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Splitting methods for non-autonomous linear systems

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We present splitting methods for numerically solving a certain class of explicitly time-dependent linear differential equations. Starting from an efficient method for the autonomous case and making use of the formal solution obtained with the Magnus expansion, we show how to get the order conditions for the non-autonomous case. We also build a family of sixth-order integrators whose performance is clearly superior to previous splitting methods on several numerical examples.

Keywords: Splitting methods; Non-autonomous systems; Magnus expansion

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1. Introduction

Composition methods constitute a widespread procedure for numerically integrating differential equations, especially in the context of geometric integration. In this work we consider a particular case of partitioned linear systems that frequently appear when discretizing many partial differential equations (PDEs). Specifically,

$$x' = M(t)y, \quad y' = -N(t)x, \tag{1}$$

with $x(t_0) = x_0 \in \mathbb{R}^{d_1}$, $y(t_0) = y_0 \in \mathbb{R}^{d_2}$, $M: \mathbb{R} \to \mathbb{R}^{d_1 \times d_2}$ and $N: \mathbb{R} \to \mathbb{R}^{d_2 \times d_1}$. Systems of the form

$$\bar{x}' = \bar{M}(t)\bar{y} + f(t), \quad \bar{y}' = -\bar{N}(t)\bar{x} + g(t), \tag{2}$$

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are also of type (1), since the solution $(\bar{x}(t), \bar{y}(t))$ of (2) corresponds to the solution $x(t) = (\bar{x}(t)^{\mathrm{T}}, 1)^{\mathrm{T}}$, $y(t) = (\bar{y}(t)^{\mathrm{T}}, 1)^{\mathrm{T}}$ of an enlarged system (1) with

$$M(t) = \begin{pmatrix} \bar{M}(t) & f(t) \\ 0^{\mathrm{T}} & 0 \end{pmatrix}, \quad N(t) = \begin{pmatrix} \bar{N}(t) & -g(t) \\ 0^{\mathrm{T}} & 0 \end{pmatrix} \tag{3}$$

and initial conditions $x(t_0) = (\bar{x}(t_0)^{\mathrm{T}}, 1)^{\mathrm{T}}$, $y(t_0) = (\bar{y}(t_0)^{\mathrm{T}}, 1)^{\mathrm{T}}$. Similarly, the second-order differential equation

$$x'' = D(t)x + g(t) \tag{4}$$

with $D: \mathbb{R} \to \mathbb{R}^{d\times d}$, $f: \mathbb{R} \to \mathbb{R}^d$, can be considered as a special case of (1) with

$$M(t) = \begin{pmatrix} I_d & 0 \\ 0^{\mathrm{T}} & 0 \end{pmatrix}, \quad N(t) = \begin{pmatrix} -D(t) & -g(t) \\ 0^{\mathrm{T}} & 0 \end{pmatrix}. \tag{5}$$

Equation (1) describes the evolution of many relevant physical systems. In particular, the space discretization of the Schrödinger equation can be reformulated as an N-degrees of freedom classical linear Hamiltonian system with Hamiltonian equations of the form (1) [1–3] and also the time-dependent Maxwell equations can be expressed in this way [4]. On the other hand, the numerical integration of some nonlinear PDEs (such as the nonlinear Schrödinger equation) is frequently done by solving separately the linear component, which in many cases can be written as (1) and constitutes the most problematic part of the procedure.

Denoting $z = (x, y)^{\mathrm{T}}$, one may write (1) as

$$z' = \Lambda(t)z, \quad \text{where} \quad \Lambda(t) = A(t) + B(t), \tag{6}$$

and

$$A(t) = \begin{pmatrix} 0 & M(t) \\ 0 & 0 \end{pmatrix}, \quad B(t) = \begin{pmatrix} 0 & 0 \\ -N(t) & 0 \end{pmatrix}. \tag{7}$$

This system can be numerically solved by using, for instance, Magnus integrators [5–7]. These methods require computing the exponential of matrices of dimension $(d_1 + d_2) \times (d_1 + d_2)$. If $(d_1 + d_2) \gg 1$ then the exponentiation can be prohibitively costly. For this reason, new methods which only involve matrix-vector products of the form $M(t)y$ and $N(t)x$ are highly desirable.

The purpose of the present work is to adapt to equation (1) the procedure presented in [8] in a more general setting. The approach combines the Magnus expansion with efficient splitting methods for autonomous problems. Here we summarize the main ideas involved and illustrate the technique by constructing several integrators for equations (6)–(7) which outperform previous algorithms.

The new methods have the form (for a time step of size h)

$$z(t + h) \approx \mathrm{e}^{A_m(t,h)}\mathrm{e}^{B_m(t,h)} \ldots \mathrm{e}^{A_1(t,h)}\mathrm{e}^{B_1(t,h)}z(t), \tag{8}$$

where the matrices $A_i(t, h)$ and $B_i(t, h)$ are given by

$$A_i(t, h) = h\sum_{j=1}^{k} \rho_{ij} A(t + c_j h), \quad B_i(t, h) = h\sum_{j=1}^{k} \sigma_{ij} B(t + c_j h), \tag{9}$$

with appropriately chosen real parameters $c_i, \rho_{ij}, \sigma_{ij}$. Since in our case

$$\mathrm{e}^{A_i(t,h)} = \begin{pmatrix} I & M_i(t,h) \\ 0 & I \end{pmatrix}, \quad \mathrm{e}^{B_i(t,h)} = \begin{pmatrix} I & 0 \\ -N_i(t,h) & I \end{pmatrix},$$

then (8) can be written as $z(t+h) \approx K(t,h)z(t)$, where

$$K(t,h) = \mathrm{e}^{A_m(t,h)}\mathrm{e}^{B_m(t,h)} \cdots \mathrm{e}^{A_1(t,h)}\mathrm{e}^{B_1(t,h)}$$

$$= \begin{pmatrix} I & M_m \\ 0 & I \end{pmatrix} \begin{pmatrix} I & 0 \\ -N_m & I \end{pmatrix} \cdots \begin{pmatrix} I & M_1 \\ 0 & I \end{pmatrix} \begin{pmatrix} I & 0 \\ -N_1 & I \end{pmatrix}, \tag{10}$$

and obviously

$$M_i = h \sum_{j=1}^{k} \rho_{ij} M(t + c_j h), \quad N_i = h \sum_{j=1}^{k} \sigma_{ij} N(t + c_j h) \tag{11}$$

for $i = 1, \ldots, m$. Notice that when $M(t)$ and $N(t)$ are constant, then $K(t,h)$ reduces to

$$K(h) = \mathrm{e}^{ha_m A}\mathrm{e}^{hb_m B} \cdots \mathrm{e}^{ha_1 A}\mathrm{e}^{hb_1 B}$$

$$= \begin{pmatrix} I & a_m h M \\ 0 & I \end{pmatrix} \begin{pmatrix} I & 0 \\ -b_m h N & I \end{pmatrix} \cdots \begin{pmatrix} I & a_1 h M \\ 0 & I \end{pmatrix} \begin{pmatrix} I & 0 \\ -b_1 h N & I \end{pmatrix}, \tag{12}$$

where

$$a_i = \sum_{j=1}^{k} \rho_{ij}, \quad b_i = \sum_{j=1}^{k} \sigma_{ij}, \quad i = 1, \ldots, m. \tag{13}$$

In the autonomous case there exists an extensive list of splitting methods for separable systems in the literature (see [9–13] and references therein). In addition, for partitioned linear systems extremely efficient methods can be constructed due to the special structure of the system [1, 14, 15]. Our goal here is to start from a set of coefficients a_i, b_i $(i = 1, \ldots, m)$ which provides an efficient method for the autonomous case, and then to find appropriate values for $c_i, \rho_{ij}, \sigma_{ij}$ such that (13) holds and (10) leads to a good method for the non-autonomous system (1).

For the convenience of the reader (and potential user of the new class of integration methods) we collect in table B1 two algorithms implementing schemes (12) and (10) for the numerical integration of equation (1) in the autonomous and the non-autonomous case, respectively. In the last situation, the proposed algorithm requires the computation and storage of $M(t + c_j h)$, $N(t + c_j h)$, $j = 1, \ldots, k$, at each step. We assume that the linear combination (11) is efficiently computed. This is the case, in particular, when $M(t) = \sum_{i=1}^{l} f_i(t) M^{[i]}$ with $M^{[i]}$ constant matrices and $f_i(t)$ scalar functions, for a small value of l (and similarly for $N(t)$).

2. Order conditions

One possible approach for deriving the conditions to be satisfied by the coefficients $c_i, \rho_{ij}, \sigma_{ij}$ of a method of order, say, p, is formally to build a solution of equation (6) with the Magnus expansion.

It is well known that $z(t)$ can be formally written as

$$z(t+h) = \mathrm{e}^{\Omega(t,h)} z(t), \tag{14}$$

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 $\Lambda(t)$ [5]. This constitutes the so-called Magnus expansion of the solution. An important feature of this expansion is that, when the solution of (6) evolves into a Lie group $\mathcal{G}$, then $\mathrm{e}^{\Omega(t,h)}$ stays on $\mathcal{G}$ even if the series is truncated, provided that $\Lambda(t)$ belongs to the Lie algebra associated with $\mathcal{G}$ [16].

It is possible to get $\Omega_k(t,h)$ explicitly by inserting into the recurrence defining the Magnus expansion a Taylor series of the matrices $A(t)$ and $B(t)$. In fact, to take advantage of the time-symmetry property of the solution, which implies that

$$\Omega(t+h,-h) = -\Omega(t,h), \tag{15}$$

it is more convenient to expand around $t+h/2$. More specifically, if we denote

$$\alpha_i = \frac{1}{(i-1)!} \frac{\mathrm{d}^{i-1} A(s)}{\mathrm{d}s^{i-1}}\bigg|_{s=t+(h/2)}, \quad \beta_i = \frac{1}{(i-1)!} \frac{\mathrm{d}^{i-1} B(s)}{\mathrm{d}s^{i-1}}\bigg|_{s=t+(h/2)}$$

so that

$$\begin{aligned} A\left(t+\frac{h}{2}+\tau\right) &= \alpha_1 + \alpha_2\tau + \alpha_3\tau^2 + \cdots \\ B\left(t+\frac{h}{2}+\tau\right) &= \beta_1 + \beta_2\tau + \beta_3\tau^2 + \cdots, \end{aligned} \tag{16}$$

then $\Omega(t,h)$ in (14) can be expanded as

$$\Omega(t,h) = \sum_{n\geq 1} h^n \sum_{k=1}^{n} \Omega_{k,n}(t,h), \tag{17}$$

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, $\Omega_{n,k}(t,h) = 0$ 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]

$$\Omega = h\Omega_{1,1} + h^3(\Omega_{1,3} + \Omega_{2,3}) + h^5(\Omega_{1,5} + \Omega_{2,5} + \Omega_{3,5} + \Omega_{4,5}) + \mathcal{O}(h^7), \tag{18}$$

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

$$\Omega_{1,1} = \alpha_1 + \beta_1, \quad \Omega_{1,3} = \frac{1}{12}(\alpha_3 + \beta_3), \quad \Omega_{2,3} = \frac{1}{12}([\alpha_2, \beta_1] + [\beta_2, \alpha_1]),$$

$$\Omega_{1,5} = \frac{1}{80}(\alpha_5 + \beta_5), \quad \Omega_{2,5} = \frac{1}{240}([\alpha_2, \beta_3] + [\beta_2, \alpha_3]) + \frac{1}{80}([\alpha_4, \beta_1] + [\beta_4, \alpha_1]),$$

$$\Omega_{3,5} = \frac{1}{360}(-[\alpha_1, \beta_3, \alpha_1] + [\alpha_1, \beta_1, \alpha_3] - [\beta_1, \alpha_3, \beta_1] + [\beta_1, \alpha_1, \beta_3])$$

$$+ \frac{1}{240}([\alpha_1, \beta_2, \alpha_2] - [\alpha_2, \beta_1, \alpha_2] + [\beta_1, \alpha_2, \beta_2] - [\beta_2, \alpha_1, \beta_2]),$$

$$\Omega_{4,5} = \frac{1}{720}([\alpha_1, \beta_1, \alpha_1, \beta_2] - [\beta_1, \alpha_1, \beta_2, \alpha_1] + [\beta_1, \alpha_1, \beta_1, \alpha_2] - [\alpha_1, \beta_1, \alpha_2, \beta_1]).$$

If, on the other hand, one applies the Baker–Campbell–Hausdorff (BCH) formula repeatedly in (8), it is possible to write $K(t,h)$ formally as the exponential of only one operator, $K(t,h) = \exp(\tilde{\Omega}(t,h))$, depending on $A_i(t,h)$, $B_i(t,h)$ $(i = 1,\ldots,m)$ and nested commutators of these matrices. The numerical scheme will be of order p if

$$\tilde{\Omega}(t,h) - \Omega(t,h) = \mathcal{O}(h^{p+1}) \quad \text{as } h \longrightarrow 0.$$

One can then obtain explicitly the order conditions as follows. First, we expand $A_i(t,h)$, $B_i(t,h)$ in terms of α_j, β_j,

$$A_i(t,h) = \sum_{n\geq 1} h^n a_i^{(n)} \alpha_n, \quad B_i(t,h) = \sum_{n\geq 1} h^n b_i^{(n)} \beta_n, \tag{19}$$

where

$$a_i^{(n)} = \sum_{j=1}^{k} \rho_{ij} \left(c_j - \frac{1}{2}\right)^{n-1}, \quad b_i^{(n)} = \sum_{j=1}^{k} \sigma_{ij} \left(c_j - \frac{1}{2}\right)^{n-1}, \tag{20}$$

for each $i = 1,\ldots,m$, $n \geq 1$.

Then, we substitute the expressions (19) in the corresponding $\tilde{\Omega}(t,h)$, thus obtaining an expansion of the form

$$\tilde{\Omega}(t,h) = \sum_{n\geq 1} h^n \sum_{k=1}^{n} \tilde{\Omega}_{k,n}(t,h), \tag{21}$$

where each $\tilde{\Omega}_{k,n}(t,h)$ is a linear combination of terms $[\mu_{i_1}, \mu_{i_2} \ldots, \mu_{i_k}]$ with $i_1 + \cdots + i_k = n$ and $\mu_j = \alpha_{i_j}$ or $\mu_j = \beta_{i_j}$ for $j = 1,\ldots,k$. Finally, we compare the truncated (up to $n = p$) expansion (21) with the corresponding expression (17) for $\Omega(t,h)$, so that the numerical scheme is of order p if

$$\sum_{k=1}^{n} \tilde{\Omega}_{k,n} = \sum_{k=1}^{n} \Omega_{k,n} \quad \text{for } n = 1,\ldots,p. \tag{22}$$

A usual assumption imposed on the scheme (8) that simplifies the analysis considerably (and also leads to integrators with better preservation of qualitative properties) is the time-symmetry of the composition (10). That is, $K(t+h,-h) = K(t,h)^{-1}$, 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 symmetry is automatically satisfied (and thus all order conditions at even orders) if either

$$A_{m+1-i}(t+h,-h) = -A_i(t,h), \quad B_{m-i}(t+h,-h) = -B_i(t,h), \quad B_m(t,h) = 0, \tag{23}$$

or

$$B_{m+1-i}(t+h,-h) = -B_i(t,h), \quad A_{m-i}(t+h,-h) = -A_i(t,h), \quad A_m(t,h) = 0, \tag{24}$$

for $i = 1,2,\ldots,m$. In the first case, the scheme will be said to be of type ABA, whereas in the second, of type BAB. For our problem, A and B play the same role and they can be interchanged so, without loss of generality, we only consider ABA schemes. Since the first (or last) exponential is cancelled and one exponential can be concatenated in two consecutive

steps, these symmetric schemes are referred as $(m-1)$-stage methods. The symmetry (23) is achieved if

$$c_{k-j+1} = 1 - c_j, \quad \rho_{m+1-i,k-j+1} = \rho_{ij}, \quad \sigma_{m+1-i,k-j+1} = \sigma_{ij}, \tag{25}$$

for $j = 1, \ldots, k$, $i = 1, 2, \ldots, m$, which implies that

$$a^{(n)}_{m+1-i} = (-1)^{n+1}\, a^{(n)}_i, \quad b^{(n)}_{m-i} = (-1)^{n+1}\, b^{(n)}_i, \quad b^{(n)}_m = 0, \tag{26}$$

for $n \geq 1$, $i = 1, 2, \ldots, m$,

If in addition to the time-symmetry, we assume that the method is of order at least six for the autonomous case (that is, $K(h)$ in (12) is such that $K(h) = \mathrm{e}^{h(A+B)+\mathcal{O}(h^7)}$) then, by applying the above procedure, we get $\tilde{\Omega}(t, h)$ as

$$\tilde{\Omega} = h\tilde{\Omega}_{1,1} + h^3(\tilde{\Omega}_{1,3} + \tilde{\Omega}_{2,3}) + h^5(\tilde{\Omega}_{2,5} + \tilde{\Omega}_{3,5} + \tilde{\Omega}_{4,5}) + \mathcal{O}(h^7), \tag{27}$$

where

$$\begin{aligned}
&\tilde{\Omega}_{1,1} = \alpha_1 + \beta_1, \quad \tilde{\Omega}_{1,3} = \lambda_3\alpha_3 + \mu_3\beta_3,\\
&\tilde{\Omega}_{2,3} = \lambda_{21}[\alpha_2, \beta_1] + \mu_{21}[\beta_2, \alpha_1], \quad \tilde{\Omega}_{1,5} = \lambda_5\alpha_5 + \mu_5\beta_5,\\
&\tilde{\Omega}_{2,5} = \lambda_{23}[\alpha_2, \beta_3] + \mu_{23}[\beta_2, \alpha_3] + \lambda_{41}[\alpha_4, \beta_1] + \mu_{41}[\beta_4, \alpha_1],\\
&\tilde{\Omega}_{3,5} = \lambda_{131}[\alpha_1, \beta_3, \alpha_1] + \lambda_{113}[\alpha_1, \beta_1, \alpha_3] + \mu_{131}[\beta_1, \alpha_3, \beta_1] + \mu_{113}[\beta_1, \alpha_1, \beta_3]\\
&\qquad + \lambda_{122}[\alpha_1, \beta_2, \alpha_2] + \lambda_{212}[\alpha_2, \beta_1, \alpha_2] + \mu_{122}[\beta_1, \alpha_2, \beta_2] + \mu_{212}[\beta_2, \alpha_1, \beta_2],\\
&\tilde{\Omega}_{4,5} = \lambda_{1112}[\alpha_1, \beta_1, \alpha_1, \beta_2] + \lambda_{1121}[\beta_1, \alpha_1, \beta_2, \alpha_1] + \mu_{1112}[\beta_1, \alpha_1, \beta_1, \alpha_2]\\
&\qquad + \mu_{1121}[\alpha_1, \beta_1, \alpha_2, \beta_1],
\end{aligned} \tag{28}$$

and the coefficients $\lambda_{i_1\cdots i_l}$, $\mu_{i_1\cdots i_l}$, are polynomials in $a^{(n)}_i$, $b^{(n)}_i$, $i = 1, \ldots, m$, $n = 1, \ldots, 5$. Their explicit expressions are collected in Appendix A.

Since in the autonomous case $\alpha_j = \beta_j = 0$, $j > 1$, we take $a^{(1)}_i = a_i$, $b^{(1)}_i = b_i$ (the coefficients of the splitting method we have previously chosen). The coefficients $a^{(n)}_i$, $b^{(n)}_i$, $n = 2, \ldots, 5$, $i = 1, \ldots, m$, must be chosen in such a way that the time-symmetry assumption (26) holds and the following 22 additional order conditions are satisfied:

$$\lambda_3 = \mu_3 = \frac{1}{12}, \quad \lambda_{21} = \mu_{21} = \frac{1}{12}, \quad \lambda_{23} = \mu_{23} = \frac{1}{240}, \tag{29}$$

$$\lambda_{131} = \mu_{131} = -\frac{1}{360}, \quad \lambda_{113} = \mu_{113} = \frac{1}{360}, \quad \lambda_{122} = \mu_{122} = \frac{1}{240}, \tag{30}$$

$$\lambda_{212} = \mu_{212} = -\frac{1}{240}, \quad \lambda_{1112} = \mu_{1112} = \frac{1}{720}, \quad \lambda_{1121} = \mu_{1121} = -\frac{1}{720}, \tag{31}$$

$$\lambda_5 = \mu_5 = \frac{1}{80}, \quad \lambda_{41} = \mu_{41} = \frac{1}{80}. \tag{32}$$

Once a set of values for $a^{(n)}_i, b^{(n)}_i$, $n = 2, \ldots, 5$, $i = 1, \ldots, m$, satisfying the symmetry condition (26) and the order conditions (29)–(32) is chosen, a sixth-order time-symmetric scheme (8)–(9) with $k = 5$ will be obtained for each set of arbitrarily fixed values of the nodes $c_1 < c_2 < c_3 = 1/2 < c_4 = 1 - c_2 < c_5 = 1 - c_1$ by determining the coefficients ρ_{ij}, σ_{ij} uniquely from the linear equations (20).

However, for $k < 5$ and an arbitrary set of nodes $c_1 < \cdots < c_k$ satisfying the symmetry condition (25), no sixth-order scheme exists, unless the nodes $c_1 < \cdots < c_k$ correspond to a quadrature rule of order six for the interval [0, 1], i.e. unless

$$0 = \int_0^1 t(t - c_1) \cdots (t - c_k)\, \mathrm{d}t. \tag{33}$$

In that case, $\lambda_5 = \mu_5 = 1/80$ automatically holds if the remaining order conditions in (29)–(32) are imposed. For $k = 3$ one has that (33) holds if and only if

$$c_1 = \frac{1}{2} - \frac{\sqrt{15}}{10}, \quad c_2 = \frac{1}{2}, \quad c_3 = \frac{1}{2} + \frac{\sqrt{15}}{10}, \tag{34}$$

i.e. if they are the nodes of the Gaussian quadrature rule. Now the four conditions (32) are automatically satisfied if the eighteen conditions (29)–(31) hold. Thus, a sixth-order time-symmetric scheme (8)–(9) with Gaussian nodes (34) can be constructed by first obtaining a solution of the conditions (29)–(31) for the unknowns $a_i^{(n)}, b_i^{(n)}, n = 2, 3, i = 1, \ldots, m$ (satisfying the symmetry condition (26)), and then determining the coefficients ρ_{ij}, σ_{ij} from (20), or equivalently, from

$$\begin{pmatrix} \rho_{i1} & \sigma_{i1} \\ \rho_{i2} & \sigma_{i2} \\ \rho_{i3} & \sigma_{i3} \end{pmatrix} = \begin{pmatrix} 0 & -\dfrac{\sqrt{15}}{3} & \dfrac{10}{3} \\ 1 & 0 & -\dfrac{20}{3} \\ 0 & \dfrac{\sqrt{15}}{3} & \dfrac{10}{3} \end{pmatrix} \begin{pmatrix} a_i^{(1)} & b_i^{(1)} \\ a_i^{(2)} & b_i^{(2)} \\ a_i^{(3)} & b_i^{(3)} \end{pmatrix}.$$

More generally, it can be seen [7, 8] that, if the nodes $c_1 < \cdots < c_k$ correspond to a sixth-order symmetric quadrature rule with weights d_i, then, given $a_i^{(n)}, b_i^{(n)}, n = 2, 3, i = 1, \ldots, m$, satisfying the symmetry condition (26) and the 18-order conditions (29)–(31), the coefficients ρ_{ij}, σ_{ij} of the scheme (8)–(9) can be explicitly determined as

$$\rho_{ij} = \sum_{n=1}^{3} \sum_{l=1}^{3} a_i^{(n)} r_{nl} d_j \left(c_j - \frac{1}{2}\right)^{l-1}, \quad \sigma_{ij} = \sum_{n=1}^{3} \sum_{l=1}^{3} b_i^{(n)} r_{nl} d_j \left(c_j - \frac{1}{2}\right)^{l-1}, \tag{35}$$

where

$$(r_{n,l}) = \begin{pmatrix} 9/4 & 0 & -15 \\ 0 & 12 & 0 \\ -15 & 0 & 180 \end{pmatrix}. \tag{36}$$

3. Construction of methods of order six

The first step in the construction of new sixth-order methods for equation (1) is to choose symmetric splitting methods which perform efficiently in the autonomous case. This simplifies the search for coefficients and usually leads to efficient methods also for the non-autonomous problem. We must bear in mind, however, that the most efficient method for the autonomous problem does not necessarily show the best performance on the non-autonomous case. For equation (1) in the time-independent case, a good starting point is the family of splitting methods proposed in [1]. These are m-stage schemes of order m for $m = 4, 6, 8, 10, 12$, and

are denoted by $\Phi_m(h)$. They are not time-symmetric, so that to apply the above procedure, we have to build symmetrized versions by composing half a step of the method with half a step of its adjoint (the same composition, but in the reverse order), $\Psi_{2m-1}(h) = \Phi_m(h/2) \circ \Phi_m^*(h/2)$. This also allows saving one stage and, as a result, we have $(2m-1)$-stage methods of order m for the same values of m.

We have analysed the order conditions associated to the methods $\Psi_{2m-1}(h)$ for $m = 6, 8, 10, 12$ and found several sets of solutions (except for $m = 6$, where no real coefficients have been located). Among them, we have chosen those $a_i^{(n)}, b_i^{(n)}, n = 2, 3, i = 1, \ldots, m$ with the smallest absolute values.

Although the schemes $\Psi_{2m-1}(h)$ perform quite satisfactorily in the autonomous case, it is still possible to design other symmetric splitting methods which are even more efficient in a wide range of time step values [17]. Here, for the sake of illustration, we consider an 11-stage sixth-order integrator of this new family and build the corresponding scheme for the non-autonomous problem (1).

In the next section we show how the new methods behave in practice by applying them to several numerical examples. In all cases the $\Psi_{2m-1}(h)$ method with $m = 8$ and the new sixth-order integrator show the best performance. For completeness, we collect the coefficients of the method based on $\Psi_{15}(h)$ in table B2, whereas those corresponding to the new scheme are available from the authors upon request. Notice that the coefficients $a_i^{(1)}, b_i^{(1)}$ for the scheme $\Psi_{15}(h)$ are taken from [1] for $\Phi_8(h)$ and are divided by two because $\Psi_{15}(h) = \Phi_8(h/2) \circ \Phi_8^*(h/2)$.

4. Numerical examples

Here we compare the new especially adapted splitting methods for partitioned linear systems with standard splitting methods for separable systems on some relatively simple problems.

It is known that the system (1) can be written as an autonomous nonlinear separable system [3]

$$\hat{x}' = f^{[A]}(\hat{y}), \quad \hat{y}' = f^{[B]}(\hat{x}) \tag{37}$$

with $\hat{x} = (x, x_t)^{\mathrm{T}} \in \mathbb{R}^{d_1+1}$, $\hat{y} = (y, y_t)^{\mathrm{T}} \in \mathbb{R}^{d_2+1}$ and $f^{[A]}(\hat{y}) = (M(y_t)y, 1)^{\mathrm{T}}$, $f^{[B]}(\hat{x}) = (-N(x_t)x, 1)^{\mathrm{T}}$. Equation (37) is separable in solvable parts, but since $N(x_t)$ and $M(y_t)$ are in general nonlinear functions of x_t and y_t, respectively, the schemes presented in [1] are not appropriate. On the other hand, standard splitting methods can be used in a straightforward way. We consider the six-stage fourth-order method (BM_4) and the 10-stage sixth-order method (BM_6) designed in [18] for general separable systems (the coefficients are also collected in [8, 10–12]). We can also build a second-order symmetric method, say $S_2(h) = \Phi^{[A]}(h/2) \circ \Phi^{[B]}(h) \circ \Phi^{[A]}(h/2)$, where $\Phi^{[A]}(t)$, $\Phi^{[B]}(t)$ denote the t-flow associated with $f^{[A]}$ and $f^{[B]}$, respectively. Then, by composing S_2 with different time steps, it is possible to build methods of order $m > 2$, denoted here by $S_m^{(2)}$. We can find in the literature schemes with up to 35 stages to build methods up to order 10 [9, 11, 19, 20]. We choose the five-stage fourth order, the nine-stage sixth-order, the 17-stage eighth-order and the 35-stage tenth-order methods whose coefficients are collected in [9].

We denote by SGM_m with $m = 8, 10, 12$ the symmetrized methods $\Psi_{2m-1}(h)$ adapted to the non-autonomous case, whereas the new symmetric 11-stage sixth-order integrator is referred to as S_6. In all the examples the sixth-order Gaussian quadrature rule has been chosen, since it minimizes the number of evaluations of $M(t)$ and $N(t)$.

The computational cost of the methods is measured by the number of stages required. It is important to mention, however, that this number is, for the new methods, several times

higher than the number of time-dependent function evaluations (using the sixth-order Gaussian quadrature only three evaluations per step are required).

Perturbed harmonic oscillators. Time dependent linear harmonic oscillators constitute a very simple example where the preceding integrators can be tested.

(i) First we consider the time-dependent Hamiltonian

$$H(q,\,p,t) = \mathrm{e}^{-\epsilon t}\,\frac{1}{2}p^2 + \mathrm{e}^{\epsilon t}\left(\frac{1}{2}q^2 - \delta\cos(\omega t)q\right), \tag{38}$$

$q,\,p \in \mathbb{R}$, with associated equations of motion

$$q' = \mathrm{e}^{-\epsilon t}\,p, \quad p' = -\mathrm{e}^{\epsilon t}\,(q - \delta\cos(\omega t))\,, \tag{39}$$

(or equivalently $q'' + \epsilon q' + q = \delta\cos(\omega t)$). This system corresponds to a modification of the well-known Duffing oscillator. We take as initial conditions $q(0) = 1.75,\ p(0) = 0$, integrate up to $t = 40\,\pi/\omega$ and measure the average error in phase space (at $t = 2\pi/\omega, 4\pi/\omega, \ldots, 40\pi/\omega$) in terms of the number of force evaluations for different time steps (in logarithmic scale).

In figure B1(a) (see Appendix B) we show the results achieved by standard splitting methods for the autonomous case ($\epsilon = \delta = 0$) in order to choose the most efficient integrators in this case. The curves correspond to the schemes BM_4, BM_6 (dashed lines) and $\mathrm{S}_m^{(2)},\ m = 4, 6, 8, 10$ (solid lines). The order of the method can be easily identified with the slope of the respective curve. For comparison with the schemes proposed in this paper we choose those showing the best efficiency: BM_4, BM_6 and $\mathrm{S}_{10}^{(2)}$ (dashed lines from now on). In figure B1(b) we collect, in addition, the results achieved with SGM_8 (lines with circles), SGM_{10} (lines with $\times$), SGM_{12} (lines with $+$) and S_6 (thick solid lines) also in the autonomous case. Figures B1(c) and B1(d), finally, show the results for $\delta = \omega = 1/2$ with $\epsilon = 2 \times 10^{-5}$ and $\epsilon = 2 \times 10^{-2}$. In the last case, the curves obtained SGM_{10} and SGM_{12} are not included, because now these methods are less efficient than SGM_8.

(ii) As a second perturbed harmonic oscillator we choose the Mathieu equation, $q'' + (\omega^2 + \epsilon\cos(t))q = 0$, with $q \in \mathbb{R}$. We take the same initial conditions and period of integration as before and compare the relative error for $\epsilon = 1/4$ with $\omega = 2$ and $\omega = 5$. In the last case, the system corresponds to a highly oscillatory system with a relatively small time-dependent perturbation, which frequently occurs after semidiscretizing many PDEs. The results obtained are shown in figure B2, where the same coding as before has been used for the curves.

The Schrödinger equation. To illustrate the interest of the new integrators proposed here, we consider now (as a less trivial example) the Walker–Preston model of a diatomic molecule in a strong laser field [21]. This system is described by the one-dimensional Schrödinger equation (in units where $\hbar = 1$)

$$\mathrm{i}\frac{\partial}{\partial t}\psi(x,t) = \left(-\frac{1}{2\mu}\frac{\partial^2}{\partial x^2} + V(x) + f(t)x\right)\psi(x,t), \tag{40}$$

with $\psi(x,0) = \psi_0(x)$. Here $V(x) = D\left(1 - \mathrm{e}^{-\alpha x}\right)^2$ is the Morse potential and $f(t)x = A\cos(\omega t)x$ accounts for the laser field. This problem is used as a test bench for the numerical methods presented in [2,3] and we take the same values for the parameters as those authors: $\mu = 1745$ au, $D = 0.2251$ au and $\alpha = 1.1741$ au (corresponding to the HF molecule), $A = 0.011025$ au 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, equation (40) leads to the complex linear equation

$$u' = H(t)u, \tag{41}$$

with $u \in \mathbb{C}^N$ and $u_k(t) = \psi(x_k, t)(\Delta x)^{1/2}$. Here $x_k = x_0 + (k-1)\Delta x$ and $H(t) = T + \hat{V}(t)$ is an Hermitian matrix (real and symmetric). If we split $u = x + \mathrm{i}y$, the N-dimensional linear complex system (41) can be written as

$$x' = H(t)y, \quad y' = -H(t)x, \tag{42}$$

which corresponds to (1) with $M(t) = N(t) = H(t)$ and appropriate dimensions. As initial conditions we take the ground state of the Morse potential, $\phi(x) = \sigma \exp\left[-(\gamma - 1/2)\alpha x\right] \exp\left(-\gamma \mathrm{e}^{-\alpha x}\right)$, with $\gamma = 2D/w_0$, $w_0 = \alpha\sqrt{2D/\mu}$ and σ is a normalizing constant.

To check accuracy, we consider the instantaneous mean energy of the diatomic molecule, $E(t) = u^{\mathrm{T}}(t)H(t)u(t)$, for the time range $t \in [0, 100\tau]$ with $\tau = 2\pi/\omega$. As usual, the exact solution is accurately approximated using a sufficiently small time step. We measure the averaged relative error in $E(t)$ evaluated at $t = \tau, 2\tau, \ldots, 100\tau$. The algorithm requires the repeated computation of products Hx and Hy. Here $\hat{V}(t)$ is a diagonal matrix with elements $\hat{V}_{jj} = V(x_j) + f(t)x_j$, and Tx, Ty can be efficiently computed using FFTs [1,14]. Notice also that in (11) we now have

$$M_i = h\sum_{j=1}^{k} \rho_{ij} H(t + c_j h) = h a_i^{(1)} T + h a_i^{(1)} V + hX \sum_{j=1}^{k} \rho_{ij} f(t + c_j h) \tag{43}$$

when $H(t)$ plays the role of $M(t)$ and

$$N_i = h\sum_{j=1}^{k} \sigma_{ij} H(t + c_j h) = h b_i^{(1)} T + h b_i^{(1)} V + hX \sum_{j=1}^{k} \sigma_{ij} f(t + c_j h) \tag{44}$$

when $H(t)$ plays the role of $N(t)$. Here X is a diagonal matrix with diagonal elements $X_{jj} = x_j$. Observe that the products $H_i x$ and $H_i y$ only require one FFT and its inverse and thus an m-stage method requires $4m$ FFTs per step. In [3] a fourth-order method for the system (42) is considered (the system was previously converted into an autonomous system as shown in (37)), showing a clear improvement with respect to the second-order Magnus integrator (combined with a third-order splitting scheme) given in [2]. The results achieved by the fourth-order BM_4 are very similar to those obtained by the scheme considered in [3] (with slightly better stability limit). Figure B3 shows the efficiency plots for the methods. The largest time step (i.e. the smaller number of FFTs) corresponds to the stability limit of the method (an overflow appears if the time step is slightly increased). The superiority of the new splitting methods (and especially, of the scheme S_6) is manifest both with respect to efficiency and the stability limit.

5. Conclusions and outlook

There exists in the literature a large number of excellent splitting methods for numerically integrating partitioned linear systems. Nevertheless, most of these methods cannot be used

when there is an explicit time dependency in the equations, since the usual strategy of treating the time variable as an additional coordinate often modifies the special structure of the system.

In this paper we have presented a procedure for adapting efficient splitting schemes when the system is explicitly time-dependent by considering the formal solution obtained with the Magnus expansion. In particular, from the symmetrized version of the methods designed in [1] we have built a new family of sixth-order integrators for the problem defined by equation (1). The new schemes are shown to be more efficient than previous families of algorithms in all cases analysed here. In any case, we should remark that their accuracy decreases in comparison with the original schemes applied to autonomous problems. This motivates the search of new and more powerful integration methods for time independent partitioned linear systems, a problem currently under investigation. In fact, the scheme S_6 presented in this paper may be considered as a first step in that approach, whose ultimate goal is to construct splitting methods showing a high efficiency both in autonomous and non-autonomous linear equations of the form (1). This family of algorithms could be extremely useful in the numerical integration of this kind of problem.

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Appendix A: Explicit polynomial expressions

In this appendix, for the convenience of the reader, we collect the explicit expressions of the polynomials $\lambda_{i_1\cdots i_l}$, $\mu_{i_1\cdots i_l}$ appearing in (28).

Introducing

$$s_j^{(n)} = \sum_{l=1}^{j} a_l^{(n)}, \quad u_j^{(n)} = \sum_{l=j}^{m} b_l^{(n)}, \quad n = 1, \ldots, 5,$$

the consistency conditions are simply $s_m^{(1)} = u_{m+1}^{(1)} = 1$. Taking into account these equalities, one has

$$\lambda_3 = s_m^{(3)}, \quad \lambda_5 = s_m^{(5)}, \quad \lambda_{21} = \sum_{j=1}^{m} a_j^{(2)} u_j^{(1)},$$

$$\lambda_{23} = \sum_{j=1}^{m} a_j^{(2)} u_j^{(3)}, \quad \lambda_{41} = \sum_{j=1}^{m} a_j^{(4)} u_j^{(1)},$$

$$\lambda_{131} = -\frac{1}{12} \sum_{j=1}^{m} b_j^{(3)} \left[\left(-1 + 2 s_j^{(1)} \right)^2 + 2 s_j^{(1)} \left(s_j^{(1)} - 1 \right) \right],$$

$$\lambda_{113} = \frac{1}{2} \sum_{j=1}^{m} b_j^{(1)} s_j^{(3)} \left(1 - 2 s_j^{(1)} \right), \quad \lambda_{122} = \frac{1}{2} \sum_{j=1}^{m} b_j^{(2)} s_j^{(2)} \left(1 - 2 s_j^{(1)} \right),$$

$$\lambda_{212} = -\frac{1}{2} \sum_{j=1}^{m} b_j^{(1)} \left(s_j^{(2)} \right)^2,$$

$$\lambda_{1112} = -\frac{1}{6} \sum_{l=1}^{m} \left(a_l^{(1)} \right)^2 u_l^{(2)} - \frac{1}{6} \sum_{l=1}^{m-1} a_l^{(1)} \sum_{j=l+1}^{m} a_j^{(1)} \left(-1 - 3 u_l^{(1)} + 3 u_j^{(1)} \right) \left(u_l^{(2)} + u_j^{(2)} \right),$$

$$\lambda_{1121} = -\frac{1}{12} \sum_{l=2}^{m} \left(a_l^{(1)} \right)^2 u_l^{(2)} - \frac{1}{6} \sum_{l=1}^{m-1} a_l^{(1)} \sum_{j=l+1}^{m} a_j^{(1)} \left(2 u_l^{(1)} u_l^{(2)} \right.$$

$$\left. - u_l^{(2)} u_j^{(1)} - 3 u_l^{(1)} u_j^{(2)} - u_l^{(2)} + 2 u_j^{(2)} \right),$$

and the expressions for $\mu_{i_1\cdots i_l}$ are obtained from the corresponding $\lambda_{i_1\cdots i_l}$ by interchanging the roles of $a_i^{(n)}$ and $b_i^{(n)}$.

Appendix B: Tables and figures

Table B1. Algorithms for the numerical integration of (1) using J steps of length $h = t/J$: (Algorithm 1) with scheme (12) for the autonomous case, and (Algorithm 2) with scheme (10) for the non-autonomous case.

Algorithm 1–Autonomous	Algorithm 2–Non-autonomous
$x_0 = x(0); \quad y_0 = y(0)$	$x_0 = x(0); \quad y_0 = y(0); \quad t_n = t_0$
do $n = 1, J$	**do** $n = 1, J$
do $i = 1, m$	**do** $i = 1, k$
$y_i = y_{i-1} - b_i h N x_{i-1}$	$M_i = M(t_n + c_i h); \quad N_i = N(t_n + c_i h)$
$x_i = x_{i-1} + a_i h M y_i$	**enddo**
enddo	**do** $i = 1, m$
$x_0 = x_m; \quad y_0 = y_m$	$\hat{M} = \rho_{i1} M_1 + \cdots + \rho_{ik} M_k$
If (output) then	$\hat{N} = \sigma_{i1} N_1 + \cdots + \sigma_{ik} N_k$
$x_{\text{out}}(t_n) = x_0; \quad y_{\text{out}}(t_n) = y_0$	$y_i = y_{i-1} - h\hat{N} x_{i-1}$
endif	$x_i = x_{i-1} + h\hat{M} y_i$
enddo	**enddo**
	$x_0 = x_m; \quad y_0 = y_m; \quad t_n = t_n + h$
	If (output) then
	$x_{\text{out}}(t_n) = x_0; \quad y_{\text{out}}(t_n) = y_0$
	endif
	enddo

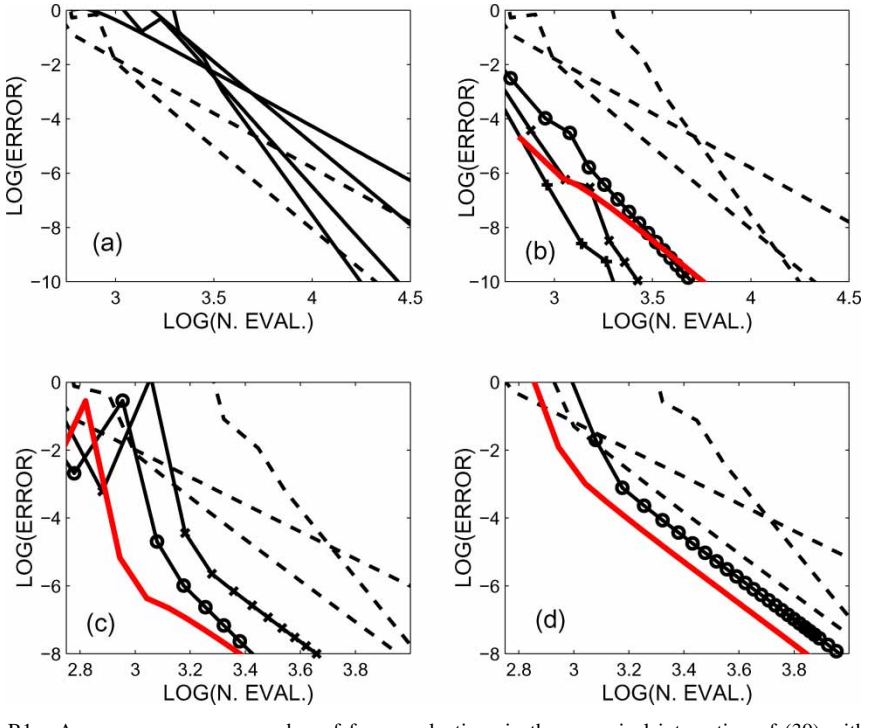

Figure B1. Average error versus number of force evaluations in the numerical integration of (39) with initial conditions $q(0) = 1.75$, $p(0) = 0$. For the autonomous case ($\epsilon = \delta = 0$) we consider: (a) standard methods for the separable system (37), BM_4 and BM_6 (dashed lines) and $\text{S}_4^{(2)}$, $\text{S}_6^{(2)}$, $\text{S}_8^{(2)}$, $\text{S}_{10}^{(2)}$ (solid lines), and (b) BM_4, BM_6, $\text{S}_{10}^{(2)}$ (dashed lines) versus SGM_8 (lines with circles), SGM_{10} (lines with $\times$), SGM_{12} (lines with $+$) and S_6 (thick solid lines). For the non-autonomous case we take $\delta = \omega = 1/2$ with: (c) $\epsilon = 2 \times 10^{-5}$; and (d) $\epsilon = 2 \times 10^{-2}$.

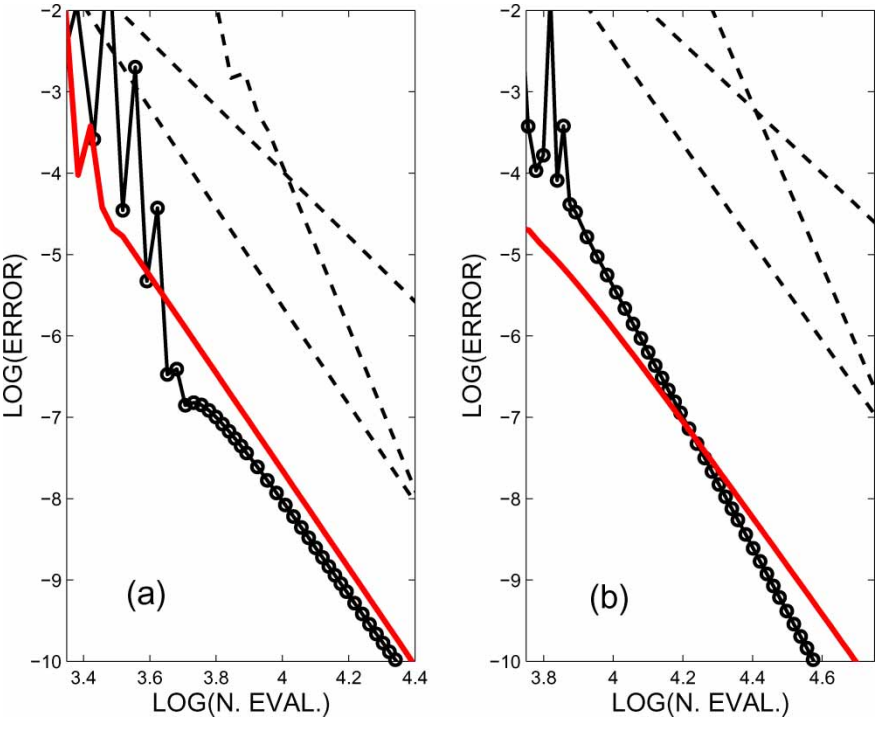

Figure B2. Same as figure B1 but for the Mathieu equation $q'' + (\omega^2 + \epsilon\cos(t))q = 0$ with $\epsilon = 1/4$ and (a) $\omega = 2$, (b) $\omega = 5$.

Table B2. Coefficients $a_i^{(j)}$, $b_i^{(j)}$ for the method SGM_8.

$a_1^{(1)} = 0.0406820423192522/2$	$a_1^{(2)} = -0.009222020674782949$	$a_1^{(3)} = 0.042062087251634246$
$b_1^{(1)} = a_8^{(1)}$	$b_1^{(2)} = -0.027214664019007236$	$b_1^{(3)} = 0.01203916935966199523$
$a_2^{(1)} = 0.1895126902355599/2$	$a_2^{(2)} = -0.043751041846595763$	$a_2^{(3)} = -0.043165966713163549$
$b_2^{(1)} = a_7^{(1)}$	$b_2^{(2)} = -0.046523437710806227$	$b_2^{(3)} = 0.018721555200024248$
$a_3^{(1)} = 0.3242803211745088/2$	$a_3^{(2)} = -0.048031113572426925$	$a_3^{(3)} = 0.046527834673773506$
$b_3^{(1)} = a_6^{(1)}$	$b_3^{(2)} = 0.027749195139632094$	$b_3^{(3)} = -0.007127646651729842$
$a_4^{(1)} = -0.0394120731572997/2$	$a_4^{(2)} = 0.006708367822842748$	$a_4^{(3)} = -0.003757288545577531$
$b_4^{(1)} = a_5^{(1)}$	$b_4^{(2)} = -0.057311963541271888$	$b_4^{(3)} = 0.018033588758710264$
$a_5^{(1)} = 0.2560570296317553/2$	$a_5^{(2)} = -0.03179575697272915$	$a_5^{(3)} = 0$
$b_5^{(1)} = a_4^{(1)}$	$b_5^{(2)} = -0.001087310633678879$	$b_5^{(3)} = 0$
$a_6^{(1)} = -0.1376837011836700/2$	$a_6^{(2)} = 0.017021775197289018$	$a_6^{(3)} = 0$
$b_6^{(1)} = a_3^{(1)}$	$b_6^{(2)} = -0.015640480519270482$	$b_6^{(3)} = 0$
$a_7^{(1)} = 0.2474725260224518/2$	$a_7^{(2)} = -0.014452573126795444$	$a_7^{(3)} = 0$
$b_7^{(1)} = a_2^{(1)}$	$b_7^{(2)} = 0$	$b_7^{(3)} = 0$
$a_8^{(1)} = 1/2 - (a_1^{(1)} + \cdots + a_7^{(1)})$	$a_8^{(2)} = -0.001311755029957398$	$a_8^{(3)} = 0$
$b_8^{(1)} = 2a_1^{(1)}$	$b_8^{(2)} = 0$	$b_8^{(3)} = 0$
$a_{8+i}^{(1)} = a_{9-i}^{(1)}$	$a_{8+i}^{(2)} = -a_{9-i}^{(2)}$	$a_{8+i}^{(3)} = a_{9-i}^{(3)}$
$b_{8+i}^{(1)} = b_{8-i}^{(1)}$	$b_{8+i}^{(2)} = -b_{8-i}^{(2)}$	$b_{8+i}^{(3)} = b_{8-i}^{(3)}$
$i = 1, \ldots, 8$		

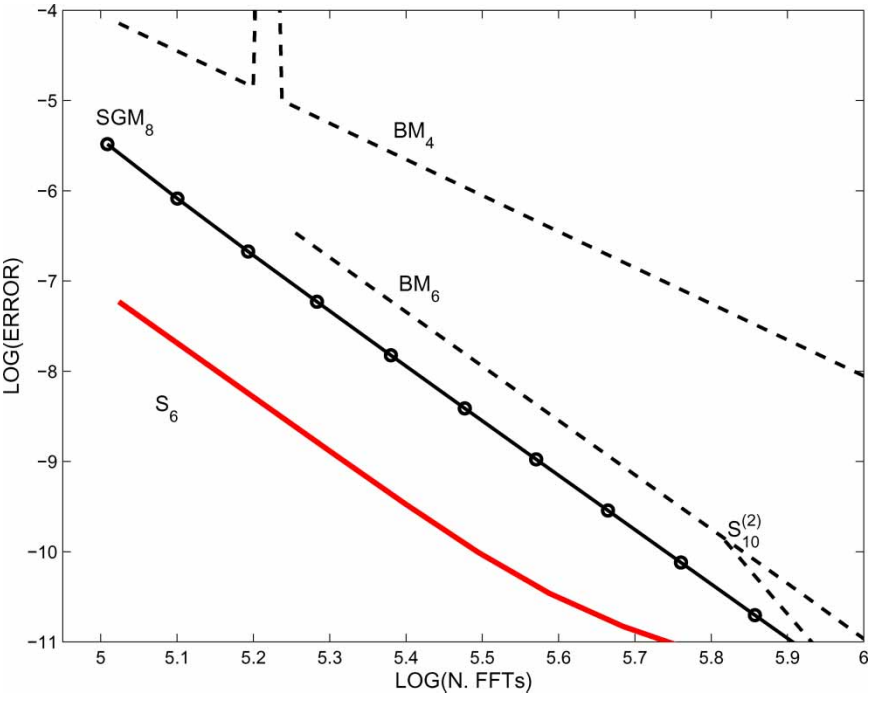

Figure B3. Average relative error in $E(t)$ versus the number of FFTs for the one-dimensional Schrödinger equation (40) written in the form (42) after space discretization.