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S. Blanes and P.C. Moan

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Department of Applied Mathematics and Theoretical Physics
Silver Street
Cambridge
England CB3 9EW

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S. Blanes and P.C. Moan

Department of Applied Mathematics and Theoretical Physics,

University of Cambridge, Silver Street,

Cambridge CB3 9EW, England.

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Abstract

A new fourth order splitting method is presented which in a certain measure is optimal. In combination with a new way of handling non-autonomous problems, the schemes we present are based on Magnus expansions and they show very promising results when applied to Hamiltonian ODEs.

Keywords: Non-linear time-dependent differential equations; Initial value problems; Numerical methods; Free Lie algebra; Magnus expansion

AMS classification: 65L05; 65L70; 65D30

1 Introduction

In the last two decades or so *geometric integration* (GI) of ODEs has been a research area spinning of many useful results. The focus of GI is the construction of numerical methods that retain algebraic and differential algebraic structures of the solutions, hence imposing, in a natural way, constraints on the approximations which are hoped to lead to an improved numerical accuracy. Maybe most importantly structures that lend them self to backward error analysis results which can be used to predict and analyse error growth of numerical methods[24]. Hamiltonian systems whose phase space possess a symplectic structure are maybe the most important of such systems and so called symplectic integrators that retain this structure have been constructed specifically for them. The most successful symplectic integrators are *splitting methods* [13, 15, 25], that work by splitting the vector fields into a sum whose elements are exactly integrable. Another branch of GI is the construction and analysis of numerical methods whose approximate solutions evolve on the same homogenous spaces as the exact solutions. These so called Lie-group methods utilise the fact that one can avoid the generally non-linear structure of the Lie groups associated with the homogenous space by doing the analysis and construction in the corresponding Lie algebras[21]. Central in this development is the so-called Magnus expansion which represents the solution of a linear differential equation $Y' = A(t)Y$ as an exponential $Y(t) = \exp(\Omega(t))Y(0)$.

In this paper we present new numerical methods for solving non-linear differential equations

$$\frac{d\mathbf{x}}{dt} = \mathbf{f}(\mathbf{x}, t) \tag{1}$$

with $\mathbf{x} \in \mathbb{R}^n$ and $\mathbf{f} \in \mathbb{R}^n \times \mathbb{R} \to \mathbb{R}^n$, using the Magnus series which was originally constructed for linear systems. The time-dependent part in $\mathbf{f}(\mathbf{x}, t)$ plays an important role for many problems and it seems of importance to have numerical methods which take special care of it. The simplest and most used trick for avoiding the use of time-dependent functions is to consider t as a new coordinate, x_t, thus increasing the dimension of the phase space, whereupon one solves the transformed equation

$$\frac{d\mathbf{y}}{dt} = \mathbf{F}(\mathbf{y}) \tag{2}$$

numerically with a standard method, where $\mathbf{y} = (\mathbf{x}, x_t)$ and $\mathbf{F}(\mathbf{y}) = (\mathbf{f}(\mathbf{y}), 1)$. In many cases such transformations do not lead to efficient numerical methods, and in some cases, do not lead to accurate methods at all.

Examples of problems where this can be the case are:

- If the explicit time-dependence of $\mathbf{f}$ has a relatively short time scale, then the main contribution to the error will originate from it. Thus it is very important to have numerical methods which efficiently manage the time-dependent part.

- If the time-dependent functions $\mathbf{f}$ are expensive to evaluate, the methods for solving (2) will in general be expensive since they do not attempt to minimise the number of time-evaluations.

- There are many numerical methods which are especially efficient for solving (1) if $\mathbf{f}$ were time-independent and had some special structure.

In (2) the time-dependency is eliminated, but the structure of the equation can be destroyed and one has to resort to more general and less efficient methods. Also the dimension of the phase space has been increased, thus allowing computational errors to accumulate in a larger space.

In order to avoid these problems, we present numerical methods based on the Magnus series. For one time-step, h, the Magnus approximation can be considered as an averaging method for the explicitly time-dependent part. For example the standard averaging of (1) gives

$$\frac{d\hat{\mathbf{x}}}{dt} = \hat{\mathbf{f}}(\hat{\mathbf{x}}), \qquad\qquad \hat{\mathbf{x}}(t_0) = \mathbf{x}(t_0) \tag{3}$$

with $\hat{\mathbf{f}}(\hat{\mathbf{x}}) = \frac{1}{h}\int_{t_0}^{t_0+h} \mathbf{f}(\hat{\mathbf{x}}, s)ds,$ which leads to a second order approximation to the solution $\hat{\mathbf{x}}(t_0+h) = \mathbf{x}(t_0+h) + O(h^3)$. This corresponds to truncating the Magnus series after the first term. In this paper we will generalise the Magnus expansion to non-linear systems and we will rewrite this expansion in order to get fourth order methods which have more or less the same complexity as those methods used to solve eq. (3).

This paper is organised as follows. Section 2 contains a short review of the Magnus series for linear systems and how it can be used to construct numerical methods for such systems. In section 3 we take the formalism of linear systems a step further and use the Magnus series as a representation of the solution of non-linear non-autonomous ODEs. Section 4 introduces a factorisation of the Magnus series in the general case based on the Baker–Campbell–Hausdorff formula, which removes the otherwise difficult commutators. In order to complete the construction of the numerical approximations, section 5 introduces splitting methods for non-autonomous separable systems. That section also summarises the know fourth order methods from the literature, in addition we present a novel method that performs very well. The last section contains a set of numerical experiments showing the efficacy of the proposed schemes, in addition to a conclusion of this work.

2 Magnus series for linear systems

We start by looking at linear systems

$$\frac{d}{dt}X = A(t)X \qquad\qquad X(t_0) = X_0, \tag{4}$$

for which the Magnus series was first introduced, where $X \in \mathbb{R}^{n\times r}$ and $A \in \mathbb{R}^{n\times n}$, and let us introduce the evolution matrix, $X(t) = M(t, t_0)X(t_0)$ with $M \in \mathbb{R}^{n\times n}$. It then follows that M also satisfies a evolution equation

$$\frac{d}{dt}M = A(t)M \qquad\qquad M(t_0) = I. \tag{5}$$

One of the most popular perturbative methods for solving (5), while preserving the qualitative properties of the exact solution, can be obtained through the Magnus expansion [17]. Magnus assumed that the solution was written in the form

$$M(t) = e^{\Omega(t)} \tag{6}$$

with $\Omega = \sum_{i=1}^{\infty} \Omega_i$, also giving the first few terms explicitly. Physicists have studied this problem in connection with Quantum physics, maybe most notably Feynman [8], even though he does not explicitly give the terms.

Recursive expressions for the Ω_ks were presented in [10, 11, 7] using various techniques. While explicit solutions of the recursion relations have been presented in [23, 6, 18]. In particular the low order terms are given by

$$\Omega_1(t) = \int_{t_0}^{t} A(s_1)ds_1; \qquad \Omega_2(t) = \frac{1}{2}\int_{s_0}^{t} ds_1 \int_{t_0}^{s_1} ds_2[A(s_1), A(s_2)]. \tag{7}$$

If A belongs to a Lie algebra, $\mathfrak{g}$ then $\Omega \in \mathfrak{g}$ and the solution will belong to the Lie group, $\mathfrak{G}$, associated with the Lie algebra. Considering that $\Omega_k \in \mathfrak{g} \quad \forall k$, the approximate solutions obtained when truncating the Magnus series will stay in the same Lie group as the exact solution. This seems to us like an important property when manipulating differential equations since the flow of the transformed equation will be restricted to the same space as the exact flow, giving similar global properties of the solutions. Provided that $A(t)$ is a bounded matrix, the series is absolutely convergent for a sufficiently small t [1, 20] and we can expect very accurate approximations in this region, even for a moderate number of terms in the series expansion. In this case the Magnus series seems like a good candidate for constructing numerical methods. One of the main problems with the series is the evaluation of multidimensional integrals. This problem was studied in [10] where it was shown that it is possible to evaluate all multidimensional integrals using standard unidimensional quadratures derived from collocation principles. For example, using a Gauss-Legendre quadrature with n points (n evaluations of $A(t)$ per step) it is possible to obtain a numerical method of order $2n$ in the time-step. In order to improve the efficiency and to simplify the methods the Magnus series is written in terms of unidimensional integrals so the application of quadrature becomes even more transparent[4].

For example, if we consider a time-step, $t = h$, and we define the integrals

$$A^{(0)}(h) = \int_{t_0}^{t_0+h} A(s)ds; \qquad A^{(1)}(h) = \frac{1}{h}\int_{-h/2}^{h/2} sA(s + t_0 + h/2)ds, \tag{8}$$

then

$$\begin{aligned} \Omega(h) &= \Omega_1(h) + \Omega_2(h) + O(h^5) \\ &= A^{(0)} + [A^{(1)}, A^{(0)}] + O(h^5), \end{aligned} \tag{9}$$

corresponds to a fourth order approximation. Higher order methods in terms of unidimensional integrals or Gaussian quadratures can be found in [4, 19].

3 Magnus series for non-linear systems

Let us now return to the non-linear differential equation

$$\frac{d\mathbf{x}}{dt} = \mathbf{f}(\mathbf{x}, t), \tag{10}$$

which can be rewritten in the form

$$\frac{d\mathbf{x}}{dt} = L_{\mathbf{f}(\mathbf{x},t)}\mathbf{x} \tag{11}$$

where $L_{\mathbf{f}}$ is the Lie operator

$$L_{\mathbf{f}} = \sum_{i=1}^{n} f_i(\mathbf{x}, t)\frac{\partial}{\partial x_i}, \tag{12}$$

with $\mathbf{f} = (f_1, \ldots, f_n)$. Applying the Magnus series directly to (11) leads to an immediate difficulty: $L_{\mathbf{f}(\mathbf{x},t)}$ depends on the solution $\mathbf{x}(t)$, which is implicitly time-dependent. This can easily be solved using the properties of Lie operators and Lie transformations.

Denote the solution of (11) as $\mathbf{x}(t) = \mathcal{M}(\mathbf{x}_0, t)$, where $\mathcal{M}$ is a Lie transform giving the evolution of $\mathbf{x}_0$ to $\mathbf{x}(t)$. In order to simplify notation further we will write $\mathcal{M}(\mathbf{x}_0, t) = \mathcal{M}(t)\mathbf{x}_0$, keeping in mind that $\mathcal{M}$ is a non-linear transformation. Then, it is easy to see that eq. (11) can be written as

$$\begin{aligned} \dot{\mathcal{M}}(t)\mathbf{x}_0 &= L_{\mathbf{f}(\mathcal{M}(t)\mathbf{x}_0,t)}\mathcal{M}(t)\mathbf{x}_0 \\ &= \mathcal{M}(t)L_{\mathbf{f}(\mathbf{x_0},t)}\mathbf{x}_0 \end{aligned} \tag{13}$$

where the dot indicates derivative respect to t, and $\mathcal{M}$ satisfies the following differential equation

$$\dot{\mathcal{M}}(t) = \mathcal{M}(t)L_{\mathbf{f}(\mathbf{x_0},t)}, \tag{14}$$

where both $\mathcal{M}$ and $L_{\mathbf{f}(\mathbf{x_0},t)}$ are operators acting on the initial conditions. Observe that $L_{\mathbf{f}(\mathbf{x_0},t)}$ is now only explicitly dependent on t, and we can use the Magnus series as in the previous section. Basically the same result can be obtained through considering all diffeomorphism $\varphi : \mathbb{R}^n \mapsto \mathbb{R}$, in which we use that $\varphi(\hat{\mathbf{x}})$ satisfies the quasi-linear PDE $\frac{\partial}{\partial t}\varphi(\hat{\mathbf{x}}) = L_{\mathbf{f}(\hat{\mathbf{x}},t)}\varphi(\hat{\mathbf{x}})$, a device introduced by Cauchy.

At this point it seems appropriate to introduce classical Hamiltonian systems. If we denote the Hamiltonian $H(\mathbf{q}, \mathbf{p}, t)$ were $\mathbf{q}$, $\mathbf{p} \in \mathbb{R}^n$ are the coordinates and momenta of the system, then the Hamiltonian equations are

$$\dot{\mathbf{q}} = \frac{\partial H}{\partial \mathbf{p}}; \qquad \dot{\mathbf{p}} = -\frac{\partial H}{\partial \mathbf{q}}. \tag{15}$$

If we now introduce the notation $\mathbf{z} = (\mathbf{q}, \mathbf{p}) = (q_1, \ldots, q_n, p_1, \ldots, p_n)$, then (15) can be simplified to

$$\dot{\mathbf{z}} = L_{H(\mathbf{z},t)}\mathbf{z} \tag{16}$$

where we now are using the standard notation in Hamiltonian systems

$$L_H = \sum_{i=1}^{n} \left(\frac{\partial H}{\partial p_i}\frac{\partial}{\partial q_i} - \frac{\partial H}{\partial q_i}\frac{\partial}{\partial p_i} \right) = \sum_{i,j=1}^{n} \frac{\partial H}{\partial z_i} J_{i,j} \frac{\partial}{\partial z_j} \tag{17}$$

with $J = \begin{pmatrix} 0 & -I \\ I & 0 \end{pmatrix}$ and I is the $n \times n$ identity matrix. Observe that $L_H\mathbf{z} = \{\mathbf{z}, H\}$, where $\{\cdot, \cdot\}$ is the usual Poisson bracket, and the evolution operator $\mathbf{z}(t) = \mathcal{M}(\mathbf{z}_0, t)$ satisfies the linear differential equation (14) after exchanging $L_{H(\mathbf{z}_0,t)}$ for $L_{\mathbf{f}(\mathbf{x_0},t)}$ (see [22]). In order to use the results of the previous section, we take the time derivative of $\mathcal{M}\mathcal{M}^{-1} = I$, and by using (16) we obtain

$$\dot{\mathcal{M}}^{-1} = -L_{\mathbf{f}}\mathcal{M}^{-1} \tag{18}$$

so if we denote $\mathcal{M}^{-1} = e^{-L_\Omega}$ then $\mathcal{M} = e^{L_\Omega}$ with $L_\Omega = \sum_i L_{\Omega_i}$. Using (7) we have

$$L_{\Omega_1(t)} = \int_{t_0}^{t} L_{\mathbf{f}_1} ds_1; \qquad L_{\Omega_2(t)} = -\frac{1}{2}\int_{t_0}^{t} ds_1 \int_{t_0}^{s_1} ds_2 [L_{\mathbf{f}_1}, L_{\mathbf{f}_2}] \tag{19}$$

where $\mathbf{f}_i \equiv \mathbf{f}(\mathbf{x}_0, s_i)$. Observe that the sign of $L_{\Omega_{2n}}$ is changed when compared with (7). Finally, if we want to write the solution in terms of unidimensional integrals we define

$$\mathbf{f}^{(0)}(\mathbf{x}_0, h) = \int_{t_0}^{t_0+h} \mathbf{f}(\mathbf{x}_0, s) ds; \qquad \mathbf{f}^{(1)}(\mathbf{x}_0, h) = \frac{1}{h} \int_{-h/2}^{h/2} s\mathbf{f}(\mathbf{x}_0, s+t_0+h/2) ds, \tag{20}$$

and have

$$L_{\Omega(h)} = L_{\mathbf{f}^{(0)}} + [L_{\mathbf{f}^{(0)}}, L_{\mathbf{f}^{(1)}}] + O(h^5). \tag{21}$$

For Hamiltonian systems we have that

$$[L_{H_1}, L_{H_2}] = L_{\{H_1, H_2\}} \tag{22}$$

with $H_i \equiv H(\mathbf{z}_0, t_i)$, while in the general case

$$[L_{\mathbf{f}_1}, L_{\mathbf{f}_2}] = L_{\mathbf{g}} \tag{23}$$

where $\mathbf{g} = (g_1, \ldots, g_n)$ and

$$g_i = \sum_{j=1}^{n} \left(\frac{\partial f_i(s_1)}{\partial x_j} f_j(s_2) - \frac{\partial f_i(s_2)}{\partial x_j} f_j(s_1) \right), \tag{24}$$

so all the operations can be carried out on the Hamiltonian function. Thus solving (10) over one time step, h, using the Magnus series is equivalent to solving an autonomous system

$$\dot{\hat{\mathbf{x}}} = \mathbf{F}(\hat{\mathbf{x}}, h). \tag{25}$$

over the same time step h. Now considering only the first term in the Magnus series then we have

$$\mathbf{F}(\hat{\mathbf{x}}, h) = \frac{1}{h} \int_{t_0}^{t_0+h} \mathbf{f}(\hat{\mathbf{x}}, t) dt, \tag{26}$$

(or equivalently, $\mathbf{F}(\hat{\mathbf{x}}, h) = \frac{1}{h}\mathbf{f}^{(0)}(\hat{\mathbf{x}}_0, h)$) giving a second order approximation to $x(t)$ in h. Higher order methods involve more terms in the Magnus series. In this case the expression for $\mathbf{F}(\hat{\mathbf{x}}, h)$ will have terms like the integral of (24), and it is impractical to compute the commutator. This is the reason why Magnus' series has not been a popular method for solving nonlinear differential equations.

4 Splitting the Magnus series

For many problems, it is very easy to solve eq. (25) in the particular case that $\mathbf{F} = \alpha_1 \mathbf{f}^{(0)} + \alpha_2 \mathbf{f}^{(1)}$, with α_1 and α_2 constants. Considering that $\exp\left(\alpha_1 L_{\mathbf{f}^{(0)}} + \alpha_2 L_{\mathbf{f}^{(1)}}\right)$ is easy to evaluate, we will try to write the Magnus expansion as a product of this class of simple flows. In particular we will consider fourth order methods in the form

$$e^{L_{\Omega(h)}} = \prod_{i=1}^{m} e^{L_{\alpha_i \mathbf{f}^{(0)} + \beta_i \mathbf{f}^{(1)}}} + O(h^5). \tag{27}$$

In [5] we presented the following factorisations in the linear case

$$\begin{aligned} e^{\Omega(h)} = e^{A^{(0)} + [A^{(1)}, A^{(0)}] + O(h^5)} &= e^{\frac{1}{2}A^{(0)} + 2A^{(1)}} \, e^{\frac{1}{2}A^{(0)} - 2A^{(1)}} + O(h^5) \qquad (28) \\ &= e^{A^{(1)}} \, e^{A^{(0)}} \, e^{-A^{(1)}} + O(h^5) \qquad (29) \end{aligned}$$

which are derived by using the Baker–Campbell–Hausdorff (BCH) formula. In the case of non-linear equations the equivalent result is

$$\begin{aligned} \exp\left(L_{\Omega(h)}\right) &= \exp\left(L_{\mathbf{f}^{(0)}} + [L_{\mathbf{f}^{(0)}}, L_{\mathbf{f}^{(1)}}] + O(h^5)\right) \\ &= \exp\left(L_{\frac{1}{2}\mathbf{f}^{(0)} - 2\mathbf{f}^{(1)}}\right) \exp\left(L_{\frac{1}{2}\mathbf{f}^{(0)} + 2\mathbf{f}^{(1)}}\right) + O(h^5) \qquad (30) \\ &= \exp\left(-L_{\mathbf{f}^{(1)}}\right) \exp\left(L_{\mathbf{f}^{(0)}}\right) \exp\left(L_{\mathbf{f}^{(1)}}\right) + O(h^5), \qquad (31) \end{aligned}$$

but observe that in (30) and (31) the order of the factors are the reverse of (28) and (29). This is so because of the way Lie transformations act on the initial conditions. For example, if we denote $\mathbf{x}_1 \equiv \mathbf{x}_1(\mathbf{x}_0) = e^{L_{\mathbf{f}_1(\mathbf{x}_0)}}\mathbf{x}_0$ and $\mathbf{x}_2 \equiv \mathbf{x}_2(\mathbf{x}_0) = e^{L_{\mathbf{f}_2(\mathbf{x}_0)}}\mathbf{x}_0$ then

$$\begin{aligned} e^{L_{\mathbf{f}_1(\mathbf{x}_0)}} \, e^{L_{\mathbf{f}_2(\mathbf{x}_0)}} \mathbf{x}_0 &= e^{L_{\mathbf{f}_1(\mathbf{x}_0)}} \mathbf{x}_2(\mathbf{x}_0) = \mathbf{x}_2(e^{L_{\mathbf{f}_1(\mathbf{x}_0)}} \mathbf{x}_0) = \mathbf{x}_2(\mathbf{x}_1) \\ &= e^{L_{\mathbf{f}_2(\mathbf{x}_1)}} \mathbf{x}_1. \qquad (32) \end{aligned}$$

If $L_{\mathbf{f}}$ was a Lie operator associated with a linear operator, then (30) and (31) would be equal to (28) and (29).

As a simple example to follow we consider the scalar equation

$$\dot{x} = 1 + \beta(t) x^2, \tag{33}$$

which corresponds to solving (25) with $\mathbf{F}(\mathbf{x}) = \bar{\alpha} + \bar{\beta} x^2$, $\bar{\alpha}$ and $\bar{\beta}$ now constant, thus $\mathbf{f}^{(0)} = h + \beta^{(0)} x^2$ and $\mathbf{f}^{(1)} = \beta^{(1)} x^2$ where $\beta^{(i)}$, $i = 0, 1$ are given by (8), after substituting for the matrix A the function β. For example, to apply scheme (30) is equivalent to solving the following sequence of two exactly solvable autonomous equations

$$\begin{array}{lll} \dot{x}_1 = \frac{1}{2} + \frac{1}{h}\left(\frac{1}{2}\beta^{(0)} - 2\beta^{(1)}\right)x_1^2 & x_1(0) = x_0 & t \in [0,h] \\ \dot{x}_2 = \frac{1}{2} + \frac{1}{h}\left(\frac{1}{2}\beta^{(0)} + 2\beta^{(1)}\right)x_2^2 & x_2(0) = x_1(h) & t \in [0,h]. \end{array} \tag{34}$$

where $x_2(h)$ is the approximate solution at $t = h$. If the integrals for $\beta^{(i)}$ are not explicitly available, one can freely use numerical quadratures of sufficient accuracy to obtain approximations.

It seems to us clear that important information of the original equation is retained, while at the same time the most expensive part in the calculation is reduced. Thus, a method like (34), based on the average of β seems to be an efficient alternative to known methods in analogous cases.

The main motivation of geometric integration is to reduce the global error growth by taking advantage of structural stability results. If we let $\tilde{y}_n$ denote the numerical approximation to $y(t_n)$ obtained after n steps it is known that the global error can be bounded as

$$\|y(t_n) - \tilde{y}_n\| = C_1 h^p t_n + C_2 h^p t_n^2.$$

While for special cases like e.g. periodic problems one can get a linear error bound

$$\|y(t_n) - \tilde{y}_n\| = C_1^* h^p t_n.$$

It is well known that one of the most important properties of symplectic integrators is that they present a linear error growth in the coordinates (when applied on bounded Hamiltonian systems) as opposed to quadratic like for many standard numerical methods. The new methods presented in this paper are geometric integrators and we expect better than quadratic error growth when applying them to systems with bounded solutions. In order to illustrate this fact let us consider the forced pendulum

$$\ddot{x} + \sin(x) = F\cos(w\,t) \tag{35}$$

with F and w constants. This equation is associated to the Hamiltonian $H = \frac{1}{2}p^2 - \cos(q) - F\cos(w\,t)q$, and is one of the most popular equations in textbooks on non-linear systems because of its simplicity as well as its richness in qualitative properties.

Solving (35) using our method (30) for one time step, h, is equivalent to solving the equations obtained through the autonomous Hamiltonian

$$H = \frac{1}{4}p^2 - \frac{1}{2}\cos(q) - F_1 q \tag{36}$$

followed by the Hamiltonian

$$H = \frac{1}{4}p^2 - \frac{1}{2}\cos(q) - F_2 q \tag{37}$$

where $F_{1,2} = \frac{1}{h}F\left(\frac{1}{2}c^{(0)} \mp 2c^{(1)}\right)$ and $c^{(i)}, \quad i = 0, 1$ are given by (8), substituting the function $\cos(w\,t)$ for the matrix A.

At this moment we are only interested in the error growth of the Magnus truncation so we will solve the equations for (36) and (37) numerically to machine accuracy, e.g. splitting the time step in a number of subintervals and using an accurate method in each subinterval. The computational cost as well as the best implementation will be analysed in later sections. The solution will be compared with results obtained using the standard fourth order Runge-Kutta method. We considered $F = 1/10$ and $w = 1$, with initial conditions $(q,p) = (0,1)$. In figure 1 we give the average error in (q,p) along the interval $t \in [0, 5000 \cdot 2\pi]$ for the schemes (30), (31) together with the classical RK method using the same time step $h = 2\pi/100$. Observe that all methods use the same number of time evaluations.

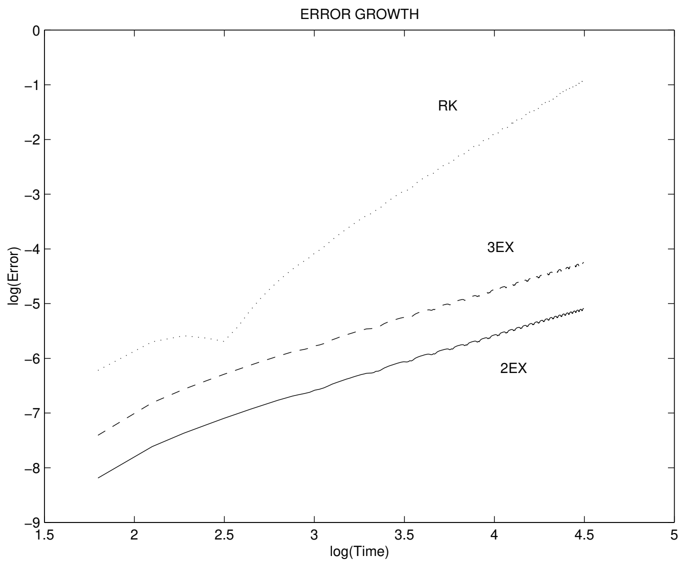

Figure 1: Average errors in position vs. time for the forced pendulum problem using the Runge-Kutta method, and the schemes 2-EX (30) and 3-EX (31) based on Magnus expansions.

The main point of figure 1 is the linear error growth introduced by the factored Magnus expansion, as opposed to quadratic for a 'non-geometric' approximation. Hence by approximating the flows of the autonomous vectorfields produced by schemes (30) and (31) using a geometric scheme retains the linear error growth sought after in geometric integration.

After applying schemes (30) and (31) to several examples in section 6, it will become clear when the various methods lead to more efficient algorithms.

4.1 Preservation of Time-symmetry

Time-symmetry is one important qualitative property of the exact solution and it is some times important to preserve it in numerical approximations. This has been shown in case of ODEs with periodic solutions and small perturbations of such. Numerical experiments show that time-symmetry is a geometric quality on equal footing with symplecticity for Hamiltonian ODE systems, and we now wish to show that (28)-(31) satisfy this condition.

Definition: A one step method $\mathbf{x}_h = \Phi(t_0 + h, t_0, \mathbf{x}_0)$, is time-symmetric if it satisfies $\mathbf{x}_0 = \Phi(t_f - h, t_f, \mathbf{x}_h)$ with $t_f = t_0 + h$.

In other words, if we integrate an ODE numerically over one step, h, followed by an integration of the same ODE backwards in time using the same method but with time step $-h$, we recover the initial condition. If we use the short notation $\Phi(h)$ for the method, then Φ is time-symmetric if

$$\Phi^{-1}(h) = \Phi(-h). \tag{38}$$

From definition (8) we have $A^{(0)}(-h) = -A^{(0)}(h)$, $A^{(1)}(-h) = A^{(1)}(h)$, and similarly from (20), $\mathbf{f}^{(0)}(\mathbf{x}_0, -h) = -\mathbf{f}^{(0)}(\mathbf{x}_0, h)$, $\mathbf{f}^{(1)}(\mathbf{x}_0, -h) = \mathbf{f}^{(1)}(\mathbf{x}_0, h)$. Let us consider (28), then

$$\begin{aligned} \Phi(-h) &\equiv e^{\frac{1}{2}A^{(0)}(-h)+2A^{(1)}(-h)}\, e^{\frac{1}{2}A^{(0)}(-h)-2A^{(1)}(-h)} && (39)\\ &= e^{-\frac{1}{2}A^{(0)}(h)+2A^{(1)}(h)}\, e^{-\frac{1}{2}A^{(0)}(h)-2A^{(1)}(h)} \equiv \Phi^{-1}(h), && (40) \end{aligned}$$

so, it is time-symmetric. A similar proof holds for (29). However, for the nonlinear case it is not so straight forward. If we consider (30), then

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

and we have to prove that, using the same method on $\mathbf{x}_h$ with a time step

$-h$, we recover the initial condition $\mathbf{x}_0$. Taking into account (32) we have

$$\begin{aligned}
&\Phi(t_f-h,t_f,x_h)\\
&\equiv \exp\left(L_{\frac{1}{2}\mathbf{f}^{(0)}(\mathbf{x}_h,-h)-2\mathbf{f}^{(1)}(\mathbf{x}_h,-h)}\right)\,\exp\left(L_{\frac{1}{2}\mathbf{f}^{(0)}(\mathbf{x}_h,-h)+2\mathbf{f}^{(1)}(\mathbf{x}_h,-h)}\right)\mathbf{x}_h\\
&=\exp\left(-L_{\frac{1}{2}\mathbf{f}^{(0)}(\mathbf{x}_h,h)+2\mathbf{f}^{(1)}(\mathbf{x}_h,h)}\right)\,\exp\left(-L_{\frac{1}{2}\mathbf{f}^{(0)}(\mathbf{x}_h,h)-2\mathbf{f}^{(1)}(\mathbf{x}_h,h)}\right)\mathbf{x}_h\\
&=\left(\exp\left(L_{\frac{1}{2}\mathbf{f}^{(0)}(\mathbf{x}_0,h)-2\mathbf{f}^{(1)}(\mathbf{x}_0,h)}\right)\,\exp\left(L_{\frac{1}{2}\mathbf{f}^{(0)}(\mathbf{x}_0,h)+2\mathbf{f}^{(1)}(\mathbf{x}_0,h)}\right)\right)\\
&\times\left(\exp\left(-L_{\frac{1}{2}\mathbf{f}^{(0)}(\mathbf{x}_0,h)+2\mathbf{f}^{(1)}(\mathbf{x}_0,h)}\right)\,\exp\left(-L_{\frac{1}{2}\mathbf{f}^{(0)}(\mathbf{x}_0,h)-2\mathbf{f}^{(1)}(\mathbf{x}_0,h)}\right)\mathbf{x}_0\right)=\mathbf{x}_0,
\end{aligned}$$

and similarly for (31).

Finally, it is important to say that, because $A^{(0)}(h)=O(h)$ and $A^{(1)}(h)=O(h^2)$ then (28) and (29) would agree with the exact solution up to order h^3 but since time-symmetry is preserved they will agree with the exact solution up to order h^4 as has been indicated, the same follows for the nonlinear schemes (30) and (31). In addition to being a geometric quality time-symmetry also considerably simplifies the search of numerical methods in terms of the number order-conditions needed.

5 Separable systems

Frequently equation (1) is separable in two parts, $\mathbf{f}(\mathbf{x},t)=\mathbf{f}_A(\mathbf{x},t)+\mathbf{f}_B(\mathbf{x},t)$, such that

$$\dot{\mathbf{x}_\mathbf{a}}=\alpha_1\mathbf{f}_A^{(0)}(\mathbf{x}_\mathbf{a})+\alpha_2\mathbf{f}_A^{(1)}(\mathbf{x}_\mathbf{a});\qquad\qquad \dot{\mathbf{x}_\mathbf{b}}=\beta_1\mathbf{f}_B^{(0)}(\mathbf{x}_\mathbf{b})+\beta_2\mathbf{f}_B^{(1)}(\mathbf{x}_\mathbf{b}) \tag{42}$$

are exactly solvable (or at least easy to evaluate up to the desired order). This is the case, for example, for Hamiltonian systems separable in the kinetic and potential energies, $H(\mathbf{q},\mathbf{p},t)=T(\mathbf{p},t)+V(\mathbf{q},t)$. In this case, when using (30) we have

$$\frac{1}{2}\mathbf{f}^{(0)}\pm 2\mathbf{f}^{(1)}=\left(\frac{1}{2}\mathbf{f}_A^{(0)}\pm 2\mathbf{f}_A^{(1)}\right)+\left(\frac{1}{2}\mathbf{f}_B^{(0)}\pm 2\mathbf{f}_B^{(1)}\right). \tag{43}$$

and we can apply a splitting method for the numerical approximation. Splitting methods introduce additional errors, and it is important to keep them as small as possible. If the the main contribution to the error comes from the Magnus approximation we should use cheap splitting methods. Under this assumption it seems more useful to look for methods requiring fewer factors in product

$$e^{L_{\Omega(h)}}=\prod_{i=1}^{m}\exp\left(L_{a_1\mathbf{f}_A^{(0)}+c_1\mathbf{f}_A^{(1)}}\right)\exp\left(L_{b_1\mathbf{f}_B^{(0)}+d_1\mathbf{f}_B^{(1)}}\right)+O(h^5), \tag{44}$$

were a_i, b_i, c_i and d_i are constants to be determined. If we assume that $\mathbf{f}_A^{(1)} = \mathbf{f}_B^{(1)} = 0$ and consider one of the splitting methods of section 5.1 then

$$\prod_{i=1}^{m} \exp\left(a_i L_{\mathbf{f}_A^{(0)}}\right) \exp\left(b_i L_{\mathbf{f}_B^{(0)}}\right) = \exp\left(L_{\mathbf{f}_A^{(0)}+\mathbf{f}_B^{(0)}}\right) + O(h^5), \tag{45}$$

thus $\{a_i, b_i\}_{i=1}^m$ are the coefficients of a splitting method in the autonomous case. If we suppose that $\mathbf{f}_A^{(0)}$ and $\mathbf{f}_A^{(1)}$ commute as well as $\mathbf{f}_B^{(0)}$ and $\mathbf{f}_B^{(1)}$, then the composition

$$\exp\left(-L_{\mathbf{f}_A^{(1)}}\right) \exp\left(-L_{\mathbf{f}_B^{(1)}}\right) \left(\prod_{i=1}^{m} \exp\left(a_i L_{\mathbf{f}_A^{(0)}}\right) \exp\left(b_i L_{\mathbf{f}_B^{(0)}}\right)\right) \exp\left(L_{\mathbf{f}_B^{(1)}}\right) \exp\left(L_{\mathbf{f}_A^{(1)}}\right)$$

satisfies (44). However, if (45) is symmetric it is still more efficient to consider the composition

$$\begin{aligned} &\exp\left(L_{a_1\mathbf{f}_A^{(0)}-\mathbf{f}_A^{(1)}}\right) \exp\left(L_{b_1\mathbf{f}_B^{(0)}-d\mathbf{f}_B^{(1)}}\right) \exp\left(a_2 L_{\mathbf{f}_A^{(0)}}\right) \ldots \\ &\ldots \exp\left(a_2 L_{\mathbf{f}_A^{(0)}}\right) \exp\left(L_{b_1\mathbf{f}_B^{(0)}+d\mathbf{f}_B^{(1)}}\right) \exp\left(L_{a_1\mathbf{f}_A^{(0)}+\mathbf{f}_A^{(1)}}\right) \end{aligned} \tag{46}$$

where a_i, b_i are the coefficients of the symmetric splitting method and $d = 1/(1-2a_1)$.

5.1 Fourth-order splitting methods

Considering that the new methods based on Magnus series are of fourth order, we are interested in looking for splitting methods of this accuracy. In the literature we can find a huge number of methods, many specially tailored for particular structures of A and B. In order to avoid the use of different methods for each problem, we will present a new fourth order method which works more efficiently for the important case of quadratic kinetic energies ('RKN' problems) than any other one we found in the literature. In addition, it will work as efficiently as the best methods we know for the most general case of A and B and will be competitive for other structures assumed on A and B.

Let us consider a fourth order composition

$$\prod_{i=1}^{m} e^{ha_iA} e^{hb_iB} = e^{h(A+B)+h^5R+O(h^6)}, \tag{47}$$

where R contains the main error terms. Such a method is completely determined by the vectors $\mathbf{a} = (a_1, \ldots, a_m)$ and $\mathbf{b} = (b_1, \ldots, b_m)$, and can be considered as a partitioned Runge–Kutta method. In the following we will consider different structures for A and B and in each separate case, we will look for the most efficient splitting method.

To compare the different methods, it is interesting to study the case when no special structure is assumed on A and B (the FLA (Free Lie Algebra) case). Let $L(A,B)$ denote the algebra whose elements are A, B and all elements obtained through the vector space operations of addition and multiplication by scalars in addition to the commutator. The subset $L^5(A,B)$ of commutators with 5 operators can be represented by the six dimensional basis

$$\begin{array}{ll} E_{5,1}=[A,[A,[A,[A,B]]]], & E_{5,6}=[B,[B,[B,[B,A]]]], \\ E_{5,2}=[B,[A,[A,[A,B]]]], & E_{5,5}=[A,[B,[B,[B,A]]]], \\ E_{5,3}=[A,[A,[B,[B,A]]]], & E_{5,4}=[B,[B,[A,[A,B]]]] \end{array}$$

thus we can write $R=\sum_{i=1}^{6} r_i E_{5,i}$. It is usual to define the leading error coefficient of (47) as the Euclidian norm of the vector $\mathbf{r}=(r_1,\ldots,r_6)$, i.e. $\mathcal{E}=\sqrt{\sum_i r_i^2}$. Next, in order to compare the efficiency of different method one can consider its cost per step. In (47) m is usually proportional to the cost of one step, but not always. For example, the second order leapfrog method $e^{\frac{h}{2}A}e^{B}e^{\frac{h}{2}A}$ would correspond to $m=2$ with $\mathbf{a}=(1/2,1/2)$ and $\mathbf{b}=(1,0)$ but since $\mathbf{b}_2=0$ the first and the last "A-exponential" can be concatenated. Thus effectively the cost per step is lowered by one function evaluation. In such and similar cases we will assume that the cost is proportional to $m-1$ instead of m. With these assumptions the standard definition for the effective error is $E_f=\mu\mathcal{E}^{1/4}$, where $\mu=m$ or $\mu=m-1$ accordingly. We will take as the most efficient method the one with the smaller effective error. It is important to notice that the adjoint composition of (47) (obtained through reversing the order of the exponentials) has exactly the same order and error and therefore we need not consider those cases.

The following cases are studied:

1– RKN: corresponds to the special case in which $[B,[B,[B,A]]]=0$. Considering that now $E_{5,5}=E_{5,6}=0$ so a complete description of the leading error term is described by the vector $\mathbf{r}=(r_1,\ldots,r_4)$. In this case A and B are qualitatively different and can not be interchanged. For example, if we take $a_1=0$ we will find methods with different value of E_f than considering $b_m=0$. In [24] a non symmetric composition with $m=5$ and $a_1=0$ is presented whose effective error constant is $E_f=0.476$. With $m=4$ a method with $E_f=0.509$ has been found [13]. Symmetric compositions with $b_m=0$ can also be found in [13] for $m=5$ and $m=6$ with $E_f=0.634$ and $E_f=0.527$, respectively. We found no other symmetric compositions with

$a_1 = 0$, hence a search for methods with $m = 5$ and $m = 6$ was initiated. In the first case no improved methods were found, while for $m = 6$ a new method with $E_f = 0.360$ was discovered, let us denote it S^*. S^* is the most efficient method known to us of this type and it is given by the coefficients

$$\mathbf{a} = (0, a_2, a_3, a_4, a_3, a_2); \qquad \mathbf{b} = (b_1, b_2, b_3, b_3, b_2, b_1) \tag{48}$$

with

$$\begin{array}{lll} a_2 = 0.254 & a_3 = -0.032290201410934288448 & a_4 = 1 - 2(a_2 + a_3) \\ b_1 = 0.084 & b_2 = 0.682281125946589406371 & b_3 = \frac{1}{2} - (b_1 + b_2). \end{array} \tag{49}$$

The error coefficients of the method are given by

$$\mathbf{r} = 10^{-5} \times (-0.82,\ 2.13,\ -0.65,\ -1.28,\ 23.07,\ 9.95). \tag{50}$$

Observe that, for this problem B commutes with $[B, [B, A]]$ and for many problems both operators represent exactly solvable ODEs. On can in this case obtain schemes by composing exponentials of not only B and A but instead of the Bs, $C_{b_i,c_i} = b_i B + h^2 c_i [B, [B, A]]$ (referred to as a modified potential). If the commutator is not very expensive to evaluate, such methods could possibly lead to very efficient schemes, and one scheme of this type is found in [12];

$$\mathbf{a} = (0, \frac{1}{2}, \frac{1}{2}); \qquad \mathbf{b} = (\frac{1}{6}, \frac{2}{3}, \frac{1}{6}); \qquad \mathbf{c} = (0, -\frac{1}{72}, 0). \tag{51}$$

The effective error of the method is $E_f = \mu_m \mathcal{E}^{1/4} = \mu_m\, 0.164$, where μ_m will depend on the cost of the modified potentials. It is usual to take into consideration the cost as a number in the interval $\mu_m \in (\mu, \mu + \pi)$, where π is the number of modified potentials appearing in the scheme. With this criterium we find $E_f \in (0.327, 0.491)$ and in practice it does not improve the previous method by much. We have analysed the uniparametric family of solutions in the case $c_1 = c_3 \neq 0$, obtaining the minimum very close to $c_1 = c_3 = 0$, with error $\mu_m \mathcal{E}^{1/4} = \mu_m\, 0.156$. This improvement is also too small to compensate for the presence of extra modified potentials. The case $b_3 = c_3 = 0$ gave two solutions but also these had a bigger error constant.

2− Free Lie Algebra (FLA): corresponds to the general case where no simplification in the algebra is possible. In this case, it seems preferable to consider only symmetric compositions since A and B are interchangeable. The Ruth/Yoshida method with $m = 4$ given in [25] has $E_f = 1.335$. For $m = 5$ and $m = 6$ we found two methods with $E_f = 0.708$ and $E_f = 0.623$, respectively [13]. The RKN scheme S^*, being symmetric, turns by a stroke of luck to be a fourth order method also for this case with $E_f = 0.630$. It is, essentially, as efficient as the best method and has the additional property of being much better in the RKN case so we conclude this paragraph by recommending scheme S^*.

3– RKN2: corresponds to the case $[B,[B,[B,A]]] = [A,[A,[A,B]]] = 0$. We will take $\mathbf{r} = (r_3, r_4)$ in the definition of the error, because $E_{5,1} = E_{5,2} = E_{5,5} = E_{5,6} = 0$. Observe that now A and B can be considered qualitatively equivalent and they are interchangeable. In [9] they present several families of non-symmetric methods where the coefficients of (47) satisfy the relation $b_{m+1-i} = a_i, \quad i = 1, \ldots, m$. This symmetry imposes that $r_3 = r_4$, being an useful property in some cases. For example in [5] these schemes were applied to a particular representation of the Schrödinger equation where the uniticity was not exactly preserved (as was the case for other symplectic integrators) but was retained at higher order than the order of the method because $r_3 = r_4$. The most efficient fourth order methods of [9], denoted by $(m = 4, n = 4)$ and $(m = 6, n = 4)$, have $E_f = 0.342$ and $E_f = 0.322$, respectively.

Using symmetric or non-symmetric compositions does not alter the situation by much. We have also studied the use of modified potentials in this case but the reduction in the number of exponentials per step do not compensate the extra cost. S^* has for this problem $E_f = 0.308$, thus we again conclude by recommending S^*.

4– Near-Integrable (NI): This is the case in which $\|B\| \ll \|A\|$ for some norm. It is therefore natural to optimise the accuracy with this priori information, hence one can consider a smaller number of order conditions when constructing the method. It is now the case that $\|E_{5,i}\| \ll \|E_{5,1}\|, \quad i = 2, \ldots, 6$ and an efficient method will be the one that minimises the coefficient of $E_{5,1}$. For this problem it is difficult to define a useful effective error because one has to consider h as well as the size of $\|B\|$ in the measure. Again, A and B are qualitatively different and the number of possible methods is higher. For example, in [14] we found two symmetric second order methods (taking $m = 3$ and $a_1 = 0$ or $b_3 = 0$) which work in practice as fourth order methods for many problems. One of them is given by (51) taking $c_2 = 0$. Even more efficient symmetric fourth order methods are presented in [14] cancelling the coefficients of $E_{5,1}$, $[A, E_{5,1}]$, $[A,[A,E_{5,1}]]$ and $[A,[A,[A,E_{5,1}]]]$, and the most efficient corresponds to the "(8,4) BAB" method. The error coefficients of this method are

$$\mathbf{r} = 10^{-5} \times (0,\ 1.08,\ -44.79,\ \ldots), \tag{52}$$

where the coefficients of $E_{5,2}$ and $E_{5,3}$ (containing two B operators) give the main contribution to the overall error. From these coefficients and comparing with the coefficient of $E_{5,1}$ in (50), $-0.82 \cdot 10^{-5}$, we can see that, unless $\|B\| \leq \|A\|/50$, the method S^* will be more efficient[1]. If $\|B\|$ was even smaller it would be sufficient to use the second order method (51) with $c_2 = 0$ because the main contribution to the error would come from the Magnus approximation.

In conclusion, we have presented a new method which works very efficiently under many assumptions on the vectorfields. It is at least as accurate as other methods which were specially designed for the special cases. In our opinion, for most of the problems, it is highly recommended to use only the new method.

In this section we have considered only one step splitting methods because we are dealing with a time-dependent problem. That means A and B will change with time. One class of very efficient methods are schemes based on processing techniques [2, 3, 16] but they would be efficient for our problem only if the evaluation of each exponential in (28)-(30) was split in a relatively large number of sub steps which is the case only for extremely slowly varying vectorfields.

6 Numerical examples

In this section we present numerical experiments that highlight the efficency of the proposed schemes. The first subsection contains experiments showing the performance of the new splitting method applied to several different separable vectorifield, each of which there exist specially tailored schemes with which we compare our method with. In the second subsection we apply the factored Magnus series to a non-autonomous version of the duffing oscillator to produce an autonomous approximation which in turn is solved using the new splitting scheme presented in Section 4. In the third subsection we study how the new methods perform for oscillatory vectorfields with different time-scales.

6.1 Performance of the new splitting method

In the following, we will test S^* on four different systems which are of the types separable (FLA), quadratic kinetic energy (RKN), quadratic Hamilto-

[1]The error coefficient $[A,[A,E_{5,1}]]$ of S^* is $9.64 \cdot 10^{-7}$ also being very small

nian (RKN2) and near integrable (NI). We will compare S^* with the most efficient schemes in each case accordingly. In particular, we will consider the following methods:

- FLA: The most efficient fourth order symmetric method given in [15] we denote this S_{FLA}. (Triangles joined by lines).
- RKN: The most efficient fourth order symmetric method given in [15], denoted by us S_{RKN}. (Squares joined by lines).
- RKN2: The $(m = 4, n = 4)$ scheme presented in [9], denoted S_{RKN2}, (asterisks joined by lines).
- NI: The scheme $(8, 4) - BAB$ presented in [14], denoted S_{NI} (diamonds joined by lines).
- The new scheme S^* (circles joined by broken lines).
- The well known symmetric fourth order method of Ruth/Yoshida [25] (crosses joined by lines). This is used as a reference method, because is the most well known and has been used in many papers.

First we consider four autonomous Hamiltonian systems and use the average error in energy as measure of accuracy. The interval of integration is not of great importance since the average error in energy is always bounded by constants for all methods and problems studied.

(a)- FLA: The Hamiltonian considered is

$$H = \frac{1}{2}(p^2 + q^2) + \frac{1}{2}p^2q^2, \tag{53}$$

being separable in two exactly solvable parts with no possible simplification in the algebra. The initial conditions used are $(q, p) = (2, 0)$ and we integrated the system along the interval $t \in [0, 20 \cdot 2\pi]$. Taking into account that all symmetric methods considered are also fourth order methods for FLA problems we present the average error in energy versus the number of function evaluations for different time-steps(figure 2a). The numerical experiment agree very well with the theoretical result from the effective error analysis.

(b)- RKN: The simple Hamiltonian associated with the pendulum will be used as a system suitable for RKN methods,

$$H = \frac{1}{2}p^2 - cos(q). \tag{54}$$

The initial conditions used are $(q,p) = (0,1)$ and we integrated the system along the interval $t \in [0, 20 \cdot 2\pi]$. In figure 2b we give the average error in energy versus the number of function evaluations for several time-steps. In this case the new method clearly shows its superiority. Observe that it is approximately three orders of magnitude more accurate at the same computational cost than the Ruth/Yoshida method. While it is one order of magnitude more accurate than the previously most efficient method, S_{RKN}.

(b)- RKN2: The simplest Hamiltonian suitable for RKN2 methods is the harmonic oscillator, $H = p^2/2 + q^2/2$. But, in order to better understand the interest in RKN2 methods we will study a less trivial system. Let us consider the Schrödinger equation with the Morse potential

$$i\frac{d}{dt}\psi(x,t) = \left(-\frac{1}{2\mu}\frac{\partial^2}{\partial x^2} + D\left(1 - e^{-\alpha x}\right)^2\right)\psi(x,t), \qquad \psi(x,0) = \psi_0(x) \tag{55}$$

with parameters: $\mu = 1745$ $a.u.$, $D = 0.2251$ $a.u.$ and $\alpha = 1.1741$ $a.u.$, corresponding to the HF molecule. As initial conditions we will take the ground state whose energy is $E_0 = w_0/2 - w_0^2/(16D)$, where $w_0 = \alpha\sqrt{2D/\mu}$, and we integrate along the interval $t \in [0, 20 \cdot 2\pi/w_0]$. We assume that the system is defined in the interval $x \in [-0.8, 4.32]$ and we split this interval in $N = 64$ parts of length $\triangle x = 0.08$. Next, we consider $c_n = \psi(x_n, t)$ where $x_n = x_0 + n\,\triangle x$, $n = 1, \ldots, N$, thus obtaining the finite dimensional linear equation

$$i\,\dot{\mathbf{c}} = \mathbf{H}\,\mathbf{c} \qquad\qquad \mathbf{c}(0) = \mathbf{c}_0, \tag{56}$$

where $\mathbf{c} = (c_1, \ldots, c_N)^T \in \mathbb{C}^N$ and $\mathbf{H} = \mathbf{T} + \mathbf{V} \in \mathbb{C}^{N\times N}$. Here $\mathbf{V}$ is a diagonal matrix associated with the potential and with diagonal values $V(x_i)$, $i = 1, \ldots, N$ and $\mathbf{T}$ is a full matrix associated with the kinetic energy. However, Fast Fourier Transforms (FFT) gives a way of evaluating $\mathbf{T}\,\mathbf{c} = \mathbf{F^{-1}D_T F}\,\mathbf{c}$ where $\mathbf{D_T}$ is diagonal and $\mathbf{Fc}$ and $\mathbf{F^{-1}c}$ in only $O(Nlog(N))$ operations. If we define the real vectors: $\mathbf{q} = \mathrm{Re}\,\mathbf{c}$ and $\mathbf{p} = \mathrm{Im}\,\mathbf{c}$ then solving (56) is equivalent to solving

$$\frac{d}{dt}\left\{\begin{array}{c}\mathbf{q}\\ \mathbf{p}\end{array}\right\} = \left(\begin{array}{cc}0 & \mathbf{H}\\ -\mathbf{H} & 0\end{array}\right)\left\{\begin{array}{c}\mathbf{q}\\ \mathbf{p}\end{array}\right\} \tag{57}$$

which can be considered as the system associated to the N-dimensional Hamiltonian $\mathcal{H} = \frac{1}{2}\mathbf{p}^T\mathbf{H}\mathbf{p} + \frac{1}{2}\mathbf{q}^T\mathbf{H}\mathbf{q}$. Evaluating the exponential of (57) is prohibitively expensive and one has to look for alternative techniques. Since in this case the Hamiltonian is separable in two solvable parts, the exponentiation can be done with RKN2 methods.

	$E_{f,FLA}$	$E_{f,RKN}$	$E_{f,RKN2}$	$10^5 \mathcal{E}_{NI}$[1]
FLA	0.623	0.618	0.573	$12.7 + 15.6\epsilon$
RKN	0.727	0.527	0.454	$1.00 + 12.2\epsilon$
RKN2	-	-	0.342	-
NI	0.812	0.799	0.799	$0.00 + 44.8\epsilon$
S^*	0.630	0.360	0.308	$0.82 + 2.22\epsilon$
Ruth-Y	1.335	1.231	1.216	$60.7 + 483.\epsilon$

Table 1: Effective error of the methods used in the numerical examples. For NI methods we use a different definition for the error: $\mathcal{E}_{NI} = |r_{5,1}| + \epsilon\sqrt{r_{5,2}^2 + r_{5,3}^2}$ ($\epsilon \approx \|B\|/\|A\|$).

In figure 2c we present the relative average error in energy versus the number of FFTs for different time-steps. The biggest time-step taken corresponds to be the stability limit of each method. Observe the advantage of S^* versus the other methods not especially designed for RKN2 problems. The good performance of the specially tailored RKN2 method can be explained from the fact that the solutions of (56) and (57) evolve through a unitary and an orthogonal transform, respectively. The splitting methods used preserve symplecticity but not orthogonality for this problem. However, this particular RKN2 method preserves uniticity to fifth order as can be seen from the the slope of its curve. This method has been used in [5], in a time-dependent problem. Finally, we have to say that the RKN2 method works this efficiently only if one uses the error in energy as a measure of accuracy. The error in position on the other hand behaves as predicted by the effective error analysis.

(d)- NI: As a Hamiltonian suitable for NI methods we will consider the one used by Hénon-Heiles,

$$H = \frac{1}{2}\left(p_x^2 + p_y^2 + x^2 + y^2\right) + \left(x^2 y - \frac{1}{3}y^3\right). \tag{58}$$

We will study the evolution near the origin with initial conditions $x = y = p_x = p_y = 1/100$, where the cubic term can be considered as a small perturbation. In figure 2d we give the average relative error in energy versus the number of evaluations. S_{NI} is the most efficient but S_{RKN} and S^* have very similar performance since in both those cases r_1 is very small.

[1] The coefficients for Yoshidas method are divided by $(5/3)^4$ since that method requires less function evaluations per step than the other methods.

In order to better compare the results obtained in the numerical examples with the results theoretically expected, we have collected the effective error of the various methods in table 1.

Before concluding this section, it is important to notice that for time-dependent Hamiltonians of the form $H = A(t) + B(t)$ the nature of the system might change as time evolves between the classes: Separable, RKN-type , RKN2-type and Near integrable. Thus the new splitting method presented seems like a very natural candidate, being nearly optimal for all these cases.

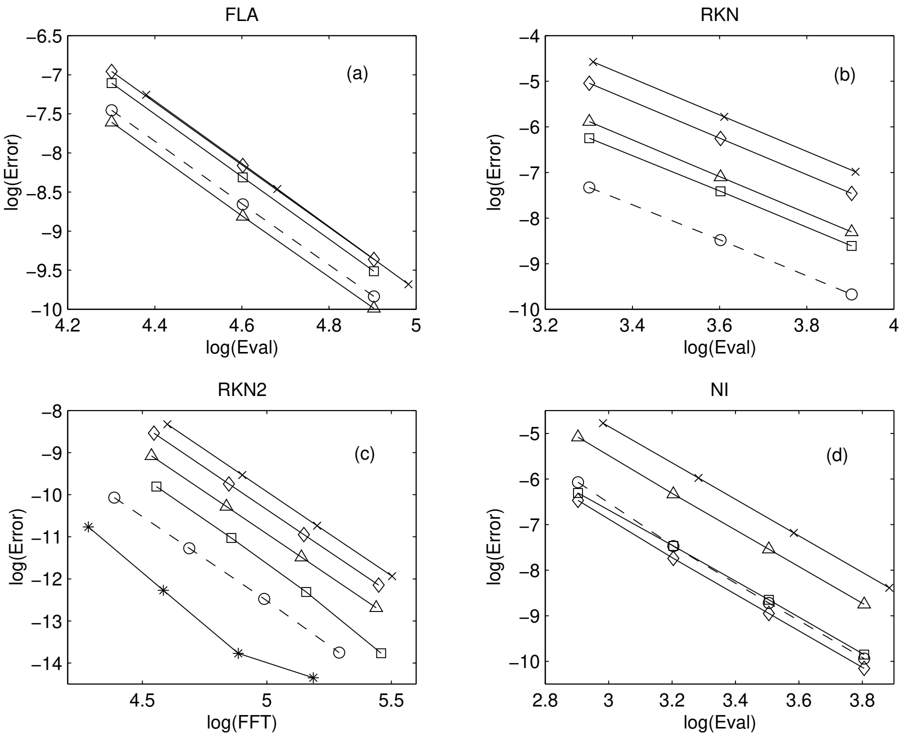

Figure 2: Average relative errors in energy vs. number of evaluations for the Hamiltonians suitable for FLA (fig. 2a), RKN (fig. 2b), RKN2 (fig. 2c) and NI (fig. 2d).

6.2 An non-autonomous example

As a simple example we choose to look at the Duffing problem with the Hamiltonian

$$H = \exp(-\epsilon\delta t)\frac{p^2}{2} + \exp(\epsilon\delta t)\left\{\frac{q^4}{4} - \frac{q^2}{2} - \epsilon\gamma\cos(\omega t)\right\}, \tag{59}$$

where the parameters are chosen as $\epsilon = 1/1000$, $\delta = 1/10$, $\gamma = 1$ and $\omega = 1/2$, while the initial values are given by $p(0) = 0.0$ and $q(0) = 1.75$. In order to apply standard splitting methods to this problem it is common practice to expand the phase-space by introducing dummy coordinates q_+, q_- to produce the autonomous Hamiltonian in the extended phase-space $(p, p_+, p_-, q, q_+, q_-)$

$$H = \left(\exp(-\epsilon\delta q_+)\frac{p^2}{2} + p_-\right) + \left(\exp(\epsilon\delta q_-)\left\{\frac{q^4}{4} - \frac{q^2}{2} - \epsilon\gamma\cos(\omega q_-)\right\} + p_+\right), \tag{60}$$

hereby retaining the separability of the Hamiltonian at the cost of altering the quadratic kinetic energy to a general non-linear form. In the experiment we will apply the optimal fourth order method, S_{FLA}, to this autonomous Hamiltonian problem, while the new optimised RKN method will be used to solve the autonomous approximate problem obtained by using the factored Magnus method 2-EX. For reference we include the errors of the classical RK method of order 4, and Yoshida/Ruths' splitting method of order 4. The plot is normalised so the computational cost in terms of execution time is the same for all schemes (on the machines we used).

Figure 3 clearly shows the advantage of handling the time dependency explicitly when solving non-autonomous problems. The computational saving in this problem comes from reducing the number of function evaluations in addition to allowing a specialised RKN method to be applied. In addition the plot show clearly that the Yoshida/Ruth method has effective error orders of magnitude larger than the most optimised methods, while S_{FLA} gives an error approximately two and a half orders of magnitude larger than the Magnus based splitting method. Also in this case the error of the RK method is larger than for the optimal symplectic method. For reference the number of time dependent function evaluations for the Magnus based method, S_{FLA}, Ruth/Yoshida and Runge–Kutta is for this example 2, 5, 3 and 2 per step.

6.3 Performance for different time scales

In this paper we have presented three new methods, (30), (31) and (46) based in Magnus series for time dependent problems. The error of these methods will come from the Magnus series truncation as well as from the particular factorisation considered, and it is ultimately dependent on the smoothness of the vectorfield $f(y, t)$. In order to have a better idea about the performance of the new methods in problems with different time scales we will consider

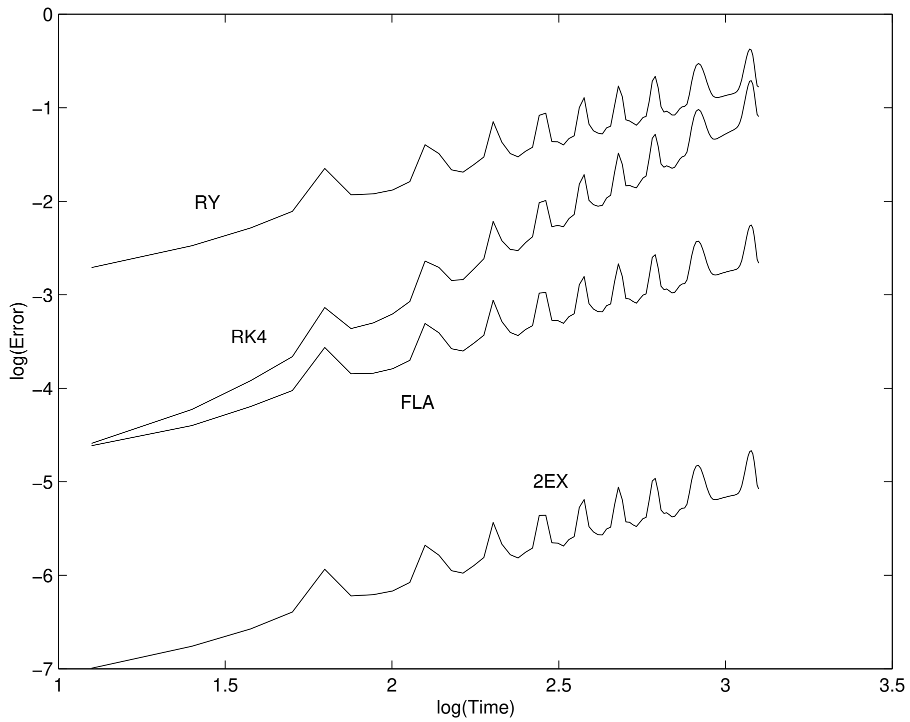

Figure 3: Relative errors in position vs. time at the same computational cost.

again the forced pendulum

$$H = \frac{1}{2}p^2 - \cos(q) - F\cos(\omega\, t)q \tag{61}$$

with $F = 1/10$, initial conditions $(q, p) = (0, 1)$ and we will study the error of the methods for $\omega \in [1/10, 100]$ and $t \in [0, 100 \cdot 2\pi]$.

Considering that all methods are of the same order and qualitatively the same error growth, we will for each value of w look for the number of evaluations required in order to reach a given accuracy. The various methods are all implemented using the new splitting method. Taking into account that (61) is of the form $H = T(p) + V(q, t)$, schemes (31) and (46) are equivalent for this problem and the qualitative results will be the same for both methods. We will also consider the symmetric RKN method considered in section 6.1.

In figure 4 we give the number of evaluations against w at fixed accuracy 10^{-8} in (q, p). Figure 4a shows the number of evaluations of the potential plus the number of time dependent functions evaluations, a number which is for this example proportional to the computational time.

In figure 4b we present the same computation but the cost is given as the number of time-dependent function evaluations, which is the case for e.g. the Duffing problem. The schemes (31) and (46) are superior only if evaluating the potential is expensive and when values of ω are around the resonance but its performance deteriorates as $\omega \to \infty$. If the time dependent part is expensive or the frequency is particularly high or low compared to the natural frequency of the autonomous systems ($F = 0$) then (30) with two exponentials is always the best scheme. In the region $\omega \in [0, 1/2]$ the Magnus approximation is very accurate (in the limit $\omega \to 0$ the system would be autonomous) and the error comes only from the splitting method used. Thus if the evaluation of the potential is cheaper than the time-dependent part it is more efficient to use high order splitting methods or to split the time step and to use the fourth order splitting method repeatedly.

Observe that according to figure 4b 2EX is approximately 7 times faster than the standard symplectic RKN in case the time dependent part is the most expensive to evaluate.

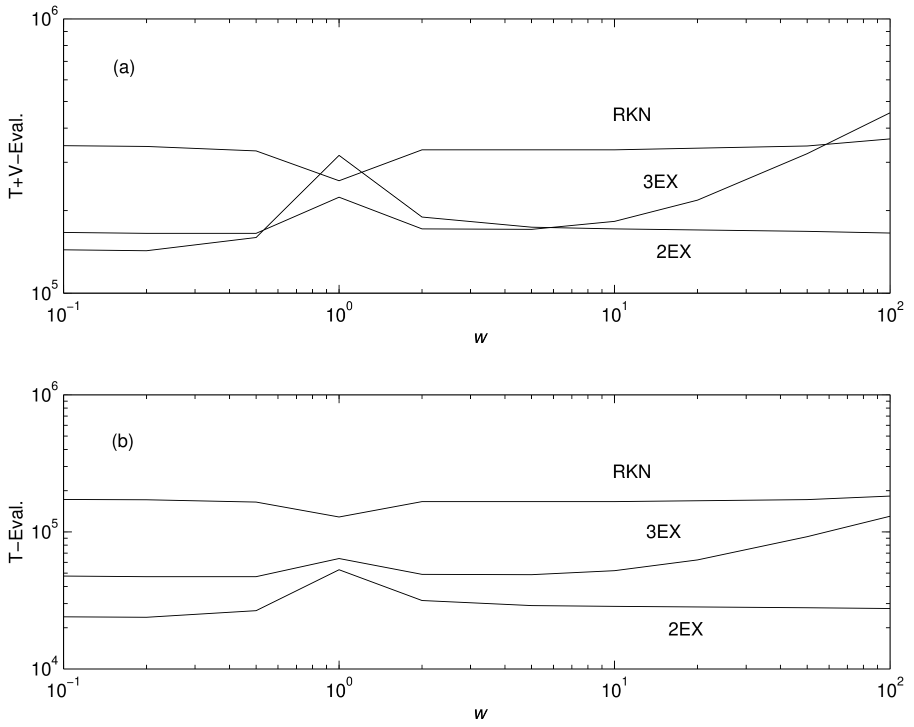

Figure 4: Number of evaluations vs. w for the forced pendulum (61) for the new methods based in Magnus and a standard symplectic integrator: (a) number of evaluations of the potential plus the time dependent evaluations (is equivalent to the CPU time); (b) number of time dependent evaluations.

7 Conclusions

We have presented new numerical integration schemes for ordinary differential equations which evolve in the same solution manifold as the exact solution. These methods are based on Magnus expansions and can be considered *Geometric Integrators*, retaining many of the qualitative properties of the exact solution. In order to avoid the presence of the troublesome commutators we split the Magnus series over a product of simple exponential factors. Such an approach seem to be attractive for e.g. separable Hamiltonian systems.

In order to implement these schemes in a optimal way we also presented a new fourth order symmetric splitting method. This method works more efficiently than other fourth order methods we found in the literature for RKN problems. At the same time it works as nearly as efficiently as the best methods specially designed for general separable problems, linear problems and near integrable problems.

The numerical experiments show the high performance of the new methods, in particular when the time-dependent part of the system is expensive to evaluate. The high accuracy obtained comes both from the efficient management of the time-dependent functions, using the averaging technique, as well as from the efficiency of the new splitting method.

The good results obtained encourage us to look for higher order methods as well as more sophisticated schemes for different types of problems. At the same time, we are interested in looking for good methods for evaluating the exponentials for the cases where the splitting methods can not be used or are expensive. This will be the subject of a future work.

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