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Practical Symplectic Partitioned Runge–Kutta and Runge–Kutta–Nyström Methods

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Abstract

We present new symmetric fourth and sixth-order symplectic Partitioned Runge–Kutta and Runge–Kutta–Nyström methods. We studied compositions using several extra stages, optimising the efficiency. An effective error, E_f, is defined and an extensive search is carried out using the extra parameters. The new methods have smaller values of E_f than other methods found in the literature. When applied to several examples they perform up to two orders of magnitude better than previously known method, which is in very good agreement with the values of E_f.

Key words: Differential equations; Geometric Integrators; Partitioned Runge–Kutta; Runge–Kutta–Nyström; Optimised efficiency
AMS classification: 34A50;34A34;65L05 ;65L06

1 Introduction

During the last few years, there has been special interest in the search of efficient methods for numerically solving ordinary differential equations, while preserving some of the qualitative properties of the exact solution [20]. For most physical problems the vector field is separable in a number of exactly solvable parts. In such cases the exact solution can be approximated by a composition of flows associated to each part of the vector field.

In this paper we will consider the particular case in which the vector field is separable in only two parts

$$\frac{dy}{dt} = f_A(y) + f_B(y), \qquad\qquad y_0 = y(0) \in \mathbb{R}^d \tag{1}$$

with $f_A,\ f_B : \mathbb{R}^d \to \mathbb{R}^d$, and where the systems

$$\frac{dy}{dt} = f_A(y), \qquad\qquad \frac{dy}{dt} = f_B(y) \tag{2}$$

can be integrated in closed form. Let us denote by e^{tA} and e^{tB} the exact flows of the systems (2). Then, for a time-step h the composition

$$\Phi_s = \prod_{i=1}^{s} e^{a_i hA}\, e^{b_i hB} = e^{h(A+B)} + O(h^{p+1}) \tag{3}$$

(with appropriate coefficients a_i, b_i) is a numerical method of order p and usually is referred as a Partitioned Runge–Kutta method (PRK). For instance, the system

$$\frac{dq}{dt} = g_1(p), \qquad\qquad \frac{dp}{dt} = g_2(q), \tag{4}$$

where $y = (q,p),\ q \in \mathbb{R}^l$ and $p \in \mathbb{R}^{d-l}$ can be separated into two solvable parts, e.g. $f_A = (g_1(p), 0)$ and $f_B = (0, g_2(q))$. Denoting by (q_n, p_n) an approximation to the exact solution $(q(nh), p(nh))$, the composition (3) is equivalent to the following algorithm for advancing (q_n, p_n) to (q_{n+1}, p_{n+1})

Observe that such an implementation requires only one l-dimensional

$P_0 = p_n \qquad Q_0 = q_n$

do i=1,s

$$Q_i = Q_{i-1} + a_i h g_1(P_{i-1})$$

$$P_i = P_{i-1} + b_i h g_2(Q_i)$$

enddo

$q_{n+1} = Q_s \quad p_{n+1} = P_s$.

and one $(d-l)$-dimensional vectors for storage. In the particular case of a Hamiltonian system with the Hamiltonian function $H(q,p) = T(p) + V(q)$ we have $d = 2l$, and $g_1(p) = \frac{\partial}{\partial p} T(p)$ and $g_2(q) = -\frac{\partial}{\partial q} V(q)$.

Taking s sufficiently large, in [21,25] they proved in a simple and elegant way that it is possible to get p as high as desired. Since then, a number of papers appeared in order to find the most efficient composition at each order [22,23,17,13,18].

A particular equation which frequently appear in many physical problems is

$$\frac{d^2x}{dt^2} = g(x), \qquad\qquad x_0 = x(0) \in \mathbb{R}^l \tag{5}$$

with $g : \mathbb{R}^l \to \mathbb{R}^l$. If we consider $y = (x, v)$ with $v = \frac{dx}{dt}$ then, eq. (5) can be written as (1) with the exactly solvable vector fields $f_A = (v, 0)$ and $f_B = (0, g(x))$. This equation appears, for example, when considering most non-relativistic Hamiltonian systems with quadratic kinetic energy. The particular structure of f_A simplifies the analysis. The number of order conditions to be satisfied by the coefficients $\{a_i, b_i\}_{i=1}^s$ is considerably reduced for $p > 4$, and more efficient methods for this particular equation can be obtained [16,4,19,17,15]. They will be referred as Runge–Kutta–Nyström (RKN) methods.

The efficiency of a method depends on its cost (usually the number of stages, s) and how large the $O(h^{p+1})$ term is. The experience shows that, in the PRK and RKN cases, compositions with the minimum number of stages (to reach a given order) usually do not give the most efficient algorithms.

Symplectic PRK and RKN methods have been successfully used for numerically solving problems in celestial mechanics [11,24,14], quantum mechanics [12], plasma physics [6], accelerator physics and optics [8], chaos [7], etc. However, in spite of its interest, we realised that the search for numerical methods was far from complete. And that there is still room for more efficient methods, in particular when the order $p \geq 4$.

In this paper we present new fourth and sixth-order symplectic PRK and RKN methods. We consider symmetric compositions using more stages that strictly necessary for solving order conditions. We define the effective error, E_f, of a method taking into account the number of stages, s, and the size of $O(h^{p+1})$. If a composition has more variables than order conditions, an infinite number of solutions will exist and we will look for solutions which minimising E_f. The number of stages is increased until E_f is not decreased by the possible solutions, or an higher order method is found. For RKN methods we have to bear in mind that f_A and f_B are qualitatively different and are not interchangeable so, all types of compositions have to be analysed. While for the more general PRK methods we make no special assumtions on f_A and f_B, making them interchangable.

This search allowed us to find new methods which, according to the effective error, should perform up half order of magnitude more efficient for the fourth-order methods and nearly two orders of magnitude for the sixth-order methods (at the same computational cost). These figures perfectly agree with the numerical results obtained for different examples and initial conditions. On the other hand, it seems clear that the processing technique can provide more efficient methods. Unfortunately, this technique cannot be used efficiently in several cases, for example, if at each step the solution is approximated using more than one exponential, as in [2,3]. Then, it is important to have composition methods without processing and very good performances.

2 Symmetric Compositions and Effective Error

It is well known that the composition of an odd order method with its adjoint is equivalent to a symmetric method of higher order, and in some cases the computational cost is reduced. For instance, if we consider one step with the first order method $\Phi_1 = e^{hA}\, e^{hB}$ and in the next step we use its adjoint $\tilde{\Phi}_1 = e^{hB}\, e^{hA}$ then it is equivalent to use the well known leap-frog or Strang symmetric second order method (for one step $2h$)

$$\Phi_2 = e^{hA}\, e^{2hB}\, e^{hA} = e^{2h(A+B)} + O(h^3). \qquad (6)$$

The method is of second order but requires only one evaluation of e^A and e^B (instead of two) per step because it is possible to concatenate terms and the *First Same As Last* (FSAL) property

.

For this reason, in this paper we will only consider symmetric compositions. In addition, the number of order conditions for high order methods is considerably reduced. This makes the numerical search of solutions for the coefficients $\{a_i, b_i\}$ much easier and faster, allowing a more careful numerical study when extra stages (or exponentials) are introduced in the composition.

The following types of symmetric compositions are considered:

- **PRK**: this is the case when f_A and f_B play the same role and are interchangeable. The family of compositions considered is

$$\mathrm{S}_s = e^{a_1 hA}\, e^{b_1 hB} \ldots e^{a_s hA}\, e^{b_s hB}\, e^{a_{s+1} hA} \tag{7}$$

  with $a_{s+2-i} = a_i$ and $b_{s+1-i} = b_i$. Because the FSAL property, this composition requires s evaluations of e^A and e^B.
- **RKN**: they are compositions to solve (5) where f_A and f_B are qualitatively different. Then, the following two compositions have to be considered:

$$\mathrm{SRKN}_s^a = e^{a_1 hA}\, e^{b_1 hB} \ldots e^{a_s hA}\, e^{b_s hB}\, e^{a_{s+1} hA} \tag{8}$$

  with $a_{s+2-i} = a_i$ and $b_{s+1-i} = b_i$, and

$$\mathrm{SRKN}_s^b = e^{b_1 hB}\, e^{a_1 hA} \ldots e^{b_s hB}\, e^{a_s hA}\, e^{b_{s+1} hB} \tag{9}$$

  with $a_{s+1-i} = a_i$ and $b_{s+2-i} = b_i$, where again both compositions require s evaluations of e^A and e^B.

Assuming that h is sufficiently small and f is sufficiently smooth, it becomes clear that the main contribution to the error in the numerical solution originates from the leading error term

$$\mathbf{E}_p = h^{p+1} \sum_{i=1}^{\#\mathfrak{L}_{p+1}} c_i \mathbf{D}_{p+1,i}(A, B), \tag{10}$$

where $\mathbf{D}_{p+1,i}$ correspond to independent elementary differentials or commutators of $f \cdot \nabla$ and $g \cdot \nabla$ (for example a basis of the subspace of order $p+1$ of the Lie algebra generated by $f \cdot \nabla$ and $g \cdot \nabla$), whose dimension we denote by $\#\mathfrak{L}_{p+1}$. The coefficients c_i only depend on the parameters $\{a_i, b_i\}$. To avoid dependence on the vector fields it has become standard practise to consider

$$\mathfrak{e}_2 = \sqrt{\sum_{i=1}^{\#\mathfrak{L}_{p+1}} c_i^2} \tag{11}$$

as a measure of the error

Finally, we define the effective error of the method as $E_f := s\mathfrak{e}_2^{1/p}$.

Observe that this definition is based on the assumption that all the elements $\mathbf{D}_{p+1,i}$ are of equal magnitude. In addition, different choices of basis give different values of E_f and the method giving the minimum value of E_f can depend on the basis chosen. We considered two: a Hall basis and the basis given in [1]. In the PRK case the differences we observed were relatively small. Surprisingly, if we interchange A and B the numerical value of E_f for $p > 4$ usually changes because the basis are not symmetric under this change, especially for the Hall basis. We found higher differences in the RKN case and $p > 4$, mainly because the smaller number of independent terms at leading order and because f_A and f_B are now qualitatively different so, a more careful search has to be carried out.

2.1 Optimisation Algorithm

Assume that we are searching for splitting pth-order methods with k parameters (k independent values of a_i, b_i) used to satisfy the $N_p := \sum_{j=1}^{\lfloor p/2 \rfloor} \#\mathfrak{L}_{2j-1}$ order conditions ($k \geq N_p$). Then, we have $r = k - N_p$ free parameters, and for each particular value of these free parameters we have a number of solutions of the order conditions to be used for minimising the value of E_f. Thus we have a constrained optimisation problem with non-linear equality constraints and objective function. The problem of finding a global minimum of E_f hence, will be quite problematic. We chose a randomised approach to search for the minima. We start by taking a random initial guess for the k variables and the Powell hybrid method (*NAG* routine C05NBF) is then evoked for solving the N_p order conditions, using N_p of the k variables. If a solution is found, we optimise (using the *NAG* routine E04JYF) along the particular solution manifold, alternating between the solving routine and the optimisation routine, and eventually finding a local minimum. After verifying that it is indeed a local minimum, a new random initial guess is generated and the process is repeated. For each type of splitting method this process was repeated with 10000 random initial values. At the end of the computations we selected those methods that had the smallest scaled leading error constants for each type of scaling function. The numerical values we show for E_f are obtained using the basis given in [1].

3 Optimised Methods

In this section we present the optimised schemes we found during our search. The coefficients of the methods are collected in Tables 1 and 2. We compare the effective error of the new optimised methods with other composition methods of the same order we found in the literature.

3.1 Partitioned Runge–Kutta methods

In this case we considered the family of symmetric compositions (7) where no structural assumptions on f_A and f_B was made.

3.1.1 Fourth order methods

For a fourth order method it is necessary to take at least $s = 3$. The well known solution for $s = 3$ was given in [10,25,21,5] but this method has a large effective error, $E_f = 1.33$. Only few attempts for optimising such methods are known to us [22,17]. The best results were presented in [17] for $s = 4$ and $s = 5$ with $E_f = 0.71$ and $E_f = 0.62$, respectively. Our search resulted in a new method with $s = 6$ and $E_f = 0.56$, whose coefficients correspond to the S_6 scheme given in Table 1. With $s = 7$ it is possible to get a sixth order method due to some very fortunate circumstances (when an special symmetric composition is considered [25]).

3.1.2 Sixth order methods

Ten order conditions have to be satisfied, and in order to have as many variables as order conditions one has to take at least $s = 9$. Although this is a rather moderate number there are 18 terms in the leading error constant. Thus it is highly possible that the error constants have a large number of local minima and carrying out an exhaustive search for methods becomes almost impossible with our approach. The only attempt we know for getting sixth-order methods using (7) and $s = 9$ was done by Forest [9] obtaining a solution with $E_f = 3.40$. On the other hand, using symmetric compositions of a symmetric second order method, Yoshida [25] found solutions with only $s = 7$. If this second order method is the leap-frog then the best one (solution A) has $E_f = 2.55$. In the same way, but using $s = 9$, McLachlan [17] found one method with $E_f = 2.13$. Because of difficulties when optimising under determined problems we were only able to carry out our search for $s \geq 9$, and we did it up to $s = 15$. The most efficient method we found has $E_f = 1.12$ and corresponds to S_{10} given in Table 1. According to the effective error this method is nearly twice as cheap or, equivalently, at the same computational cost the error is a factor $(2.13/1.12)^6 \simeq 47$ smaller when comparing with the best method known from the literature.

3.2 Runge–Kutta–Nyström methods

Now A and B are qualitatively different. For such systems one can show that $[B,[B,[B,A]]] = 0$, where $[A,B] = AB - BA$, leading to reductions in the number of order conditions and error terms. So, more efficient methods can be obtained for this family of problems. It is clear that now A and B are not interchangeable, and we have to consider the two types of symmetric splitting methods (8) and (9).

3.2.1 Fourth order RKN methods

The same number of order conditions as in the general case has to be solved for symmetric compositions. However, the number of error terms is reduced from six to four, and an optimisation taking into account only these terms has to be considered. Non-symmetric RKN methods with $s = 4$ were studied by Calvo and Sanz-Serna [4] and by Atela and McLachlan [16] giving solutions with $E_f = 0.47$ and $E_f = 0.50$, respectively. However, in the last case, if the non-symmetric method is composed with its adjoint, the effective error is reduced to $E_f = 0.44$ because the concatenation of one exponential allows to reduce the cost. SRKN_s^a methods with $s = 4$ and $s = 5$ can be found in [17] with $E_f = 0.63$ and $E_f = 0.53$, respectively (in the last case it is possible to get a method with $E_f = 0.46$. Next, RKN_s^b methods with $s = 4$ and

$s = 5$ were studied in [3] and an improved method was found for $s = 5$ with $E_f = 0.36$. So, in this work we considered methods with $s = 6$ and the best one we found corresponds to the SRKN_6^b given in Table 2, with $E_f = 0.29$. As in the general splitting case, it is possible to find sixth-order RKN methods with $s = 7$ so, we stopped here our search for fourth-order methods.

3.2.2 *Sixth order RKN methods*

For sixth-order $\mathrm{SRKN}_s^{a,b}$ methods there are eight order conditions, hence it is necessary to take $s \geq 7$. The only symplectic RKN methods we know from the literature are given in [9,19], corresponding to the $\mathrm{SRKN}_7^{a,b}$ families. Out of the sixteen solutions for the SRKN_7^a presented in [19], McLachlan [17] showed the optimal, which has $E = 1.023$. In [9] two of the $SRKN_7^a$ solutions were presented and one for SRKN_7^b, with $E_f = 1.69$. Several fifth-order non-symmetric RKN methods can be found in the literature [16,19,15]. If these schemes are composed with their adjoint new sixth-order symmetric RKN methods can be obtained. However, we find that none of these compositions improve the previous best value of E_f.

Next, we carried out a search for $\mathrm{SRKN}_s^{a,b}$ methods with $7 \leq s \leq 15$. A task which was complicated by the more unruly nature of the error coefficients compared to fourth-order methods. The best methods we found were the SRKN_{11}^b and SRKN_{14}^a given in Table 2, with $E_f = 0.78$ and $E_f = 0.63$, respectively. We present these two methods because since the performance of RKN methods for solving (5) depend highly on $g(x)$. On the other hand, although SRKN_{14}^a has better efficiency, its large number of stages can make it more unstable for big time-steps. We will test these two methods in a number of examples and different conditions,

Table 1
New PRK methods using composition (7).

Order 4; S_6, $E_f = 0.56$

$a_1 = 0.0792036964311957$	$b_1 = 0.209515106613362$
$a_2 = 0.353172906049774$	$b_2 = -0.143851773179818$
$a_3 = -0.0420650803577195$	$b_3 = 1/2 - (b_1 + b_2)$
$a_4 = 1 - 2(a_1 + a_2 + a_3)$	

Order 6; S_{10}, $E_f = 1.12$

$a_1 = 0.0502627644003922$	$b_1 = 0.148816447901042$
$a_2 = 0.413514300428344$	$b_2 = -0.132385865767784$
$a_3 = 0.0450798897943977$	$b_3 = 0.067307604692185$
$a_4 = -0.188054853819569$	$b_4 = 0.432666402578175$
$a_5 = 0.541960678450780$	$b_5 = 1/2 - (b_1 + \ldots + b_4)$
$a_6 = 1 - 2(a_1 + \ldots + a_5)$	

in order to shed light on how they perform in different situations.

Finally, for illustrating the benefits of using extra parameters in the numerical schemes, we present in Table 3 the results we obtained for all types of fourth-order methods studied. For each type of compositions and number of stages, we give the smallest value of E_f we were able to get. For $s = 7$ it is possible to get $E_f = 0$ in all cases (obtaining six-order methods) so, we stopped our search for fourth-order methods at $s = 6$. From this table it is clear the benefits obtained when considering more variables in the composition. The extra cost is compensated by the reduction in the leading error term.

Table 2
New RKN methods using compositions (8) and (9).

Order 4; SRKN_6^b, $E_f = 0.28$	
$b_1 = 0.0829844064174052$	$a_1 = 0.245298957184271$
$b_2 = 0.396309801498368$	$a_2 = 0.604872665711080$
$b_3 = -0.0390563049223486$	$a_3 = 1/2 - (a_1 + a_2)$
$b_4 = 1 - 2(b_1 + b_2 + b_3)$	

Order 6; SRKN_{11}^b, $E_f = 0.78$	
$b_1 = 0.0414649985182624$	$a_1 = 0.123229775946271$
$b_2 = 0.198128671918067$	$a_2 = 0.290553797799558$
$b_3 = -0.0400061921041533$	$a_3 = -0.127049212625417$
$b_4 = 0.0752539843015807$	$a_4 = -0.246331761062075$
$b_5 = -0.0115113874206879$	$a_5 = 0.357208872795928$
$b_6 = 1/2 - (b_1 + \ldots + b_5)$	$a_6 = 1 - 2(a_1 + \ldots + a_5)$

Order 6; SRKN_{14}^a, $E_f = 0.63$	
$a_1 = 0.0378593198406116$	$b_1 = 0.09171915262446165$
$a_2 = 0.102635633102435$	$b_2 = 0.183983170005006$
$a_3 = -0.0258678882665587$	$b_3 = -0.05653436583288827$
$a_4 = 0.314241403071447$	$b_4 = 0.004914688774712854$
$a_5 = -0.130144459517415$	$b_5 = 0.143761127168358$
$a_6 = 0.106417700369543$	$b_6 = 0.328567693746804$
$a_7 = -0.00879424312851058$	$b_7 = 1/2 - (b_1 + \ldots + b_6)$
$a_8 = 1 - 2(a_1 + \ldots + a_7)$	

s	3	4	5	6
S_s	1.33	0.71	0.62	0.56
SRKN_s^a	1.23	0.63	0.46	0.42
SRKN_s^b	1.32	0.64	0.36	0.29

Table 3
The best effective error we obtained for PRK and RKN fourth-order methods using symmetric compositions with s-stages.

4 Numerical Experiments

In the previous section, we presented a number of methods which have been obtained considering the criterion of minimising E_f. From the definition of E_f one can see that its value will depend on the basis chosen. On the other hand, the same weight has been given to all elements of the basis in the leading error term, but this is not a realistic situation for typical problems and initial conditions. Then, it is important to test the performance of the methods in different kind of equations and initial conditions. We will compare with the best splitting methods we found in the literature. These methods are denoted by:

- LF2: the leap-frog or Strang splitting method. It is used as a reference.
- M4: the fourth order (S,$m = 5$) given by McLachlan [17].
- Y4: the well known three stages fourth-order method presented in [25]. It is also used as a reference because is a very well known method.
- O4: the fourth-order method S_6 from Table 1.
- Y6: the best sixth-order method presented in [25] (solution A).
- M6: the sixth-order (SS,$m = 9$) method given in [17].
- O6: the sixth-order method S_{10} from Table 1.
- M8: the eight-order (SS,$m = 17$) method given in [17].

In addition to reference methods we will consider, for the RKN case:

- AM4: the symmetric fourth order method obtained from the non-symmetric scheme given in [16], and composed with its adjoint.
- O6-4: the fourth-order method SRKN_6^b from Table 2.
- OS6: the best sixth-order method presented in [19] (method 13).
- O11-6: the sixth-order method SRKN_{11}^b from Table 2.
- O14-6: the sixth-order method SRKN_{14}^a from Table 2.

4.1 PRK Methods

In this section we test the performance of the new optimised PRK methods O4 and O6 in several systems which are separable in exactly solvable parts.

Example 1: As a first example, let us consider the simple Volterra-Lotka problem

$$\dot{u} = u(v-2); \qquad \dot{v} = v(1-u), \tag{12}$$

which has the first integral $I(u,v) = \ln(uv^2) - (u+v)$. The vector field $f(u,v) = (u(v-2), v(1-u))$ is separable in two solvable parts, i.e. $f_A = (u(v-2), 0)$ and $f_B = (0, v(1-u))$. Then, it is possible to use the splitting methods for the general case. In the region $0 < u, v$ the system has periodic trajectories around $(u,v) = (1,2)$. In order to measure how sensible the methods are to the initial conditions we considered as initial conditions $(u_0, v_0) = (\alpha, 2\alpha)$ for $\alpha \in (0,1)$. We integrated up to $t = 100 \times 2\pi$ and measured the average error in $I(u,v)$. Figures 1(a) and 1(b)

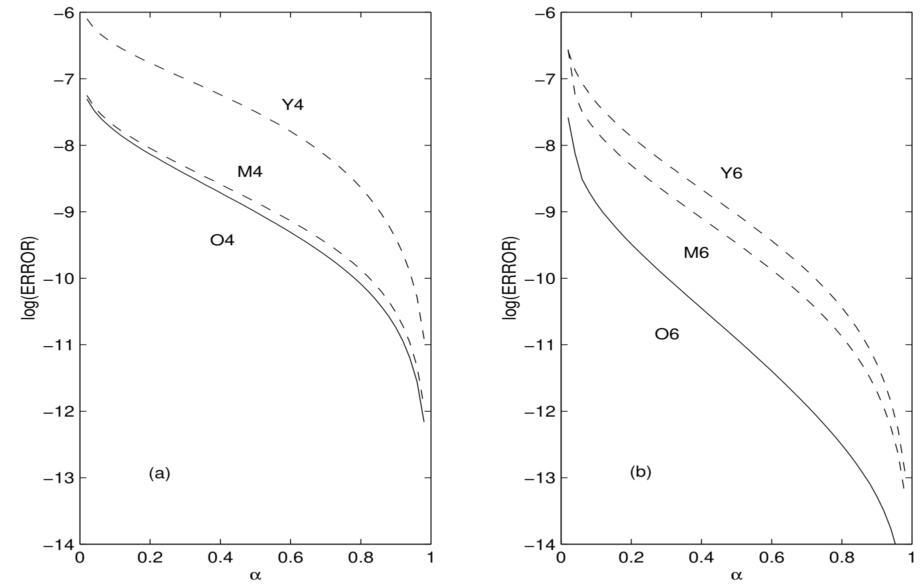

Fig. 1. Average error in $I(u, v)$ for initial conditions $(u_0, v_0) = (\alpha, 2\alpha)$.

show the result obtained for the fourth and sixth-order methods. The time-step was chosen such that all methods require the same computational cost. If we increase the number of evaluations the error decreases according to the order of each method so, the errors correspond, essentially, to the leading term.

In order to appreciate how methods of different order perform at the same computational cost, we took $(u_0, v_0) = (1, 1)$, integrated until $t = 100 \times 2\pi$ and measured the average relative error in position along $t \in [80 \times 2\pi, 100 \times 2\pi]$. Figure 2(a) shows the results obtained for different time-steps. For this problem and initial conditions, M4 and O4 perform similarly, and the new sixth-order method O6 is the best one if the desired error is between 10^{-3} and 10^{-11}. Observe that the relative performance between methods of the same order agree, approximately, according to the results theoretically predicted from the effective error.

Example 2: Next, we consider the Lorenz system. The equations

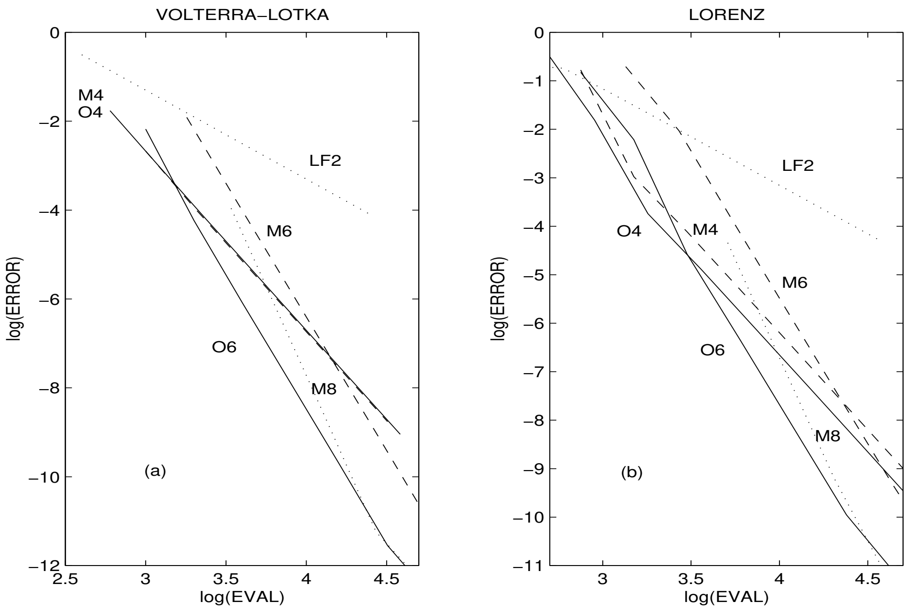

Fig. 2. Average error in position vs. number of evaluations.

can be written as follows:

$$\frac{d}{dt}\begin{bmatrix} x \\ y \\ z \end{bmatrix} = \begin{bmatrix} -\sigma & \sigma & 0 \\ r & -1 & 0 \\ 0 & 0 & b \end{bmatrix}\begin{bmatrix} x \\ y \\ z \end{bmatrix} + \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & -x \\ 0 & x & 0 \end{bmatrix}\begin{bmatrix} x \\ y \\ z \end{bmatrix}, \tag{13}$$

and it is a clear example in which the system is separable in the linear and non-linear part, both being exactly solvable. We will consider $\sigma = 10$, $b = 8/3$ and $r = 28$, and initial conditions $(x_0, y_0, z_0) = (0, 1, 0)$. We integrated the system until $t = 15 \times 2\pi$ and measured (in $t \in [5 \times 2\pi, 15 \times 2\pi]$) the average relative error for different time-steps. We choose as the exact solution the numerical result obtained with different methods and sufficiently small time-steps. Figure 2(b) shows the results obtained. Now, O4 works slightly better than M4 and O6 performs similarly to the previous example.

Example 3: Let us now consider the ABC-flow, whose equations are given by

$$\begin{aligned} x' &= \mathfrak{B}\cos y + \mathfrak{C}\sin z \\ y' &= \mathfrak{C}\cos z + \mathfrak{A}\sin x \\ z' &= \mathfrak{A}\cos x + \mathfrak{B}\sin y. \end{aligned} \tag{14}$$

where the vector field is separable in three solvable parts, i.e.

$$\begin{aligned} f &= f_A + f_B + f_C \\ &= \mathfrak{A}(0, \sin x, \cos x) + \mathfrak{B}(\cos y, 0, \sin y) + \mathfrak{C}(\sin z, \cos z, 0). \end{aligned}$$

Let us consider a first order method, i.e. $\Phi(h) = e^{hA}\ e^{hB}\ e^{hC}$ and its adjoint $\tilde{\Phi}(h) = e^{hC}\ e^{hB}\ e^{hA}$. Then it is known that with the coefficients of a method for a system separable in two parts ($\{a_i, b_i\}_{i=1}^s$ from (3)) it is possible to build a method of the same order using the following composition of Φ and $\tilde{\Phi}$ [17]:

$$\Psi(h) = \prod_{i=1}^{s} \Phi(c_i h)\tilde{\Phi}(d_i h), \qquad c_i = a_i - d_{i-1}, \quad d_i = b_i - c_i$$

for $i = 1, \ldots, s$ with $d_0 = 0$. The methods we presented in this paper are not optimised for this particular problem. However, we expect they will give very efficient results. We compare our new sixth-order method with Y6 and M6, which correspond to symmetric compositions of 7 and 9 symmetric second-order methods, respectively. As the basic second-order method for Y6 and M6 we take $S_2(h) = \Phi(h/2)\tilde{\Phi}(h/2)$.

We consider as initial conditions $(x_0, y_0, z_0) = (3.14, 2.77, 0)$ and integrated the system until $t = 20 \times 2\pi$. In order to appreciate the efficiency in different regimes we considered $B = C = 1$ and $A = \alpha$ with $\alpha \in [0, 1]$. In the limit $\alpha \to 0$ the system can be considered as separable in only two parts, and in the limit $\alpha \to 1$ we have a general case. The time-step used for each method is such that all

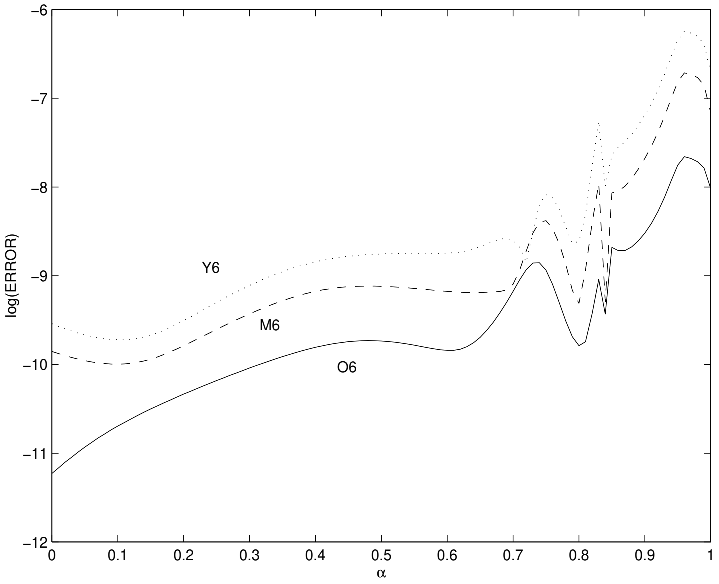

Fig. 3. Error for different values of the parameter A.

methods require the same number of evaluations. Figure 3 shows the results obtained. The new method clearly performs better although, as expected, its best performance happens when the system is separable in only two parts ($\alpha = 0$). The behaviour of the numerical errors around $\alpha \approx 0.8$ indicate less regular motion for this value of the parameter.

4.2 RKN Methods

In the RKN case, the system is separable in two parts which are qualitatively different. For this reason, the performance of the methods can be highly dependent on the problem and initial conditions. Then, in this section we will make several tests in order to see if, in average, the performance of the methods agree with the theoretically predicted from the effective error. The following Hamiltonian systems with quadratic energy are studied:

Example 4. Let us consider the well known Hénon-Heiles Hamiltonian

$$H(\mathbf{q},\mathbf{p}) = \frac{1}{2}(p_x^2 + p_y^2) + \frac{1}{2}(x^2 + y^2) + x^2 y - \frac{1}{3}y^3. \qquad (15)$$

We considered the set of initial conditions $(x_0, y_0, p_{x0}, p_{y0}) = (\alpha, 0, 0, \alpha/2)$, with $\alpha \in [0, 1/2]$ and we integrated the system until $t = 100 \times 2\pi$. The time-step is such that all methods require 20000 evaluations of the potential. Figures 4(a) and 4(c) show the average error in energy for fourth and sixth-order methods, respectively.

Example 5: Next we consider the simple Hamiltonian associated to the pendulum

$$H = \frac{1}{2}p^2 - cos(q). \qquad (16)$$

We choose the set of initial conditions $(q, p) = (0, \alpha)$ with $\alpha \in [0, 3.5]$, and integrated the system until $t = 100 \times 2\pi$. The time-step is such that all methods require 40000 evaluations of the potential. Figures 4(b) and 4(d) show the average error in energy.

From these two examples it seems clear that the relative performance of the methods depend on the initial conditions. Among the fourth-order methods O6-4 is the best and at order six it is not so clear, but it seems that O14-6 gives the best results.

Example 6: As an example of a Hamiltonian where the potential has a singularity we choose the Kepler problem. Its Hamiltonian is given by

$$H(\mathbf{q},\mathbf{p}) = \frac{1}{2}\left(p_x^2 + p_y^2\right) - \frac{1}{\sqrt{q_x^2 + q_y^2}}, \qquad (17)$$

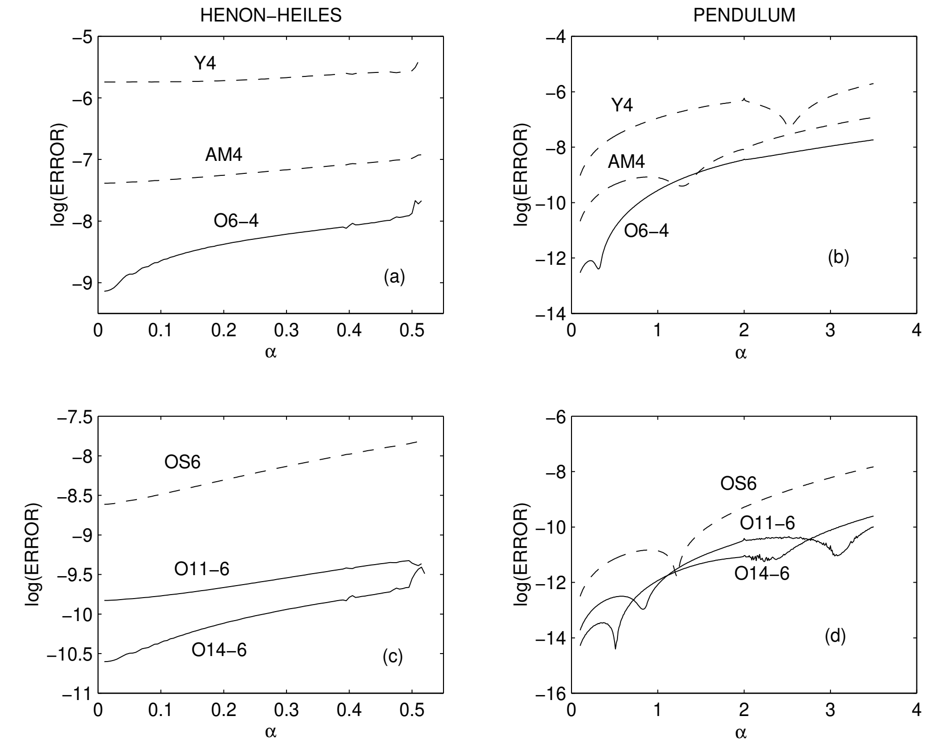

Fig. 4. Average error in energy for the initial conditions: $(q_0, p_0) = (0, \alpha)$ (pendulum) and $(x_0, y_0, p_{x0}, p_{y0}) = (\alpha/2, 0, 0, \alpha/4)$.

and we take as initial conditions $p_x = 0,\ p_y = \sqrt{\frac{1+e}{1-e}},\ q_x = 1 - e,\ q_y = 0$, where e is the eccentricity. These correspond to an orbit of period 2π and energy $-1/2$. We integrated the system for 10 periods and measured the average error in position (along the last 2 periods) for different values of the eccentricity. Figures 5(a) and 5(b) show the results obtained for fourth and sixth-order methods. The time-step is such that all methods require the same number of evaluations of the potential. Very similar results are obtained when measuring the average error in energy, and the same comments as in the previous examples are still valid.

Example 7: Next, we consider the Toda-lattice Hamiltonian

$$H = \frac{1}{2}\sum_{i=1}^{N} p_i^2 + \sum_{i=1}^{N-1}\left(e^{q_i - q_{i+1}} - 1\right) + \left(e^{q_N - q_1} - 1\right). \qquad (18)$$

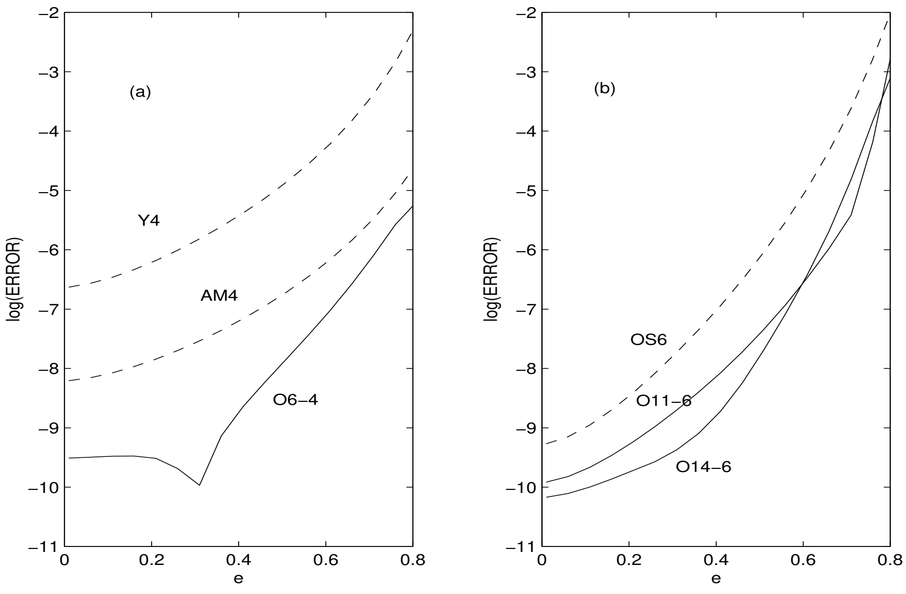

Fig. 5. Average error for different values of the eccentricity.

This system has several conserved quantities. One of them, $I = \sum_{i=1}^{N} p_i$, is exactly preserved by the splitting methods. We will take $N = 10$, initial conditions $q_0 = 0$, $p_0 = -1$, $q_i = 0$, $p_i = 1/9, \quad i = 2, \ldots, 10$, and integrated until $t = 100 \times 2\pi$. The average error in energy is measured for different time-steps. Figure 6(a) shows the results obtained. The scheme O11-6 works slightly worse than O14-6, and does not appear in the figure for clarity.

Example 8: Finally, we measure the performance of the new RKN methods in the one-dimensional non-linear Schrödinger equation

$$\begin{aligned} i\frac{\partial}{\partial t}\Psi(x,t) &= -\frac{1}{2}\frac{\partial^2}{\partial x^2}\Psi(x,t) - \alpha|\Psi(x,t)|^2\Psi(x,t) \\ &= (\mathfrak{T} + \mathfrak{V})\Psi. \end{aligned} \tag{19}$$

This system is separable in two exactly solvable parts. We will solve the system for $\mathfrak{V}\Psi = -|\Psi|^2\Psi$ in the coordinate space and $\mathfrak{T}\Psi = -\frac{1}{2}\partial_x^2\Psi$ in the momentum space. Periodic boundary conditions are assumed for Ψ, and Fast Fourier Transformations, FFT, are used to carry out the coordinate transforms. Observe that $\{\mathfrak{V}, \{\mathfrak{V}, \{\mathfrak{V}, \mathfrak{T}\}\}\} = 0$, where $\{\Psi^*(x,t), \Psi(y,t)\} = i\delta(x-y)$ and Ψ^* is the complex conjugate of Ψ so, it is possible to use RKN methods.

As initial conditions we take $\Psi(x,0) = 2\sin(x)$ and we split the interval $x \in [0, 2\pi]$ in $N = 128$ parts, where periodic boundary conditions are assumed. We integrated the system until $t = 5 \times 2\pi$ for different time-steps. The system has many preserved quantities (norm, energy, momentum, etc.). The splitting methods preserve the norm and momentum of the wave function up to round off, so we measured the average error in energy

$$E = \frac{1}{2} \int \left(\left| \frac{\partial \Psi}{\partial x} \right|^2 - |\Psi|^4 \right) dx. \tag{20}$$

as an indication of the computational error. Figure 6(b) shows the results obtained. Observe that the same algorithm can be used for a more general potential $\mathfrak{V}(|\Psi(x,t)|, x, t)$, which includes the linear Schrödinger equation.

We observe from the figures that the value of E_f do not explain exactly the relative performance between methods of same order, for each particular problem studied. However, if we estimate an average for different problems and initial conditions, we see that E_f is a good indicator of the performance of a method. On the other hand, if a method has too many stages per step it is possible that the method suffers from stability problems, and this is not reflected in the value of E_f, being this an interesting open problem.

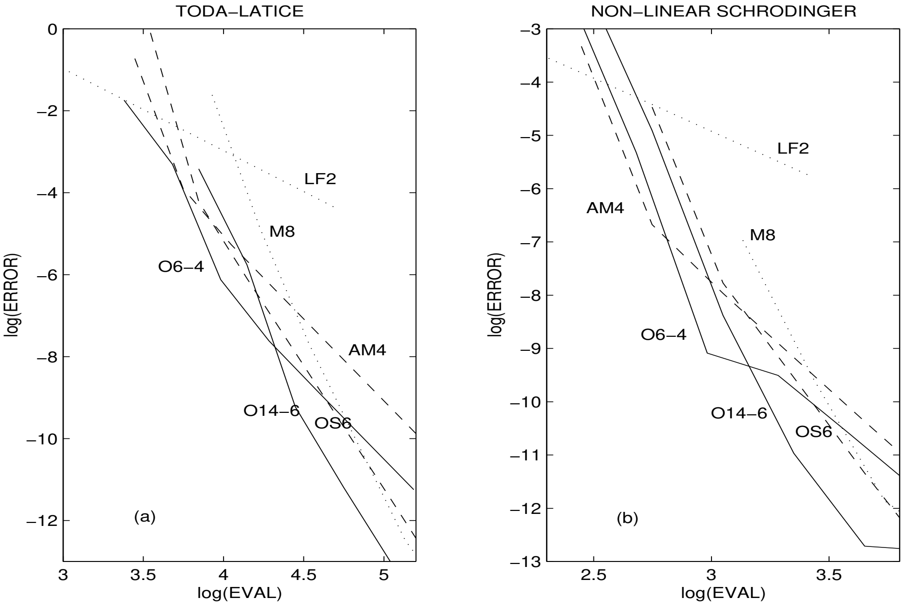

Fig. 6. Average error in energy vs. number of evaluations.

5 Conclusions

In this paper we presented new symmetric fourth and sixth-order PRK and RKN methods. The methods are specially designed for the case in which the vector field is separable in two parts $f = f_A + f_B$, but still can be applied efficiently if it is separable in more than two parts. If the flows associated to f_A and f_B retain some of the properties of the flow associated to f (i.e. same Lie group) then, the new methods will preserve several qualitative properties: in a classical Hamiltonian problem the symplecticity is preserved, in quantum mechanics the unitarity is preserved, etc. So, the methods are *Geometric Integrators*.

We have studied symmetric composition methods considering up to 15 stages both for the PRK and RKN cases. Given a composition, if we have more variables than order conditions (for obtaining a given order p) but still not enough for having one of order $p+1$, then we look for pth-order methods where the extra parameters are used for minimising the effective error. This search allowed to find new methods with smaller effective error than previous methods.

A number of examples using different initial conditions have been studied. We observed that, for most of the problems, the new methods clearly perform more efficiently (than other methods found in the literature) and in accordance with the effective error. Then, it seems clear the benefits in using extra parameters when building a numerical method.

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