# An almost symmetric Strang splitting scheme for nonlinear evolution equations ${ }^{\text {* }}$ 

Lukas Einkemmer*, Alexander Ostermann<br>Department of Mathematics, University of Innsbruck, Austria

## ARTICLE INFO

Article history:
Available online 20 March 2014

## Keywords:

Splitting methods
High order
Evolution equations
Time integration
Approximate flows


#### Abstract

In this paper we consider splitting methods for the time integration of parabolic and certain classes of hyperbolic partial differential equations, where one partial flow cannot be computed exactly. Instead, we use a numerical approximation based on the linearization of the vector field. This is of interest in applications as it allows us to apply splitting methods to a wider class of problems from the sciences.

However, in the situation described, the classic Strang splitting scheme, while still being a method of second order, is not longer symmetric. This, in turn, implies that the construction of higher order methods by composition is limited to order three only. To remedy this situation, based on previous work in the context of ordinary differential equations, we construct a class of Strang splitting schemes that are symmetric up to a desired order.

We show rigorously that, under suitable assumptions on the nonlinearity, these methods are of second order and can then be used to construct higher order methods by composition. In addition, we illustrate the theoretical results by conducting numerical experiments for the Brusselator system and the KdV equation.


© 2014 The Authors. Published by Elsevier Ltd. This is an open access article under the CC BY-NC-ND license (http://creativecommons.org/licenses/by-nc-nd/3.0/).

## 1. Introduction

In this paper we consider the time discretization of parabolic and certain classes of hyperbolic partial differential equations. More specifically, we assume that the considered problem can be written as the following abstract Cauchy problem

$$
\begin{equation*}
u^{\prime}=A u+B(u), \quad u(0)=u_{0} \tag{1}
\end{equation*}
$$

on some Banach space $X$, where $A$ is a linear (but possibly unbounded) operator. In order that a solution to the initial value problem (1) is well defined, we have to assume that $A+B$ generates a one-parameter semigroup. To consider splitting methods we further have to assume that $A$ and $B$ generate semigroups as well.

In this context splitting methods can be applied if the partial flows generated by $A$ and $B$ have an analytical representation, or if an efficient algorithm for finding their exact solution is known. For a review of splitting methods we refer the reader to [1]. However, the assumption that the partial flow generated by the nonlinear operator $B$ can be computed exactly is usually a very strong requirement. Most partial differential equations which are drawn from the sciences do neither admit an analytical solution nor can they be computed exactly in an efficient manner by some algorithm from the literature.

[^0]To remedy this deficiency of classic splitting methods, we propose and analyze splitting schemes which approximate the partial flow generated by B, i.e.

$$
\begin{equation*}
u^{\prime}=B(u) \tag{2}
\end{equation*}
$$

by that of an inhomogeneous linear differential equation. That is, instead of Eq. (2), we consider the linearized problem given by

$$
\begin{equation*}
u^{\prime}=b\left(u_{\star}\right) u+d \tag{3}
\end{equation*}
$$

where for consistency reasons we have to assume that

$$
B(u)=b(u) u+d
$$

That is, once a value $u_{\star}$ is substituted, the flow corresponding to (3) can be computed efficiently. That such a linearized problem can be computed exactly is a much less stringent condition and thus splitting methods can potentially be applied to a larger class of problems.

For the remainder of the paper let us denote the flow corresponding to Eq. (3) by $\varphi_{t}^{b\left(u_{\star}\right)}$. Note that this notation suggests that, once $u_{\star}$ is fixed, the evolution equation given by (3) generates a semigroup. This assumption is not necessarily satisfied for each $u_{\star} \in X$ (even if $B$ generates a semigroup). We will discuss this point further at the beginning of Section 2 . In the framework developed there the flow $\varphi_{t}^{b\left(u_{\star}\right)}$ can be written explicitly (for a $u_{\star}$ chosen in an appropriate subspace of $X$ ), by employing the exponential and $\phi_{1}$ function, as follows

$$
\begin{equation*}
\varphi_{t}^{b\left(u_{\star}\right)}(u(0))=\mathrm{e}^{t b\left(u_{\star}\right)} u(0)+t \phi_{1}\left(t b\left(u_{\star}\right)\right) d, \quad t \geq 0, \tag{4}
\end{equation*}
$$

where the $\phi_{1}$ function is given by

$$
\begin{equation*}
\phi_{1}(z)=\frac{\mathrm{e}^{z}-1}{z} \tag{5}
\end{equation*}
$$

In this context we can formulate the (classic) Strang splitting scheme as follows

$$
\begin{align*}
& u_{1 / 2}=\varphi_{\frac{\tau}{2}}^{b\left(u_{0}\right)}\left(\mathrm{e}^{\frac{\tau}{2} A} u_{0}\right),  \tag{6}\\
& u_{1}=M_{\tau}\left(u_{0}\right)=\mathrm{e}^{\frac{\tau}{2} A} \varphi_{\tau}^{b\left(u_{1 / 2}\right)}\left(\mathrm{e}^{\frac{\tau}{2} A} u_{0}\right) .
\end{align*}
$$

Such a splitting scheme has been employed, for example, to numerically solve the Vlasov-Poisson equations (see e.g. [2,3]) or the Davey-Stewartson equation (see e.g. [4]). Note, however, that in both of these cases the underlying structure of the equations guarantees that the Strang splitting scheme, as stated above, is still symmetric. Therefore, the usual construction of composition methods (as described in [5], for example) can be carried out without modification.

However, for many problems arising in the sciences, such as nonlinear reaction-diffusion equations or the KdV equation (both of which are discussed in Section 6), such a simplification cannot be assumed. Then the Strang splitting scheme above is, unfortunately, no longer symmetric. The lacking symmetry of the method does not severely affect performance; however, if composition is used as a means to construct higher order methods, symmetry is usually a necessary condition.

To remedy this situation a family of Strang splitting schemes were introduced in the context of ordinary differential equation (see [6]). The construction of these schemes is based on the fact that the Lie splitting algorithm

$$
\begin{equation*}
L_{\frac{\tau}{2}}=\varphi_{\frac{\tau}{2}}^{b\left(u_{0}\right)} \circ \mathrm{e}^{\frac{\tau}{2} A} \tag{7}
\end{equation*}
$$

composed with its adjoint method, which we denote by $L_{\frac{\tau}{2}}^{*}$, is a method of second order and symmetric. It is given by

$$
\begin{equation*}
S_{\tau}=L_{\frac{\tau}{2}}^{*} \circ L_{\frac{\tau}{2}} . \tag{8}
\end{equation*}
$$

However, for our purpose it is more convenient to represent $u_{1}=S_{\tau} u_{0}$ as the solution of the following implicit equation

$$
u_{1}=\mathrm{e}^{\frac{\tau}{2} A} \circ \varphi_{\frac{\tau}{2}}^{b\left(u_{1}\right)}\left(u_{1 / 2}\right), \quad u_{1 / 2}=L_{\frac{\tau}{2}} u_{0}
$$

Note that solving this equation is computationally not attractive in practice. Therefore, it has been suggested to employ $i \in \mathbb{N}$ fixed-point iterations to compute an approximation to $u_{1}$. Let us denote the resulting scheme by $S_{\tau}^{(i)}$. The corresponding starting value (for the fixed-point iteration) is given by

$$
\begin{equation*}
S_{\tau}^{(1)} u_{0}=\mathrm{e}^{\frac{\tau}{2} A} \circ \varphi_{\frac{\tau}{2}}^{b\left(u_{1 / 2}\right)} \circ \varphi_{\frac{\tau}{2}}^{b\left(u_{0}\right)} \circ \mathrm{e}^{\frac{\tau}{2} A}\left(u_{0}\right) \tag{9}
\end{equation*}
$$

The one-step methods $S_{\tau}^{(i)}$ are not symmetric but they are symmetric up to order $i$; that is, they satisfy the following relation $\left(S_{\tau}^{(i)}\right)^{*}=S_{\tau}^{(i)}+\mathcal{O}\left(\tau^{i}\right)$ (for the non-stiff case this result can be found in [6]; for the stiff case we will consider this in more detail in Section 2). Therefore, it is possible to construct composition methods of arbitrary (even) order, where $i$, and thus the computational cost of $S_{\tau}^{(i)}$, increases linearly with the desired order $p$. For a more detailed description we refer the reader to [6].

In this paper, we will provide a rigorous convergence analysis which shows that for parabolic and certain classes of hyperbolic partial differential equations the method $S_{\tau}^{(i)}$ is of second order, if $i \geq 2$. This analysis in the context of partial differential equations is significantly more involved than the analysis provided in [6]. The assumptions we make in order to prove the main result will be that the classic Strang splitting scheme given in Eq. (6) is convergent of order two (i.e., that the classic Strang splitting scheme can be successfully applied to the problem under consideration) and that up to three applications of $b(\tilde{u})$ and its derivatives to the exact solution are bounded in a suitable norm; here $\tilde{u}$ is a generic function that is, in a sense to be made precise, close to the exact solution $u(t)$. Note that in the linear case this assumption is equivalent to the fact that $b^{3} u(t)$ can be bounded; i.e., we have to bound three applications of the operator $b$ to the exact solution. It is useful to keep that in mind in order to compare the assumptions made here to, for example, [7], where an analysis of the exact Strang splitting scheme in the linear case is provided.

To that end, we will discuss the fixed-point iteration in the stiff case (Section 2), and show second order convergence of $S_{\tau}^{(i)}$ for the hyperbolic (Section 3) and parabolic case (Section 4). In Section 5 we discuss the construction of higher order composition methods. Finally, we will show in Section 6 that in the case of the KdV equation as well as the Brusselator system the predicted behavior agrees well with the numerical experiments conducted.

## 2. Fixed-point iteration in the stiff case

The purpose of this section is to discuss the fixed-point iteration necessary to compute $S_{\tau}^{(i)}$, as outlined in Section 1 , in more detail. In the non-stiff case an appropriate step size $\tau$ can always be found such that the iteration converges. However, in the present discussion it is necessary to employ a condition on the, in general, unbounded nonlinearity $b$. We will assume that $b(v) w$ satisfies a Lipschitz condition with respect to $v$ in the Banach space $(X,\|\cdot\|)$, whenever $v$ and $w$ are chosen from a bounded subset of some subspace $\left(V,\|\cdot\|_{V}\right)$, where the norm in $V \subset X$ is stronger than that in $X$.

Note that all the convergence results in this paper are formulated in the Banach space $X$. However, the second Banach space $V$ is necessary as in most problems it is not possible to show the required Lipschitz results for arbitrary elements in $X$. However, in many instances an assumption on the regularity of the initial value (i.e. $u_{0} \in V$ ) does result in the same regularity of the solution at later times (i.e. $u(t) \in V$ ). This, in turn, allows us to assume additional regularity in order to show consistency in a weaker space $X$. A similar approach for the $K d V$ equation can be found, for example, in [8]. In all the considerations that follow, we assume that $A, B$, and $b\left(u_{\star}\right)$, for $u_{\star} \in V$, generate one-parameter semigroups on $V$ as well as on $X$.

Before proceeding, let us note that for the Brusselator system (discussed in Section 6.1) using $X=V=H^{2}$ would constitute an appropriate choice as in this case the nonlinearity is polynomial in the solution (and, in particular, does not include spatial derivatives of the solution). The multiplications necessary such that $B$ and $b$ form a self-map on $V$ can be carried out as $H^{2}$ forms an algebra in two space dimensions (in addition to the Banach space structure). However, for the KdV equation (discussed in Section 6.2) the spaces $X$ and $V$ have to be chosen to be distinct (see [8], where $X=H^{1}$ and $V=H^{6}$, and Example 2).

Now, let us formulate a mathematically rigorous theorem that gives assumptions under which the fixed-point iteration used to define $S_{\tau}$ converges.

Theorem 1. Let $u_{0} \in V \subset X$, and let $N_{V}$ be a closed neighborhood of $u_{0}$ in $V$, such that the map

$$
\begin{equation*}
F(u)=\mathrm{e}^{\frac{\tau}{2} A} \varphi_{\frac{\tau}{2}}^{b(u)}\left(u_{1 / 2}\right) \tag{10}
\end{equation*}
$$

is a self-map on $N_{V}$, and $\varphi_{s}^{b(u)}\left(u_{1 / 2}\right) \in N_{V}$ for all $u \in N_{V}$ and $0 \leq s \leq \tau / 2$. Recall that $u_{1 / 2}$ is defined in (6). Further suppose that the map $b(\cdot)$ is Lipschitz continuous for arguments in $N_{V}$, i.e., there exists a constant $L$ such that

$$
\left\|b\left(v_{1}\right)-b\left(v_{2}\right)\right\|_{X \leftarrow V} \leq L\left\|v_{1}-v_{2}\right\|
$$

for all $v_{1}, v_{2} \in N_{V}$. Then there exists a step size $\tau_{0}>0$, which depends only on the Lipschitz constant $L$ and on bounds of the partial flows, such that for all $\tau \in\left[0, \tau_{0}\right)$ the fixed-point iteration with starting value $u_{1 / 2}$ converges to an element $S_{\tau} u_{0} \in X$. In particular, it holds that

$$
\begin{equation*}
\left\|S_{\tau}^{(i)} u_{0}-S_{\tau} u_{0}\right\| \leq\left(C_{1} L\right)^{i-1} \tau^{i-1}\left\|S_{\tau}^{(1)} u_{0}-S_{\tau} u_{0}\right\|, \quad i \geq 1 \tag{11}
\end{equation*}
$$

Proof. We have to consider the fixed-point iteration given by

$$
u=F(u),
$$

with starting values in $N_{V}$. By employing the variation-of-constants formula, we can write

$$
\varphi_{\frac{\tau}{2}}^{b\left(v_{1}\right)}\left(u_{1 / 2}\right)=\varphi_{\frac{\tau}{2}}^{b\left(v_{2}\right)}\left(u_{1 / 2}\right)+\int_{0}^{\frac{\tau}{2}} \mathrm{e}^{\left(\frac{\tau}{2}-s\right) b\left(v_{2}\right)}\left(b\left(v_{1}\right)-b\left(v_{2}\right)\right) \varphi_{s}^{b\left(v_{1}\right)}\left(u_{1 / 2}\right) \mathrm{d} s
$$

and by using the Lipschitz continuity of $b$, we get

$$
\left\|F\left(v_{1}\right)-F\left(v_{2}\right)\right\| \leq C_{1} L \tau\left\|v_{1}-v_{2}\right\|
$$

since $w=\varphi_{s}^{b\left(v_{1}\right)}\left(u_{1 / 2}\right) \in N_{V}$. Note that $C_{1}$ does depend on the $V$ norm of $w$.

Thus, the fixed-point iteration with starting value $u_{1 / 2}$ provides a sequence in $N_{V}$, which is a Cauchy sequence in $X$, if $\tau_{0}$, as given in the statement of the theorem, satisfies $C_{1} L \tau_{0}<1$. Since the fixed-point iteration converges in $X$ and the Lipschitz constant of $F$ is proportional to $\tau$, we obtain (11) by a standard induction argument.

It should be duly noted that although the step size is limited by the above theorem this is not a CFL condition. In our case the step size does only depend on local properties of $b(u)$, the exact solution as well as the scheme under consideration. However, the bound holds independently of the specific space discretization under consideration. In fact, the above result is what one would expect for a stable numerical scheme; namely that the step size is limited by the Lipschitz constant of the right-hand side.

Example 2. To illustrate Theorem 1 let us consider the following operators

$$
A=0, \quad b(u) w=u \partial_{x} w
$$

In this case we choose $X=L^{1}(\mathbb{R})$ and $V=W^{1,1}(\mathbb{R})$. Now in Section 3.2 we are interested to apply the above theorem to some $u(k \tau)$. Let us use $u_{0}$ to denote this value for a fixed $k$. Then for a sufficiently small $\delta>0$, we take for $N_{V}$ the corresponding ball of radius $\delta$. To verify the assumptions of Theorem 1 let us note that clearly, for $\tau$ sufficiently small, $F$ is a self-map in $N_{V}$. This follows from the fact that $F(u)$ is the solution of an advection equation with velocity $u$ at time $\tau / 2$. (This can be elaborated, for example, with the method of characteristics.) Furthermore, by the same argument, since both $u_{1 / 2}$ and $u$ lie in $N_{V}$, we follow that

$$
\varphi_{s}^{b(u)} u_{1 / 2} \in N_{V}
$$

which is needed in the proof of Theorem 1.
In the next section we will employ heavily the following result; it states that a time step conducted by applying $S_{\tau}$ to some $u_{0}$ results in a value that is different from $u_{0}$ by at most an order of $\tau$. For the convenience of the reader we state and prove this well-known result in the next theorem.

Corollary 3. If the Lie splitting algorithm (7) is consistent of order 1 and $\tau$ is chosen such that the fixed-point iteration (10) converges, then

$$
\left\|S_{\tau}\left(u_{0}\right)-u_{0}\right\| \leq C \tau
$$

where the constant $C$ is independent of $\tau$.
Proof. From Eq. (9) we know that $S_{\tau}^{(1)}$ is the composition of two Lie steps. Therefore, it holds that

$$
\left\|S_{\tau}^{(1)}\left(u_{0}\right)-u_{0}\right\| \leq C_{2} \tau
$$

By employing standard estimates for the fixed-point iteration, we get

$$
\left\|S_{\tau}^{(i)}\left(u_{0}\right)-u_{0}\right\| \leq\left\|S_{\tau}^{(1)}\left(u_{0}\right)-u_{0}\right\| \sum_{k=0}^{i-1}\left(C_{1} L \tau\right)^{k} \leq \frac{C_{2}}{1-C_{1} L \tau} \tau
$$

for any $i \geq 2$. This bound gives the desired result, since under the assumptions of convergence of the fixed-point iteration we know that $C_{1} L \tau<1$ (see Theorem 1 ).

For later use, we formulate a result on the nonlinear operator $M_{\tau}$.
Lemma 4. Let $u_{k}, \bar{u}_{k} \in V$. Then we have

$$
\begin{equation*}
M_{\tau} u_{k}-M_{\tau} \bar{u}_{k}=\mathrm{e}^{\frac{\tau}{2} A} \mathrm{e}^{\tau b\left(\bar{u}_{k+1 / 2}\right)} \mathrm{e}^{\frac{\tau}{2} A}\left(u_{k}-\bar{u}_{k}\right)+R_{k} \tag{12}
\end{equation*}
$$

where the remainder $R_{k}$ satisfies the bound

$$
\left\|R_{k}\right\| \leq C \tau\left\|u_{k}-\bar{u}_{k}\right\|
$$

with a constant $C$ that depends on $\left\|u_{k}\right\|_{V}$ and $\left\|\bar{u}_{k}\right\|_{V}$.
Proof. From (6) we infer the representation (12) with remainder

$$
R_{k}=\mathrm{e}^{\frac{\tau}{2} A}\left(\mathrm{e}^{\tau b\left(u_{k+1 / 2}\right)}-\mathrm{e}^{\tau b\left(\bar{u}_{k+1 / 2}\right)}\right) \mathrm{e}^{\frac{\tau}{2} A} u_{k}+\tau \mathrm{e}^{\frac{\tau}{2} A}\left(\phi_{1}\left(\tau b\left(u_{k+1 / 2}\right)\right)-\phi_{1}\left(\tau b\left(\bar{u}_{k+1 / 2}\right)\right)\right) d .
$$

The result follows by applying the variation-of-constants formula several times and from the Lipschitz continuity of $b$, see the proof of Theorem 1.

## 3. Convergence for hyperbolic differential equations

First, we study how the spatial regularity of the initial value influences the temporal regularity of the solution. This will give us an idea of the required regularity assumptions on the initial value, which is needed for the schemes described here to be convergent of second order. To accomplish this, in Section 3.1, a suitable toy model is analyzed. In Section 3.2 we will
derive, for the hyperbolic case, the conditions under which the splitting scheme $S_{\tau}^{(i)}$, for $i \geq 2$, is convergent of order two. We will formulate a condition that depends on the regularity of the exact solution. More formally, we have to bound a number of applications of $b\left(u_{\star}\right)$ and its derivatives to the exact solution and assume that the (classic) Strang splitting scheme $M_{\tau}$ is convergent of order two. For hyperbolic systems which do not change the regularity of the initial value this is equivalent to assuming some regularity for the initial value.

### 3.1. Regularity in time

An interesting question is how much regularity on the initial value is required such that a scheme can be convergent of second order in time. To elaborate on this question let us consider the following (nonlinear) advection equation

$$
\begin{equation*}
\partial_{t} u(t, x)+u(t, 0) \partial_{x} u(t, x)=0 \tag{13}
\end{equation*}
$$

The solution of this toy model can be written as

$$
\begin{equation*}
u(t, x)=u_{0}(x-v(t)) \tag{14}
\end{equation*}
$$

where the advection speed depends on the solution as follows

$$
v(t)=\int_{0}^{t} u(\sigma, 0) \mathrm{d} \sigma
$$

Now, let us investigate the time regularity of the solution $u(t, x)$. To that end let us assume that the initial value satisfies $u_{0} \in \mathcal{C}^{1, \alpha}$ for some $\alpha \in(0,1)$. From (13) we deduce that $u(t, x)$ is at least once differentiable in time. The resulting function $\partial_{t} u(t, \cdot)$ lies in $\mathcal{C}^{0, \alpha}$; this can be easily deduced from Eq. (14). Our goal is to show that

$$
\frac{\left|\left(\partial_{t} u\right)(t, x)-\left(\partial_{t} u\right)(s, x)\right|}{|t-s|^{\beta}}
$$

is not bounded for any $\beta>\alpha$ as $s$ tends to $t$. Rewriting the above expression we get

$$
\left(\partial_{t} u\right)(t, x)-\left(\partial_{t} u\right)(s, x)=(u(t, 0)-u(s, 0)) \partial_{x} u(t, x)+u(s, 0)\left(\left(\partial_{x} u\right)(t, x)-\left(\partial_{x} u\right)(s, x)\right) .
$$

The first term is Lipschitz continuous in time and therefore can be bounded. However, for the second term we can write

$$
\frac{\left|\left(\partial_{x} u\right)(t, x)-\left(\partial_{x} u\right)(s, x)\right|}{|t-s|^{\beta}}=\frac{\left|u_{0}^{\prime}(x-v(t))-u_{0}^{\prime}(x-v(s))\right|}{|t-s|^{\beta}}
$$

where by defining $z=x-v(t)$ and $w=x-v(s)$ and using the estimate

$$
|z-w|=\left|\int_{s}^{t} u(\sigma, 0) \mathrm{d} \sigma\right| \geq \min _{\sigma \in[0, t]}|u(\sigma, 0)||t-s|
$$

we get

$$
\frac{\left|u_{0}^{\prime}(x-v(t))-u_{0}^{\prime}(x-v(s))\right|}{|t-s|^{\beta}} \geq \frac{\left|u_{0}^{\prime}(z)-u_{0}^{\prime}(w)\right| \cdot \min _{\sigma \in[0, t]}|u(\sigma, 0)|^{\beta}}{|z-w|^{\beta}} .
$$

If we now choose a $u_{0} \in \mathcal{C}^{1, \alpha}$ that nowhere can be improved to a better Hölder exponent $\beta>\alpha$ and is bounded away from zero (which then also holds true for $u(t, \cdot)$ ), then the term on the right-hand side diverges as $z$ tends to $w$ and thus we have shown that the regularity of $u(t, x)$ in time is at most $\mathcal{C}^{1, \alpha}$. That such an initial value exists is shown in [9].

As a numerical approximation to the solution of (13), we consider the exact solution of

$$
\begin{equation*}
\partial_{t} u(t, x)=u\left(\frac{\tau}{2}, 0\right) \partial_{x} u(t, x) \tag{15}
\end{equation*}
$$

on the interval $[0, \tau]$. This is not a practical numerical method as we have, in general, no algorithm that allows us to compute $v(\tau / 2)$ exactly. However, it can be seen as the limit of a scheme, where we approximate $v$ by approximating $u(t, 0)$ in some suitable manner. In this case the numerical solution, i.e. the exact solution of Eq. (15), is given by the midpoint rule, i.e.

$$
u_{1}=u_{0}\left(x-\tau u\left(\frac{\tau}{2}, 0\right)\right)
$$

which has to be compared to the exact solution, given in (14). By using the method of characteristics we can estimate the error as follows

$$
\left\|u(\tau, x)-u_{1}\right\| \leq \tau L\left\|u\left(\frac{\tau}{2}, 0\right)-\frac{1}{\tau} \int_{0}^{\tau} u(t, 0) \mathrm{d} t\right\|,
$$

where $L$ is the Lipschitz constant of $u_{0}$. Therefore, the numerical scheme can be seen as the midpoint rule approximating an integral. It is well-known that the midpoint rule yields an approximation with a local error of $\operatorname{size} C \tau^{\min (3, k+\alpha)}$, if and only if the integrand lies in $\mathcal{C}^{k, \alpha}$.

### 3.2. Convergence of the iterated Strang splitting scheme

The discussion in the previous section shows that we can expect the Strang splitting scheme to be second order accurate in time only if we require that $u_{0} \in \mathcal{C}^{2,1}$. In the framework discussed in Section 1 this means that we have to bound at least three applications of the operator $b\left(u_{\star}\right)$ to the exact solution. In fact our assumption, which we will state in this section, will turn out to be slightly more complicated due to the fact that we have to bound certain derivatives of $b(\cdot)$ as well.

Before stating the assumption that is used to prove the consistency result, we recall the following fact. Let $U, W$, and $Z$ be Banach spaces and $f: U \times W \rightarrow Z$ a function, which is Fréchet differentiable with respect to the first component. Then it holds that

$$
\left\|\left(\partial_{1} f\right)\left(u_{0}, w\right) d\right\|_{z} \leq\left\|\left(\partial_{1} f\right)\left(u_{0}, w\right)\right\|_{z \leftarrow U}\|d\|_{U}
$$

Thus, we can separate the condition on the function $f$ from the direction of the derivative. We will see below that this fact simplifies the condition needed to establish the correct order of the scheme significantly.

Note that, clearly, this also holds true if the function $f$ is linear in the second component and we employ the notation outlined in Section 1. In this instance we have $f(u, w)=b(u) w$ and thus $W=V$ and $Z=X$. In fact, we assume the following bounds

$$
\begin{align*}
& \sup _{t \in[0, T]}\left\|b^{i}(\tilde{u}) u(t)\right\|_{X} \leq C, \quad i \leq 3,  \tag{16a}\\
& \sup _{t \in[0, T]}\left\|b^{i}(\tilde{u}) b^{\prime}(\tilde{u}) b^{j}(\tilde{u}) u(t)\right\|_{X \leftarrow V} \leq C, \quad i+j \leq 2,  \tag{16b}\\
& \sup _{t \in[0, T]}\left\|b^{i}(\tilde{u}) b^{\prime \prime}(\tilde{u}) b^{j}(\tilde{u}) u(t)\right\|_{X \leftarrow V^{2}} \leq C, \quad i+j \leq 1, \tag{16c}
\end{align*}
$$

where $i, j \in \mathbb{N}$. The functions $\tilde{u}$ are generic, i.e. different occurrences of such functions do not need to be indistinguishable, linear combinations of the exact solution $u(s)$ as well as $L_{\frac{\tau}{2}}(u(s))$ and $S_{\tau}(u(s))$ for some $s \in[0, T]$.

The following theorem shows consistency under the additional assumption that the (classic) Strang splitting scheme $M_{\tau}$ is of the expected order.

Theorem 5 (Consistency). Let us consider the following abstract initial value problem

$$
u^{\prime}=A u+b(u) u+d, \quad u(0)=u_{0}
$$

and suppose that assumption (16) is satisfied. If, in addition, the Strang splitting scheme $M_{\tau}$ is consistent of order two, we can conclude that $S_{\tau}^{(i)}$, for $i \geq 2$, is consistent of order two, i.e.

$$
\left\|S_{\tau}^{(i)} u_{0}-u(\tau)\right\| \leq C \tau^{3}
$$

Proof. First, let us consider a single time step of the implicit scheme $S_{\tau}$, i.e. $u_{1}=S_{\tau} u_{0}$, which can be written as (note that $u_{0}$ is not to be confused with the initial value; it is the exact solution at a point in time to which a splitting operator is applied)

$$
u_{1}=\mathrm{e}^{\frac{\tau}{2} A} \circ \varphi_{\frac{\tau}{2}}^{b\left(u_{1}\right)} \circ \varphi_{\frac{\tau}{2}}^{b\left(u_{0}\right)} \circ \mathrm{e}^{\frac{\tau}{2} A}\left(u_{0}\right) .
$$

Now let us proceed by comparing our method, i.e. $S_{\tau}$, to the Strang splitting scheme $M_{\tau}$. The difference can be estimated as follows

$$
\left\|\mathrm{e}^{\frac{\tau}{2} A} \circ \varphi_{\tau}^{b\left(u_{1 / 2}\right)} \circ \mathrm{e}^{\frac{\tau}{2} A}\left(u_{0}\right)-\mathrm{e}^{\frac{\tau}{2} A} \circ \varphi_{\frac{\tau}{2}}^{b\left(u_{1}\right)} \circ \varphi_{\frac{\tau}{2}}^{b\left(u_{0}\right)} \circ \mathrm{e}^{\frac{\tau}{2} A}\left(u_{0}\right)\right\| \leq\left\|\mathrm{e}^{\frac{\tau}{2} A}\right\|\left\|\varphi_{\tau}^{b\left(u_{1 / 2}\right)}\left(v_{0}\right)-\varphi_{\frac{\tau}{2}}^{b\left(u_{1}\right)} \circ \varphi_{\frac{\tau}{2}}^{b\left(u_{0}\right)}\left(v_{0}\right)\right\|
$$

with $v_{0}=\mathrm{e}^{\frac{\tau}{2} A} u_{0}$. By substituting $t=\tau$ into (4), we can write the semiflow $\varphi_{\tau}^{b\left(u_{\star}\right)}$ as

$$
\varphi_{\tau}^{b\left(u_{\star}\right)}\left(u_{0}\right)=\mathrm{e}^{\tau b\left(u_{\star}\right)} u_{0}+\tau \phi_{1}\left(\tau b\left(u_{\star}\right)\right) d
$$

Therefore, we have to compare

$$
\begin{equation*}
\varphi_{\frac{\tau}{2}}^{b\left(u_{1}\right)} \circ \varphi_{\frac{\tau}{2}}^{b\left(u_{0}\right)}\left(v_{0}\right)=\mathrm{e}^{\frac{\tau}{2} b\left(u_{1}\right)} \mathrm{e}^{\frac{\tau}{2} b\left(u_{0}\right)} v_{0}+\frac{\tau}{2}\left(\mathrm{e}^{\frac{\tau}{2} b\left(u_{1}\right)} \phi_{1}\left(\frac{\tau}{2} b\left(u_{0}\right)\right)+\phi_{1}\left(\frac{\tau}{2} b\left(u_{1}\right)\right)\right) d \tag{17}
\end{equation*}
$$

to the following expression

$$
\begin{equation*}
\varphi_{\tau}^{b\left(u_{1 / 2}\right)}\left(v_{0}\right)=\mathrm{e}^{\tau b\left(u_{1 / 2}\right)} v_{0}+\tau \phi_{1}\left(\tau b\left(u_{1 / 2}\right)\right) d \tag{18}
\end{equation*}
$$

Let us first compare the homogeneous parts. By expanding this part in Eq. (18) we get

$$
\mathrm{e}^{\tau b\left(u_{1 / 2}\right)}=I+\tau b\left(u_{1 / 2}\right)+\frac{\tau^{2}}{2} b^{2}\left(u_{1 / 2}\right)+\tau^{3} b^{3}\left(u_{1 / 2}\right) \phi_{3}\left(\tau b\left(u_{1 / 2}\right)\right)
$$

where the $\phi_{k}$ functions are defined recursively by

$$
\begin{aligned}
& \phi_{k}(\tau z)=\frac{1}{k!}+\tau z \phi_{k+1}(\tau z), \\
& \phi_{0}(\tau z)=\mathrm{e}^{\tau z}
\end{aligned}
$$

To expand Eq. (17) let us first define $g(\tau)=\mathrm{e}^{\frac{\tau}{2} b\left(u_{1}\right)} \mathrm{e}^{\frac{\tau}{2} b\left(u_{0}\right)}$. Then

$$
\begin{aligned}
& g^{\prime}(\tau)=\frac{1}{2}\left(b\left(u_{1}\right) g(\tau)+g(\tau) b\left(u_{0}\right)\right), \\
& g^{\prime \prime}(0)=\frac{1}{4}\left(b^{2}\left(u_{1}\right)+2 b\left(u_{1}\right) b\left(u_{0}\right)+b^{2}\left(u_{0}\right)\right),
\end{aligned}
$$

which gives the desired expansion

$$
\mathrm{e}^{\frac{\tau}{2} b\left(u_{1}\right)} \mathrm{e}^{\frac{\tau}{2} b\left(u_{0}\right)}=I+\frac{\tau}{2}\left(b\left(u_{0}\right)+b\left(u_{1}\right)\right)+\frac{\tau^{2}}{8}\left(b^{2}\left(u_{1}\right)+2 b\left(u_{1}\right) b\left(u_{0}\right)+b^{2}\left(u_{0}\right)\right)+R_{3},
$$

where

$$
R_{3}=\tau^{3} \sum_{i=0}^{3} c_{i} \int_{0}^{1}(1-\theta)^{2} b^{i}\left(u_{1}\right) \mathrm{e}^{\frac{\theta \tau}{2} b\left(u_{1}\right)} \mathrm{e}^{\frac{\theta \tau}{2} b\left(u_{0}\right)} b^{3-i}\left(u_{0}\right) \mathrm{d} \theta
$$

for appropriately chosen constants $c_{i}$. Now we have to compare the corresponding terms of equal order.
Terms of first order. By employing the fundamental theorem of calculus we can show that

$$
\begin{aligned}
b\left(u_{0}+\theta\left(u_{1 / 2}-u_{0}\right)\right)-b\left(u_{0}\right) & =\int_{0}^{\theta} \frac{\mathrm{d}}{\mathrm{~d} \eta} b\left(u_{0}+\eta\left(u_{1 / 2}-u_{0}\right)\right) \mathrm{d} \eta \\
& =\int_{0}^{\theta} b^{\prime}\left(u_{0}+\eta\left(u_{1 / 2}-u_{0}\right)\right)\left(u_{1 / 2}-u_{0}\right) \mathrm{d} \eta \\
& =\theta b^{\prime}\left(u_{0}\right)\left(u_{1 / 2}-u_{0}\right)+\int_{0}^{\theta}(\theta-\eta) b^{\prime \prime}\left(u_{0}+\eta v_{1 / 2}\right)\left(v_{1 / 2}, v_{1 / 2}\right) \mathrm{d} \eta
\end{aligned}
$$

where $v_{1 / 2}=u_{1 / 2}-u_{0}$. For $\theta=1$ this gives the following operator identity

$$
b\left(u_{1 / 2}\right)=b\left(u_{0}\right)+b^{\prime}\left(u_{0}\right)\left(u_{1 / 2}-u_{0}\right)+\int_{0}^{1}(1-\eta) b^{\prime \prime}\left(u_{0}+\eta v_{1 / 2}\right)\left(v_{1 / 2}, v_{1 / 2}\right) \mathrm{d} \eta
$$

The same expansion can be carried out for $b\left(u_{1}\right)$. Finally, we have to bound

$$
b\left(u_{1 / 2}\right)-\frac{1}{2}\left(b\left(u_{0}\right)+b\left(u_{1}\right)\right)=b^{\prime}\left(u_{0}\right)\left(u_{1 / 2}-\frac{1}{2}\left(u_{0}+u_{1}\right)\right)+R_{2},
$$

where for the sake of brevity the remainder term is denoted by $R_{2}$. This remainder can be bounded by assumption (16). Furthermore, to estimate the expression above, we have to use the fact that $\left\|u_{1 / 2}-\frac{1}{2}\left(u_{0}+u_{1}\right)\right\| \leq C \tau^{2}$. This follows easily by employing the triangle inequality and Theorem 1 (note that $u_{0}, u_{1 / 2} \in V$ ).

Terms of second order. We have to estimate

$$
\begin{aligned}
& b^{2}\left(u_{1}\right)+2 b\left(u_{1}\right) b\left(u_{0}\right)+b^{2}\left(u_{0}\right)-4 b^{2}\left(u_{1 / 2}\right) \\
& \quad=\left(b^{2}\left(u_{1}\right)-b^{2}\left(u_{1 / 2}\right)\right)+\left(b^{2}\left(u_{0}\right)-b^{2}\left(u_{1 / 2}\right)\right)+2\left(b\left(u_{1}\right) b\left(u_{0}\right)-b^{2}\left(u_{1 / 2}\right)\right) .
\end{aligned}
$$

A bound for the first and the second term can easily be found. The third term can be rewritten as

$$
2\left(b\left(u_{1}\right)-b\left(u_{1 / 2}\right)\right) b\left(u_{0}\right)+2 b\left(u_{1 / 2}\right)\left(b\left(u_{0}\right)-b\left(u_{1 / 2}\right)\right)
$$

which together with the estimate

$$
\left\|\left(b\left(u_{0}\right)-b\left(u_{1 / 2}\right)\right) u_{0}\right\| \leq \sup _{\eta \in[0,1]}\left\|b^{\prime}\left(u_{0}+\eta\left(u_{1 / 2}-u_{0}\right)\right) u_{0}\right\|\left\|u_{0}-u_{1 / 2}\right\|,
$$

Corollary 3 as well as assumption (16) is sufficient to show the desired bound.
Terms of third order. We have to bound $R_{3}$ as well as $b^{3}\left(u_{1 / 2}\right) \phi_{3}\left(\tau b\left(u_{1 / 2}\right)\right)$. The first bound is immediate, for the second we note that since the commutator $\left[b^{3}\left(u_{1 / 2}\right), \phi_{3}\left(\tau b\left(u_{1 / 2}\right)\right)\right]$ vanishes, the desired result follows easily.

Finally, let us compare the two inhomogeneous terms which are given by

$$
\begin{aligned}
\phi_{1}\left(\tau b\left(u_{1 / 2}\right)\right) & =I+\tau b\left(u_{1 / 2}\right) \phi_{2}\left(\tau b\left(u_{1 / 2}\right)\right) \\
& =I+\frac{\tau}{2} b\left(u_{1 / 2}\right)+\tau^{2} b^{2}\left(u_{1 / 2}\right) \phi_{3}\left(\tau b\left(u_{1 / 2}\right)\right)
\end{aligned}
$$

and

$$
\begin{aligned}
\frac{1}{2}\left(\mathrm{e}^{\frac{\tau}{2} b\left(u_{1}\right)} \phi_{1}\left(\frac{\tau}{2} b\left(u_{0}\right)\right)+\phi_{1}\left(\frac{\tau}{2} b\left(u_{1}\right)\right)\right)= & \frac{1}{2}\left(I+\mathrm{e}^{\frac{\tau}{2} b\left(u_{1}\right)}\right)+\frac{\tau}{8}\left(\mathrm{e}^{\frac{\tau}{2} b\left(u_{1}\right)} b\left(u_{0}\right)+b\left(u_{1}\right)\right) \\
& +\frac{\tau^{2}}{8}\left(\mathrm{e}^{\frac{\tau}{2} b\left(u_{1}\right)} b^{2}\left(u_{0}\right) \phi_{3}\left(\frac{\tau}{2} b\left(u_{0}\right)\right)+b^{2}\left(u_{1}\right) \phi_{3}\left(\frac{\tau}{2} b\left(u_{1}\right)\right)\right) \\
= & I+\frac{\tau}{8}\left(b\left(u_{0}\right)+3 b\left(u_{1}\right)\right) \\
& +\frac{\tau^{2}}{8}\left(b^{2}\left(u_{1}\right) \phi_{2}\left(\frac{\tau}{2} b\left(u_{1}\right)\right)+\frac{1}{2} b\left(u_{1}\right) \phi_{1}\left(\frac{\tau}{2} b\left(u_{1}\right)\right) b\left(u_{0}\right)\right) \\
& +\frac{\tau^{2}}{8}\left(\mathrm{e}^{\frac{\tau}{2} b\left(u_{1}\right)} b^{2}\left(u_{0}\right) \phi_{3}\left(\frac{\tau}{2} b\left(u_{0}\right)\right)+b^{2}\left(u_{1}\right) \phi_{3}\left(\frac{\tau}{2} b\left(u_{1}\right)\right)\right) .
\end{aligned}
$$

The term of first order vanishes and the term of second order is easily shown to yield an additional order. In addition, we can easily bound the remainder terms.

To show second order consistency of $S_{\tau}$ we have to estimate

$$
\begin{equation*}
\left\|S_{\tau} u_{0}-u(\tau)\right\| \leq\left\|S_{\tau} u_{0}-M_{\tau} u_{0}\right\|+\left\|M_{\tau} u_{0}-u(\tau)\right\| \tag{19}
\end{equation*}
$$

where the first term on the right-hand side of (19) has the right order by the argument provided above. Furthermore, the appropriate bound for the second term follows from the assumption that the (classic) Strang splitting scheme is consistent of order two.

Therefore, we have shown consistency for $S_{\tau}$. The extension of this result to $S_{\tau}^{(i)}$, for $i \geq 2$, follows immediately from Theorem 1.

In the previous theorem we have established consistency and are thus in a position to show convergence. Before stating the result we formulate a nonlinear stability assumption that enables us to control the numerical solution obtained by the iterated Strang splitting in $V$ : for $T>0$ there exist constants $R>0$ and $C>0$ such that for all $\tau>0$ and $n \in \mathbb{N}$ with $0 \leq n \tau \leq T$ and all $v_{j} \in V$ with $\left\|v_{j}\right\|_{V} \leq R$ it holds

$$
\begin{equation*}
\left\|\prod_{j=1}^{n} \mathrm{e}^{\frac{\tau}{2} A} \varphi_{\tau / 2}^{b\left(v_{j}\right)}\right\|_{V \leftarrow V} \leq C \tag{20}
\end{equation*}
$$

Much effort has been devoted to provide an analysis of nonlinear stability for a variety of partial differential equations found in the literature (see e.g. [3] for the Vlasov-Poisson equations, [10] for the Schrödinger-Poisson and cubic nonlinear Schrödinger equations, and [8] for the KdV equation). For our examples presented in Section 6, assumption (20) can easily be verified (see also Example 2).

Theorem 6 (Convergence in the Hyperbolic Case). Suppose that the assumptions (16) and (20) are satisfied, and that $M_{\tau}$ is second order convergent. Then, the iterated Strang splitting applied to (1) is convergent of order two, i.e., for $i \geq 2$, it holds that

$$
\left\|\left(S_{\tau}^{(i)}\right)^{k} u_{0}-u(k \tau)\right\| \leq C \tau^{2}
$$

where $C$ depends on the problem and the final time $T$, but not on $k$ and $\tau$ for $0 \leq k \tau \leq T$.
Proof. For fixed $\tau>0$ and integer $k \geq 0$, let

$$
\bar{u}_{k}=\left(M_{\tau}\right)^{k}\left(u_{0}\right) \quad \text { and } \quad u_{k}=\left(S_{\tau}^{(i)}\right)^{k}\left(u_{0}\right)
$$

denote the numerical solutions, obtained with $k$ steps (of length $\tau$ ) by the classic and the iterated Strang splitting, respectively. Then we have

$$
\left\|S_{\tau}^{(i)} u_{k}-u((k+1) \tau)\right\| \leq\left\|S_{\tau}^{(i)} u_{k}-M_{\tau} \bar{u}_{k}\right\|+\left\|M_{\tau} \bar{u}_{k}-u((k+1) \tau)\right\|
$$

By using the assumption that the classic Strang splitting scheme is convergent of order two, we can show the desired bound for the second term. Therefore, we once again proceed by comparing $S_{\tau}^{(i)}$ to $M_{\tau}$. For this purpose, let us write

$$
S_{\tau}^{(i)} u_{k}-M_{\tau} \bar{u}_{k}=S_{\tau}^{(i)} u_{k}-M_{\tau} u_{k}+M_{\tau} u_{k}-M_{\tau} \bar{u}_{k}
$$

and denote $e_{k}=u_{k}-\bar{u}_{k}$. Employing Lemma 4 this shows that

$$
\begin{equation*}
e_{k+1}=\left(S_{\tau}^{(i)}-M_{\tau}\right) u_{k}+\mathrm{e}^{\frac{\tau}{2} A} \mathrm{e}^{\tau b\left(\bar{u}_{k+1 / 2}\right)} \mathrm{e}^{\frac{\tau}{2} A} e_{k}+R_{k} \tag{21}
\end{equation*}
$$

with $\left\|R_{k}\right\| \leq C \tau\left\|e_{k}\right\|$. As we can control the $V$ norm of the numerical solution $u_{k}$ by assumption (20), we can estimate

$$
\left\|\left(S_{\tau}^{(i)}-M_{\tau}\right) u_{k}\right\| \leq C \tau^{3}
$$

with the help of Theorem 5. Recursion (21) has thus the form of the error recursion for the classic Strang splitting. Since this method is convergent, we infer the stability of this recursion. By successively eliminating the $e_{k}$ from the linear part (the second term in Eq. (21)) and treating $R_{k}$ as a perturbation, we obtain a non-linear recursion for $e_{k}$. Now, we can easily show the desired result by applying Gronwall's inequality.

## 4. Convergence for parabolic differential equations

Let us note that Theorems 5 and 6 have an immediate extension to the parabolic case. Due to the parabolic smoothing property we can weaken assumption (16). Following the ideas presented in [7], we can show second order convergence even if the right-hand side of (16) is replaced by $C / t^{\alpha}$ for $0 \leq \alpha<1$. However, we will not work this out in detail here.

For notational simplicity, we consider only the particular case where the nonlinearity $b(u)$ is a bounded operator. Note that in this case, we can take $X=V$. As $A$ is the generator of an analytic semigroup, we can choose (by standard arguments) an equivalent norm on $X$, again denoted by $\|\cdot\|$, such that

$$
\left\|\mathrm{e}^{\tau A}\right\| \leq 1, \quad \tau \geq 0, \quad \text { and } \quad\left\|\varphi_{\tau}^{b(u)}\right\| \leq 1+C \tau
$$

for $\|u\| \leq R$ and $|\tau| \leq \tau_{0}$ with a constant $C$ that depends on $b, R$, and $\tau_{0}$. These bounds imply at once the stability assumption (20).

The following theorem states second order convergence of the iterated Strang splitting in this situation.
Corollary 7 (Convergence in the Parabolic Case). Let A be the generator of an analytic semigroup and B a bounded operator. Further assume that the classic Strang splitting $M_{\tau}$ is second order convergent. Then, for $i \geq 2$, the iterated Strang splitting is convergent of order two, i.e., it holds that

$$
\left\|\left(S_{\tau}^{(i)}\right)^{k} u_{0}-u(k \tau)\right\| \leq C \tau^{2}
$$

where $C$ depends on the problem and the final time $T$, but not on $k$ and $\tau$ for $0 \leq k \tau \leq T$.
Proof. To show this corollary, we only have to verify the assumptions of Theorem 6. However, this is immediate from the discussion above.

## 5. High order composition methods

In the previous sections we have exclusively considered the iterated Strang splitting scheme $S_{\tau}^{(i)}$. Now, we will describe how this (almost) symmetric Strang splitting scheme can be used to construct splitting methods of higher order. To that end we will first discuss composition for a symmetric one-step method.

Suppose that a symmetric one-step method $\Phi_{\tau}$ is of even order $p$. Then a method of order $p+2$ can be constructed by composition (see e.g. [5, p. 43]). More specifically, under suitable conditions on $\gamma_{1}, \gamma_{2}, \gamma_{3}$, the method $\Phi_{\gamma_{3} \tau} \circ \Phi_{\gamma_{2} \tau} \circ \Phi_{\gamma_{1} \tau}$ is of order $p+2$. Therefore, we are able to construct methods of arbitrarily high even order. For $p=2$, i.e. starting with Strang splitting, the corresponding fourth order method is the well-known triple jump scheme. The cost, in terms of a single evaluation of the Strang splitting scheme, is given by $3^{p / 2-1}$, where $p$ is the desired order of the composition method constructed.

That such an approach can be extended to the case of the almost symmetric Strang splitting method $S_{\tau}^{(i)}$ has been shown, in the case of non-stiff ordinary differential equations, in [6]. In this section we will extend the results presented in the before mentioned paper to the time integration of partial differential equations. Recall that if the following system of equations is satisfied

$$
\begin{align*}
& \gamma_{1}+\gamma_{2}+\gamma_{3}=1  \tag{22}\\
& \gamma_{1}^{p+1}+\gamma_{2}^{p+1}+\gamma_{3}^{p+1}=0 \tag{23}
\end{align*}
$$

the composition results in a scheme of order at least $p+1$. By a symmetry argument we can then deduce that the order is indeed $p+2$. This symmetry argument requires that $\Phi_{\tau}^{*}-\Phi_{\tau}=\mathcal{O}\left(\tau^{p+3}\right)$, where we have used $\Phi_{\tau}^{*}$ to denote the adjoint method of $\Phi_{\tau}$, and $\gamma_{1}=\gamma_{3}$ (see [6]).

The single real solution that simultaneously satisfies (22) and (23) is given by

$$
\gamma_{1}=\gamma_{3}=\frac{1}{2-2^{1 /(p+1)}}, \quad \gamma_{2}=-2^{1 /(p+1)} \gamma_{1}
$$

Note that in order to perform this scheme we have to compute at least one negative time step. In fact, this is shown to be necessary if the desired order of the composition method is strictly larger than two (see e.g. [11]). While it is possible to take negative time steps in the case of hyperbolic equations, in parabolic problems this almost certainly leads to numerical instabilities as, for example, roundoff errors are exponentially amplified in each backward step. To remedy this situation in $[12,13]$ it has been pointed out that the system of equations given by (22) and (23) admits complex solutions with positive real part. We will discuss the efficiency ramifications of using complex values in the entire computation in Section 6.1.

Now, let us turn to the main result of this section. That is, we will indicate how the analysis conducted above can be extended from the non-stiff ordinary differential equations considered in [6] to the partial differential equations considered in this paper. For such an analysis appropriate regularity assumptions are indispensable. In particular we have to control the
remainder terms in the expansions. Now, under the assumption that the symmetric splitting scheme is consistent of order $p$, it holds that the local errors $e_{i}$ of $\Phi_{\gamma_{i} \tau}$ satisfy

$$
\begin{aligned}
& e_{1}=C\left(u_{0}\right)\left(\gamma_{1} \tau\right)^{p+1}+\tau^{p+2} R_{1}\left(u_{0}\right), \\
& e_{2}=C\left(u\left(\gamma_{1} \tau\right)\right)\left(\gamma_{2} \tau\right)^{p+1}+\tau^{p+2} R_{2}\left(u\left(\gamma_{1} \tau\right)\right), \\
& e_{3}=C\left(u\left(\left(\gamma_{1}+\gamma_{2}\right) \tau\right)\right)\left(\gamma_{3} \tau\right)^{p+1}+\tau^{p+2} R_{3}\left(u\left(\left(\gamma_{1}+\gamma_{2}\right) \tau\right)\right),
\end{aligned}
$$

where $R_{i}(\cdot)$ denotes the (bounded) remainder term. Note that this, in fact, requires additional applications of the $b$ operator as computed in the previous section. However, it should be clear that if the solution is sufficiently regular, such an expansion can be accomplished by the straightforward, but tedious, extension of Sections 3 and 4 . Then it is possible to generalize the proof given above by employing Corollary 3 . Let $E_{i}$ denote the full errors, i.e.

$$
\begin{aligned}
& E_{1}=\Phi_{\gamma_{1} \tau}\left(u_{0}\right)-u\left(\gamma_{1} \tau\right) \\
& E_{2}=\Phi_{\gamma_{2} \tau} \circ \Phi_{\gamma_{1} \tau}\left(u_{0}\right)-u\left(\left(\gamma_{1}+\gamma_{2}\right) \tau\right) \\
& E_{3}=\Phi_{\gamma_{3} \tau} \circ \Phi_{\gamma_{2} \tau} \circ \Phi_{\gamma_{1} \tau}\left(u_{0}\right)-u(\tau)
\end{aligned}
$$

Now we can employ the same argument as is provided in [5, Chapter II.4] to show that the composition method is in fact of order $p+1$.

To conclude this section, let us note that the argument provided establishes that, under suitable assumptions on the regularity of the solution, the composition method is of order $p+1$. Due to the fact that $S_{\tau}^{(p+2)}$ is symmetric up to order $p+2$, the method is in fact of order $p+2$.

## 6. Numerical simulations

Having established the theoretical convergence rates for the Strang splitting scheme $S_{\tau}^{(i)}$ and its composition in the previous sections, we now turn our attention to illustrate these results by conducting numerical simulations. To that end we have chosen the well-known Brusselator as a parabolic system. The Brusselator consists of two coupled reaction-diffusion equations and provides a valuable prototype for many similar, but often considerably more complicated, systems that model the interaction of chemical species. As an example for a hyperbolic system we have chosen the KdV equation in a single dimension. This equation is then split in such a manner that the Burgers type nonlinearity can be treated as a positiondependent but linear advection. For each of these examples a $\mathrm{C}++$ program has been written that employs the fftw library and is parallelized using OpenMP.

### 6.1. A parabolic system: the Brusselator

As an example of a parabolic system we consider the Brusselator (see e.g. [14, p. 152]). This system is given by

$$
\begin{aligned}
& \partial_{t} u=\alpha \Delta u+(u v-\beta) u+\delta, \\
& \partial_{t} v=\alpha \Delta v-u^{2} v+\gamma u
\end{aligned}
$$

where $u(t, x, y)$ and $v(t, x, y)$ are the two unknowns that usually represent the concentration of chemical species. We have chosen the reaction parameters as $\beta=4.4, \gamma=3.4, \delta=1$, and employ a relatively weak diffusion with $\alpha=10^{-2}$. The equations above have to be supplemented by suitable initial conditions. For the purpose of the numerical simulations conducted in this section, the following initial values are used

$$
\begin{gathered}
u_{0}(x, y)=22 y(1-y)^{3 / 2}(1+\cos (10 \pi x)) \\
v_{0}(x, y)=27 x(1-x)^{3 / 2}(1+\sin (10 \pi x))
\end{gathered}
$$

and all computations are carried out on the domain $[0,1]^{2}$ with periodic boundary conditions.
In the context of the splitting scheme outlined in Section 1, let us define

$$
A\left[\begin{array}{l}
u \\
v
\end{array}\right]=\left[\begin{array}{l}
\alpha \Delta u \\
\alpha \Delta v
\end{array}\right]
$$

The corresponding flow can be computed efficiently by employing two discrete Fourier transforms. In addition, the nonlinearity is represented by (note that this choice is not unique)

$$
b\left(u_{\star}, v_{\star}\right)=\left[\begin{array}{cc}
u_{\star} v_{\star}-\beta & 0 \\
\gamma & -u_{\star}^{2}
\end{array}\right]
$$

and

$$
d=\left[\begin{array}{l}
\delta \\
0
\end{array}\right]
$$



Fig. 1. Order plot for the Brusselator integrated up to $T=0.25$ with $2^{10}$ grid points per dimension (in total we have $2^{21}$ grid points). The error at the final time (measured in the discrete infinity norm) is computed by comparing the numerical solution for a given $\tau$ with a reference solution for which a sufficiently small time step is chosen. For the triple jump and implicit triple jump scheme complex arithmetics is employed. In addition, for each scheme a line with slope equal to the expected order is displayed as well.


Fig. 2. Work-precision plot for the Brusselator integrated up to $T=0.25$ with $2^{10}$ grid points per dimension (in total we have $2^{21}$ grid points). The error at the final time (measured in the discrete infinity norm) is computed by comparing the numerical solution for a given $\tau$ with a reference solution for which a sufficiently small time step is chosen.

Thus, we have to compute the solution of a linear system in two variables which can be done analytically. Note that in this case we could, in fact, find, by a rather tedious calculation, an analytical solution for the complete nonlinearity. However, this is no longer possible if one considers either additional variables, i.e. additional chemical species, or alternatively a more complicated nonlinearity. In such a case, the splitting scheme outlined here would not suffer any further difficulty or even a loss of efficiency as the nonlinearity in question still reduces to a linear system that is easily solved by standard methods.

In the numerical simulation we will compare three splitting schemes: the (classic) Strang splitting scheme $M_{\tau}$ which is expected to be of order two; the naive triple jump scheme which is constructed by composition from $M_{\tau}$. Since $M_{\tau}$ is not symmetric we expect this to be a third order scheme. Finally, we will consider the triple jump scheme constructed by composition from $S_{\tau}^{(4)}$. Since $S_{\tau}^{(4)}$ is symmetric up to order four we expect that this approach results in a fourth order scheme. In fact, this is the main motivation for our approach as it enables us to construct high order (for example, fourth or sixth order methods) by employing the well known composition rules. The numerical results shown in Fig. 1 confirm the expected order for all numerical schemes considered.

From Fig. 1 we can clearly see that if similar step sizes are taken the error made by the fourth order iterated triple jump scheme is significantly less than the error of both the third order triple jump scheme as well as the second order (classic) Strang splitting scheme. However, to discuss whether the high order schemes constructed here can also provide a significant gain in efficiency we have to plot the simulation time as a function of the error. This is done in Fig. 2.

It is shown that for high precision requirement (or equivalently long integration times) the use of the fourth order iterated triple jump scheme (with 4 iterations, i.e. $S_{\tau}^{(4)}$ ) results in a significant increase in efficiency. However, due to the overhead involved in the use of complex arithmetics for small precision requirements and short integration intervals the Strang splitting scheme is clearly the preferred choice. Also note that our fourth order scheme is superior to the naive triple
jump scheme for almost any precision requirements that go beyond the region where the (classic) Strang splitting scheme is superior in terms of efficiency.

### 6.2. A hyperbolic system: the KdV equation

As an example of a hyperbolic system we consider the KdV (Korteweg-de Vries) equation in a single dimension. It is given by

$$
\partial_{t} u(t, x)+\partial_{x}^{3} u(t, x)+u(t, x) \partial_{x} u(t, x)=0
$$

It is shown in $[15,16]$ that for sufficiently regular initial values the regularity of the solution to the KdV equation is not diminished as it is evolved in time (although this does not rule out the appearance of high frequency oscillations). For the purpose of this section, we will consider two initial values with extremely different dynamical behavior.

First, let us consider the following initial value

$$
\begin{equation*}
u_{0}(x)=u(0, x)=\frac{12}{\cosh ^{2} x} \tag{24}
\end{equation*}
$$

The exact solution is a soliton that travels to the right with speed 4, i.e., the solution is given by (see e.g. [17])

$$
u(t, x)=u_{0}(x-4 t)
$$

For our numerical studies we consider the domain $[-20,20]$ in order to limit artifacts which originate from the fact that periodic boundary conditions are imposed on the domain of finite length that is used in the numerical simulations. We integrate up to a final time $T=0.4$.

Second, we consider an initial value where oscillations appear. The so called Schwartzian initial value is given by (see e.g. [4])

$$
\begin{equation*}
u_{0}(x)=\frac{12 x \tanh |x|}{|x| \cosh ^{2} x} \tag{25}
\end{equation*}
$$

In this instance we integrate only up to $T=0.05$ and employ the domain $[-4 \pi, 4 \pi]$ with periodic boundary conditions (following the same argument as given above).

Now let us turn our attention to the splitting scheme employed. In the framework of Section 1 the linear problem is defined as

$$
A=-\partial_{x}^{3}
$$

and can be solved efficiently by employing two discrete Fourier transforms. Instead of the full nonlinearity we numerically compute the evolution corresponding to

$$
\begin{equation*}
b\left(u_{\star}\right)=u_{\star}(x) \partial_{x}, \quad d=0 \tag{26}
\end{equation*}
$$

This is significantly less involved than the case with the full Burgers type nonlinearity. In fact, [4] states that using the full nonlinearity invalidates splitting as a viable approach to numerically solve the KP (Kadomtsev-Petviashvili) equation (note that, compared to the KdV equation, the two dimensional KP equation includes an additional diffusive term in the second variable). However, the linear problem given by Eq. (26) can be computed numerically to high precision, for example, by using the (exact) exponential of a finite difference stencil (as it is often done in the context of exponential integrators, for example). We intended to employ the Expokit package to compute the exponential of a seven-point stencil that is used to approximate the first derivative. However, in case of the soliton solution the results were not satisfactory except for very small step sizes. Therefore, we used the SUNDIALS CVODE solver, with a prescribed tolerance of $10^{-12}$, for this example. ${ }^{1}$

The numerical results are shown in Fig. 3 (for the soliton initial value given in Eq. (24)) and in Fig. 4 (for the Schwartzian initial value given in Eq. (25)). Note that the numerical simulations match the predicted orders of the schemes studied very well. Thus, we conclude that the data obtained are clearly consistent with the analysis conducted in Sections 3 and 5.

## 7. Conclusion and outlook

We have rigorously shown that the proposed iterated Strang splitting scheme is of second order in time and due to its symmetry properties can be used to construct methods of arbitrary (even) order by composition. The main assumption we have made is that the classic Strang splitting method is convergent of order two (i.e., we deal with a problem for which applying a splitting scheme of second order is sensible). Further, a technical assumption on the nonlinearity is made. This assumption reduces, in the linear limit, to the statement that we have to bound an appropriate number of application of the

[^1]

Fig. 3. Order plot for the KdV equation integrated up to $T=0.4$ with $2^{10}$ grid points for the soliton initial value given in (24). The error at the final time (measured in the discrete $L^{2}$ norm) is computed by comparing the numerical solution for a given $\tau$ with a reference solution for which a sufficiently small time step has been chosen. In addition, for each scheme a line with slope equal to the expected order is displayed as well.


Fig. 4. Order plot for the KdV equation integrated up to $T=0.05$ with $2^{11}$ grid points for the Schwartzian initial value given in (25). The error at the final time (in the discrete $L^{2}$ norm) is computed by comparing the numerical solution for a given $\tau$ with a reference solution for which a sufficiently small time step has been chosen. In addition, for each scheme a line with slope equal to the expected order is displayed as well.
operator in question to the exact solution (assumptions of a similar type have been used in much of the literature to show convergence of splitting methods for linear partial differential equations).

In addition, we have provided an argument demonstrating that our iterated Strang splitting can be used, similar to the case of ordinary differential equations, to construct higher order methods by composition if sufficient regularity of the exact solution can be assumed. This has been verified up to order four for both the Brusselator system (a parabolic problem) and the KdV equation (a hyperbolic partial differential equation). In both instances the iterated fourth order method is shown to provide superior performance, in case of medium to high precision requirements (or equivalently long integration times), as compared to the (classic) Strang splitting. In addition, we observe superior performance for high precision requirements when the iterated fourth order method is compared to the (classic) triple jump scheme (which is a method of order three). We also conclude that the necessity of using complex precision arithmetics, in the case of parabolic problems, does not negate the performance gain we expect from higher order methods.

In this paper we have only considered methods of order up to four. However, composition can be used to construct methods of arbitrary (even) order. To provide a clear picture of the efficiency gain expected for such high order methods, longer integration times as well as more complicated partial differential equations have to be considered. Since we have not considered parallelization and other computing aspects in this paper, we will consider such investigations as a subject of further research.

## References

[1] R.I. McLachlan, On the numerical integration of ordinary differential equations by symmetric composition methods, SIAM J. Sci. Comput. 16 (1) (1995) 151-168.
[2] C.Z. Cheng, G. Knorr, The integration of the Vlasov equation in configuration space, J. Comput. Phys. 22 (3) (1976) 330-351.
[3] L. Einkemmer, A. Ostermann, Convergence analysis of Strang splitting for Vlasov-type equations, SIAM J. Numer. Anal. 52 (2014) 140-155.
[4] C. Klein, K. Roidot, Fourth order time-stepping for Kadomtsev-Petviashvili and Davey-Stewartson equations, SIAM J. Sci. Comput. 33 (6) (2011) 3333-3356.
[5] E. Hairer, C. Lubich, G. Wanner, Geometric Numerical Integration: Structure-Preserving Algorithms for Ordinary Differential Equations, Springer Verlag, 2006.
[6] L. Einkemmer, A. Ostermann, An almost symmetric Strang splitting scheme for the construction of high order composition methods, 2013, arXiv preprint. arXiv:1306.1169.
[7] T. Jahnke, C. Lubich, Error bounds for exponential operator splittings, BIT Numer. Math. 40 (4) (2000) 735-744.
[8] H. Holden, C. Lubich, N.H. Risebro, Operator splitting for partial differential equations with Burgers nonlinearity, Math. Comp. 82(281)(2013) 173-185.
[9] N.I. Katzourakis, A Hölder continuous nowhere improvable function with derivative singular distribution, 2010, arXiv preprint. arXiv: 1011.6071 .
[10] C. Lubich, On splitting methods for Schrödinger-Poisson and cubic nonlinear Schrödinger equations, Math. Comp. 77 (2008) $2141-2153$.
[11] S. Blanes, F. Casas, On the necessity of negative coefficients for operator splitting schemes of order higher than two, Appl. Numer. Math. 54 (1) (2005) 23-37.
[12] E. Hansen, A. Ostermann, High order splitting methods for analytic semigroups exist, BIT Numer. Math. 49 (3) (2009) $527-542$.
[13] F. Castella, P. Chartier, S. Descombes, G. Vilmart, Splitting methods with complex times for parabolic equations, BIT Numer. Math. 49 (3) (2009) 487-508.
[14] E. Hairer, G. Wanner, Solving Ordinary Differential Equations II: Stiff and Differential-Algebraic Problems, second ed., Springer Verlag, 1996.
[15] Y. Kametaka, Korteweg-de Vries equation, I. Global existence of smooth solutions, Proc. Japan Acad. Ser. A Math. Sci. 45 (7) (1969) $552-555$.
[16] J.L. Bona, R. Smith, The initial-value problem for the Korteweg-de Vries equation, Phil. Trans. R. Soc. A 278 (1287) (1975) 555-601.
[17] C. Klein, C. Sparber, P. Markowich, Numerical study of oscillatory regimes in the Kadomtsev-Petviashvili equation, J. Nonlinear Sci. 17 (5) (2007) 429-470.


[^0]:    This work is supported by the Austrian Science Fund (FWF)-project id: P25346.

    * Corresponding author.

    E-mail addresses: lukas.einkemmer@uibk.ac.at (L. Einkemmer), alexander.ostermann@uibk.ac.at (A. Ostermann).
    http://dx.doi.org/10.1016/j.camwa.2014.02.027
    0898-1221/© 2014 The Authors. Published by Elsevier Ltd. This is an open access article under the CC BY-NC-ND license (http://creativecommons.org/ licenses/by-nc-nd/3.0/).

[^1]:    1 Unfortunately, to our knowledge, there are no packages that are written in C++ available to compute the matrix exponential. We have tried both Expokit as outlined above and the (unsupported) matrix exponential provided by the SPARSEKIT package (using our own Fortran to C bindings). Even though the source code of SPARSEKIT is much more readable, it is only able to compute an approximation up to a tolerance of $10^{-6}$. This, is even true for the diagonal example provided as part of the package. None of these packages are parallelized. However, let us mention here, for the sake of completeness, that there are a number of Python and Matlab implementations available.

