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Splitting methods in the numerical integration of non-autonomous dynamical systems

Sergio Blanes, Fernando Casas, and Ander Murua

Abstract.

We analyze several strategies to adapt previously existing splitting methods to explicitly time dependent differential equations without deteriorating their efficiency. In the relevant case of linear differential equations originating in the space discretization of partial differential equations of evolution, a new, especially tailored procedure is devised which allows us to design splitting methods much more efficient than other previously available.

Métodos de escisión en la integración numérica de sistemas dinámicos no autónomos

Resumen.

En este trabajo se analizan diferentes estrategias para adaptar algunos de los métodos de escisión ya existentes a ecuaciones diferenciales con dependencia explícita del tiempo sin deteriorar su eficiencia. En el importante caso de ecuaciones diferenciales lineales provenientes de la discretización espacial de ecuaciones diferenciales en derivadas parciales de evolución, presentamos un nuevo procedimiento especialmente adaptado que permite diseñar métodos de escisión mucho más eficientes que otros previamente existentes.

1. Introduction

The evolution of many physical systems is usually described by an ordinary differential equation (ODE)

$$x' = f(x), \qquad x(t_0) = x_0 \in \mathbb{R}^d, \tag{1}$$

whose formal solution can be written as

$$x(t) = \varphi_t(x_0) = \exp((t - t_0)\, D_f)x_0.$$

Here D_f stands for the Lie derivative associated with $f(x)$, i.e. $D_f \equiv f(x) \cdot \nabla$. Describing the physical problem at hand requires then to formulate an appropriate mathematical model in this setting. In other words, a suitable function $f(x)$ such that (1) can reproduce the most salient features of the real system. In this respect, since the real system often involves one or more symmetries and these symmetries can

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be mathematically formulated in terms of Lie groups, a necessary condition is that the Lie derivative D_f possess the appropriate Lie algebraic structure.

Of course, one is also interested in solving (1), but with the exception of a very few simple cases, only numerical approximations are usually obtained. Generally speaking, standard numerical integrators (Runge–Kutta formulae, linear multistep methods) produce approximate solutions that do not take into account the special algebraic structure of f and therefore do not preserve the corresponding symmetries. In consequence, much effort has been devoted during the last two decades to the design of numerical integrators preserving those qualitative (geometric) properties of the exact solution. Examples of such algorithms include symplectic integrators, volume preserving methods, Lie group integrators, variational methods in mechanics, etc. [11, 12, 18]. All of them are now put into the more general category of *geometric numerical integrators*. In geometric integration, in fact, it is crucial to identify significant (geometric) properties of the dynamical system (1) and construct numerical integration algorithms that preserve those features. In addition, of course, one is interested in building efficient methods with the usual properties of accuracy and stability.

Although research in geometric numerical integrators for differential equations has experienced a tremendous boost during the last decades, it is fair to say that this has been mainly restricted to autonomous problems, whereas nonlinear systems of the form

$$x' = f(x,t), \qquad x(t_0) = x_0 \in \mathbb{R}^d, \tag{2}$$

i.e., when time appears explicitly in the formulation of the problem, have been up to some point disregarded. In the linear case $X' = A(t)X$, with A and X $n \times n$ matrices, several options have been widely explored and indeed the Magnus expansion has shown to be an extremely useful device to get analytical as well as numerical approximations [6].

A usual procedure in the numerical analysis of explicitly time-dependent problems consists in transforming (2) into an autonomous differential equation by the introduction of a new variable,

$$\left\{ \begin{array}{rcl} x' & = & f(x, x_t) \\ x_t' & = & 1 \end{array} \right. \tag{3}$$

or, equivalently,

$$y' = F(y), \qquad y(t_0) = (x_0, t_0) \in \mathbb{R}^{d+1}, \tag{4}$$

and $F(y) = (f(x, x_t), 1)$. Notice that formulation (3) introduces the auxiliary variable x_t aimed at eliminating the explicit time dependence, so that numerical integrators designed for (1) can, in principle, be used in this setting. This process exhibits, nevertheless, several drawbacks. First, the algebraic structure of D_f and D_F may differ, so that methods specifically designed for (1) cannot simply be used for the integration of the new enlarged system (4). Second, even when they can be applied, very often their efficiency reduces considerably.

In this work we explore other alternatives to cope with non autonomous differential equations from a computational point of view. They can be applied when dealing with splitting methods, and the goal is to adapt to this setting highly efficient methods previously designed for autonomous systems. We will analyze in detail the case of linear differential equations for simplicity and illustrate how in this particular situation our goal can be achieved.

2. Splitting methods and their generalization to non autonomous systems

2.1. General treatment

Although splitting methods have been used for a long time in the numerical treatment of differential equations, they have experienced a revival with the advent of geometric integration. In fact, a good deal of

geometric integrators are based on the idea of splitting. The idea is fairly simple: suppose f in equation (1) can be decomposed as $f(x) = f^{[A]}(x) + f^{[B]}(x)$ in such a way that systems

$$x' = f^{[A]}(x), \qquad x' = f^{[B]}(x) \tag{5}$$

can either be solved in closed form or accurately integrated. Then one combines these partial solutions into an approximate solution for (1), often of high accuracy. To make this sentence precise, let us denote by

$$\varphi_t^{[A]} = \exp((t-t_0)\, D_A), \qquad \varphi_t^{[B]} = \exp((t-t_0)\, D_B)$$

the flows corresponding to equations (5), where D_A and D_B represent the Lie derivatives associated with $f^{[A]}(x)$ and $f^{[B]}(x)$, respectively. Then one considers the composition

$$\psi_h \equiv \varphi^{[A]}_{a_{m+1}h} \circ \varphi^{[B]}_{b_{m+1}h} \circ \varphi^{[A]}_{a_m h} \circ \varphi^{[B]}_{b_m h} \circ \varphi^{[A]}_{a_{m-1}h} \circ \cdots \circ \varphi^{[B]}_{b_2 h} \circ \varphi^{[A]}_{a_1 h} \circ \varphi^{[B]}_{b_1 h} \tag{6}$$

with appropriately chosen real coefficients a_i, b_i to ensure that ψ_h is an approximation to the exact solution φ up to order $\mathcal{O}(h^p)$ with respect to the time step h, i.e. $\psi_h = \varphi_h + \mathcal{O}(h^{p+1})$. A great deal of methods of this class exist in the literature, of different orders and tailored for different structures of the vector field: general separable problems, systems arising from second order differential equations $x'' = g(x)$, near-integrable systems, etc. (see [4, 11, 13, 15] and references therein). One could said that the performance of the different splitting methods strongly depends on the particular problem at hand, so that a previous analysis is highly recommended to select the most appropriate scheme for its numerical treatment [4]. The non-autonomous separable problem

$$x' = f^{[A]}(x,t) + f^{[B]}(x,t). \tag{7}$$

is indeed a case in point.

One might think of two procedures to adapt the scheme (6) in this setting. The first one consists in replacing the maps $\varphi^{[A]}_{a_i h}$, $\varphi^{[B]}_{b_i h}$ by the maps associated to the exact flow defined by the equations

$$x' = f^{[A]}(x,t), \qquad t \in [t_0 + c_i h, t_0 + (c_i + a_i)h] \tag{8}$$

$$x' = f^{[B]}(x,t), \qquad t \in [t_0 + d_i h, t_0 + (d_i + b_i)h]. \tag{9}$$

Here $c_i = \sum_{j=0}^{i-1} a_j$, $d_i = \sum_{j=0}^{i-1} b_j$, $a_0 = 0$, $b_0 = 0$, and the initial conditions are given by the solution obtained from the previous flow. This approach can be considered as a time-average on each stage of the composition. Obviously, obtaining the exact solution of the non-autonomous equations (8) and (9) is by no means trivial due to the explicit time-dependence. In any case, the formal solution can be obtained by using the Magnus expansion, as shown in [6].

The second procedure is perhaps simpler. It consists in taking the maps $\varphi^{[A]}_{a_i h}$, $\varphi^{[B]}_{b_i h}$ in (6) as the $(a_i h)$-flow and $(b_i h)$-flow associated respectively to the autonomous equations

$$x' = f^{[A]}(x, t_0 + d_i h), \qquad t \in [t_0 + c_i h, t_0 + (c_i + a_i)h] \tag{10}$$

$$x' = f^{[B]}(x, t_0 + c_i h), \qquad t \in [t_0 + d_i h, t_0 + (d_i + b_i)h]. \tag{11}$$

Notice that the coefficients c_i, d_i appear interchanged in the vector fields with respect to (8) and (9).

These two strategies, which could be dubbed 'averaging' and 'frozen' techniques, respectively, may differ considerably both in the accuracy reached by the methods and also in their computational cost. Let us illustrate them on a simple but important example arising in applications.

2.2. Linear non autonomous separable systems

When discretizing in space the time dependent Schrödinger equation involving a time dependent potential $V(t)$ (for instance, with a pseudospectral method), the following system of ODEs arises:

$$iu' = H(t)u, \tag{12}$$

where $u \in \mathbb{C}^N$ and H is a real symmetric matrix. If the real and imaginary parts in u are considered, $u = q + ip$, the N-dimensional linear complex system (12) can be written as the $2N$-dimensional real system

$$q' = H(t)p, \qquad p' = -H(t)q. \tag{13}$$

These, in fact, can be interpreted as the classical Hamilton equations corresponding to the Hamiltonian

$$\mathcal{H}(q,p,t) = \frac{1}{2}p^T H(t)p + \frac{1}{2}q^T H(t)q. \tag{14}$$

Although we limit ourselves to this problem, most of the discussion is also valid with minor modifications for the more general system

$$q' = M(t)p, \qquad p' = N(t)q, \tag{15}$$

for $q \in \mathbb{R}^{d_1},\ p \in \mathbb{R}^{d_2}$. Equation (15) arises, in particular, when the Maxwell equations are discretized in space [17].

Equations (13) can be written in the compact form

$$z' = (A(t) + B(t))z, \tag{16}$$

where $z = (q,p)^T$ and

$$A(t) = \begin{pmatrix} 0 & H(t) \\ 0 & 0 \end{pmatrix}, \qquad B(t) = \begin{pmatrix} 0 & 0 \\ -H(t) & 0 \end{pmatrix}. \tag{17}$$

Let us consider first the autonomous problem, i.e., when H does not depend explicitly on t, in which case the corresponding equations

$$q' = Hp, \quad p' = -Hq \tag{18}$$

possess the formal solution

$$z(t) = \mathrm{e}^{t(A+B)}z(0). \tag{19}$$

Typically, as a result of the discretization in space, the value of N is large, and thus the exact computation of the exponential is exceedingly costly. In consequence, it makes sense to construct approximations requiring a much reduced computational effort. This can be achieved when the scheme only involves the computation of Hq and Hp in a particular sequence and only a few times per step. But this is precisely what splitting methods effectively do, as it is evident if one writes the composition (6) for this particular problem:

$$\begin{aligned} K(h) &\equiv \mathrm{e}^{ha_{m+1}A}\mathrm{e}^{hb_mB}\mathrm{e}^{ha_mA}\cdots\mathrm{e}^{hb_1B}\mathrm{e}^{ha_1A} \\ &= \begin{pmatrix} I & ha_{m+1}H \\ 0 & I \end{pmatrix}\begin{pmatrix} I & 0 \\ -hb_mH & I \end{pmatrix}\cdots\begin{pmatrix} I & 0 \\ -hb_1H & I \end{pmatrix}\begin{pmatrix} I & ha_1H \\ 0 & I \end{pmatrix}. \end{aligned} \tag{20}$$

The scheme requires m matrix-vector products Hq and Hp (the last product at each step can be reused in the first stage at the following step) and is referred as an m-stage method. Although any of the splitting methods for separable systems collected in [11, 13, 15, 16] can be used for carrying out numerical integrations here, equation (16) in the autonomous case possesses the following crucial simplifying property:

$$[A,[A,[A,B]]] = [B,[B,[B,A]]] = 0, \tag{21}$$

where $[\cdot,\cdot]$ stands for the usual commutator: $[A,B] = AB - BA$. This feature allows one to build very efficient methods indeed [9, 1, 2]. Moreover, it has been shown that any non-symmetric method for this problem is conjugate to a symmetric method [3], so that one may restrict the analysis to symmetric compositions, i.e., when $a_{m+2-i} = a_i,\ b_{m+1-i} = b_i$. The resulting scheme is sometimes referred to as an

ABA composition. Since the role of A and B can be naturally interchanged, BAB compositions are not separately studied.

Let us turn our attention now to the time dependent case. As is well known, the Magnus expansion allows one to formally write the solution of (16) as

$$z(t) = \mathrm{e}^{\Omega(t)} z(0), \tag{22}$$

where $\Omega(t)$ is given by an infinite series involving $A(t)$, $B(t)$, multivariate integrals and nested commutators with a finite radius of convergence [14, 6]. Although it is indeed possible to derive numerical integration algorithms from the Magnus expansion, they still require the computation of the exponential of a full matrix of high dimension involving iterate integrals and commutators. We apply instead the two procedures pointed out in section 2.1.

The first one uses composition (6) with maps corresponding to the exact solutions of (8)-(9), which for this particular problem read (taking $t_0 = 0$)

$$\varphi_{a_i h}^{[A_1]}(q,p) = \left(q + \int_{c_i h}^{c_{i+1} h} H(\tau) d\tau \, p, \;\; p \right), \qquad \varphi_{b_i h}^{[B_1]}(q,p) = \left(q, \;\; p - \int_{d_i h}^{d_{i+1} h} H(\tau) d\tau \, q \right). \tag{23}$$

Notice that the resulting scheme can be seen as the composition method (6) applied to the autonomous Hamiltonian

$$\mathcal{H}(q, q_1, q_2, p, p_1, p_2) = \left(\frac{1}{2} p^T H(q_1) p + p_1 \right) + \left(\frac{1}{2} q^T H(q_2) q + p_2 \right) \equiv A_1 + B_1, \tag{24}$$

where we have considered time as *two* different additional coordinates.

On the other hand, with the 'frozen' technique (10)-(11) one has

$$\varphi_{a_i h}^{[A_2]}(q,p) = (q + H(d_i h), \; p), \qquad \varphi_{b_i h}^{[B_2]}(q,p) = (q, \; p - H(c_i h)), \tag{25}$$

and the corresponding scheme, as before, is nothing but composition (6) applied to the Hamiltonian

$$\mathcal{H}(q, q_1, q_2, p, p_1, p_2) = \left(\frac{1}{2} p^T H(q_2) p + p_1 \right) + \left(\frac{1}{2} q^T H(q_1) q + p_2 \right) \equiv A_2 + B_2. \tag{26}$$

Now the Hamilton equations are no longer linear and, moreover,

$$\{A_i, \{A_i, \{A_i, B_i\}\}\} \neq 0, \qquad \{B_i, \{B_i, \{B_i, A_i\}\}\} \neq 0, \qquad i = 1, 2$$

in terms of the Poisson bracket. In consequence, the highly efficient schemes of type (20) designed for systems verifying (21) lose their appealing accomplishments when applied in the non autonomous case.

Another possibility is suggested in [8]. One might consider a combination of (24) and (26) in the form

$$\mathcal{H}(q, q_1, q_2, p, p_1, p_2) = \left(\frac{1}{2} p^T H(q_1) p + p_1 \right) + \left(\frac{1}{2} q^T H(q_1) q + p_2 \right) \tag{27}$$

or equivalently

$$\mathcal{H}(q, q_1, p, p_1) = \left(\frac{1}{2} p^T H(q_1) p + p_1 \right) + \left(\frac{1}{2} q^T H(q_1) q \right) \equiv A_3 + B_3, \tag{28}$$

with associated maps

$$\varphi_{a_i h}^{[A_3]}(q,p) = \left(q + \int_{c_i h}^{c_{i+1} h} H(\tau) d\tau \, p, \;\; p \right), \qquad \varphi_{b_i h}^{[B_3]}(q,p) = (q, \; p - H(c_i h)). \tag{29}$$

Now $\{B_3, \{B_3, \{B_3, A_3\}\}\} = 0$ so that Runge–Kutta–Nyström methods can be used (even with modified potentials) [4], and thus significant improvements in the efficiency with respect to the previous choices can be achieved.

At this point a natural question arises: is it possible to directly adapt the extremely efficient schemes of type (20) constructed for the autonomous case to the more general problem (16), so that the resulting splitting methods do not suffer from a degradation in their performance? The answer is provided in the next section.

3. A new class of splitting methods for non autonomous linear systems

Our purpose here is to generalize the 'averaging' technique (23) by using the Magnus expansion and formulate directly the splitting method (20) in terms of the new maps. More specifically, the new methods have the form (for a time step of size h)

$$z(t+h) \approx \mathrm{e}^{\tilde{A}_{m+1}} \mathrm{e}^{\tilde{B}_m} \mathrm{e}^{\tilde{A}_m} \cdots \mathrm{e}^{\tilde{B}_1} \mathrm{e}^{\tilde{A}_1} z(t), \tag{30}$$

where the matrices $\tilde{A}_i \equiv A_i(t,h)$ and $\tilde{B}_i \equiv B_i(t,h)$ are taken as

$$\tilde{A}_i = h \int_{-1/2}^{1/2} p_i^a(\tau)\, A(t_{1/2} + h\tau)\, d\tau, \qquad \tilde{B}_i = h \int_{-1/2}^{1/2} p_i^b(\tau)\, B(t_{1/2} + h\tau)\, d\tau. \tag{31}$$

Here $t_{1/2} = t + \frac{h}{2}$ and $p_i^a(\tau)$, $p_i^b(\tau)$ are *filters* (scalar functions). As we will see in the sequel, to get integrators of even order $n = 2s$, it is enough to consider p_i^a, p_i^b as polynomials of degree $s-1$, i.e.,

$$p_i^a(\tau) = \mathrm{a}_i^{[0]} + \mathrm{a}_i^{[1]}\tau + \cdots + \mathrm{a}_i^{[s-1]}\tau^{s-1}, \qquad p_i^b(\tau) = \mathrm{b}_i^{[0]} + \mathrm{b}_i^{[1]}\tau + \cdots + \mathrm{b}_i^{[s-1]}\tau^{s-1}.$$

Since in our case

$$\mathrm{e}^{\tilde{A}_i} = \begin{pmatrix} I & \tilde{H}_i^A \\ 0 & I \end{pmatrix}, \qquad \mathrm{e}^{\tilde{B}_i} = \begin{pmatrix} I & 0 \\ -\tilde{H}_i^B & I \end{pmatrix},$$

then (30) can be written as $z(t+h) \approx K(t,h) z(t)$, where

$$\begin{aligned} K(t,h) &= \mathrm{e}^{\tilde{A}_{m+1}} \mathrm{e}^{\tilde{B}_m} \mathrm{e}^{\tilde{A}_m} \cdots \mathrm{e}^{\tilde{B}_1} \mathrm{e}^{\tilde{A}_1} \\ &= \begin{pmatrix} I & \tilde{H}_{m+1}^A \\ 0 & I \end{pmatrix} \begin{pmatrix} I & 0 \\ -\tilde{H}_m^B & I \end{pmatrix} \begin{pmatrix} I & \tilde{H}_m^A \\ 0 & I \end{pmatrix} \cdots \begin{pmatrix} I & 0 \\ -\tilde{H}_1^B & I \end{pmatrix} \begin{pmatrix} I & \tilde{H}_1^A \\ 0 & I \end{pmatrix}, \end{aligned} \tag{32}$$

and

$$\tilde{H}_i^A = h \int_{-1/2}^{1/2} p_i^a(\tau)\, H(t_{1/2} + h\tau)\, d\tau, \qquad \tilde{H}_i^B = \int_{-1/2}^{1/2} p_i^b(\tau)\, H(t_{1/2} + h\tau)\, d\tau. \tag{33}$$

These integrals can either be computed analytically or numerically approximated by using some appropriate quadrature rule. If the method (32) is of order $2s$, then a quadrature rule of order $2s$ or higher must be used to retain the original order.

The numerical scheme is then determined by the values of the coefficients $\mathrm{a}_i^{[k]}$, $\mathrm{b}_i^{[k]}$ ($k = 0, 1, \ldots, s-1$, $i = 1, \ldots, m$). The problem of designing efficient methods of a prescribed order $2s$ is then equivalent to determining coefficients such that the composition (30) achieve the desired order of accuracy and, at a given cost, provide the most accurate results among a number of possible choices. The method is of order $2s$ if the coefficients $\mathrm{a}_i^{[k]}$, $\mathrm{b}_i^{[k]}$ satisfy a system of algebraic equations (the order conditions), which have to be first formulated and then solved (usually by numerical tools). A subset of such order conditions correspond

precisely to the particular case where $H(t)$ actually does not depend on t, so that the matrix (32) reduces to the matrix $K(h)$ in (20) with a_i, b_i related to $\mathrm{a}_i^{[k]}$, $\mathrm{b}_i^{[k]}$. When constructing a method of order $2s$, we proceed as follows: (i) we first determine the values of the coefficients a_i, b_i in such a way that (20) gives a good method of order $2s$ for the autonomous case, (ii) and then choose the coefficients $\mathrm{a}_i^{[k]}$, $\mathrm{b}_i^{[k]}$, so that the remaining order conditions hold (once the relation between the coefficients a_i, b_i and $\mathrm{a}_i^{[k]}$, $\mathrm{b}_i^{[k]}$ is taken into account).

3.1. Order conditions for the autonomous case

When considering the matrix (20) used to propagate the numerical solution in the autonomous case (18), one observes that diagonalizing the matrix H with an appropriate linear change of variables transforms the system into N uncoupled harmonic oscillators with frequencies $\omega_1, \ldots, \omega_N$. Although in practice one wants to avoid diagonalizing the matrix H, numerically solving the system (18) by a splitting method is mathematically equivalent to applying the splitting method to each of such harmonic oscillators (and then rewritting the result in the original variables). Clearly, the exact solution of each individual harmonic oscillator with frequency ω is propagated by 2×2 matrix $O(\omega h)$, where

$$O(x) = \begin{pmatrix} \cos x & \sin x \\ -\sin x & \cos x \end{pmatrix}. \tag{34}$$

As for the numerical solution, it is propagated by a matrix $K(\omega h)$ defined as

$$K(x) = \begin{pmatrix} 1 & a_{m+1}x \\ 0 & 1 \end{pmatrix} \begin{pmatrix} 1 & 0 \\ -b_m x & 1 \end{pmatrix} \begin{pmatrix} 1 & a_m x \\ 0 & 1 \end{pmatrix} \cdots \begin{pmatrix} 1 & 0 \\ -b_1 x & 1 \end{pmatrix} \begin{pmatrix} 1 & a_1 x \\ 0 & 1 \end{pmatrix}.$$

It is straightforward to check that

$$K(x) = \begin{pmatrix} K_1(x) & K_2(x) \\ K_3(x) & K_4(x) \end{pmatrix} = \begin{pmatrix} 1 + \sum_{i=1}^{m} k_{1,i}\, x^{2i} & \sum_{i=1}^{m+1} k_{2,i}\, x^{2i-1} \\ \sum_{i=1}^{m} k_{3,i}\, x^{2i-1} & 1 + \sum_{i=1}^{m} k_{4,i}\, x^{2i} \end{pmatrix}, \tag{35}$$

where $k_{i,j}$ are homogeneous polynomials in the parameters a_i, b_i.

The integrator (35) typically will be stable for $|h\omega| < x_*$ for some value x_* (that we call stability threshold) depending on the coefficients a_i, b_i. It has been shown [3] that if for a given splitting method $x_* > 0$, then the method applied to (18), for H a constant matrix, is conjugate, for $h\rho(H) < x_*$, to the solution of a modified system

$$q' = \tilde{H}(h)p, \qquad p' = -\tilde{H}(h)q, \tag{36}$$

where

$$h\tilde{H}(h) = hH + \phi_{2s+1}(hH)^{2s+1} + \phi_{2s+3}(hH)^{2s+3} + \cdots \tag{37}$$

for some constants $\phi_{2i+1},\ i = 1, 2, \ldots$, provided that the method is of order $2s$ for the harmonic oscillator (see [3] for more details).

We thus intend to construct accurate symmetric schemes with large stability intervals $(-x_*, x_*)$. Notice that for a fair comparison of the stability interval for splitting methods with different number of stages, one must consider the relative stability threshold x_*/m. For this class of schemes, the elements of the stability matrix have to satisfy

$$K_1(x) = K_4(x) \approx \cos x, \tag{38}$$

$$K_2(x) \approx \sin x, \qquad K_3(x) \approx -\sin x, \tag{39}$$

$$K_1(x)^2 - K_2(x)K_3(x) = 1. \tag{40}$$

Since we are dealing with symmetric compositions, we found more appropriate (due to the ill conditioned equations to be numerically solved) to consider the decomposition

$$K(x) = U(-x)^{-1}U(x), \quad \text{where} \quad U(x) = \begin{pmatrix} U_1(x) & U_2(x) \\ U_3(x) & U_4(x) \end{pmatrix} \tag{41}$$

with U_1, U_4 even polynomial functions and U_2, U_3 odd polynomial functions. Since we are interested in matrices K, U to be decomposed as products (35), then it is clear that they must satisfy $\det(K) = \det(U) = 1$. Clearly, conditions (38)-(40) are equivalent to $O(x) \approx U(-x)^{-1}U(x)$ together with

$$U_1(x)U_4(x) - U_2(x)U_3(x) \equiv 1. \tag{42}$$

Whence, one has an approximation of order $2s$ if

$$\begin{aligned} U_3(x)\cos(x/2) + U_4(x)\sin(x/2) &= \mathcal{O}(x^{2s+1}) \\ U_1(x)\sin(x/2) - U_2(x)\cos(x/2) &= \mathcal{O}(x^{2s+1}). \end{aligned} \tag{43}$$

Observe that to obtain a method of order $2s$ one needs a composition with $m \geq 2s-1$ stages, as already noticed in [9]. The matrix U has $4s-2$ parameters that can be used to solve the required system of $4s-2$ equations: indeed, equations (43) originate $2s$ linear equations and condition (42) gives $2s-2$ quadratic equations. However, the methods with minimal number of stages obtained by solving these $4s-2$ equations have stability thresholds $x_* \approx \pi$, and thus the relative stability threshold $x_*/m \approx \pi/(4s-2)$ becomes very small for high order methods.

A simple trick to get methods with larger relative stability threshold is to add the condition

$$O(j\pi) = K(j\pi), \qquad j = 1, \ldots, l \tag{44}$$

for some positive integer l. For moderate values of l relative to s, this typically gives a method with stability threshold $x_* > l\pi$. In addition to improving stability, due to its interpolatory nature, condition (44) contributes to improve the precision of the method when applied to (18).

In terms of the matrix $U(x)$, condition (44) reads

$$U_1((2j-1)\pi) = U_4((2j-1)\pi) = 0, \qquad U_1(j\pi) = U_3(2j\pi) = 0, \qquad j \leq l/2. \tag{45}$$

Given positive integers s, l, we impose conditions (42), (43), and (45) to the matrix $U(x)$, which gives a system of $4(n+l)-2$ linear and quadratic equations in terms of the coefficients of the polynomials $U_j(x)$, $j = 1, 2, 3, 4$. The required number of free parameters can be obtained by considering

$$\begin{aligned} d(U_1) &= 2(n+l-1), \qquad & d(U_4) &= 2(n+l), \\ d(U_2) &= 2(n+l)-1, \qquad & d(U_3) &= 2(n+l)-1, \end{aligned}$$

where $d(P(x))$ denotes de degree of the polynomial $P(x)$. For a given matrix $U(x)$ satisfying the required conditions, if there exists a splitting method associated to the matrix (41) (if it exists, is unique [3]), then in general will have $m = 2(n+l)-1$ stages.

We have obtained (with the help of the software *Mathematica*) all the solutions of the equations corresponding to moderate values of n and l ($n + l \leq 6$). For each s and l, we choose among all the real solutions of the corresponding system of polynomial equations the best methods with respect to suitable criteria based on the rigorous error estimates (for the application of (18)) derived in [5]. Once an appropriate matrix $U(x)$ is chosen for given s and l, we compute the coefficients $\{a_1, b_1, a_2, b_2, \ldots\}$ of the splitting scheme corresponding to $K(x) = U(-x)^{-1}U(x)$ by following the algorithm presented in [3]. We collect in Table 1 the coefficients of one of the best methods obtained in this way ($s = l = 3$, $m = 11$, and relative stability threshold $x_* = 1.07$).

3.2. Order conditions for the non autonomous case

In the following, we analyze the order conditions to be satisfied by the coefficients $\mathrm{a}_i^{[k]}, \mathrm{b}_i^{[k]}$, $i, k = 0, 1, \ldots, s-1$ for the polynomials in the scheme (33) to give a method of order $p = 2s$. To this purpose, we first consider the formal solution of equations (16) as furnished by the Magnus expansion.

As is well known, for a time step h we can write

$$z(t+h) = \mathrm{e}^{\Omega(t,h)} z(t), \tag{46}$$

where $\Omega(t,h) = \sum_{k=1}^{\infty} \Omega_k(t,h)$ and each $\Omega_k(t,h)$ is a multiple integral of combinations of nested commutators containing k matrices $A(t)$ and $B(t)$ [6, 14].

The explicit expression of $\Omega_k(t,h)$ can be obtained by inserting into the recurrence defining the Magnus expansion a Taylor series of the matrices $A(t)$ and $B(t)$ around the midpoint $t + h/2$ (to take advantage of the time-symmetry property of the solution), i.e.,

$$A(t+\tfrac{h}{2}+\tau) = \alpha_1 + \alpha_2\tau + \alpha_3\tau^2 + \cdots, \qquad B(t+\tfrac{h}{2}+\tau) = \beta_1 + \beta_2\tau + \beta_3\tau^2 + \cdots$$

Then $\Omega(t,h)$ in (46) can be expanded as

$$\Omega(t,h) = \sum_{n\geq 1} h^n \sum_{k=1}^{n} \Omega_{k,n}(t,h), \tag{47}$$

where each $\Omega_{k,n}(t,h)$ is a linear combination of terms of the form $[\mu_{i_1}, \mu_{i_2} \ldots, \mu_{i_k}]$ with $\mu_j = \alpha_{i_j}$ or $\mu_j = \beta_{i_j}$ for each $j = 1, \ldots, k$, and $i_1 + \cdots + i_k = n$. Furthermore, $\Omega_{k,n}(t,h) = 0$ for even values of n, $\Omega_{k,k}(t,h) = 0$ for $k > 1$ and $\Omega_{1,1}(t,h) = \alpha_1 + \beta_1$.

In particular, up to order h^6 one has [7]

$$\Omega = h\Omega_{1,1} + h^3(\Omega_{1,3} + \Omega_{2,3}) + h^5(\Omega_{1,5} + \Omega_{2,5} + \Omega_{3,5} + \Omega_{4,5}) + \mathcal{O}(h^7), \tag{48}$$

where (for simplicity, we omit the arguments (t,h))

$$\begin{aligned}
\Omega_{1,1} &= \alpha_1 + \beta_1, \qquad \Omega_{1,3} = \frac{1}{12}(\alpha_3 + \beta_3), \qquad \Omega_{2,3} = \frac{1}{12}\big([\alpha_2, \beta_1] + [\beta_2, \alpha_1]\big), \\
\Omega_{1,5} &= \frac{1}{80}(\alpha_5 + \beta_5), \quad \Omega_{2,5} = \frac{1}{240}\left([\alpha_2, \beta_3] + [\beta_2, \alpha_3]\right) + \frac{1}{80}\left([\alpha_4, \beta_1] + [\beta_4, \alpha_1]\right), \\
\Omega_{3,5} &= \frac{1}{360}\big(- [\alpha_1, \beta_3, \alpha_1] + [\alpha_1, \beta_1, \alpha_3] - [\beta_1, \alpha_3, \beta_1] + [\beta_1, \alpha_1, \beta_3]\big) \\
&\quad + \frac{1}{240}\big([\alpha_1, \beta_2, \alpha_2] - [\alpha_2, \beta_1, \alpha_2] + [\beta_1, \alpha_2, \beta_2] - [\beta_2, \alpha_1, \beta_2]\big), \\
\Omega_{4,5} &= \frac{1}{720}\big([\alpha_1, \beta_1, \alpha_1, \beta_2] - [\beta_1, \alpha_1, \beta_2, \alpha_1] + [\beta_1, \alpha_1, \beta_1, \alpha_2] - [\alpha_1, \beta_1, \alpha_2, \beta_1]\big).
\end{aligned}$$

Notice that, due to the structure of the matrices $A(t), B(t)$, we have that $[\alpha_i, \alpha_j, \alpha_k, \beta_l] = [\beta_i, \beta_j, \beta_k, \alpha_l] = 0$ for any value of i, j, k, l.

Once the exact solution is constructed up to the desired order, we analyze the order conditions to be satisfied by the composition (30) to approximate the formal solution at different orders. This can be done by applying the Baker–Campbell–Hausdorff (BCH) formula repeatedly to (30), so that $K(t,h)$ is expressed as the exponential of only one operator,

$$K(t,h) = \exp(\tilde{\Omega}(t,h)),$$

depending on $\tilde{A}_i(t,h)$, $\tilde{B}_i(t,h)$ $(i = 1, \ldots, m)$ and nested commutators of these matrices. The numerical scheme will be of order p if $\tilde{\Omega}(t,h) - \Omega(t,h) = \mathcal{O}(h^{p+1})$ as $h \to 0$. One can then obtain explicitly the order conditions as follows. First, we expand $\tilde{A}_i(t,h)$, $\tilde{B}_i(t,h)$ in (31) in terms of α_j, β_j,

$$\tilde{A}_i(t,h) = \sum_{n\geq 1} h^n a_i^{(n)} \alpha_n, \qquad \tilde{B}_i(t,h) = \sum_{n\geq 1} h^n b_i^{(n)} \beta_n, \tag{49}$$

where $a_i^{(n)}, b_i^{(n)}$ have to be determined and subsequently the coefficients $\mathrm{a}_i^{[j]}, \mathrm{b}_i^{[j]}$.

We substitute the expressions (49) in the corresponding $\tilde{\Omega}(t,h)$, thus obtaining an expansion of the form

$$\tilde{\Omega}(t,h) = \sum_{n\geq 1} h^n \sum_{k=1}^{n} \tilde{\Omega}_{k,n}(t,h), \tag{50}$$

where each $\tilde{\Omega}_{k,n}(t,h)$ is also a linear combination of terms $[\mu_{i_1}, \mu_{i_2} \ldots, \mu_{i_k}]$ with $\mu_j = \alpha_{i_j}$ or $\mu_j = \beta_{i_j}$ for $j = 1, \ldots, k$. Finally, we compare the truncated (up to $n = p$) expansion (50) with the corresponding expression (47) for $\Omega(t,h)$, so that the numerical scheme is of order p if

$$\sum_{k=1}^{n} \tilde{\Omega}_{k,n} = \sum_{k=1}^{n} \Omega_{k,n} \qquad \text{for} \quad n = 1, \ldots, p. \tag{51}$$

The analysis is simplified by imposing time symmetry to the composition (32): $K(t+h,-h) = K(t,h)^{-1}$, or equivalently, $\tilde{\Omega}(t+h-h) = -\tilde{\Omega}(t,h)$, which implies that $\tilde{\Omega}_{k,n}(t,h) = 0$ for even values of n. This procedure, in addition, leads to integrators with better preservation of qualitative properties.

The time symmetry is automatically satisfied (and thus all order conditions at even orders) if

$$\tilde{A}_{m+2-i}(t+h,-h) = -\tilde{A}_i(t,h), \qquad \tilde{B}_{m+1-i}(t+h,-h) = -\tilde{B}_i(t,h), \qquad B_{m+1}(t,h) = 0, \tag{52}$$

for $i = 1, 2, \ldots, m$, which in turn is satisfied as soon as

$$a_{m+1-i}^{(n)} = (-1)^{n+1}\, a_i^{(n)}, \qquad b_{m-i}^{(n)} = (-1)^{n+1}\, b_i^{(n)}, \qquad b_m^{(n)} = 0, \tag{53}$$

for $n \geq 1,\ i = 1, 2, \ldots, m$. As a result we have

$$\tilde{\Omega} = h\tilde{\Omega}_{1,1} + h^3(\tilde{\Omega}_{1,3} + \tilde{\Omega}_{2,3} + \tilde{\Omega}_{3,3}) + h^5(\tilde{\Omega}_{2,5} + \tilde{\Omega}_{3,5} + \tilde{\Omega}_{4,5} + \tilde{\Omega}_{5,5}) + \mathcal{O}(h^7), \tag{54}$$

where

$$\begin{aligned}
\tilde{\Omega}_{1,1} &= \alpha_1 + \beta_1, & \tilde{\Omega}_{1,3} &= \lambda_3\alpha_3 + \mu_3\beta_3, \\
\tilde{\Omega}_{2,3} &= \lambda_{21}[\alpha_2,\beta_1] + \mu_{21}[\beta_2,\alpha_1], & \tilde{\Omega}_{3,3} &= \epsilon_{31}[\alpha_1,\beta_1,\alpha_1] + \epsilon_{32}[\beta_1,\alpha_1,\beta_1] \\
\tilde{\Omega}_{1,5} &= \lambda_5\alpha_5 + \mu_5\beta_5, \\
\tilde{\Omega}_{2,5} &= \lambda_{23}[\alpha_2,\beta_3] + \mu_{23}[\beta_2,\alpha_3] + \lambda_{41}[\alpha_4,\beta_1] + \mu_{41}[\beta_4,\alpha_1], \\
\tilde{\Omega}_{3,5} &= \lambda_{131}[\alpha_1,\beta_3,\alpha_1] + \lambda_{113}[\alpha_1,\beta_1,\alpha_3] + \mu_{131}[\beta_1,\alpha_3,\beta_1] + \mu_{113}[\beta_1,\alpha_1,\beta_3] \\
&\quad +\lambda_{122}[\alpha_1,\beta_2,\alpha_2] + \lambda_{212}[\alpha_2,\beta_1,\alpha_2] + \mu_{122}[\beta_1,\alpha_2,\beta_2] + \mu_{212}[\beta_2,\alpha_1,\beta_2], \\
\tilde{\Omega}_{4,5} &= \lambda_{1112}[\alpha_1,\beta_1,\alpha_1,\beta_2] + \lambda_{1121}[\beta_1,\alpha_1,\beta_2,\alpha_1] + \mu_{1112}[\beta_1,\alpha_1,\beta_1,\alpha_2] \\
&\quad +\mu_{1121}[\alpha_1,\beta_1,\alpha_2,\beta_1], \\
\tilde{\Omega}_{5,5} &= \epsilon_{51}[\alpha_1,\beta_1,\alpha_1,\beta_1,\alpha_1] + \epsilon_{52}[\beta_1,\alpha_1,\beta_1,\alpha_1,\beta_1],
\end{aligned} \tag{55}$$

and the coefficients $\lambda_{i_1\cdots i_l}$, $\mu_{i_1\cdots i_l}, \epsilon_{ij}$, are polynomial functions depending on $a_i^{(n)}$, $b_i^{(n)}$, $i = 1, \ldots, m$, $n = 1, \ldots, 5$. The explicit expressions for $\lambda_{i_1\cdots i_l}$, $\mu_{i_1\cdots i_l}$ up to order six can be found in [2].

Notice that while for the exact solution $\Omega_{n,n} = 0$, $n > 1$, now $\tilde{\Omega}_{n,n} \neq 0,\ n > 1$ unless the coefficients $\mathrm{a}_i^{[j]}$, $\mathrm{b}_i^{[j]}$ are chosen so that $\epsilon_{ij} = 0$. Therefore, to build a method of order p it is necessary that $\epsilon_{ni} = 0$, $n \leq p$. In this respect, notice that the polynomials ϵ_{ni} multiply elements generated only by $\{\alpha_1, \beta_1\}$ and their nested commutators. These are precisely the terms appearing in the autonomous case.

In most cases of practical interest, the dominant terms at each step correspond to the constant part, i.e. in general $\|\alpha_1\| \gg \|\alpha_i\|$ and $\|\beta_1\| \gg \|\beta_i\|$, $i > 1$. For this reason, it makes sense to analyze separately the error contributions coming from $\Omega_{n,n}$.

3.3. Determining the coefficients for the non autonomous case

As we said before, in the autonomous case one has $\alpha_1 = hA$, $\beta_1 = hB$ and $\alpha_j = \beta_j = 0$, $j > 1$ so that the scheme reduces to

$$K(h) = \mathrm{e}^{a_{m+1}^{(1)}\alpha_1}\mathrm{e}^{b_m^{(1)}\beta_1}\mathrm{e}^{a_m^{(1)}\alpha_1}\cdots\mathrm{e}^{b_m^{(1)}\beta_1}\mathrm{e}^{a_1^{(1)}\alpha_1}, \tag{56}$$

which corresponds to eq. (20) with $a_i^{(1)} = a_i$, $b_i^{(1)} = b_i$. From (56) it is clear that $a_i^{(1)}, b_i^{(1)}$ can be taken separately from the remaining coefficients. For instance, from (31) we have

$$a_i^{(1)} = h\int_{-1/2}^{1/2} p_i^a(\tau)\,d\tau, \qquad b_i^{(1)} = h\int_{-1/2}^{1/2} p_i^b(\tau)\,d\tau. \tag{57}$$

In any case, the actual choice of $a_i^{(1)}, b_i^{(1)}$ plays an essential role to get the coefficients $\mathrm{a}_i^{[j]}, \mathrm{b}_i^{[j]}$ leading to efficient methods, since the constant parts $\alpha_1 = hA(t_{1/2})$, $\beta_1 = hB(t_{1/2})$ usually represent the dominant contributions to the evolution of the system.

Once a set of values for $a_i^{(1)}$, $b_i^{(1)}$, $i = 1,\ldots,m$, satisfying the symmetry condition (53) is chosen, we have to determine the coefficients, $a_i^{(n)}, b_i^{(n)}$, $n \geq 2$, $i = 1,\ldots,m$, which satisfy the remaining order conditions. This can produce different methods with the same values for the coefficients $a_i^{(1)}, b_i^{(1)}$. If we compare (55) with the formal solution, one can easily identify the order conditions at different orders of accuracy.

Let us now write $\tilde{A}_i,\ \tilde{B}_i$ as follows:

$$\tilde{A}_i = \sum_{j=0}^{s-1} \mathrm{a}_i^{[j]} A^{(j)}, \qquad \tilde{B}_i = \sum_{j=0}^{s-1} \mathrm{b}_i^{[j]} B^{(j)}, \tag{58}$$

where

$$A^{(j)} \equiv h\int_{-1/2}^{1/2} \tau^j A(t_{1/2}+h\tau)\,d\tau, \qquad B^{(j)} \equiv h\int_{-1/2}^{1/2} \tau^j B(t_{1/2}+h\tau)\,d\tau \tag{59}$$

for $j = 0,\ldots,s-1$.

At this point the following remark is worth to be stated. Suppose that $\bar{b}_i$, c_i, $(i = 1,\ldots,k)$, are the weights and nodes of a particular quadrature rule for integrals. Then it is possible to approximate all the integrals $A^{(i)}$ (up to the required order) just by using only the evaluations A_i at the nodes c_i of the quadrature rule required to compute $A^{(0)}$:

$$A^{(i)} = h\sum_{i=1}^{k} \bar{b}_j \left(c_j - \frac{1}{2}\right)^i A_j. \qquad i = 0,\ldots,s-1, \tag{60}$$

with $A_i \equiv A(t_n + c_i h)$.

In particular, if fourth and sixth order Gauss-Legendre quadrature rules are considered, we have $s = k = 2$ and $\bar{b}_1 = \bar{b}_2 = 1/2$, $c_1 = 1/2 - \sqrt{3}/6$, $c_2 = 1/2 + \sqrt{3}/6$. To order six we have $s = k = 3$ and $\bar{b}_1 = \bar{b}_3 = 5/18$, $\bar{b}_2 = 4/9$, $c_1 = 1/2 - \sqrt{15}/10$, $c_2 = 1/2$, $c_3 = 1/2 + \sqrt{15}/10$.

Now, a simple relationship can be established between the coefficients $\mathrm{a}_i^{[j]}, \mathrm{b}_i^{[j]}$ for a given method and the coefficients $a_i^{(n)}, b_i^{(n)}$ by taking into account how the matrices $A^{(i)}$, $B^{(i)}$ and α_i, β_i are related. Specifically, by substituting (47) into (59) one has (neglecting higher order terms)

$$A^{(i)} = \int_{-1/2}^{1/2} \sum_{j=1}^{s} h^j \alpha_j \tau^{i+j-1} d\tau = \sum_{j=1}^{s} \left(T^{(s)}\right)_{ij} h^j \alpha_j \ \equiv\ \sum_{j=1}^{s} \frac{1-(-1)^{i+j}}{(i+j)2^{i+j}} h^j \alpha_j, \tag{61}$$

$0 \leq i \leq s-1$, and and analogous expression relating $B^{(i)}$ with β_i. If this relation is inverted (to order four, $s = 2$, and six, $s = 3$) we get

$$(r_{ij}^{(2)}) \equiv (T^{(2)})^{-1} = \begin{pmatrix} 1 & 0 \\ 0 & 12 \end{pmatrix}, \qquad (r_{ij}^{(3)}) = \begin{pmatrix} \frac{9}{4} & 0 & -15 \\ 0 & 12 & 0 \\ -15 & 0 & 180 \end{pmatrix} \tag{62}$$

respectively. If we consider (49)

$$\begin{aligned}\tilde{A}_i &= \sum_{n=1}^{s} a_i^{(n)} h^n \alpha_n = \sum_{n=1}^{s} a_i^{(n)} \sum_{j=1}^{s} r_{nj}^{(s)} A^{(j-1)} \\ \tilde{B}_i &= \sum_{n=1}^{s} b_i^{(n)} h^n \alpha_n = \sum_{n=1}^{s} b_i^{(n)} \sum_{j=1}^{s} r_{nj}^{(s)} B^{(j-1)},\end{aligned} \tag{63}$$

and compare with (58) then

$$\mathrm{a}_i^{[j]} = \sum_{n=1}^{s} a_i^{(n)} r_{n,j+1}^{(s)}, \qquad \mathrm{b}_i^{[j]} = \sum_{n=1}^{s} b_i^{(n)} r_{n,j+1}^{(s)}. \tag{64}$$

From this analysis, we proceed as follows. We first compute the coefficients a_i, b_i by applying the procedure shown before for the autonomous case. Then, we take $a_i^{(1)} = a_i$, $b_i^{(1)} = b_i$ and then we get the coefficients $a_i^{(k)}, b_i^{(k)},\ k > 1$.

In this work we have considered symmetric methods of order six. For the autonomous case the schemes have necessarily $m \geq 5$ stages. In consequence, we have analyzed compositions with $m = 5, 7, 9, 11$ which corresponds to take $n = 3$ and $l = 0, 1, 2, 3$ in section 3.1.. In each case we have taken the optimal choices according to the criterion considered before.

Table 1. Coefficients $a_i^{(j)}$, $b_i^{(j)}$ for the 11-stage sixth-order method with $n = 3, l = 3$. The scheme is written as an ABA time-reversible composition. The corresponding coefficients $\mathrm{a}_i^{[j]}, \mathrm{b}_i^{[j]}$ can be obtained from (64) for $s = 3$, and then using the coefficients from $r_{i,j}^{(3)}$ given in (62).

$\mathrm{S}_{11}6$	
$a_1^{(1)} = 0.046487454790863130865306186 9817$	$b_1^{(1)} = 0.184330483502665563472197717881$
$a_2^{(1)} = -0.060691671165642935309132549 4096$	$b_2^{(1)} = -0.041056903297711462374776749 0040$
$a_3^{(1)} = 0.218466526463406810473052519699$	$b_3^{(1)} = 0.133755679666750330706128392342$
$a_4^{(1)} = 0.168053579483092703041517425135$	$b_4^{(1)} = 0.203764547132354738209957028584$
$a_5^{(1)} = 0.314392364170353486741817155744$	$b_5^{(1)} = -0.011760166914960043722445217 9216$
$a_6^{(1)} = \frac{1}{2} - (a_1^{(1)} + \cdots + a_5^{(1)})$	$b_6^{(1)} = 1 - 2(b_1^{(1)} + \cdots + b_5^{(1)})$
$a_{13-i}^{(1)} = a_i^{(1)}, \quad i = 1, \ldots, 6$	$b_{12-i}^{(1)} = b_i^{(1)}, \quad i = 1, \ldots, 5$
$a_1^{(2)} = 0.021932662014222435543552799908$	$a_1^{(3)} = 0.010774353196216145701968912508$
$b_1^{(2)} = 0.076265342985813349737917161509$	$b_1^{(3)} = 0.030142125018327940937414989541$
$a_2^{(2)} = -0.020398565920802831959213582992$	$a_2^{(3)} = -0.005427130288899774421764282115$
$b_2^{(2)} = -0.012596890479914684316312760274$	$b_2^{(3)} = -0.004372117757445952771769239956$
$a_3^{(2)} = 0.082852466619572947024295608947$	$a_3^{(3)} = 0.029554036305343044582330966298$
$b_3^{(2)} = 0.027320232738183409571021354736$	$b_3^{(3)} = 0.013314214993014633059427728923$
$a_4^{(2)} = 0.033874531967335174405681619187$	$a_4^{(3)} = 0.006765407454007250804131069975$
$b_4^{(2)} = 0.057518598444719069538561641736$	$b_4^{(3)} = 0.002582444412770045441593188157$
$a_5^{(2)} = -0.002750880801534023845247809420$	$a_5^{(3)} = 0$
$b_5^{(2)} = 1/100$	$b_5^{(3)} = 0$
$a_6^{(2)} = 0.002702345260889928730160405903$	$a_6^{(3)} = 0$
$b_6^{(2)} = 0$	$b_6^{(3)} = 0$
$a_{6+i}^{(2)} = -a_{7-i}^{(2)}$	$a_{6+i}^{(3)} = a_{7-i}^{(3)}$
$b_{6+i}^{(2)} = -b_{6-i}^{(2)}$	$b_{6+i}^{(3)} = b_{6-i}^{(3)}, \quad i = 1, \ldots, 6$

On the other hand, getting sixth-order methods for the non-autonomous case requires to solve a system of 10 nonlinear equations in the variables $a_i^{(2)}, b_i^{(2)}$ and an additional linear system of 8 equations to be

solved in $a_i^{(3)}, b_i^{(3)}$, with the symmetry (53). To obtain real solutions for these equations it was necessary to consider methods with at least 11 stages. Among all solutions obtained, we selected the set of coefficients which minimized the sum of the absolute values of the coefficients.

In Table 1 we collect the coefficients for the method which shows in practice the best performance. The corresponding coefficients $\mathrm{a}_i^{[j]}, \mathrm{b}_i^{[j]}$ can be obtained from (64) for $s = 3$, and then using the coefficients from $(r_{i,j}^{(3)})$ given in (62).

4. Numerical examples

Our purpose in this section is to illustrate the performance of the new specially adapted 11-stage sixth-order ($SM_{11}6$) splitting methods for partitioned non-autonomous linear systems. To do so, we carry out some comparison with some other well established general purpose geometric schemes. Given a basic symmetric second order method, these schemes are built by a symmetric composition of this basic method with fractional steps. The algorithms considered are the following: the 9-stage sixth-order ($S_9 6$), the 17-stage eighth-order ($S_{17}8$), and the 35-stage tenth-order ($S_{35}10$) methods whose coefficients are collected, for instance, in [11, chapter V]. As basic second order scheme we take the well known leapfrog composition: $\psi^{[2]}{}_h \equiv \varphi_{h/2}^{[B]} \circ \varphi_h^{[A]} \circ \varphi_{h/2}^{[B]}$. The explicit time dependence is treated by taking the time as two new coordinates as shown in (25).

Since the main interest of this family of methods lies in the numerical integration of differential equations originated from space discretizations of PDEs, the computational cost of the methods is measured by the number of stages required. The integrals (31) appearing in the new scheme are approximated by the sixth-order Gauss-Legendre quadrature rule, as indicated in (58) and (60). Notice that using this quadrature rule only three evaluations for the time dependent functions are required per step, whereas 11 is the number used to count the cost of the algorithm.

Perturbed Harmonic Oscillators. We first consider as a simple test bench problem the Mathieu equation,

$$q'' + (\omega^2 + \epsilon \cos(t))q = 0,$$

with $q \in \mathbb{R}$, which corresponds to a time dependent linear harmonic oscillator with Hamiltonian

$$H = \frac{1}{2}p^2 + \frac{1}{2}(\omega^2 + \epsilon \cos(t))q^2.$$

We take as initial condition $q(0) = 1, p(0) = 1$, integrate up to $t = 200\,\pi/\omega$ and measure the average error in phase space (at $t = 2\pi/\omega, 4\pi/\omega, \ldots, 200\pi/\omega$) in terms of the number of force evaluations for different time steps (in logarithmic scale). We compare the relative error for $\omega = 3/2$ and $\omega = 5$, and in each case for $\epsilon = 1/40$ and $\epsilon = 1/4$. The superiority of the new scheme is manifest for all accuracies of practical interest. We can also observe that this superiority is more relevant when the dominant contribution from the Hamiltonian originates from the constant part, since the new scheme is built to be highly efficient for small perturbations of the autonomous harmonic oscillator.

The Schrödinger equation. Let us now consider the one-dimensional Schrödinger equation (in units where $\hbar = 1$)

$$i\frac{\partial}{\partial t}\psi(x,t) = \left(-\frac{1}{2\mu}\frac{\partial^2}{\partial x^2} + V(x) + f(t)x\right)\psi(x,t), \tag{65}$$

with $\psi(x,0) = \psi_0(x)$. We take the Morse potential $V(x) = D\left(1 - \mathrm{e}^{-\alpha x}\right)^2$ in a laser field described by $f(t)x = A\cos(\omega t)x$. It corresponds to the Walker–Preston model of a diatomic molecule in a strong laser field [20]. This problem is used as a test bench for the numerical methods presented in [10] and [19] and the same values for the parameters are taken (in atomic units): $\mu = 1745\ a.u.$, $D = 0.2251\ a.u.$ and $\alpha =$

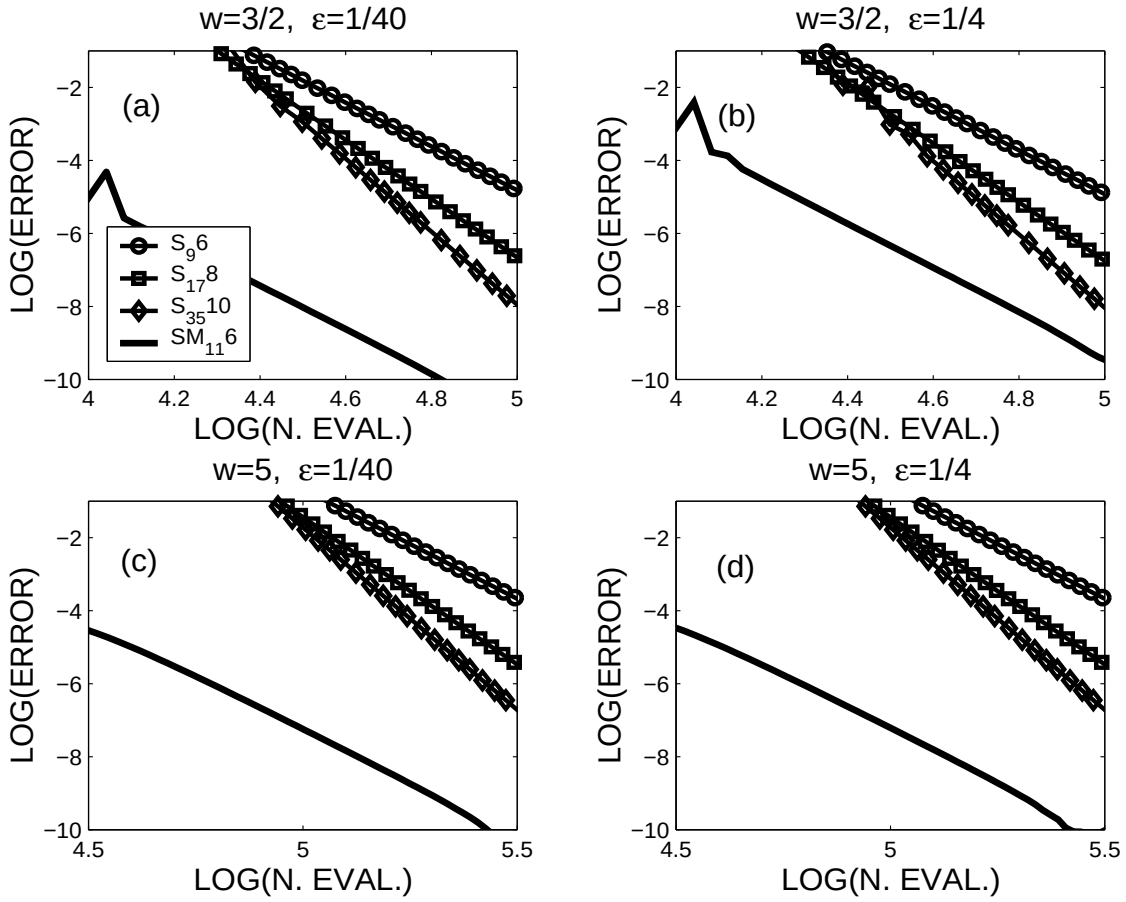

Figure 1. Average error in phase space (at $t = 2\pi/\omega, 4\pi/\omega, \ldots, 100\pi/\omega$) vs. the number of force evaluations for different time steps (in logarithmic scale) for the Mathieu equation for different values of ω and ϵ.

$1.1741\ a.u.$ (corresponding to the HF molecule), $A = 0.011025\ a.u.$ and laser frequency $w = 0.01787$. We assume that the system is defined in the interval $x \in [-0.8, 4.32]$, which is split into $N = 64$ parts of length $\Delta x = 0.08$, and impose periodic boundary conditions.

After space discretization, eq. (65) leads to the complex linear equation (12) with $u \in \mathbb{C}^N$ and $u_k(t) = \psi(x_k, t)(\Delta x)^{1/2},\ k = 0, 1, \ldots, N-1$. Here $x_k = x_0 + k\Delta x$ and $H(t) = T + \hat{V}(t)$ is an Hermitian matrix (real and symmetric). As initial conditions we take the ground state of the Morse potential,

$$\phi(x) = \sigma \exp\big(-(\gamma - 1/2)\alpha\, x\big) \exp\big(-\gamma \mathrm{e}^{-\alpha x}\big),$$

with $\gamma = 2D/w_0$, $w_0 = \alpha\sqrt{2D/\mu}$ and σ is a normalizing constant.

Notice that $\hat{V}(t)$ is a diagonal matrix with elements $\hat{V}_{jj} = V(x_j) + f(t)x_j$, and Tq, Tp can be efficiently computed using FFTs [1, 9]. Notice also that in (33) we now have

$$H_i^A = h \int_{-1/2}^{1/2} p_i^a(\tau) H(t_{1/2} + h\tau)\, d\tau = h a_i^{(1)} T + h a_i^{(1)} V + hXF_a(t, h) \tag{66}$$

and

$$H_i^B = h\int_{-1/2}^{1/2} p_i^b(\tau) H(t_{1/2}+h\tau)\, d\tau = hb_i^{(1)} T + hb_i^{(1)} V + hXF_b(t,h), \tag{67}$$

where $F_{a/b}(t,h) = h\int_{-1/2}^{1/2} p_i^{a/b}(\tau)\, f(t_{1/2}+h\tau)\, d\tau$. Here X is a diagonal matrix with diagonal elements $X_{jj} = x_j$. The products $H_i q$ and $H_i p$ only require one FFT and its inverse and thus an m-stage method requires $4m$ FFTs per step. The split (25) used for the general purpose methods $S_m p$ was already proposed in [19], showing a clear improvement with respect to the second order Magnus integrator (combined with a third order splitting scheme) given in [10].

First, we integrate the system in the time interval $t \in [0, 2\tau]$ with $\tau = 2\pi/\omega$. The exact solution, $u_{ex}(2\tau)$, at the final time is obtained numerically using a sufficiently small time step. We measure the error in the wave function, $\|u_{ex}(2\tau) - u(2\tau)\|$ versus the number of FFTs required for each method, and this is repeated for different values of the time step, starting with a very small time step and increasing it until reaching a time step close to the stability limit of the method (an overflow appears if the time step is slightly increased). We repeated the same experiment taking a larger time integration, $t \in [0, 200\tau]$.

Figure 2 shows the efficiency plots for the methods. The superiority of the new splitting method is manifest both with respect to efficiency and the stability limit. In addition, we observe that this superiority increases when taking a longer time integration. This constitutes indeed an interesting property of the new methods which is currently under investigation [5].

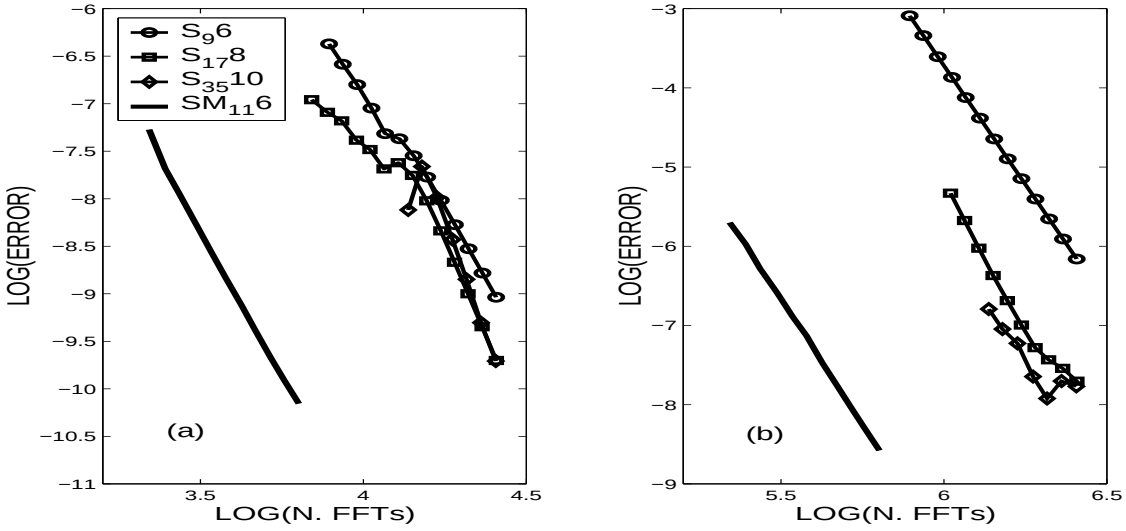

Figure 2. Error in the wave function versus the number of FFTs for the one-dimensional Schrödinger equation (65) written in the form (13) after space discretization: (a) for the time integration $t \in [0, 2\tau]$, and (b) for $t \in [0, 200\tau]$ with $\tau = 2\pi/\omega$.

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Sergio Blanes: Instituto de Matemática Multidisciplinar, Universidad Politécnica de Valencia, E-46022 Valencia, Spain. Email: `serblaza@imm.upv.es`
Fernando Casas: Departament de Matemàtiques and Institut de Matemàtiques i Aplicacions de Castelló, Universitat Jaume I, E-12071 Castellón, Spain. Email: `Fernando.Casas@uji.es`
Ander Murua: Konputazio Zientziak eta A.A. saila, Informatika Fakultatea, EHU/UPV, Donostia/San Sebastián, Spain. Email: `Ander.Murua@ehu.es`