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Fourth- and sixth-order commutator-free Magnus integrators for linear and non-linear dynamical systems

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Abstract

We present a family of numerical integrators based on the Magnus series expansions which is designed for solving non-autonomous differential equations. The main difference with standard Magnus integrators is that no commutators are involved. This property allows, in a simple way, to use the methods on non-linear ODEs. Fourth- and sixth-order methods for non-stiff differential equations are studied and new methods are presented. This type of method can easily be tailored to preserve geometric properties of the solutions, and we show through several examples that the performance and error behaviour is significantly better than known methods.

Keywords: Time-dependent differential equations; Initial value problems; Numerical methods; Magnus expansion

1. Introduction

In this paper we consider numerical methods for systems of ODEs

$$\dot{\mathbf{x}} = \mathbf{f}(t, \mathbf{x}), \qquad \mathbf{x}(t_0) = \mathbf{x}_0 \in \mathbb{R}^d \tag{1}$$

where the dot indicates derivative respect to t. In particular, we are interested in problems where the vector field $\mathbf{f}(t, \mathbf{x})$ is explicitly time-dependent. For simplicity of presentation, and without much loss of generality we assume that the vector field $\mathbf{f}$ can be factored, that is, $\mathbf{f}(t, \mathbf{x}) = B(t)\mathbf{F}(\mathbf{x})$, so (1) can be written as

$$\dot{\mathbf{x}} = B(t)\,\mathbf{F}(\mathbf{x}), \qquad \mathbf{x}(t_0) = \mathbf{x}_0, \tag{2}$$

with $B(t) \in \mathbb{R}^{d\times m}$ and $\mathbf{F}: \mathbb{R}^d \to \mathbb{R}^m$. Note that this is often the case in applications. This includes the following cases: (i) the linear problem

$$\dot{\mathbf{x}} = A(t)\mathbf{x}, \qquad \mathbf{x}(t_0) = \mathbf{x}_0, \tag{3}$$

with $A(t) \in \mathbb{R}^{d\times d}$, corresponding to the particular case $m = d$, $B(t) = A(t)$ and $\mathbf{F}(\mathbf{x}) = \mathbf{x}$; (ii) the non-homogeneous problem, $\mathbf{f}(\mathbf{x}, t) = A(t)\mathbf{x} + \mathbf{b}(t)$ which corresponds to $B(t) = (A(t), \mathbf{b}(t))$ and $\mathbf{F}(\mathbf{x}) = (\mathbf{x}, 1)^{\mathrm{T}}$; (iii) the non-linear

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systems where the vector field is given by $\mathbf{f}(\mathbf{x},t)=\sum_i \alpha_i(t)\mathbf{g}_i(\mathbf{x})$, with $\alpha_i(t)$ scalar functions, can also be rewritten in this form, being the case, for instance, of all time-dependent polynomial vector fields. This form is also very common in control theory, where the α_is are the controls. (iv) When dealing with perturbed problems of the form $\dot{\mathbf{x}}=\mathbf{f}_0(\mathbf{x})+\epsilon\mathbf{f}_1(\mathbf{x})$ where the solution of $\mathbf{f}_0$ is explicitly known, a change of coordinates can be carried out leading to a new ODE, $\dot{\mathbf{y}}=\epsilon\tilde{\mathbf{f}}_1(t,\mathbf{y})$, giving the motion of the system relative to the unperturbed motion $\dot{\mathbf{x}}_0=\mathbf{f}_0(\mathbf{x}_0)$. In some important cases such as when $\mathbf{f}_0$ is linear in $\mathbf{x}$ and $\mathbf{f}_1$ is a polynomial, $\tilde{\mathbf{f}}_1$ can be written as (2). Although the analysis is presented for (2) only minor modifications are needed in the general case (1).

On the other hand, geometric integrators (GIs) are numerical methods especially designed to retain qualitative properties of the exact dynamics. It is known that preserving certain properties lead to improved stability and errorgrowth, thus making such methods vastly more efficient for some types of simulations [13]. Handling non-autonomous problems has not been viewed a particular difficulty, but loss of efficiency often result if such problems are not treated in a good way. Methods based on Magnus series have addressed the linear problem (3), and some highly efficient general purpose Magnus integrators up to order ten [23,6,17] as well as modified versions for highly oscillatory systems [16], adiabatic systems [19], eigenvalue problems [23,1], etc. have been derived. These methods involve the exponential of nested commutators of $A(t)$ evaluated at different instants. It is straightforward to formally use these Magnus integrators also for the non-linear problem (1). In this case the exponential of a matrix corresponds to the computation of a flow-map (associated with a Lie transformation or exponential of a Lie operator) and the commutator of matrices corresponds to the Lie bracket of Lie operators [8]. To avoid the presence of commutators we consider Magnus integrators using a composition technique and new methods at order four and six are obtained.

In Section 2 we present a composition technique and present the basic form of the methods proposed. In Section 3 we show how such methods can be constructed using the Magnus series expansion for linear problems and in Section 4 we adapt the methods to non-linear problem. Section 5 contains several illustrative examples.

2. Composition methods

Let us briefly consider the standard and maybe the simplest procedure to convert Eq. (1) into autonomous. We introduce a new coordinate x_t as follows

$$\frac{\mathrm{d}}{\mathrm{d}t}\begin{Bmatrix}\mathbf{x}\\ x_t\end{Bmatrix}=\underbrace{\begin{Bmatrix}\mathbf{0}\\ 1\end{Bmatrix}}_{X}+\underbrace{\begin{Bmatrix}B(x_t)\mathbf{F}(\mathbf{x})\\ 0\end{Bmatrix}}_{Y} \tag{4}$$

which we write in this separable form for later convenience. Then to solve this extended autonomous system is equivalent to solve Eq. (2), where now we can use an standard method for autonomous systems. However, this procedure has several drawbacks: (i) it usually requires many evaluations of $B(t)$, thus making it computationally expensive for some problems; (ii) depending on the structure of $B(t)$ (for example, if it evolves slowly or fast with respect to the evolution of $\mathbf{F}(\mathbf{x})$) it can be convenient to evaluate the matrices at certain points to reduce the error; (iii) let us suppose that for the autonomous problem

$$\dot{\mathbf{x}}=D\mathbf{F}(\mathbf{x}) \tag{5}$$

with $D\in\mathbb{R}^{d\times m}$ a constant matrix, it is known a map, ψ_D^h, which approximates the solution, φ_D^t up to order q in the time step h, i.e. $\psi_D^h=\varphi_D^h+\mathcal{O}(h^{q+1})$ ($\mathbf{x}(t)=\varphi_D^\tau(\mathbf{x}_0)$ with $\tau=t-t_0$ and φ_D^0 the identity map, e.g. for the linear case $\varphi_D^t=\exp(\tau D)$). We can think, for example, that (1) is a Hamiltonian system, then Eq. (5) is an averaged autonomous Hamiltonian system and ψ_D^h is a symplectic integrator for autonomous Hamiltonian systems. Then, in general, the map ψ_D^h cannot be used for solving (4), and another (frequently less efficient) integrator has to be used.

This last drawback (iii) can be solved making use of the splitting and composition methods frequently used in geometric integration. Given X, Y two non-commutative operators, consider the splitting scheme given by

$$\Psi_k^{[q]}\equiv e^{hb_kY}e^{ha_kX}\cdots e^{hb_1Y}e^{ha_1X}=e^{h(X+Y)}+\mathcal{O}\big(h^{q+1}\big) \tag{6}$$

where many solutions for the parameters a_i, b_i at different orders and for a number of problems can be found in the literature (see [20] and references therein).

We can adapt the scheme (6) to solve (2), and this corresponds to the composition

$$\Psi_k^{[q]}\equiv\psi_{b_kB_k}^h\circ\cdots\circ\psi_{b_1B_1}^h \tag{7}$$

with $B_i = B(t_0 + c_i h)$ where $c_i = a_1 + \cdots + a_i$ and $\psi^h_{b_i B_i}$ is, as mentioned, a map which approximates the h-flow solution of the autonomous equation $\dot{\mathbf{x}} = b_i B_i \mathbf{F}(\mathbf{x})$. If the map ψ^h_D preserves the qualitative properties of the exact solution then $\Psi^{[q]}_k$ will retain these properties too. However, the main problem with the composition (7) is that k takes relatively large values ($k \geqslant 3$ for $q = 4$ and $k \geqslant 9$ for $q = 6$) and the drawbacks mentioned in (i) and (ii) still remain.

To solve this problem, in this paper we propose a new family of composition schemes given by

$$\Psi^{[q]}_m \equiv \psi^h_{D_m} \circ \cdots \circ \psi^h_{D_1} \tag{8}$$

where $\Psi^{[q]}_k = \varphi^h_B + \mathcal{O}(h^{q+1})$ with $q = 4, 6$ and

$$D_i = h \sum_{j=1}^{r} \rho_{i,j} B_j, \quad i = 1, \ldots, m, \tag{9}$$

with $B_j = B(t_0 + c_j h)$ where now c_j are the nodes of a previously chosen quadrature rule of order q and $\rho_{i,j}$ are constants to be determined once m and c_j are fixed. We will show that $m \geqslant 2$, $r \geqslant 2$ for $q = 4$ and $m \geqslant 5$, $r \geqslant 3$ for $q = 6$ so, a significant reduction in the cost of the methods can be obtained.

In addition, the new schemes can be adapted (or optimized) for different problems depending where the main source of error comes from. For instance, we can increase m (the number of map evaluations) while keeping the evaluation of $B(t)$ at the same quadrature points by changing appropriately the constants $\rho_{i,j}$, and vice-versa, we can look for a more appropriate quadrature rule for the coefficients c_j while keeping m (and changing properly the $\rho_{i,j}$).

Solutions for the $\rho_{i,j}$ can be easily (up to order six) be obtained making use of the Magnus series expansion and, since (8) does not contain commutators they will be referred as commutator-free (CF) Magnus integrators. They can lead to efficient integrators for the non-linear equation (2) for a number of problems as well as for many linear systems even if the computation of the exponential of commutators is not a problem. In [7] two fourth-order CF Magnus integrators were presented, showing their performances on the Schrödinger equation [7,3], and their efficiencies on non-linear problems is shown in [8,29]. A similar technique has been also considered in [11,22] to avoid commutators in the Runge–Kutta–Munthe-Kaas methods [26,17].

The scheme (8)–(9) can also be used to solve (1), and the scheme reads

$$\Psi^{[q]}_{m,\mathbf{f}} \equiv \psi^h_{\mathbf{f}_m} \circ \cdots \circ \psi^h_{\mathbf{f}_1} \tag{10}$$

where

$$\mathbf{f}_i(\mathbf{x}) = h \sum_{j=1}^{r} \rho_{i,j} \mathbf{f}(t_0 + c_j h, \mathbf{x}), \quad i = 1, \ldots, m, \tag{11}$$

for the same values of the parameters c_j and $\rho_{i,j}$ as in (9) and $\psi^h_{\mathbf{f}_i}$ is a map which approximates the 1-flow solution of the autonomous equation

$$\dot{\mathbf{x}} = \mathbf{f}_i(\mathbf{x}). \tag{12}$$

As mentioned, the parameters $\rho_{i,j}$ depend on the choice of c_j and the number of maps m considered, but they are the same for linear and non-linear problems. Then, for simplicity, we solve this problem for the linear case.

3. CF Magnus integrators for linear systems

The Magnus expansion [21] is a popular perturbative method for solving the linear system (3) while preserving the qualitative properties of the exact solution. Magnus assumed the solution can be written in the form

$$\mathbf{x}(t) = \exp\big(\Omega(t, t_0)\big)\mathbf{x}_0 \tag{13}$$

with $\Omega = \sum_{i=1}^{\infty} \Omega_i$. The first four terms are given by

$$\Omega_1 = \int_{t_0}^{t} A_1 \, \mathrm{d}s_1,$$

$$\Omega_2 = \frac{1}{2}\int_{t_0}^{t} \mathrm{d}s_1 \int_{t_0}^{s_1} \mathrm{d}s_2\,[A_1, A_2],$$

$$\Omega_3 = \frac{1}{6}\int_{0}^{t} \mathrm{d}s_1 \int_{0}^{s_1} \mathrm{d}s_2 \int_{0}^{s_2} \mathrm{d}s_3\big(\big[[A_1, A_2], A_3\big] + \big[A_1, [A_2, A_3]\big]\big),$$

$$\Omega_4 = \frac{1}{12}\int_{0}^{t} \mathrm{d}s_1 \int_{0}^{s_1} \mathrm{d}s_2 \int_{0}^{s_2} \mathrm{d}s_3 \int_{0}^{s_3} \mathrm{d}s_4 \big(\big[\big[[A_1, A_2], A_3\big], A_4\big] + \big[A_1, \big[[A_2, A_3], A_4\big]\big] + \big[A_1, \big[A_2, [A_3, A_4]\big]\big] + \big[A_2, \big[A_3, [A_4, A_1]\big]\big]\big) \tag{14}$$

with $A_i \equiv A(s_i)$ and $[A, B] = AB - BA$. Recently, the Magnus expansion has been used as a basis for obtaining efficient numerical integrators [6,18,23] because the approximate solution is restricted to the same space as the exact flow, giving it similar geometric properties of the exact solutions. Provided that $A(t)$ is a bounded matrix, the series is absolutely convergent for a sufficiently small $(t - t_0)$ [5,25,24] and accurate approximations can be expected for such interval. In this case the Magnus series is a good candidate for constructing numerical methods. For some problems like the Schrödinger equation, for which the norm of the matrices take large values, Magnus integrators have been shown to be efficient even outside the convergence domain of the Magnus expansion [14]. Due to their particular structure, it is possible to evaluate all multidimensional integrals using standard unidimensional quadratures derived from collocation principles [18]. For example, using a Gauss–Legendre quadrature with s points (s evaluations of $A(t)$ per step) it is possible to obtain a numerical method of order $2s$ in the time-step.

To evaluate the solution of (3) is then equivalent to compute the exponential (13). For $t = t_0 + h$, this is equivalent to evaluate the h-flow associated to the autonomous equation ($\Omega_A^h \equiv \Omega(t_0 + h, t_0)$)

$$\dot{\mathbf{x}} = \frac{1}{h}\Omega_A^h \mathbf{x} \tag{15}$$

with solution

$$\mathbf{x}(h) = \varphi_\Omega^h(\mathbf{x}_0) = \exp\big(\Omega_A^h\big)\mathbf{x}_0 \tag{16}$$

(it can also be considered as the 1-flow solution of the equation $\dot{\mathbf{x}} = \Omega_A^h \mathbf{x}$). In other words, this corresponds to consider the vector field $\mathbf{f} = A(t)\mathbf{x}$ with $\mathbf{x}$ frozen at the initial instant and then to take this particular average only on the time-dependent functions. This point of view helps to understand how Magnus integrators apply on non-linear systems.

3.1. Standard Magnus integrators

Since the solution of (3) is time-symmetric (i.e. $\varphi_h = \varphi_{-h}^{-1}$) it is clear that $\Omega(t_0 + h, t_0) = -\Omega(t_0, t_0 + h)$. To take advantage of this symmetry we consider the Taylor expansion of $A(t)$ around $t_{1/2} = t_0 + \frac{h}{2}$,

$$A(t) = \sum_{i=0}^{\infty} a_i (t - t_{1/2})^i, \tag{17}$$

where $a_i = \frac{1}{i!}\frac{\mathrm{d}^i A(t)}{\mathrm{d}t^i}|_{t=t_{1/2}}$, and then compute the corresponding expression for the terms $\Omega_k(t_0 + h, t_0)$ in the Magnus expansion. Hereafter throughout the work we assume $t_0 = 0$.

To get methods up to order $n = 2s$ it is only necessary to consider $\Omega_1, \ldots, \Omega_{2s-2}$ and the algebra generated by the terms $a_1, \ldots, a_s$ [23,17,27,6] (if a quadrature of order $2s$ is finally considered to approximate the integrals). Since we are interested in methods up to order $2s = 6$, we have to consider Ω_k, $k = 1, \ldots, 4$. Let us denote $b_i \equiv a_{i-1}h^i$, $i = 1, 2, 3$ then up to order six we can write

$$\begin{aligned}\Omega &= \Omega_1 + \Omega_2 + \Omega_3 + \Omega_4 + \mathcal{O}\big(h^7\big) \\ &= b_1 + \frac{1}{12}b_3 - \frac{1}{12}[1, 2] + \frac{1}{240}[2, 3] + \frac{1}{360}[1, 1, 3] - \frac{1}{240}[2, 1, 2] + \frac{1}{720}[1, 1, 1, 2] + \mathcal{O}\big(h^7\big).\end{aligned} \tag{18}$$

Here we denote $[i_1, i_2, \ldots, i_{l-1}, i_l] \equiv [b_{i_1}, [b_{i_2}, [\ldots, [b_{i_{l-1}}, b_{i_l}]\ldots]]]$, being an element of order $\mathcal{O}(h^{i_1+\cdots+i_l})$. Since $b_i = \mathcal{O}(h^i)$, $i = 1, 2, 3$ then b_1, b_2, b_3 can be considered as the generators of a graded free Lie algebra with grades 1, 2, 3 [27].

We can also consider the following unidimensional integrals [6]

$$A^{(i)}(h) \equiv \frac{1}{h^i}\int_0^h (t - t_{1/2})^i A(t)\,\mathrm{d}t = \frac{1}{h^i}\int_{-h/2}^{h/2} t^i A(t + t_{1/2})\,\mathrm{d}t, \tag{19}$$

$i = 0, 1, \ldots, s-1$. If their analytical evaluation is not possible or is computationally expensive, a numerical quadrature may be used instead. In fact, the integrals $A^{(i)}$, $i \geqslant 1$, can be approximated up to the required order just by evaluating A at the nodes c_i of the quadrature rule required to compute $A^{(0)}$. Denoting these by $A_i \equiv A(t_0 + c_i h)$, $i = 1, \ldots, r$, one can write (terms of order greater than the order of the method itself are omitted)

$$A^{(i)} = h\sum_{j=1}^{r} \big(Q_C^{(s,r)}\big)_{ij} A_j, \quad i = 0, \ldots, s-1, \tag{20}$$

with

$$Q_C^{(s,r)} = \begin{pmatrix} b_1 & \ldots & b_r \\ \vdots & \ddots & \vdots \\ b_1(c_1 - \frac{1}{2})^{s-1} & \ldots & b_r(c_r - \frac{1}{2})^{s-1} \end{pmatrix} \tag{21}$$

and $Q_C^{(s,r)} \in \mathbb{R}^{s\times r}$. Here b_i, c_i are the weights and nodes, respectively, of a quadrature referred as C. For instance, using the fourth and sixth order Gauss–Legendre quadrature rules we obtain

$$Q_G^{(2,2)} = \begin{pmatrix} \frac{1}{2} & \frac{1}{2} \\ -\frac{\sqrt{3}}{12} & \frac{\sqrt{3}}{12} \end{pmatrix}, \qquad Q_G^{(3,3)} = \begin{pmatrix} \frac{5}{18} & \frac{4}{9} & \frac{5}{18} \\ -\frac{\sqrt{15}}{36} & 0 & \frac{\sqrt{15}}{36} \\ \frac{1}{24} & 0 & \frac{1}{24} \end{pmatrix}. \tag{22}$$

On the other hand, it is clear that $A^{(i)}(-h) = (-1)^{i+1}A^{(i)}(h)$, and

$$A^{(i)} = \sum_{j=1}^{s} \big(T^{(s)}\big)_{ij} b_j \equiv \sum_{j=1}^{s} \frac{1 - (-1)^{i+j}}{(i+j)2^{i+j}} b_j, \quad i = 0, 1, \ldots, s-1. \tag{23}$$

If this relation is inverted (to order four, $s = 2$, and six, $s = 3$) one has

$$R^{(2)} \equiv \big(T^{(2)}\big)^{-1} = \begin{pmatrix} 1 & 0 \\ 0 & 12 \end{pmatrix}, \qquad R^{(3)} = \begin{pmatrix} \frac{9}{4} & 0 & 15 \\ 0 & 12 & 0 \\ -15 & 0 & 180 \end{pmatrix}, \tag{24}$$

and the corresponding expression of b_i in terms of $A^{(k)}$ or A_j is then given by

$$b_i = \sum_{j=1}^{s} \big(R^{(s)}\big)_{ij} A^{(j-1)} = h\sum_{j=1}^{r} \big(R^{(s)} Q_C^{(s,r)}\big)_{ij} A_j. \tag{25}$$

Then, making use of (25) we can write $\Omega(h)$ in terms of the univariate integrals (19) and also in terms of any desired quadrature rule. For example, we can get the following fourth- and sixth-order approximations ($\Omega^{[2s]} = \Omega_1 + \cdots + \Omega_{2s-2} + \mathcal{O}(h^{2s+1}) = \Omega + \mathcal{O}(h^{2s+1})$)

$$\Omega^{[4]} = A^{(0)} + \big[A^{(1)}, A^{(0)}\big], \tag{26}$$

$$\Omega^{[6]} = A^{(0)} + \left[A^{(1)}, \frac{3}{2}A^{(0)} - 6A^{(2)}\right] + \frac{1}{2}\big[A^{(0)}, A^{(0)}, A^{(2)}\big] + \frac{3}{5}\big[A^{(1)}, A^{(1)}, A^{(0)}\big] + \frac{1}{60}\big[A^{(0)}, A^{(0)}, A^{(0)}, A^{(1)}\big]. \tag{27}$$

3.2. CF Magnus integrators

We have seen that $e^{\Omega^{[4]}}$ and $e^{\Omega^{[6]}}$ from (26) and (27) correspond to fourth- and sixth-order methods, respectively, which contain commutators. Alternatively, approximations up to the same order can be obtained by a product of exponentials of linear combinations of the $A^{(i)}$ which avoids the presence of commutators. For example, we can consider

$$\Psi_m^{[4]} \equiv \prod_{i=1}^{m} \exp\bigl(\alpha_i^{(0)} A^{(0)} + \alpha_i^{(1)} A^{(1)}\bigr) = \exp\bigl(\Omega^{[4]}\bigr) + \mathcal{O}\bigl(h^5\bigr), \tag{28}$$

$$\Psi_m^{[6]} \equiv \prod_{i=1}^{m} \exp\bigl(\alpha_i^{(0)} A^{(0)} + \alpha_i^{(1)} A^{(1)} + \alpha_i^{(2)} A^{(2)}\bigr) = \exp\bigl(\Omega^{[6]}\bigr) + \mathcal{O}\bigl(h^7\bigr), \tag{29}$$

where the coefficients $\alpha_k^{(i)}$ have to be determined. To work with the Lie algebra generated by the $A^{(i)}$s (or the A_is) is equivalent to work with the Lie algebra generated by the b_i. However, in the last case the problem simplifies considerably since the number of terms of the Lie algebra is reduced [27]. To get fourth- and sixth-order integrators it suffices to consider the graded free Lie algebra generated by $\{b_1, b_2\}$ and $\{b_1, b_2, b_3\}$, respectively. Then, the problem reduces to solve the equations (see (18))

$$\Psi_m^{[4]} \equiv \prod_{i=1}^{m} \exp(x_{i,1} b_1 + x_{i,2} b_2) = \exp\left(b_1 - \frac{1}{12}[b_1, b_2]\right) + \mathcal{O}\bigl(h^5\bigr), \tag{30}$$

$$\begin{aligned}\Psi_m^{[6]} &\equiv \prod_{i=1}^{m} \exp(x_{i,1} b_1 + x_{i,2} b_2 + x_{i,3} b_3) \\ &= \exp\left(b_1 + \frac{1}{12} b_3 - \frac{1}{12}[1,2] + \frac{1}{240}[2,3] + \frac{1}{360}[1,1,3] - \frac{1}{240}[2,1,2]\right. \\ &\quad \left. + \frac{1}{720}[1,1,1,2]\right) + \mathcal{O}\bigl(h^7\bigr).\end{aligned} \tag{31}$$

Here we can use, for example, the Baker–Campbell–Hausdorff (BCH) formula

$$e^A e^B = e^Z,$$

with

$$Z = A + B + \frac{1}{2}[A, B] + \frac{1}{12}\bigl([A, [A, B]] + [B, [B, A]]\bigr) + \frac{1}{24}\bigl[A, \bigl[B, [B, A]\bigr]\bigr] + \cdots. \tag{32}$$

Notice that the exact solution $\Omega(h)$ is time-symmetric and only odd terms appear in the equation. For example, the fourth-order commutators $[b_1, b_3] \equiv [1, 3]$ and $[b_1, [b_1, b_2]] \equiv [1, 1, 2]$ do not appear. Then those terms at even orders up to the order of the method have to be cancelled with a proper choice of the parameters $x_{i,j}$.

An integrator, ψ_h, is time-symmetric if $\psi_{-h}^{-1} = \psi_h$. Then the following symmetry for the coefficients

$$x_{m+1-i,j} = (-1)^{j+1} x_{i,j}, \quad j = 1, 2, 3 \tag{33}$$

makes the schemes (30) and (31) time-symmetric and all even order terms are cancelled. This constraint reduces the number of free parameters to solve the equations but, in general, it is compensated by the number of equations which are automatically solved. There are four order conditions for non-symmetric fourth-order methods but only two if the composition is time-symmetric. Similarly, there are fourteen order conditions for non-symmetric sixth-order methods but only seven if the composition is time-symmetric. Then, the minimum value of m in (30) and (31) remains the same if we consider either a symmetric or a non-symmetric composition. From the number of free parameters and order conditions it is clear that $m \geqslant 2$ to obtain fourth-order integrators and $m \geqslant 5$ to obtain sixth-order integrators. In addition, time-symmetry is an important property which in many cases is important to be preserved. For these reasons, in this paper we only consider time-symmetric compositions.

3.3. Fourth-order methods

In this section we present the order conditions to be satisfied by the coefficients $x_{i,j}$ for several time-symmetric fourth-order CF Magnus integrators. First, we illustrate in detail the procedure to obtain the methods (we neglect terms of order $\mathcal{O}(h^5)$). The order conditions are easily obtained from the recurrence given by the following time-symmetric composition

$$e^{xb_1+yb_2}\, e^{C(\beta^{(k)})} e^{xb_1-yb_2} = e^{C(\beta^{(k+1)})}, \tag{34}$$

where $\beta^{(k)} = (\beta_1^{(k)}, \beta_2^{(k)})$, $k = 0, 1, \ldots, N = \lfloor \frac{m}{2} \rfloor$ with $\lfloor x \rfloor$ the integer part of x, and

$$C\big(\beta^{(k)}\big) = \beta_1^{(k)} b_1 + \beta_2^{(k)} [b_1, b_2]. \tag{35}$$

The recurrence relations are then

$$\begin{cases} \beta_1^{(k+1)} = \beta_1^{(k)} + 2x, \\ \beta_2^{(k+1)} = \beta_2^{(k)} - y(\beta_1^{(k)} + x) \end{cases} \tag{36}$$

for $k = 0, 1, \ldots, N$. This recurrence has to be started with $\beta^{(0)} = (0, 0)$ if m is even or with $\beta^{(0)} = (\beta_1^{(0)}, 0)$ if m is odd and the exponential in the middle is $e^{\beta_1^{(0)} b_1}$. Finally we have to equate to the coefficients given in (18)

$$\big(\beta_1^{(N)}, \beta_2^{(N)}\big) = \left(1, -\frac{1}{12}\right).$$

Then we find the following order conditions for the coefficients $x_{i,1}, x_{i,2}$ for symmetric compositions with $m = 2, 3$ exponentials

$$\Psi_2^{[4]} \equiv \exp(x_{1,1} b_1 + x_{1,2} b_2) \exp(x_{1,1} b_1 - x_{1,2} b_2)$$

$$\left.\begin{aligned} 2x_{1,1} &= 1 \\ -x_{1,2} x_{1,1} &= -\tfrac{1}{12} \end{aligned}\right\} \implies x_{1,1} = \frac{1}{2}, \quad x_{1,2} = \frac{1}{6}, \tag{37}$$

$$\Psi_3^{[4]} \equiv \exp(x_{1,1} b_1 + x_{1,2} b_2) \exp(x_{2,1} b_1) \exp(x_{1,1} b_1 - x_{1,2} b_2)$$

$$\left.\begin{aligned} x_{2,1} + 2x_{1,1} &= 1 \\ -x_{1,2}(x_{2,1} + x_{1,1}) &= -\tfrac{1}{12} \end{aligned}\right\} \tag{38}$$

and if we take $x_{1,1} = 0$ then $x_{2,1} = 1, x_{1,2} = 1/12$. The solutions (37) and (38) (with $x_{1,1} = 0$) correspond to the fourth-order methods with two and three exponentials given in [7].

Example 1. To illustrate how to apply the CF Magnus integrator presented in this section we consider the simple example

$$\ddot{y} + f(t) y = 0, \qquad y(0) = y_0 \in \mathbb{R}, \tag{39}$$

which can be written in matrix form $\dot{\mathbf{x}} = A(t)\mathbf{x}$ with $\mathbf{x} = (y, \dot{y})^{\mathrm{T}}$ and

$$A(t) = \begin{pmatrix} 0 & 1 \\ -f(t) & 0 \end{pmatrix}. \tag{40}$$

If the fourth-order Gauss–Legendre quadrature rule is used then we have to compute $f_i = f(t_0 + c_i h)$, $c_i = \frac{1}{2} \mp \frac{\sqrt{3}}{6}$, $i = 1, 2$ to obtain $A_i = A(t_0 + c_i h)$, $i = 1, 2$. Finally, the two- and three-exponential CF Magnus integrators read

$$\mathbf{x}_h = \exp\left(\frac{1}{2} A^{(0)} + 2A^{(1)}\right) \exp\left(\frac{1}{2} A^{(0)} - 2A^{(1)}\right) \mathbf{x}_0, \tag{41}$$

$$\mathbf{x}_h = \exp\big(A^{(1)}\big) \exp\big(A^{(0)}\big) \exp\big(-A^{(1)}\big) \mathbf{x}_0, \tag{42}$$

with $\mathbf{x}_h \equiv \mathbf{x}(t_0 + h)$, or in terms of A_1, A_2 (where up to order four $A^{(0)} = \frac{h}{2}(A_1 + A_2)$, $\quad A^{(1)} = \frac{\sqrt{3}h}{12}(A_2 - A_1)$, using $A^{(i)} = (Q_G^{(2,2)})_{i,j} A_j$ from (22))

$$\mathbf{x}_h = \exp(\alpha_1 h A_1 + \alpha_2 h A_2)\exp(\alpha_2 h A_1 + \alpha_1 h A_2)\mathbf{x}_0, \tag{43}$$

$$\mathbf{x}_h = \exp\left(\frac{\sqrt{3}}{12}h(A_2 - A_1)\right)\exp\left(\frac{h}{2}(A_1 + A_2)\right)\exp\left(-\frac{\sqrt{3}}{12}h(A_2 - A_1)\right)\mathbf{x}_0 \tag{44}$$

with $\alpha_1 = \frac{3-2\sqrt{3}}{12}$, $\alpha_2 = \frac{3+2\sqrt{3}}{12}$.

Let us consider, for example, the Mathieu equation $\ddot{y} + (\omega^2 + \varepsilon\cos(t))y = 0$, with initial conditions $t_0 = 0$ and $(y(0), \dot{y}(0)) = (1, 0)$. The solutions can be either bounded and oscillating or unbounded, depending on the parameters ω and ε. This system is Hamiltonian with Hamiltonian function $H(q, p) = \frac{1}{2}p^2 + f(t)\frac{1}{2}q^2$ where $(q, p) = (y, \dot{y})$. If we consider, for example, the extended Hamiltonian system (we can avoid working with the momentum associated to x_t)

$$\frac{\mathrm{d}}{\mathrm{d}t}\begin{Bmatrix} q \\ p \\ x_t \end{Bmatrix} = \begin{Bmatrix} p \\ 0 \\ 1 \end{Bmatrix} + \begin{Bmatrix} 0 \\ -f(x_t)q \\ 0 \end{Bmatrix} \tag{45}$$

then splitting symplectic integrators as given in (6) can be used.

We now consider $\varepsilon = 1/4$ and $\varepsilon = 10/4$ for different values of ω and integrate along the interval $t \in [0, 20\pi]$. We assume that the evaluation of $f(t)$ is the most consuming part of the methods (although for this very simple problem it is not necessarily the case) and we use a time step h such that the whole integration is reached with 800 evaluations of the function f. The following fourth-order methods are compared: (i) the symplectic integrators given by the standard 3-stage method for a general splitting (S_4) and the 6-stage scheme for Nyström problems ($SRKN_4$) and the splitting (45) [9,20,13]; (ii) the standard 4-stage Runge–Kutta method (RK_4) (it uses the Lobatto quadrature, i.e. two evaluations of the time-dependent functions); (iii) the standard Magnus integrator (M_4) given by (26) and the integrals approximated as mentioned above; (iv) the CF Magnus integrators (43) ($CF2_4$) and (44) ($CF3_4$).

We measure the error of $(y, \dot{y})$ at $t = 20\cdot\pi$ in Euclidean norm. The exact solution has been accurately approximated using a sufficiently small time step. The results obtained are shown in Fig. 1. We observe that the accuracy of the splitting symplectic and RK methods highly deteriorate with ω. Obviously, the accuracy of all methods also diminishes in the zones of parametric resonances in the $\omega^2 - \varepsilon$ plane [2]. The RK_4 method is the only one which is not a GI having a larger error growth along the time, and it will be the least efficient after a few more periods. The error growth with ω for the symplectic splitting methods can be largely reduced if we consider the splitting $H = H_1 + H_2$ with $H_1 = \frac{1}{2}(p^2 + \omega^2 q^2)$ and $H_2 = \frac{1}{2}\varepsilon\cos(t)q^2$. However, the errors are still higher than for the Magnus methods and the efficient methods for Nyström problems cannot be used if, for example, ω depends on t.

This example clearly illustrates that CF Magnus integrators can be of similar or even higher accuracy than standard Magnus integrators. Notice that $A^{(0)} = \mathcal{O}(h)$ while $A^{(1)} = \mathcal{O}(h^2)$, so $A^{(0)}$ carries the main contribution to the solution. The scheme $CF2_4$ distributes this terms equally into the two exponentials allowing to get more accurate results for this

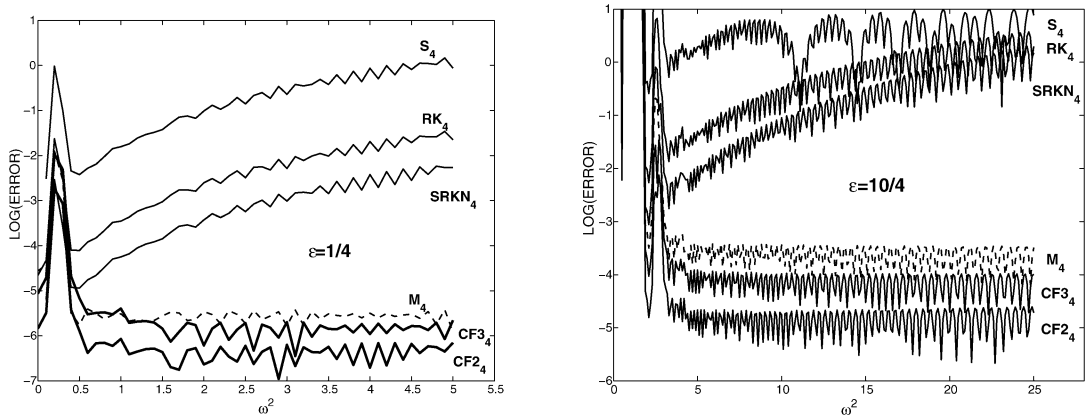

Fig. 1. Error of different numerical methods for the Mathieu equation $\ddot{y} + (\omega^2 + \varepsilon\cos(t))y = 0$ at $t = 20\cdot\pi$ with $\varepsilon = 1/4$ and $\varepsilon = 10/4$ for different values of ω. All methods require the same number of evaluations of $f(t) = \omega^2 + \varepsilon\cos(t)$.

problem, in agreement with the error analysis carried out in [8]. The advantage of $CF3_4$ comes from the simplicity in the computation of the exponentials of $A^{(1)}$ or $A_2 - A_1$ although for this problem this is not much relevant. In addition, as we show later, these methods can be easily adapted to a large number of non-linear equations. This justifies the interest to look for other fourth-order CF methods as well as to look for higher order methods.

From (30) and (33) it is clear that a time symmetric composition with m exponentials contains $m-2$ free parameters, and many different criterions to choose the free parameters can be considered. The simplicity of the order conditions up to order four allow us to build many different schemes tailored for different purposes. In Appendix A we illustrate some procedures to obtain other fourth-order CF methods which can be of interest for some particular problems.

3.4. Sixth-order methods

To build sixth-order CF Magnus integrators we first look for the order conditions to be satisfied by the coefficients of the method. For this purpose we consider the recurrence relations given by the time-symmetric composition

$$e^{xb_1+yb_2+zb_3} e^{C(\beta^{(k)})} e^{xb_1-yb_2+zb_3} = e^{C(\beta^{(k+1)})}, \tag{46}$$

where now $\beta^{(k)} = (\beta_1^{(k)}, \ldots, \beta_7^{(k)})$, $k = 0, 1, \ldots, N$ with

$$\begin{aligned} C(\beta^{(k)}) = {} & \beta_1^{(k)} b_1 + \beta_2^{(k)} b_3 + \beta_3^{(k)}[1,2] + \beta_4^{(k)}[2,3] + \beta_5^{(k)}[1,1,3] \\ & + \beta_6^{(k)}[2,1,2] + \beta_7^{(k)}[1,1,1,2]. \end{aligned} \tag{47}$$

Here we have neglected terms of order $\mathcal{O}(h^7)$. The order conditions are easily obtained from (46) if we consider

$$e^{xb_1+yb_2+zb_3}\ e^{C(\beta^{(k)})} = e^{C(\beta^{(k+1)})}\ e^{-xb_1+yb_2-zb_3}. \tag{48}$$

Notice that the composition is time-symmetric and we need only to consider odd order terms up order five. The recurrence relations can be obtained using the BCH formula (32) up fourth order because the element with the higher number of nested commutators is $[b_1,[b_1,[b_1,b_2]]] = \mathcal{O}(h^5)$. Then, equating terms we obtain

$$\begin{aligned} \beta_1^{(k+1)} &= \beta_1^{(k)} + 2x, \\ \beta_2^{(k+1)} &= \beta_2^{(k)} + 2z, \\ \beta_3^{(k+1)} &= \beta_3^{(k)} - \frac{1}{2}\big(\beta_1^{(k+1)} + \beta_1^{(k)}\big)y, \\ \beta_4^{(k+1)} &= \beta_4^{(k)} + \frac{1}{2}\big(\beta_2^{(k+1)} + \beta_2^{(k)}\big)y, \\ \beta_5^{(k+1)} &= \beta_5^{(k)} + \frac{1}{12}\big(x - \beta_1^{(k)}\big)\big(\beta_2^{(k)}x - \beta_1^{(k)}z\big) - \frac{1}{12}\big(x + \beta_1^{(k+1)}\big)\big(\beta_2^{(k+1)}x - \beta_1^{(k+1)}z\big), \\ \beta_6^{(k+1)} &= \beta_6^{(k)} + \frac{1}{2}\big(\beta_3^{(k+1)} + \beta_3^{(k)}\big)y + \frac{1}{12}\big(\beta_1^{(k+1)} - \beta_1^{(k)}\big)y^2, \\ \beta_7^{(k+1)} &= \beta_7^{(k)} + \frac{1}{12}\big(\big(x - \beta_1^{(k)}\big)\beta_3^{(k)}x - \big(\beta_1^{(k+1)} + x\big)\beta_3^{(k+1)}x\big) + \frac{1}{24}\big(\big(\beta_1^{(k)}\big)^2 - \big(\beta_1^{(k+1)}\big)^2\big)xy. \end{aligned} \tag{49}$$

This recurrence has to be started with $\beta^{(0)} = (0, \ldots, 0)$ if m is even or with $\beta^{(0)} = (\beta_1^{(0)}, \beta_2^{(0)}, 0, \ldots, 0)$ if m is odd and the exponential in the middle is $e^{\beta_1^{(0)}b_1 + \beta_2^{(0)}b_3}$. The final equations are obtained by equating to the coefficients in (18), i.e.

$$\big(\beta_1^{(N)}, \ldots, \beta_7^{(N)}\big) = \left(1, \frac{1}{12}, -\frac{1}{12}, \frac{1}{240}, \frac{1}{360}, -\frac{1}{240}, \frac{1}{720}\right).$$

A symmetric composition with 4 exponentials has only 6 free parameters for the seven order conditions, so at least $m \geqslant 5$ exponentials has to be considered. If $m = 5$, we have 8 coefficients and one of them can be considered as a free parameter. In general, a composition with $m \geqslant 5$ exponentials has $\lfloor \frac{3}{2}(m-5)+1 \rfloor$ free parameters. Since $b_i = \mathcal{O}(h^i)$, it is clear that the coefficients $x_{i,1}$ of b_1 in (31) play the most important role. With the constraint $\sum_{i=1}^m x_{i,1} = 1$ we

Table 1
Coefficients for time-symmetric sixth-order CF Magnus integrators given by the composition (31) with 5 and 6 exponentials

$\Psi_5^{[6]}$		
$x_{1,1} = 0.2$	$x_{1,2} = 0.08734395950888931101$	$x_{1,3} = 0.03734395950888931101$
$x_{2,1} = 0.34815492558797391479$	$x_{2,2} = 0.053438272547684150$	$x_{2,3} = 0.00584269157837031012$
$x_{3,1} = 1 - 2(x_{1,1} + x_{2,1})$	$x_{3,2} = 0$	$x_{3,3} = 1/12 - 2(x_{1,3} + x_{2,3})$
$\Psi_6^{[6]}$		
$x_{1,1} = 0.208$	$x_{1,2} = 0.09023186422416794596$	$x_{1,3} = 0.03823186422416794596$
$x_{2,1} = 0.312$	$x_{2,2} = 0.04467385661651479788$	$x_{2,3} = 0.00439421553992544024$
$x_{3,1} = 1/2 - (x_{1,1} + x_{2,1})$	$x_{3,2} = 0.01407960659498524468$	$x_{3,3} = 1/24 - (x_{1,3} + x_{2,3})$

can try, for example, to minimize the value $\sum_{i=1}^{m} |x_{i,1} - \frac{1}{m}|$, keeping the other coefficients still small. This can be done, for example, if we define the objective function $\mathcal{E} = \sum_i (|x_{i,1} - \frac{1}{m}| + \alpha_1 |x_{i,2}| + \alpha_2 |x_{i,3}|)$ for some appropriate values α_1 and α_2. Some values which gave acceptable results in practice are $\alpha_1 = 4$ and $\alpha_2 = 10$. The coefficients of the schemes with 5 and 6 exponentials given in Table 1 correspond, approximately, to local minima of $\mathcal{E}$. Obviously, other criterions as well as additional exponentials can be considered which can lead to more efficient methods for some problems. Other schemes with a higher number of exponentials have been also analyzed but not much more accurate methods for the numerical experiments considered have been found. Finally the parameters $\rho_{i,j}$ of (9) or (11) are given by

$$\rho_{i,j} = \left(X R^{(s)} Q_C^{(s,r)}\right)_{i,j} \tag{50}$$

with $X_{i,j} = x_{i,j}$. Here, $R^{(s)}$ is given by (23)–(24) for methods of order $q = 2s$, then $Q_C^{(s,r)}$ is obtained once the quadrature is chosen and X depends only on m and q.

4. CF Magnus integrators for non-linear systems

Let us first consider the autonomous equation

$$\dot{\mathbf{x}} = \mathbf{f}(\mathbf{x}) \tag{51}$$

or, in order to follow the same notation as in the previous section, it is preferable to consider

$$\dot{\mathbf{x}} = D\mathbf{F}(\mathbf{x}) \tag{52}$$

where D can be the identity matrix. If φ_D^t denotes the exact flow of (52) (with $t_0 = 0$), i.e. $\mathbf{x}(t) = \varphi_D^t(\mathbf{x}_0)$, then for each infinitely differentiable map $g : \mathbb{R}^d \to \mathbb{R}$, $g(\varphi_D^t(\mathbf{y}))$ admits the representation

$$g\left(\varphi_D^t(\mathbf{y})\right) = \Phi_D^t[g](\mathbf{y}) \tag{53}$$

where Φ_D^t acts on differentiable functions (it is a Lie transform). Φ_D^t is the solution of a differential equation closely related to (52) which can be written as

$$\frac{\mathrm{d}}{\mathrm{d}t} Id_j(\mathbf{x}) = L_{\mathbf{f}(\mathbf{x})} Id_j(\mathbf{x}), \quad j = 1, \ldots, d \tag{54}$$

where $Id_j(\mathbf{x}) = x_j$ is the projection onto the jth component and $L_{\mathbf{f}}$ is the Lie derivative (or Lie operator) associated to $\mathbf{f}$ given by

$$L_{\mathbf{f}} = \sum_{i=1}^{d} f_i \frac{\partial}{\partial x_i} \tag{55}$$

acting on differentiable functions (see [2, Chapter 8] for more details). If we consider the map φ_D^t as a change of coordinates $\mathbf{z} = \varphi_D^t(\mathbf{y})$ (where at the end we can take $\mathbf{z} = \mathbf{x}$ and $\mathbf{y} = \mathbf{x}_0$) then (54) can be written as

$$\frac{\mathrm{d}}{\mathrm{d}t} \Phi_D^t[Id_j](\mathbf{y}) = \Phi_D^t L_{\mathbf{f}(\mathbf{y})}[Id_j](\mathbf{y}), \quad j = 1, \ldots, d, \quad \mathbf{y} = \mathbf{x}_0 \tag{56}$$

or, shortly, we can write

$$\frac{\mathrm{d}}{\mathrm{d}t}\Phi_D^t = \Phi_D^t L_{\mathbf{f}(\mathbf{y})}, \quad \mathbf{y} = \mathbf{x}_0, \tag{57}$$

with formal solution

$$\Phi_D^t = \exp(t L_{\mathbf{f}(\mathbf{y})}) \equiv \left(\sum_{k=0}^{\infty} \frac{t^k}{k!} L_{\mathbf{f}(\mathbf{y})}^k \right), \quad \mathbf{y} = \mathbf{x}_0 \tag{58}$$

with $L_{\mathbf{f}}^i \psi = L_{\mathbf{f}}(L_{\mathbf{f}}^{i-1}\psi)$ and $L_{\mathbf{f}}^0 \psi = \psi$. Here $\exp(t L_{\mathbf{f}})$ is the Lie transform associated with $\mathbf{f}$.

Suppose now that φ_D^t can be decomposed as $\varphi_D^t = \varphi_{D_1}^{t_1} \circ \varphi_{D_2}^{t_2}$ with

$$g\big(\varphi_{D_i}^{t_i}(\mathbf{y})\big) = \exp(L_{\mathbf{f}_i})[g](\mathbf{y}), \quad i = 1, 2 \tag{59}$$

where we use the notation from (5) with $\mathbf{f}_i = D_i \mathbf{F}$. Then it is clear that

$$g\big(\varphi_{D_1}^{t_1} \circ \varphi_{D_2}^{t_2}(\mathbf{y})\big) = \exp(L_{\mathbf{f}_2}) \exp(L_{\mathbf{f}_1})[g](\mathbf{y}), \tag{60}$$

i.e. the Lie transforms appear in the reverse order as their corresponding maps. This is also manifest on Eq. (57), which is an infinite-dimensional linear system where the linear operator $L_{\mathbf{f}}$ is now on the right side of Φ_D^t.

We can follow the same steps for the non-autonomous equation (1) or (2). The exact solution is denoted by $\mathbf{x}(t) = \varphi_B^t(\mathbf{x}_0)$ where $g(\varphi_B^t(\mathbf{y})) = \Phi_B^t[g](\mathbf{y})$ and Φ_B^t is the solution of the time-dependent linear equation [8]

$$\frac{\mathrm{d}}{\mathrm{d}t}\Phi_B^t = \Phi_B^t L_{\mathbf{f}(t,\mathbf{y})}, \quad \mathbf{y} = \mathbf{x}_0. \tag{61}$$

To simplify notation, from now on we consider $\mathbf{x}_0$ as a set of coordinates such that $\mathbf{f}(t, \mathbf{x}_0)$ is a differentiable function on the coordinates $\mathbf{x}_0$.

We can then use the Magnus series expansion to obtain the formal solution $\Phi_{\mathbf{f}}^t = \exp(L_{\mathbf{w}(t,\mathbf{x_0})})$, with $\mathbf{w} = \sum_i \mathbf{w}_i$. The first two terms are now

$$\mathbf{w}_1(t, \mathbf{x}_0) = \int_0^t \mathbf{f}(s, \mathbf{x}_0)\,\mathrm{d}s; \qquad \mathbf{w}_2(t, \mathbf{x}_0) = -\frac{1}{2}\int_0^t \mathrm{d}s_1 \int_0^{s_1} \mathrm{d}s_2 \big(\mathbf{f}(s_1, \mathbf{x}_0), \mathbf{f}(s_2, \mathbf{x}_0)\big).$$

Here we have considered the following property: given the vector fields $\mathbf{f}$ and $\mathbf{g}$ then

$$[L_{\mathbf{f}}, L_{\mathbf{g}}] = L_{\mathbf{f}} L_{\mathbf{g}} - L_{\mathbf{g}} L_{\mathbf{f}} = L_{\mathbf{h}}, \tag{62}$$

where $\mathbf{h}$ is another vector field corresponding to the Lie bracket of the vector fields, $\mathbf{h} = (\mathbf{f}, \mathbf{g})$, whose components are

$$h_i = (\mathbf{f}, \mathbf{g})_i = L_{\mathbf{f}} g_i - L_{\mathbf{g}} f_i = \sum_{j=1}^{n} \left(f_j \frac{\partial g_i}{\partial x_j} - g_j \frac{\partial f_i}{\partial x_j} \right). \tag{63}$$

Observe that the sign of $\mathbf{w}_2$ is changed when compared with Ω_2 in (14).

Then, if we can write (1) as in (2) it is straightforward to adapt the Magnus integrators studied for the linear problem in the previous section to the non-linear problem. Let us denote $\mathbf{f}^{(i)}(\mathbf{x}_0) = D^{(i)}\mathbf{F}(\mathbf{x}_0)$ with $L_{D^{(i)}}$ the associated Lie operator and $D^{(i)}$ defined similarly to $A^{(i)}$ in (19)

$$D^{(i)} = \frac{1}{h^i} \int_{-h/2}^{h/2} t^i B(t + t_{1/2})\,\mathrm{d}t. \tag{64}$$

Then, the fourth-order Magnus integrator $\exp(\Omega^{[4]})$ given by (26) corresponds now to the Lie transform $\exp(L_{\mathbf{w}^{[4]}})$ with

$$L_{\mathbf{w}^{[4]}} = L_{D^{(0)}} - [L_{D^{(1)}}, L_{D^{(0)}}] \tag{65}$$

which is the Lie operator associated to the vector field

$$\mathbf{w}^{[4]}(\mathbf{x}_0) = \mathbf{f}^{(0)}(\mathbf{x}_0) - \big(\mathbf{f}^{(1)}(\mathbf{x}_0), \mathbf{f}^{(0)}(\mathbf{x}_0)\big). \tag{66}$$

Similarly to (15) and (16), to evaluate this Lie transform is equivalent to compute the 1-flow solution of the autonomous differential equation

$$\dot{\mathbf{x}} = \mathbf{w}^{[4]}(\mathbf{x}), \qquad \mathbf{x}(0) = \mathbf{x}_0. \tag{67}$$

However, the Lie bracket involved in $\mathbf{w}^{[4]}$ makes very difficult, in general, the computation of the solution or to obtain an approximation to it.

On the other hand, as we mentioned, it could be possible to have efficient integrators for Eq. (2) when the time is frozen and this is the case for a large number of problems of practical interest.

Given the autonomous equation

$$\dot{\mathbf{x}} = \mathbf{f}^{(i)}(\mathbf{x}) = D^{(i)}\mathbf{F}(\mathbf{x}) \tag{68}$$

we denote its solution by $\mathbf{x}(t) = \varphi_{D^{(i)}}(\mathbf{x}_0)$ and an appropriate numerical method by $\mathbf{x}(t) = \psi_{D^{(i)}}(\mathbf{x}_0)$. If we cannot write (1) as in (2) the same results remain still valid by considering the autonomous vector fields

$$\mathbf{f}^{(i)}(\mathbf{x}) = \frac{1}{h^i}\int_{-h/2}^{h/2} t^i \mathbf{f}(t + t_{1/2}, \mathbf{x})\,\mathrm{d}t \tag{69}$$

or we can take numerical approximations for the integrals as previously.

In this case CF Magnus integrators are a viable alternative. The same methods obtained for the linear problem can also be used, and the fourth- and sixth-order methods (28) and (29) are given by

$$\Psi_m^{[4]} \equiv \prod_{i=m}^{1} \exp(L_{\alpha_i^{(0)} D^{(0)} + \alpha_i^{(1)} D^{(1)}}) = \exp(L_{\mathbf{w}^{[4]}}) + \mathcal{O}\big(h^5\big), \tag{70}$$

$$\Psi_m^{[6]} \equiv \prod_{i=m}^{1} \exp(L_{\alpha_i^{(0)} D^{(0)} + \alpha_i^{(1)} D^{(1)} + \alpha_i^{(2)} D^{(2)}}) = \exp(L_{\mathbf{w}^{[6]}}) + \mathcal{O}\big(h^7\big) \tag{71}$$

with the same coefficients $\alpha_k^{(i)}$. Notice that due to property (60) the exponentials appear in the reverse order.

Let us denote

$$D_i = \sum_{k=1}^{s} \big(X R^{(s)}\big)_{i,k} D^{(k)} = \sum_{j=1}^{r} \big(X R^{(s)} Q_C^{(s,r)}\big)_{i,j} B_j \tag{72}$$

with $B_j = B(c_j h)$, $(X R^{(s)})_{i,k} = \alpha_i^{(k)}$ and $X \in \mathbb{R}^{m\times s}$ is the matrix with coefficients $X_{i,j} = x_{i,j}$. Then, it is clear that

$$g\big(\psi_{D_1} \circ \cdots \circ \psi_{D_m}(\mathbf{y})\big) = \exp(L_{D_m}) \cdots \exp(L_{D_1})[g](\mathbf{y}). \tag{73}$$

In other words, the maps ψ_{D_i} act in the same order as the exponentials of the matrices for the linear problem.

To sum up, the methods proposed are:

(i) For the linear problem $\dot{\mathbf{x}} = A(t)(\mathbf{x})$ with solution $\mathbf{x}(t) = \exp(\Omega)\mathbf{x}_0$ we propose the methods

$$\Psi_m^{[q]} \equiv \exp(D_1) \cdots \exp(D_m) \tag{74}$$

where $\Psi_m^{[q]} = \exp(\Omega) + \mathcal{O}(h^{q+1})$ with $q = 4, 6$ and the matrices are given by (72) replacing the matrices B_i by A_i.

(ii) For the non-linear problem $\dot{\mathbf{x}} = \mathbf{f}(t, \mathbf{x})$ or $\dot{\mathbf{x}} = B(t)\mathbf{F}(\mathbf{x})$ with formal solution $\mathbf{x}(t) = \varphi_B^t(\mathbf{x}_0)$ we propose

$$\Psi_m^{[q]} \equiv \psi_{D_1} \circ \cdots \circ \psi_{D_m} \tag{75}$$

where $\Psi_m^{[q]} = \varphi_B^t + \mathcal{O}(h^{q+1})$ with $q = 4, 6$. As mentioned, ψ_{D_i} is a map which approximates the autonomous equation $\dot{\mathbf{x}} = \mathbf{f}_i(\mathbf{x})$ or $\dot{\mathbf{x}} = D_i\mathbf{F}(\mathbf{x})$.

Example 2. (i) In order to illustrate how the CF Magnus integrators apply to non-linear systems, we consider the Abel's equation

$$\dot{x} = a_0(t) + a_1(t)x + a_2(t)x^2 + a_3(t)x^3 + a_4(t)x^4, \qquad x(0) = x_0 \in \mathbb{R} \tag{76}$$

with $a_i(t)$ sufficiently smooth functions. Obviously, this equation can be written as (2) with $B(t) = (a_0, \ldots, a_4)$, $\mathbf{F}(\mathbf{x}) = (1, x, \ldots, x^4)^{\mathrm{T}}$. We denote the solution we intend to approximate by $x(t) = \varphi_B^t(x_0)$. Let us now consider the autonomous equation

$$\dot{x} = \alpha_0 + \alpha_1 x + \alpha_2 x^2 + \alpha_3 x^3 + \alpha_4 x^4, \tag{77}$$

with α_i, $i = 0, \ldots, 4$ constants. The solution of this equation for one time step h, ψ_D^h, with $D = (\alpha_0, \ldots, \alpha_4)$ can be computed either exactly or accurately approximated with a numerical integrator. Notice that, contrarily to Eq. (76), the right-hand side of (77) is very cheap to compute because it is an autonomous polynomial function, and a high order numerical integrator can be used cheaply to get an accurate approximation. For example, $\mathrm{CF2}_4$ is now given by

$$\psi_2^{[4]}(x_0) = \psi_{D_1} \circ \psi_{D_2}(x_0) \tag{78}$$

where

$$D_{1/2} = \frac{1}{2} D^{(0)} \pm D^{(1)} \quad \text{with } D^{(i)} = \big(a_0^{(i)}, \ldots, a_4^{(i)}\big), \tag{79}$$

and $a_j^{(i)}$ are approximations to the unidimensional integrals. Using the fourth-order Gaussian quadrature we obtain

$$a_j^{(0)} = \frac{h}{2}(a_{j,1} + a_{j,2}), \qquad a_j^{(1)} = \frac{\sqrt{3}h}{12}(a_{j,2} - a_{j,1})$$

and $a_{j,i} = a_j(t_0 + c_i h)$, $c_i = \frac{1}{2} \mp \frac{\sqrt{3}}{6}$, $j = 0, 1, 2, 3, 4$, $i = 1, 2$. This method requires then two evaluations of each function $a_j(t)$ and two evaluations of the map ψ_D. Notice the similarity with (41). Other fourth- and sixth-order schemes apply similarly.

(ii) Let us consider the linear non-homogeneous equation

$$\frac{\mathrm{d}\mathbf{x}}{\mathrm{d}t} = A(t)\mathbf{x} + \mathbf{b}(t), \quad \mathbf{x}, \mathbf{b} \in \mathbb{R}^d, \ A \in \mathbb{R}^{d \times d}, \tag{80}$$

where, for sufficiently small t, the solution can be written as

$$\mathbf{x}(t) = \varphi_B^t(\mathbf{x}_0) \equiv e^{\Omega(t,0)}\mathbf{x}_0 + \int_0^t e^{\Omega(t,\tau)}\mathbf{b}(\tau)\,\mathrm{d}\tau, \tag{81}$$

and $\mathbf{x}(t) = e^{\Omega(t,0)}\mathbf{x}_0$ denotes the solution of the homogeneous system. It is well known that the solution of the autonomous equation (A, $\mathbf{b}$ constants) is given by

$$\mathbf{x}(t) = \psi_{A,\mathbf{b}}^t(\mathbf{x}_0) \equiv e^{tA}\mathbf{x}_0 + \frac{e^{tA} - I}{A}\mathbf{b}. \tag{82}$$

Then, one step with $\mathrm{CF2}_4$ is given by the composition

$$\psi_2^{[4]}(\mathbf{x}_0) = \psi_{D_1,\mathbf{d}_1} \circ \psi_{D_2,\mathbf{d}_2}(\mathbf{x}_0) = \varphi_B^t(\mathbf{x}_0) + \mathcal{O}\big(h^5\big), \tag{83}$$

with

$$D_{1/2} = \frac{1}{2}A^{(0)} \pm 2A^{(1)}, \qquad \mathbf{d}_{1/2} = \frac{1}{2}\mathbf{b}^{(0)} \pm 2\mathbf{b}^{(1)}$$

and if desired we can use different quadrature rules to approximate $A^{(i)}$ and $\mathbf{b}^{(i)}$.

5. Numerical examples

In this section we analyze the performance of the CF methods on some numerical examples. We compare with explicit fourth- and sixth-order RK methods which require the minimum number of time-dependent function evaluations per step. Let us consider the general RK scheme

$$\mathbf{k}_l = \mathbf{f}\left(t_n + c_l h, \mathbf{x}_n + h\sum_{j=1}^{\nu} a_{l,j}\mathbf{k}_j\right), \quad l = 1,\ldots,\nu, \tag{84}$$

$$\mathbf{x}_{n+1} = \mathbf{x}_n + h\sum_{l=1}^{\nu} b_l \mathbf{k}_l, \tag{85}$$

with $c_l = \sum_{j=1}^{\nu} a_{l,j}$, $l = 1,\ldots,\nu$. Using Lobatto III quadrature points one can build implicit methods of order $2\nu-2$. On the other hand, it is known that using the same quadrature points for the c_l, explicit methods of the same order (but with a higher number of stages [12,10]) can be obtained. For example, the standard four-stage fourth-order RK method has $c_1 = 0$, $c_2 = c_3 = 1/2$, $c_4 = 1$. A seven-stage sixth-order method using $c_1 = 0$, $c_2 = \frac{5-\sqrt{5}}{10}$, $c_3 = \frac{5+\sqrt{5}}{10}$, $c_4 = c_2$, $c_5 = c_3$, $c_6 = c_2$, $c_7 = 1$ can be obtained [10]. Notice that since $c_1 = 0$ and $c_\nu = 1$ the last evaluation in one step can be reused in the next step saving one evaluation, and we count only n evaluations for a method of order $2n$.

5.1. Example I: the non-homogeneous Hill's equation

It is given by the second order equation

$$\ddot{y} + f(t)y = g(t), \quad \text{with } f(t) = \theta_0 + 2\sum_{n=1}^{\infty}\theta_n\cos(2nt). \tag{86}$$

It is clear that, in general, the most costly part of the numerical integrators will come from the evaluations of $f(t)$ and $g(t)$. This system has a Hamiltonian structure and then some geometric properties are preserved. The methods presented in this paper are GI when applied to this problem, and are optimal with respect to the number of evaluations of f and g. We consider the following particular cases:

(i) For simplicity we first consider $g = 0$ and $\theta_n = 0$, $n \geqslant 2$ which corresponds to the Mathieu equation. To follow the notation used in Example 1, we consider (with a simple transformation) $f(t) = \omega^2 + \varepsilon\cos(t)$. We repeat the same experiment as in Fig. 1 for $\varepsilon = 1/4$ and include the results obtained for the sixth-order RK (RK_6) and CF Magnus methods with 5 exponentials ($\mathrm{CF5}_6$) and with 6 exponentials ($\mathrm{CF6}_6$). The results obtained are shown in Fig. 2. The results for $\mathrm{CF6}_6$ are very similar to those of $\mathrm{CF5}_6$ and, for simplicity, they are not shown in the following.

Next, we take $\omega^2 = 5$ and measure the average error at $t = k\cdot 2\pi$, $k = 1,\ldots,10$ for different time steps. Fig. 3 shows, in a logarithmic scale, this error versus the number of evaluations of $f(t)$, N_t. This figure clearly illustrates the superiority of the CF Magnus integrators. It is also worth to remark the excellent stability property of the Magnus integrators (the largest time step shown is $h = 2\pi$ although even larger time steps give stable solutions). We must remember that this difference with respect to RK methods increases for longer times because they are not GIs. The splitting symplectic integrators (with the splitting considered in Fig. 1) have similar stability properties as RK methods.

(ii) We now consider the case $\theta_n = 0$, $n \geqslant 3$ which corresponds to the Wittaker–Hill's equation and we include the non-homogeneous term $g = 10/\cosh^2(t/10)$. This system can be rewritten as in Example 2(ii) with $\mathbf{b}(t) = (0, g(t))^{\mathrm{T}}$ and CF Magnus integrators can be easily implemented using the map (82). We take $\theta_0 = 10$, $\theta_1 = \theta_2 = 1/20$ with initial conditions $(y(0), \dot{y}(0)) = (1, 0)$ and integrated the system until $t = 20\pi$ using different time steps. Fig. 4 shows the efficiency curves obtained with the RK and CF Magnus integrators.

5.2. Example II

Let us now consider the following Abel's equation

$$\dot{x} = ax - \big(b + c\cos(\pi t)\big)x^3 \tag{87}$$

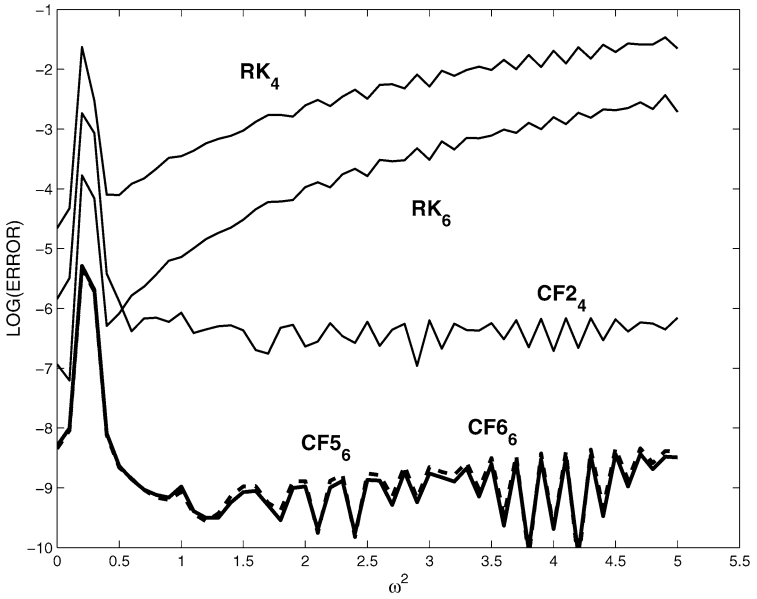

Fig. 2. Same numerical experiments as in Fig. 1 for $\varepsilon = 1/4$ but including the sixth-order RK (RK_6) method and the sixth-order CF Magnus integrators with 5 exponentials ($CF5_6$) and with 6 exponentials ($CF6_6$).

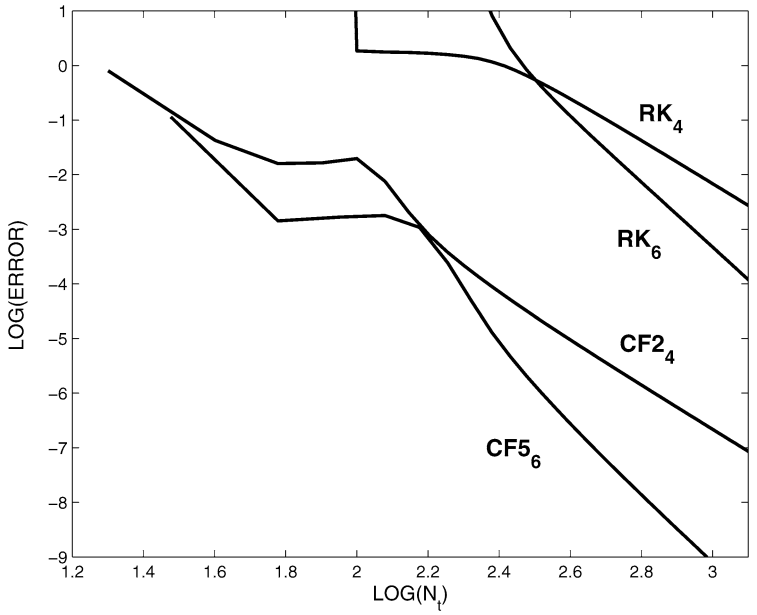

Fig. 3. Error versus number of time-dependent function evaluations, N_t, in logarithmic scale, for the RK and the CF Magnus integrators.

with initial conditions $x(0) = 1$. The exact solution is given by

$$x(t) = \left[\frac{b}{a} + A\cos(\pi t) + B\sin(\pi t) - Ce^{-2at}\right]^{-1/2},$$

with $A = 4ac/D$, $B = 2c\pi/D$, $C = (4a^2(a-b-c) + (a-b)\pi)/(aD)$, $D = 4a^2 + \pi^2$, corresponding to a solution which has an exponentially decaying term, it is asymptotically oscillatory and can blow-up at a given instant depending on the values of the parameters a, b, c. We take $a = 1/10$, $b = 1$ and different values of c, where for $c > 4.92\ldots$ the solution has a singularity.

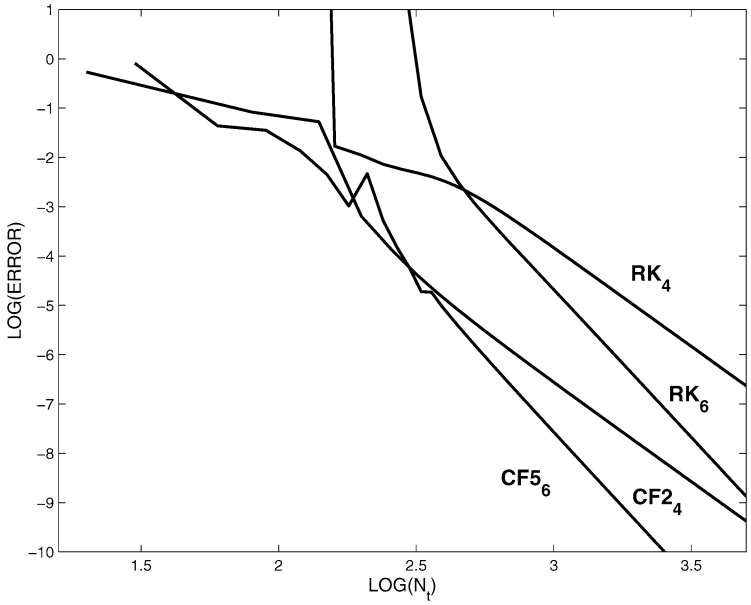

Fig. 4. Error versus N_t for the RK and the CF Magnus integrators for the Wittaker–Hill's equation (86) where $f(t) = \theta_0 + 2(\theta_1 \cos(2t) + \theta_2 \cos(4t))$ with $\theta_0 = 10$, $\theta_1 = \theta_2 = 1/20$ and $g = 10/\cosh^2(t/10)$.

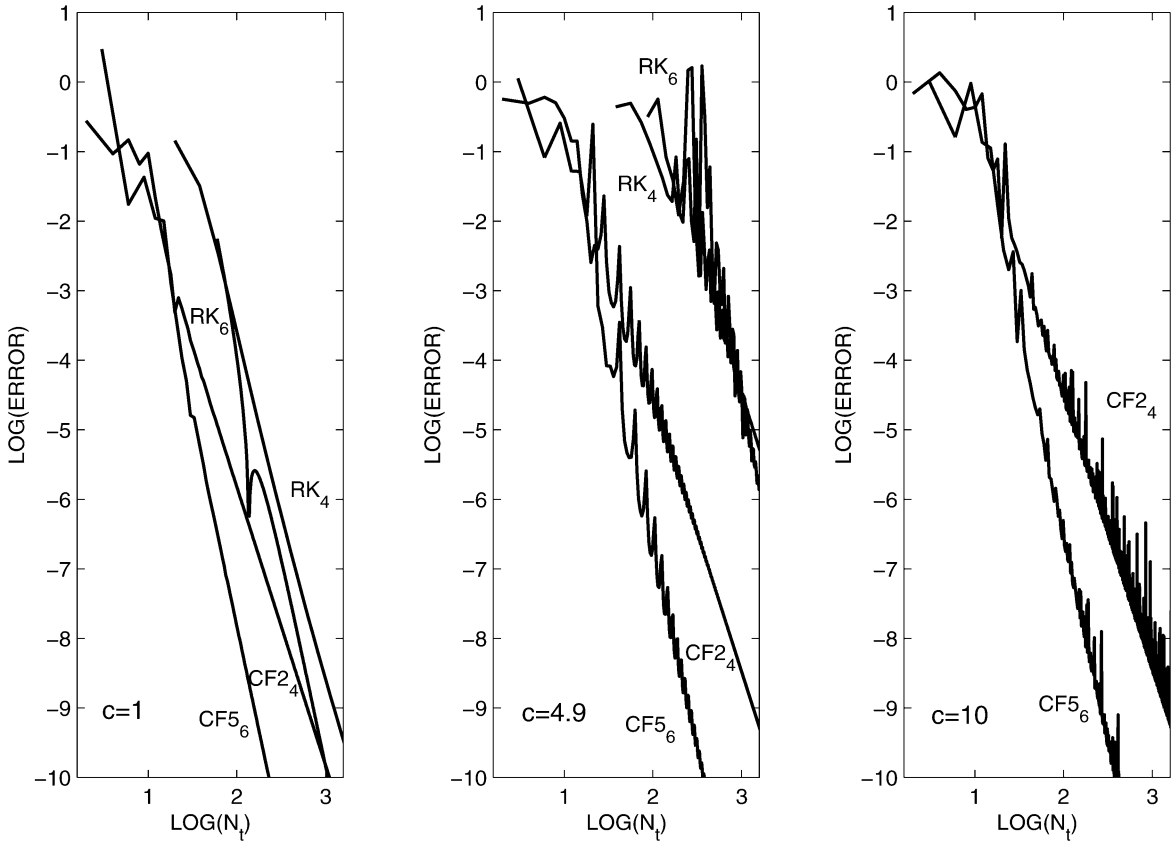

Fig. 5. Error versus number of time-dependent function evaluations for the RK and the CF Magnus integrators for the Abel's equation (87) with $a = 1/10$, $b = 1$, and $c = 1, 4.9, 10$. In the last case, the RK methods break-down at the singularity and do not give any solution.

Let us now consider the autonomous equation $\dot{x} = ax - bx^3$ with solution given by the map

$$x(t) = \psi^t_{a,b}(x_0, t_0) = \left[\frac{b}{a} - C(x_0, t_0)e^{-2at}\right]^{-1/2}, \tag{88}$$

with $C(x_0, t_0) = e^{2at_0}(\frac{b}{a} - \frac{1}{x_0^2})$. We integrate the system (87) until $t = 10$ and measure the average relative error for different time steps. Fig. 5 show the results obtained with the RK and the CF Magnus integrators (using the map (88)) for $c = 1$, $c = 4.9$ and $c = 10$. Notice that in the last case the exact solution blow-up at a given instant and after that the solution is oscillatory. Obviously, the RK methods fail to give any result and, surprisingly, the CF Magnus integrators are able to cross the singularity and still give accurate results. Notice that the efficiency curves are not much deteriorated when increasing the value of c. The small pics are due to the fact that for some values of the time step some discretised times, $t_n = t_0 + nh$, can stay very close to the singular point.

6. Conclusions and outlook

Starting with the Magnus integrators for linear systems, we have obtained factored methods of order 4 and 6 which through simulations have proven themselves as efficient. By avoiding the nested commutators of standard Magnus methods, the new methods can easily be applied to non-linear problems. The removal of the commutators implied factorizations into flows/exponentials which, depending on the particular application might not be a significant cost. Clearly, before a definite assessment of the performance of the new methods can be made, much additional numerical experimentation is needed. However, from the preliminary results obtained, we believe the CF Magnus integrators can be of interest for the numerical integration of many ODEs and PDEs.

As mentioned, Magnus integrators have proved to be efficient for the linear time dependent Schrödinger equation [7,14] for time steps outside the convergence interval of the Magnus series [5,23,24]. Then, a similar analysis for CF Magnus integrators would also be of interest[1] as it might shed some light on how to improve such methods.

Since Magnus integrators can be considered as exponential integrators, it is also interesting to analyze the performance of the CF Magnus integrators on stiff differential equations. For instance, time-dependent semilinear parabolic problems of the form

$$\dot{\mathbf{x}} = A(t)\mathbf{x} + \mathbf{g}(t, \mathbf{x}), \tag{89}$$

and for which efficient (possibly Runge–Kutta) exponential integrators for the autonomous problem are known (see [15,28] and references therein for more information on exponential integrators). The CF Magnus integrator with two exponentials and Gauss–Legendre quadrature then requires the solution of two autonomous parabolic equations which can efficiently be done using e.g. an exponential integrator.

It is worth to mention that for separable non-linear differential equations it is possible to adapt the methods presented to non-autonomous separable systems [4], obtaining e.g. very efficient symplectic schemes.

Finally, the following problems are under consideration at this moment:

(i) as mentioned, symmetric schemes of order four and six require the same minimum number of exponentials as non-symmetric methods. However, the numerical solutions for their parameters could lead to efficient methods for some particular problems;
(ii) higher order methods can also be obtained following this procedure. For instance, eight-order schemes require to consider the Lie algebra generated by $\{b_1, b_2, b_3, b_4\}$, where a symmetric method has to solve 22 order conditions. A symmetric composition with $m \geqslant 11$ exponentials has $2(m - 11)$ free parameters. The complexity of these schemes is significant and it is not clear if they can lead to efficient methods.

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[1] After the submission of this work Ref. [28] appeared where this problem is addressed for the CF Magnus integrators with two exponentials and Gauss–Legendre quadrature.

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Appendix A. Some optimized fourth-order CF methods

As analyzed in [23] the accuracy of Magnus integrators can be hampered when time-steps approximate the length of the natural period of the exact solution. This situation is not unique to Magnus schemes, and such resonances are well known for most numerical approximation schemes. If we assume that the main cause of the oscillation is the constant term of $A(t)$, i.e. b_1, as it is often the case, then the error will be dominated by the commutators $[b_1,\ldots,b_1,b_2]$ in (18), so we can rearrange the expansion in the form

$$\Omega = b_1 - \frac{1}{12}[b_1,b_2] + \frac{1}{720}[b_1,b_1,b_1,b_2] + \cdots + c_j[\overbrace{b_1,\ldots,b_1}^{jb_1's},b_2] + \cdots + \frac{1}{12}b_3 + \frac{1}{240}[b_2,b_3] + \cdots \tag{A.1}$$

where the coefficients c_k are given by

$$\sum_{k\geqslant 0} c_k x^k = \frac{1-\frac{x}{2}-\frac{x}{e^x-1}}{x} = g(x).$$

The highest value of c_j which is considered depends on how the discrete Magnus series is truncated. In this case, the dominating error term is given by

$$E_1^j = c_j[b_1,\ldots,b_1,b_2] + c_{j+1}[b_1,\ldots,b_1,b_1,b_2] + \cdots.$$

The main problem pinpointed by E_1^j are the singularities at multiples of $2\pi i$ ($i^2=-1$) in $g(x)$. In particular if b_1 has two eigenvalues whose difference is a multiple of $2\pi i$ then we expect severe loss of accuracy when using the truncated Magnus series as an approximation. In [23] this difficulty was resolved by explicitly computing the dominating error term E_1^j and adding it to the discrete approximation to the Magnus expansion, improving the accuracy by several orders of magnitude. For moderately small problems this approach seems to be reasonably good, while for large systems as well as for non-linear problems the computation of E_1^j will totally dominate the cost of the algorithm. This procedure is closely related to the modified Magnus integrators in [16] where the dominant constant term is factorized. Modified Magnus integrators have proved to be very efficient for oscillatory linear equation but, its direct application to non-linear systems turn into very complicated procedures.

To avoid computing E_1^j we can seek to find coefficients $x_{i,j}$ such that our factored scheme renders a good approximation to E_1^j. For example, in (38) we can choose the extra parameter to cancel the term at order five $[1,1,1,2]$ which for many problems is the dominant error term. The solution is given by

$$x_{1,1} = \frac{5-\sqrt{5}}{10}, \qquad x_{1,2} = \frac{5}{30+6\sqrt{5}}, \qquad x_{2,1} = 1-2x_{1,1}.$$

Clearly since E_1^j has an infinite number of singularities, corresponding to resonances of different orders, it is not possible to remove all of them with a finite number of coefficients. Then, another criterion for optimization is to add more factors to the numerical scheme to have free parameters to remove the singularities closest to the origin $2\pi i, 4\pi i \ldots$. For instance, a method with 5 exponentials which removes the two first singularities is given by

$$x_{1,1} = 0.08320595238621673655, \qquad x_{2,1} = 0.26469874860518009962, \qquad x_{3,1} = 1-2(x_{1,1}+x_{2,1})$$
$$x_{1,2} = 0.04160297618650280498, \qquad x_{2,2} = 0.07943895007147464695.$$

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