

Splitting methods with complex times for parabolic equations

F. Castella · P. Chartier · S. Descombes · G. Vilmart

Received: 25 September 2008 / Accepted: 3 July 2009 / Published online: 28 July 2009
© Springer Science + Business Media B.V. 2009

Abstract Using composition procedures, we build up high order splitting methods to solve evolution equations posed in finite or infinite dimensional spaces. Since high-order splitting methods with real time are known to involve large and/or negative time steps, which destabilizes the overall procedure, the key point of our analysis is, we develop splitting methods that use *complex* time steps having *positive real part*: going to the complex plane allows to considerably increase the accuracy, while keeping small time steps; on the other hand, restricting our attention to time steps with positive real part makes our methods more stable, and in particular well adapted in the case when the considered evolution equation involves unbounded operators in infinite dimensional spaces, like parabolic (diffusion) equations.

Communicated by Christian Lubich.

Note: Similar results are derived independently by E. Hansen & A. Ostermann in [15].

F. Castella

IRMAR and INRIA Rennes, Université de Rennes 1, Campus Beaulieu, 35042 Rennes Cedex, France
e-mail: francois.castella@univ-rennes1.fr

P. Chartier (✉)

INRIA Rennes and Ecole Normale Supérieure de Cachan, Antenne de Bretagne,
Avenue Robert Schumann, 35170 Bruz, France
e-mail: Philippe.Chartier@inria.fr

S. Descombes

Université de Nice–Sophia Antipolis, Parc Valrose, 06108 Nice Cedex 02, France
e-mail: sdescomb@unice.fr

G. Vilmart

Section de mathématiques, University of Geneva, 2-4, rue du Lièvre, CP 64, 1211, Genève 4,
Switzerland
e-mail: Gilles.Vilmart@unige.ch

We provide a thorough analysis in the case of linear equations posed in general Banach spaces. We also numerically investigate the nonlinear situation. We illustrate our results in the case of (linear and nonlinear) parabolic equations.

Keywords Splitting · Complex time steps · Composition method · Higher order · Parabolic equations

Mathematics Subject Classification (2000) 65M12 · 47D06

1 Introduction

The goal of the present text is to derive *high-order* splitting methods, obtained by using *complex* time steps. These methods are obtained through composition procedures. For stability purposes, the retained methods only involve time steps that have positive real part: our motivation is to recover methods which can be used in the case when unbounded operators are involved, associated with propagators that are C^0 semi-groups only (instead of C^0 groups). Our paradigm is the case of diffusion equations.

Let us make our statement precise.

Consider a linear evolution equation of the form

$$\frac{d}{dt}u(t) = Au(t) + Bu(t), \quad (1.1)$$

where the right-hand-side involves the sum of two well identified operators A and B . Here, the unknown $u(t)$ is assumed to belong to some finite or infinite dimensional Banach space X , while A and B are linear, possibly unbounded, operators. In the case when A and B are unbounded, we assume A , B , and $A + B$ generate C^0 semi-groups of propagators over X , denoted by e^{tA} , e^{tB} and $e^{t(A+B)}$, respectively, whenever $t \geq 0$. The prototype we have in mind is the linear heat equation with potential

$$\partial_t u(t, x) = \Delta u(t, x) + V(x)u(t, x),$$

where $t \geq 0$ is time and $x \in \mathbb{R}^d$ (or $x \in \mathbb{T}^d$) is the space variable, Δ denotes the standard Laplacian in x , while the potential $V(x)$ is assumed bounded. In that case one may choose $X = L^2(\mathbb{R}^d)$ and define the unbounded operator $(Au)(x) = \Delta u(x)$ with domain $D(A) = H^2(\mathbb{R}^d)$, together with the bounded operator $(Bu)(x) = V(x)u(x)$ (other choices are obviously possible for the Banach space X at this level, depending on the assumed smoothness of the potential: X may as well measure Sobolev regularity, or Hölder regularity of the solution u).

It is well-known that a possible approach to numerically solve (1.1) is to use a splitting method, *i.e.* to approximate the propagator of the full operator $u \mapsto Au + Bu$ by using an appropriate combination of the propagators $u \mapsto Au$ and $u \mapsto Bu$, both assumed to be numerically cheaper to evaluate. In the finite dimensional setting, splitting methods basically rely on the identity

$$e^{h(A+B)} = e^{hA} e^{hB} + \mathcal{O}(h^2),$$

where h is some small time-step. Higher order approximations may be obtained by writing

$$e^{h(B+A)} = e^{b_1hA} e^{a_1hB} e^{b_2hA} e^{a_2hB} \dots e^{b_s hA} e^{a_s hB} + \mathcal{O}(h^{r+1}),$$

where a_1, \dots, a_s and b_1, \dots, b_s are (to be chosen) real or complex numbers, and s is usually referred to as the number of steps of the method. The exponent r depends on the chosen values of the a_i 's and b_i 's.

The above procedure immediately extends to the case when the operators A and B become nonlinear. In this case indeed, the above formulae remain unchanged, provided the factors $e^{h(A+B)}$, $e^{a_i hA}$, and $e^{b_i hB}$ are replaced by the true flows $\Phi_{A+B}(h)$, $\Phi_A(a_i h)$, and $\Phi_B(b_i h)$ respectively, or by appropriate approximations of them. Here we have defined, for any y_0 , the flow $\Phi_A(t)(y_0)$ as the solution to the differential equation

$$\frac{d}{dt}(\Phi_A(t)(y_0)) = A(\Phi_A(t)(y_0)),$$

supplemented with the initial condition $\Phi_A(0)(y_0) = y_0$ (and the similar definition is used to prescribe the flows $\Phi_{A+B}(t)$ and $\Phi_B(t)$). In this context however, it needs to be assumed that the vector fields A and B possess enough smoothness to have well-defined flows $\Phi_{A+B}(h)$, $\Phi_A(h)$, and $\Phi_B(h)$ for small values of h . Note also that if a_i is complex, the definition of $\Phi_A(a_i h)$ requires, say, that for any y_0 the differential equation $\frac{d}{dt}(\Phi_A(t)(y_0)) = A(\Phi_A(t)(y_0))$ be solvable along the complex line $t = a_i t'$ ($t' \in \mathbb{R}$) whenever $0 \leq t' \leq h$ and h is small enough (and similarly for B).

The *formal* extension of all above formulae in the infinite dimensional setting is easy as well, keeping in mind that the existence and well definiteness of all involved propagators over the retained Banach space X should then be carefully checked. In the paradigmatic case when $A = \Delta$, for instance, we recall that the propagator $e^{z\Delta}$ ($z \in \mathbb{C}$) is well-defined, in any reasonable distribution sense, if and only if $\text{Re}(z) \geq 0$. Naturally, another key difficulty in the infinite dimensional situation is to check that the remainder terms indeed have size $\mathcal{O}(h^2)$ resp. $\mathcal{O}(h^{r+1})$ in the correct norm.

Now, the derivation of *high-order* splitting methods is not straightforward in general, even in the finite dimensional case. The simplest, high-order splitting methods involve large negative time steps alternating with large positive time steps (*i.e.* large positive values of the a_i 's or b_i 's alternating with large negative values of the same coefficients), which eventually leads to poor accuracy in practice. Even more, a disappointing result shows that all splitting methods (or composition methods—see below for the definition) with *real* coefficients must have some negative coefficients a_i and b_i in order to achieve order 3 or more. The existence of at least one negative coefficient was shown in [20, 21], and the existence of a negative coefficient for both operators was proved in [12]. An elegant geometric proof can also be found in [2]. As a consequence, such high-order splitting methods *cannot* be used in general when one operator A or B has large negative spectrum, or when it only generates a C^0 *semi-group* of propagators—and not a group (like the Laplacian).

In order to circumvent this order-barrier, there are two possibilities. One can use a linear, convex combination (see [1, 10, 11] for methods of orders 3 and 4) or non-convex combination (see [6, 19] where an extrapolation procedure is exploited), of

elementary, low order splitting methods (some of the above mentioned works use elementary methods which involve one or two complex time steps). Another possibility is to systematically consider splitting methods with *complex* coefficients a_i and b_i , having yet *positive real parts* (see [3] in celestial mechanics). In 1962/1963, Rosenbrock [18] considered complex coefficients in a similar context. We may also quote the text [23]—see also [1]—, where some low order methods with complex coefficients are derived (one can find here an alternative proof of the existence of negative coefficients when only real time steps are allowed).

This is the route we chose here.

In this article, we consider splitting methods of the form

$$e^{h(B+A)} = \prod_{i=1}^s e^{b_i h A} e^{a_i h B} + \mathcal{O}(h^{r+1}),$$

and we derive new high-order splitting methods (up to order fourteen), which involve complex time steps having positive real part. We state and prove error estimates that are valid both in the finite and in the infinite dimensional setting. We last investigate *numerically* the behaviour of the retained methods both in the case of the linear heat equation with bounded potential (the setting is one-dimensional with periodic boundary conditions), and in the case of nonlinear versions of the heat equation (in the similar setting).

Our derivation uses composition techniques that were originally developed for the geometric numerical integration of ordinary differential equations [13].

The main advantages of our approach are the following:

- the splitting method inherits the stability property of exponential operators;
- in the retained methods, we can always replace the costly exponentials of the operators e^{hA} etc. by cheap low order approximations of the latter, without altering the overall order of accuracy;
- using complex coefficients allows to reduce the number of compositions needed to achieve any given order.

This paper is organized as follows. In Sect. 2, we derive new high-order splitting methods. In Sect. 3 we give a rigorous order estimate in the linear case, obtained as a direct consequence of the recent results by Hansen & Ostermann [14]. Section 4 presents several numerical simulations, confirming the formally expected order of accuracy in the non-linear case.

2 Deriving high order splitting/composition methods

2.1 Composition methods in the finite dimensional case

Composition methods were mainly developed in the 90's in the papers of Suzuki [22], Yoshida [24] and McLachlan [16] in the context of ordinary differential equations. They rely on the following observation.

Consider a (linear or nonlinear) ordinary differential equation of the form

$$\frac{d}{dt}u(t) = f(u(t)),$$

where $u(t) \in \mathbb{R}^d$ belongs to some finite dimensional space. Denote by $\phi(t)$ the flow of the above equation, namely $\phi(t) : \mathbb{R}^d \rightarrow \mathbb{R}^d$ satisfies

$$u(t) = \phi(t)(u(0)).$$

On the other hand take a time step $h > 0$, and consider any approximation ϕ_h of $\phi(h)$ at order p , for some value of $p \in \mathbb{N}$. In other words, $\phi_h : \mathbb{R}^d \rightarrow \mathbb{R}^d$ is assumed to satisfy

$$\phi_h = \phi(h) + \mathcal{O}(h^{p+1}).$$

The above identity is assumed to hold between mappings on \mathbb{R}^d . It means that whenever $K \subset \mathbb{R}^d$ is a compact set, there is a constant $C > 0$ and a small $h_0 > 0$, such that for any $u \in K$, and any $0 < h < h_0$, we have $\|\phi_h(u) - \phi(h)(u)\| \leq Ch^{p+1}$.

Lastly, take an integer s and choose (real or complex) coefficients $\gamma_1, \dots, \gamma_s$ (in the classical theory, only real coefficients were considered).

Under these circumstances, a composition method is defined as the operator

$$\psi_h = \phi_{\gamma_s h} \circ \dots \circ \phi_{\gamma_1 h}, \tag{2.1}$$

i.e. as the composition of the method ϕ_h , successively used with time steps $\gamma_1 h, \gamma_2 h, \dots, \gamma_s h$. Naturally, if the γ_i 's are complex, we implicitly assume here that the operators $\phi_{\gamma_i h}$ are well-defined for small values of $h > 0$, in the following sense: for any compact set $K \subset \mathbb{R}^d$, there is an $h_0 > 0$ such that the operator $\phi_{\gamma_i h}$ is well-defined over K whenever $0 < h < h_0$. Similarly, we also assume that the operators $\phi(\gamma_i h)$ are well-defined for small values of $h > 0$, and that the estimates $\phi_{\gamma_i h} = \phi(\gamma_i h) + \mathcal{O}(h^{p+1})$ hold for small $h > 0$ as well (in the above sense).

The following classical result in numerical integration illustrates that the composition procedure allows to transform a method ϕ_h of order p , into a higher-order method ψ_h of order $p + 1$.

Theorem 2.1 (see, [13, Theorem II.4.1]) *With the above notation and assumptions, let ϕ_h be an approximation of $\phi(h)$ of order p , namely*

$$\phi_h = \phi(h) + \mathcal{O}(h^{p+1}).$$

If the γ_i 's satisfy

$$\gamma_1 + \dots + \gamma_s = 1 \quad \text{and} \quad \gamma_1^{p+1} + \dots + \gamma_s^{p+1} = 0, \tag{2.2}$$

*then the composition method $\psi_h = \phi_{\gamma_s h} \circ \dots \circ \phi_{\gamma_1 h}$ approximates $\phi(h)$ at order $p + 1$, *i.e.**

$$\psi_h = \phi(h) + \mathcal{O}(h^{p+2}).$$

Remark 2.1 Whenever p is even and the composition is symmetric (i.e. $\gamma_{s-i+1} = \gamma_i$ for any i), then ψ_h is of order $p + 2$.

Proof The idea of proof is to show that if the basic method has order p , i.e.

$$\phi_h(y) = \phi(h)(y) + C(y)h^{p+1} + \mathcal{O}(h^{p+2}),$$

where $\phi(h)$ denotes the exact flow, then, using the fact that the sum of the γ_i 's is one, we have

$$\phi_{\gamma_s h} \circ \dots \circ \phi_{\gamma_1 h}(y) = \phi(h)(y) + C(y)(\gamma_1^{p+1} + \dots + \gamma_s^{p+1})h^{p+1} + \mathcal{O}(h^{p+2}).$$

Here, the constant $C(y)$ denotes a quantity that remains bounded whenever y belongs to a given compact set. The result follows. □

Given the above theorem, a classical idea is the following. Starting from a low order method ϕ_h , we may increase the order by one, by appropriately choosing the γ_i 's; iterating the process, and choosing therefore possibly different γ_i 's at each stage of the whole procedure, we may eventually come up with a high-order method.

This is the program we intend to follow, in the very case of splitting methods. The point is, such a program fails past order 2 when the γ_i 's are restricted to only take real values: past order 2 indeed, negative γ_i 's, as well as large γ_i 's come up in the analysis, which makes the so-obtained methods have poor accuracy in practice.

We therefore rely on the use of complex γ_i 's. In that perspective, our main constraint is to obtain high-order method for which the γ_i 's all have positive real part: our goal is to eventually apply the methods in the case of diffusion equations. Secondly, we try to keep the number of stages (the integer s in formula (2.1)) reasonably small (to reduce the computational cost), and the moduli $|\gamma_i|$ as small as possible as well (to reduce the size of the time steps). Lastly, we also try to keep the quantities $|\arg(\gamma_i)|$ as small as possible. In the context of splitting methods, all these constraints are fairly natural, since the reader should keep in mind that one step of the full evolution equation $\dot{y} = A(y) + B(y)$, along a time step h , is here approximated by s steps of either $\dot{y} = A(y)$ or $\dot{y} = B(y)$, along the successive time steps $\gamma_1 h, \dots, \gamma_s h$ (see e.g. Fig. 1).

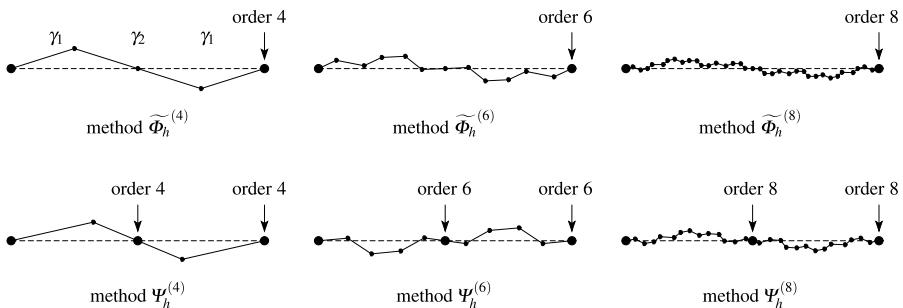


Fig. 1 Diagrams of coefficients for compositions methods (2.10) and (2.13)

A last, important remark is in order. Throughout this text, we will restrict our attention to the case of *symmetric* methods. The reason for this choice is, as stated in Remark 2.1, that symmetric composition methods applied to symmetric procedures allow to gain two orders of accuracy each time one applies Theorem 2.1. We nevertheless stress that this choice is arbitrary, and considering non-symmetric methods is relevant as well. For instance, we may quote the work of Hansen and Ostermann [15] where non-symmetric methods are considered.

2.2 Building up high-order splitting/composition methods with complex coefficients—the linear, finite-dimensional case

Throughout this paragraph, we take fixed matrices A and B acting on \mathbb{R}^d , and introduce new splitting/composition methods to solve the linear ODE

$$\dot{y} = Ay + By.$$

Though A and B are finite dimensional matrices here, the reader may keep in mind that we will eventually consider the infinite dimensional situation where A is the Laplace operator, while B denotes the multiplication by a bounded potential V (see introduction). Hence A may be typically thought of as a matrix with 'large' negative eigenvalues.

Following the general methodology described in the previous paragraph, we first need to choose some low-order approximation of the true propagator $\exp(h(A + B))$. We retain the simplest symmetric splitting algorithm, namely the Strang splitting operator, and we set

$$\Phi_h = \exp\left(\frac{hB}{2}\right) \exp(hA) \exp\left(\frac{hB}{2}\right), \tag{2.3}$$

a symmetric second order approximation of $\exp(h(A + B))$. While the methods we propose below are all based on this particular choice of a basic low order method, we readily mention that the analysis we provide remains unchanged when starting from *any* other symmetric second order method. For instance, the following

$$\Phi_h^P = \underbrace{\left(\text{Id} - \frac{h}{2}B\right)^{-1}}_{\text{implicit Euler}} \underbrace{\left[\left(\text{Id} - \frac{h}{2}A\right)^{-1} \left(\text{Id} + \frac{h}{2}A\right) \right]}_{\text{implicit midpoint}} \underbrace{\left(\text{Id} + \frac{h}{2}B\right)}_{\text{explicit Euler}} \tag{2.4}$$

would provide such a basic choice. In the infinite dimensional setting and when formally choosing A as the Laplace operator while B is the multiplication by the bounded potential V , the method Φ_h^P coincides with the Peaceman-Rachford formula [17] originally developed for the heat equation, and extended to reaction-diffusion problems in [7]. Note that the use of an implicit midpoint approximation for the operator A corresponds to a standard Crank-Nicolson scheme when A is the Laplace operator, a standard choice.

2.2.1 Triple jump procedures

Starting from the basic, second order, Strang splitting algorithm Φ_h , we wish to derive various higher order *symmetric* methods by applying Theorem 2.1. Since the symmetry requirement anyhow prevents the choice $s = 2$ in Theorem 2.1 (system (2.2) for $s = 2$ and symmetric γ_i 's imposes $\gamma_1 = \gamma_2 = 0$), the simplest choice is to set $s = 3$ in Theorem 2.1 and to look for a three steps, symmetric composition procedure. Such a method is usually called ‘Triple jump composition procedure’. Note in passing that double jump composition procedures (with complex time steps) have been considered in [14], where methods of order 6 are derived.

In the case when $s = 3$, and starting from an arbitrary, symmetric method ϕ_h of order p (p is an arbitrary even integer here), a triple jump composition procedure is provided by a triple $(\gamma_{1,p}, \gamma_{2,p}, \gamma_{3,p}) \in \mathbb{C}^3$ such that

$$\begin{aligned} \gamma_{1,p} &= \gamma_{3,p} \quad (\text{symmetry}), \\ \gamma_{1,p} + \gamma_{2,p} + \gamma_{3,p} &= 1, \quad \gamma_{1,p}^{p+1} + \gamma_{2,p}^{p+1} + \gamma_{3,p}^{p+1} = 0 \quad (\text{Theorem 2.1}), \end{aligned} \tag{2.5}$$

and the associated improved method is $\psi_h = \phi_{\gamma_{3,p}h} \circ \phi_{\gamma_{2,p}h} \circ \phi_{\gamma_{1,p}h}$. The set of all complex solutions to (2.5) is given by the $p + 1$ values

$$\begin{aligned} \gamma_{1,p}^{(k)} &= \gamma_{3,p}^{(k)} = \frac{1}{2 - 2^{1/(p+1)} e^{2ik\pi/(p+1)}}, \\ \gamma_{2,p}^{(k)} &= -\frac{2^{1/(p+1)} e^{2ik\pi/(p+1)}}{2 - 2^{1/(p+1)} e^{2ik\pi/(p+1)}} \quad (k = 0, \dots, p). \end{aligned} \tag{2.6}$$

Setting $k = 0$ above provides the unique *real* solution to (2.5), namely

$$\gamma_{1,p}^{(0)} = \gamma_{3,p}^{(0)} = \frac{1}{2 - 2^{1/(p+1)}}, \quad \gamma_{2,p}^{(0)} = -\frac{2^{1/(p+1)}}{2 - 2^{1/(p+1)}}. \tag{2.7}$$

Unsurprisingly, the coefficient $\gamma_{2,p}^{(0)}$ is negative. In any circumstance, if ϕ_h has order 2, then the method $\psi_h^{(4)} := \phi_{\gamma_{3,2}h} \circ \phi_{\gamma_{2,2}h} \circ \phi_{\gamma_{1,2}h}$ reaches order 4 using three steps of ϕ_h , while, repeating the method at any order, the method $\psi_h^{(6)} := \psi_{\gamma_{3,4}h}^{(4)} \circ \psi_{\gamma_{2,4}h}^{(4)} \circ \psi_{\gamma_{1,4}h}^{(4)}$ reaches order 6 with 9 steps of ϕ_h , and so on. These methods are originally due to Creutz & Gocksch [4], Forest [9], Suzuki [22], Yoshida [24], the name ‘Triple Jump composition methods’ was given in [13, Example II.4.2]. However, since $\gamma_{2,p}^{(0)} < 0$, these methods cannot be extended, in the infinite dimensional situation, to problems where A only generates a C^0 semi-group of propagators, and where the basic method of choice ϕ_h coincides with the Strang splitting method Φ_h , or with any low order splitting method. On top of that, and even in the finite dimensional setting, the estimate $|\gamma_{j,p}^{(0)}| > 1$, valid for any $j = 1, 2, 3$, implies a terrible zig-zag in the coefficients of the methods. Thus, the above technique is not even very efficient in the finite dimensional case.

Another choice of k is therefore in order in (2.6).

Setting $k = \pm p/2$ (recall that p is even), provides the two conjugate solutions of (2.5) which minimize the quantity $|\gamma_{1,p}^{(k)}| + |\gamma_{2,p}^{(k)}| + |\gamma_{3,p}^{(k)}|$. These two conjugate solutions also minimize the quantity $\max_{i=1,2,3} |\arg(\gamma_{i,p}^{(k)})|$. In order to keep notation simple, we drop the upper index “ $\pm p/2$ ” for the associated coefficients, and simply define $(\gamma_{1,p}, \gamma_{2,p}, \gamma_{3,p})$ as

$$\gamma_{1,p} = \gamma_{3,p} = \frac{e^{i\pi/(p+1)}}{2e^{i\pi/(p+1)} + 2^{1/(p+1)}}, \quad \gamma_{2,p} = \frac{2^{1/(p+1)}}{2e^{i\pi/(p+1)} + 2^{1/(p+1)}}. \tag{2.8}$$

Needless to say, these γ_i 's have positive real part.

A triple jump composition strategy: reaching order 8 Symmetric composition methods $\Phi_h^{(p)}$ of order p (p even) can be constructed by induction, setting

$$\Phi_h^{(2)} = \Phi_h, \quad \Phi_h^{(p+2)} = \Phi_{\gamma_{3,p}h}^{(p)} \circ \Phi_{\gamma_{2,p}h}^{(p)} \circ \Phi_{\gamma_{1,p}h}^{(p)} \quad \text{for } p \geq 2, \tag{2.9}$$

where $\gamma_{1,p}, \gamma_{2,p}, \gamma_{3,p}$ are given in (2.8). The method $\Phi_h^{(p)}$ requires $s = 3^{p/2-1}$ compositions of the basic method Φ_h . Taking care of the non-commuting products (product signs should be read from the right to the left), we may write

$$\Phi_h^{(2)} = \Phi_h = \exp\left(\frac{hB}{2}\right) \exp(hA) \exp\left(\frac{hB}{2}\right),$$

together with

$$\Phi_h^{(4)} = \prod_{j=1}^3 \Phi_{\gamma_{j,2}h}, \quad (= \Phi_{\gamma_{3,2}h} \circ \Phi_{\gamma_{2,2}h} \circ \Phi_{\gamma_{1,2}h}),$$

$$\Phi_h^{(6)} = \prod_{k=1}^3 \left(\prod_{j=1}^3 \Phi_{\gamma_{k,4}\gamma_{j,2}h} \right),$$

$$\Phi_h^{(8)} = \prod_{\ell=1}^3 \left(\prod_{k=1}^3 \left(\prod_{j=1}^3 \Phi_{\gamma_{\ell,6}\gamma_{k,4}\gamma_{j,2}h} \right) \right),$$

and so on. In summary, each method $\Phi_h^{(p)}$ reads

$$\Phi_h^{(p)} = \prod_{j=1}^{3^{(p/2)-1}} \Phi_{\alpha_{j,p}h},$$

for some coefficients $\alpha_{j,p}$ that are obtained as products of the $\gamma_{k,p-2}$'s, $\gamma_{k,p-4}$'s, ..., $\gamma_{k,2}$'s. This defines the coefficients $\alpha_{j,p}$.

Remark 2.2 Coming back to the value of Φ_h in turn allows to write

$$\Phi_h^{(p)} = \prod_{j=1}^{3^{(p/2)-1}} \exp(b_{j,p}hA) \exp(a_{j,p}hB),$$

where $a_{1,p} = \alpha_{1,p}/2$, $b_{1,p} = \alpha_{1,p}$, while $a_{j,p} = (\alpha_{j,p} + \alpha_{j-1,p})/2$, $b_{j,p} = \alpha_{j,p}$ whenever $2 \leq j \leq 3^{(p/2)-1} - 1$, and lastly $a_{j,p} = \alpha_{j,p}/2$, $b_{j,p} = 0$ in the particular case when $j = 3^{(p/2)-1}$.

Now, the important point is

Proposition 2.1 *The above defined method $\Phi_h^{(p)}$ has order p .*

Besides, for $p = 2, 4, 6, 8$, the coefficients $\alpha_{j,p}$ ($j = 1, \dots, 3^{(p/2)-1}$) satisfy

$$\text{Re}(\alpha_{j,p}) > 0.$$

This property ceases to hold whenever $p \geq 10$.

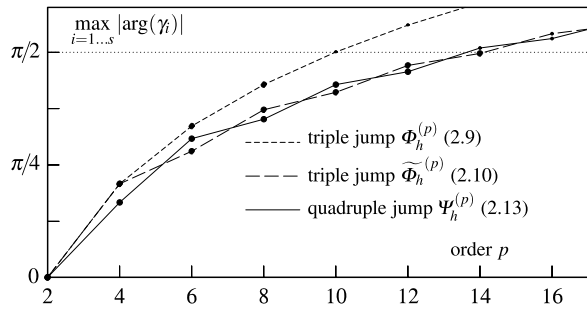
Remark 2.3 The fact that the method $\Phi_h^{(p)}$ reaches order p is here presented in the case of a linear equation $\dot{y} = Ay + By$, and when the basic method Φ_h is the Strang splitting algorithm. Naturally the same result holds when the chosen basic method is any symmetric method of order 2. *Mutatis mutandis* (see introduction), and provided the appropriate assumptions described in the introduction are met, the same result holds in the nonlinear setting as well, where $y \mapsto A(y)$ and $y \mapsto B(y)$ become nonlinear operators.

As a consequence, starting from a second order symmetric method ϕ_h (be it the Strang splitting algorithm Φ_h as above, or any symmetric second order algorithm), the present composition technique can only improve numerical accuracy up to order 8, while preserving the use of time steps $\alpha_{j,p}h$ that all have non-negative real part. This property may be somewhat precised. We observe in Fig. 2 that the quantity $\max_j |\arg(\alpha_{j,p})|$ increases with the order p of the composition methods in (2.9). For the method (2.9) of order $p = 10$ this quantity is greater than $\pi/2$: it involves 81 factors $\Phi_{\alpha_{j,10}}$ and the middle coefficient $\alpha_{41,10}$ has a negative real part, namely $\text{Re}(\alpha_{41,10}) \approx -5 \cdot 10^{-5} < 0$. Thus, this method cannot be used, in general, when the operator A or B has large negative eigenvalues, nor can it be extended, in the infinite dimensional case, when the operator A coincides with the Laplacian.

Another triple jump composition strategy: reaching order 14 Before concluding this paragraph about triple jump procedures, we mention an improvement of the above method.

To reduce the quantity $\max_{i=1\dots s} |\arg(\alpha_{i,p})|$, an idea is to alternate the coefficients $(\gamma_{1,p}, \gamma_{2,p}, \gamma_{3,p})$ by $(\bar{\gamma}_{1,p}, \bar{\gamma}_{2,p}, \bar{\gamma}_{3,p})$ in (2.9). In other words, we propose here to

Fig. 2 Values of $\max_{i=1,\dots,s} |\arg \gamma_i|$ for various composition methods



set

$$\begin{aligned} \tilde{\Phi}_h^{(2)} &= \Phi_h, \\ \tilde{\Phi}_h^{(p+2)} &= \widetilde{\Phi}_{\gamma_{3,p}h}^{(p)} \circ \widetilde{\Phi}_{\gamma_{2,p}h}^{(p)} \circ \widetilde{\Phi}_{\gamma_{1,p}h}^{(p)} \quad \text{if } p/2 \text{ odd,} \\ \tilde{\Phi}_h^{(p+2)} &= \widetilde{\Phi}_{\bar{\gamma}_{3,p}h}^{(p)} \circ \widetilde{\Phi}_{\bar{\gamma}_{2,p}h}^{(p)} \circ \widetilde{\Phi}_{\bar{\gamma}_{1,p}h}^{(p)} \quad \text{else.} \end{aligned} \tag{2.10}$$

This yields a family of composition methods which again reads

$$\tilde{\Phi}_h^{(p)} = \prod_{j=1}^{3^{(p/2)-1}} \Phi_{\tilde{\alpha}_{j,p}h}$$

for some coefficients $\tilde{\alpha}_{j,p}$ that can be explicitly computed. In that situation we have

Proposition 2.2 *The above defined method $\tilde{\Phi}_h^{(p)}$ has order p .*

Besides, for $p = 2, 4, 6, 8, 10, 12, 14$, the coefficients $\tilde{\alpha}_{j,p}$ ($j = 1, \dots, 3^{(p/2)-1}$) satisfy

$$\text{Re}(\tilde{\alpha}_{j,p}) > 0.$$

This property ceases to hold whenever $p \geq 16$.

Remark 2.4 Surprisingly, the sum of the moduli of coefficients $\sum_{j=1}^{3^{(p/2)-1}} |\alpha_{j,p}|$ and $\sum_{j=1}^{3^{(p/2)-1}} |\tilde{\alpha}_{j,p}|$ in the considered composition methods $\Phi_h^{(p)}$ or $\tilde{\Phi}_h^{(p)}$ is bounded as the order p goes to infinity. It is estimated by

$$\begin{aligned} \prod_{k=1}^{\infty} (|\gamma_{1,2k}| + |\gamma_{2,2k}| + |\gamma_{3,2k}|) &\leq \prod_{k=1}^{\infty} \frac{2 + 2^{1/(2k+1)}}{|2e^{i\pi/(2k+1)} + 2^{1/(2k+1)}} \\ &= \prod_{k=1}^{\infty} \left(1 + \frac{\pi^2}{36k^2} + \mathcal{O}\left(\frac{1}{k^3}\right) \right) < +\infty. \end{aligned}$$

This means that the length of the family of polygons in Fig. 1 is bounded (this limit is ≈ 1.315).

2.2.2 Quadruple jump composition methods

In the similar way we have derived symmetric, triple jump composition methods, we investigate here the symmetric quadruple jump case. To do so, for any even integer p , we need to find complex quadruples $(\gamma_{1,p}, \gamma_{2,p}, \gamma_{3,p}, \gamma_{4,p})$, still denoted by the letters $\gamma_{j,p}$ not to overweight notation, such that

$$\begin{aligned} \gamma_{1,p} &= \gamma_{4,p}, & \gamma_{2,p} &= \gamma_{3,p} \quad (\text{symmetry}), \\ \gamma_{1,p} + \gamma_{2,p} + \gamma_{3,p} + \gamma_{4,p} &= 1, \\ \gamma_{1,p}^{p+1} + \gamma_{2,p}^{p+1} + \gamma_{3,p}^{p+1} + \gamma_{4,p}^{p+1} &= 0 \quad (\text{Theorem 2.1}). \end{aligned} \tag{2.11}$$

Starting from any basic symmetric method ϕ_h of order p , the symmetric method $\phi_{\gamma_{4,p}h} \circ \phi_{\gamma_{3,p}h} \circ \phi_{\gamma_{2,p}h} \circ \phi_{\gamma_{1,p}h}$ automatically has order $p + 2$. Now, the set of all complex solutions to (2.11) is given by the p values

$$\gamma_{1,p}^{(k)} = \bar{\gamma}_{2,p}^{(k)} = \bar{\gamma}_{3,p}^{(k)} = \gamma_{4,p}^{(k)} = \frac{1}{2 - 2e^{2ki\pi/(p+1)}} \quad (k = 1, \dots, p). \tag{2.12}$$

The two complex conjugate solutions with minimal sum of moduli are obtained with $k = \pm p/2$. These solutions also have minimal value of $\max_{i=1,\dots,4} |\arg(\gamma_{i,p}^{(k)})|$. Therefore, we set

$$\gamma_{1,p} = \bar{\gamma}_{2,p} = \bar{\gamma}_{3,p} = \gamma_{4,p} = \frac{1}{4} + i \frac{\sin(\pi/(p+1))}{4 + 4 \cos(\pi/(p+1))}.$$

With this notation we define the quadruple jump procedure

$$\begin{aligned} \Psi_h^{(2)} &= \Phi_h, \\ \Psi_h^{(p+2)} &= \widetilde{\Phi}_{\gamma_{4,p}h}^{(p)} \circ \widetilde{\Phi}_{\gamma_{3,p}h}^{(p)} \circ \widetilde{\Phi}_{\gamma_{2,p}h}^{(p)} \circ \widetilde{\Phi}_{\gamma_{1,p}h}^{(p)}, \end{aligned} \tag{2.13}$$

where the method $\widetilde{\Phi}_h^{(p)}$ has been defined before in (2.10). Naturally, each method $\Psi_h^{(p)}$ reads

$$\Psi_h^{(p)} = \prod_{j=1}^{4 \times 3^{(p/2)-2}} \Phi_{\beta_{j,p}h},$$

for some coefficients $\beta_{j,p}$ that can be explicitly computed. We draw the reader’s attention to the fact that $\Psi_h^{(p+2)}$ is here defined recursively using $\widetilde{\Phi}_h^{(p)}$ as a building block (instead of $\Psi_h^{(p)}$ —in other words, we *do not* define $\Psi_h^{(p+2)}$ as the composition $\Psi_{\gamma_{4,p}h}^{(p)} \circ \Psi_{\gamma_{3,p}h}^{(p)} \circ \Psi_{\gamma_{2,p}h}^{(p)} \circ \Psi_{\gamma_{1,p}h}^{(p)}$). This choice is made to reduce the total number of compositions of the basic method Φ_h needed to build up the method $\Psi_h^{(p)}$: in our case, $\Psi_h^{(p)}$ requires $4 \times 3^{(p/2)-2}$ compositions of Φ_h (instead of $4^{(p/2)-1}$).

We have the

Proposition 2.3 *The above defined method $\Psi_h^{(p)}$ has order p .*

Besides, for $p = 2, 4, 6, 8, 10, 12$, the coefficients $\beta_{j,p}$ ($j = 1, \dots, 4 \times 3^{(p/2)-2}$) satisfy

$$\operatorname{Re}(\beta_{j,p}) > 0.$$

This property ceases to hold whenever $p \geq 14$.

Another advantage of this composition procedure is that we obtain an accurate approximation of the solution at intermediate time steps as well. More precisely, we have the

Proposition 2.4 *Take an initial condition y_0 and an even integer p . Define for any integer n the sequence of vectors y_n ($n \geq 0$) by the recursion $y_{n+1} = \Psi_h^{(p)}(y_n)$. Lastly, define $y(t)$ as the solution to the ODE $\dot{y}(t) = A y(t) + B y(t)$ with initial condition $y(0) = y_0$.*

Then, y_n approximates $y(nh)$ to within $\mathcal{O}(h^p)$. Moreover, writing

$$\Psi_h^{(p)} = \widetilde{\Phi}_{\gamma_{4,p-2}h}^{(p-2)} \circ \widetilde{\Phi}_{\gamma_{3,p-2}h}^{(p-2)} \circ \widetilde{\Phi}_{\gamma_{2,p-2}h}^{(p-2)} \circ \widetilde{\Phi}_{\gamma_{1,p-2}h}^{(p-2)},$$

and setting

$$y_{n+1/2} = \widetilde{\Phi}_{\gamma_{2,p-2}h}^{(p-2)} \circ \widetilde{\Phi}_{\gamma_{1,p-2}h}^{(p-2)}(y_n),$$

we also have that

$$y_{n+1/2} \text{ approximates } y((n + 1/2)h) \text{ to within } \mathcal{O}(h^p).$$

More generally, the same result holds, with the obvious change of notation, taking any symmetric method $\phi_h^{(p-2)}$ of order $p - 2$ and defining the improved symmetric method of order p as $\psi_h^{(p)} = \phi_{\gamma_{4,p-2}h}^{(p-2)} \circ \phi_{\gamma_{3,p-2}h}^{(p-2)} \circ \phi_{\gamma_{2,p-2}h}^{(p-2)} \circ \phi_{\gamma_{1,p-2}h}^{(p-2)}$.

The proof of this fact simply comes from observing that $\gamma_{1,p} + \gamma_{2,p} = 1/2$ for any p , so that the two couples $(2\gamma_{1,p}, 2\gamma_{2,p})$ and $(2\gamma_{2,p}, 2\gamma_{1,p})$ satisfy the order equations (2.2) with $s = 2$. Hence the recursion $y_{n+1/2} = \widetilde{\Phi}_{\gamma_{2,p-2}h}^{(p-2)} \circ \widetilde{\Phi}_{\gamma_{1,p-2}h}^{(p-2)}(y_n)$ yields an approximation of the true solution at time $t = nh + h/2$ with local error $\mathcal{O}(h^p)$. Since this error is not propagated (it is only an inner stage), we obtain an approximation of order p both for y_{n+1} at time $(n + 1)h$ and for $y_{n+1/2}$ at time $(n + 1/2)h$.

3 Convergence analysis for unbounded operators

In this section, we extend the analysis of the previous paragraph, valid in the finite dimensional case, to the infinite dimensional situation. We first give a general state-

ment, next specify the assertions in the case of splitting algorithms applied to linear diffusion equations.

3.1 A general statement

Hansen and Ostermann in [14] have provided an elegant and general framework, valid for linear equations, and which allows to assert that *if* a splitting method is p -th order accurate in the finite dimensional case, *then* the same method is p -th order accurate in the infinite dimensional case as well, provided some natural functional analytic assumptions are met.

The Hansen and Ostermann result states the following.

Theorem 3.1 (see Hansen and Ostermann [14]) *Let X be an arbitrary complex Banach space with norm $\|\cdot\|$. Denote by the same symbol $\|\cdot\|$ the norm on the space of bounded linear operators over X . Consider s linear unbounded operators A_j ($j = 1, \dots, s$). Lastly, take a time $T \geq 0$, an integer p , and an initial datum $u_0 \in X$. Assume that the following assumptions are met:*

(i) (semi-group property).

The linear operators A_j ($j = 1, \dots, s$) and $A_1 + \dots + A_s$ generate C_0 semi-groups on X . Moreover there exist a real ω and s real numbers ω_j ($j = 1, \dots, s$) such that

$$\forall t \geq 0, \quad \|e^{t(A_1+\dots+A_s)}\| \leq e^{\omega t} \quad \text{and} \quad \|e^{tA_j}\| \leq e^{\omega_j t}. \quad (3.1)$$

(ii) (smoothness assumption).

For any operator E_{p+1} that is obtained as the product of exactly $p + 1$ factors chosen amongst the A_j 's, there is a constant $C > 0$ such that

$$\forall 0 \leq t \leq T, \quad \|E_{p+1} e^{t(A_1+\dots+A_s)} u_0\| \leq C. \quad (3.2)$$

(iii) (splitting method).

Take a splitting method S of the form

$$S = \prod_{j=1}^m (e^{\gamma_{j,1}hA_1} e^{\gamma_{j,2}hA_2} \dots e^{\gamma_{j,s}hA_s}),$$

where $\gamma_j, 1 \leq j \leq m$, are nonnegative reals, while m is an integer. Assume this splitting method is a p -th order approximation of $e^{h(A_1+\dots+A_s)}$. This means that whenever the A_j 's are replaced by finite dimensional matrices M_j , say, we have $\prod_{j=1}^s (e^{\gamma_{j,1}hM_1} \dots e^{\gamma_{j,s}hM_s}) = e^{h(M_1+\dots+M_s)} + \mathcal{O}(h^{p+1})$, in the sense of matrix norms.

Under all these assumptions, the following holds. There exists a constant $C > 0$ such that for any integer $n \geq 0$ and any time step $h > 0$ satisfying $nh \leq T$, we have,

$$\|(S^n - e^{nh(A_1+\dots+A_s)}) u_0\| \leq Ch^p.$$

Using this theorem, the following is easily deduced

Corollary 3.1 (Banach space formulation) *Let X be an arbitrary complex Banach space with norm $\|\cdot\|$. Denote by the same symbol $\|\cdot\|$ the norm on the space of bounded linear operators over X . Take two linear unbounded operators A and B . Lastly, take a time $T \geq 0$, an integer p , and an initial datum $u_0 \in X$. Assume that the following assumptions are met:*

(i) (semi-group property).

The operator $A + B$ generates a C_0 semigroup on X . Besides, for any $z \in \mathbb{C}$ such that $\operatorname{Re}(z) > 0$, the linear operators zA and zB , generate C_0 semigroups on X . Lastly, for any given $z \in \mathbb{C}$ with $\operatorname{Re}(z) > 0$, there exists a real number ω such that

$$\forall t \geq 0, \quad \|e^{t(A+B)}\| \leq e^{\omega t}, \quad \text{and} \quad \|e^{tzA}\| + \|e^{tzB}\| \leq e^{\omega|z|t}. \quad (3.3)$$

(ii) (smoothness assumption).

For any operator E_{p+1} that is obtained as the product of exactly $p + 1$ factors chosen amongst A and B , there is a constant $C > 0$ such that

$$\forall 0 \leq t \leq T, \quad \|E_{p+1} e^{t(A+B)} u_0\| \leq C. \quad (3.4)$$

(iii) (splitting method).

Next, consider s complex numbers $a_1, \dots, a_s, b_1, \dots, b_s$, and take a splitting method S of the form

$$S = \prod_{j=1}^s e^{b_j h A} e^{a_j h B}.$$

Assume this splitting method is a p -th order approximation of $e^{h(A+B)}$, meaning that whenever A and B are replaced by finite dimensional matrices M and N we have $\prod_{j=1}^s e^{b_j h M} e^{a_j h N} = e^{h(M+N)} + \mathcal{O}(h^{p+1})$, in the sense of matrix norms.

Under all these assumptions, the following holds. There exists a constant $C > 0$ such that for any integer $n \geq 0$ and any time step $h > 0$ satisfying $nh \leq T$, we have,

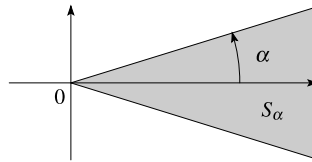
$$\|(S^n - e^{nh(A+B)}) u_0\| \leq Ch^p. \quad (3.5)$$

In particular, under the present assumptions on A, B , and u_0 , the methods $\Phi_h^{(p)}$, $\widetilde{\Phi}_h^{(p)}$, and $\Psi_h^{(p)}$ discussed in the previous paragraphs satisfy estimate (3.5) for $0 \leq nh \leq T$, with S replaced by $\Phi_h^{(p)}$, resp. $\widetilde{\Phi}_h^{(p)}$, resp. $\Psi_h^{(p)}$, whenever $p = 2, 4, 6, 8$, resp. $p = 2, 4, 6, 8, 10, 12, 14$, resp. $p = 2, 4, 6, 8, 10, 12$.

Before ending this paragraph, we propose a slightly different formulation, adopting a Hilbert space setting: so-called $m\alpha$ -dissipative operators are well-adapted in the present context, where we eventually wish to derive splitting methods that are adapted to parabolic equations.

Let α belong to $[0, \pi/2]$ and define the sector S_α in the complex plane by

$$S_\alpha = \{z \in \mathbb{C}, z = 0 \text{ or } |\arg z| \leq \alpha\}.$$



Let H be a complex Hilbert space with scalar product denoted by (\cdot, \cdot) . Take a linear, unbounded operator A on H , with domain $D(A)$, a dense subspace of H . We recall that A is said $m\alpha$ -dissipative whenever for all u in $D(A)$, the quantity $(-Au, u)$ belongs to S_α , and if for all complex $z \notin S_\alpha$, the operator $z\text{Id} + A$ is an isomorphism from $D(A)$ to H . A nice introduction to $m\alpha$ -accretive operators¹ can be found in [5]. It is known that an $m\alpha$ -dissipative operator generates a C_0 semigroup on H , denoted by e^{tA} ($t \geq 0$), and e^{tA} is a contraction operator from H to H . Besides, if an operator A is such that there exists a real number c for which $A + c\text{Id}$ is $m\alpha$ -dissipative for some $\alpha \in [0, \pi/2]$, then A generates a C^0 semi-group as well, and we have the estimate $\|e^{tA}\| \leq e^{+ct}$ whenever $t \geq 0$.

Corollary 3.2 (Hilbert space formulation) *Let H be a complex Hilbert space with scalar product (\cdot, \cdot) and associated norm $\|\cdot\|$. Take an initial datum $u_0 \in H$, a time $T \geq 0$, and an integer p . Assume the following:*

- (i) *Let A resp. B be such that there exist two real numbers a and b for which $A + a\text{Id}$ resp. $B + b\text{Id}$ are $m\alpha$ -dissipative resp. $m\beta$ -dissipative operator for some $\alpha \in [0, \pi/2]$ resp. $\beta \in [0, \pi/2]$. Lastly, assume that there is a real number c for which $A + B + c\text{Id}$ is $m\gamma$ -dissipative for some $\gamma \in [0, \pi/2]$.*
- (ii) *Assume that for any operator E_{p+1} that is obtained as the product of exactly $p + 1$ factors chosen amongst A and B , that there is a constant $C > 0$ such that*

$$\forall 0 \leq t \leq T, \quad \|E_{p+1} e^{t(A+B)} u_0\| \leq C. \tag{3.6}$$

Then, the methods $\Phi_h^{(p)}$, $\widetilde{\Phi}_h^{(p)}$, and $\Psi_h^{(p)}$ discussed in the previous paragraphs satisfy estimate (3.5) for $0 \leq nh \leq T$, with S replaced by $\Phi_h^{(p)}$, resp. $\widetilde{\Phi}_h^{(p)}$, resp. $\Psi_h^{(p)}$, whenever $p = 2, 4, 6, 8$, resp. $p = 2, 4, 6, 8, 10, 12, 14$, resp. $p = 2, 4, 6, 8, 10, 12$.

3.2 Application to linear diffusion equations

In this paragraph, we apply the above results in the case of the linear heat equation with potential

$$\partial_t u(t, x) = \Delta u(t, x) + V(x)u(t, x), \quad u(0, x) = u_0(x).$$

¹An operator A is said $m\alpha$ -accretive whenever $-A$ is $m\alpha$ -dissipative.

To fix ideas, consider the case when x belongs to the whole space \mathbb{R}^d . There are many settings adapted to this equation, and one may either seek solutions u having Hölder smoothness, or $L^p(\mathbb{R}^d)$ smoothness, or Sobolev regularity (in turn based either on L^p — $p \neq 2$ —or on L^2). In order to keep a simple presentation, we choose to work in an L^2 -based Sobolev space setting.

Therefore, we introduce the Hilbert space $H = L^2(\mathbb{R}^d)$, and the two operators $A : u \mapsto \Delta u$ and $B : u \mapsto Vu$. The operator A with domain $D(A) = H^2(\mathbb{R}^d)$ is m_0 -dissipative on H . Whenever $V \in L^\infty(\mathbb{R}^d)$, the operator B is bounded on H . Lastly, the operator $A + B$ is such that $A + B - \|V\|_{L^\infty} \text{Id}$ is m_0 -dissipative. Hence assumption (i) in Corollary 3.2 is met.

To ensure assumption (ii), namely the smoothness assumption, we take an integer p , and assume that $u_0 \in H^{2(p+1)}(\mathbb{R}^d)$ and $V \in W^{p,\infty}(\mathbb{R}^d)$. This ensures that assumption (ii) in Corollary 3.2 is met.

We are in position to state the

Theorem 3.2 *Under all these assumptions, considering either the method $\Phi_h^{(p)}$ ($2 \leq p \leq 8$) or $\widetilde{\Phi}_h^{(p)}$ ($2 \leq p \leq 14$) or $\Psi_h^{(p)}$ ($2 \leq p \leq 12$), estimate (3.5) with S replaced by one of the above methods holds true.*

Needless to say, the similar result holds when the heat equation is considered on the Torus as well, or on a bounded domain with appropriate boundary conditions and smooth enough boundary, etc.

4 Numerical results

In this section, we numerically illustrate the above convergence results.

4.1 The linear case

We consider the one-dimensional linear heat equation with potential on the Torus \mathbb{T} (identified with $[0, 1]$)

$$\partial_t u(t, x) = \Delta u(t, x) + V(x) u(t, x), \quad u(0, x) = u_0(x),$$

where the potential V is taken as

$$V(x) = 2 + \sin(2\pi x).$$

In order to discretize the equation in space, we take a (large) integer N and choose a finite differences procedure on the regular grid $0, 1/N, 2/N, \dots, N/N$. The original heat equation then becomes

$$\dot{u} = Au + Bu,$$

where the vector $u(t)$ belongs to \mathbb{R}^N , and has the form

$$u(t) = (u^1(t), \dots, u^N(t)),$$

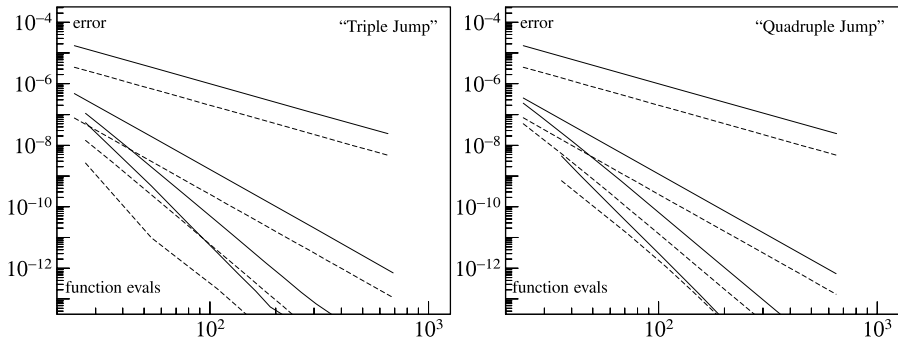


Fig. 3 Plot: Linear potential $V(x) = 2 + \sin(2\pi x)$. Error (L^2 norm at time T) of composition methods versus number of evaluations of the basic method Φ_h . *Left picture*: “triple jump” composition methods $\widetilde{\Phi}_h^{(p)}$, $p = 2, 4, 6, 8$. *Right picture*: “quadruple jump” composition methods $\Psi_h^{(p)}$, $p = 2, 4, 6, 8$. For all these pictures, *solid lines*: basic method is the Strang splitting with exponential maps (2.3)—*dashed lines*: basic method is Peaceman-Rachford formula (2.4)

and $u^j(t)$ is an approximation of $u(t, \frac{j}{N})$, while the Laplacian Δ is approximated by the $N \times N$ matrix A given by

$$A = (N + 1)^2 \begin{pmatrix} -2 & 1 & & & 1 \\ 1 & -2 & 1 & & \\ & 1 & -2 & 1 & \\ & & \ddots & \ddots & \ddots \\ 1 & & & 1 & -2 \end{pmatrix},$$

and the vector Bu stands for

$$Bu = \left(V\left(\frac{1}{N}\right)u^1, \dots, V\left(\frac{j}{N}\right)u^j, \dots, V\left(\frac{N}{N}\right)u^N \right).$$

We take the C^∞ initial condition $u_0(x) = \sin(2\pi x)$, and consider a spatial discretization with $N = 100$ points.² In Fig. 3, we compare the accuracy of the composition methods introduced in this article (“triple” (2.10) and “quadruple” (2.13) jump compositions) on the time interval $[0, T]$, where $T = 0.2$. We plot for many stepsizes the solution error at time T as a function of the number of evaluations of the basic method. As a basic method, we consider (in solid lines) alternatively the Strang splitting Φ_h involving exact flows (where the terms $e^{hB/2}$ are replaced by half a time step of the exact flow of the nonlinear differential equation $\dot{y} = F(y)$), and (in dashed lines) the Peaceman-Rachford method Φ_h^P . The ‘exact’ solution is computed with a very small time step. We observe the expected orders (lines of slopes 2, 4, 6, 8). Surprisingly, composition methods using the Peaceman-Rachford formula are slightly more accurate than the one using exponentials.

²This number of discretization points is naturally arbitrary. The fact that, with this value of N , the extrapolation method (4.2) diverges, as expected—see below—, while it converges for smaller values of N , indicates that the value $N = 100$ is enough for our purposes.

4.2 The nonlinear case

At least *formally*, all above results immediately extend to the nonlinear situation, provided all exponentials e^{hA} etc. are replaced by the appropriate nonlinear flows (see introduction).

In that perspective, we consider the one-dimensional, non-linear heat equation on the Torus \mathbb{T} (identified with $[0, 1]$)

$$\partial_t u(t, x) = \Delta u(t, x) + F(u(t, x)), \quad u(0, x) = u_0(x),$$

where $F(u)$ is a non-linear reaction term and, for the purpose of testing our methods, we have retained Fisher’s potential

$$F(u) = u(1 - u).$$

The differential equation

$$\frac{\partial u}{\partial z} = u(1 - u), \quad u(0) = u_0$$

can be solved analytically as

$$u(z) = u_0 + u_0(1 - u_0) \frac{(e^z - 1)}{1 + u_0(e^z - 1)},$$

which is well defined for small complex time z . We discretize the equation in space as in the linear case. The original nonlinear heat equation becomes

$$\dot{u} = Au + F(u), \tag{4.1}$$

where the vector $u(t)$ is as in the linear case, the Laplacian Δ is approximated by the above $N \times N$ matrix A , and the vector $F(u)$ stands for

$$F(u) = (u^1(1 - u^1), \dots, u^N(1 - u^N)).$$

The experimental conditions are the ones we used to illustrate the linear case. In Fig. 4, we compare the accuracy of the composition methods introduced in this article (“triple” (2.10) and “quadruple” (2.13) jump compositions). We plot for many stepsizes the solution error at time T as a function of the number of evaluations of the basic method. As a basic method, we consider (in solid lines) alternatively the Strang splitting Φ_h involving exact flows (where the terms $e^{hB/2}$ are replaced by half a time step of the exact flow of the nonlinear differential equation $\dot{y} = F(y)$), and (in dashed lines) the Peaceman-Rachford formula Φ_h^P (where the implicit Euler and explicit Euler operators are replaced by the appropriate nonlinear operators obtained by applying the explicit and/or implicit Euler algorithm to the nonlinear equation $\dot{y} = F(y)$).

In Fig. 5, we compare the “quadruple jump” composition method of order 4 with two extrapolation methods. We also give the results for the Strang splitting of order 2.

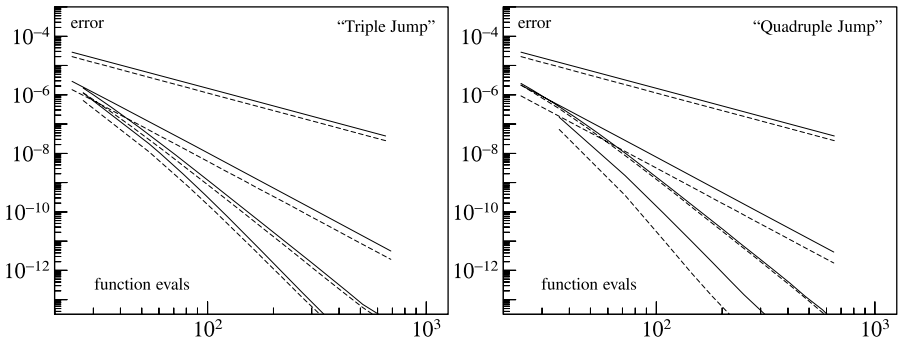


Fig. 4 Plot: Nonlinear case—Error (L^2 norm at time T) of composition methods versus number of evaluations of the basic method Φ_h . *Left picture*: “triple jump” composition methods $\widetilde{\Phi}_h^{(p)}$, $p = 2, 4, 6, 8$. *Right picture*: “quadruple jump” composition methods $\Psi_h^{(p)}$, $p = 2, 4, 6, 8$. For all these pictures, solid lines: basic method is the Strang splitting with exponential maps (2.3)—dashed lines: basic method is the Peaceman-Rachford formula (2.4)

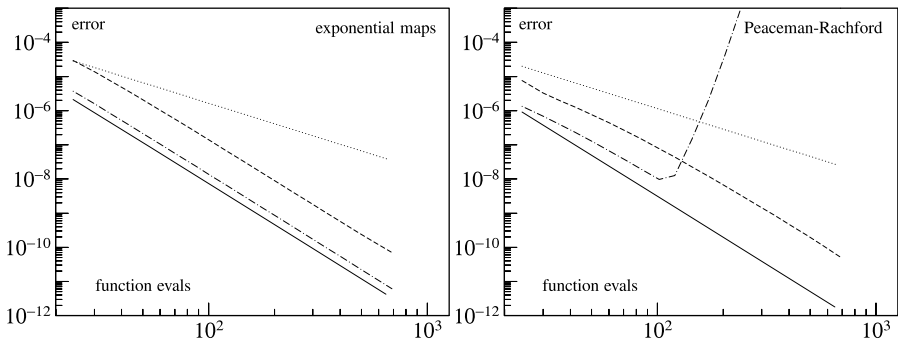


Fig. 5 Plot: Nonlinear case—Error (L^2 norm at time T) versus number of evaluations of the basic method Φ_h . Strang splitting (dotted lines), “quadruple jump” composition method $\Psi_h^{(4)}$ (solid line), extrapolation method (4.2) (dashed-dotted line), extrapolation method (4.3) (dashed lines). *Left picture*: Basic method is the Strang splitting with exponential maps (2.3). *Right picture*: Peaceman-Rachford formula (2.4)

We use the same initial data and parameters as before. The first extrapolation formula we consider is

$$\frac{4}{3}\Phi_{h/2} \circ \Phi_{h/2} - \frac{1}{3}\Phi_h, \tag{4.2}$$

where for the basic method Φ_h , we take alternatively the Strang splitting Φ_h with the exact flows, see left picture in Fig. 5, or the—conveniently adapted, see above—Peaceman-Rachford formula, see right picture. However, as pointed out in [19, Sect. 6] this scheme is not stable and does not converge in the second case (see dashed-dotted line in right picture). Another extrapolation method (dashed lines) is considered in [19] and taken from [8],

$$\frac{45}{64}\Phi_{h/3} \circ \Phi_{h/3} \circ \Phi_{h/3} + \frac{1}{2}\Phi_{h/2} \circ \Phi_{h/2} - \frac{13}{64}\Phi_h. \tag{4.3}$$

Although the formal order of this method is 4, it is said in [19] that the true order of convergence of this method is not clearly understood, and in the numerical experiments for linear problems in [8], “the formal order is not reached; the experimental precision is smaller than the theoretical precision, and the difference is smaller than 1”.

Finally, and for a fair comparison in Fig. 5, it should be mentioned that computations using complex numbers are actually about four times more expensive than computations with real numbers (because of the cost of a multiplication).

5 Conclusion

We have constructed new high-order composition methods and splitting methods using complex coefficients for parabolic linear and non-linear parabolic partial differential equations. Based on the results of Hansen & Osterman [14], a convergence analysis is provided in the linear case. The methods we have derived are all based on a composition procedure with complex time steps; they actually allow to build up high order methods which are based on the composition of possibly cheap low order algorithms.

Going a bit further, we may stress here that it is also possible to construct high-order *splitting* methods for which only one operator carries complex time steps. Such methods are however *not* based on the composition technique we have presently developed. For instance, the following splitting method is symmetric and of order 4,

$$e^{b_1hV} e^{a_1hA} e^{b_2hV} e^{a_2hA} e^{b_3hV} e^{a_2hA} e^{b_2hV} e^{a_1hA} e^{b_1hV}, \tag{5.1}$$

where $b_1 = 1/10 - i/30$, $b_2 = 4/15 + 2i/15$, $b_3 = 4/15 - i/5$ are complex, and $a_1 = a_2 = a_3 = a_4 = 1/4$ are all reals. Such a decomposition is interesting when the evolution along A carries the most computational cost and the evolution with V is cheap to compute (*e.g.* when V is a diagonal matrix): in that case the extra cost due to the complex numbers is marginal. This type of splitting method is also of great interest in the case where one operator has its eigenvalues close to the imaginary axis, like *e.g.* the Ginzburg-Landau equation. Note however that in this very case, and because this algorithm is not based on a composition procedure, the true exponentials cannot be replaced, in general, by low order approximations: the exponential needs to be approximated to within the appropriate order in any circumstance here.

Independently, note that a systematic study of *optimal* composition methods (*i.e.* methods with optimal error constants) is out of the scope of this paper and will be the subject of a future article by the same authors. It requires the resolution in \mathbb{C} of the polynomial systems of order conditions for composition methods and splitting methods. Also, a theoretical analysis in the case of a non-linear source is in preparation.

Acknowledgements The authors are grateful to Ernst Hairer for useful discussions and comments. The fourth author was partially supported by the Fonds National Suisse, project No. 200020-109158.

References

1. Bandrauk, A., Dehghanian, E., Lu, H.: Complex integration steps in decomposition of quantum exponential evolution operators. *Chem. Phys. Lett.* **419**, 346–350 (2006)
2. Blanes, S., Casas, F.: On the necessity of negative coefficients for operator splitting schemes of order higher than two. *Appl. Numer. Math.* **54**, 23–37 (2005)
3. Chambers, J.E.: Symplectic integrators with complex time steps. *Astron. J.* **126**, 1119–1126 (2003)
4. Creutz, M., Gocksch, A.: Higher-order hybrid Monte Carlo algorithms. *Phys. Rev. Lett.* **63**, 9–12 (1989)
5. Crouzeix, M.: Approximation of parabolic equations. Lecture notes available at <http://perso.univ-rennes1.fr/michel.crouzeix/> (2005)
6. Descombes, S.: Convergence of a splitting method of high order for reaction-diffusion systems. *Math. Comput.* **70**, 1481–1501 (2001) (electronic)
7. Descombes, S., Ribot, M.: Convergence of the Peaceman-Rachford approximation for reaction-diffusion systems. *Numer. Math.* **95**, 503–525 (2003)
8. Dia, B.O.: Méthodes de directions alternées d'ordre élevé en temps. PhD Thesis, Université Claude Bernard Lyon 1 (1996)
9. Forest, E.: Canonical integrators as tracking codes. *AIP Conf. Proc.* **184**, 1106–1136 (1989)
10. Gegechkori, Z., Rogava, J., Tsiklauri, M.: High degree precision decomposition method for the evolution problem with an operator under a split form. *M2AN Math. Model. Numer. Anal.* **36**, 693–704 (2002)
11. Gegechkori, Z., Rogava, J., Tsiklauri, M.: The fourth order accuracy decomposition scheme for an evolution problem. *M2AN Math. Model. Numer. Anal.* **38**, 707–722 (2004)
12. Goldman, D., Kaper, T.J.: N th-order operator splitting schemes and nonreversible systems. *SIAM J. Numer. Anal.* **33**, 349–367 (1996)
13. Hairer, E., Lubich, C., Wanner, G.: *Geometric Numerical Integration. Structure-Preserving Algorithms for Ordinary Differential Equations*, 2nd edn. Springer Series in Computational Mathematics, vol. 31. Springer, Berlin (2006)
14. Hansen, E., Ostermann, A.: Exponential splitting for unbounded operators. *Math. Comput.* **78**, 1485–1496 (2009)
15. Hansen, E., Ostermann, A.: High order splitting methods for analytic semigroups exist. *BIT Numer. Math.* (2009). doi:10.1007/s.10543.003-0236-x
16. McLachlan, R.I.: Composition methods in the presence of small parameters. *BIT Numer. Math.* **35**, 258–268 (1995)
17. Peaceman, D.W., Rachford, H.H. Jr.: The numerical solution of parabolic and elliptic differential equations. *J. Soc. Ind. Appl. Math.* **3**, 28–41 (1955)
18. Rosenbrock, H.H.: Some general implicit processes for the numerical solution of differential equations. *Comput. J.* **5**, 329–330 (1962/1963)
19. Schatzman, M.: Numerical integration of reaction-diffusion systems. In: *Numerical Methods for Ordinary Differential Equations* (Auckland, 2001). *Numer. Algorithms* **31**, 1–4 (2002)
20. Sheng, Q.: Solving linear partial differential equations by exponential splitting. *IMA J. Numer. Anal.* **9**, 199–212 (1989)
21. Sussman, G.J., Wisdom, J.: Chaotic evolution of the solar system. *Science* **257**, 56–62 (1992)
22. Suzuki, M.: Fractal decomposition of exponential operators with applications to many-body theories and Monte Carlo simulations. *Phys. Lett. A* **146**, 319–323 (1990)
23. Suzuki, M.: General theory of fractal path integrals with applications to many-body theories and statistical physics. *J. Math. Phys.* **32**, 400–407 (1991)
24. Yoshida, H.: Construction of higher order symplectic integrators. *Phys. Lett. A* **150**, 262–268 (1990)