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Abstract

In this paper new integration algorithms for linear differential equations up to eighth order are obtained. Starting from Magnus expansion, methods based on Cayley transformation and Fer expansion are also built. The structure of the exact solution is retained while the computational cost is reduced compared to similar methods. Their relative performance is tested on some illustrative examples.

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1 Introduction

In recent years there has been a renewed interest in designing numerical schemes for solving the linear matrix differential equation

$$\frac{dX}{dt} = A(t)X, \qquad X(t_0) = X_0, \tag{1}$$

particularly in the context of geometric integration. The main goal in this field is to discretize equation (1) in such a way that important geometric and qualitative properties of the exact solution are retained by the numerical approximation. Here $A(t)$ stands for a sufficiently smooth matrix to ensure existence and unicity of a n-by-n matrix solution $X(t)$.

It is generally recognised that geometric integrators provide a better description of the original system than standard integration algorithms, both in the preservation of invariant quantities and in the accumulation of numerical errors along the evolution [4]. For this reason there has been a systematic search of efficient geometric integrators for equation (1), especially when it evolves in Lie groups or a homogeneous space (see [11] for a review). In particular, the classical Magnus [13] and Fer [7] analytic expansions have been turned into very effective numerical methods, even for nonlinear matrix differential equations in Lie groups and homogeneous spaces [8, 18, 19], whereas other schemes based on the use of the Cayley transform [10, 14] and (conveniently modified) Runge-Kutta methods [15] have also been proposed.

Although some preliminary analysis of complexity issues related to this class of integration algorithms are already available [5], it is clear that much work along this direction is still to be done. In particular, a detailed study is needed in order to clarify under which circumstances a particular method is preferable to others. This requires, as a first step, some optimization strategy to bring to a minimum the computational cost of the different geometric integrators, in particular by reducing the number of function evaluations and matrix operations (products and/or commutators) involved.

In a recent publication [3], the authors have presented a technique that, at present, gives the least number of commutators required for methods based on the Magnus expansion up to order eight. Here we extend those results to geometric integrators based on the Fer expansion and the Cayley transform. We show how this class of integration methods (optimal with respect to the number of commutators) can be easily constructed from the Magnus expansion, both in terms of univariate analytic integrals and symmetric quadrature rules. We also discuss the use of diagonal Padé approximants to evaluate the matrix exponential and report on our experience when the new methods are applied to some illustrative examples.

Given the initial value problem (1), it is well known that the matrix solution

X can, in a neighborhood of t_0, be written in the following forms:

$$\begin{aligned} X(t_0+h) &= e^{\Omega(h)} X_0 && \text{Magnus} && (2) \\ &= e^{F_1(h)} e^{F_2(h)} \cdots X_0 && \text{Fer} && (3) \\ &= e^{S_1(h)} e^{S_2(h)} \cdots e^{S_2(h)} e^{S_1(h)} X_0 && \text{Symmetric Fer I} && (4) \\ &= \cdots e^{T_2(h)} e^{T_1(h)} e^{T_2(h)} \cdots X_0 && \text{Symmetric Fer II} && (5) \\ &= \left(I - \frac{1}{2} C(h)\right)^{-1} \left(I + \frac{1}{2} C(h)\right) X_0 && \text{Cayley} && (6) \end{aligned}$$

and these expansions are convergent for sufficiently small values of h [2, 10, 19]. Observe that if $A(t)$ belongs to a Lie algebra $\mathfrak{g}$ then schemes (2)-(5) and the numerical integrators based on them provide approximate solutions staying in the corresponding Lie group G if $X_0 \in G$, whereas this is true for the Cayley transform (6) only when G is a J-orthogonal (also called quadratic) Lie group [16]. The choice of the representation (2)-(6) is dictated by the requirement that the solution stays in G. If on the other hand this requirement is abandoned one has a much larger class of representations to choose from.

The plan of the paper is the following: in section 2 we collect some numerical integration schemes of order 4, 6 and 8 based on the Magnus expansion. These methods are used in section 3 in combination with the Fer expansion and the Cayley transformation to get new and optimized geometric integrators for the differential equation (1) up to order 8. The idea is to write the functions F_i, S_i and C in terms of the successive approximations to Ω, thus obtaining methods which involve considerably fewer matrix commutators than other previously available. Also some considerations about the computational cost of the algorithms are incorporated in this section. In section 4 we apply these methods to several illustrative examples in order to compare their relative performance and elucidate when it is preferable to use one particular scheme to the others. Finally, section 5 contains some conclusions.

2 Review of Magnus methods

Several $2n$-th order integration algorithms for eq. (1) based on the Magnus expansion (2) have been obtained recently in [3]. These methods, for a given time interval $[t_k, t_k+h]$ and step-size h, read

$$\begin{aligned} \Omega^{[2n]} &\equiv \sum_{i=0}^{n-1} w_{2i+1} = \Omega + O(h^{2n+1}) \\ X(t_k+h) &= \exp(\Omega^{[2n]})\, X(t_k), \end{aligned} \qquad (7)$$

where the functions $w_j = O(h^j)$ are expressed in terms of the univariate integrals

$$B^{(i)} = \frac{1}{h^{i+1}} \int_{t_k}^{t_k+h} \left(t - (t_k + \frac{h}{2})\right)^i A(t)\, dt \qquad i = 0, 1, 2, \ldots \qquad (8)$$

and (the minimum number of) nested commutators. In particular, we have

$$\Omega^{[2]} = w_1 = hB^{(0)}$$

and farther approximations to Ω are obtained from:

Order 4 $(n = 2)$

$$w_3 = -h^2[B^{(0)}, B^{(1)}] \tag{9}$$

Order 6 $(n = 3)$

$$\begin{aligned} w_3 &= h^2[B^{(1)}, \frac{3}{2}B^{(0)} - 6B^{(2)}] \\ w_5 &= [w_1, [w_1, \frac{1}{2}hB^{(2)} - \frac{1}{60}w_3]] + \frac{3}{5}h[B^{(1)}, w_3] \end{aligned} \tag{10}$$

Order 8 $(n = 4)$

$$\begin{aligned} w_3 &= h^2(Q_1 + Q_2) \\ w_5 &= h^3(Q_3 + Q_4) + h^4(Q_5 + Q_6 - hP) \\ w_7 &= h^5(Q_7 + P) \end{aligned} \tag{11}$$

with

$$\begin{aligned} &Q_1 = [-\tfrac{38}{5}B^{(0)} + 24B^{(2)}, B^{(3)}] \qquad Q_2 = [\tfrac{63}{5}B^{(0)} - 84B^{(2)}, -\tfrac{5}{28}B^{(1)} + B^{(3)}] \\ &Q_3 = [\frac{19}{28}B^{(0)} - \frac{15}{7}B^{(2)}, [B^{(0)}, B^{(2)} + h(\frac{61}{588}Q_1 - \frac{1}{12}Q_2)]] \\ &Q_4 = [B^{(3)}, \tfrac{20}{7}Q_1 + 10Q_2] \qquad Q_5 = [-\tfrac{6025}{4116}B^{(0)} + \tfrac{2875}{343}B^{(2)}, [B^{(2)}, Q_1]] \\ &Q_6 = [B^{(3)}, \tfrac{20}{7}(Q_3 + Q_4) + \tfrac{820}{189}hQ_5] \qquad Q_7 = [B^{(0)}, -\tfrac{1}{42}[B^{(0)}, Q_3 - \tfrac{1}{3}Q_4 + hQ_5]] \end{aligned} \tag{12}$$

and the explicit expression of P in (11) is not required for the practical implementation of the method because only the total sum $w_5 + w_7$ has to be computed. Observe that schemes (9), (10) and (11) involve 1, 4 and 10 commutators, respectively. In addition, due to the dependence of the single integrals $B^{(i)}$ on h and the structure of the approximations w_j, they are self-adjoint. This property is also preserved when $B^{(i)}$ are replaced by symmetric quadratures.

3 Lie-group solvers obtained from Magnus methods

3.1 Cayley-transform methods

When the differential equation (1) evolves on the so-called J-orthogonal Lie group [16]

$$\mathrm{O}_J(n) = \{A \in \mathrm{GL}_n(\mathbb{R}) \, : \, A^T J A = J\}, \tag{13}$$

where $\mathrm{GL}_n(\mathbb{R})$ is the group of all $n \times n$ nonsingular real matrices and J is some constant matrix in $\mathrm{GL}_n(\mathbb{R})$, numerical methods based on the Cayley transformation constitute a valid option preserving the Lie group structure of the equation [6, 10, 14].

Familiar examples of the J-orthogonal group $\mathrm{O}_J(n)$ are the orthogonal group (when $J = I$, the $n \times n$ identity matrix), the symplectic group $\mathrm{Sp}(n)$ (when J is the basic symplectic matrix) and the Lorentz group (corresponding to $J = \mathrm{diag}(1, -1, -1, -1)$).

A natural complexification process of (13) leads to the notion of J-unitary matrices A of order n, which are characterized by the relation

$$A^\dagger J A = J,$$

where $J \in \mathrm{GL}_n(\mathbb{C})$ and $A^\dagger = \bar{A}^T$. They form also a Lie group $\mathrm{U}_J(n)$. An important example is the unitary group $\mathrm{U}(n)$, which corresponds to $J = I$.

As is well known, A is a J-orthogonal matrix if

$$B = -\frac{1}{\alpha}(I + A)^{-1}(I - A)$$

is a J-skew-symmetric matrix, i.e., if $B^T J + JB = 0$ and $\alpha \neq 0$. In fact, the set

$$\mathrm{o}_J(n) = \{B \in \mathfrak{gl}_n(\mathbb{R}) \ : \ B^T J + JB = 0\}, \tag{14}$$

where $\mathfrak{gl}_n(\mathbb{R})$ is the Lie algebra of all $n \times n$ real matrices, is the matrix Lie algebra associated with $\mathrm{O}_J(n)$ [16]. Conversely, if $B \in \mathrm{o}_J(n)$, then its Cayley transform

$$A = (I - \alpha B)^{-1}(I + \alpha B) \tag{15}$$

is J-orthogonal. Thus, for $\mathrm{O}_J(n)$ the Cayley transform (15) provides a useful alternative to the exponential mapping relating the Lie algebra to the Lie group. This fact is particularly important for numerical methods where the evaluation of the exponential matrix is the most computation-intensive stage of the algorithm.

It has been shown that the solution of eq. (1) can be written ($\alpha = 1/2$) as

$$X(t) = \left(I - \frac{1}{2}C(t)\right)^{-1} \left(I + \frac{1}{2}C(t)\right) X_0 \tag{16}$$

in a neighborhood of t_0, with $C(t) \in \mathrm{o}_J(n)$ satisfying the so-called 'decayinv equation' [10]

$$\frac{dC}{dt} = A - \frac{1}{2}[C, A] - \frac{1}{4}CAC, \qquad t \geq t_0, \qquad C(t_0) = 0. \tag{17}$$

Time-symmetric methods of order 4 and 6 have been obtained based on the Cayley transform (16) by expanding the solution of (17) in a recursive manner and constructing quadrature formulae for the multivariate integrals that appear in the procedure [10, 14]. Then the recently introduced notion of graded free hierarchical algebra is applied to reduce the number of terms in the quadrature formula [12]. Here we show how efficient Cayley based methods can be built directly from Magnus based integrators.

Equations (2) and (6) lead to

$$\frac{1}{2}C(h) = \left(e^{\Omega(h)} + I\right)^{-1}\left(e^{\Omega(h)} - I\right)$$

and thus

$$C(h) = \Omega(h) - \frac{1}{12}\Omega(h)^3 + \frac{1}{120}\Omega(h)^5 - \frac{17}{20160}\Omega(h)^7 + \cdots \tag{18}$$

When approximations (9), (10) and (11) for Ω are inserted in (18) we obtain optimized schemes of order 4, 6 and 8. It is worth noticing that the approximate expressions we get for $C(h)$ when the series (18) is truncated belong to the Lie algebra and the corresponding methods are time-symmetric.

Order 4. Now $\Omega^3 = w_1^3 + O(h^5) = (hB^{(0)})^3 + O(h^5)$, so that

$$C^{[4]} = hB^{(0)} + h^2[B^{(1)}, B^{(0)}] - \frac{h^3}{12}(B^{(0)})^3 = C(h) + O(h^5). \tag{19}$$

If we consider the Gauss-Legendre quadrature of order 4 for approximating the univariate integrals $B^{(0)}$ and $B^{(1)}$,

$$A_1 \equiv A\left(t_k + \left(\frac{1}{2} - \frac{\sqrt{3}}{6}\right)h\right), \qquad A_2 \equiv A\left(t_k + \left(\frac{1}{2} + \frac{\sqrt{3}}{6}\right)h\right),$$

and define

$$B_0 \equiv \frac{1}{2}(A_1 + A_2), \qquad B_1 \equiv \sqrt{3}(A_2 - A_1),$$

then $B_0 = B^{(0)} + O(h^4)$, $B_1 = 12B^{(1)} + O(h^3)$, so that

$$C^{[4]} = hB_0 + \frac{h^2}{12}[B_1, B_0] - \frac{h^3}{12}B_0^3 + O(h^5), \tag{20}$$

which coincides with the result obtained by Iserles [10] and Marthinsen & Owren [14]. Observe that $C^{[4]}$ requires, in general, the computation of 4 matrix-matrix products. In fact, this number can be reduced to 3 by writing

$$C^{[4]} = hB^{(0)} + h^2\left(B^{(1)} - \frac{h}{12}(B^{(0)})^2\right)B^{(0)} - h^2B^{(0)}B^{(1)}. \tag{21}$$

Order 6. From (18) we have

$$C(h) = w_1 + w_3 + w_5 - \frac{1}{12}(w_1 + w_3)^3 + \frac{1}{120}(w_1 + w_3)^5 + O(h^7).$$

If we denote $W \equiv w_1 + w_3$ and take into account (10),

$$\begin{aligned} C^{[6]} &= W + w_5 + \frac{1}{120}W^3(W^2 - 10) = C(h) + O(h^7) \\ &= W + W\left(\frac{1}{120}W^2(W^2 - 10) + [w_1, \frac{1}{2}hB^{(2)} - \frac{1}{60}w_3]\right) \\ &\quad -[w_1, \frac{1}{2}hB^{(2)} - \frac{1}{60}w_3]W + \frac{3}{5}h[B^{(1)}, w_3] + O(h^7) \end{aligned} \tag{22}$$

with w_3 given in (10). Notice that the computation of $C^{[6]}$ according to eq. (22) requires only 10 matrix-matrix products per step, in contrast with other 6-th order schemes previously available (18 and 23 matrix-matrix products). Of course, these same results can in principle be achieved through a careful analysis and simplification of the expressions obtained in [11] by applying the theory of hierarchical algebras.

With respect to the 8th-order case, the corresponding approximation to $\Omega(h)$ involves 10 commutators, whereas eq. (18) for $C(h)$ can be expressed in terms of 4 matrix-matrix products:

$$C^{[8]} = \Omega \left(I - \frac{1}{12}\Omega^2 \left(I - \frac{1}{10}\Omega^2 \left(I - \frac{17}{168}\Omega^2 \right) \right) \right) = C(h) + O(h^9).$$

Thus, in principle, we have an 8-th order integrator based on Cayley requiring 24 matrix-matrix products.

The resulting n-th order ($n = 4, 6, 8$) numerical methods for eq. (1) are then given by

$$X(t_k + h) = \left(I - \frac{1}{2}C^{[n]} \right)^{-1} \left(I + \frac{1}{2}C^{[n]} \right) X(t_k) \tag{23}$$

and, in particular, they preserve time-symmetry because $C^{[n]}$ involves expressions (9), (10) and (11).

3.2 Magnus-Padé methods

As is well known, diagonal Padé approximants map the Lie algebra $\mathrm{o}_J(n)$ to the Lie group $\mathrm{O}_J(n)$ and thus constitute also a valid alternative to the evaluation of the exponential matrix in Magnus based methods for this particular Lie group. More specifically, if $B \in \mathrm{o}_J(n)$, then $\psi_{2m}(tB) \in \mathrm{O}_J(n)$ for sufficiently small $t \in \mathbb{R}$, with

$$\psi_{2m}(\lambda) = \frac{P_m(\lambda)}{P_m(-\lambda)}, \tag{24}$$

provided the polynomials P_m are generated according to the recurrence

$$\begin{aligned} P_0(\lambda) &= 1, \qquad\qquad P_1(\lambda) = 2 + \lambda \\ P_m(\lambda) &= 2(2m-1)P_{m-1}(\lambda) + \lambda^2 P_{m-2}(\lambda). \end{aligned}$$

Moreover, $\psi_{2m}(\lambda) = e^{\lambda} + O(\lambda^{2m+1})$ and ψ_2 corresponds to the Cayley transform, whereas for $m = 2, 3$ we have

$$\begin{aligned} \psi_4(\lambda) &= \left(1 + \frac{1}{2}\lambda + \frac{1}{12}\lambda^2\right) \Big/ \left(1 - \frac{1}{2}\lambda + \frac{1}{12}\lambda^2\right) \\ \psi_6(\lambda) &= \left(1 + \frac{1}{2}\lambda + \frac{1}{10}\lambda^2 + \frac{1}{120}\lambda^3\right) \Big/ \left(1 - \frac{1}{2}\lambda + \frac{1}{10}\lambda^2 - \frac{1}{120}\lambda^3\right). \end{aligned}$$

Thus, we can combine the optimized approximations to Ω collected in section 2 for Magnus based methods with diagonal Padé approximants up to the corresponding order to obtain time-symmetric integration schemes preserving the algebraic structure of the problem without computing the matrix exponential. In addition, it is not difficult to show that the methods thus obtained, at least for orders 4 and 6, require exactly the same number of matrix-matrix products than the optimized integrators based on the Cayley transform collected in section 3.1 (3 and 10, respectively), whereas the 8-th order scheme only involve 23 matrix-matrix products and the inversion of one matrix. Therefore, these 'Magnus-Padé methods' are, in principle, as efficient as the Cayley-transform integrators and constitute, thus, a computationally very attractive alternative to them.

3.3 Fer based methods

The procedure carried out for generating optimized Cayley-transform methods from the Magnus expansion can be extended to more general matrix Lie groups and other geometric integrators, such as those based on the Fer factorization. More specifically, we now construct Fer based integrators of order 4, 6 and 8 involving considerably fewer commutators than other schemes recently published [5]. The analysis is based on the optimized expressions for the Magnus expansion and the use of the Baker-Campbell-Hausdorff (BCH) formula.

Taking into account the Magnus and the Fer expansions (eqs. (2) and (3)) we can, in their domain of convergence, write

$$e^{\Omega(h)} = e^{F_1(h)}\, e^{\bar{F}(h)}$$

where $F_1 = w_1$ and $e^{\bar{F}(h)} = e^{F_2(h)}\, e^{F_3(h)} \cdots$. In this way

$$e^{\bar{F}(h)} = e^{-F_1(h)}\, e^{\Omega(h)}$$

with $\Omega(h) = w_1 + W + O(h^9)$ and $W = w_3 + w_5 + w_7$, so that, by applying the BCH formula and grouping terms, we get

$$\begin{aligned} \bar{F}(h) &= W - \frac{1}{2}[w_1, W] + \frac{1}{6}[w_1,[w_1,W]] - \frac{1}{24}[w_1,[w_1,[w_1,W]]] \\ &\quad + \frac{1}{12}[W,[w_1,W]] + \frac{1}{120}[w_1,[w_1,[w_1,[w_1,W]]]] - \frac{1}{24}[w_1,[W,[w_1,W]]] \\ &\quad - \frac{1}{720}[w_1,[w_1,[w_1,[w_1,[w_1,W]]]]] + O(h^9) \end{aligned} \tag{25}$$

and the different approximations follow:

Order 4. As is well known, $F_2(h) = O(h^3)$ and $F_3(h) = O(h^7)$, so that

$$F_2^{[4]} \equiv w_3 - \frac{1}{2}[w_1, w_3] = \bar{F}(h) + O(h^5) \tag{26}$$

or, in terms of univariate integrals,

$$F_2^{[4]}(h) = -h^2[B^{(0)}, B^{(1)}] + \frac{h^3}{2}[B^{(0)},[B^{(0)},B^{(1)}]]. \tag{27}$$

Order 6. In this case, from (25) we have

$$F_2^{[6]}(h) = W_{35} - \frac{1}{2}[w_1, W_{35}] + \frac{1}{6}[w_1,[w_1,W_{35}]] - \frac{1}{24}[w_1,[w_1,[w_1,W_{35}]]] \tag{28}$$

with $W_{35} = w_3 + w_5$ as given by (10) and $F_2^{[6]}(h) = \bar{F}(h) + O(h^7)$.

Order 8. Taking into account the dependence of W on h, it is clear from (25) that $e^{\bar{F}(h)} = e^{F_2(h)}\, e^{F_3(h)} + O(h^9)$, with

$$
\begin{aligned}
F_2(h) &= W - \frac{1}{2}[w_1, W] + \frac{1}{6}[w_1,[w_1,W]] - \frac{1}{24}[w_1,[w_1,[w_1,W]]] \\
F_3(h) &= \frac{1}{12}[W,[w_1,W]] + \frac{1}{120}[w_1,[w_1,[w_1,[w_1,W]]]] - \frac{1}{24}[w_1,[W,[w_1,W]]] \\
&\quad -\frac{1}{720}[w_1,[w_1,[w_1,[w_1,[w_1,W]]]]]
\end{aligned}
$$

and thus the corresponding integration scheme

$$X(t_k + h) = e^{F_1(h)}\, e^{F_2(h)}\, e^{F_3(h)}\, X(t_k)$$

requires 7 additional commutators, for a total of 17. This number can be reduced to 15, however, if we write $\bar{F}(h)$ in the form

$$
\begin{aligned}
F_2^{[8]}(h) &\equiv W + R_1 + R_2 + R_3 + R_4 + R_5 \\
&= \bar{F}(h) + O(h^9)
\end{aligned} \tag{29}
$$

with

$$
\begin{array}{ll}
R_1 = -\frac{1}{2}[w_1, W] & R_2 = -\frac{1}{3}[w_1 + \frac{1}{2}W, R_1] \\
R_3 = -\frac{1}{4}[w_1 + \frac{1}{2}W, R_2] & R_4 = -\frac{1}{5}[w_1, R_3] \\
R_5 = -\frac{1}{6}[w_1, R_4] &
\end{array} \tag{30}
$$

and the expressions of w_j are given by eq. (11). In addition, only the computation ot two matrix exponentials is needed. The resulting n-th order algorithms, $n = 4, 6, 8$, based on the Fer expansion are

$$X(t_k + h) = e^{F_1(h)}\, e^{F_2^{[n]}(h)}\, X(t_k) \tag{31}$$

and they require 2, 7 and 15 commutators, respectively. This represents a significant saving with respect to the estimates presented in [5], especially for the 8-th order scheme (45 commutators).

3.4 Symmetric Fer methods

A drawback of the Lie-group solvers based on the Fer expansion is that, contrarily to Magnus methods, they do not preserve the time-symmetry of the exact solution. For this reason Zanna [19] has proposed recently a self-adjoint version of the Fer factorization in the form (4), which can be implemented as time-symmetric Lie-group numerical integrators with essentially the same computational cost than conventional Fer methods. In the following we get optimized symmetric Fer methods up to order 8 by expressing $S_i(h)$ in terms of w_i as given in section 2. It is shown explicitly that the new methods require exactly the same number of commutators as Magnus based solvers.

Although we consider only the first symmetric Fer expansion (eq. (4)), it is clear that the same results can be achieved from eq. (5), and thus a new family of symmetric Fer methods can be obtained with the same properties and computational cost.

We can write (4) in the form

$$X(t_0+h) = e^{S_1(h)} e^{V(h)} e^{S_1(h)} X_0$$

with

$$S_1 = \frac{1}{2} w_1 \tag{32}$$

and $e^V = e^{S_2} e^{S_3} \cdots e^{S_3} e^{S_2}$. Here, as for the conventional Fer expansion, $S_1 = O(h)$, $S_2 = O(h^3)$ and $S_3 = O(h^7)$.

For sufficiently small h we have

$$e^V = e^{-S_1} e^{\Omega} e^{-S_1},$$

where Ω is given by eq. (7). Then, application of the symmetric Baker-Campbell-Hausdorff formula [17] allows to write, after some algebra,

$$V(h) = W + \frac{1}{24}[w_1,[w_1,W]] + \frac{1}{12}[W,[w_1,W]] + \frac{1}{1920}[w_1,[w_1,[w_1,[w_1,W]]]] + O(h^9) \tag{33}$$

where, as in the previous section, $W = w_3 + w_5 + w_7$. From this equation we obtain the following approximations up to the order considered.

Order 4. It is true that $V(h) = w_3 + O(h^5)$ and thus

$$S_2^{[4]}(h) = w_3 = -h^2[B^{(0)}, B^{(1)}]. \tag{34}$$

This method has been considered previously in [19].

Order 6. In this case

$$V(h) = w_3 + w_5 + \frac{1}{24}[w_1,[w_1,w_3]] + O(h^7) = S_2(h) + O(h^7).$$

The commutator $[w_1,[w_1,w_3]]$ can be inserted in the expression of w_5 (eq. (10)), thus leading to

$$S_2^{[6]}(h) = w_3 + [w_1,[w_1,\frac{1}{2}hB^{(2)} + \frac{1}{40}w_3]] + \frac{3}{5}h[B^{(1)}, w_3]. \tag{35}$$

Order 8. In this approximation $e^V = e^{S_2}\, e^{S_3}\, e^{S_2}$, with

$$\begin{aligned} S_2 &= \frac{1}{2}\left(w_3 + w_5 + \frac{1}{24}[w_1,[w_1,w_3]]\right) \\ S_3 &= w_7 + \frac{1}{24}[w_1,[w_1,w_5]] + \frac{1}{12}[w_3,[w_1,w_3]] + \frac{1}{1920}[w_1,[w_1,[w_1,[w_1,w_3]]]]. \end{aligned}$$

Here also the total number of commutators and matrix exponentials is reduced by following the same procedure leading to equations (11) and (12) for the 8-th order Magnus method [3]. Indeed, (33) can be written in the form

$$\begin{aligned} S_2^{[8]}(h) &\equiv h^2(U_1+U_2) + h^3(U_3+U_4) + h^4(U_5+U_6) + h^5 U_7 \\ &= V(h) + O(h^9) \end{aligned} \tag{36}$$

with

$$
\begin{array}{ll}
U_1 = [-\frac{38}{5}B^{(0)} + 24B^{(2)}, B^{(3)}] & U_2 = [\frac{63}{5}B^{(0)} - 84B^{(2)}, -\frac{5}{28}B^{(1)} + B^{(3)}] \\
U_3 = \frac{1}{7}[\frac{19}{4}B^{(0)} - 15B^{(2)}, [B^{(0)}, B^{(2)} + h\frac{55}{294}U_1] & \\
U_4 = [B^{(3)}, \frac{20}{7}U_1 + 10U_2] & U_5 = \frac{25}{343}[-23B^{(0)} + 150B^{(2)}, [B^{(2)}, U_1]] \\
U_6 = \frac{1}{7}[B^{(3)}, 20(U_3 + U_4) - \frac{80}{3}hU_5] & U_7 = \frac{1}{56}[B^{(0)}, [B^{(0)}, U_3 - 5U_4 + \frac{37}{30}hU_5]]
\end{array}
\tag{37}
$$

The resulting n-th order ($n = 4, 6, 8$) time-symmetric integration algorithms read

$$
X(t_k + h) = e^{S_1(h)}\, e^{S_2^{[n]}(h)}\, e^{S_1(h)} X(t_k) \tag{38}
$$

requiring 1, 4 and 10 commutators, respectively, i.e. the same number than Magnus based Lie-group solvers.

3.5 Computational cost

In order to compare the efficiency of the different geometric integrators obtained in this paper, we must estimate their computational cost. It is made up of the cost of evaluating the single integrals $B^{(i)}$ (or, instead, the number of A evaluations if quadratures are used), the total number of commutators (or matrix-matrix products) involved and eventually the exponential or the inverse of a matrix. Although the actual cost is highly dependent on the Lie algebra in question and the structure of the matrix differential equation, it is clear, however, that the factors above enumerated could serve as a good indicator of the practical performance of the different methods. These numbers are collected in Table 1, in a similar form to reference [5]: F stands for the number of function evaluations, C is the number of commutators, P indicates the total number of matrix-matrix products (commutators included), E is the number of matrix exponentials and In the number of inversions per time step for each class of methods when they are applied to the linear equation (1).

4 Numerical examples

Here we show some of the properties of the Lie-group solvers collected in section 3 and test their efficiency on some examples, chosen to embrace different kinds of physically relevant behavior.

Example 1. First we consider the Mathieu equation

$$
\ddot{x} + (\omega_0 - 2\epsilon \cos 2t)x = 0 \tag{39}
$$

with $\omega_0 > 0$, $\epsilon > 0$. This corresponds to eq. (1) with coefficient matrix

$$
A(t) = \begin{pmatrix} 0 & 1 \\ -\omega_0 + 2\epsilon \cos 2t & 0 \end{pmatrix},
$$

Method	Order	F	C	P	E	In
Magnus	4	2	1	2	1	
	6	3	4	8		
	8	4	10	20		
Cayley (Magnus-Padé)	4	2		3		1
	6	3		10		
	8	4		24(23)		
Fer	4	2	2	4	2	
	6	3	7	14		
	8	4	15	30		
Symmetric Fer	4	2	1	2	3	
	6	3	4	8		
	8	4	10	20		

Table 1: Computational cost of different Lie-group solvers for the linear differential equation (1). P also includes the matrix-matrix products coming from the commutators.

whose solution evolves in the Lie group $\mathrm{Sp}(2) \approx \mathrm{SL}(2)$. With this example we illustrate the qualitative behavior of the methods, the error growth in the numerical solution and, in particular, the different properties of Cayley based integration algorithms and Magnus-Padé schemes, both qualitative and quantitative.

As is well known, the space of parameters (ω_0, ϵ) is divided into stable and unstable regions, depending on the character of the solutions of (39): the point (ω_0, ϵ) belongs to an unstable region when there exists at least one solution which is unbounded with time, whereas it belongs to a stable region when the two linearly independent solutions are bounded. Therefore it is interesting to check if the different integration algorithms provide numerical approximations which share with the exact solution this important feature.

We take $\omega_0 = 3.9869$, $\epsilon = 0.4$, which corresponds to an unstable region [1], and initial conditions $x(0) = 1$, $\dot{x}(0) = 0$. We solve numerically equation (1) with the 4-th order algorithms considered in this paper (with step-size $h = \pi/15$ and univariate integrals) and, for the purpose of comparison, also the popular 4-th order Runge-Kutta method (with $h = \pi/20$). The final time is $t_{\mathrm{f}} = 400\pi$ and the output is depicted once per period π.

In Figure 1 we show the exact solution $x(t)$ (solid line E) and the approximations obtained by the following schemes: Magnus (M4), Magnus-Padé (MP4), Cayley (C4), Fer (F4), symmetric Fer (SF4) and Runge-Kutta (RK4). It is clear that, with these step sizes, C4, MP4 and RK4 provide oscillatory and bounded numerical solutions and therefore a wrong qualitative behavior for the dynamics of the system. It is worth noticing, however, that if the exponential $e^{\Omega^{[4]}}$ in the Magnus scheme is substituted by the 6-th order Padé approximant $\Psi_6(\Omega^{[4]})$, then the curve for the numerical solution obtained with the resulting scheme (MP46) matchs exactly the line M4.

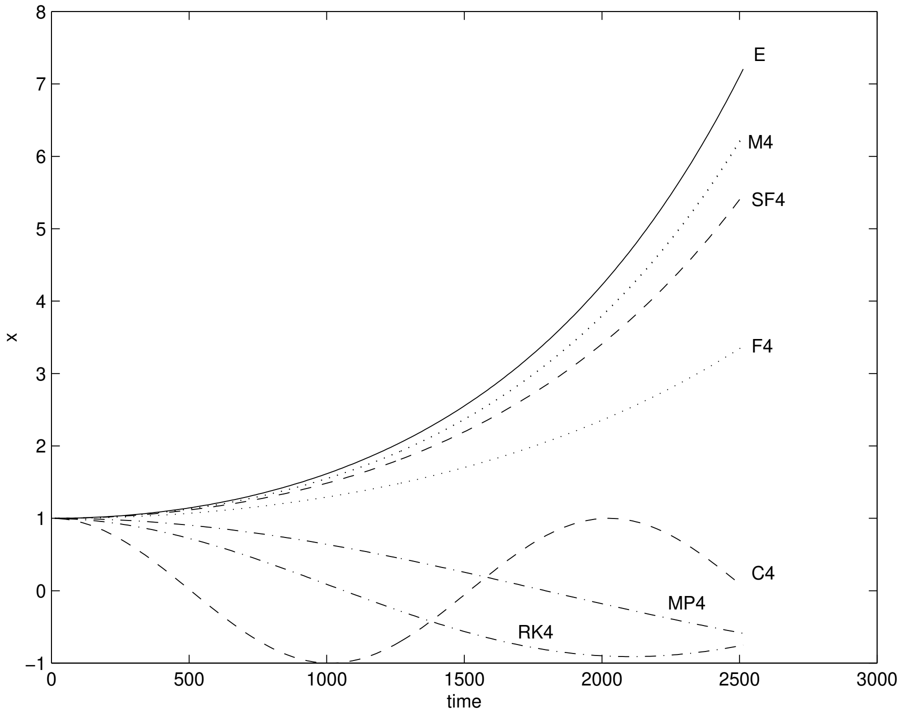

Figure 1: Solution $x(t)$ of the Mathieu equation with $\omega_0 = 3.9869$, $\epsilon = 0.4$ and initial conditions $x(0) = 1$, $\dot{x}(0) = 0$ obtained with different 4-th order integration methods.

Next we compute the error in the solution, $[(x_{\rm ex} - x_{\rm appr})^2 + (\dot{x}_{\rm ex} - \dot{x}_{\rm appr})^2]^{1/2}$ as a function of time for $\omega_0 = 3$, $\epsilon = 0.4$ with the same initial condition and step-sizes. The results are shown in Figure 2. As before, the curve obtained by MP46 coincides with M4.

We observe how the schemes based on Magnus and Fer provide better results than Cayley for this example and step-size.

As a third test we fix $\epsilon = 4$ and compute the relative error

$$\left[\frac{(x_{\rm ex} - x_{\rm appr})^2 + (\dot{x}_{\rm ex} - \dot{x}_{\rm appr})^2}{(x_{\rm ex}^2 + \dot{x}_{\rm ex}^2)}\right]^{1/2}$$

as a function of the parameter $\omega_0 \in [6, 50]$ at the final time $t_{\rm f} = 200\pi$ with initial condition $x(0) = \dot{x}(0) = 1$. Now we consider the 6-th order Lie-group solvers of section 3 with the univariate integrals replaced by Gauss-Legendre quadratures and step-size $h = \pi/25$, so that all the schemes require the same number of A evaluations.

Here also Magnus provides much better results than Fer and Cayley, independently of the value of ω_0 and the stability or unstability of the solution. In fact, the relative error achieved by Magnus (M6) is always bounded by $6 \cdot 10^{-3}$, whereas Cayley (C6) yields an error for $\omega_0 = 50$ which is about three orders of magnitude greater and the error of Magnus-Padé (MP6) is less than 0.16. Here also, if the exponential $e^{\Omega^{[6]}}$ is substituted by the 8-th order Padé approx-

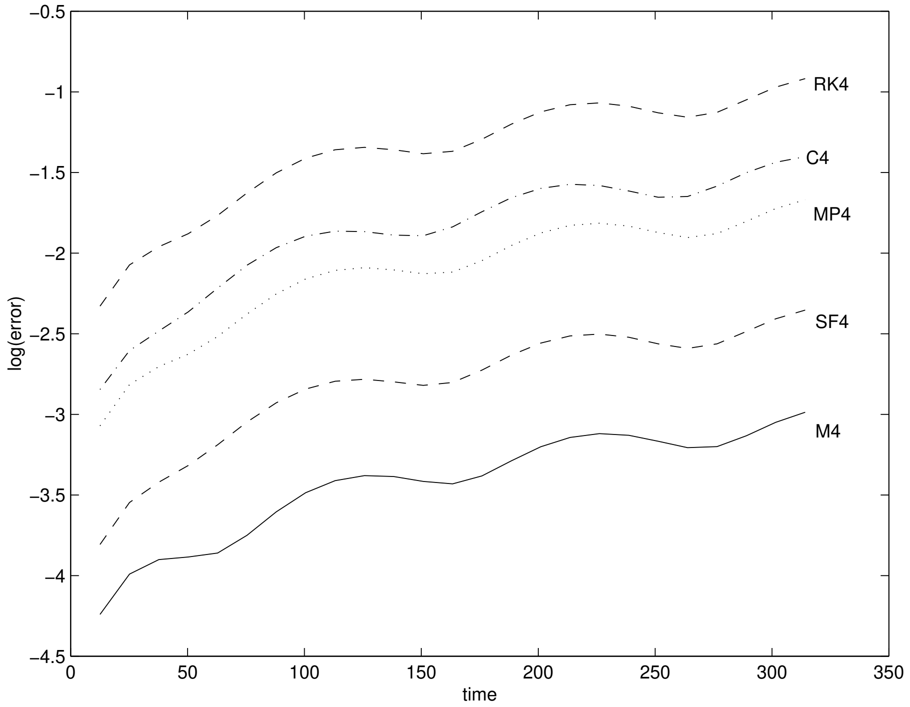

Figure 2: Error of the approximate solutions obtained by different 4-th order integrators for the Mathieu equation with $\omega_0 = 3$, $\epsilon = 0.4$ and initial conditions $x(0) = 1$, $\dot{x}(0) = 0$. The exact solution is bounded.

imant (thus providing the new scheme MP68), then the results are similar to M6. On the other hand, the bounds for the relative errors given by the Fer based schemes F6 and SF6 are, respectively, 0.08 and 0.025 for the range of ω_0 considered. As illustration, in Figure 3 we collect the results obtained with M6 (and MP68), MP6 and C6.

Example 2. Next we consider the coefficient matrix

$$A(t) = -i\frac{\omega_0}{2}\sigma_3 - i\beta(\sigma_1 \cos \omega t + \sigma_2 \sin \omega t), \tag{40}$$

where σ_j, $j = 1, 2, 3$, denote the Pauli matrices and β, ω_0, ω are real parameters. Then the corresponding initial value problem (1) with $X(0) = I$ has the exact solution

$$X(t) = \exp\left(-\frac{1}{2}i\omega t\sigma_3\right) \exp\left(-it\left(\frac{1}{2}(\omega_0 - \omega)\sigma_3 + \beta\sigma_1\right)\right), \tag{41}$$

which belongs to SU(2) for all t. This example is well known in the theory of nuclear magnetic resonance (NMR) and is useful to check the behavior of numerical schemes over very long integration intervals by comparing approximate solutions with the exact result. In particular, we analyze the efficiency of the 6-th and 8-th order algorithms described in section 3, both in terms of analytic integrals $B^{(i)}$ and symmetric quadratures. We compute the global error in the

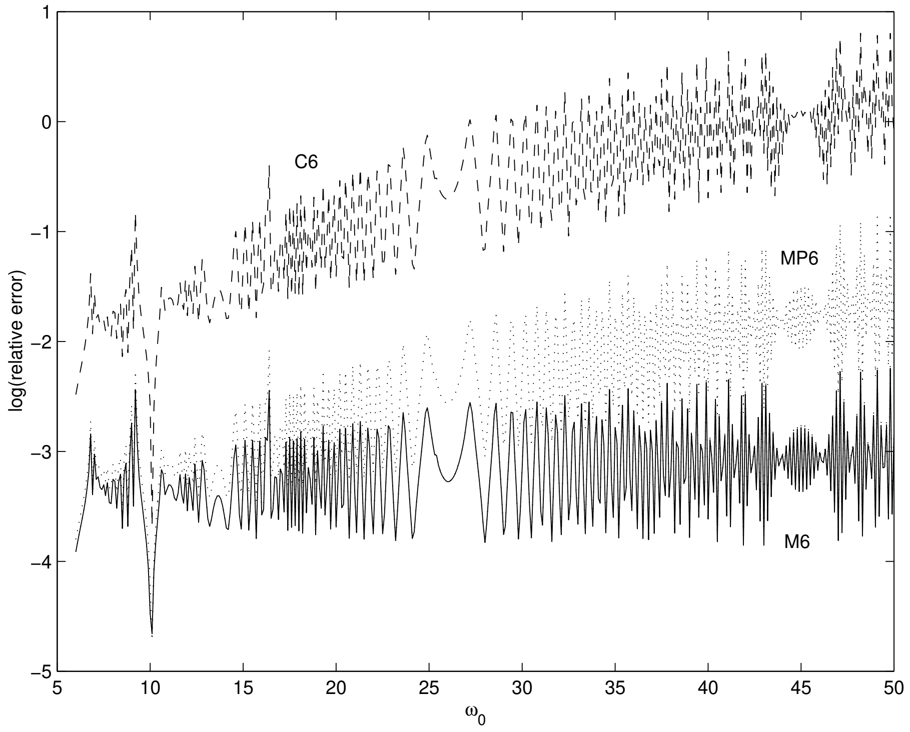

Figure 3: Relative error of the approximate solutions obtained by 6-th order schemes as a function of ω_0 for the Mathieu equation with $\epsilon = 4$. There are stable and unstable regions in this range of parameters.

solution as a function of the computational effort measured in CPU time for $\omega_0 = \omega = 1$ and $\beta = 0.8$. The global error is measured by computing the Frobenius norm of the difference between approximate and the exact solution matrices at time $t_{\rm f} = 5000\frac{2\pi}{\omega'}$, with $\omega' = \sqrt{(\omega_0-\omega)^2+4\beta^2}$, although similar conclusions can be attained by determining the quantum mechanical transition probability

$$|(X(t))_{21}| = \left(\frac{2\beta}{\omega'}\sin\frac{\omega' t}{2}\right)^2. \tag{42}$$

In Figure 4(a) we plot (in a log-log scale) the efficiency curves for the 6-th order integration methods based on Magnus with exact univariate integrals (M6) and quadratures (M6c), Magnus-Padé (MP6), and standard and symmetric Fer expansions (F6 and SF6, respectively). The graph exhibits clearly the order of consistency of the algorithms and the advantages of implementing Magnus with the integrals $B^{(i)}$ instead of quadratures, at least for this example. This conclusion remains also valid for the other schemes. Notice that the optimized version (22) of C6 is the most efficient method, although MP6 proves to be a quantitatively valid alternative to Cayley.

With respect to the 8-th order algorithms of section 3, their efficiency curves for this problem are shown in Figure 4(b), where a similar notation has been

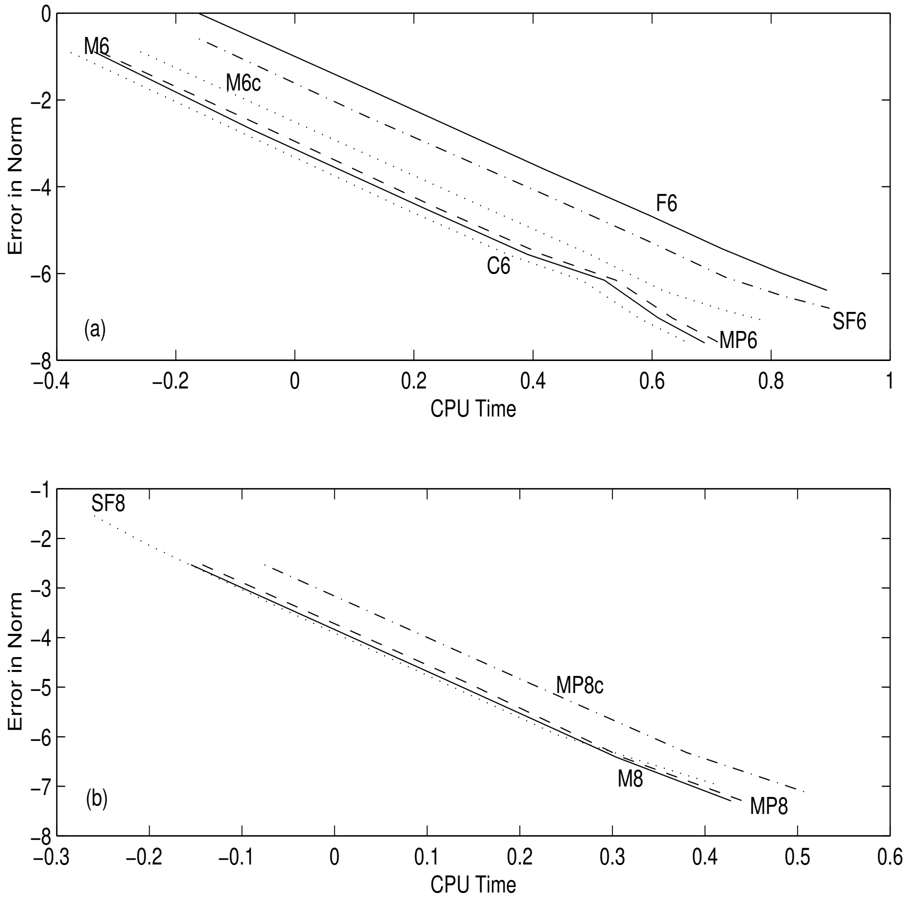

Figure 4: Efficiency diagram corresponding to the optimized 6-th (a) and 8-th (b) Lie-group solvers of section 3 when they are applied to the second example with $\omega_0 = \omega = 1$, $\beta = 0.8$, both with exact integrals $B^{(i)}$ and Gauss-Legendre quadratures.

used for the methods. Essentially, the same comments apply, but now SF8 is as efficient as M8 (the cost of computing one additional matrix exponential is almost negligeable in comparison with the number of evaluations and commutators required).

Example 3. As a final illustration we consider a skew-symmetric coefficient matrix $A(t)$ and $X_0 = I$, so that the solution $X(t)$ is orthogonal for all t. In particular we take as upper triangular elements of $A(t)$ the following:

$$A_{ij} = \sin\left(t(i^2 - j^2)\right) \qquad 1 \le i < j \le N \tag{43}$$

$$A_{ij} = \log\left(1 + t\frac{i-j}{i+j}\right) \tag{44}$$

with $N = 10, 20$. In both cases $X(t)$ oscillates with time, mainly due to the time-dependence of $A(t)$ (in (43)) or the norm of the coefficient matrix (with (44)).

The integration is carried out in the interval $t \in [0, 10]$ and the approximate solutions are compared with the exact one at the final time $t = 10$, where the corresponding error is computed for different h. The Lie-group solvers presented in this paper are implemented with Gauss-Legendre quadratures and constant step size.

In contrast with the above examples, now there is not a closed formula for the matrix exponentials appearing in the Magnus and Fer based integrators, so that some alternative procedure must be applied. Here we compute e^C by splitting and squaring, i.e. we take

$$e^C = \left(e^{C/2^k}\right)^{2^k}$$

for some integer k and estimate $e^{C/2^k}$ by a diagonal Padé approximant of a sufficiently high order m, so that the result is correct up to round-off. Although k and m are clearly h-dependent we have found that, for the integration methods and step sizes h considered in this paper, the pair $k = 2$, $m = 8$ provides succesful results if C has the form $C = \alpha_1 h + O(h^2)$, whereas $k = 0$, $m = 4$ lead to the same result than the procedure implemented in Matlab when $C = \alpha_3 h^3 + O(h^4)$, as is the case with Fer methods.

In Figure 5 we present, for simplicity, the efficiency curves corresponding to the most and less effective 6-th and 8-th order Lie-group solvers for the particular skew-symmetric matrices (43) and (44). These are the Magnus (solid lines) and Cayley (broken lines) based methods. For comparison we also include the result obtained with the explicit 6-th order Runge-Kutta method RK6 considered in [9], which requires six evaluations of $A(t)$ per step (dotted lines). We should mention that the relative position of the curves corresponding to the Runge-Kutta method and the geometric integrators considered in this paper does not depend significantly on the dimension of $A(t)$. This is mainly due to the following reasons: (i) when N increases then also does the intricacy of the solution, so that the better preservation of its structure by the geometric integrators compensates their higher computational cost, and (ii) the number of $A(t)$ evaluations is reduced to a minimum for the Lie-group solvers of this paper. In order to stress the importance of this issue we also include for $N = 20$ an estimate of the efficiency of an 8-th order Magnus method involving 45 commutators instead of 10 (circles joined by a solid line in Figures 5 (c) and (d)). The resulting loss of accuracy is nearly two orders of magnitude for the same computational effort.

It is also worth noticing that the efficiency achieved by Fer and symmetric Fer methods is very similar to that of Magnus in all cases analyzed if the matrix exponentials are evaluated accurately up to machine precision. This is so for the matrix (43) even if Padé approximants of the corresponding order are used to replace the exponentials. In fact, all the geometric integrators provide essentially the same results at each order. On the other hand, the efficiency of Magnus-Padé methods (and also of Fer when the exponentials are replaced by Padé approximants) is highly deteriorated for the matrix (44), although it is always better than the corresponding to Cayley schemes.

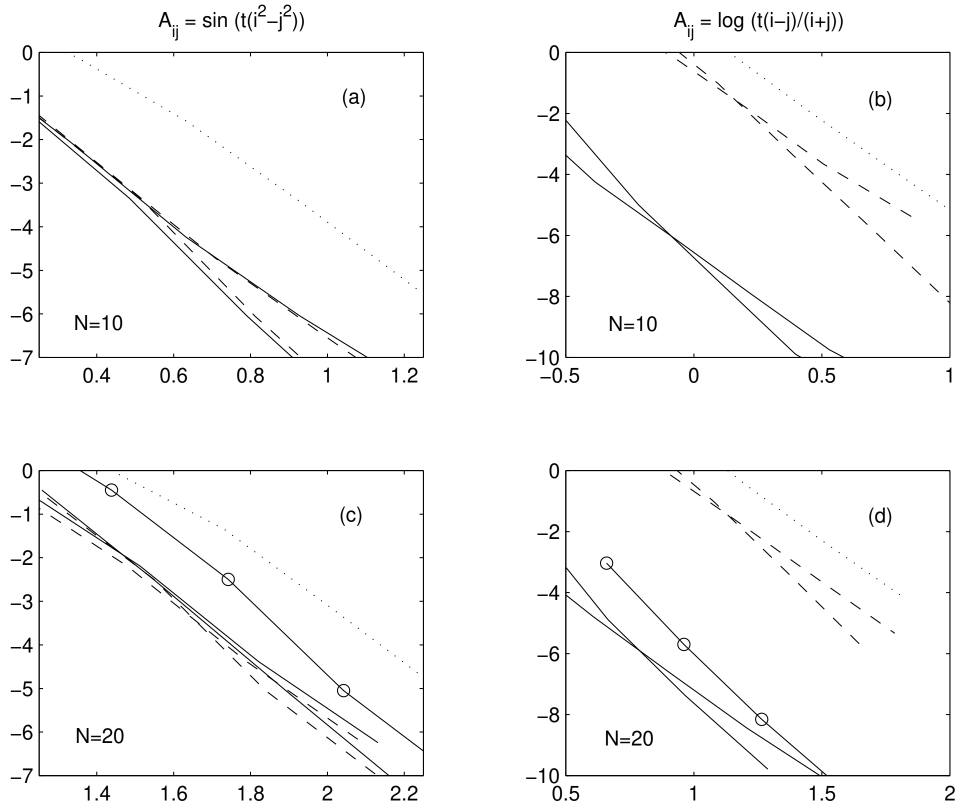

Figure 5: Error versus CPU time (in logarithmic scale) obtained with the 6-th and 8-th order integrators based on Magnus (solid lines), Cayley (broken lines) and RK6 (dotted lines). We have also included an 8-th order method based on Magnus with 45 commutators (circles joined by lines).

To better illustrate all these results, in Figure 6 we display the error in the solution corresponding to (43) and (44) as a function of time in the interval $t \in [0, 100]$ obtained with the 6-th order Lie-group solvers and RK6. We take $N = 10$ and $h = 1/20$, all methods requiring the same number of A evaluations, except RK6, which duplicates this number. Observe the great importance of evaluating the exponential as accurately as possible for the matrix (44): by increasing slightly the computational cost per step in the computation of the matrix exponential it is possible to improve dramatically the accuracy of the methods. On the contrary, for matrix (43) the meaningful fact seems to be that the integration scheme provide a solution in the corresponding Lie group.

It is well known than the implicit s-stage Runge-Kutta-Gauss-Legendre (RKGL) method of order $2s$ can be considered a geometric integrator if $A \in \mathfrak{o}_J(n)$. In fact, for the linear equation (1) this method can be written in an explicit form: one has to invert an $sn \times sn$ matrix, but in fact its block structure leads to a rational expression similar to Magnus-Padé, involving $n \times n$ matrices and (possibly) more matrix-matrix products. The results achieved by RKGL

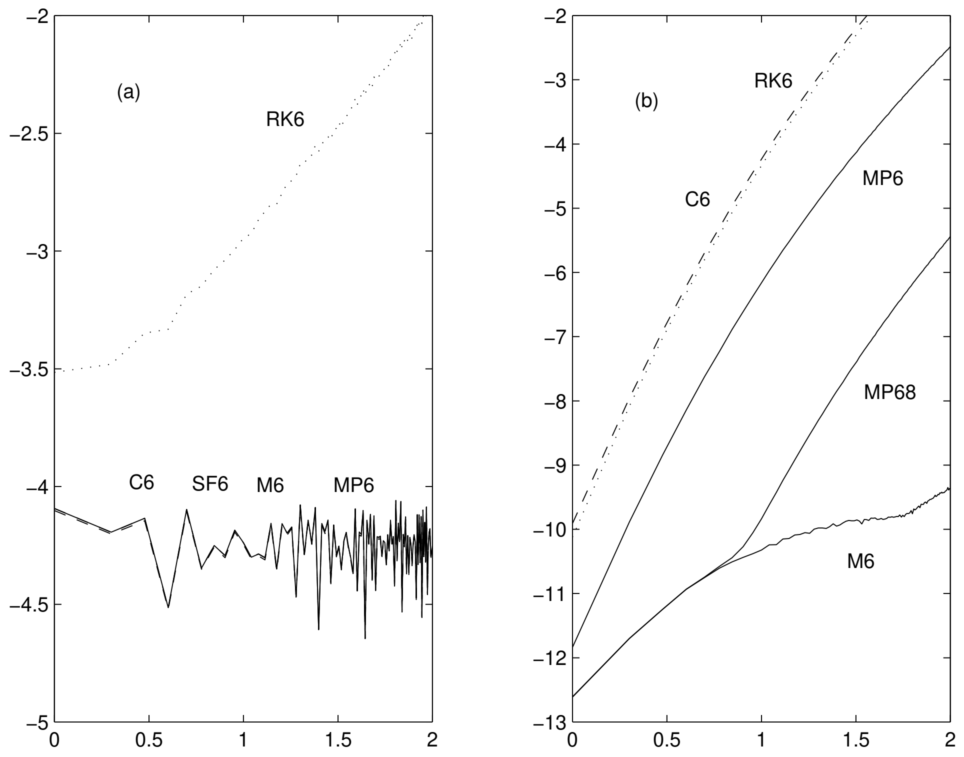

Figure 6: Error as a function of time (in logarithmic scale) obtained with different 6-th order integrators: (a) problem (43); (b) problem (44).

methods for the matrix (43) are slightly less efficient than the other geometric integrators, whereas for the matrix (44) are very similar to Magnus-Padé schemes of the same order. This is not very surprising, because in the particular case when A is a constant matrix both methods are equivalent, when neglecting machine accuracy.

5 Final comments

In this paper we have presented different families of 6-th and 8-th order geometric integrators for linear differential equations based on the Cayley transform and the Magnus and Fer analytical expansions. The methods are optimized in the sense that the number of commutators and matrix-matrix products is reduced to a minimum, so that they are far more efficient than other schemes of similar type found in the literature.

Although only J-orthogonal matrices are considered in this paper, the integration methods based on Magnus and Fer we present here can be applied to more general Lie groups than $O_J(n)$ if the matrix exponentials are evaluated up to machine precision.

We have also studied the applicability of these integration algorithms to several examples involving different algebraic structure. Our purpose was not to compare them exhaustively with other integrators but to establish when the use of one particular Lie-group solver is recommended, based on criteria such as their relative efficiency, the preservation of additional qualitative properties of the exact solution, etc.

From the previous analysis of the examples considered we can draw some tentative conclusions:

- There are problems where the preservation of the Lie group by the numerical solution seems to be the only crucial feature. Then no particular geometric integrator is preferred to the others, because all of them provide the correct qualitative and also quantitative behavior at approximately the same computational cost. In this case Magnus-Padé methods can be considered as an interesting alternative to both Magnus and Cayley solvers.

- On the contrary, for other problems the presence of the exponential in the numerical scheme seems to be essential. It is precisely the matrix exponential which allows to recover accurately the main features of the exact solution, and not only the Lie algebraic structure of the problem. Indeed, a more accurate approximation to the matrix exponential leads directly to a better overall description. In this case it is worthwile to calculate accurately the matrix exponential even if the computational cost increases. In this respect we should remark that the combined use of the Magnus expansion and high order Padé approximants leads to integration schemes clearly superior to those based on the Cayley transform.

- High order Lie-group solvers based on the symmetric Fer expansion are as efficient as those built from Magnus, at least in the examples considered. Perhaps in problems where e^{w_1} is easier to compute than $e^{\Omega^{[2n]}}$ the use of symmetric Fer methods is advantageous. On the other hand, schemes based on the standard Fer expansion are clearly less efficient and, in addition, do not preserve time-symmetry.

- If the elements of the matrix $A(t)$ are simple enough so as to render feasible the exact evaluation of the integrals $B^{(i)}$, then it is convenient to incorporate them into the algorithms instead of numerical quadratures because the corresponding integration schemes are more efficient.

It has been argued [11] that one of the reasons which explains the superior performance of Lie-group solvers might be that standard methods invariably employ the ansatz that locally the solution behaves like a polynomial in t, whereas the former are based on a representation of the solution as an exponential of a matrix with polynomial entries (or a product of such exponentials). Unlike polynomials, exponentials of matrices with polynomial entries can describe adecuately high oscillations, exponential changes, etc. From our analysis we could say that, at least in some situations, these exponentials provide also a better qualitative and quantitative description than rational functions of matrices with polynomials entries.

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