



Splitting and composition methods for explicit time dependence in separable dynamical systems[☆]

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ABSTRACT

We consider splitting methods for the numerical integration of separable non-autonomous differential equations. In recent years, splitting methods have been extensively used as geometric numerical integrators showing excellent performances (both qualitatively and quantitatively) when applied on many problems. They are designed for autonomous separable systems, and a substantial number of methods tailored for different structures of the equations have recently appeared. Splitting methods have also been used for separable non-autonomous problems either by solving each non-autonomous part separately or after each vector field is frozen properly. We show that both procedures correspond to introducing the time as one or more further coordinates. We generalize these results by considering the time as one or more further coordinates which can be integrated following either of the previous two techniques. We show that the performance as well as the order of the final method can strongly depend on the particular choice. We present a simple analysis which, in many relevant cases, allows one to choose the most appropriate split to retain the high performance the methods show on the autonomous problems. This technique is applied to different problems and its performance is illustrated for several numerical examples.

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1. Introduction

In recent years, great interest has been devoted to searching and analysing efficient numerical methods for dynamical systems, which are able to preserve qualitative features of the exact solution (see [1–3] and references therein). In particular, growing attention is being paid to splitting procedures aimed at numerically solving ordinary differential equations (ODEs) as well as evolutionary partial differential equations (PDEs) whose vector field is separable in a number of exactly solvable parts. Thus, the solution flow is approximated by a composition of flows related to each part which are exactly solved. Splitting methods have been developed in order to approximate the solution of autonomous separable problems

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

where the forcing term $f : \mathbb{R}^d \rightarrow \mathbb{R}^d$ is split into solvable parts. For simplicity in the presentation, we consider the system is separable into only two parts, $f(x) = f^{[A]}(x) + f^{[B]}(x)$. In this respect, great effort has been made in searching for the independent order conditions and the algebraic structure of the problem [4,5] as well as in building new numerical methods,

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featured by different accuracy orders and accounting for different structures of the vector field [6–15] (see, for instance, the reviews [16,12,17]). Let us assume that both the systems

$$x' = f^{[A]}(x), \quad x' = f^{[B]}(x) \tag{2}$$

can be either solved in closed form or accurately integrated. We denote by φ_t the exact global flow of (1), i.e. $x(t) = \varphi_t(x_0)$, or equivalently, $\varphi_t = \exp((t - t_0) (D_A + D_B))$, where D_A and D_B are the Lie derivatives related to the vector fields $f^{[A]}(x)$ and $f^{[B]}(x)$, respectively, i.e. $D_A \equiv f^{[A]}(x) \cdot \nabla$ and $D_B \equiv f^{[B]}(x) \cdot \nabla$. If $\varphi_t^{[A]}, \varphi_t^{[B]}$ represent the exact flows associated to (2), then it is well known that different splitting methods in the form

$$\psi_h = \varphi_{a_{m+1}h}^{[A]} \circ \varphi_{b_{m+1}h}^{[B]} \circ \varphi_{a_mh}^{[A]} \circ \varphi_{b_mh}^{[B]} \circ \varphi_{a_{m-1}h}^{[A]} \circ \dots \circ \varphi_{b_2h}^{[B]} \circ \varphi_{a_1h}^{[A]} \circ \varphi_{b_1h}^{[B]} \tag{3}$$

are constructed by choosing coefficients $a_i, b_i \in \mathbb{R}$ to ensure that the numerical integrator ψ_h is an approximation up to order $\mathcal{O}(h^p)$ with respect to the time step h , i.e. $\psi_h = \varphi_h + \mathcal{O}(h^{p+1})$. Closely connected to the splitting technique are the composition methods. It can be proved (see [12,1]) that any splitting scheme can be interpreted as a composition procedure. In this respect, there exists a strong relationship between the order conditions for both approaches, whenever splitting is considered as a special case of composition. Splitting and composition methods have been adapted to integrate different classes of problem such as general separable autonomous systems, first-order systems arising from second-order problems, $x'' = g(x)$, the so-called near-integrable systems, etc. Indeed, the performance of the different composition methods strongly depends on the particular problem to be solved and, as a consequence, a previous analysis is needed in order to choose an appropriate procedure for approximating the solution [16]. This is the case of the non-autonomous separable problem

$$x' = f^{[A]}(x, t) + f^{[B]}(x, t). \tag{4}$$

It is well known that the formal solution is given neither by

$$\varphi_t = \exp\left((t - t_0) (D_A(t) + D_B(t))\right)$$

nor by

$$\varphi_t = \exp\left(\int_{t_0}^t (D_A(\tau) + D_B(\tau))d\tau\right).$$

Then, to use the splitting method (3) requires some appropriate considerations. There are two simple procedures to circumvent this drawback. One of them corresponds to replacing the maps $\varphi_{a_ih}^{[A]}, \varphi_{b_ih}^{[B]}$ by the maps associated to the exact flow of the equations

$$x' = f^{[A]}(x, t), \quad t \in [t_0 + c_ih, t_0 + (c_i + a_i)h], \tag{5}$$

$$x' = f^{[B]}(x, t), \quad t \in [t_0 + d_ih, t_0 + (d_i + b_i)h], \tag{6}$$

where $c_i = \sum_{j=0}^{i-1} a_j, d_i = \sum_{j=0}^{i-1} b_j, a_0 = 0, b_0 = 0$, and the initial conditions are given by the solution obtained from the previous stage. This procedure can be considered as a time-average on each stage of the composition. Obviously, the exact solution of the non-autonomous Eqs. (5) and (6) are not always trivial due to the explicit time dependence. The formal solution for these two equations can be obtained, for instance, using the Magnus series expansion for nonlinear differential equations [18].

There is a simpler alternative, which we refer to as the “frozen” technique, where the maps $\varphi_{a_ih}^{[A]}, \varphi_{b_ih}^{[B]}$ correspond to the (a_ih) -flow and (b_ih) -flow associated to the autonomous vector fields

$$x' = f^{[A]}(x, t_0 + d_ih), \quad t \in [t_0 + c_ih, t_0 + (c_i + a_i)h] \tag{7}$$

$$x' = f^{[B]}(x, t_0 + c_ih), \quad t \in [t_0 + d_ih, t_0 + (d_i + b_i)h] \tag{8}$$

(notice that the coefficients c_i, d_i appear interchanged in the vector fields with respect to (5) and (6)).

Given a method characterized by the coefficients $\{a_i, b_i\}$, the averaging and frozen techniques can differ considerably both in the accuracy reached by the methods, as well as their computational cost. We illustrate this fact in a simple example.

Example 1. Let us consider the perturbed system

$$x' = f^{[A]}(x) + \varepsilon \sum_{i=1}^k f^{[B,i]}(x), \tag{9}$$

with $|\varepsilon| \ll 1$. The composition

$$\psi_h = \varphi_{h/2}^{[B,1]} \circ \dots \circ \varphi_{h/2}^{[B,k]} \circ \varphi_h^{[A]} \circ \varphi_{h/2}^{[B,k]} \circ \dots \circ \varphi_{h/2}^{[B,1]} \tag{10}$$

corresponds to a symmetric second-order method which exploits the fact of being a perturbed system, and the local error is of order $\mathcal{O}(\epsilon h^3)$. For the non-autonomous problem

$$x' = f^{[A]}(x, t) + \epsilon \sum_{i=1}^k f^{[B,i]}(x, t), \quad (11)$$

there are many different ways to freeze and average the vector fields, and then to use the second-order symmetric composition (10). We advance to the reader that all these combinations except one show a local error $\mathcal{O}(h^3)$. To keep the local error $\mathcal{O}(\epsilon h^3)$ obtained for the autonomous case, we will show that one has to take the average of the vector field $f^{[A]}(x, t)$ and to keep all remaining ones frozen. \square

There are also some problems where the time dependence can appear in different parts of the vector fields and/or on different time scales, e.g.

$$x' = f^{[A]}(x, \epsilon_1 t, \dots, \epsilon_k t) + f^{[B]}(x, \epsilon_1 t, \dots, \epsilon_m t), \quad (12)$$

and each time dependence can be treated separately using either the averaging or the frozen technique. Let us illustrate this case also in a simple example.

Example 2. Let us now consider the system

$$x' = \cos(t/\epsilon) f^{[A]}(x, t) + f^{[B]}(x, t), \quad (13)$$

with $|\epsilon| \ll 1$, corresponding to a highly oscillatory system. Standard splitting methods which freeze both parts present a local error depending on the time derivative of the highly oscillatory function, $\cos(t/\epsilon)$. To reduce this error contribution, we can integrate exactly the autonomous equation $x' = \cos(t/\epsilon) f^{[A]}(x, t)$, but this can be quite involved in practice. We will show that similar performance can be obtained with a proper combination of the average considered in (5)–(6) and the frozen technique (7)–(8), i.e.

$$x' = \cos(t/\epsilon) f^{[A]}(x, t_0 + d_i h), \quad t \in [t_0 + c_i h, t_0 + (c_i + a_i) h] \quad (14)$$

$$x' = f^{[B]}(x, t_0 + c_i h), \quad t \in [t_0 + d_i h, t_0 + (d_i + b_i) h], \quad (15)$$

where the first equation requires the integral (or average) of the oscillatory function, and the remaining time-dependent functions on the vector fields are kept frozen. \square

This provides a great flexibility to adapt the splitting methods to separable non-autonomous problems in an efficient way.

The frozen and averaging techniques transform the original non-autonomous problem into an autonomous problem, but in an extended phase space. Then, to apply splitting methods which have been tailored for problems with particular structures in a naive way can lead to numerical solutions with unexpected degradation in their performance and even in accuracy order (with respect to the same methods applied to the corresponding autonomous problem) as is proved in [19]. This is explored in the present work in order to understand the origin of this problem and then to look for the more appropriate combination of averaging and/or frozen techniques to reach the highest performance.

In this paper we analyse different ways to introduce these procedures which allow one, in many cases, to use in a straightforward way splitting schemes for non-autonomous separable systems while preserving the good behaviour the schemes show for similar autonomous problems.

The analysis for separable Hamiltonian systems is similar, due to the relationship between Lie brackets of vector fields and the Poisson brackets of functions associated to vector fields [20]. The time can be considered as a new set of coordinates, and we have to introduce the associated momenta properly. We found the Hamiltonian formalism easier to understand, and for this reason, when required, we will illustrate the results using this formalism, but we must keep in mind that the results presented in this work are valid for general separable differential equations.

2. Different splitting techniques

Given the general equation

$$x' = f(x, t), \quad x(t_0) = x_0 \in \mathbb{R}^d, \quad (16)$$

a usual procedure which enormously simplifies the numerical analysis on the order conditions is to transform (16) into an autonomous form by appending t to the dependent variables

$$\begin{cases} x' = f(x, t) \\ t' = 1. \end{cases} \quad (17)$$

The averaging and frozen techniques previously mentioned correspond to generalizations to this procedure by taking the time as two different coordinates, as follows. The averaging technique corresponds to the following split of the vector field

in the enlarged system:

$$\frac{d}{dt} \begin{pmatrix} x \\ t_A \\ t_B \end{pmatrix} = \begin{pmatrix} f^{[A]}(x, t_B) \\ 0 \\ 1 \end{pmatrix} + \begin{pmatrix} f^{[B]}(x, t_A) \\ 1 \\ 0 \end{pmatrix}. \tag{18}$$

This system is now autonomous in the enlarged system, and separable into solvable parts (if we assume that both the equations $x' = f^{[A]}(x, t)$ and $x' = f^{[B]}(x, t)$ are solvable).

The frozen technique corresponds, however, to the split

$$\frac{d}{dt} \begin{pmatrix} x \\ t_A \\ t_B \end{pmatrix} = \begin{pmatrix} f^{[A]}(x, t_B) \\ 1 \\ 0 \end{pmatrix} + \begin{pmatrix} f^{[B]}(x, t_A) \\ 0 \\ 1 \end{pmatrix}, \tag{19}$$

which is also autonomous and separable in solvable parts (if we assume that both the equations $x' = f^{[A]}(x, t)$ and $x' = f^{[B]}(x, t)$ are solvable when the time is frozen).

These splittings easily generalize to the case where the vector fields present several time-dependent sources or time scales, $f^{[A]}(x, \epsilon_1 t, \dots, \epsilon_k t)$, $f^{[B]}(x, \epsilon_1 t, \dots, \epsilon_m t)$, simply by introducing new coordinates for the times, $\epsilon_1 t, \dots, \epsilon_k t, \epsilon_1 t, \dots, \epsilon_m t$, which are then treated as in any of the previous ways.

For simplicity, and without loss of generality, we consider the vector fields containing only two different time-dependent contributions and $k = m = 2$ (i.e. $f^{[A]}(x, \epsilon_1 t, \epsilon_2 t)$, $f^{[B]}(x, \epsilon_1 t, \epsilon_2 t)$). For clarity in the presentation and to avoid confusion, we assume that one of the time dependences in each vector field can be factorized as follows:

$$f^{[A]}(x, t) = A(t)g^{[A]}(x, t), \quad f^{[B]}(x, t) = B(t)g^{[B]}(x, t) \tag{20}$$

with $A(t) \in \mathbb{R}^{d \times n_1}$, $B(t) \in \mathbb{R}^{d \times n_2}$ and $g^{[A]} : \mathbb{R}^d \times \mathbb{R} \rightarrow \mathbb{R}^{n_1}$, $g^{[B]} : \mathbb{R}^d \times \mathbb{R} \rightarrow \mathbb{R}^{n_2}$. Moreover, we suppose that the matrix functions $A(t)$ and $B(t)$ are exactly integrable or, at least, the integrals can be approximated with low computational cost. We present the cases where the time-dependent functions in $g^{[A]}(x, t)$, $g^{[B]}(x, t)$ are always frozen, and only the most easy to deal with, $A(t)$, $B(t)$, can be either frozen or exactly solved in the associated non-autonomous equations.

As a first step, we account for the most frequent approach which arises from formulation (19) by considering the forcing term split into the sum of

$$F^{(A_1)}(y) = \begin{pmatrix} A(t_B)g^{[A]}(x, t_B) \\ 1 \\ 0 \end{pmatrix}, \quad F^{(B_1)}(y) = \begin{pmatrix} B(t_A)g^{[B]}(x, t_A) \\ 0 \\ 1 \end{pmatrix} \tag{21}$$

in order to study the equivalent autonomous problem $y' = F^{(A_1)}(y) + F^{(B_1)}(y)$ with $y = (x, t_A, t_B)^T$, where $y' = F^{(A_1)}(y)$ and $y' = F^{(B_1)}(y)$ can be solved exactly by means of their related flows $\varphi_t^{[A_1]}$, $\varphi_t^{[B_1]}$. The solution approximation, given by the composition method

$$\psi_h^{(1)} = \varphi_{a_{m+1}h}^{[A_1]} \circ \varphi_{b_{m+1}h}^{[B_1]} \circ \varphi_{a_mh}^{[A_1]} \circ \varphi_{b_mh}^{[B_1]} \circ \varphi_{a_{m-1}h}^{[A_1]} \circ \dots \circ \varphi_{b_2h}^{[B_1]} \circ \varphi_{a_1h}^{[A_1]} \circ \varphi_{b_1h}^{[B_1]},$$

is obtained by advancing in time with step sizes $a_i h, b_i h$ ($i = 1, 2, \dots, m + 1$) and maintaining the time variable frozen in both the forcing terms.

As an alternative to this numerical scheme, we provide different approaches in the framework of splitting procedures. In particular, we notice that in the case when either $A(t)$ or $B(t)$ can be exactly integrated, other schemes can be formulated, as follows.

First, under the assumption that $B(t)$ is exactly integrable, we consider the forcing split

$$F^{(A_2)}(y) = \begin{pmatrix} A(t_B)g^{[A]}(x, t_B) \\ 1 \\ 0 \end{pmatrix}, \quad F^{(B_2)}(y) = \begin{pmatrix} B(t_B)g^{[B]}(x, t_A) \\ 0 \\ 1 \end{pmatrix}, \tag{22}$$

which corresponds to a combination of both (18) and (19), and provides the equivalent system $y' = F^{(A_2)}(y) + F^{(B_2)}(y)$. In this way, the alternative numerical scheme may be developed as

$$\psi_h^{(2)} = \varphi_{a_{m+1}h}^{[A_2]} \circ \varphi_{b_{m+1}h}^{[B_2]} \circ \varphi_{a_mh}^{[A_2]} \circ \varphi_{b_mh}^{[B_2]} \circ \varphi_{a_{m-1}h}^{[A_2]} \circ \dots \circ \varphi_{b_2h}^{[B_2]} \circ \varphi_{a_1h}^{[A_2]} \circ \varphi_{b_1h}^{[B_2]},$$

where flows $\varphi_t^{[A_2]}$ and $\varphi_t^{[B_2]}$ are composed at suitable step lengths. It is worthwhile noticing that, at each step, term $B(t)$ evolves during the first integration related to $\varphi_{b_ih}^{[B_2]}$, i.e. $\varphi_{b_ih}^{[B_2]}$ corresponds to the $(b_i h)$ -flow of $y' = F^{(B_i)}(y)$ or, equivalently, to the exact solution of

$$x' = B(t)g^{[B]}(x, t_A)$$

for a time step $b_i h$ and where t_A is frozen. As mentioned, the formal solution for this problem can be obtained by using the Magnus series expansion for nonlinear differential equations [18], and in the following sections we present some cases

where this problem is exactly solvable or easy to approximate numerically. For the computation of the flow $\varphi_{a_i h}^{[A_2]}$, the time variable t_B is kept frozen in the forcing term $F^{(A_2)}(y)$. This argument can be inverted in the approximation process: indeed, supposing the exact integral is available for $A(t)$, we set

$$F^{(A_3)}(y) = \begin{pmatrix} A(t_A)g^{[A]}(x, t_B) \\ 1 \\ 0 \end{pmatrix}, \quad F^{(B_3)}(y) = \begin{pmatrix} B(t_A)g^{[B]}(x, t_A) \\ 0 \\ 1 \end{pmatrix} \tag{23}$$

and we discretize the differential equation $y' = F^{(A_3)}(y) + F^{(B_3)}(y)$. In this different approach, the numerical algorithm consists of keeping the time variable completely frozen in the integration at the first step and accounting for time evolution in the successive integration. The resulting scheme is obtained by the composition

$$\psi_h^{(3)} = \varphi_{a_{m+1}h}^{[A_3]} \circ \varphi_{b_{m+1}h}^{[B_3]} \circ \varphi_{a_m h}^{[A_3]} \circ \varphi_{b_m h}^{[B_3]} \circ \varphi_{a_{m-1}h}^{[A_3]} \circ \dots \circ \varphi_{b_2 h}^{[B_3]} \circ \varphi_{a_1 h}^{[A_3]} \circ \varphi_{b_1 h}^{[B_3]}, \tag{24}$$

where exact flows $\varphi_t^{[A_3]}, \varphi_t^{[B_3]}$ are involved.

In addition, we assume that both $A(t)$ and $B(t)$ are exactly integrable, and consider the system $y' = F^{(A_4)}(y) + F^{(B_4)}(y)$, where

$$F^{(A_4)}(y) = \begin{pmatrix} A(t_A)g^{[A]}(x, t_B) \\ 1 \\ 0 \end{pmatrix}, \quad F^{(B_4)}(y) = \begin{pmatrix} B(t_B)g^{[B]}(x, t_A) \\ 0 \\ 1 \end{pmatrix}. \tag{25}$$

This formulation leads to the alternative numerical scheme

$$\psi_h^{(4)} = \varphi_{a_{m+1}h}^{[A_4]} \circ \varphi_{b_{m+1}h}^{[B_4]} \circ \varphi_{a_m h}^{[A_4]} \circ \varphi_{b_m h}^{[B_4]} \circ \varphi_{a_{m-1}h}^{[A_4]} \circ \dots \circ \varphi_{b_2 h}^{[B_4]} \circ \varphi_{a_1 h}^{[A_4]} \circ \varphi_{b_1 h}^{[B_4]}.$$

In this procedure, the vector field related to $F^{(B_4)}(y)$ is first integrated by accounting for an explicit time dependence in term $B(t)$, then the second integration related to $F^{(A_4)}(y)$ is performed by letting $A(t)$ evolve in time; therefore, a full integration is performed with respect to the time variable.

Notice that all the schemes we have just considered reduce to the classical one $\psi_h^{(1)}$ when the matrices A and B are constants. On the other hand, the performance of a splitting method depends on the choice of the set of coefficients, a_i, b_i , and the most appropriate one depends on the Lie algebra generated by the Lie operators, $\mathcal{L}_i = \{D_{A_i}, D_{B_i}\}, i = 1, \dots, 4$. Unfortunately, in most cases, the Lie algebra generated by \mathcal{L}_i does not have the simplified structure which characterizes the autonomous problem, with the Lie algebra generated by $\{D_A, D_B\}$. For example, there are separable problems where the vector fields satisfy the simplifying relation, $[D_B, [D_B, [D_B, D_A]]] = 0$. This is the case of second-order problems, $x'' = g(x)$, when written as a first-order ODE system, and such a system can be efficiently solved numerically by Nyström methods. Many other separable problems share the same algebraic structure (e.g. in classical and quantum mechanics) and, for brevity, in this work we will refer to them as Nyström problems. On the other hand, for near-integrable systems we have $\|D_B\| \ll \|D_A\|$. We analyse these algebraic structures and look for those cases where the algebraic structure is recovered by the non-autonomous problem.

2.1. Near-separable systems

As an example of integration, we consider the following time-dependent system:

$$q' = M_1(t)g_2(p, t), \quad p' = M_2(t)g_1(q, t),$$

$q \in \mathbb{R}^s, p \in \mathbb{R}^{d-s}$, which is separable with respect to q and p variables but joint by the time variable. Notice that, in contrast with the general case (20), both equations are solvable, i.e.

$$\begin{cases} q' = M_1(t)g_2(p, t) \\ p' = 0 \end{cases} \Rightarrow \begin{cases} q(t) = q_0 + \int_{t_0}^t M_1(\tau)g_2(p_0, \tau)d\tau \\ p(t) = p_0 \end{cases},$$

and similarly for the other equation. In our presentation we have considered the case where the time in $g_2(p, t), g_1(q, t)$ is kept frozen.

The solution approximation provided by the classical composition method $\psi_h^{(1)}$ allows one to recover the whole separability of the system since it maintains the time variable frozen in both the forcing terms. The resulting algorithm is given by

$$\begin{aligned} P_0 &= p_n, & Q_0 &= q_n, & T_0^A &= t_n, & T_0^B &= t_n, \\ \text{Do } i &= 1, m + 1 \\ &P_i &= P_{i-1} + h b_i M_2(T_{i-1}^A) g_1(Q_{i-1}, T_{i-1}^A), & T_i^B &= T_{i-1}^B + h b_i, \\ &Q_i &= Q_{i-1} + h a_i M_1(T_i^B) g_2(P_i, T_i^B), & T_i^A &= T_{i-1}^A + h a_i, \\ \text{enddo} \\ P_{n+1} &= P_{m+1}, & Q_{n+1} &= Q_{m+1}, & t_{n+1} &= T_{m+1}^A = T_{m+1}^B = t_n + h. \end{aligned} \tag{26}$$

Under the assumption that $M_2(t)$ is exactly integrable, the alternative numerical scheme, denoted by $\psi_h^{(2)}$, is obtained by replacing P_i in (26) with

$$P_i = P_{i-1} + \int_{T_{i-1}^B}^{T_i^B} M_2(s) ds g_1(Q_{i-1}, T_{i-1}^A). \quad (27)$$

On the other hand, supposing that the exact integral is available for $M_1(t)$, the algorithm $\psi_h^{(3)}$ is obtained by replacing Q_i in (26) with

$$Q_i = Q_{i-1} + \int_{T_{i-1}^A}^{T_i^A} M_1(s) ds g_2(P_i, T_i^B). \quad (28)$$

Finally, if we assume that both $M_1(t)$ and $M_2(t)$ are exactly integrable, it is possible to build the alternative numerical scheme, denoted by $\psi_h^{(4)}$, by replacing both P_i and Q_i in (26) with relationships defined in (27) and (28), respectively.

2.2. Nyström-like problems

In the class of the near-separable problems, let us focus on what we are going to refer as a Nyström-like problem:

$$q' = M(t)p, \quad p' = g_1(q, t). \quad (29)$$

We remark that a Nyström problem is recovered when $M(t) = I$ and g_1 does not explicitly depend on time; therefore, $f^{[A]}(x) = Ag^{[A]}(x) = (p, 0)$ and $f^{[B]}(x) = Bg^{[B]}(x) = (0, g_1(q))$, where we can take for example A, B as identity matrices. In this case, the specific structure of $f^{[A]}$ simplifies the analysis of accuracy for the composition method (3); indeed, as mentioned before, $[D_B, [D_B, [D_B, D_A]]] = 0$. Therefore, for orders $p > 4$, a significant reduction holds both in the error terms and in the number of order conditions satisfied by the coefficients a_i, b_i . In this respect, Runge–Kutta Nyström methods represent highly efficient numerical integrators provided in the literature in order to discretize the problem. The following question remains: is it possible to split system (29) appropriately such that the nested commutators still vanish?

Under the assumption that time is accounted for, the classical splitting $\psi_h^{(1)}$ can be exploited in the solution approximation: it recovers the separability of variables (q, t_A) and (p, t_B) in the system

$$\begin{aligned} q' &= M(t_B)p, & t'_A &= 1, \\ p' &= g_1(q, t_A), & t'_B &= 1. \end{aligned}$$

Unfortunately, by performing the Lie derivatives D_{A_1} and D_{B_1} related to the enlarged vector fields $F^{(A_1)}$ and $F^{(B_1)}$ as in (21), it is possible to prove that $[D_{B_1}, [D_{B_1}, [D_{B_1}, D_{A_1}]]]$ does not nullify any longer. For this reason, it is expected that this approach cannot gain in applying numerical integrators suitably built for Nyström problems. Moreover, we notice that $\psi_h^{(2)}$ is equivalent to $\psi_h^{(1)}$, whereas $\psi_h^{(4)}$ corresponds to $\psi_h^{(3)}$; thus, the unique alternative splitting is given by $\psi_h^{(3)}$, which is related to the integration of system

$$\begin{aligned} q' &= M(t_A)p, & t'_A &= 1, \\ p' &= g_1(q, t_A). \end{aligned}$$

It is possible to verify that $[D_{B_3}, [D_{B_3}, [D_{B_3}, D_{A_3}]]]$ vanishes: this feature suggests that the above system structure is Nyström-like and it makes the described approach able to recover all the advantages of using Runge–Kutta Nyström methods. We are going to point out this issue in the framework of time-dependent Hamiltonian systems, where the use of the Poisson brackets allows us to get the previous results in an easier way.

3. Separable time-dependent Hamiltonian systems

The previous analysis applies to separable Hamiltonian systems with Hamiltonian function $H(q, p, t) = H_1(q, p, t) + \dots + H_k(q, p, t)$, where $q, p \in \mathbb{R}^d$ represent the coordinates and associated conjugate momenta, respectively. For simplicity in the presentation we consider the case of a Hamiltonian separable into kinetic (quadratic in momenta) and potential components, i.e.

$$H(p, q, t) = \frac{1}{2}p^T M(t)p + V(q, t).$$

$M^T = M$, and the evolution depends on both maps $M : \mathbb{R} \rightarrow \mathbb{R}^{d \times d}$ and $V : \mathbb{R}^d \times \mathbb{R} \rightarrow \mathbb{R}$. This class of problem, with a time-dependent kinetic part, can be found, for example, in quantum mechanics [21–23] or in celestial mechanics [24]. According to the canonical equations

$$q'(t) = \frac{\partial H}{\partial p}, \quad p'(t) = -\frac{\partial H}{\partial q},$$

the problem represents a specific case of Nyström-like problem (29). We extend the phase space by introducing the variables λ_A, λ_B , conjugate with respect to t_A, t_B , in the enlarged Hamilton function $\tilde{H} = H^{(A_1)}(p, \lambda_A, t_B) + H^{(B_1)}(q, t_A, \lambda_B)$ which is split by defining

$$H^{(A_1)}(p, \lambda_A, t_B) = \frac{1}{2}p^T M(t_B)p + \lambda_A, \quad H^{(B_1)}(q, t_A, \lambda_B) = V(q, t_A) - \lambda_B \tag{30}$$

(here (q, t_A, λ_B) can be seen as coordinates and (p, λ_A, t_B) their associated momenta). In this way we obtain the canonical equations

$$\begin{aligned} q' &= \frac{\partial H^{(A_1)}}{\partial p}, & t'_A &= \frac{\partial H^{(A_1)}}{\partial \lambda_A} = 1, \\ p' &= -\frac{\partial H^{(B_1)}}{\partial q}, & t'_B &= -\frac{\partial H^{(B_1)}}{\partial \lambda_B} = 1, \end{aligned}$$

which are equivalent to the first splitting procedure (21); we remark that the relationships $\lambda'_B = \frac{\partial H^{(A_1)}}{\partial t_B}$ and $\lambda'_A = -\frac{\partial H^{(B_1)}}{\partial t_A}$ are struck out since they have no relevance to our purposes. We evaluate the Poisson brackets, and thus we obtain

$$\begin{aligned} \{H^{(B_1)}, H^{(A_1)}\} &= V_q^T(q, t_A)M(t_B)p + V_{t_A}(q, t_A) - \frac{1}{2}p^T M'(t_B)p, \\ \{H^{(B_1)}, \{H^{(B_1)}, H^{(A_1)}\}\} &= V_q^T(q, t_A)M(t_B)V_q(q, t_A) - 2V_q^T(q, t_A)M'(t_B)p + \frac{1}{2}p^T M''(t_B)p, \\ \{H^{(B_1)}, \{H^{(B_1)}, \{H^{(B_1)}, H^{(A_1)}\}\}\} &= -3V_q^T(q, t_A)M'(t_B)V_q(q, t_A) + 3V_q^T(q, t_A)M''(t_B)p - \frac{1}{2}p^T M'''(t_B)p, \end{aligned}$$

where $(V_q(q, t_A), V_{t_A}(q, t_A))$ represents the gradient of the function V . Observe that the error depends on the derivatives of $M(t)$. As mentioned, due to the relationship holding between Poisson and Lie brackets, this result can be extended to the corresponding commutator of the Lie derivatives on the vector fields $F^{(A_1)}$ and $F^{(B_1)}$ in order to verify that $[D_{B_1}, [D_{B_1}, [D_{B_1}, D_{A_1}]]]$ does not vanish. Again, we point out that no advantage is expected when Runge–Kutta Nyström integrators are applied to approximate the above problem, unless M is constant ($M' = M'' = M''' = 0$), as previously mentioned.

On the other hand, as an alternative, we are going to focus on the other approach related to formulation (23); then, the treatment of the time variable as a new coordinate leads to the enlarged Hamilton function $\tilde{H} = H^{(A_3)}(p, t_A, \lambda_A) + H^{(B_3)}(q, t_A)$, which we split into the following parts:

$$H^{(A_3)}(p, t_A, \lambda_A) = \frac{1}{2}p^T M(t_A)p + \lambda_A, \quad H^{(B_3)}(q, t_A) = V(q, t_A),$$

whose canonical equations are

$$\begin{aligned} q' &= \frac{\partial H^{(A_3)}}{\partial p}, & t'_A &= \frac{\partial H^{(A_3)}}{\partial \lambda_A} = 1, \\ p' &= -\frac{\partial H^{(B_3)}}{\partial q}, \end{aligned}$$

where $\lambda'_A = -\frac{\partial H^{(A_3)}}{\partial t_A} - \frac{\partial H^{(B_3)}}{\partial t_A}$ is disregarded since it does not take part in our numerical integration. In this case, in the evaluation of the Poisson brackets we have

$$\begin{aligned} \{H^{(B_3)}, H^{(A_3)}\} &= V_q^T(q, t_A)M(t_A)p + V_{t_A}(q, t_A), \\ \{H^{(B_3)}, \{H^{(B_3)}, H^{(A_3)}\}\} &= V_q^T(q, t_A)M(t_A)V_q(q, t_A) \equiv \hat{V}(q, t_A). \end{aligned} \tag{31}$$

Then, since both $H^{(B_3)}$ and $\{H^{(B_3)}, H^{(A_3)}\}$ are functions depending only on the coordinates, (q, t_A) , they commute, i.e.

$$\{H^{(B_3)}, \{H^{(B_3)}, \{H^{(B_3)}, H^{(A_3)}\}\}\} = 0.$$

In addition, the term (31) can be added to the flow associated to $H^{(B_3)}$ allowing one to build splitting methods with a reduced number of flows. In (24), one can replace the flows $\varphi_{b_i/h}^{[B_3]}$ by the more general maps $\varphi_{b_i h, c_i h^3}^{[C_3]}$, which correspond to the h -flow for the autonomous Hamiltonian

$$H^{(C_3)} = b_i H^{(B_3)} + c_i h^2 \{H^{(B_3)}, \{H^{(A_3)}, H^{(B_3)}\}\}. \tag{32}$$

If the computational cost to compute $\nabla \hat{V}(q, t_A)$ is not significant (once $\nabla V(q, t_A)$ has been already computed) the schemes obtained are usually more efficient (see [9,10,14]).

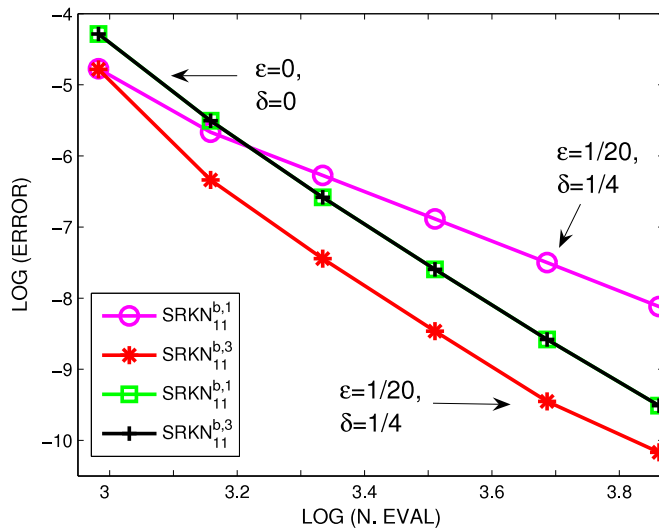


Fig. 1. Efficiency comparison between algorithms $SRKN_{11}^{b,1}$ and $SRKN_{11}^{b,3}$ at different choices for parameters ϵ, δ .

By exploiting the relation between Poisson and Lie brackets, it follows that the third Lie commutator $[D_{B_3}, [D_{B_3}, [D_{B_3}, D_{A_3}]]$, related to vector fields $F^{(A_3)}$ and $F^{(B_3)}$ given in (23), nullifies. Therefore, as we already remarked, in this framework it should be convenient to use numerical methods suitably built for solving Nyström problems. In order to test the effectiveness of the procedures we have provided, we illustrate some numerical examples where the issues discussed so far can be confirmed.

Example 3. Consider the well-known Duffing oscillator (see [25])

$$q' = e^{-\epsilon t} p, \quad p' = -e^{\epsilon t} (q^3 - q - \delta \cos(\omega t)).$$

This scalar problem is related to the time-dependent Hamilton function

$$H = \frac{1}{2} e^{-\epsilon t} p^2 + e^{\epsilon t} \left(\frac{1}{4} q^4 - \frac{1}{2} q^2 - q \delta \cos(\omega t) \right),$$

which can be split according to the different rules we have just discussed.

In our tests, we start from the Runge–Kutta Nyström $SRKN_{11}^b$ scheme provided in [8]: it is a symmetric 11-stage Runge–Kutta method with general fourth order, which gains an accuracy of the sixth order when it is applied to solve Nyström problems. We use its coefficients a_i, b_i in $\psi_h^{(1)}$ and $\psi_h^{(3)}$ in order to build the corresponding numerical schemes $SRKN_{11}^{b,1}$ and $SRKN_{11}^{b,3}$, respectively.

The integration is performed in the interval $[0, 10\pi]$, with initial step $h = \frac{\pi}{8}$, by defining initial conditions $q(0) = 1.75$ and $p(0) = 0$. Moreover, as is usual, the efficiency for every method considered is expressed in terms of the maximal error versus the total number of function evaluations.

In Fig. 1, we compare the performance and the efficiency of both the schemes $SRKN_{11}^{b,1}$ and $SRKN_{11}^{b,3}$ we are interested in. In particular, two different choices for parameters ϵ and δ are considered. First, the time dependence is disregarded and we suppose that $\epsilon = \delta = 0$; therefore, the Nyström structure is recovered on the problem at hand and both the numerical schemes reduce to the classical Runge–Kutta Nyström $SRKN_{11}^b$. In Fig. 1 we observe that algorithms $SRKN_{11}^{b,1}$ and $SRKN_{11}^{b,3}$ behave in the same way as a method with the sixth order of accuracy.

As a second choice, we set $\epsilon = 1/20$ and $\delta = 1/4$ in order to account for time dependence. In [19] the authors already proved that the classical splitting $SRKN_{11}^{b,1}$ loses the extra gain in order, achieved on Nyström structures, and it is featured by fourth-order behaviour. These results are in agreement with the tests shown in Fig. 1. In contrast, we stress that in the same figure it is evident how scheme $SRKN_{11}^{b,3}$ outperforms splitting $SRKN_{11}^{b,1}$ since it is able to preserve the sixth order of accuracy; indeed, this algorithm relies on the use of ad hoc Runge–Kutta coefficients for solving a problem with a suitable structure.

The performance of the new scheme $SRKN_{11}^{b,3}$ is similar to the one obtained in [19] (for this problem and when the CPU time for computing the time dependent functions are not significant). Its main advantage is that it is possible to use the coefficients a_i, b_i from any splitting methods for Nyström problems in a straightforward way and without the need to look for additional order conditions for each splitting method we intend to use.

We have seen that order reduction can happen for Nyström problems because we are applying Nyström methods to problems which have lost this particular structure. We have shown a procedure to recover this structure and then to avoid

this loss of accuracy. This fact can also happen for other families of methods where an order reduction or, at least, a significant loss of accuracy may occur. This is the case of perturbed or near-integrable systems, which are now considered.

4. Perturbed systems

Let us consider a perturbed non-autonomous system

$$x' = f^{[A]}(x, t) + \varepsilon f^{[B]}(x, t). \quad (33)$$

The standard splitting (19) applied to the enlarged system corresponds to

$$\frac{d}{dt} \begin{pmatrix} x \\ t_A \\ t_B \end{pmatrix} = \begin{pmatrix} f^{[A]}(x, t_B) \\ 1 \\ 0 \end{pmatrix} + \begin{pmatrix} \varepsilon f^{[B]}(x, t_A) \\ 0 \\ 1 \end{pmatrix}, \quad (34)$$

which, as previously, is separable, but the parameter ε can not be factorized in the second term. This is also the case for the split (18). Splitting methods tailored for near-integrable problems have shown to be highly efficient for autonomous perturbed problems. However, these methods lose their excellent performances when applied to a general separable system. The near-integrable structure is recovered if we consider the time as a new coordinate as follows (which corresponds to the case (23)):

$$\frac{d}{dt} \begin{pmatrix} x \\ t_A \end{pmatrix} = \begin{pmatrix} f^{[A]}(x, t_A) \\ 1 \end{pmatrix} + \varepsilon \begin{pmatrix} f^{[B]}(x, t_A) \\ 0 \end{pmatrix}. \quad (35)$$

This split requires one on the one hand to solve the non-autonomous problem $x' = f^{[A]}(x, t)$ exactly (or numerically with sufficient accuracy) and, on the other, to solve the autonomous problem $x' = \varepsilon f^{[B]}(x, t_A)$ (where t_A has been frozen). This procedure can be of interest for problems where, for instance, $f(x, t)$ is close to being linear, where $f^{[A]}(x, t)$ corresponds to the linear part (accurate and relatively fast methods exist for this problem) and $\varepsilon f^{[B]}(x, t_A)$ is a small nonlinear part.

In Hamiltonian formalism, this problem would correspond to the case $H(q, p, t) = H_0(q, p, t) + \varepsilon H_1(q, p, t)$. Let us consider, for example, the case $H_0 = T(p, t) + V_0(q, t)$ with $T = \frac{1}{2}p^T M(t)p$ (we assume that H_0 is integrable or easy to integrate numerically) and $H_1 = V_1(q, t)$.

The standard procedure given by (34) corresponds to considering the enlarged Hamiltonian system

$$\tilde{H} = \left(T(p, t_A) + V_0(q, t_A) + \lambda_B \right) + \left(\varepsilon V_1(q, t_B) + \lambda_B \right) = H^{(A_1)} + H^{(B_1)}. \quad (36)$$

The scheme given by (35) corresponds to considering the Hamiltonian

$$\tilde{H} = \left(T(p, t_A) + V_0(q, t_A) + \lambda_A \right) + \varepsilon V_1(q, t_A) = H^{(A_3)} + H^{(B_3)}. \quad (37)$$

Then, one has to evolve separately the flow associated to the autonomous Hamiltonian $H^{(B_3)}$ where the time is frozen, and to solve accurately the evolution for $H^{(A_3)}$, which is equivalent to considering the evolution for the non-autonomous system

$$H_0(q, p, t) = T(p, t) + V_0(q, t).$$

Then, we can choose coefficients a_i, b_i for splitting methods addressed for near-integrable problems (see [11]). Notice also that

$$\{H^{(B_3)}, \{H^{(B_3)}, H^{(A_3)}\}\} = \varepsilon^2 (V_1)_q^T(q, t_A) M(t_A) (V_1)_q(q, t_A) \equiv \varepsilon^2 V_2(q, t_A), \quad (38)$$

i.e. $V_2(q, t_A)$ is a function depending only on coordinates, similarly to $V_1(q, t_A)$, and this term can be added to the flow associated to $H^{(B_3)}$ in order to construct $H^{(C_3)}$ as described in Section 3.

In addition, it is worth mentioning that, since the time has been considered as a new coordinate in an enlarged system, the system can be treated as autonomous, and the processing technique can also be used, allowing one to obtain an additional improvement in the numerical integration (see [15,6,7]). A processed method is given by the composition

$$\psi_h = \left(\varphi_h^{[P]} \right)^{-1} \circ \varphi_h^{[K]} \circ \varphi_h^{[P]}, \quad (39)$$

where $\varphi_h^{[K]}$ is the kernel and $\varphi_h^{[P]}$, $\left(\varphi_h^{[P]} \right)^{-1}$ are the pre- and post-processor or corrector, respectively. For N steps, we have

$$\psi_h^N = \left(\varphi_h^{[P]} \right)^{-1} \circ \left(\varphi_h^{[K]} \right)^N \circ \varphi_h^{[P]}, \quad (40)$$

so the computational cost is dominated by the cost of the kernel. Then, we can build an accurate method, ψ_h , at the hopefully low cost of the kernel, $\varphi_h^{[K]}$.

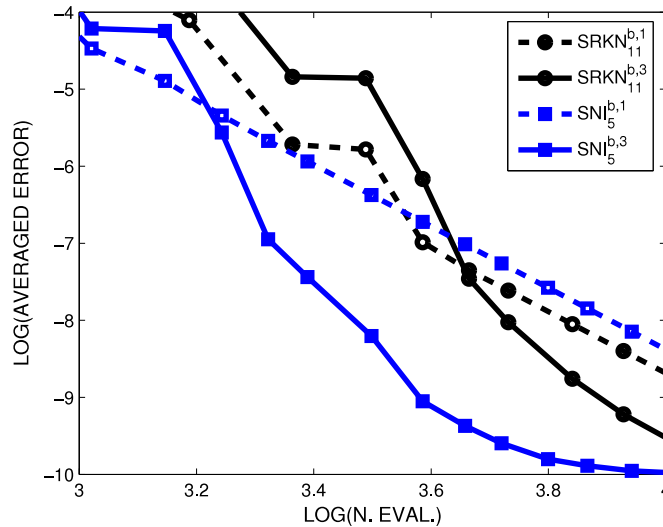


Fig. 2. Efficiency comparison between algorithms $SRKN_{11}$ and SNI_5 .

We illustrate with a simple example the application of these schemes and their relative performance.

Example 4. Let us consider the Hamiltonian

$$H(q, p, t) = \frac{1}{2}p^2 + \frac{1}{2}f(t)q^2 + \varepsilon \sum_{j=1}^s \cos(q - \omega_j t), \tag{41}$$

where $q, p \in \mathbb{R}$, which describes the motion of a charged particle in a magnetic field perturbed by s electrostatic plane waves, each with the same wavenumber and amplitude, but with different temporal frequencies ω_j . We set $f(t) = 1 + g(t)$, where the case $g = 0$ corresponds to the problem analysed in [26]. In our experiments, we consider the more general case $g(t) \neq 0$, and we also illustrate the performance of the proposed schemes.

We analyse the splittings (36) and (37). In the last case, the evolution of the Hamiltonian $H^{(A_3)}$ requires one to solve the linear system for q, p

$$\frac{d}{dt} \begin{pmatrix} q \\ p \end{pmatrix} = M(t) \begin{pmatrix} q \\ p \end{pmatrix} \quad \text{with} \quad M(t) = \begin{pmatrix} 0 & 1 \\ -f(t) & 0 \end{pmatrix} \tag{42}$$

with sufficient accuracy. This can be easily accomplished using a high-order numerical method for this part (or dividing the step for its integration).

For the numerical integration of this problem, we consider (in addition to $SRKN_{11}$) the symmetric five-stage fourth-order (8, 4) BAB method (SNI_5) given in [11] and designed for near-integrable systems. This is a method which also cancels the error terms of order $\mathcal{O}(\varepsilon h^n)$ up to $n = 8$.

We take $f(t) = 1 + \frac{1}{2} \cos(\frac{3}{2}t)$, $\varepsilon = \frac{1}{100}$, and the remaining parameters and initial conditions as given in [26]:

$$q_0 = 0, \quad p_0 = 11.2075, \quad \omega_j = j\omega_0, \quad \omega_0 = 7, \quad s = 3.$$

We integrate the system along the interval $t \in [0, 20\pi]$ and measure the exact solution numerically (using an accurate numerical method and taking a sufficiently small time step) at the following instants: $t_n = n\frac{2\pi}{7}$, $n = 1, 2, \dots, 70$. In order to analyse the performance of the numerical methods, we choose a time step given by $h_m = \frac{2\pi}{7m}$, with $m \in \mathbb{N}$, and we can compare the approximation obtained with the “exact” solution at the previous mesh. Then, the average value

$$\varepsilon_m = \left(\frac{1}{N} \sum_{n=1}^N (q(t_n) - q_n)^2 + (p(t_n) - p_n)^2 \right)^{1/2},$$

with $N = 70$, is taken as the resulting error. Fig. 2 shows the efficiency plots for the sixth-order Nyström method $SRKN_{11}$ and the fourth-order near-integrable method SNI_5 , plotting the error versus the number of flows $\varphi^{[B]}$. In this numerical experiment, the flows associated with the linear part are computed up to round-off accuracy, so the error corresponds to the composition scheme.

We observe that, for this near-integrable problem, methods tailored for this structure are superior. In addition, it is evident from the figure that considering the time as a parameter in the standard form does not reduce the order of the method $SNI_5^{b,1}$ (it is still of fourth order) but its accuracy decays considerably.

Table 1
Coefficients of the processor for the kernel (43) for a near-integrable system.

$y_1 = 0.1659120515409654$	$z_1 = 0.9125829692505096$
$y_2 = 0.1237659000825160$	$z_2 = 0.3605243318856133$
$y_3 = -0.0250397323738759$	$z_3 = -0.7354063037876117$
$y_4 = -0.2269372219010943$	$z_4 = -1/2$

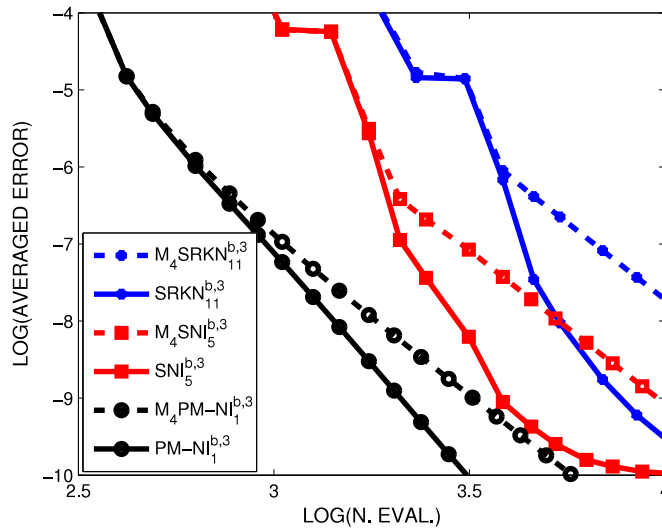


Fig. 3. Efficiency comparison between algorithms $SRKN_{11}$, SNI_5 and $PM-NI_1$ when the time-dependent linear part is integrated using the fourth-order integrators (44) (labelled with M_4) or accurately up to round-off error (this extra cost is not reflected in the plots).

To illustrate how the processing technique can be used to solve this problem, we consider a one-stage fourth-order processed method for Nyström and near-integrable problems which uses one modified potential (the processor is taken, in this case, as appropriate for near-integrable problems) and is given by the composition (39), where

$$\begin{aligned} \varphi_h^{[K]} &\simeq \varphi_{h/2}^{[A_3]} \circ \varphi_{h,h^3/24}^{[C_3]} \circ \varphi_{h/2}^{[A_3]}, \\ \varphi_h^{[P]} &= \varphi_{z_4h}^{[A_3]} \circ \varphi_{y_4h}^{[B_3]} \circ \varphi_{z_3h}^{[A_3]} \circ \varphi_{y_3h}^{[B_3]} \circ \varphi_{z_2h}^{[A_3]} \circ \varphi_{y_2h}^{[B_3]} \circ \varphi_{z_1h}^{[A_3]} \circ \varphi_{y_1h}^{[B_3]}, \\ \left(\varphi_h^{[P]}\right)^{-1} &= \varphi_{-y_1h}^{[B_3]} \circ \varphi_{-z_1h}^{[A_3]} \circ \varphi_{-y_2h}^{[B_3]} \circ \varphi_{-z_2h}^{[A_3]} \circ \varphi_{-y_3h}^{[B_3]} \circ \varphi_{-z_3h}^{[A_3]} \circ \varphi_{-y_4h}^{[B_3]} \circ \varphi_{-z_4h}^{[A_3]}. \end{aligned} \tag{43}$$

We take the coefficients from [6] corresponding to a fourth-order method; these also cancel the error terms at orders εh^5 and εh^6 (for the convenience of the reader, the coefficients are collected in Table 1). The method will be denoted by $(PM-NI_1)$. More elaborated sets of coefficients (which cancel more nested commutators of order εh^n) can be found in [15].

Next, we analyse how the error changes when the flow associated with $H^{(A_3)}$ is approximated instead of being computed with accuracy up to round-off error. To approximate this linear problem, we have considered the fourth-order commutator-free Magnus integrator given by the following product of exponentials:

$$\varphi_h^{[A_3]} = \exp\left(\frac{h}{2}(\alpha M_1 + \beta M_2)\right) \exp\left(\frac{h}{2}(\beta M_1 + \alpha M_2)\right), \tag{44}$$

with $M_i = M(t_n + c_i h)$, $c_1 = \frac{1}{2} - \frac{\sqrt{3}}{2}$, $c_2 = \frac{1}{2} + \frac{\sqrt{3}}{2}$, and $\alpha = \frac{1}{2} - \frac{\sqrt{3}}{3}$, $\beta = 1 - \alpha$ (for more details as well as how to consider different quadrature rules, see [27,18] and references therein). We have chosen this scheme because it has shown a high performance for time-dependent linear problems and at the same time it can be used for solving nonlinear problems. The results are shown in Fig. 3. We also show the results obtained by the fourth-order processed method (43), where the number of evaluations corresponds to the flow $\varphi^{[C_3]}$ in the kernel. From the figure, the superiority of the methods which incorporate the most information on the scheme is clear. $PM-NI_1$ is addressed for Nyström problems and for near-integrable systems; it uses modified potentials (cost-free for this problem) and it exploits the processing technique. It is also important to mention that the loss of accuracy, when the flow $\varphi_h^{[A_3]}$ is approximated using a fourth-order method, can be significant. Then, it is important to analyse if it is possible to approximate this part using low-cost schemes and without losing much accuracy.

5. The integral approximation

The approach described so far can be extended to the general case when the explicit linear time dependence in (20) cannot be treated by the exact integration of $A(t)$ or $B(t)$. In a more general framework, the exact integral solution can be replaced with a first-order approximation without any loss of accuracy. In this respect, each $\Theta_h^{(i)} = \varphi_h^{[A_i]} \circ \varphi_h^{[B_i]}$ and its adjoint $\Theta_h^{(i)*} = \varphi_h^{[B_i]} \circ \varphi_h^{[A_i]}$ can be considered as the basis for the composition method

$$\psi_h^{(i)} = \Theta_{\alpha_m h}^{(i)*} \circ \Theta_{\beta_m h}^{(i)} \circ \Theta_{\alpha_{m-1} h}^{(i)*} \circ \dots \circ \Theta_{\beta_2 h}^{(i)} \circ \Theta_{\alpha_1 h}^{(i)*} \circ \Theta_{\beta_1 h}^{(i)} \tag{45}$$

with suitable coefficients α_j, β_j . The resulting algorithms are in a close connection with $\psi_h^{(i)}$ and, in the case when $a_{m+1} = 0$, the equivalence is obtained by the following choice for the method parameters: $\beta_1 = b_1, \alpha_m = b_{m+1}$ and $\alpha_i = a_i - \beta_i, \beta_{i+1} = b_{i+1} - \alpha_i$ for $i = 1, \dots, m - 1$. It is known that the accuracy can be retained whenever both exact and numerical flows are combined so that they appear in a composition of methods with their corresponding adjoint ones (see [1] for more details). We exploit this property with the aim of formulating composition schemes for the case at hand. Notice that, since the classical splitting approach does not require explicit time integration, scheme $\psi_h^{(1)}$ is not modified, while the other approaches are formulated by mixing numerical and exact flows. Indeed, we denote by $\Phi_h^{[A_i]}$ and $\Phi_h^{[B_i]}$ any first-order integrator to $y' = F^{(A_i)}(y)$ ($i = 3, 4$) and $y' = F^{(B_i)}(y)$ ($i = 2, 4$), respectively, and we limit ourselves to the indices corresponding to distinct cases where the time integrals are needed. The basis of each modified composition method can be recast as follows:

$$\begin{aligned} \Theta_h^{(2)} &= \varphi_h^{[A_2]} \circ \Phi_h^{[B_2]}, & \Theta_h^{(2)*} &= \Phi_h^{[B_2]*} \circ \varphi_h^{[A_2]}, \\ \Theta_h^{(3)} &= \Phi_h^{[A_3]} \circ \varphi_h^{[B_3]}, & \Theta_h^{(3)*} &= \varphi_h^{[B_3]} \circ \Phi_h^{[A_3]*}, \\ \Theta_h^{(4)} &= \Phi_h^{[A_4]} \circ \Phi_h^{[B_4]}, & \Theta_h^{(4)*} &= \Phi_h^{[B_4]*} \circ \Phi_h^{[A_4]*}; \end{aligned}$$

then, by means of a composition as in (45), the corresponding modified methods $\tilde{\psi}_h^{(i)}$ are defined as

$$\begin{aligned} \tilde{\psi}_h^{(2)} &= \Phi_{\alpha_m h}^{[B_2]*} \circ \varphi_{\alpha_m h}^{[A_2]} \circ \dots \circ \varphi_{\alpha_2 h}^{[A_2]} \circ \Phi_{\beta_2 h}^{[B_2]} \circ \Phi_{\alpha_1 h}^{[B_2]*} \circ \varphi_{\alpha_1 h}^{[A_2]} \circ \Phi_{\beta_1 h}^{[B_2]}, \\ \tilde{\psi}_h^{(3)} &= \varphi_{b_{m+1} h}^{[B_3]} \circ \Phi_{\alpha_m h}^{[A_3]*} \circ \Phi_{\beta_m h}^{[A_3]} \circ \dots \circ \varphi_{b_2 h}^{[B_3]} \circ \Phi_{\alpha_1 h}^{[A_3]*} \circ \Phi_{\beta_1 h}^{[A_3]} \circ \varphi_{b_1 h}^{[B_3]}, \\ \tilde{\psi}_h^{(4)} &= \Phi_{\alpha_m h}^{[B_4]*} \circ \Phi_{\alpha_m h}^{[A_4]} \circ \Phi_{\beta_m h}^{[A_4]} \circ \dots \circ \Phi_{\alpha_1 h}^{[B_4]*} \circ \Phi_{\alpha_1 h}^{[A_4]*} \circ \Phi_{\beta_1 h}^{[A_4]} \circ \Phi_{\beta_1 h}^{[B_4]}. \end{aligned}$$

In the case of near-separable problems, $\tilde{\psi}_h^{(2)}$ is built by replacing P_i in (26) with

$$P_i = P_{i-1} + h \left(\alpha_{i-1} M_2(T_{i-1}^B) + \beta_i M_2(T_i^B) \right) g_1(Q_{i-1}, T_{i-1}^A), \tag{46}$$

where we set $\alpha_0 = 0$. In a similar way, $\tilde{\psi}_h^{(3)}$ is obtained by replacing Q_i in (26) with

$$Q_i = Q_{i-1} + h \left(\beta_i M_1(T_{i-1}^A) + \alpha_i M_1(T_i^A) \right) g_2(P_i, T_i^B). \tag{47}$$

Finally, $\tilde{\psi}_h^{(4)}$ arises from (26) with P_i and Q_i replaced by (46) and (47), respectively. The following example illustrates the effectiveness of this procedure.

Example 5. We consider the Duffing oscillator as a test problem. We focus our attention on splitting procedure $\psi_h^{(3)}$, which has revealed itself to be very efficient in the treatment of this kind of problem, and on the scheme $SRKN_{11}^{b,3}$. In this framework, we replace the exact flows by the approximated ones exploiting formula (47), and we denote the resulting algorithm by $Mod_1SRKN_{11}^{b,3}$. In Fig. 4, it is evident that the advantages due to the Nyström-like structure are lost and the method recovers the fourth order for problems with generic structure. We use the second-order approximation defined by

$$Q_i = Q_{i-1} + h \left(\beta_i M_1 \left(T_{i-1}^A + \frac{h\beta_i}{2} \right) + \alpha_i M_1 \left(T_i^A - \frac{h\alpha_i}{2} \right) \right) g_2(P_i, T_i^B); \tag{48}$$

then the resulting method is denoted by $Mod_2SRKN_{11}^{b,3}$; in Fig. 4 we numerically show how it is able to preserve the sixth order of accuracy.

As a further test, we account for the sixth-order ten-stage method named S_{10} in [8]; then we exploit its coefficients in $\psi_h^{(3)}$ and we obtain the algorithm denoted by S_{10}^3 . Then the same coefficients are employed in $\tilde{\psi}_h^{(3)}$ with the approximation of the first order and the resulting algorithm is denoted by $Mod_1S_{10}^3$. As is shown in Fig. 4, the sixth order of accuracy of the original scheme is preserved when the exact integrals are replaced with their first-order approximations.

We conclude that replacing the exact integration with a first-order quadrature rule retains the general accuracy of the original method but it loses the further gain in order of the Nyström schemes. More accurate quadrature rules have to be adopted in order to recover their extra accuracy.

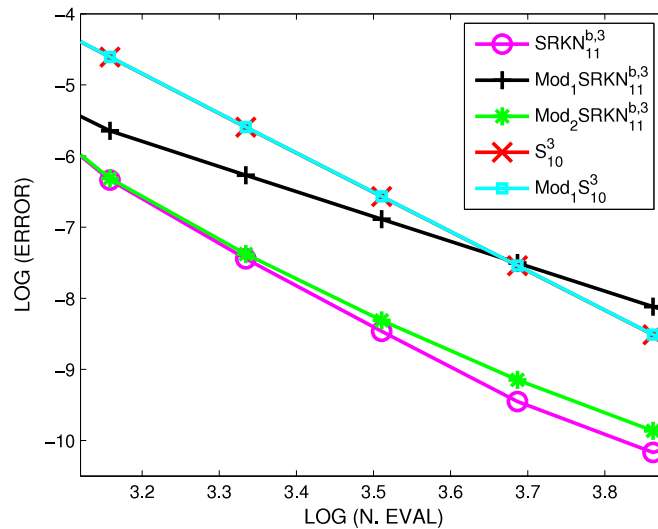


Fig. 4. Efficiency comparison among algorithms S_{10}^3 , $Mod_1 S_{10}^3$, $SRKN_{11}^{b,3}$, $Mod_1 SRKN_{11}^{b,3}$ and $Mod_2 SRKN_{11}^{b,3}$ at $\epsilon = 1/20$, $\delta = 1/4$.

6. Conclusions

We have considered splitting methods for the numerical integration of non-autonomous separable differential equations. Splitting methods are frequently used as geometric numerical integrators, and they have been designed for autonomous separable systems. A substantial number of methods tailored for different structures of the equations have recently appeared, showing excellent performances in many cases. When these methods are used on non-autonomous problems, usually their performance diminishes considerably, and they can even lose the order of accuracy observed for the corresponding autonomous problems, as shown by several numerical examples.

We have presented a simple alternative which, for many relevant cases, allows one to retain the high performance of the splitting methods using the same schemes as for the autonomous problems. We have analysed in detail near-separable systems, Nyström-like problems and near-integrable systems, as well as their corresponding Hamiltonian problems. If the time functions which appear on the vector fields are taken as coordinates in an appropriate way, it is possible to use splitting methods in those problems without losing their good performances. This technique is applied to different problems and its performance is illustrated with several numerical examples.

For those problems where the techniques proposed in this work do not allow one to recover the full structure of the associated autonomous problem, we recommend considering the more elaborate numerical methods based on Magnus series proposed for general non-autonomous dynamical systems (see [27]), as well as for Hamiltonian and separable dynamical equations (see [19,18] and references therein). They require one to choose one particular set of coefficients for a splitting method and to look for additional complementary coefficients obtained from new order conditions.

High-order splitting methods have been used in recent years for the numerical integration of an important number of evolutionary PDEs such as Maxwell equations [28,29] or linear and nonlinear Schrödinger equations [9,14,30]. In [30] the sixth-order Nyström splitting scheme $SRKN_{11}^b$ was used, showing a high performance on the Gross–Pitaevskii equation, and for the linear equation, in [9,14] we can find methods up to order eight which use the maps $\phi_{b;h,c;h^3}^{[C]}$. In a similar way as in the examples presented in this work, the performance of these methods deteriorates if they are applied to the non-autonomous case when some of the parameters are explicitly time dependent. Exactly the same procedures as presented in this work allow one to recover the high performance the splitting methods show for the autonomous case, for which the methods were originally designed.

Finally, before concluding this work, it is worth mentioning that the new autonomous systems (in the enlarged phase space) could in some cases have new algebraic structures not considered in this work, which could be interesting to analyse [4], as well as the structure preservation of the new approach.

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