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High order numerical integrators for differential equations using composition and processing of low order methods

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Abstract

In this paper we build high order integrators for solving ordinary differential equations by composition of low order methods and using the processing technique. From a basic pth-order method, Ψ_p, one can obtain high order integrators in the processed form $\overline{\Psi}_n = \mathcal{P}\mathcal{K}\mathcal{P}^{-1}$ ($n > p$) being both the processor, $\mathcal{P}$, and the kernel, $\mathcal{K}$, compositions of the basic method. The number of conditions for the kernel is drastically reduced if we compare with a standard composition. The particular case in which Ψ_p is a symmetric scheme of order 2 and 4, respectively, is analyzed, and new optimized 4th-, 6th- and 8th-order integrators are built. © 2001 IMACS. Published by Elsevier Science B.V. All rights reserved.

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1. Introduction

One of the most useful techniques for analytically solving the equation

$$\frac{\mathrm{d}\boldsymbol{y}}{\mathrm{d}t} = \boldsymbol{f}(\boldsymbol{y}), \qquad \boldsymbol{y}(0) = \boldsymbol{y}_0 \in \mathbb{R}^m, \tag{1}$$

is to look for an invertible transformation $\boldsymbol{z} = \mathcal{P}(\boldsymbol{y})$ such that the corresponding equation for $\boldsymbol{z}$,

$$\frac{\mathrm{d}\boldsymbol{z}}{\mathrm{d}t} = \boldsymbol{g}(\boldsymbol{z}), \qquad \boldsymbol{z}(0) = \mathcal{P}(\boldsymbol{y}_0) \in \mathbb{R}^m, \tag{2}$$

is exactly solvable or it is easy to obtain analytical approximations. We will refer to this transformation as the processing technique.

For instance, in classical mechanics, the evolution of an autonomous dynamical system is given by the Hamiltonian equations

$$\dot{\boldsymbol{q}} = \frac{\partial H(\boldsymbol{q},\boldsymbol{p})}{\partial \boldsymbol{p}}, \qquad \dot{\boldsymbol{p}} = -\frac{\partial H(\boldsymbol{q},\boldsymbol{p})}{\partial \boldsymbol{q}}, \tag{3}$$

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where the dot indicates derivative respect to t and $\boldsymbol{q}$, $\boldsymbol{p} \in \mathbb{R}^D$ are the canonical coordinates and associated momenta. The scalar function $H : \mathbb{R}^D \times \mathbb{R}^D \to \mathbb{R}$ is the Hamiltonian of the system. A standard technique for exactly solving (3) or to obtain analytical approximations is to look for a canonical transformation [1, 11]

$$\left.\begin{aligned} \boldsymbol{Q} &= \boldsymbol{Q}(\boldsymbol{q}, \boldsymbol{p}) \\ \boldsymbol{P} &= \boldsymbol{P}(\boldsymbol{q}, \boldsymbol{p}) \end{aligned}\right\} \quad \text{or} \quad (\boldsymbol{Q}, \boldsymbol{P}) = \mathcal{P}(\boldsymbol{q}, \boldsymbol{p}), \tag{4}$$

such that $\boldsymbol{Q}, \boldsymbol{P}$ can be considered as the coordinates and momenta of another Hamiltonian $K(\boldsymbol{Q}, \boldsymbol{P})$ which is exactly solvable (for example, if we have $K(\boldsymbol{Q})$ or $K(\boldsymbol{P})$), or it can be approximately solved (for example, if we have $K(\boldsymbol{Q}, \boldsymbol{P}) = K_1(\boldsymbol{P}) + \varepsilon K_2(\boldsymbol{Q}, \boldsymbol{P}) + \mathrm{O}(\varepsilon^2)$ and $0 < \varepsilon \ll 1$). For instance, the Hamilton–Jacobi method and the perturbative canonical theory are based in this procedure. However, this useful technique for obtaining analytical results is not an standard procedure for building numerical integrators.

Let us consider $\Psi_{t,\boldsymbol{f}}$ the exact flow of (1) and $\mathcal{K}_{t,\boldsymbol{g}}$ the corresponding flow for (2). Then, if the processing technique is used we have

$$\Psi_{t,\boldsymbol{f}} = \mathcal{P}\mathcal{K}_{t,\boldsymbol{g}}\mathcal{P}^{-1}. \tag{5}$$

In this paper we will present new one-step numerical integrators $\widehat{\Psi}_h$ for the problem (1) in the form

$$\widehat{\Psi}_h = \widehat{\mathcal{P}}_h \widehat{\mathcal{K}}_h \widehat{\mathcal{P}}_h^{-1}, \tag{6}$$

where h is the time-step and $\widehat{\mathcal{K}}_h$, $\widehat{\mathcal{P}}_h$ can be considered as numerical methods approximating $\mathcal{K}_{h,\boldsymbol{g}}$ and $\mathcal{P}$. We will refer to $\widehat{\mathcal{K}}_h$ and $\widehat{\mathcal{P}}_h$ as the kernel and processor of the method, respectively. Then, N steps can be written in the form

$$\left(\widehat{\Psi}_{h,\boldsymbol{f}}\right)^N = \widehat{\mathcal{P}}_h \left(\widehat{\mathcal{K}}_h\right)^N \widehat{\mathcal{P}}_h^{-1}. \tag{7}$$

Observe that $\widehat{\mathcal{P}}_h$ has to be evaluated only once at the beginning and $\widehat{\mathcal{P}}_h^{-1}$ only when the output is desired then, essentially, one can consider the cost of the method as the cost of $\widehat{\mathcal{K}}_h$.

The composition (6) was originally considered by Butcher [7] (see also [12, Chapter II.12]) using Runge–Kutta (RK) methods for $\widehat{\mathcal{P}}_h$ and $\widehat{\mathcal{K}}_h$. A general analysis in this line is presented in [8] but not practical methods are obtained. However, this technique has shown to be very efficient in the context of symplectic integrators for some particular cases: near-integrable systems [4,18,28], Runge–Kutta–Nyström (RKN) methods [5,16,22] and when the system is separable in two exactly solvable parts in general [2]. All these papers present methods for the case in which the vector field is separable in exactly solvable parts, but this is not strictly necessary. If one has a low order method for a given problem, in this paper we will show how to obtain high order processed methods by composition of this low order method.

The use of *Geometric Integrators* (GI) have proved very useful for solving (1) when the system has some qualitative properties which are important to retain [23]. For example, the preservation of these properties makes that, in most of the cases, the approximate solutions have smaller error growth than standard integrators. Then, it will be very important that $\widehat{\mathcal{K}}_h$ retains these properties and it will be less essential, but still interesting, for $\widehat{\mathcal{P}}_h$ to preserve them.

Let us consider now an integrator $S_p(h)$ of order p. It is well known that with a composition of this basic method it is possible to obtain high order methods in the form

$$\overline{S}_n(\boldsymbol{a}) = S_p(a_1 h) \ldots S_p(a_k h), \tag{8}$$

where $\overline{S}_n$ is a new integrator of order $n > p$. The vector $\boldsymbol{a} = (a_1, \ldots, a_k)$ characterizes the method and the a_i have to solve a number of order conditions; for instance, $\sum_{i=1}^{k} a_i = 1$ for consistency. Observe that if $S_p(h)$ is a GI then the composition will be a GI. In addition, if $S_p(h)$ is a symmetric method with p an even number, and the composition (8) is symmetric ($a_{k+1-i} = a_i,\ i = 1, 2, \ldots$) then $\overline{S}_n$ will be a symmetric integrator with n an even number. Compositions like (8) have been widely used in the literature for building high order integrators [9,13–15,17,19,20,24–27,29].

In this paper we will show that it is possible and very efficient to follow a similar strategy but using the processing technique. That means to consider

$$\widehat{\mathcal{K}}_h(\boldsymbol{b}) = S_p(b_1 h) \ldots S_p(b_r h), \tag{9}$$

$$\widehat{\mathcal{P}}_h(\boldsymbol{c}) = S_p(c_1 h) \ldots S_p(c_s h) \tag{10}$$

in such a way that $\widehat{\Psi}_h$ has effective order n. We will see that the coefficients b_i in (9) have to solve a considerably smaller number of order conditions than the coefficients a_i in (8) because some of these conditions can be solved by the c_i in (10).

An alternative technique for increasing the order of a method is to use extrapolation. The qualitative properties of the basic method are lost because the linear combinations destroy the group properties but, that happens at higher orders than the order of the final method [3,10]. This technique shows to be very efficient for increasing the order of GI when the basic method is of order four or higher. In this paper we will consider, as basic, low order methods and, for simplicity, we will take symmetric integrators, but the same idea and technique can be used for non-symmetric basic methods and different orders.

The plan of the paper is as follows. Section 2 introduces some basic concepts on Lie algebras. In Section 3 we consider symmetric basic methods and present the kernel conditions when the kernel is itself a symmetric composition. Explicit expressions for the kernel and processor are presented for moderate orders. In Section 4 we show how to obtain the kernel and processor by composition in such a way that the previous conditions are satisfied. In particular, we present new optimal processed 4th-, 6th- and 8th-order methods using S_2 and S_4. Finally, in Section 5 we present some numerical examples and we will observe that the results completely agree with the theoretically predicted.

2. Lie algebraic tools

Let us write Eq. (1) in the linear form

$$\frac{\mathrm{d}\boldsymbol{y}}{\mathrm{d}t} = F\,\boldsymbol{y}, \tag{11}$$

where $F = \boldsymbol{f} \cdot \nabla_{\boldsymbol{y}} = \sum_{i=1}^{m} f_i(\partial/\partial y_i)$ is the Lie operator associated to $\boldsymbol{f} = (f_1, \ldots, f_m)$. Then, the solution of (11) takes the formal expression [1]

$$\boldsymbol{y}(t) = \mathrm{e}^{tF}\,\boldsymbol{y}(0), \tag{12}$$

where e^{tF} is the Lie transformation associated to $\boldsymbol{f}$. In general, a numerical one-step integrator, $\widehat{\Psi}_h$, can be considered as the exact solution of a perturbed differential equation (usually divergent)

$$\frac{\mathrm{d}\widehat{\boldsymbol{y}}}{\mathrm{d}t} = \boldsymbol{f}(\widehat{\boldsymbol{y}}) + h\,\boldsymbol{f}_2(\widehat{\boldsymbol{y}}) + h^2\,\boldsymbol{f}_3(\widehat{\boldsymbol{y}}) + \cdots$$

and formally we can write

$$\widehat{\Psi}_h = \mathrm{e}^{h\widetilde{F}}, \tag{13}$$

where $\widetilde{F} = F_1 + hF_2 + h^2F_3 + \cdots$, and $F_i = \boldsymbol{f}_i \cdot \nabla_{\boldsymbol{y}}$. For consistency $F_1 = F$.

The operator F can be considered as an element of a Lie algebra $\mathfrak{g}$ and then e^{tF} is an element of the Lie group, $\mathfrak{G}$ associated to $\mathfrak{g}$. If the numerical integrator which exactly solves the perturbed equation is built such that $F_i \in \mathfrak{g},\ i = 2, 3, \ldots$, then $\mathrm{e}^{h\widetilde{F}}$ will stay in the same Lie group as the exact solution. In this case, many important qualitative properties of the exact solution are preserved by the numerical integrator [23]. This will be the case if in (8)–(10) the elementary flows belong to the same Lie group as the exact solution, being the methods referred as *Geometric Integrators*. For a method of order p, the functions $\boldsymbol{f}_2, \ldots, \boldsymbol{f}_p$ vanish identically, so $F_2, \ldots, F_p = 0$, and if it is symmetric then $F_{2i} = 0,\ i \geqslant 1$. For standard methods as RK, multistep, etc. we will find, in general, that $F_i \notin \mathfrak{g}$. However, in some cases [3,10] we can have a method of order p with $F_{p+i} \in \mathfrak{g}$ for $i = 1, \ldots, q$, but $F_{p+i} \notin \mathfrak{g}$ for $i > q$ being the method referred as pseudogeometric.

2.1. Composition of symmetric methods

Let us consider as the basic method a second-order symmetric integrator $S_2(h)$. Then, it is possible to write it as [29]

$$S_2(h) = \mathrm{e}^{h\widetilde{F}} = \exp\bigl(hF_1 + h^3F_3 + h^5F_5 + \cdots\bigr), \tag{14}$$

with $F_1 = F$. At this point the F_i can be considered as the elements of a graded Lie algebra with grade i. Then compositions (8)–(10) can be formally written, making use of the Baker–Campbell–Hausdorff (BCH) formula, in only one exponential e^C with

$$C = \sum_{i=1}^{\infty} h^i \sum_{j=1}^{\nu_i} d_{i,j} E_{i,j}, \tag{15}$$

where $d_{i,j}$ are scalar functions depending on the parameters of the method. The $E_{i,j}$ are the elements of a basis of the Lie algebra generated by $\{F_1, F_3, F_5, \ldots\}$. In particular, each $E_{i,j}$ will correspond to F_i or to a nested commutator of different F_j of grade i, i.e., $E_{i,j} = [F_k, [\ldots, [F_l, F_m]\ldots]],\ k + \cdots + l + m = i$, being ν_i the dimension of the subspace of the Lie algebra of degree i, and $[F_i, F_j]$ is the Lie bracket for vector fields. In Table 1 we present a basis up to order 9, where the notation $[i \ldots jk] \equiv [F_i, [\ldots, [F_j, F_k]\ldots]]$ has been used.

If we consider a 4th-order symmetric integrator S_4 as the basic method, then

$$S_4(h) = \mathrm{e}^{h\widetilde{F}} = \exp\bigl(hF_1 + h^5F_5 + h^7F_7 + \cdots\bigr), \tag{16}$$

and we have to consider the Lie algebra generated by $\{F_1, F_5, F_7, \ldots\}$. It corresponds to the previous algebra taking $F_3 = 0$ so, a considerably simplification happens, allowing us to analyze easily high order methods. A basis up to order 11 is given in Table 2.

In general, the most efficient methods are obtained when some information from the vector field is considered (e.g., it is separable or for the RKN case) or by composition of low order methods. However, it is very difficult to obtain efficient high order methods because the large number of order conditions makes

Table 1
Basis of the Lie algebra generated by $\{F_1, F_3, F_5, F_7, F_9\}$ up to order 9

n	ν_n	S_2			
1	1	$E_{1,1} = F_1$;			
3	1	$E_{3,1} = F_3$;			
4	1	$E_{4,1} = [13]$;			
5	2	$E_{5,1} = F_5$;	$E_{5,2} = [113]$;		
6	2	$E_{6,1} = [15]$;	$E_{6,2} = [1113]$;		
7	4	$E_{7,1} = F_7$;	$E_{7,2} = [115]$;	$E_{7,3} = [11113]$;	$E_{7,4} = [313]$;
		$E_{8,1} = [17]$;	$E_{8,2} = [1115]$;	$E_{8,3} = [111113]$;	
8	5	$E_{8,4} = [1313]$;	$E_{8,5} = [35]$;		
		$E_{9,1} = F_9$;	$E_{9,2} = [117]$;	$E_{9,3} = [11115]$;	$E_{9,4} = [1111113]$;
9	8	$E_{9,5} = [11313]$;	$E_{9,6} = [31113]$;	$E_{9,7} = [135]$;	$E_{9,8} = [315]$;

Table 2
Basis of the Lie algebra generated by $\{F_1, F_5, F_7, F_9, F_{11}\}$ up to order 11

n	ν_n	S_4		
1	1	$E_{1,1} = F_1$;		
5	1	$E_{5,1} = F_5$;		
6	1	$E_{6,1} = [15]$;		
7	2	$E_{7,1} = F_7$;	$E_{7,2} = [115]$;	
8	2	$E_{8,1} = [17]$;	$E_{8,2} = [1115]$;	
9	3	$E_{9,1} = F_9$;	$E_{9,2} = [117]$;	$E_{9,3} = [1115]$;
10	3	$E_{10,1} = [19]$;	$E_{10,2} = [1117]$;	$E_{10,3} = [11115]$;
		$E_{11,1} = F_{11}$;	$E_{11,2} = [119]$;	$E_{11,3} = [11117]$;
11	5	$E_{11,4} = [1111115]$;	$E_{11,5} = [515]$;	

the numerical search extremely difficult. On the other hand, compositions using S_4 as basic integrator can be useful for obtaining high order methods mainly for two reasons:

(i) The reduced number of equations allows a deep analysis of the numerical solutions.
(ii) It is possible to use a large quantity of different methods S_4 specially tailored for particular problems, i.e., RKN methods.

3. Kernel and processor conditions

In the same way as in [2], and for simplicity, it is possible to consider for $\widehat{\mathcal{K}}_h$ a symmetric composition, so

$$\widehat{\mathcal{K}}_h^{-1} = \widehat{\mathcal{K}}_{-h} \tag{17}$$

and for the processor we can take a scheme with only even powers of h

$$\widehat{\mathcal{P}}_{-h} = \widehat{\mathcal{P}}_h. \tag{18}$$

From (14) and (16) we see that $S_i(-h) = S_i^{-1}(h),\ i = 2, 4$, so, the composition (10) cannot satisfy condition (18) exactly. However, it is possible to preserve this condition up to h^k with k as high as desired.

Formally, we can write

$$\widehat{\mathcal{K}}_h = \exp\left(\sum_{i=1}^{\infty} h^{2i-1} \sum_{j=1}^{\nu_{2i-1}} k_{2i-1,j} E_{2i-1,j}\right) \equiv \mathrm{e}^{hK}, \tag{19}$$

$$\widehat{\mathcal{P}}_h = \exp\left(\sum_{i=1}^{\infty} h^{2i} \sum_{j=1}^{\nu_{2i}} p_{2i,j} E_{2i,j}\right) \equiv \mathrm{e}^{P}, \tag{20}$$

and using the BCH formula

$$\widehat{\Psi}_h = \widehat{\mathcal{P}}_h \widehat{\mathcal{K}}_h \widehat{\mathcal{P}}_h^{-1} = \mathrm{e}^{P} \mathrm{e}^{hK} \mathrm{e}^{-P} = \mathrm{e}^{h\widehat{F}} \tag{21}$$

with

$$\begin{aligned} h\widehat{F} &= \mathrm{e}^{P} hK \mathrm{e}^{-P} = \mathrm{e}^{[ad_P,\cdot]} hK = hK + [P, hK] + \frac{1}{2}\big[P, [P, hK]\big] + \cdots \\ &= \sum_{i=1}^{\infty} h^{2i-1} \sum_{j=1}^{\nu_{2i-1}} f_{2i-1,j} E_{2i-1,j}, \end{aligned} \tag{22}$$

where the $f_{i,j}$ are polynomial functions of $k_{r,s},\ r \leqslant i$, and $p_{r,s},\ r \leqslant i-1$. Observe that $h\widehat{F}$ does not contain even powers of h. The integrator $\widehat{\Psi}_h$ will be of order n if $\widehat{F} = F + \mathrm{O}(h^n)$ or, equivalently, if

$$\begin{aligned} &f_{1,1} = k_{1,1} = 1, \\ &f_{2i-1,j}(\boldsymbol{k}, \boldsymbol{p}) = 0, \quad i = 2, \ldots, \frac{n}{2},\ j = 1, \ldots, \nu_{2i-1}, \end{aligned} \tag{23}$$

where $\boldsymbol{k} = (k_{1,1}, \ldots, k_{n,\nu_n})$ and $\boldsymbol{p} = (p_{1,1}, \ldots, p_{n-1,\nu_{n-1}})$. The total number of order conditions is

$$N_f = \sum_{i=1}^{n/2} \nu_{2i-1}, \tag{24}$$

which agree with the number of order conditions for a non-processed symmetric composition. The main difference is that now we have a number of variables $p_{i,j}$ which can be used for solving some of the conditions.

In [2] the number of kernel conditions is given for the Lie algebra generated by $\{A, B\}$. It can be considered as a graded Lie algebra, where A and B are of grade one and all elements of grade $n+1$

can be generated from the commutator of one element of grade n and A or B. The situation is now different because the Lie algebra is generated by $\{F_1, F_3, \ldots\}$, where F_i is an element of grade i, and not all elements of grade $n+1$ can be generated from commutators with elements of grade n. However, a similar result to [2] for the number of kernel conditions is obtained:

Theorem. *Given* (19) *and* (20) *as the kernel and processor of an nth order integrator* (*n even*) *then, the number of necessary conditions to be satisfied by the kernel is given by*

$$N_k = \sum_{i=1}^{n/2} \nu_{2i-1} - \sum_{i=1}^{n/2-1} \nu_{2i} = \sum_{i=0}^{n/2-1} (\nu_{2i+1} - \nu_{2i}). \tag{25}$$

Proof. In a similar way to [2] it is possible to eliminate the $\sum_{i=1}^{n/2-1} \nu_{2i}$ variables $p_{i,j}$ from (23) solving the same number of equations. The other N_k conditions will only depend on the kernel coefficients, being the kernel conditions. □

In Table 3 we present the number of order conditions for a non-processed composition as well as for the kernel, both when considering as the basic method S_2 and S_4. From this table it is clear the great saving in the number of evaluations per step when the processing technique is used for high-order methods.

Observe that the variables $p_{2i,j}$, $i < n/2 - 1$, have been used for solving the order conditions but, we still have the ν_n variables $p_{n,j}$, $j = 1, \ldots, \nu_n$, which appear in the ν_{n+1} error functions at order h^{n+1}, $f_{n+1,j}$, $j = 1, \ldots, \nu_{n+1}$, and can be used for minimizing their value [2]. This optimization procedure will be particularly simple in some cases.

Table 3
Number of order conditions up to order n for symmetric compositions of the basic methods S_2 and S_4 for a kernel and for a non-processed composition

	S_2		S_4	
n	no-proc	proc	no-proc	proc
2	1	1	1	1
4	2	2	–	–
6	4	3	2	2
8	8	5	4	3
10	16	8	7	4
12	34	15	12	6
14			21	8

3.1. Examples

In order to illustrate how to obtain the kernel conditions, how to get the conditions for the processor and to minimize the error coefficients, we will apply this technique for obtaining optimal 4th- and 6th-order integrators using S_2 as the basic method and an 8th-order integrators using S_4.

Optimal 4th- and 6th-order integrators with S_2. Let us consider the kernel and processor up to order 7:

$$\begin{aligned} hK &= hk_{1,1}E_{1,1} + h^3k_{3,1}E_{3,1} + h^5(k_{5,1}E_{5,1} + k_{5,2}E_{5,2}) \\ &\quad + h^7(k_{7,1}E_{7,1} + k_{7,2}E_{7,2} + k_{7,3}E_{7,3} + k_{7,4}E_{7,4}), \end{aligned} \tag{26}$$

$$P = h^4p_{4,1}E_{4,1} + h^6(p_{6,1}E_{6,1} + p_{6,2}E_{6,2}), \tag{27}$$

where the $E_{i,j}$ correspond to the basis in Table 1. After a simple algebraic manipulation we have

$$\begin{aligned} h\widehat{F} &= \mathrm{e}^P h K \mathrm{e}^{-P} = hK + [P, hK] + \mathrm{O}(h^9) \\ &= hk_{1,1}E_{1,1} + h^3k_{3,1}E_{3,1} + h^5\big(k_{5,1}E_{5,1} + (k_{5,2} - p_{4,1})E_{5,2}\big) \\ &\quad + h^7\big(k_{7,1}E_{7,1} + (k_{7,2} - p_{6,1})E_{7,2} + (k_{7,3} - p_{6,2})E_{7,3} + (k_{7,4} - p_{4,1}k_{3,1})E_{7,4}\big), \end{aligned} \tag{28}$$

then, the conditions for a 6th-order method are

$$f_{1,1} = k_{1,1} = 1, \qquad f_{3,1} = k_{3,1} = 0, \tag{29}$$

$$f_{5,1} = k_{5,1} = 0, \qquad f_{5,2} = k_{5,2} - p_{4,1} = 0, \tag{30}$$

so, the three kernel conditions at order 6 we see from Table 3 correspond to: $k_{1,1} = 1,\ k_{3,1} = 0,\ k_{5,1} = 0$, and the processor condition is $p_{4,1} = k_{5,2}$. Substituting these results into the error functions we have

$$f_{7,1} = k_{7,1}, \qquad f_{7,2} = k_{7,2} - p_{6,1}, \qquad f_{7,3} = k_{7,3} - p_{6,2}, \qquad f_{7,4} = k_{7,4},$$

and taking $p_{6,1} = k_{7,2}$ and $p_{6,2} = k_{7,3}$ we obtain $f_{7,2} = f_{7,3} = 0$, corresponding to the optimization with the processor previously mentioned. Now, $f_{7,1}$ and $f_{7,4}$ depend only on $k_{i,j}$. Then, the conditions $k_{7,1} = 0$ and $k_{7,4} = 0$ will correspond to the two new kernel conditions if we want to obtain an 8th-order integrator. In this case, more conditions on the processor can be used for optimization.

If we are looking for a 4th-order method then conditions (29) have to be satisfied and, if $p_{4,1} = k_{5,2}$, the only error function will be $f_{5,1} = k_{5,1}$. In this case, the number of order conditions is not reduced with respect to a non-processed composition but we can get smaller leading error terms.

Optimal 8th-order integrator with S_4. Following the same procedure we can write, keeping terms up to order h^9,

$$\begin{aligned} hK &= hk_{1,1}E_{1,1} + h^5k_{5,1}E_{5,1} + h^7(k_{7,1}E_{7,1} + k_{7,2}E_{7,2}) \\ &\quad + h^9(k_{9,1}E_{9,1} + k_{9,2}E_{9,2} + k_{9,3}E_{9,3}), \end{aligned} \tag{31}$$

$$P = h^6p_{6,1}E_{6,1} + h^8(p_{8,1}E_{8,1} + p_{8,2}E_{8,2}), \tag{32}$$

where now the $E_{i,j}$ correspond to the basis in Table 2. From the order conditions we have the kernel and processor conditions:

$$k_{1,1} = 1, \qquad k_{5,1} = k_{7,1} = 0, \qquad p_{6,1} = k_{7,2}, \tag{33}$$

and considering $p_{8,1} = k_{9,2}$ and $p_{8,2} = k_{9,3}$ we have for the error functions

$$f_{9,1} = k_{9,1}, \qquad f_{9,2} = f_{9,3} = 0, \tag{34}$$

being $k_{9,1} = 0$ the only new kernel condition for 10th-order methods.

4. Obtaining the kernel and processor by composition

Using the analysis of the previous section we can obtain the conditions to be satisfied by the coefficients $k_{i,j}$ and $p_{i,j}$. From (9) and (10), and using the BCH formula we have:

$$S_p(b_1 h) \dots S_p(b_r h) = \mathrm{e}^{hK(\boldsymbol{b})}, \tag{35}$$

$$S_p(c_1 h) \dots S_p(c_s h) = \mathrm{e}^{P(\boldsymbol{c})}, \tag{36}$$

with $\boldsymbol{b} = (b_1, \dots, b_r)$ and $\boldsymbol{c} = (c_1, \dots, c_s)$ being the unknowns. The $k_{i,j}$ and $p_{i,j}$ are polynomial functions of b_k and c_k, respectively. Here, we have to evaluate $\boldsymbol{b}$ such that the $k_{i,j}$ satisfy the kernel conditions. Once the kernel is chosen we have to evaluate $\boldsymbol{c}$ in such a way that the $p_{i,j}$ satisfy the required conditions for this particular kernel.

Observe that the computational cost of the method as well as the leading error term will depend exclusively on $\boldsymbol{b}$. At the same time, we can find many solutions for (35). Among all these solutions we will choose the one which minimize the error terms. There is a problem at this point. The leading error term of an nth-order method is given by

$$E_r^{(n)} = \sum_{j=1}^{\nu_{n+1}} f_{n+1,j} E_{n+1,j}, \tag{37}$$

where (after the optimization with the processor parameters) the $f_{n+1,j}$ depend only on the kernel coefficients. We are interested in a solution which minimizes $\|E_r^{(n)}\|$ for a given norm but, the relative value of the different elements $\|E_{n+1,j}\|$ is strongly dependent on the basic method used. For instance, the error of the 6th-order method presented in the last section is given by

$$E_r^{(6)} = k_{7,1}(\boldsymbol{b}) F_7 + k_{7,4}(\boldsymbol{b}) \big[F_3, [F_1, F_3]\big], \tag{38}$$

where $k_{7,1}$ and $k_{7,4}$ depend on the particular solution $\boldsymbol{b}$ for the kernel conditions and $\|F_7\|$, $\|[F_3, [F_1, F_3]]\|$ depend on the basic method chosen. On the other hand, for the processor we only need a solution which satisfy the required conditions.

From Table 3 it is clear that the processing technique will be very useful for obtaining high order methods because the reduction on the number of conditions. However, in order to illustrate this procedure we will consider 4th- and 6th-order methods using S_2 and 8th-order methods using S_4 as in the previous section, where the saving versus non-processed methods is minimum. We will show explicitly how to get an optimal kernel and how to obtain a processor for this particular kernel.

As mentioned, the polynomial functions $k_{i,j}(\boldsymbol{b})$ and $p_{i,j}(\boldsymbol{c})$ can be obtained using the BCH formula. If the kernel is a symmetric composition using S_2, we can take the recurrence formulae presented in [29] based on the symmetric BCH formula or, alternatively, to consider the expressions presented in [26]. If S_4 is used, small modifications on the previous expressions are necessary.

For the processor we will consider the BCH formula

$$\mathrm{e}^X\mathrm{e}^Y = \exp\big(X+Y+\tfrac{1}{2}[X,Y]+\tfrac{1}{12}\big([X,[X,Y]]+[Y,[Y,X]]\big)+\tfrac{1}{24}[X,[Y,[Y,X]]]+\cdots\big). \tag{39}$$

Considering the general term

$$Q\big(\alpha^{(k)}\big) = \exp\left(\sum_{i=1}^{\infty} h^i \sum_{j=1}^{\nu_i} \alpha_{i,j}^{(k)} E_{i,j}\right) \tag{40}$$

we are interested in the recurrence expression

$$Q\big(\alpha^{(k+1)}\big) = S_p(xh)\,Q\big(\alpha^{(k)}\big) \tag{41}$$

for $p=2,4$. Using (39) and S_2, and after some algebra we have, up to order 6,

$$\begin{aligned}
\alpha_{1,1}^{(k+1)} &= \alpha_{1,1}^{(k)} + x,\\
\alpha_{3,1}^{(k+1)} &= \alpha_{3,1}^{(k)} + x^3,\\
\alpha_{4,1}^{(k+1)} &= \alpha_{4,1}^{(k)} + \tfrac{1}{2}\big(x\alpha_{3,1}^{(k)} - x^3\alpha_{1,1}^{(k)}\big),\\
\alpha_{5,1}^{(k+1)} &= \alpha_{5,1}^{(k)} + x^5,\\
\alpha_{5,2}^{(k+1)} &= \alpha_{5,2}^{(k)} + \tfrac{1}{2}x\alpha_{4,1}^{(k)} + \tfrac{1}{12}\big(x^2\alpha_{3,1}^{(k)} - x^4\alpha_{1,1}^{(k)} + x^3(\alpha_{1,1}^{(k)})^2 - x\alpha_{1,1}^{(k)}\alpha_{3,1}^{(k)}\big),\\
\alpha_{6,1}^{(k+1)} &= \alpha_{6,1}^{(k)} + \tfrac{1}{2}\big(x\alpha_{5,1}^{(k)} - x^5\alpha_{1,1}^{(k)}\big),\\
\alpha_{6,2}^{(k+1)} &= \alpha_{6,2}^{(k)} + \tfrac{1}{2}x\alpha_{5,2}^{(k)} + \tfrac{1}{12}\big(x^2\alpha_{4,1}^{(k)} - x\alpha_{1,1}^{(k)}\alpha_{4,1}^{(k)}\big) + \tfrac{1}{24}\big(x^4(\alpha_{1,1}^{(k)})^2 - x^2\alpha_{1,1}^{(k)}\alpha_{3,1}^{(k)}\big).
\end{aligned} \tag{42}$$

If we take S_4 then

$$\begin{aligned}
\alpha_{1,1}^{(k+1)} &= \alpha_{1,1}^{(k)} + x,\\
\alpha_{5,1}^{(k+1)} &= \alpha_{5,1}^{(k)} + x^5,\\
\alpha_{6,1}^{(k+1)} &= \alpha_{6,1}^{(k)} + \tfrac{1}{2}\big(x\alpha_{5,1}^{(k)} - x^5\alpha_{1,1}^{(k)}\big),\\
\alpha_{7,1}^{(k+1)} &= \alpha_{7,1}^{(k)} + x^7,\\
\alpha_{7,2}^{(k+1)} &= \alpha_{7,2}^{(k)} + \tfrac{1}{2}x\alpha_{6,1}^{(k)} + \tfrac{1}{12}\big(x^2\alpha_{5,1}^{(k)} - x^6\alpha_{1,1}^{(k)} + x^5(\alpha_{1,1}^{(k)})^2 - x\alpha_{1,1}^{(k)}\alpha_{5,1}^{(k)}\big),\\
\alpha_{8,1}^{(k+1)} &= \alpha_{8,1}^{(k)} + \tfrac{1}{2}\big(x\alpha_{7,1}^{(k)} - x^7\alpha_{1,1}^{(k)}\big),\\
\alpha_{8,2}^{(k+1)} &= \alpha_{8,2}^{(k)} + \tfrac{1}{2}x\alpha_{7,2}^{(k)} + \tfrac{1}{12}\big(x^2\alpha_{6,1}^{(k)} - x\alpha_{1,1}^{(k)}\alpha_{6,1}^{(k)}\big) + \tfrac{1}{24}\big(x^6(\alpha_{1,1}^{(k)})^2 - x^2\alpha_{1,1}^{(k)}\alpha_{5,1}^{(k)}\big).
\end{aligned} \tag{43}$$

Considering (36) and taking $\alpha_{i,j}^{(0)} = 0$ as initial conditions we will have that $p_{i,j}(\boldsymbol{c}) = \alpha_{i,j}^{(s)}$.

4th-order, S_2. It is necessary to use a 4th-order method for solving the two kernel conditions. Special care has to be taken to the error term $f_{5,1} = k_{5,1}$. If we use the well known three stages 4th-order composition [29] $\boldsymbol{b} = (b_2, b_1, b_2)$ with $b_2 = (2-2^{1/3})^{-1}$, $b_1 = 1-2b_2$ then $k_{5,1}$ takes a very large value. With the kernel $\boldsymbol{b} = (b_3, b_2, b_1, b_2, b_3)$ it is possible to get $f_{5,1} = k_{5,1} = 0$ and a higher order method is allowed but, as we will see, the big coefficients of the method makes it useless. On the other hand, taking b_3 as a free parameter we can find a minimum for $k_{5,1}$ with small values for the b_i. This minimum happens for $b_3 = b_2 = (4-4^{1/3})^{-1}$, $b_1 = 1-2(b_2+b_3)$ and corresponds to the 4th-order method obtained by Suzuki [24,25]. If we take the processor $\boldsymbol{c} = (c_1, c_2, c_3, -c_1, -c_2, -c_3)$, we will have many solutions such that $p_{4,1} = k_{5,2}$, and one of them is $c_3 = -0.3$, $c_2 = -0.0322132492397077$, $c_1 = -(c_2+c_3)$.

The best 4th-order methods we know corresponds to the symmetric five-stages of Suzuki [24,25] and of McLachlan [17]. If the leapfrog method is used as S_2 in a separable problem then both have very similar error terms but, using the previous processor the leading error terms are reduced by a factor two. As expected, the processed 4th-order method has only a marginal improvement with respect to the non-processed algorithms.

6th-order, S_2. Let us consider $\boldsymbol{b} = (b_3, b_2, b_1, b_2, b_3)$ for the five-stages kernel of a 6th-order integrator. The kernel conditions are

$$k_{1,1} = b_1 + 2(b_2 + b_3) = 1, \qquad k_{3,1} = b_1^3 + 2\big(b_2^3 + b_3^3\big) = 0, \qquad k_{5,1} = b_1^5 + 2\big(b_2^5 + b_3^5\big) = 0.$$

As mentioned, the two real solutions have large error functions: $f_{7,1} = 56.03$ in both cases and $f_{7,4} = 2.112,\ -51.99$. These error functions can be considerably reduced considering a seven-stages composition, $\boldsymbol{b} = (b_4, b_3, b_2, b_1, b_2, b_3, b_4)$, with b_4 as a free parameter. The computational cost increases from five to seven stages so, it will be interesting only if the error functions are reduced at least by a factor $(7/5)^6 = 7.529\ldots$.

In Fig. 1 we present the values of $|f_{7,1}|$ and $|f_{7,4}|$ versus b_4. We observe that the value of $|f_{7,1}|$ at the minimum is more than two orders of magnitude smaller than its value for $b_4 = 0$. On the other hand, the two different solutions for $|f_{7,4}|$ can be canceled at several points. Observe that one of the zeros of $|f_{7,4}|$ is very close to the minimum of $|f_{7,1}|$. Then, we will chose the closest value of b_4 to the minimum of $|f_{7,1}|$ such that $f_{7,4} = 0$. The solution is given in Table 4.

Finally, we have to find a processor which satisfy all the the required conditions. For example, we will take $\boldsymbol{c} = (c_1, c_2, c_3, c_4, c_5, -c_1, -c_2, -c_3, -c_4, -c_5)$, where a solution is given in Table 4. For this solution, the processor has not odd powers of h up to order 9. That means for the whole method we have $h\widehat{F} = hF + h^7 k_{7,1} E_{7,1} + \mathrm{O}(h^9)$ and it will work in practice as a symmetric integrator.

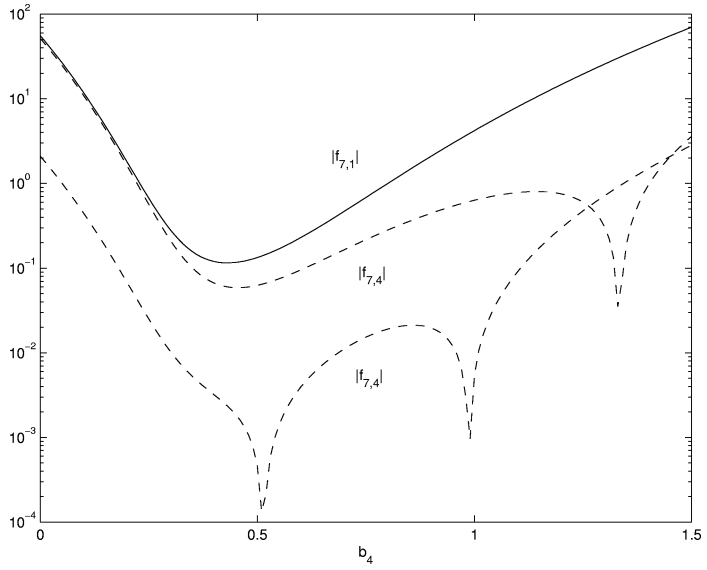

Fig. 1. Error functions $|f_{7,1}|$ and $|f_{7,4}|$ versus b_4, for the seven-stages processed method using S_2.

Table 4
Coefficients for the new processed 6th- and 8th-order methods with kernel $\boldsymbol{b} = (b_4, b_3, b_2, b_1, b_2, b_3, b_4)$ and processor $\boldsymbol{c} = (c_1, c_2, c_3, c_4, c_5, -c_1, -c_2, -c_3, -c_4, -c_5)$, using S_2 and S_4, respectively

6th-order: S_2	
	$c_5 = 0.375012038697862$
$b_4 = 0.513910778424374$	$c_4 = 0.384998538774070$
$b_3 = 0.364193022833858$	$c_3 = -0.074332422810238$
$b_2 = -0.867423280969274$	$c_2 = -0.461165940466494$
$b_1 = 1 - 2(b_2 + b_3 + b_4)$	$c_1 = -(c_2 + c_3 + c_4 + c_5)$
8th-order: S_4	
	$c_5 = 0.1$
$b_4 = 0.3836$	$c_4 = 0.153884390967272$
$b_3 = 0.38378409898601552832$	$c_3 = 0.295715027608753$
$b_2 = -0.58571608011635309034$	$c_2 = -0.182295174329697$
$b_1 = 1 - 2(b_2 + b_3 + b_4)$	$c_1 = -(c_2 + c_3 + c_4 + c_5)$

Table 5
Error terms for the non-processed and processed methods. The numerical values correspond to $f^*_{7,i} = (m/7)^6 f_{7,i}$, where m is the number of stages per step for each method

Method-stages	$f^*_{7,1}$	$f^*_{7,2}$	$f^*_{7,3}$	$f^*_{7,4}$
Yos-7	0.88839	0.02987	0.0001961	−0.01798
McL-9	0.40799	0.01254	0.0001012	−0.02451
Proc-5	7.44179	0	0	0.28046
Proc-7	0.14135	0	0	0

In order to better appreciate the efficiency of the new method, we present in Table 5 the error terms of the most efficient 6th-order methods we found in the literature which take (8) using S_2. These coefficients are normalized in order to take into account the different number of stages. The methods are: the best 7-stages of [29] and the optimized 9-stages of [17]. We must say that in spite of the small values of $f_{7,i}$, $i = 2, 3, 4$, their corresponding $\|E_{7,i}\|$ usually take greater values than $\|E_{7,1}\|$. This is the case, for instance, if we consider the well known leapfrog method as S_2 in a separable problem. From the results of this table we already appreciate the benefits of using the processing technique.

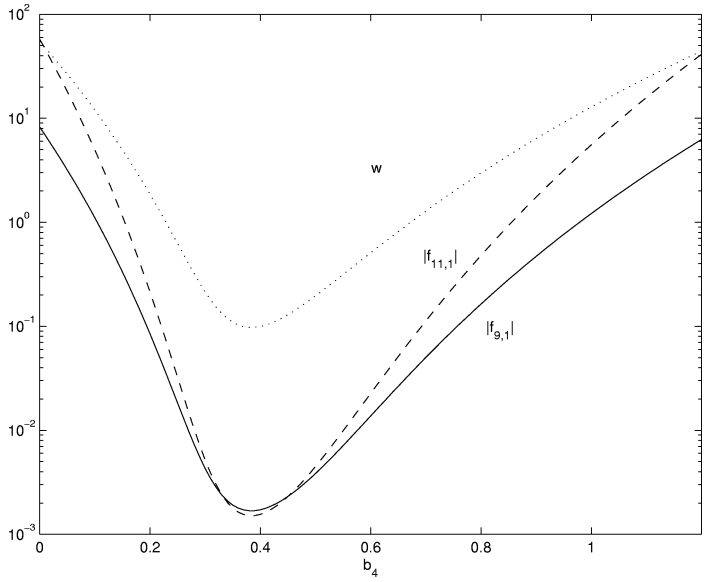

Fig. 2. Absolute value of the coefficients w and error functions $|f_{9,1}|$ and $|f_{11,1}|$ versus b_4. In order to appreciate the position of the minimum for the coefficients of the method we display $w = (\mu^2/20)^4$ with $\mu = \sum_i |b_i|$.

8th-order, S_4. In the same way, for an 8th-order integrator we can consider $\boldsymbol{b} = (b_3, b_2, b_1, b_2, b_3)$ and S_4 as the basic method. Now, we have only one error term, $f_{9,1}$. The two real solutions give $f_{9,1} = 8.22\ldots$. This large value can be considerably reduced considering, as previously, $\boldsymbol{b} = (b_4, b_3, b_2, b_1, b_2, b_3, b_4)$ which has one free parameter. It seems interesting to minimize $f_{9,1}$ as well as $\mu = \sum_i |b_i|$ in order the higher order terms do not take extremely large values. In Fig. 2 we represent $|f_{9,1}|$ and μ versus b_4 as well as $|f_{11,1}|$ as representative of higher order error terms. All of them have the minimum at the same point. Observe that the value of the error functions is reduced around four orders of magnitude at the minimum if we compare with their values at $b_4 = 0$.

A solution for b_4 near the minimum is given in Table 4. For the processor we can take $\boldsymbol{c} = (c_1, c_2, c_3, c_4, c_5, -c_1, -c_2, -c_3, -c_4, -c_5)$ and one solution is given in Table 4. Again, with this processor we have that $h\widehat{F} = hF + h^9 k_{9,1} E_{9,1} + \mathrm{O}(h^{11})$ and the method is, for practical purposes equivalent to a symmetric integrator.

In order to appreciate the improvement obtained using the processing technique, let us consider a non-processed 8th-order composition. It requires at least seven stages, i.e., $\boldsymbol{a} = (a_4, a_3, a_2, a_1, a_2, a_3, a_4)$. We found several solutions and the one with smaller error coefficients is

$$a_4 = 0.846121147469682, \qquad a_3 = 0.158012845800852,$$
$$a_2 = -1.09020666054393, \qquad a_1 = 1 - 2(a_2 + a_3 + a_4),$$

where the error terms are given in Table 6. This method has exactly the same computational cost as the seven-stages processed method but, the error coefficients are more than two orders of magnitude greater.

From the results of this section and Table 3 we expect that higher order processed methods will be considerably more efficient than the corresponding non-processed integrators. However, higher order methods are technically more involved both for getting the kernel and optimal processor conditions

Table 6
Error terms for the non-processed and processed methods. The numerical values correspond to $f^*_{9,i} = (m/7)^8 f_{9,i}$, where m is the number of stages per step for each method, and $f^*_{11,1} = (m/7)^{10} f_{11,1}$

Method-stages	$f^*_{9,1}$	$f^*_{9,2}$	$f^*_{9,3}$	$f^*_{11,1}$
no-proc-7	0.270047	0.0100179	0.0000904	0.88511
Proc-5	0.556848	0	0	1.99022
Proc-7	0.0016815	0	0	0.001506

as well as due to the numerical implementation for obtaining the best solution. This problem is under consideration and the results will be published elsewhere.

5. Numerical experiments

In order to illustrate the efficiency of the new processed methods we will compare their performances versus standard integrators (of the same family) on the following two examples:

Example 1 (Volterra–Lotka problem). Let us consider the simple differential equations

$$\dot{u} = u(v-2), \qquad \dot{v} = v(1-u) \tag{44}$$

which correspond to (1) with $\boldsymbol{y} = (u, v)$ and $\boldsymbol{f}(\boldsymbol{y}) = (u(v-2), v(1-u))$. The system has the first integral: $I(u, v) = \ln(u) - u + 2\ln(v) - v = \text{Const}$. Several second order symmetric methods can be used as the basic scheme S_2. The following two methods will be considered:

(i) *Implicit midpoint rule*:

$$\boldsymbol{y}_{k+1} = S_2 \boldsymbol{y}_k = \boldsymbol{y}_k + h\boldsymbol{f}\left(\frac{\boldsymbol{y}_k + \boldsymbol{y}_{k+1}}{2}\right), \tag{45}$$

where $\boldsymbol{y}_k$ is an approximation to the exact solution $\boldsymbol{y}(kh)$.

(ii) *Leapfrog method*. The vector field is separable in two exactly solvable parts $\boldsymbol{f} = \boldsymbol{f}_A + \boldsymbol{f}_B$ with $\boldsymbol{f}_A = (u(v-2), 0)$ and $\boldsymbol{f}_B = (0, v(1-u))$. If we denote by $\mathrm{e}^{t\,A}$ and $\mathrm{e}^{t\,B}$ the exact flows of $\dot{\boldsymbol{y}}_A = \boldsymbol{f}_A$ and $\dot{\boldsymbol{y}}_B = \boldsymbol{f}_B$, respectively, we have that

$$S_2 = \mathrm{e}^{(h/2)A}\,\mathrm{e}^{hB}\,\mathrm{e}^{(h/2)A} \tag{46}$$

corresponds to the second-order leapfrog method, and it is symmetric.

The 6th-order numerical integrators considered are: the best seven-stages of [29] (NP-7) and the new seven-stages processed method (P-7). The result of the numerical experiments is shown in Fig. 3 considering as basic methods (45) and (46). As initial values we choose $(u_0, v_0) = (1, 1)$ at $t = 0$, and we integrated up to $t = 100$. The figures show the average error in the first integral $|(I(u, v) - I(u_0, v_0))|$, versus the number of evaluations in the Newton iteration which was used in the implementation of the midpoint rule, Fig. 3(a), and versus the number of S_2 evaluations in the leapfrog case, Fig. 3(b), for different time-steps. The figures agree with the results presented in Table 5. The nine-stages McL-9 stays

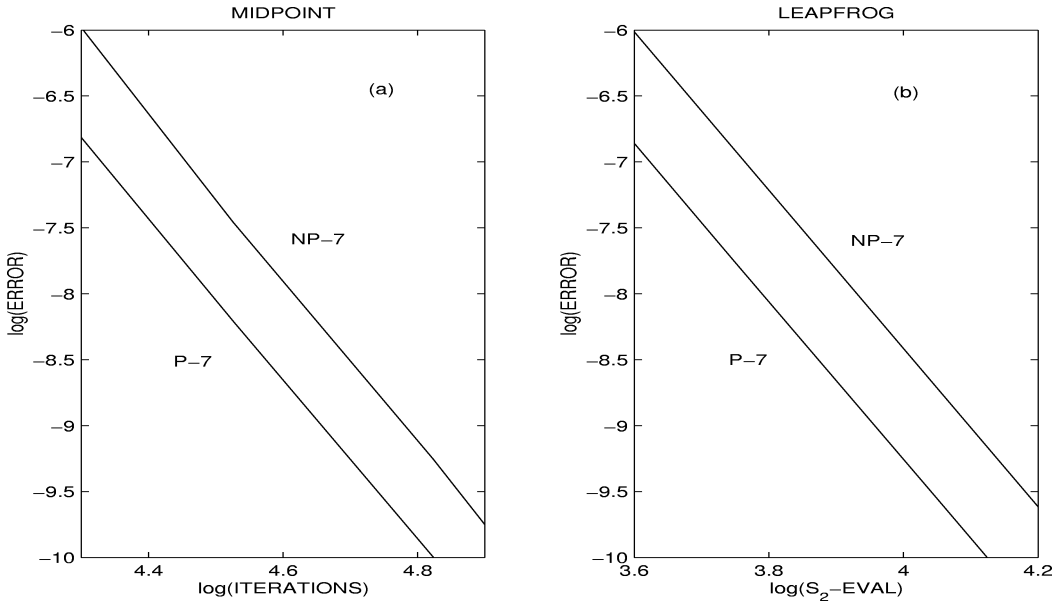

Fig. 3. Average error for the non-processed (NP-7) and processed (P-7) seven stages 6th-order methods: (a) vs. the number of iterations when the implicit midpoint rule is used, and (b) vs. number of S_2 evaluations, where S_2 is the leap-frog.

between the two previous methods, again in agreement with the error terms in Table 5. We must say that with nine stages it could be possible to get a high order processed method or a method with smaller error coefficients. On the other hand, the improvement of the fourth-order processed method is only marginal, as predicted.

Example 2 (Kepler problem). Let us consider the Hamilton equations (3) associated to the Hamiltonian

$$H(\boldsymbol{q},\boldsymbol{p}) = \frac{1}{2}\left(p_x^2 + p_y^2\right) - \frac{1}{\sqrt{q_x^2 + q_y^2}}, \tag{47}$$

where $\boldsymbol{q} = (q_x, q_y)$ and $\boldsymbol{p} = (p_x, p_y)$. We take as initial conditions $p_x = 0,\ p_y = \sqrt{(1+e)/(1-e)},\ q_x = 1-e,\ q_y = 0$, and eccentricity $e = 0.5$. These correspond to an orbit of period 2π and energy $-\frac{1}{2}$. The Hamiltonian is separable in the kinetic and potential energy. For this particular problem it is possible to use symplectic RKN methods and the most efficient we know (up to order 8) are given in [5]. However, the goal of this test is to present an example where different symmetric methods, S_4, can be used and to show that the method obtained with processing is considerably better than using a non-processed composition. For S_4 we will consider the three-stages method of [29]. Many symmetric fourth-order methods, specially tailored for RKN problems, can be used as S_4 [6]. The relative efficiency between the 8th-order methods has to be nearly independent of S_4 but, using more efficient RKN algorithms we reach machine accuracy before clearly appreciate this result. The 8th-order numerical integrators considered correspond to the seven-stages processed (P-7) and non-processed (NP-7).

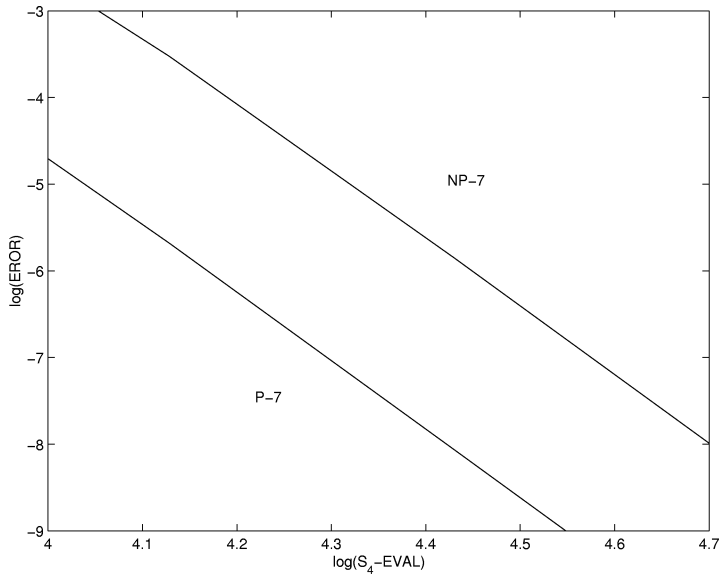

Fig. 4. Average error in position of the non-processed (NP-7) and processed (P-7) seven stages 8th-order methods vs. number of S_4 evaluations.

We integrated the system along 10 periods and measured the average error in position versus the number of evaluations of S_4. Fig. 4 shows the results obtained which perfectly agree with the values of the error terms presented in Table 6. Similar results are obtained when applying the methods to (44) using as S_4 a symmetric composition of S_2 with three or five stages as in [17,24,29]. Observe that now it is not possible to use RKN methods as in the Kepler problem.

6. Conclusions

We have shown that it is possible and very efficient to increase the order of a basic method using both the composition and the processing techniques. This efficiency comes because the kernel has to satisfy a considerable smaller number of conditions than a non-processed composition. The processor is used for solving some of the order conditions as well as for minimizing the leading error terms.

If the basic method is symmetric and a symmetric compositions for the kernel is used, the number of kernel conditions is given. In this case, the whole method will be equivalent to a symmetric integrator up to a given order if the processor is chosen properly.

From the analysis of the paper it seems clear that the relative efficiency of the processed technique versus the standard composition increases with the order. For 4th-, 6th- and 8th-order methods using S_2 and S_4 we show explicitly that the improvement is already considerable so, higher order methods are very promising. These methods are technically more involved and are, at this moment, under consideration.

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