finite-dimensional setting dissipativity (2.2) implies maximality (2.1).

As we saw in Section 2.2, to get orders in time, the splitting schemes require some regularity from the solution. However, in our linear, finite-dimensional setting Assumption 4 is valid without any further assumptions. Indeed, the domain condition of Assumption 4 is trivially fulfilled for the discrete operators. Additionally, since L_h is linear and $\eta_h \in \mathcal{H}_h = \mathcal{D}(L_h)$ we have that $u_h(t) = \mathrm{e}^{tL_h}\eta_h$ is a classical solution of the ODE (2.6), see Section 2.1. Furthermore we have

$$\|A_h \ddot{u}_h\|_{L^1(0,T;\mathcal{H}_h)} = \int_0^T \|A_h e^{tL_h} L_h^2 \eta_h\|_h \,\mathrm{d}t \leq T\|A_h L_h^{-1}\|_h \|L_h^3 \eta_h\|_h, \qquad (2.8)$$

where we have used the Lipschitz continuity (2.5) and the commutativity of L_h and e^{tL_h}. The last statement of the equation is trivially fulfilled for finite-dimensional operators. With similar reasoning for the other regularity requirements in Assumption 4 we conclude that the assumption is fulfilled. However, not to lose order we need bounds that are uniform in h for the factors $\|A_h L_h^{-1}\|_h$ and $\|L_h^3 \eta_h\|_h$. The latter bound can be translated to regularity requirements on the initial data η whereas the former bound need to be stated as a separate assumption.

ASSUMPTION 7. *The discrete operators A_h and L_h satisfy one of the following two sets of uniform bounds:*

1. $\|A_h L_h^{-1}\|_h \leq C$ *for all* $h \in (0, h_{max}]$,
2. $\|A_h L_h^{-1}\|_h \leq C$ *and* $\|A_h^2 L_h^{-2}\|_h \leq C$ *for all* $h \in (0, h_{max}]$,

where the constant C is independent of h.

Under these assumptions we can state the central theorem of Paper II. Let $S_{k,h}$ be the numerical flow given by applying a temporal discretization to the semi-discretization (2.6). That is the PR and DR full discretizations are given by replacing all occurrences of A and B with A_h and B_h, respectively, in Equations (1.9) and (1.10), respectively. Additionally, let s and q be positive numbers, where s is the convergence order of the spatial discretization. See Paper II for the meaning of q.

Theorem 4. *Let the numerical flow $S_{k,h}$ be defined by either the PR* (1.9) *or the DR* (1.10) *scheme and (for the sake of simplicity) assume that L and L_h are invertible. Assume that Assumptions 1 and 6 of this chapter are valid. Further, assume that A_h and B_h are dissipative, that Equation* (2.7) *holds for some q and s, and that the technical assumptions 2.1, 2.2 and 2.4 in Paper II are valid. Then, if additionally $\eta \in \mathcal{D}(L^{p+q+1})$, we have*

$$\|u(nk) - S_{k,h}^n \eta_h\| \leq C(h^s + k^p) \sum_{i=1}^{p+q+1} \|L^i \eta\|,$$

with first order convergence, $p = 1$, for both schemes under Assumption 7.1 or second order convergence, $p = 2$, for the PR scheme under Assumption 7.2. The approximate initial data η_h is assumed to be the Ritz projection $\eta_h = L_h^{-1} P_h L \eta$. The constant C can be chosen uniformly on bounded time intervals and, in particular, independently of h, k and n.

Remark 3. As we mentioned earlier Theorem 4 also holds for non-invertible L and L_h, confer Remark 3 of Paper II for the necessary modifications of the assumptions and proofs.

2.4 Application to a linear parabolic PDE

As we have previously mentioned, parabolic PDEs constitute common examples of dissipative evolution equations. We give an example here on how a linear PDE, taken from Section 4 of Paper II, can be fit into the dissipative framework of abstract evolution equations. This construction is generally known as the Friedrichs extension, for more details see for example [9, Sections 1–2] or [53, Chapter 19]. For introductions to partial differential equations and Sobolev spaces confer [1, 42].

Consider the two-dimensional diffusion equation

$$\dot{u} = \frac{\partial}{\partial x}(a_1 \frac{\partial}{\partial x} u) + \frac{\partial}{\partial y}(a_2 \frac{\partial}{\partial y} u), \quad u(0) = \eta, \tag{2.9}$$

defined on $\Omega = (0,1)^2$ and equipped with homogeneous Dirichlet boundary conditions. The continuously differentiable coefficient functions fulfill $a_i(x,y) \geq a_0 > 0$ for all $(x,y) \in \Omega$, $i = 0, 1$. To interpret Equation (2.9) in a weak setting let $\mathcal{H} = L^2(\Omega)$ and define the chain of imbeddings

$$H_0^1(\Omega) \hookrightarrow L^2(\Omega) \cong L^2(\Omega)' \hookrightarrow H^{-1}(\Omega)$$

where $L^2(\Omega)'$ denotes the dual space of $L^2(\Omega)$ and $H^{-1}(\Omega)$ that of $H_0^1(\Omega)$. We define on $H_0^1(\Omega)$ the bilinear form

$$b(v,w) = (a_1 \frac{\partial}{\partial x} v, \frac{\partial}{\partial x} w)_{L^2(\Omega)} + (a_2 \frac{\partial}{\partial y} v, \frac{\partial}{\partial y} w)_{L^2(\Omega)},$$

which is bounded and coercive, confer [33, Section 3.5]. That is, there are some positive constants C_1 and C_2 such that

$$b(v,w) \leq C_1 \|v\|_{H^1(\Omega)} \|w\|_{H^1(\Omega)} \quad \text{and} \quad b(v,v) \geq C_2 \|v\|^2_{H^1(\Omega)},$$

for all $v, w \in H_0^1(\Omega)$. Define the associated operator $\hat{L} : H_0^1(\Omega) \to H^{-1}(\Omega)$ by

$$\hat{L}v = -b(v, \cdot).$$

For a positive constant C we get from the coercivity of b that

$$((I - k\hat{L})v)v = \|v\|^2_{L^2(\Omega)} + kb(v,v) \geq C\|v\|^2_{H^1(\Omega)},$$

for all $v \in H_0^1(\Omega)$ and for any $k > 0$. Since additionally the operator $I - k\hat{L}$ is bounded it is a bijection according to Lax-Milgram's lemma, [42, Theorem 9.14].

To interpret $\hat{L}$ as an unbounded operator on $L^2(\Omega)$ we introduce the space

$$\mathcal{D}(L) = \{v \in H_0^1(\Omega);\ \hat{L}v \in L^2(\Omega)'\},$$

and define L as the restriction of $\hat{L}$ to $\mathcal{D}(L)$. We note that the restriction of $I - k\hat{L}$ is a surjection to $L^2(\Omega)'$, and thus, by identifying $L^2(\Omega)$ with its dual $L^2(\Omega)'$, we have that $L : \mathcal{D}(L) \subset L^2(\Omega) \to L^2(\Omega)$ is maximal. The dissipativity follows from the coercivity of b. Thus, L fulfills Assumption 1 and the $L^2(\Omega)$-interpretation of the parabolic PDE (2.9) is then given by Equation (1.1). We note that in the current setting we can characterize $\mathcal{D}(L)$ as

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

This is proven in [19, Theorem 9.1.22], see also [18] for more on regularity of elliptic PDEs.

In Section 4 of Paper II the above construction is used to apply the abstract results of Theorem 4 to dimension splitting where the spatial discretization is given by a quadrature finite element method. Confer [5, 7, 49, 50] for introductions to finite element methods in general and [8] for quadrature finite elements in particular.

Chapter 3

An Application to Axonal Growth

In Paper III we propose a continuum model for axon growth in nerve cells. Stability of steady-states is studied using numerical computations with the explicit Euler as temporal discretization. In the current chapter we will instead make an argument for using the PR scheme in the study of the time-evolution of the axon growth model. The presentation is based on preliminary results from a work in progress. The model is presented in Section 3.1 and numerical results are given in Section 3.2.

3.1 A continuum model for axonal growth

The axon growth model of Paper III is a one-dimensional moving-boundary problem consisting of an advection-diffusion-reaction PDE coupled with two nonlinear ODEs. Consider the schematic illustration of an idealized growing axon in Figure 3.1. 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 a model output 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 the differential equations

$$\begin{cases} \dot{c} = D\dfrac{\partial c^2}{\partial x^2} - a\dfrac{\partial c}{\partial x} - gc, \\ \dot{c}_{\mathrm{c}} = [(a - gl_{\mathrm{c}})c_{\mathrm{c}} - Dc_x^- - (r_{\mathrm{g}}c_{\mathrm{c}} + \tilde{r}_{\mathrm{g}}l_{\mathrm{c}})(c_{\mathrm{c}} - c_\infty)]/l_{\mathrm{c}}, \\ \dot{l} = r_{\mathrm{g}}(c_{\mathrm{c}} - c_\infty), \end{cases} \tag{3.1}$$

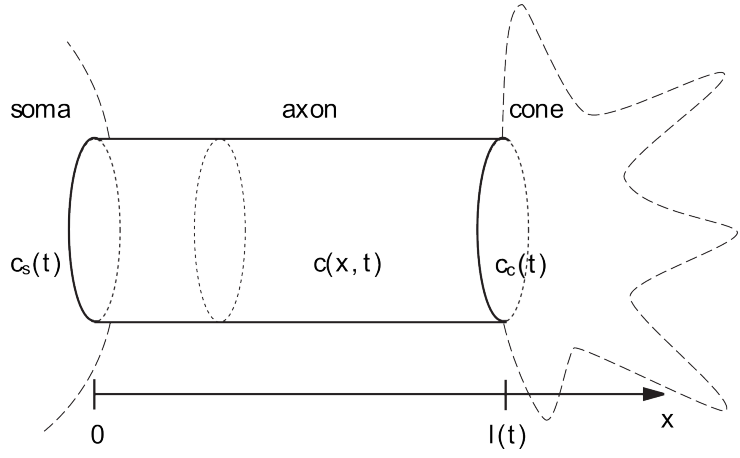


Figure 3.1: Schematic illustration of a nerve cell. The soma produces tubulin which is transported along the axon to the growth cone. There the axon is expanded by tubulin polymerization.

coupled with the boundary and initial conditions

$$\begin{cases} c(0,t) = c_{\mathrm{s}}(t), \\ c(l(t),t) = c_{\mathrm{c}}(t), \\ c(x,0) = c_0(x), \\ c_{\mathrm{c}}(0) = c_0(l_0), \\ l(0) = l_0, \end{cases} \tag{3.2}$$

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 III for relevant references and for a detailed derivation of the model and the values of its parameters.

The model (3.1), (3.2) exhibit some challenges that a successful numerical method must address, especially when studying convergence to steady-states. We summarize these in a wish list. The applied numerical method should be able to handle:

1. The moving boundary of the domain $(0, l(t))$.

2. Big variations in axon length scales as steady-state lengths 10^5 times bigger than initial lengths are expected.

3. The coupling of the PDE to the nonlinear ODEs through the tubulin concentration and its flow at the moving boundary.

4. The stiffness of the PDE.

5. Marching towards steady-states, that is the method should preserve fixed points.

The expanding (or contracting) domain was considered already in [38] where a spatial scaling was proposed. For short axon lengths the advection and diffusion effects are big in relation to the size of the domain. Therefore, the performance of a numerical method is to a big extend determined by these short length scales. Big time steps may be possible late in the simulation but for many methods this cannot be utilized since the step has to be small to accurately resolve the initial evolution of the model. To alleviate, we propose a temporal scaling in addition to the spatial scaling. Assuming that $l(t) > 0$ at all times, we define the coordinate transformation

$$\begin{cases} y = \dfrac{x}{l(t)}, \\ \tau = g(t) = a\displaystyle\int_0^t \frac{1}{l(s)}\mathrm{d}s, \end{cases} \qquad 0 \le x \le l(t),\, t \ge 0. \tag{3.3}$$

Since $\mathrm{d}g/\mathrm{d}t = a/l > 0$ for all $t \ge 0$, the inverse of g exists, thus Equation (3.3) is equivalent to

$$\begin{cases} x = y\bar{l}(\tau), \\ t = g^{-1}(\tau), \end{cases} \qquad 0 \le y \le 1,\, \tau \ge 0, \tag{3.4}$$

where $\bar{l}(\tau) = l(g^{-1}(\tau)) = l(t)$. Hence we can expand the dynamical system (3.1), (3.2) with the ODE

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

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 dynamical model (3.1), (3.2) can be transformed and expanded into

$$\begin{cases} \dfrac{\partial \bar{c}}{\partial \tau} = \dfrac{D}{a}\dfrac{1}{\bar{l}}\dfrac{\partial^2 \bar{c}}{\partial y^2} - (1 - \dfrac{r_{\mathrm{g}}}{a}y(\bar{c}_{\mathrm{c}} - c_\infty))\dfrac{\partial \bar{c}}{\partial y} - \dfrac{g}{a}\bar{l}\bar{c}, \\ \dfrac{\mathrm{d}\bar{c}_{\mathrm{c}}}{\mathrm{d}\tau} = \dfrac{(a - gl_{\mathrm{c}})\bar{l}\bar{c}_{\mathrm{c}} - D\bar{c}_y^- - \bar{l}(r_{\mathrm{g}}\bar{c}_{\mathrm{c}} + \tilde{r}_{\mathrm{g}}l_{\mathrm{c}})(\bar{c}_{\mathrm{c}} - c_\infty)}{al_{\mathrm{c}}}, \\ \dfrac{\mathrm{d}\bar{l}}{\mathrm{d}\tau} = \dfrac{r_{\mathrm{g}}}{a}\bar{l}(\bar{c}_{\mathrm{c}} - c_\infty), \\ \dfrac{\mathrm{d}t}{\mathrm{d}\tau} = \dfrac{1}{a}\bar{l}, \end{cases} \tag{3.5}$$

which is defined for $\tau \ge 0$ and $y \in (0,1)$ and where the boundary and initial conditions are given by

$$\begin{cases} \bar{c}(0,\tau) = c_{\mathrm{s}}(t(\tau)), \\ \bar{c}(1,\tau) = \bar{c}_{\mathrm{c}}(\tau), \\ \bar{c}(y,0) = c_0(yl_0), \\ \bar{c}_{\mathrm{c}}(0) = c_0(l_0), \\ \bar{l}(0) = l_0, \\ t(0) = 0. \end{cases} \tag{3.6}$$

With the two first items of the wish list addressed we move on to Item 3 and 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. Therefore, to take advantage of this linearity, we propose the splitting

$$\begin{aligned} F_1 : \begin{pmatrix} \bar{c} \\ \bar{c}_{\mathrm{c}} \\ \bar{l} \\ t \end{pmatrix} &\mapsto \begin{pmatrix} \frac{D}{a}\frac{1}{\bar{l}}\frac{\partial^2 \bar{c}}{\partial y^2} - (1 - \frac{r_{\mathrm{g}}}{a} y(\bar{c}_{\mathrm{c}} - c_\infty))\frac{\partial \bar{c}}{\partial y} - \frac{g}{a}\bar{l}\bar{c} \\ 0 \\ 0 \\ 0 \end{pmatrix}, \\ F_2 : \begin{pmatrix} \bar{c} \\ \bar{c}_{\mathrm{c}} \\ \bar{l} \\ t \end{pmatrix} &\mapsto \begin{pmatrix} 0 \\ \frac{(a - g l_{\mathrm{c}})\bar{l}\bar{c}_{\mathrm{c}} - D\bar{c}_y^- - \bar{l}(r_{\mathrm{g}}\bar{c}_{\mathrm{c}} + \tilde{r}_{\mathrm{g}} l_{\mathrm{c}})(\bar{c}_{\mathrm{c}} - c_\infty)}{a l_{\mathrm{c}}} \\ \frac{r_{\mathrm{g}}}{a}\bar{l}(\bar{c}_{\mathrm{c}} - c_\infty) \\ \frac{1}{a}\bar{l} \end{pmatrix}. \end{aligned} \tag{3.7}$$

The domain of F_1 consists of functions fulfilling the boundary conditions of Equation (3.6). With this splitting the PDE fully decouples from the ODEs. Due to the parabolic nature of the model and the results of Section 2.2 we expect the PR scheme to be unconditionally stable when used for time discretization of Equations (3.5), (3.6). Therefore, also the stiffness of the problem, Item 4, would be taken care of. However, we have not provided an analytic framework in which Equations (3.5), (3.6) with the splitting (3.7) fulfills Assumptions 1–4. Thus, we cannot use Theorem 1 to conclude unconditional stability. We consider this analysis to be future work and, for now, content ourselves with some numerical experiments confirming our expectations. To conclude the section, we note that since the PR scheme preserves fixed points, also Item 5 of the wish list is fulfilled, see Section 1.1.3.

3.2 Numerical experiments

In the previous section we listed five requirement on numerical methods for successful discretization of the axon growth problem (3.1), (3.2). In the current section we will use numerical experiments to illustrate that our expectations stated in the previous section are

fulfilled. To this end we discretize the transformed evolution equation (3.5), (3.6) using the method of lines. To discretize the spatial derivatives of the PDE we apply standard, second order, central finite differences with mesh width $h = 1/(M+1)$, where M is a positive integer. For $j = 1, \ldots, M$ let $\bar{c}_{h,j}$ denote this semi-discretization of $\bar{c}$ at $y = jh$. For the left derivative in the ODE of the growth cone we use the one-sided difference formula

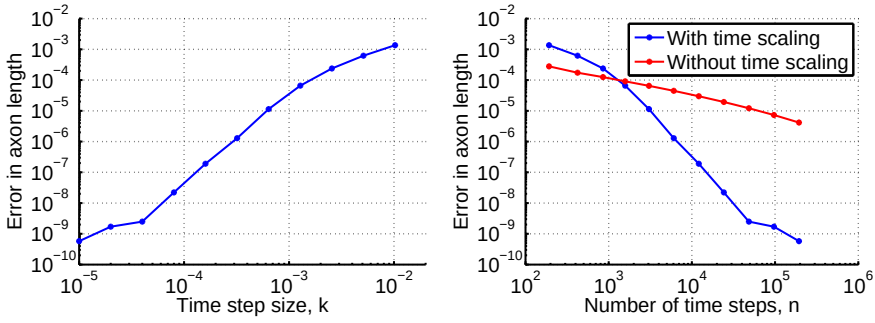
$$\bar{c}_y^- \approx \frac{3\bar{c}_c - 4\bar{c}_{h,M} + \bar{c}_{h,M-1}}{2h},$$

which is also second order. We note that the application of an explicit temporal discretization method to the semi-discretization comes with a CFL condition of the type $k < Ch^2$ due to the parabolic nature of the model (3.5), (3.6). However, an implicit method must, in each time step, solve a big, non-linear system of equations. The splitting (3.7) resolves the latter issue and employing an (expectedly) unconditionally stable splitting scheme, like the PR scheme, resolves the former.

The experiments presented in Figure 3.2(a) are made with nominal values on the physical parameters, see Table 1 of Paper III. For the left boundary condition we use the constant soma concentration $c_s(t) = 2c_\infty$. The initial length l_0 is set to 10^{-6} and the initial concentration profile c_0 is chosen to be the second degree polynomial in x such that $c_0(0) = 2c_\infty$, $c_0(l_0) = c_\infty$, and $(\partial c_0/\partial x)(l_0) = (a - gl_c)c_\infty/D$. With this initial value the boundary conditions are fulfilled and the cone concentration ODE is initially at an steady-state. The axon growth is terminated after one day, $T = 86400$, which covers the transient part of the growth, confer also Figure 3.3(a). After retrieving a semi-discretization on a fine spatial grid, $M = 10^5$, we discretize in time using the PR scheme. In Figure 3.2(a) the maximal error in axon length is plotted for different values of k. The reference solution is found by using the same discretization method on a very fine grid, $M = 10^6$ and $k = 10^{-6}$.

Our experiments seem to indicate that our discretization successfully address Item 4 in the wish list of Section 3.1. In Figure 3.2(a) we see the errors of stable numerical computations that indeed indicate the absence of a CFL condition for values of k/h^2 far bigger than allowed by the explicit Euler scheme. In the experiments we get $k/h^2 \approx 10^6$ on the coarsest temporal mesh whereas for explicit Euler to be stable it is required that $k/h^2 < a\bar{l}/(2D)$, which is initially $10^{-3}/2$. Thus, explicit Euler is not a viable choice for discretization of Equations (3.5), (3.6). Neither is implicit Euler due to its extremely expensive time steps. The same conclusions may be drawn for any explicit method or implicit method that consider the whole system (3.5), (3.6) at once. Unconditionally stable splitting schemes seem to be the ideal choices for addressing Items 3 and 4.

The blue graph in Figure 3.2(b) represent results from the same PR computations as earlier discussed. However, here the axon length errors are instead plotted over the number of time steps used, n. This is done to be able to address Item 2 of the wish list, that is, highlighting the impact of time scaling. Consider the equation system (3.1), (3.2) after transforming it only with the spatial scaling $y = x/l(t)$. The red graph in Figure 3.2(b)

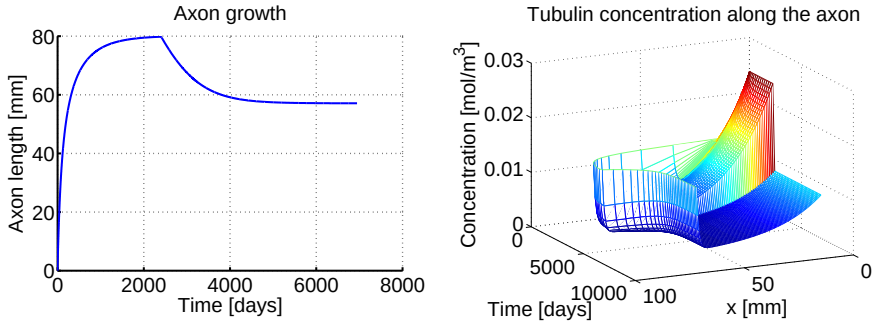


(a) (b)

Figure 3.2: Convergence for the PR scheme used as temporal discretization of the axon growth model. In (a) results are shown for discretizations of Equations (3.5), (3.6) where different values of k are used. We observe higher convergence order than the expected order two. In (b) the same results are compared to similar computations with the only difference that the equation to be discretized has not been scaled in time. The results are plotted over the number of time steps for easy comparison. Without the time scaling we do not observe the expected order two. This is due to the fast transient behavior of the cone concentration which is not properly resolved.

is created by using the same setup for the discretization of this partially scaled problem as we used for the fully scaled one. However, we have to pay extra attention to the time step k which has different meanings for the two models: Δt in the former and $\Delta\tau$ in the latter. To get comparable result we instead focus on the number of time steps taken. To this end, for each value of k ($= \Delta\tau$) 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. We see prominent order drops when time scaling is not used. This happens since the relatively large time steps are not able to resolve the transient behavior of the cone concentration. In future work we will study these order drops closer.

To conclude the chapter we plot in Figure 3.3 a numerical solution of the axon growth problem. This also serves the purpose of illustrating the PR scheme's ability to march towards steady-states, Item 5 of the wish list. Here we use the same settings as was used for the simulations giving the results plotted in Figure 3.2(a). The exceptions are the end time which is chosen much bigger, $T = 6 \cdot 10^8$, and the time step $k = 5 \cdot 10^{-4}$. Additionally we let the soma concentration be time dependent to illustrate our models ability to handle axon shrinkage. Initially $c_s(t)$ is constant $2c_\infty$, but at $t = 2 \cdot 10^8$ it drops to the new constant value $2c_\infty/3$. At end time the axon length is approximately $57 \cdot 10^{-3}$ with an error of $14 \cdot 10^{-6}$ compared to the exact value given by Equation (23) of Paper III. The error comes almost exclusively from the space discretization. Also note



(a) (b)

Figure 3.3: Numerical solution of the axon growth problem discretized in time by the PR scheme. The piecewise constant soma concentration c_s drops to one third of its initial value at time $2 \cdot 10^8$ s $\approx 2.3 \cdot 10^3$ days. In (a) we see the axon length growing towards a steady-state before the c_s drop and then shrinking towards a new steady-state. In (b) the axon tubulin concentration c along the axon is plotted as a function of time and space. Note the characteristic concentration profile which was studied in Section 4 of Paper III. The plots illustrate that our discretization scheme is a viable choice when marching towards steady-states.

in Figure 3.3(b) the characteristic spatial profile of the tubulin concentration c along the axon. Compare with the figures of Section 4 in Paper III.

Chapter 4

Conclusions and Outlook

4.1 Conclusions

The research presented in this Licentiate thesis is concerned with splitting methods. These methods are known to be superior choices in several applications where the vector field can be split into several parts. Done correctly a set of subproblems are generated which are far easier to solve than the original problem. The long term objective of our research is the analysis of ADI splitting methods for dissipative evolution equations and their application to relevant models found within science and technology.

We are particularly interested in convergence with orders in the infinite-dimensional setting. In this case simple Taylor expansions cannot be used for error analysis since the vector fields are usually unbounded. Instead we have seen that the maximal dissipative framework summarized in Section 2.1 gives the necessary tools to perform convergence studies. As has been previously discussed in the literature we have seen that analyses in this general setting give theoretical results that are both applicable to a wide range of problems and are independent of potential spatial discretizations. Examples of equations that fit into this framework of infinite-dimensional dissipative evolution equations can be found among the parabolic and hyperbolic PDEs. Among the former we find our axon growth model which has proven to be a good example of an application where the benefits of our splitting schemes come to good use.

We continue by separately considering the three research topics stated in Section 1.2.

Research topic 1. In the semilinear unbounded setting we have proven the full spectrum of convergence orders for the PR and DR splitting schemes. The analysis provides $o(1)$-convergence for nonsmooth solutions of the evolution equation, then first and second order convergence for successively smoother solutions. Earlier convergence studies in the abstract setting have either considered fully linear problems [23, 26], Lipschitz continuous nonlinearities [10], convergence of suboptimal order [29], or convergence without

orders [34]. With our results convergence with optimal orders are assured for a variety of semilinear equations that can be found in applications. In Section 6 of Paper I we exemplify with two reaction-diffusion systems: a solidification model and a pattern formation model.

Research topic 2. We have considered full space-time discretizations when either the PR or the DR scheme is used as temporal discretization method. Optimal orders simultaneously in space and time have been proven when linear, dissipative evolution equations are discretized. As we saw in the introduction similar results exist in the literature for other temporal methods, for example implicit Euler and Crank-Nicholson are considered in [9, 50] whereas IMEX methods are considered in [2, 32, 50]. With our results we are able to consider splitting applications that do not fit into the framework of semi-implicit methods, for example the frequently used dimension splittings.

Research topic 3. The axon growth model developed in Paper III consists of two nonlinear ODEs and a parabolic PDE defined on an expanding (or contracting) domain. The application of a numerical method has proven to be non-trivial. However, in the current research we have seen that an efficient scheme can be constructed by using intelligent space and time scalings, splitting the ODEs from the PDE, and then employing an unconditionally stable method like the PR scheme.

In the application there is an interest to examine the effects of the physical and biological parameters on the behavior of the model. Such parameter studies require a big amount of computations. With our scheme these studies can be performed with big accuracy in short time using an ordinary desktop computer. This is not possible with of-the-shelf numerical methods.

4.2 Future work

A number of questions appeared during the research work. We present some of them here as possible future work.

- In our convergence studies for full space-time discretizations we consider only linear evolution equations. It is natural to propose an extension to semilinear equations, especially since we prove convergence for temporal semi-discretizations of these problems already in Paper I. However, a completely different proof technique would probably be required. The reason is that our present analysis, in the linear setting, is heavily dependent on the commutativity of the flow and the vector field. Generally we do not have this commutativity when considering nonlinear vector fields.

- We have seen that the advantageous local error structure and the thereof implied fixed point preservation are useful properties of the PR and DR schemes. Also other splitting methods exhibit these properties, for example IMEX Euler and some other

IMEX Runge–Kutta methods. We are interested in the construction and analysis of high order IMEX Runge–Kutta methods with similar advantageous error structures implying fixed point preservation.

- For many dissipative evolution equations the ADI schemes exhibit more favorable stability properties than the IMEX methods. For example, when integrating the dimension splitting mentioned in Section 2.4, the IMEX methods suffer from stability problems whereas both ADI methods considered in this thesis converge. However, since the PR and DR schemes are of low order, an interesting future line of research would be the construction and analysis of high-order methods that approximate the partial flows, preserve fixed points, and are similar to the the PR and DR schemes in their stability properties and local error structure.

- In Section 2.3 we saw that the advantageous error structures of the PR and DR schemes were useful in the analysis of full discretizations. In Paper II we consider an application to dimension splitting in two spatial dimensions. An extension to three dimensions is natural and the DR scheme is suitable for splittings with more than two operators. The analysis of such an extension would be of interest where a crucial question is whether there are similarly good error structures when several operators are present.

- Due to their fixed point preservation the PR and DR schemes can be used as iterative methods for finding approximate solutions of nonlinear, stationary equations $Fv = 0$. As these methods carry over the possibility of splitting F they are expected to be more efficient than standard methods whenever the resolvents of F_1 and F_2 are significantly simpler than the resolvent of their sum. We are interested in the analysis of this solution technique in the abstract dissipative setting.

- The axon growth model (3.5), (3.6) is by and large a parabolic problem. However, we have not yet been able to fit the problem into the setting of dissipative evolution equations. To achieve this we need to perform further analysis on the special boundary condition coupling and how to treat the left derivative $\bar{c}_y^-$.

- Our PR simulations of the axon growth model generated several questions that need to be considered more carefully. The cone concentration tends very fast to its steady-state whereas the axon length converges very slowly. A deeper understanding of why this happens and how the physical parameters affect is desirable. This could also grant a better understanding of the untypical behavior of our numerical solutions; confer Figure 3.2 where we see third order convergence with time scaling and less than first order without.

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