Splitting methods with complex coefficients for some classes of evolution equations

S. Blanes[1], F. Casas[2], P. Chartier[3] and A. Murua[4]

[1] *Instituto de Matemática Multidisciplinar, Universitat Politécnica de Valencia, 46022 Valencia, Spain*
email: serblaza@imm.upv.es

[2] *Departament de Matemàtiques and IMAC, Universitat Jaume I, 12071 Castellón, Spain*
email: Fernando.Casas@mat.uji.es

[3] *INRIA Rennes and Ecole Normale Supérieure de Cachan, Antenne de Bretagne,*
Avenue Robert Schumann, 35170 Bruz, France.
email: Philippe.Chartier@inria.fr

[4] *EHU/UPV, Konputazio Zientziak eta A.A. saila, Informatika Fakultatea, 12071 Donostia/San Sebastián, Spain*
email: Ander.Murua@ehu.es

January 24, 2011

Abstract

We are concerned with the numerical solution obtained by *splitting methods* of certain parabolic partial differential equations. Splitting schemes of order higher than two with real coefficients necessarily involve negative coefficients. In [HO09b] and in [CCDV09], the authors demonstrated the possibility to overcome this second-order barrier by considering splitting methods with *complex-valued* coefficients and built up methods of orders 3 to 14. In this paper, we reconsider the technique employed therein and show that it is inherently bound to order 14 and largely sub-optimal with respect to error constants. As an alternative, we solve directly the algebraic equations arising from the order conditions and construct several methods of orders 4, 6, 8 and 16 that are the most accurate ones available at present time.

Keywords: composition methods, splitting methods, complex coefficients, parabolic evolution equations.

MSC numbers: 65L05, 65P10, 37M15

1 Introduction

In this paper, we consider linear evolution equations of the form

$$\frac{du}{dt}(t) = Au(t) + Bu(t), \qquad u(0) = u_0, \tag{1.1}$$

where the (possibly unbounded) operators A, B and $A+B$ generate C^0 semi-groups for positive t over a finite or infinite Banach space X. Equations of this form are encountered in the context of *parabolic* partial differential equations, a prominent example being the inhomogeneous *heat equation*

$$\frac{\partial u}{\partial t}(x,t) = \Delta u(x,t) + V(x)u(x,t),$$

where $t \geq 0$, $x \in \mathbb{R}^d$ or $x \in \mathbb{T}^d$ and Δ denotes the Laplacian in x.

A method of choice for solving numerically (1.1) consists in advancing the solution alternatively along the exact (or numerical) solutions of the two problems

$$\frac{du}{dt}(t) = Au(t) \qquad \text{and} \qquad \frac{du}{dt}(t) = Bu(t).$$

Upon using an appropriate sequence of steps, high-order approximations can be obtained -for instance with exact flows- as

$$\Psi(h) = \mathrm{e}^{hb_0 B}\, \mathrm{e}^{ha_1 A}\, \mathrm{e}^{hb_1 B} \cdots \mathrm{e}^{ha_s A}\, \mathrm{e}^{hb_s B}. \tag{1.2}$$

The simplest example within this class is the *Lie-Trotter splitting*

$$\mathrm{e}^{hA}\, \mathrm{e}^{hB} \qquad \text{or} \qquad \mathrm{e}^{hB}\, \mathrm{e}^{hA} \tag{1.3}$$

which is a first order approximation to the solution of (1.1), while the *symmetrized* version

$$S(h) = \mathrm{e}^{h/2\, A}\, \mathrm{e}^{hB}\, \mathrm{e}^{h/2\, A} \qquad \text{or} \qquad S(h) = \mathrm{e}^{h/2\, B}\, \mathrm{e}^{hA}\, \mathrm{e}^{h/2\, B} \tag{1.4}$$

is referred to as *Strang splitting* and is an approximation of order 2.

In [HO09a], it has been established that, under the two conditions stated below, a splitting method of the form (1.2) is of order p for problem (1.1) if and only if it is of order p for *ordinary differential equations* in finite dimension. In other words, if and only if the difference $\Psi(h) - \mathrm{e}^{h(A+B)}$ admits a formal expansion of the form

$$\Psi(h) - \mathrm{e}^{h(A+B)} = h^{p+1} E_{p+1} + h^{p+2} E_{p+2} + \cdots \tag{1.5}$$

The two referred conditions write (see [HO09a] for a complete exposition):

1. *Semi-group property*: A, B and $A+B$ generate C^0 semi-groups on X and, for all positive t,

   $$\|\mathrm{e}^{tA}\| \le \mathrm{e}^{\omega_A t}, \qquad \|\mathrm{e}^{tB}\| \le \mathrm{e}^{\omega_B t} \quad \text{and} \quad \|\mathrm{e}^{t(A+B)}\| \le \mathrm{e}^{\omega t}$$

   for some positive constants ω_A, ω_B and ω.

2. *Smoothness property for all* $t \in [0, T]$: For any pair of multi-indices $(i_1, \ldots, i_m)$ and $(j_1, \ldots, j_m)$ with $i_1 + \cdots + i_m + j_1 + \cdots + j_m = p+1$, and for all $t \in [-T, T]$,

   $$\|A^{i_1} B^{j_1} \ldots A^{i_m} B^{j_m}\, \mathrm{e}^{t(A+B)} u_0\| \le C$$

   for a positive constant C.

However, designing high-order splitting methods is not as straightforward as it might seem at first glance. As a matter of fact, A and B are only assumed to generate C^0 semi-groups (and not groups). This means in particular that the flows e^{tA} or e^{tB} may not be defined for negative times (this is indeed the case for the Laplacian in particular) and this prevents the use of methods which embed negative coefficients. Given that splitting methods with real coefficients must have some of their coefficients a_i and b_i negative[1] to achieve order 3 or more, this seems to indicate, as it has been believed for a long time within the numerical analysis community, that it is only possible to apply exponential splitting methods of at most order $p = 2$. In order to circumvent this order-barrier, the papers [HO09b] and [CCDV09] simultaneously introduced *complex-valued* coefficients[2] with positive real parts. It can indeed be checked in many situations that the propagators e^{zA} and e^{zB} are still well-defined in a reasonable distribution sense for $z \in \mathbb{C}$, provided that $\Re(z) \ge 0$.

[1]The existence of at least one negative coefficient was shown in [She89, Suz91], and the existence of a negative coefficient for both operators was proved in [GK96]. An elementary proof can be found in [BC05].

[2]Methods with complex-values coefficients have also been used in a similar context [Ros63] or in celestial mechanics [Cha03].

Using this extension from the real line to the complex plane, they built up methods of orders 3 to 14 by considering a technique known as *triple-jump composition*[3] and made popular by a series of authors: Creutz & Gocksch [CG89], Forest [For89], Suzuki [Suz90] and Yoshida [Yos90].

In this work, we continue the search for new methods by solving directly the polynomial equations arising from the order conditions. The construction will be monitored by two important parameters: the size of error constants and the size of the arguments of the complex coefficients used in the method. While the importance of error constants does not need any justification, the relevance of the second parameter is very much related to the classes of equations we focus on here. Specifically, we will consider on the one hand, reaction diffusion equations and, on the other hand, complex Ginzburg–Landau equations:

- Reaction-diffusion equations are mathematical models that describe how the population of one or several species distributed in space evolves under the action of two concurrent phenomena: *reaction* between species in which predators eat preys; *diffusion* which makes the species to spread out in space[4]. From a mathematical point of view, they belong to the class of semi-linear parabolic partial differential equations and can be represented in the general form

$$\frac{\partial u}{\partial t} = D\Delta u + F(u),$$

  where each component of the vector $u(x,t) \in \mathbb{R}^d$ represents the population of one species, D is the matrix of diffusion coefficients (often diagonal) and F accounts for all local interactions between species.[5] Strictly speaking, the theoretical framework introduced in [HO09b] does not cover this situation if F is nonlinear, so that (apart from section 5, where we successfully integrate numerically an example with nonlinear F) we will think of F as being linear. The important feature of $A = D\Delta$ here is that it has a **real** spectrum: hence, any method involving complex steps with positive real part is suitable. In principle, one could even consider splitting methods with a_i 's having positive real part and unconstrained complex b_i 's.

- More generally, the diffusion operator may involve a complex number: in this case, we obtain the Ginzburg–Landau equation, i.e. an equation of the form

$$\frac{\partial u}{\partial t} = \delta\Delta u + F(u), \tag{1.6}$$

  where δ is a complex number with $\Re(\delta) > 0$ [6]. In this situation, the values of the $\tilde{a}_i := \arg(\delta) + \arg(a_i)$ determine the stability of the method for this specific value of δ. If for all $i = 1, \ldots, s$, $\tilde{a}_i \in [-\frac{\pi}{2}, +\frac{\pi}{2}]$ the method is stable. Otherwise, it becomes unstable. In order for the method to be applicable to a wide range of equations, it is thus of importance to minimize the value of $\max_{i=1,\ldots,s} |\arg(a_i)|$. Methods such that all a_i 's are positive reals are ideal in this respect, and we will show explicitly that the corresponding class is non-empty.

Eventually, our objective is to show that for both situations, it is possible to construct more efficient methods than those built in [HO09b] and [CCDV09] by a mere application of the triple-jump (or quadruple-jump) procedure. In Section 2, we shall prove that if an s-jump construction is carried on from a basic symmetric second-order method, it is bound to order 14 and no more and we will further justify why solving directly the system of order conditions leads to more efficient methods. In Section 3 we give explicitly the order

[3] And its generalization to *quadruple-jump*.

[4] Apart from biology and ecology, systems of this sort also appear in chemistry (hence the term reaction), geology and physics.

[5] The choice $F(u) = u(1-u)$ yields Fisher's equation and is used to describe the spreading of biological populations; the choice $F(u) = u(1-u^2)$ describes Rayleigh–Benard convection; the choice $F(u) = u(1-u)(u-\alpha)$ with $0 < \alpha < 1$ arises in combustion theory and is referred to as Zeldovich equation.

[6] The choice $F(u) = \mu_3 u^3 + \mu_2 u^2 + \mu_1 u + \mu_0$ is known as the cubic Ginzburg–Landau equation [FT88].

conditions of general splitting methods of the form (1.2) and also of methods based on compositions of simple integrators. We also present a strategy to optimize the corresponding schemes based on the analysis of the leading term of the local error. In Section 4, we solve the order conditions and construct several splitting methods whose coefficients have positive real part. In particular, in subsection 4.1 we present splitting methods of order 6, 8, and 16 obtained as the composition of simpler integrators (with Strang splitting as basic integrator in the first two cases, and an eighth order splitting method as basic integrator in the second case). In subsection 4.2, we construct splitting schemes of order 4 and 6 with real and positive coefficients a_i, thus appropriate, in particular, for the numerical integration of the complex Ginzburg–Landau equation. In section 5 we describe the implementation of the various methods obtained in this paper and show their efficiency as compared to already available methods on three test problems. Finally, section 6 contains some concluding remarks.

2 An order barrier for the s-jump construction

A simple and very fruitful technique to build high-order methods is to consider compositions of low-order ones with fractional time steps. In this way, numerical integrators of arbitrarily high order can be obtained. For splitting methods aimed to integrate problems of the form (1.1), it is necessary, however, that the coefficients have positive real part. The procedure has been carried out in [CCDV09, HO09a], where composition methods up to order 14 have been constructed. We shall prove here that 14 constitutes indeed an order barrier for this kind of approach. In other words, the composition technique used in [CCDV09, HO09a] does not allow for the construction of methods having all their coefficients in $\mathbb{C}_+ := \{z \in \mathbb{C} : \Re(z) \geq 0\}$ with orders strictly greater than 14. With this goal in mind we consider the following two families of methods:

Family I. Given a method of order p, $\Phi^{[p]}(h) = \mathrm{e}^{h(A+B)} + \mathcal{O}(h^{p+1})$, a sequence of methods of orders $p+1, p+2, \ldots$ can be defined recursively by the compositions

$$\Phi^{[p+q]}(h) = \prod_{i=1}^{m_q} \Phi^{[p+q-1]}(\alpha_{q,i}h) := \Phi^{[p+q-1]}(\alpha_{q,1}h) \cdots \Phi^{[p+q-1]}(\alpha_{q,m_q}h), \tag{2.1}$$

where for all $q \geq 1$,

$$(\forall\, 1 \leq i \leq m_q,\ \alpha_{q,i} \neq 0), \quad \sum_{i=1}^{m_q} \alpha_{q,i} = 1 \quad \text{and} \quad \sum_{i=1}^{m_q} \alpha_{q,i}^{p+q} = 0.$$

(Hereafter, we will interpret the product symbol from left to right). Notice that if $p+q$ is even, the second condition has only complex solutions.

Family II. Given a **symmetric** method of order $2p$, $\tilde{\Phi}^{[2p]}(h)$, a sequence of methods of orders $2(p+1)$, $2(p+2), \ldots$ can be defined recursively by the **symmetric** compositions

$$\forall\, q \geq 1, \quad \tilde{\Phi}^{[2(p+q)]}(h) = \prod_{i=1}^{m_q} \tilde{\Phi}^{[2(p+q)-2]}(\alpha_{q,i}h) \tag{2.2}$$

where for all $q \geq 1$,

$$(\forall\, 1 \leq i \leq m_q,\ \alpha_{q,i} \neq 0), \quad \sum_{i=1}^{m_q} \alpha_{q,i} = 1 \quad \text{and} \quad \sum_{i=1}^{m_q} \alpha_{q,i}^{2(p+q)+1} = 0.$$

Methods of this class with real coefficients have been constructed by Creutz & Gocksch [CG89], Suzuki [Suz90] and Yoshida [Yos90]. However, the second condition clearly indicates that at least one of the coefficients must be negative. In contrast, there exist many complex solutions with coefficients in $\mathbb{C}_+$.

Generally speaking, starting from $\Phi^{[1]}(h)$, the $(p+1)$-th member of family I is of the form

$$\Phi^{[p+1]}(h)=\prod_{i_p=1}^{m_p}\left(\prod_{i_{p-1}=1}^{m_{p-1}}\left(\ldots\left(\prod_{i_1=1}^{m_1}\Phi^{[1]}(\alpha_{p,i_p}\alpha_{p-1,i_{p-1}}\cdots\alpha_{1,i_1}h)\right)\ldots\right)\right) \tag{2.3}$$

and has coefficients

$$\prod_{j=1}^{p}\alpha_{j,i_j} \qquad 1\leq i_1\leq m_1,\ldots,1\leq i_p\leq m_p. \tag{2.4}$$

A similar expression holds, of course, for methods of family II, starting from $\tilde{\Phi}^{[2]}(h)$. The cases $m_1=m_2=\cdots=m_p=3$ and $m_1=m_2=\cdots=m_p=4$, correspond to the triple and quadruple jump techniques, respectively.

Lemma 2.1 *Let* $\Phi(h)$ *a consistent method (i.e., a method of order* $p\geq 1$*) and assume that the method*

$$\Psi(h)=\prod_{i=1}^{l}\Phi(\alpha_i h) \tag{2.5}$$

is also consistent (i.e., $\sum_i\alpha_i=1$*). If there exists* k, $1\leq k\leq l$, *such that* $\Re(\alpha_k)<0$, *then any consistent method of the form*

$$\prod_{j=1}^{m}\Psi(\beta_j h)=\prod_{j=1}^{m}\left(\prod_{i=1}^{l}\Phi(\beta_j\alpha_i h)\right) \tag{2.6}$$

has at least one coefficient $\beta_j\alpha_k$, $1\leq j\leq m$, *such that* $\Re(\beta_j\alpha_k)<0$.

Proof: By consistency one has $\sum_{j=1}^{m}\beta_j=1$, so that

$$\sum_{j=1}^{m}\Re(\beta_j\alpha_k)=\Re\left(\sum_{j=1}^{m}\beta_j\alpha_k\right)=\Re\left(\alpha_k\sum_{j=1}^{m}\beta_j\right)=\Re(\alpha_k)<0.$$

This implies the statement. □

Lemma 2.2 *For* $k\geq 2$ *and* $r\geq 2$, *consider* $(z_1,\ldots,z_k)\in(\mathbb{C}_+)^k$ *such that* $\sum_{i=1}^{k}z_i^r=0$, $z_i\neq 0$ *for* $i=1,\ldots,k$. *Then we have*

$$\max_{i=1,\ldots,k}\operatorname{Arg}(z_i)-\min_{i=1,\ldots,k}\operatorname{Arg}(z_i)\geq\frac{\pi}{r}.$$

Proof: All the z_i's belong to the sector $K_\sigma(\theta)=\{z\in\mathbb{C}:|\sigma-\operatorname{Arg}(z)|\leq\theta\}$ with

$$\sigma=\frac{1}{2}\left(\max_{i=1,\ldots,k}\operatorname{Arg}(z_i)+\min_{i=1,\ldots,k}\operatorname{Arg}(z_i)\right)\quad\text{and}\quad\theta=\frac{1}{2}\left(\max_{i=1,\ldots,k}\operatorname{Arg}(z_i)-\min_{i=1,\ldots,k}\operatorname{Arg}(z_i)\right),$$

where Arg is the principal value of the argument (see the left picture of Figure 1). Now, assume that $\theta<\frac{\pi}{2r}$. Then, all the z_i^r's belong to $K_{r\sigma}(r\theta)$, which, since $r\theta<\frac{\pi}{2}$, is a convex set. This implies that $\sum_{i=1}^{k}z_i^r$ also belongs to $K_{r\sigma}(r\theta)$ (see the right picture of Figure 1). The inequality $r\theta<\frac{\pi}{2}$ being strict and the z_i's non-zero, we have furthermore $\sum_{i=1}^{k}z_i^r\neq 0$, which contradicts the assumption. The result follows. □

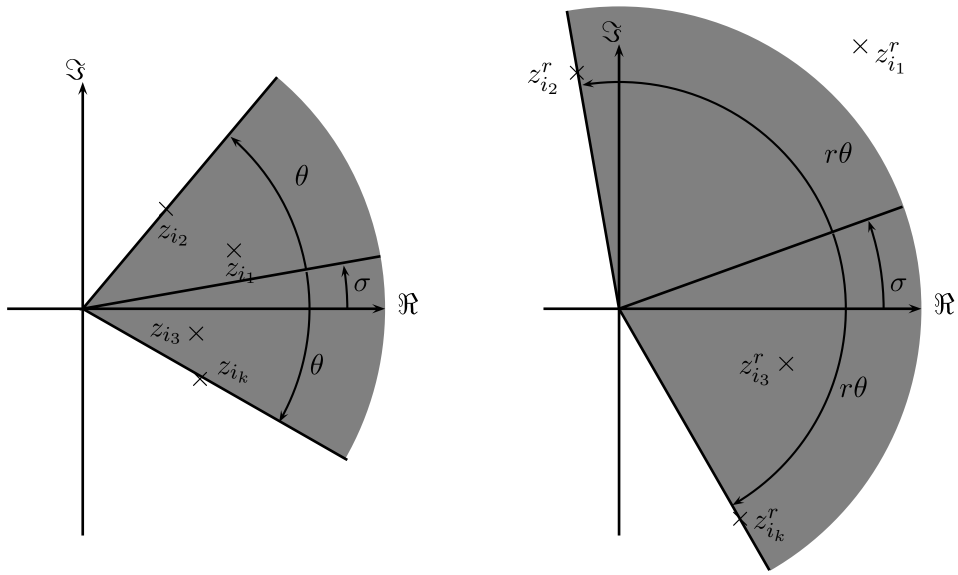

Figure 1: The enveloping sectors of $\{z_1, \ldots, z_k\} \subset \mathbb{C}_+$ and of $\{z_1^r, \ldots, z_k^r\} \subset \mathbb{C}$ (for $r = 2$).

Theorem 2.3 *(i) Starting from a first-order method $\Phi^{[1]}(h)$, all methods $\Phi^{[p]}(h)$ of order p, $p = 4, 5, \ldots$ from Family I have at least one coefficient with negative real part. (ii) Starting from a second-order symmetric method $\tilde{\Phi}^{[2]}(h)$, all methods $\tilde{\Phi}^{[2p]}(h)$ of order $2p$, $p = 8, 9, \ldots$ from Family II have at least one coefficient with negative real part.*

Proof: We prove at once the two assertions. We first notice that, according to Lemma 2.1, if method $\Phi^{[p]}(h)$ of Family I (respectively, method $\tilde{\Phi}^{[2p]}(h)$ of Family II), has a coefficient with negative real part, then all subsequent methods $\Phi^{[p+q]}(h)$, $q \geq 1$, of Family I (respectively, methods $\tilde{\Phi}^{[2(p+q)]}(h)$ of Family II), also have a coefficient with negative real part. Hence, we assume that all methods $\Phi^{[q+1]}(h)$, $q = 1, \ldots, p$ from Family I (respectively, all methods $\tilde{\Phi}^{[2q+2]}(h)$ of Family II), have all their coefficients in $\mathbb{C}_+$. Using Lemma 2.2 we have

$$\forall\, q = 1, \ldots, p, \quad \max_{i=1,\ldots,m_q} \operatorname{Arg}(\alpha_{q,i}) - \min_{i=1,\ldots,m_q} \operatorname{Arg}(\alpha_{q,i}) \geq \frac{\pi}{q+1}$$

(respectively

$$\forall q = 1, \ldots, p, \quad \max_{i=1,\ldots,m_q} \operatorname{Arg}(\alpha_{q,i}) - \min_{i=1,\ldots,m_q} \operatorname{Arg}(\alpha_{q,i}) \geq \frac{\pi}{2q+1}),$$

so that

$$\max_{1 \leq i_1 \leq m_1, \ldots, 1 \leq i_p \leq m_p} \operatorname{Arg}\left(\prod_{j=1}^{p} \alpha_{j,i_j}\right) - \min_{1 \leq i_1 \leq m_1, \ldots, 1 \leq i_p \leq m_p} \operatorname{Arg}\left(\prod_{j=1}^{p} \alpha_{j,i_j}\right) \geq \frac{\pi}{2} + \cdots + \frac{\pi}{p+1}$$

(respectively

$$\max_{1 \leq i_1 \leq m_1, \ldots, 1 \leq i_p \leq m_p} \operatorname{Arg}\left(\prod_{j=1}^{p} \alpha_{j,i_j}\right) - \min_{1 \leq i_1 \leq m_1, \ldots, 1 \leq i_p \leq m_p} \operatorname{Arg}\left(\prod_{j=1}^{p} \alpha_{j,i_j}\right) \geq \frac{\pi}{3} + \cdots + \frac{\pi}{2p+1}).$$

Now, since $\frac{1}{2} + \frac{1}{3} + \frac{1}{4} > 1$, $p = 3$ in the first case and thus the first statement follows. For Family II, since $\frac{1}{3} + \frac{1}{5} + \cdots + \frac{1}{15} > 1$), then $p = 7$, thus leading to the second statement. □

Remark 2.4 *No method of Family I with coefficients in $\mathbb{C}_+$ can have an order strictly greater than 3. Such methods of orders 2 and 3 have been constructed in [HO09a]. Similarly, no method of Family II with coefficients in $\mathbb{C}_+$ can have an order strictly greater than 14. Such methods with orders up to 14 have been constructed in [CCDV09, HO09a].*

Remark 2.5 *It is however possible to construct a composition method with coefficients in* $\mathbb{C}_+$ *of order strictly greater than* 14 *directly from a second order method. For example, in Subsection 4.1 we present a new method of sixteenth-order that we have built as*

$$\Phi^{[16]}(h) = \prod_{i=1}^{21} \Phi^{[8]}(\alpha_i h), \qquad \textit{with} \qquad \Phi^{[8]}(h) = \prod_{j=1}^{15} \Phi^{[2]}(\beta_j h) \tag{2.7}$$

and the coefficients satisfying $\Re(\alpha_i\beta_j) > 0$ *for all* $i = 1, \dots, 21$, $j = 1, \dots, 15$, *with* $\alpha_{22-i} = \alpha_i$, $\beta_{16-j} = \beta_j$, $i, j = 1, 2, \dots$. *Here,* $\Phi^{[8]}(h)$ *is a symmetric composition of symmetric second order methods, but it is not a composition of methods of order 4 or 6, and similarly for* $\Phi^{[16]}(h)$, *which is not a composition of methods of orders* 10, 12 *or* 14.

3 Order conditions and leading terms of local error

We have seen that the composition technique to construct high order methods inevitably leads to an order barrier. In addition, the resulting methods require a large number of evaluations and usually have large truncation errors. In this section we show that, as with real coefficients, it is indeed possible to build very efficient high order splitting methods whose coefficients have positive real part by solving directly the order conditions necessary to achieve a given order p. These are, roughly speaking, large systems of polynomial equations in the coefficients a_i, b_i of the method (1.2), arising by requiring that the formal expansion of the method satisfies (1.5) for arbitrary non-commuting operators A and B.

Different (equivalent) formulations of such order conditions exist in the literature [HLW06]. Here we follow the formulation introduced in [CM09] (see also [BCM08]) that can be considered as a variant of the order conditions obtained in [MSS99].

3.1 Order conditions for splitting methods

It is straightforward to check that the splitting method (1.2) is of order at least 1 if

$$\sum_{j=1}^{s} a_j = 1 = \sum_{j=0}^{s} b_j. \tag{3.1}$$

These equalities are referred to as the consistency conditions, which we hereafter assume to hold. The first step in the derivation process of the order conditions that we adopt consists in rewriting (1.2) in the form

$$\Psi(h) = X(-\alpha_1 h)^{-1} X(\alpha_2 h) \cdots X(-\alpha_{2s-1} h)^{-1} X(\alpha_{2s} h), \tag{3.2}$$

where

$$X(h) = \mathrm{e}^{hA}\,\mathrm{e}^{hB} = I + h(A+B) + h^2(\frac{1}{2}A^2 + AB + \frac{1}{2}B^2) + \cdots,$$

and for $j = 1, \dots, s$,

$$\alpha_{2j-1} = b_{j-1} - \alpha_{2j-2}, \qquad \alpha_{2j} = a_j - \alpha_{2j-1}, \tag{3.3}$$

with $\alpha_0 = \alpha_{2s+1} = 0$. Observe that $X(h) = 1 + h\,X_1 + h^2\,X_2 + \cdots$, where for each $k \geq 1$,

$$X_k = \sum_{j=0}^{k} \frac{1}{j!(k-j)!} A^j B^{k-j}. \tag{3.4}$$

The consistency conditions now reduce to

$$\sum_{j=1}^{2s} \alpha_j = 1. \tag{3.5}$$

It has been shown [BCM08, CM09] that $\Psi(h)$ can be expanded as

$$\Psi(h) = I + \sum_{n\geq 1} h^n \sum_{j_1+\cdots+j_r=n} u_{j_1,\ldots,j_r}(\alpha_1,\ldots,\alpha_{2s})\, X_{j_1}\cdots X_{j_r}, \tag{3.6}$$

where

$$\begin{aligned} u_i(\alpha_1,\ldots,\alpha_{2s}) &= \sum_{j=1}^{s}(\alpha_{2j}^i - \alpha_{2j-1}^i), & (3.7)\\ u_{i_1,\ldots,i_m}(\alpha_1,\ldots,\alpha_{2s}) &= \sum_{j=1}^{s}(\alpha_{2j}^{i_m} - \alpha_{2j-1}^{i_m})\, u_{i_1,\ldots,i_{m-1}}(\alpha_1,\ldots,\alpha_{2j-1},0,\cdots,0). & (3.8)\end{aligned}$$

Expression (3.6) has to be compared with the expansion

$$I + hX_1^2 + \frac{h^2}{2!}X_1^2 + \cdots$$

of $\mathrm{e}^{hX_1} = \mathrm{e}^{h(A+B)}$. We thus have that the method is of order p if for each multi-index $(i_1,\ldots,i_m)$ with $i_1+\cdots+i_m = n \leq r$,

$$u_{i_1,\ldots,i_m}(\alpha_1,\ldots,\alpha_{2s}) = \begin{cases} \dfrac{1}{n!} & \text{if} \quad (i_1,\ldots,i_m) = (1,\ldots,1),\\ 0 & \text{otherwise.}\end{cases} \tag{3.9}$$

However, such order conditions are not independent [CM09]. For instance, it can be checked that

$$u_{1,1} = \frac{1}{2}(u_1^2 + u_2), \qquad u_{2,1} = -u_{1,2} + u_3 + u_1 u_2, \qquad u_{1,1,1} = \frac{1}{6}u_1^3 + \frac{1}{2}u_{1,2} + \frac{1}{3}u_3,$$

which implies that the order conditions (3.9) for $u_{1,1}$, $u_{2,1}$, $u_{1,1,1}$ are fulfilled provided that the conditions for $u_1, u_2, u_3, u_{1,2}$ hold.

A set of independent order conditions can be obtained as follows. Consider the lexicographical order $<$ (i.e., the order used when ordering words in the dictionary) on the set of multi-indices. A multi-index $(i_1,\ldots,i_m)$ is a Lyndon multi-index if $(i_1,\ldots,i_k) < (i_{k+1},\ldots,i_m)$ for each $1 \leq k < m$. For each $n \geq 1$, we denote as L_n the set of polynomials $u_{i_1\cdots i_m}$ such that $(i_1,\ldots,i_m)$ is a Lyndon multi-index satisfying that $i_1+\cdots+i_m = n$. The first sets L_n are

$$\begin{aligned} L_1 &= \{u_1\}, \quad L_2 = \{u_2\}, \quad L_3 = \{u_{1,2}, u_3\}, \quad L_4 = \{u_{1,1,2}, u_{1,3}, u_4\},\\ L_5 &= \{u_{1,1,1,2}, u_{1,1,3}, u_{1,2,2}, u_{1,4}, u_{2,3}, u_5\}.\end{aligned}$$

The splitting method (1.2) is of order p if, in addition to the consistency condition (3.1),

$$u_{i_1,\ldots,i_m}(\alpha_1,\ldots,\alpha_{2s}) = 0, \quad \forall\,(i_1,\ldots,i_m)\in L_n, \quad \text{with} \quad 1 < n \leq r, \tag{3.10}$$

where the coefficients α_j are given in terms of the a_i 's and b_i 's in (3.3). It is well known [HLW06] that the number of order conditions can be reduced by restricting to splitting methods having the following symmetry in the coefficients

$$a_{s+1-j} = a_j, \qquad b_{s+1-j} = b_{j-1}. \tag{3.11}$$

(or equivalently $\alpha_{2s-j+1} = \alpha_j$). Such a symmetry condition guarantees that $\Psi(h)$ is a so-called self-adjoint method, that is, $\Psi(-h) = \Psi(h)^{-1}$. In that case, if the following conditions hold:

$$u_{i_1,\ldots,i_m}(\alpha_1,\ldots,\alpha_{2s}) = 0, \quad \forall\,(i_1,\ldots,i_m)\in L_{2j+1}, \quad \text{with} \quad 1 < 2j+1 \leq r, \tag{3.12}$$

then all the order conditions in (3.10) hold. For instance, a splitting method (1.2) is of order four if, in addition to the consistency condition (3.1) and the symmetry condition (3.12),

$$u_{1,2}(\alpha) = u_3(\alpha) = 0,$$

where we denote $\alpha = (\alpha_1, \ldots, \alpha_{2s})$. If in addition,

$$u_{1,1,1,2}(\alpha) = u_{1,1,3}(\alpha) = u_{1,2,2}(\alpha) = u_{1,4}(\alpha) = u_{2,3}(\alpha) = u_5(\alpha) = 0,$$

then the method is of order at least 6.

In the sequel we will restrict ourselves to symmetric methods, since it simplifies a great deal the procedure of construction of high order methods.

3.2 Order conditions for splitting methods based on compositions of lower order integrators

The number of order conditions for general splitting methods grows very rapidly with the order p. For instance, there are 26 independent 8th-order conditions and 82 10th-order conditions for a consistent symmetric splitting method. It makes sense, then, to consider some alternative to achieve order higher than six. This can be accomplished by taking compositions of a basic symmetric method of even order. In particular, if we consider any of the two versions of Strang splitting (1.4) as the basic method $S(h)$, then, for each $\gamma = (\gamma_1, \ldots, \gamma_m) \in \mathbb{C}^m$,

$$\Psi(h) = S(\gamma_1 h) \cdots S(\gamma_s h) \tag{3.13}$$

will be a new splitting method of the form (1.2), which can be brought into the form (3.2) (with $X(h) = \mathrm{e}^{hB}\,\mathrm{e}^{hA}$ for the first version of Strang splitting, and $X(h) = \mathrm{e}^{hA}\,\mathrm{e}^{hB}$ in the second one), with $\alpha_{2j-1} = \alpha_{2j} = \gamma_j/2$ for $j = 1, \ldots, s$. Clearly, the consistency condition now reads

$$\gamma_1 + \cdots + \gamma_s = 1. \tag{3.14}$$

As for the additional conditions to attain order p, we have the following property (see [MSS99, Theorem 5], where a superset of the order conditions (3.10) is studied). For each $n \geq 2$, let $\hat{L}_n$ denote the subset of L_n of Lyndon multi-indices having only odd indices. A composition method (3.13) with the Strang splitting as basic method $S(h)$, is of order at least p if it is consistent and

$$u_{i_1,\ldots,i_m}(\gamma) = 0, \quad \forall\, (i_1, \ldots, i_m) \in \hat{L}_n, \quad \text{with} \quad 1 < n \leq r, \tag{3.15}$$

where we have used the notation $\gamma = \frac{1}{2}(\gamma_1, \gamma_1, \ldots, \gamma_s, \gamma_s)$. If the symmetry condition

$$\gamma_{s-j+1} = \gamma_j, \qquad 1 \leq j \leq s \tag{3.16}$$

is imposed, then it is sufficient to consider multi-indices in $\hat{L}_n$ with odd n. For instance, a symmetric consistent composition method is of order six if

$$u_3(\gamma) = u_5(\gamma) = u_{1,3}(\gamma) = 0.$$

If in addition the conditions

$$u_7(\gamma) = u_{1,1,5}(\gamma) = u_{1,1,1,1,3}(\gamma) = u_{1,3,3}(\gamma) = 0$$

hold, then it is at least of order eight.[7]

[7] Actually, such order conditions are not restricted to the case where the basic method $S(h)$ is the Strang splitting. Indeed, they are valid provided that $S(h)$ is any self-adjoint second order method (that is, if $S(-h) = S(h)^{-1}$ and $S(h) = \mathrm{e}^{h(A+B)} + \mathcal{O}(h^3)$ as $h \to 0$).

Splitting methods with very high order can be constructed as (3.13) by considering as basic method $S(h)$ a symmetric method of even order $2q > 2$. In that case, it can be seen that it is sufficient to consider from (3.15) the equations corresponding to multi-indices composed of indices in the set $\{1, 2q+1, 2q+3, \ldots\}$. For instance, if $S(h)$ is a symmetric splitting method of order eight, a method (3.13) satisfying the consistency condition (3.14) and the symmetry condition (3.16) attains order sixteen if

$$\begin{aligned} u_9(\gamma) = u_{1,1,9}(\gamma) = u_{1,1,1,1,9}(\gamma) = u_{1,1,1,1,1,1,9}(\gamma) = 0, \\ u_{11}(\gamma) = u_{1,1,11}(\gamma) = u_{1,1,1,1,11}(\gamma) = 0, \\ u_{13}(\gamma) = u_{1,1,13}(\gamma) = u_{15}(\gamma) = 0. \end{aligned}$$

3.3 Leading term of the local error

To construct splitting methods of a given order p within a family of schemes, we will choose the number s of stages in such a way that the number of unknowns equals the number of order conditions, so that one typically has a finite number of isolated (real or complex) solutions, each of them leading to a different splitting method. Among them, we will be interested in methods such that, either $a_i \geq 0$ (and each b_i are arbitrary complex numbers) or $\Re(a_i) \geq 0$ and $\Re(b_i) \geq 0$. The relevant question at this point is how to choose the 'best' solution in the set of all solutions satisfying the required conditions. It is generally accepted that good splitting methods must have small coefficients a_i, b_i. Methods with large coefficients tend to show bad performance in general, which is particularly true when relatively long time-steps h are used. In addition, as mentioned in the introduction, when applying splitting methods to the class of problems considered here, the arguments of the complex coefficients a_i, b_i must also be taken into account.

In order to chose the best scheme among two methods with coefficients of similar size included in sectors with similar angle, we analyze the leading term of the local error of the splitting method. If (1.2) is of order p, then we formally have that

$$\Psi(h) - \mathrm{e}^{h(A+B)} = -\frac{h^p}{p!} X_1^{p+1} + h^{p+1} \sum_{j_1+\cdots+j_r=p+1} u_{j_1,\ldots,j_r}(\alpha)\, X_{j_1} \cdots X_{j_r} + \mathcal{O}(h^{p+2}),$$

where $\alpha = (\alpha_1, \ldots, \alpha_{2s})$ is given in terms of the original coefficients a_i, b_i of the integrator by (3.3). This can be rewritten, by taking (3.4) into account, as

$$\begin{aligned} \Psi(h) - \mathrm{e}^{h(A+B)} &= h^{p+1} E_{p+1} + \mathcal{O}(h^{p+1}), \\ E_{p+1} &:= \sum_{i_1+\cdots+i_{2m}=p+1} v_{i_1,\ldots,i_{2m}}(\alpha)\, A^{i_1} B^{i_2} \ldots A^{i_{2m-1}} B^{i_{2m}}, \end{aligned}$$

where each $v_{i_1,\ldots,i_{2m}}(\alpha)$ is a linear combination of the polynomials 1 and $u_{j_1,\ldots,j_r}(\alpha)$ with $j_1+\cdots+j_r = p$.

Incorporating that into the results in [HO09b], it can be shown that, if the smoothness assumption stated in the introduction is increased from $p+1$ to $p+2$, then for sufficiently small h, the local error is dominated by $||h^{p+1} E_{p+1} u_0||$.

Going back to the problem of choosing a suitable method among all possible choices (satisfying the required conditions, say, $a_i > 0$ or $\Re(a_i) \geq 0$ and $\Re(b_i) \geq 0$) obtained by solving the order conditions, we have adopted the following procedure: First choose a subset of solutions with reasonably small maximum norm of the coefficient vector $(\alpha_1, \ldots, \alpha_{2s})$, and then, among them, choose the one that minimizes the norm

$$\sum_{i_1+\cdots+i_{2m}=p+1} |v_{i_1\cdots i_{2m}}(\alpha)| \tag{3.17}$$

of the coefficients of the leading term of the local error. This seems reasonable if one is interested in choosing a splitting method that works fine for arbitrary operators A and B satisfying the semi-group and smoothness conditions mentioned in the introduction. Of course, this does not guarantee that a method with a smaller value of (3.17) will be more precise for any A and B than another method with a larger value of (3.17). However, we have observed in practice when solving the order conditions of different families of splitting methods, that the solution that minimizes (3.17) tend to have smaller values of most (or even all) coefficients $|v_{i_1 \cdots i_{2m}}(\alpha)|$ when compared to a solution having a larger norm (3.17) of the coefficients of the leading term of the local error.

When A and B are operators in a real Banach space X, then it makes sense to compute the approximations $u_n = u(t_n)$, as $u_n = \Re(\Psi(h))u_{n-1}$. In that case, the argument above holds with $\Psi(h)$ replaced by $\hat{\Psi}(h) = \Re(\Psi(h))$ and the local error coefficients $v_{i_1,\dots,i_{2m}}(\alpha)$ replaced by $\Re(v_{i_1,\dots,i_{2m}}(\alpha))$. In that case, (3.17) should be replaced by

$$\sum_{i_1+\cdots+i_{2m}=p+1} |\Re(v_{i_1,\dots,i_{2m}}(\alpha))| \tag{3.18}$$

as a general measure of leading term of the local error. In next section, we take into account both (3.17) and (3.18) when choosing a method among a set of candidates obtained when solving the corresponding system of order conditions.

4 Splitting methods with coefficients of positive real part

4.1 High order splitting methods obtained as a composition of simpler methods

Order 6. We first consider sixth-order symmetric splitting methods obtained as a composition (3.13) of the Strang splitting (1.4) as basic method. As we have seen in Subsection 3.2, the coefficients γ_i must satisfy three order conditions, in addition to the symmetry (3.16) and consistency requirements, to achieve order six. We thus take $s = 7$, so that we have three equations and three unknowns. Such a system of polynomial equations has 39 solutions in the complex domain (three real solutions among them), 12 of them giving a splitting method with coefficients of positive real part. According to the criteria described in Subsection 3.3, we arrive at the scheme

$$\begin{aligned}
\gamma_1 = \gamma_7 &= 0.11690003755466128438 9 + 0.04342825461606034176 2i \\
\gamma_2 = \gamma_6 &= 0.12955910128208826275 - 0.12398961218809259330i, \\
\gamma_3 = \gamma_5 &= 0.18653249281213381780 + 0.00310743071007267534i, \\
\gamma_4 &= 0.13401673670223327012 2 + 0.15490785372391915239 6i.
\end{aligned} \tag{4.1}$$

This method turns out to correspond to one of those obtained by Chambers (see Table 4 in [Cha03]).

Order 8. For consistent symmetric methods (3.13) of order eight, we have seven order conditions. By taking $s = 15$ stages, one ends up with a system of seven polynomial equations and seven unknowns. We have performed an extensive numerical search of solutions with small norm, finding 326 complex solutions. Among them, 162 lead to splitting methods whose coefficients possess positive real part. The best method, according to the criteria established in Subsection 3.3, is

$$\begin{aligned}
\gamma_1 = \gamma_{15} &= 0.05347577838761859660 6 + 0.00616935634007953251 0i, \\
\gamma_2 = \gamma_{14} &= 0.04127634284580425664 7 - 0.06994857439070781495 1i, \\
\gamma_3 = \gamma_{13} &= 0.08653355860467571028 9 - 0.02311250163691487438 4i, \\
\gamma_4 = \gamma_{12} &= 0.07964885566302104336 9 + 0.04978049545565433812 4i, \\
\gamma_5 = \gamma_{11} &= 0.06998105284632312289 9 - 0.05262393784159054128 6i, \\
\gamma_6 = \gamma_{10} &= 0.08729548075995521924 2 + 0.01003526864468873395 0i, \\
\gamma_7 = \gamma_9 &= 0.04281288641963208212 6 + 0.07605945645884352386 2i, \\
\gamma_8 &= 0.07795208894593993764 3 + 0.00728087393989420435 0i.
\end{aligned} \tag{4.2}$$

Order 16. Motivated by the results in Section 2, we have also constructed a splitting method of order 16. Our aim, rather than proposing a very efficient scheme, is to show that the barrier of order 14 existing for methods built by applying the recursive composition technique starting from order two (family II) does not apply in general.

The construction procedure can be summarized as follows. We consider a consistent symmetric composition of the form (3.13), where now the basic method $S(h)$ is any symmetric eighth order scheme. Then, as shown in Subsection 3.2, ten order conditions must be satisfied to achieve order 16. We accordingly take $s = 21$, so that we have ten polynomial equations with ten unknowns. We have performed an extensive numerical search of solutions with relatively small norm, finding 70 complex solutions with positive real part. Combined with the 162 methods of order eight, this leads to 11340 different 16 th order splitting methods with $s = 315$ stages. Among them, only 324 give rise to splitting methods with coefficients of positive real part. The coefficients of the method that we have determined as optimal can be found at `www.gicas.uji.es/Research/splitting-complex.html`.

4.2 Splitting methods with positive real a-coefficients

We consider now splitting methods specially tuned for evolution equations where one of the operators (say, A) has non-real eigenvalues in the right-hand side of the complex plane. As explained in the Introduction section, the goal is here to obtain methods such that one of the two sets of coefficients a_i 's or b_i 's is entirely contained in the positive real axis, while the other set is included in the right-hand side of the complex plane. The resulting schemes therefore are very well suited, in particular, for the numerical integration of the complex Ginzburg–Landau equation.

Order 4. We first consider symmetric methods of the form (1.2) with $s = 4$, that is,

$$\Psi(h) = \mathrm{e}^{hb_0 B}\mathrm{e}^{ha_1 A}\mathrm{e}^{hb_1 B}\mathrm{e}^{ha_2 A}\mathrm{e}^{hb_2 B}\mathrm{e}^{ha_3 A}\mathrm{e}^{hb_3 B}\mathrm{e}^{ha_4 A}\mathrm{e}^{hb_4 B}.$$

If we impose the consistency and symmetry requirements (i.e., equations (3.1) and (3.11)), and the additional restriction that the a_i 's are not only real and positive, but also all equal, then we end up with a two-parameter family of methods. As we have seen in Subsection 3.1, two order conditions must be satisfied for order four. The corresponding system of polynomial equations with two unknowns have only two solutions (complex conjugate to each other). These were previously obtained in [CCDV09] (see formula (5.1)):

$$\begin{aligned} a_1 = a_2 = a_3 = a_4 &= 1/4, \\ b_0 = b_4 &= \frac{1}{10} - \frac{i}{30}, \\ b_1 = b_3 &= \frac{4}{15} + \frac{2i}{15}, \\ b_2 &= \frac{4}{15} - \frac{i}{5}. \end{aligned} \tag{4.3}$$

Notice that methods with equal a_i 's have the potential advantage that only one matrix exponential $\mathrm{e}^{ha_1 A}$ has to be computed per step, or even for the integration of the whole interval if constant step-sizes are used. Nevertheless, this property becomes irrelevant whenever the system is so large that the matrix exponential is never computed, and the action of $\mathrm{e}^{ha_1 A}$ on vectors is computed instead (for instance, by using Krylov methods or methods that make use of the FFT algorithm).

If we allow for different a_i 's, then we have one free parameter (say, a_1), which we can determine by minimizing the objective function (3.18) for $p = 4$ under the restriction that $a_1, a_2 > 0$. This procedure leads to the scheme

$$\begin{aligned} b_0 = b_4 &= 0.060078275263542357774 - 0.060314841253378523039i, \\ a_1 = a_4 &= 0.18596881959910913140, \\ b_1 = b_3 &= 0.27021183913361078161 + 0.15290393229116195895i, \\ a_2 = a_3 &= 0.31403118040089086860, \\ b_2 &= 0.33941977120569372122 - 0.18517818207556687181i, \end{aligned} \tag{4.4}$$

which seems, according to the analysis of local error coefficients, to be about 3 times more accurate than method (4.3). We have also analyzed the corresponding minimization problem resulting from adding an additional stage, but only a marginal improvement in the efficiency is achieved, so that we omit the details of the treatment here.

Order 6. A 6th-order symmetric scheme of the form (1.2) has to satisfy 10 equations. By imposing the additional restriction of all a_i being equal, at least $s = 16$ stages are necessary to solve the remaining 9 order conditions (including consistency). We have solved these equations with a computer algebra package, thus obtaining 288 complex solutions. Among them, 228 have coefficients b_i with positive real part (114 solutions and their corresponding complex conjugates). In this set we have chosen, by applying the criteria described in Subsection 3.3, the following method:

$$\begin{aligned} a_1 = a_2 = \cdots = a_8 &= 1/16, \\ b_0 = b_{16} &= 0.024694876087018064641 - 0.0078747955629068770 58i, \\ b_1 = b_{15} &= 0.063813474021302699779 + 0.035365761034143327805i, \\ b_2 = b_{14} &= 0.068425094030316441970 - 0.062262244450748676995i, \\ b_3 = b_{13} &= 0.088047701092267837627 + 0.045473871502298704384i, \\ b_4 = b_{12} &= 0.023689611129847060696 + 0.0096243260640896 24058i, \\ b_5 = b_{11} &= 0.042729722386773382203 - 0.033994403923957610554i, \\ b_6 = b_{10} &= 0.12233468631684577296 0 - 0.010435859079752510669i, \\ b_7 = b_9 &= 0.041898432829693886044 + 0.069362492631696384275i, \\ b_8 &= 0.048732804211869708159 - 0.090518296429724730489i. \end{aligned} \tag{4.5}$$

5 Numerical tests

For our numerical experiments, we consider three different test problems: a linear reaction-diffusion equation, the semi-linear equation of Fisher, and the Ginzburg–Landau equation, which has the specificity to include complex-valued parameters. For each case, we detail the experimental setting and collect the results achieved by the different schemes.

The numerical approximations u_n obtained by each method $\Psi(h)$ are computed as $u_n = \Re(\Psi(h))u_{n-1}$. In other words, we project on the real axis after completing each time step.

5.1 A linear parabolic equation

Our first test-problem is the scalar equation in one-dimension

$$\frac{\partial u(x,t)}{\partial t} = \Delta u(x,t) + V(x,t)u(x,t), \qquad u(x,0) = u_0(x), \tag{5.1}$$

with periodic boundary conditions in the space domain $[0,1]$. We take $V(x,t) = 2 + \sin(2\pi x)$ and discretize in space

$$x_j = j(\delta x), \qquad j = 1, \ldots, N \quad \text{with} \quad \delta x = 1/(N+1),$$

thus arriving at the differential equation

$$\frac{dU}{dt} = AU + BU, \tag{5.2}$$

where $U = (u_1, \ldots, u_N) \in \mathbb{R}^N$. The Laplacian Δ has been approximated by the matrix A of size $N \times N$ given by

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

and $B = \text{diag}(V(x_1), \ldots, V(x_N))$. The solution with initial condition $u_0(x) = \sin(2\pi x)$ is represented on Figure 2.

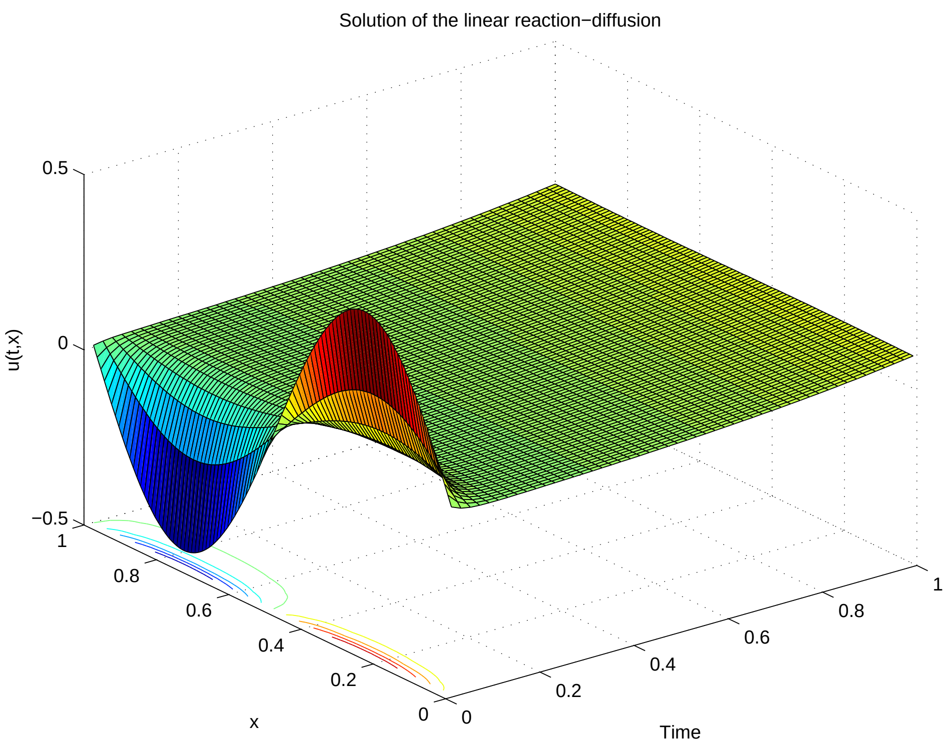

Figure 2: The solution of (5.1) with $u_0(x) = \sin(2\pi x)$ on the interval $[0, 1]$.

We discretize in space with $N = 100$ points and compare different composition methods by computing the corresponding approximate solution on the time interval $[0, 1]$. In particular, we consider the following schemes:

- **Strang**: The second-order symmetric Strang splitting method (1.4);
- **(TJ6)**: The sixth-order triple jump method (Proposition 2.1 in [CCDV09]) based on Strang's second-order method;
- **(TJ6A)**: The sixth-order triple jump method (Proposition 2.2 in [CCDV09]) based on Strang's second-order method;
- **(TJ8A)**: The eighth-order triple jump method (Proposition 2.2 in [CCDV09]) based on Strang's second-order method;

- **(P6S7)**: The sixth-order method (4.1);
- **(P8S15)**: The eighth-order method (4.2).

We compute the error of numerical solution at time $t = 1$ (in the 2-norm) as a function of the number of evaluations of the basic method (the Strang splitting) and represent the outcome in Figure 3. In the left panel we collect the results achieved by the Strang splitting and the previous sixth-order composition methods, whereas the right panel corresponds to eighth-order methods. We have also included, for reference, the curve obtained by (P6S7).

The relative cost (w.r.t. Strang) of a method composed of s steps is approximated by $4s$, where the factor 4 stands here for an average ratio between the cost of complex arithmetic compared to real arithmetic. A remarkable outcome of these experiment is that methods (P6S7) and (P8S15) outperform Strang's splitting (and actually all other methods tested here) even for low tolerances. Scheme (P8S15), in particular, proves to be the most efficient in the whole range explored. The gain with respect to triple jump methods is also very significant and completely support the approach followed here.

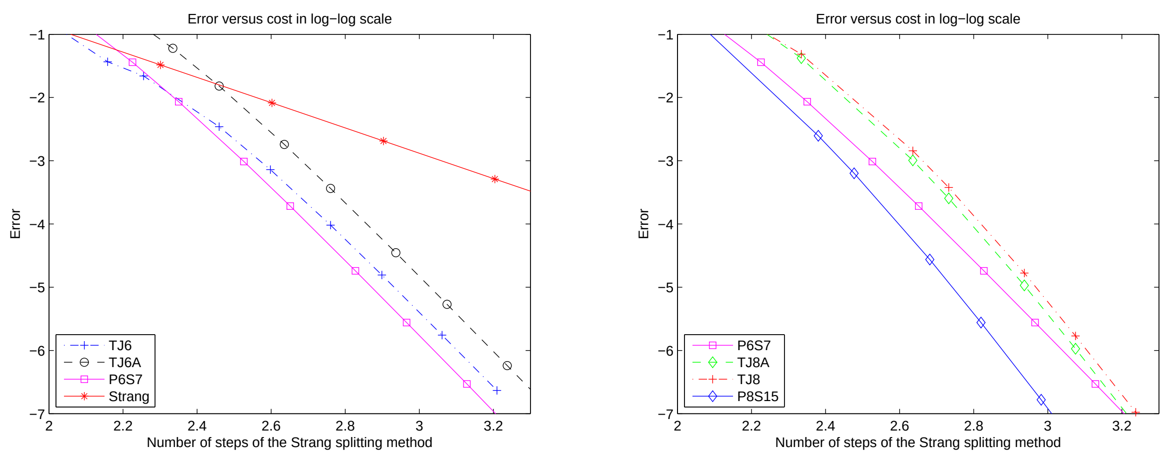

Figure 3: Error versus number of steps for the linear reaction-diffusion equation (5.1).

5.2 The semi-linear reaction-diffusion equation of Fisher

Our second test-problem is the scalar equation in one-dimension

$$\frac{\partial u(x,t)}{\partial t} = \Delta u(x,t) + F(u(x,t)), \qquad u(x,0) = u_0(x), \tag{5.3}$$

with periodic boundary conditions in the space domain $[0,1]$. We take, in particular, Fisher's potential

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

The splitting considered here corresponds to solving, on the one hand, the linear equation with the operator A being the Laplacian, and on the other hand, the nonlinear ordinary differential equation

$$\frac{\partial u(x,t)}{\partial t} = u(x,t)(1-u(x,t))$$

with initial condition

$$u(x,0) = u_0(x).$$

Note that it can be solved analytically as

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

which is well defined for small complex time t. We proceed in the same way as for the previous linear case, starting with $u_0(x)=\sin(2\pi x)$. After discretization in space, we arrive at the differential equation

$$\frac{dU}{dt} = AU + F(U), \tag{5.4}$$

where $U=(u_1,\ldots,u_N)\in\mathbb{R}^N$ and $F(U)$ is now defined by

$$F(U) = \big(u_1(1-u_1),\ldots,u_N(1-u_N)\big).$$

We choose $N=100$ and compute the error (in the 2-norm) at the final time $t=1$ by applying the same composition methods as in the linear case. The results are collected in Figure 4, where identical notation has been used. Notice that, strictly speaking, the theoretical framework upon which our strategy is based does not cover this nonlinear problem. Nevertheless, the results achieved are largely similar to the linear case. In particular, the new 8th-order composition method is the most efficient even for moderate tolerances.

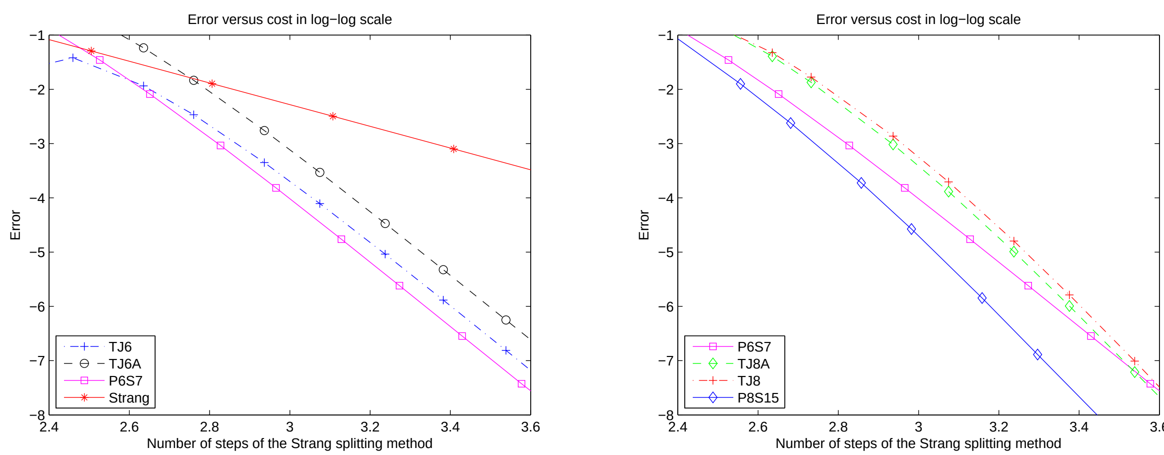

Figure 4: Error versus number of steps for the semi-linear reaction-diffusion equation (5.3).

5.3 The semi-linear complex Ginzburg–Landau equation

Our third test problem is the complex Ginzburg–Landau equation on the domain $(x,t)\in[-20,20]\times[0,100]$ with periodic boundary conditions,

$$\frac{\partial u(x,t)}{\partial t} = \alpha\,\Delta u(x,t) + \varepsilon\, u(x,t) - \beta\,|u(x,t)|^2 u(x,t), \tag{5.5}$$

with $\alpha = 1+ic_1$, $\beta = 1-ic_3$ and initial condition $u(x,0)=u_0(x)$. Here, ε, c_1 and c_3 denote **real** coefficients. In physics, the Ginzburg–Landau appears in the mathematical theory used to model superconductivity. For a broad introduction to the rich dynamics of this equation, we refer to [vS94]. Here, we will use the values $c_1=1$, $c_3=-2$ and $\varepsilon=1$, for which plane wave solutions establish themselves quickly after a transient phase (see [WMC05]). In addition, we set $u_0(x)=\frac{0.8}{\cosh(x-10)^2}+\frac{0.8}{\cosh(x+10)^2}$. The solution when $x\in[-100,100]$ is represented as in Figure 5.

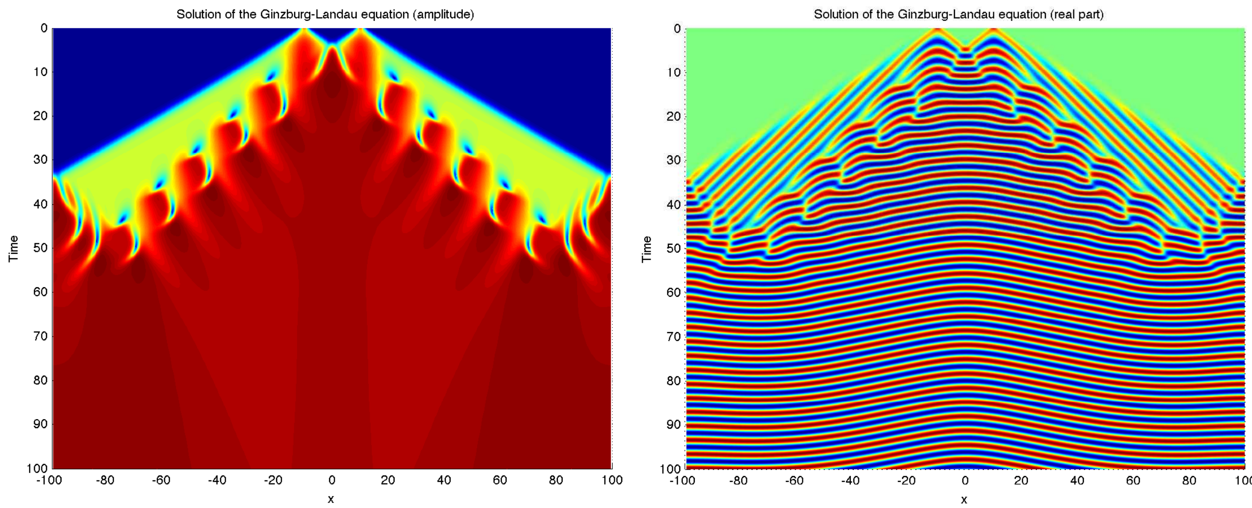

Figure 5: Colormaps of the amplitude $|u(x,t)|^2$ and real part $\Re(u(x,t))$ of the solution of (5.5).

In order to apply the splitting methods presented in Section 4, it seems natural to split equation (5.5) as

$$\frac{\partial u(x,t)}{\partial t} = (1+ic_1)\Delta u(x,t) + \varepsilon\, u(x,t), \tag{5.6}$$

whose solution is $u(x,t) = \mathrm{e}^{\varepsilon t}\mathrm{e}^{t(1+ic_1)\Delta}u_0(x)$ for $t \geq 0$, and

$$\frac{\partial u(x,t)}{\partial t} = -(1-ic_3)|u(x,t)|^2 u(x,t), \tag{5.7}$$

whose solution is for $t \geq 0$

$$u(x,t) = \mathrm{e}^{-(1-ic_3)\int_0^t M(x,s)ds}u_0(x) = \mathrm{e}^{-\frac{\beta}{2}\log(1+2tM_0(x))}u_0(x).$$

Here we have first solved the equation for $M(x,t) := |u(x,t)|^2$, given by

$$\frac{\partial M(x,t)}{\partial t} = -2M^2(x,t),$$

with solution

$$M\,(x,t) = \frac{M_0(x)}{1+2M_0(x)t}.$$

Considering t now as a complex variable with positive real part does not raise any difficulty for the first part, since $\mathrm{e}^{\varepsilon t}\mathrm{e}^{t(1+ic_1)\Delta}$ is well-defined. More care has to be taken for the second part, since $u \mapsto |u|^2 u$ is **not** a holomorphic function, and this prevents us from solving (5.5) in its current form. As a consequence, we first rewrite (5.5) as a system for $(v(x,t), w(x,t))$ where $v(x,t) = \Re(u(x,t))$ and $w(x,t) = \Im(u(x,t))$:

$$\left\{\begin{array}{rcl} \dfrac{\partial v(x,t)}{\partial t} & = & \Delta v(x,t) - c_1\Delta w(x,t) + \varepsilon\, v(x,t) - (v^2(x,t)+w^2(x,t))(v(x,t)+c_3 w(x,t)) \\ \dfrac{\partial w(x,t)}{\partial t} & = & c_1\Delta v(x,t) + \Delta w(x,t) + \varepsilon\, w(x,t) - (v^2(x,t)+w^2(x,t))(-c_3 v(x,t)+w(x,t)) \end{array}\right. \tag{5.8}$$

and now solve it for complex time $t \in \mathbb{C}$ with $\Re(t) \geq 0$. Observing that

$$\begin{pmatrix} -1 & -c_3 \\ c_3 & -1 \end{pmatrix} = PD_3P^{-1} \quad \text{and} \quad \begin{pmatrix} 1 & -c_1 \\ c_1 & 1 \end{pmatrix} = PD_1P^{-1},$$

with

$$D_1 = \begin{pmatrix} \alpha & 0 \\ 0 & \bar{\alpha} \end{pmatrix}, \quad D_3 = \begin{pmatrix} -\beta & 0 \\ 0 & -\bar{\beta} \end{pmatrix}, \quad P = \begin{pmatrix} i & 1 \\ 1 & i \end{pmatrix} \quad \text{and} \quad P^{-1} = \begin{pmatrix} -\frac{i}{2} & \frac{1}{2} \\ \frac{1}{2} & -\frac{i}{2} \end{pmatrix},$$

system (5.8) can be rewritten as

$$\begin{cases} \dfrac{\partial \tilde{v}(x,t)}{\partial t} & = & \Big(\alpha \Delta \tilde{v}(x,t) + \varepsilon \tilde{v}(x,t)\Big) - \Big(\beta \tilde{M}(x,t)\tilde{v}(x,t)\Big) \\ \dfrac{\partial \tilde{w}(x,t)}{\partial t} & = & \Big(\bar{\alpha} \Delta \tilde{w}(x,t) + \varepsilon \tilde{w}(x,t)\Big) - \Big(\bar{\beta} \tilde{M}(x,t)\tilde{w}(x,t)\Big) \end{cases} \tag{5.9}$$

where $\tilde{M}(x,t) = 4i\tilde{v}(x,t)\tilde{w}(x,t)$ and

$$\begin{pmatrix} \tilde{v} \\ \tilde{w} \end{pmatrix} = \frac{1}{2} \begin{pmatrix} -i & 1 \\ 1 & -i \end{pmatrix} \begin{pmatrix} v \\ w \end{pmatrix}.$$

It is not difficult to see that the exact solution of the second part of (5.9) is given by

$$\begin{cases} \tilde{v}(x,t) & = & \tilde{v}_0(x)\, \mathrm{e}^{-\frac{\beta}{2}\log(1+2t\tilde{M}_0(x))} \\ \tilde{w}(x,t) & = & \tilde{w}_0(x)\, \mathrm{e}^{-\frac{\bar{\beta}}{2}\log(1+2t\tilde{M}_0(x))} \end{cases} \tag{5.10}$$

where $\tilde{M}_0(x)$ is now defined as $\tilde{M}_0(x) := 4i\tilde{v}_0(x)\tilde{w}_0(x)$. Note that here, by convention, the logarithm refers to the principal value of $\log(z)$ for complex numbers: if $z = (a+ib) = r\mathrm{e}^{i\theta}$ with $-\pi < \theta \le \pi$, then

$$\log z := \ln r + i\theta = \ln|z| + i \arg z = \ln(|a+ib|) + 2i \arctan\left(\frac{b}{a+\sqrt{a^2+b^2}}\right).$$

Since $\log(z)$ is **not defined** for $z \in \mathbb{R}^-$, this means that the solution $(\tilde{v}(x,t), \tilde{w}(x,t))$ is defined only as long as $1 + 2\tilde{M}_0(x)t \notin \mathbb{R}^-$. Finally, the solution $(v(x,t), w(x,t))$ is of the form

$$\begin{cases} v(x,t) & = & v_0(x)\frac{(\mathrm{e}^{-\beta L(x,t)}+\mathrm{e}^{-\bar{\beta}L(x,t)})}{2} - w_0(x)\frac{(\mathrm{e}^{-\beta L(x,t)}-\mathrm{e}^{-\bar{\beta}L(x,t)})}{2i} \\ w(x,t) & = & v_0(x)\frac{(\mathrm{e}^{-\beta L(x,t)}-\mathrm{e}^{-\bar{\beta}L(x,t)})}{2i} + w_0(x)\frac{(\mathrm{e}^{-\beta L(x,t)}+\mathrm{e}^{-\bar{\beta}L(x,t)})}{2} \end{cases}$$

where $L(x,t) := \log(1+2t\tilde{M}_0(x)) = \log(1+2tM_0(x))$ and $M_0(x) = v_0^2(x) + w_0^2(x)$.

Denoting $V = (v_1, \ldots, v_N) \in \mathbb{R}^N$ and $W = (w_1, \ldots, w_N) \in \mathbb{R}^N$, we eventually have to numerically solve the following system:

$$\begin{cases} \dot{V} & = & AV - c_1AW + \varepsilon V - G(V + c_3W) \\ \dot{W} & = & c_1AV + AW + \varepsilon W - G(-c_3V + W) \end{cases}$$

where G is the diagonal matrix with $G_{i,i} = v_i^2 + w_i^2$ and A is the matrix corresponding to the discretized Laplacian.

One step $U_0 \mapsto U_1$ of the splitting method (1.2) is then applied as follows:

1. Initialize $V_0 = \Re(U_0)$ and $W_0 = \Im(U_0)$
2. Compute $(V_0, W_0) \mapsto (\tilde{V}_0, \tilde{W}_0)$
3. Set $k = s$
4. Compute $\tilde{V}_{1/2} := \tilde{V}(b_kh)$ and $\tilde{W}_{1/2} := \tilde{W}(b_kh)$

5. Compute $\tilde{V}_1 = \mathrm{e}^{\varepsilon a_k h} \exp(h a_k \alpha A) \tilde{V}_{1/2}$ and $\tilde{W}_1 = \mathrm{e}^{\varepsilon a_k h} \exp(h a_k \bar{\alpha} A) \tilde{W}_{1/2}$
6. Decrement k by 1
7. If $k \geq 1$, set $\tilde{V}_0 = \tilde{V}_1$, $\tilde{W}_0 = \tilde{W}_1$ and go to step 4.
8. Compute $(\tilde{V}_1, \tilde{W}_1) \mapsto (V_1, W_1)$

As we mentioned in the Introduction, for this problem the integrators designed in section 4.2 are particularly well suited. In consequence, we compare the following **splitting** methods:

- **Strang**: The second-order symmetric method of Strang (1.4);
- **(P4S4)**: The fourth-order method (4.3), already proposed in [CCDV09];
- **(P4S4opt)**: The optimized fourth-order method (4.4).
- **(P6S16)**: The sixth-order method (4.5).

The relative cost (w.r.t. Strang) of a splitting method with s steps of the diffusion part is approximated by $2s$, where the factor 2 stands here for the double dimension in the system.

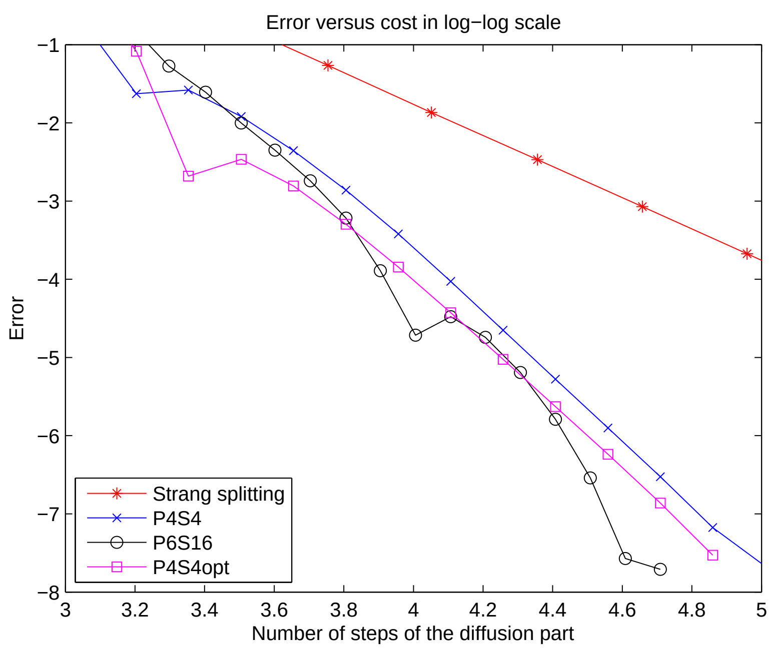

Figure 6: Error versus number of steps of the diffusion part for the complex Ginzburg–Landau equation.

We determine the matrix A by a Fourier collocation method with $N = 128$ and compute the error (in the 1-norm) at the final time $t = 100$ with respect to a reference solution obtained by integrating numerically with a much smaller time step. The results are collected in figure 6. We observe that the result achieved when using the optimized 4th-order method (4.4) is slightly better than the corresponding to (4.3) for this problem. On the other hand, the efficiency of the new scheme (4.5) is worth remarking, especially for stringent tolerances.

6 Concluding remarks

Splitting methods with real coefficients for the numerical integration of differential equations of order higher than two have necessarily some negative coefficients. This feature does not suppose any special impediment when the differential equation evolves in a group, but may be unacceptable when it is defined in a semi-group, as is the case with the evolution partial differential equations considered in this paper. One way to get around this fundamental difficulty is to consider splitting schemes with complex coefficients having positive real part. This has been recently proposed for diffusion equations in [CCDV09, HO09b]. Splitting and composition methods with complex coefficients have been considered in different contexts in the literature (see [BCM10] and references therein).

In [CCDV09, HO09b], splitting methods up to order 14 with complex coefficients with non-negative real part have been recursively constructed either by the so-called triple-jump compositions or by the quadruple-jump compositions, starting from the symmetric second-order Strang splitting. In this work we prove that there exists indeed an order barrier of 14 for methods constructed in this way. More generally, we show that no method of order higher than 14 with coefficients having non-negative real part can be constructed by sequential s-jump compositions starting from a symmetric method of order 2. We further show, by explicitly obtaining methods of order 16 (as the composition of a basic symmetric method of order 8), that this order barrier does not apply for general composition methods (non-necessarily constructed by recursive applications of s-jump compositions) with complex coefficients with non-negative real part.

In addition to this order barrier, another drawback of methods resulting from applying the s-jump composition procedure is that for high orders they require larger number of stages (i.e. number of compositions of the basic symmetric second order method) than methods obtained by directly solving the order conditions with the minimal number of stages. For instance, methods of order 6 (respectively, 8) obtained with triple jump compositions need 9 (resp. 27) compositions of the basic second order method, whereas, as we show in the present work, methods of order 6 (resp. 8) can be constructed (by directly solving for the required order conditions) with 7 (resp. 15) stages. An analysis of the local error coefficients supported by numerical tests shows that the methods proposed here are more efficient than those obtained in [CCDV09, HO09b] by applying the recursive triple jump and quadruple jump constructions.

Motivated by the application of splitting methods to problems like the complex Ginzburg-Landau equation (1.6), we further consider splitting methods of the form (1.2) such that $a_j \in \mathbb{R}$ and $\Re(b_i) \geq 0$. Such splitting methods cannot be constructed as composition methods with the Strang splitting as basic method. We construct methods of order four and six by imposing that a_j is the same for all j, and by determining the coefficients b_j from the required order conditions. Among all of the solutions with non-negative real parts obtained in this way, we choose those with smaller local error coefficients.

Based on the theoretical framework worked out in [HO09a], the integrators proposed here can be applied to the numerical integration of linear evolution equations involving unbounded operators in an infinite dimensional space, like linear diffusion equations. As a matter of fact, although the theory developed in [HO09a] does not cover the generalization to non-linear evolution equations, we have also included in our numerical tests two systems of ODEs obtained from semi-linear evolution equations with a certain space discretization. All the numerical tests show a considerable improvement in efficiency of our new methods with respect to existing splitting schemes. A remarkable feature of the new eighth order composition method when applied to both the linear and semi-linear diffusion examples is that it is more efficient than all the other integrators of order $p \leq 8$ in the whole range of tolerances explored.

Acknowledgements

The work of SB, FC and AM has been partially supported by Ministerio de Ciencia e Innovación (Spain) under the coordinated project MTM2010-18246-C03 (co-financed by the ERDF of the European Union). Additional financial support from the "Acción Integrada entre España y Francia" HF2008-0105 is also acknowledged. AM is additionally funded by project MTM2007-61572 (Universidad del País Vasco/Euskal

Herriko Unibertsitatea).

References

[BC05] S. Blanes and F. Casas. On the necessity of negative coefficients for operator splitting schemes of order higher than two. *Appl. Num. Math.*, 54:23–37, 2005.

[BCCM11] S. Blanes, F. Casas, P. Chartier, and A. Murua. Work in progress. 2011.

[BCM08] S. Blanes, F. Casas, and A. Murua. Splitting and composition methods in the numerical integration of differential equations. *Bol. Soc. Esp. Mat. Apl.*, 45:87–143, 2008.

[BCM10] S. Blanes, F. Casas, and A. Murua. Splitting methods with complex coefficients. *Bol. Soc. Esp. Mat. Apl.*, 50:47–61, 2010.

[CCDV09] F. Castella, P. Chartier, S. Descombes, and G. Vilmart. Splitting methods with complex times for parabolic equations. *BIT Numerical Analysis*, 49:487–508, 2009.

[CG89] M. Creutz and A. Gocksch. Higher-order hybrid Monte Carlo algorithms. *Phys. Rev. Lett.*, 63:9–12, 1989.

[Cha03] J. E. Chambers. Symplectic integrators with complex time steps. *Astron. J.*, 126:1119–1126, 2003.

[CM09] P. Chartier and A. Murua. An algebraic theory of order. *M2AN Math. Model. Numer. Anal.*, 43:607–630, 2009.

[For89] E. Forest. Canonical integrators as tracking codes. *AIP Conference Proceedings*, 184:1106–1136, 1989.

[FT88] S. Fauve and O. Thual. Localized structures generated by subcritical instabilities. *J. Phys. France*, 49:1829–1833, 1988.

[GK96] D. Goldman and T. J. Kaper. n th-order operator splitting schemes and nonreversible systems. *SIAM J. Numer. Anal.*, 33:349–367, 1996.

[HLW06] E. Hairer, C. Lubich, and G. Wanner. *Geometric Numerical Integration. Structure-Preserving Algorithms for Ordinary Differential Equations, Second edition*. Springer Series in Computational Mathematics 31. Springer, Berlin, 2006.

[HO09a] E. Hansen and A. Ostermann. Exponential splitting for unbounded operators. *Math. Comp.*, 78:1485–1496, 2009.

[HO09b] E. Hansen and A. Ostermann. High order splitting methods for analytic semigroups exist. *BIT Numerical Analysis*, 49:527–542, 2009.

[MSS99] A. Murua and J. M. Sanz-Serna. Order conditions for numerical integrators obtained by composing simpler integrators. *Philos. Trans. Royal Soc. London ser. A*, 357:1079–1100, 1999.

[Ros63] H. H. Rosenbrock. Some general implicit processes for the numerical solution of differential equations. *Comput. J.*, 5:329–330, 1962/1963.

[She89] Q. Sheng. Solving linear partial differential equations by exponential splitting. *IMA J. Numer. Anal.*, 9:199–212, 1989.

[Suz90] M. Suzuki. Fractal decomposition of exponential operators with applications to many-body theories and Monte Carlo simulations. *Phys. Lett. A*, 146:319–323, 1990.

[Suz91] M. Suzuki. General theory of fractal path integrals with applications to many-body theories and statistical physics. *J. Math. Phys.*, 32:400–407, 1991.

[vS94] W. van Saarloos. The complex Ginzburg–Landau equation for beginners. In P.E. Cladis and P. Palffy-Muhoray, editors, *Spatio-temporal Patterns in Nonequilibrium Complex Systems*, volume XXI of *Santa Fe Institute, Studies in the Sciences of Complexity*. Addison-Wesley, Reading, 1994.

[WMC05] D.M. Winterbottom, P.C. Mathews, and S.M. Cox. Oscillatory pattern formation with a conserved quantity. *Nonlinearity*, 18:1031–1056, 2005.

[Yos90] H. Yoshida. Construction of higher order symplectic integrators. *Phys. Lett. A*, 150:262–268, 1990.