PROCESSING SYMPLECTIC METHODS FOR NEAR-INTEGRABLE HAMILTONIAN SYSTEMS

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Abstract. Processing techniques are used to approximate the exact flow of near-integrable Hamiltonian systems depending on a small perturbation parameter. We study the reduction of the number of conditions for the kernel for this type of Hamiltonians and we build third, fourth and fifth order methods which are shown to be more efficient than previous algorithms for the same class of problems.

Key words: symplectic integrators, processing technique, near-integrable Hamiltonian systems.

1. Introduction

The use of symplectic algorithms has been rapidly growing in the last years for the numerical integration of the ordinary differential equations that arise in Hamiltonian dynamical systems. Interesting applications to relevant problems in Dynamical Astronomy can be found in [5, 6, 17, 18]. As is well known, this kind of integrators preserve qualitative properties of the exact solution, in particular the symplectic character of the evolution [22]. Basically, the problem of solving the dynamics of a classical system with Hamiltonian $H(\mathbf{q}, \mathbf{p})$ is equivalent to evaluating the action of the operator $e^{-(t-t_0)L_H}$, where t_0 is the initial time (henceforth $t_0 = 0$) and L_H is the Lie operator associated with H. It acts on an arbitrary analytic function $f(\mathbf{q}, \mathbf{p}, t)$ according to $L_H f = \{H, f\}$, where $\{H, f\}$ denotes the Poisson bracket.

When the Hamiltonian H can be split as $H = \mathcal{A} + \mathcal{B}$, so that the flows corresponding to $\mathcal{A}$ and $\mathcal{B}$ can both be computed explicitly and exactly, a usual practice is to construct a composition of these elementary flows to obtain an approximation of the true solution up to a certain given order [8, 12, 27, 28]. One particular instance where this type of methods can be applied is afforded by an exactly integrable Hamiltonian H_0 perturbed by a term H_1 which originates also an exactly computable flow [13]:

$$H(\mathbf{q}, \mathbf{p}; \varepsilon) = H_0(\mathbf{q}, \mathbf{p}) + \varepsilon H_1(\mathbf{q}, \mathbf{p}). \tag{1}$$

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In particular, the Hamiltonian of the N-body problem can be separated in the form of Equation (1) using Jacobi coordinates, with H_0 representing the Keplerian motion and εH_1 the mutual perturbations of the bodies on one another [25].

When the parameter ε is small, i.e., for the so-called near-integrable Hamiltonians, it can help to achieve methods which behave in practice as integrators of order n with less severe restrictions concerning the order conditions, so that the number of mappings to be composed decreases considerably. This approach has been used by McLachlan [13] to get several families of symplectic schemes with error terms of order εh^9 and $\varepsilon^2 h^5$.

One drawback of the procedure is that, very often, a transformation to action-angle variables of the integrable Hamiltonian H_0 must be incorporated into the algorithm [6, 21] with the resulting additional computational cost. Thus, if the numerical scheme is not very efficient and/or ε is not small enough, it could be more profitable to apply a standard symplectic integrator which does not take into account the special structure of $H(\mathbf{q}, \mathbf{p}; \varepsilon)$ [6]. The situation, then, motivates the search of methods that, while keeping the advantages of the perturbation decomposition, perform more efficiently.

Recently, a modification of the composition technique has been proposed: the use of processing. This idea was first introduced in the context of Runge–Kutta methods by Butcher [3] in 1969 and used in the last years for symplectic integrators, see for example [2, 10, 15, 20]. It has also been applied to the symplectic integration of near-integrable Hamiltonian systems by Wisdom et al. [26] and McLachlan [14]. In order to reduce the number of evaluations per time step $h = t/N$ in the integration process, the following composition is considered:

$$e^{-h\mathcal{H}(h)} \equiv e^{P} e^{-hK} e^{-P}. \tag{2}$$

Then, after N steps, we have $e^{-tL_H} \approx e^{-t\mathcal{H}(h)} = e^{P}(e^{-hK})^N e^{-P}$. At first we apply e^{P} (the corrector or processor), then e^{-hK} (the kernel) acts once per step, and e^{-P} is only evaluated when output is desired. Both the kernel and the processor are taken as compositions of the flows associated with H_0 and H_1, so that the exactly symplectic character of the integration scheme is ensured.

A general analysis of the processing technique in the context of symplectic integration has been carried out in [2]. There, the number of conditions to be satisfied by the kernel to attain a given effective order (i.e., order of the processed method) has been obtained in the general case. This figure turns out to be considerably smaller than the number of order conditions required by standard methods. In addition, it is shown that the kernel completely determines the optimal method we can obtain by processing. As a consequence of the analysis, new symplectic integrators have been constructed up to sixth order which have better efficiency than alternative symplectic schemes found in recent literature. The improvement is mainly due to the reduction in the number of evaluations of the kernel operator.

In this paper we particularize the above analysis to the near-integrable Hamiltonian (1). Recently this system has been considered by Liao [9] using implicit

symplectic algorithms. Here we approach the problem from the point of view of explicit symplectic methods. We find compositions for the kernel with as few stages as possible. Once the kernel has been fixed, we construct the processor to get more efficient symplectic schemes of effective order three, four and five than others available in the literature.

2. Kernel Conditions

2.1. GENERAL CASE

Let $L(A, B)$ be the free Lie algebra generated by $A \equiv L_{H_0}$ and $B \equiv L_{H_1}$, the Lie operators associated with the two pieces of the Hamiltonian. We denote by $[L_i, L_j]$ the commutator product of the two elements L_i and L_j of the Lie algebra and use the notation $[L_1, L_2, \ldots, L_s]$ for the nested commutator $[L_1, [L_2, \ldots, L_s]]$. Let $L^m(A, B)$ be the subspace of $L(A, B)$ generated by the independent brackets of order m, its dimension $c(m)$ being 2, 1, 2, 3, 6, 9 for $m = 1, \ldots, 6$ [11], and denote by $\{E_{m,i}\}_{i=1}^{c(m)}$ a basis of $L^m(A, B)$. Our explicit choice of basis is given in the appendix.

In this work we consider both the kernel and the processor as a composition of the readily computable evolutions governed by H_0 and H_1 (e^{-hA} and $e^{-\varepsilon hB}$, respectively). Thus, by repeated application of the Baker–Campbell–Hausdorff (BCH) formula [24] the kernel and processor generators K and P in $L(A, B)$ can be written as a power series in h:

$$K = \sum_{i=1}^{\infty} \left\{ h^{i-1} \sum_{j=1}^{c(i)} \varepsilon^{d(i,j)} k_{i,j} E_{i,j} \right\}, \quad P = \sum_{i=1}^{\infty} \left\{ h^{i} \sum_{j=1}^{c(i)} \varepsilon^{d(i,j)} p_{i,j} E_{i,j} \right\}, \quad (3)$$

where $d(i, j)$ indicates the number of B operators contained in $E_{i,j}$ and, for consistency, we take $k_{1,1} = k_{1,2} = 1$.

The basic equation (2) of the processing method will lead us to [24]

$$\mathcal{H}(h) = e^{[P,\cdot]} K = \sum_{i=1}^{\infty} \left\{ h^{i-1} \sum_{j=1}^{c(i)} \varepsilon^{d(i,j)} f_{i,j} E_{i,j} \right\} = f_{1,1} A + \varepsilon f_{1,2} B + \\ + h\varepsilon f_{2,1} [A, B] + h^2 \left\{ \varepsilon f_{3,1} [A, A, B] + \varepsilon^2 f_{3,2} [B, A, B] \right\} + \cdots . \quad (4)$$

In general there are a finite number of terms in $\mathcal{H}$ at each order in h, but an infinite number at each order in ε.

If Equations (3) are used, the $f_{i,j}$ coefficients are given in terms of polynomial relations involving $k_{i,j}$ and $p_{i,j}$ [1, 2] with $f_{1,1} = f_{1,2} = 1$. Specific nth order integration methods are obtained by requiring that $f_{i,j} = 0$ up to $i = n$. These equations cannot be solved for an arbitrary kernel using only the processor coefficients. More specifically, the kernel of a nth order ($n \geqslant 2$) symplectic processing method must satisfy exactly $k(n) = c(n) - 1$ independent conditions [2]. In the

appendix, we collect the explicit form of these conditions $N_{i,j} = 0$ up to sixth order for a general Hamiltonian $H = \mathcal{A} + \mathcal{B}$.

Concerning the near-integrable case, for most of the problems it is not necessary to cancel all the coefficients at an order h^n, and some of the conditions for the kernel will not apply. Usually, one is interested in designing methods such that

$$\mathcal{H}(h) - L_H = \mathrm{O}(\varepsilon h^{s_1} + \varepsilon^2 h^{s_2} + \varepsilon^3 h^{s_3} + \cdots). \tag{5}$$

Following McLachlan [13], a method which satisfies this condition will be said of order $(s_1, s_2, s_3, \dots)$. According to this notation, the terms up to $\varepsilon^i h^{s_i}$ are included in the numerical scheme. Termination of the list indicates that all other terms are at least of the same order as the last one. Thus, a method $(s_1, \dots, s_n)$, $s_{i+1} \leqslant s_i$, has order s_n, whereas s_1 is the order the method would have in the limit $\varepsilon \to 0$.

If we are interested in canceling only the coefficients which multiply εh^i for $i = 1, \dots, s_1$, i.e., in a $(s_1, 2)$ method, we will have to impose the conditions $f_{i,1} = 0$, $1 < i \leqslant s_1$. This is equivalent to consider only the nested commutator $[A, \dots, A, B]$ with $i - 1$ A operators, so the resulting subspace has dimension 1 and $k(i) = 0$. In other words, the kernel has not to satisfy any condition (except the consistency condition). With the leap-frog kernel

$$e^{-hK} = e^{-hA/2} e^{-\varepsilon h B} e^{-hA/2}, \tag{6}$$

one can get such a method with s_1 as high as desired, as shown by Wisdom et al. [26].

Methods which also cancel the coefficients of $\varepsilon^r h^i$ with $r > 1$ in (5) require to consider some of the conditions for the kernel. These come from the simultaneous cancellation of a number of $f_{i,j}$ coefficients at each order [1]. More specifically, Table I collects the $f_{i,j}$ coefficients to be cancelled to obtain a $(s_1, s_2, \dots, s_n)$ method. Each row gives the new coefficients to be vanished besides the ones in the preceding rows. As a result, in Table II we give the specific conditions $N_{i,j}$ to be satisfied by a kernel to generate different $(s_1, \dots, s_n)$ methods of effective order s_n.

TABLE I

Coefficients of the modified Hamiltonian $\mathcal{H}$ to be vanished to obtain a $(s_1, s_2, \dots, s_n)$ method

Method	Order conditions
$(s_1, 2)$	$\varepsilon f_{2,1} = \varepsilon f_{3,1} = \cdots = \varepsilon f_{s_1,1} = 0$
$(s_1, 4, 3)$	$\varepsilon^2 f_{3,2} = \varepsilon^2 f_{4,2} = 0$
$(s_1, 4)$	$\varepsilon^3 f_{4,3} = 0$
$(s_1, 6, 4)$	$\varepsilon^2 f_{5,2} = \varepsilon^2 f_{5,3} = \varepsilon^2 f_{6,2} = \varepsilon^2 f_{6,3} = 0$
$(s_1, 6, 5, 4)$	$\varepsilon^3 f_{5,4} = \varepsilon^3 f_{5,5} = 0$
$(s_1, 6, 5)$	$\varepsilon^4 f_{5,6} = 0$

TABLE II

Conditions to be satisfied by the kernel in order to produce different $(s_1, \ldots, s_n)$ processing methods

Method	Conditions				
	$N_{3,1}=0$	$N_{4,1}=0$	$N_{5,1}=0$	$N_{5,2}=0$	$N_{5,3}=0$
$(s_1, 2)$					
$(s_1, 4, 3)$	×				
$(s_1, 4)$	×	×			
$(s_1, 6, 4)$	×	×	×		
$(s_1, 6, 5, 4)$	×	×	×	×	
$(s_1, 6, 5)$	×	×	×	×	×

For instance, a $(7, 6, 4)$ method requires $f_{2,1} = \cdots = f_{7,1} = f_{3,2} = f_{4,2} = f_{4,3} = f_{5,2} = f_{5,3} = f_{6,2} = f_{6,3} = 0$ (Table I). Observe that $f_{3,1} = f_{3,2} = f_{4,1} = f_{4,2} = f_{4,3} = f_{5,1} = f_{5,2} = 0$ entail, according to the results presented in the appendix, $N_{3,1} = N_{4,1} = N_{5,1} = 0$. So, if the kernel satisfies these conditions then a processor that annihilates $f_{3,1}$, $f_{4,1}$, $f_{4,2}$ and $f_{5,1}$ is chosen. On the other side, $f_{2,1} = f_{5,3} = f_{6,1} = f_{6,2} = f_{6,3} = f_{7,1} = 0$ do not impose additional restrictions to the kernel and can be satisfied by means of the processor.

Table II shows, in particular, that only $(s_1, 2)$ methods can be obtained with the leap-frog kernel (6) because now $N_{3,1} = 1/24$, a feature already remarked by Suzuki [23]. If, as suggested by McLachlan [14], the symmetric kernel $e^{-\varepsilon h b_1 B} e^{-hA/2}\ e^{-\varepsilon h(1-2b_1)B}\ e^{-hA/2} e^{-\varepsilon h b_1 B}$ is considered, one can obtain more efficient processing $(s_1, 2)$ methods but, as in the previous case, it cannot be used for building up higher order schemes because $N_{3,1} = 12b_1^2 - 6b_1 + 1 \neq 0$ for all real values of b_1.

Higher order methods can be obtained by considering (a) symmetric kernels with a larger number of composed mappings, or (b) non-symmetric kernels. In the first case the effectiveness of the resulting method may be globally reduced due to the increment in the number of evaluations. On the other hand, the use of non-symmetric kernels is advantageous from the point of view of efficiency, especially when dealing with odd effective order methods [2] (for instance, with only two evaluations of B in the kernel we can build $(s_1, 4, 3)$ methods [1]), although the time-reversal symmetry of the system is no longer preserved.

As it is well known [22], a general $(2n-1)$th order non-symmetric scheme can be composed with its backward form to yield a $2n$th order symmetric method. If this procedure is applied only to the kernel K, however, the new symmetric composition thus obtained does not satisfy the kernel conditions up to order $2n-1$ $(2n)$. This can be easily seen by application of the BCH formula to the composition and taking into account the conditions verified by K.

TABLE III

Conditions to be satisfied by the kernel of $(s_1, \ldots, s_n)$ processing methods for a Hamiltonian $H = H_0(\mathbf{q}, \mathbf{p}) + \varepsilon H_1(\mathbf{q})$ with H_0 quadratic in $\mathbf{p}$

Method	Conditions		
	$N_{3,1} = 0$	$N_{5,1} = 0$	$N_{5,2} = 0$
$(s_1, 2)$			
$(s_1, 4)$	×		
$(s_1, 6, 4)$	×	×	
$(s_1, 6, 5)$	×	×	×

2.2. HAMILTONIANS WITH QUADRATIC KINETIC ENERGY

Often one finds near-integrable Hamiltonian systems as in Equation (1) with the unperturbed part $H_0(\mathbf{q}, \mathbf{p})$ quadratic in $\mathbf{p}$ and H_1 depending only on $\mathbf{q}$. The most important example is the class of Hamiltonians of the form $H_0(\mathbf{q}, \mathbf{p}) = (1/2)\mathbf{p}^T\mathbf{p} + V(\mathbf{q})$, although there may be other applications, such as Poisson systems [12]. In this case it is clear that $[B, A, B]$ only depends on $\mathbf{q}$, and therefore $[B, B, B, A] = 0$. This property reduces the number of kernel conditions to be satisfied. In particular, Table II leads in this case to Table III.

Additionally, we can consider the modified perturbation

$$C_{b,c} = bB + \varepsilon h^2 c[B, A, B], \tag{7}$$

which is exactly evaluable. Then we can replace, both in the kernel and processor compositions, all $e^{-\varepsilon h b B}$ factors by the more general ones $e^{-\varepsilon h C_{b,c}}$, which allows us to introduce two parameters with only one exponential. In fact, with the modified leap-frog kernel [20]

$$e^{-hK} = e^{-hA/2} e^{-h\varepsilon C_{1,1/24}} e^{-hA/2'} \tag{8}$$

we have $N_{3,1} = 0$, so that $(s_1, 4)$ methods can be constructed for an arbitrary s_1, and higher order schemes are possible with more evaluations in K.

3. The New Methods

In order to build new processing methods for near-integrable Hamiltonians, we consider the following processor:

$$e^P = \prod_{i=1}^{s} e^{hz_i A}\, e^{\varepsilon h y_i B}, \tag{9}$$

where the replacement $\exp(\varepsilon h y_i B) \longrightarrow \exp(\varepsilon h C_{y_i, w_i})$ can be done when $[B, B, B, A] = 0$. In any case, it is characterized by the number s of B (or C) evaluations.

As far as the kernel is concerned, the following types of composition can be used:

(i) Non-symmetric kernel with m appearances of the B operator, which will be denoted by NS-m: $\left(\sum_{i=1}^{m} a_i = \sum_{i=1}^{m} b_i = 1\right)$

$$e^{-hK} = \prod_{i=1}^{m} e^{-\varepsilon h b_i B}\, e^{-h a_i A}. \tag{10}$$

(ii) Symmetric kernel, *ABA*-type composition: $(\sum_{i=1}^{m+1} a_i = \sum_{i=1}^{m} b_i = 1)$

$$e^{-hK} = e^{-h a_1 A} e^{-\varepsilon h b_1 B} e^{-h a_2 A} \cdots e^{-h a_m A} e^{-\varepsilon h b_m B} e^{-h a_{m+1} A} \tag{11}$$

with $a_{m+2-i} = a_i$, $b_{m+1-i} = b_i$ and referred to as ABA-m.

(iii) Symmetric kernel, *BAB*-type composition: $(\sum_{i=1}^{m} a_i = \sum_{i=1}^{m+1} b_i = 1)$

$$e^{-hK} = e^{-\varepsilon h b_1 B} e^{-h a_1 A} e^{-\varepsilon h b_2 B} \cdots e^{-\varepsilon h b_m B} e^{-h a_m A} e^{-\varepsilon h b_{m+1} B} \tag{12}$$

with $a_{m+1-i} = a_i$, $b_{m+2-i} = b_i$ and denoted still by BAB-m, due to its 'first same as last' (FSAL) property [22].

We designate the whole method by the label (X-m, s), in which X = NS, ABA, BAB indicates the particular character of the kernel and, as before, we can replace $e^{-\varepsilon h b_i B}$ by $e^{-\varepsilon h C_{b_i, c_i}}$. Observe that we could also consider the non-symmetric product $e^{-hK} = \prod_i e^{-h\hat{a}_i A} e^{-\varepsilon h \hat{b}_i B}$, but then the corresponding adjoint composition is similar to (10) and thus it leads essentially to the same class of methods [22]. This is not the case of symmetric kernels because they are self-adjoint.

Once a particular (symmetric or non-symmetric) kernel is considered we proceed to the choice of a processor e^P in the form of Equation (9).

We can obtain high efficient methods if we apply some optimization algorithm to this procedure [2]. For a $(s_1, s_2, \ldots, s_n)$ processing method of order s_n we have

$$\mathcal{H}(h) - L_H = h^{s_n} \sum_{j=1}^{c(s_n+1)} \varepsilon^{d(s_n+1, j)} f_{s_n+1, j} E_{s_n+1, j} + \mathrm{O}(h^{s_n+1}), \tag{13}$$

where some of the $f_{s_n+1, j}$ coefficients have been cancelled by the kernel.

For standard symplectic integrators it is usual to define the error E_r of the method as the Euclidean norm of the vector $\mathbf{f}_{s_n+1} = (f_{s_n+1,1}, \ldots, f_{s_n+1, c(s_n+1)})$ and, to include somehow the computational cost of the algorithm, one also defines the effective error as $E_f \equiv m E_r^{1/s_n}$, where m is proportional to the cost of one step (basically, the number of A and B evaluations).

For instance, for a (7, 6, 4) scheme we have $E_r^{1/4} = (f_{5,4}^2 + f_{5,5}^2 + f_{5,6}^2)^{1/8}$. So the error is dominated by the coefficients $f_{5,4}$, $f_{5,5}$, $f_{5,6}$, but the processor can be

chosen in such a way that the coefficient $f_{5,5}$ vanishes (no additional restrictions to the kernel are necessary). Then the remaining coefficients can be written as

$$\varepsilon^3 f_{5,4} = \gamma_1 N_{5,2}, \qquad \varepsilon^4 f_{5,6} = \gamma_2 N_{5,3},$$

where γ_1 and γ_2 are now constants which are independent of the kernel and the processor. Finally, we take the kernel which minimizes the value of the coefficient $f_{5,4}$ which is multiplied by the lowest power of ε.

Thus the procedure to build a (7, 6, 4) method can be summarized as follows: first, we try to solve the system of polynomial equations $N_{3,1} = N_{4,1} = N_{5,1} = 0$ in order to determine a valid kernel. Several possibilities may occur: (i) there is no solution; (ii) there is only one solution; (iii) there are a finite set of solutions, and (iv) there is a continuous family of solutions. In the last two cases we take the solution which minimizes the value of $|N_{5,2}|$ (or equivalently, $f_{5,4}$). Then we look for a particular processor satisfying all the required conditions. In this sense the resulting method could be considered as optimal.

In order to determine z_i, y_i we apply Lie algebraic composition formulas to $(\prod_i e^{hz_i A} e^{\varepsilon h y_i B}) e^{-hK} (\prod_j e^{-\varepsilon h y_j B} e^{-hz_j A})$ to obtain, with the already known values of $k_{i,j}$,

$$f_{i,j} = f_{i,j}(\mathbf{z}, \mathbf{y}) = 0, \tag{14}$$

where a vector notation has been used for the coefficients z_i and y_i. Here, as mentioned earlier, only those values of i and j have to be considered which

(a) do not make $f_{i,j}$ identically vanish because of the kernel conditions and
(b) produce the desired effective order for the whole method.

We collect in Table IV the values of the parameters and the effective errors of some third and fourth order symplectic schemes we have obtained for the near-integrable Hamiltonian of Equation (1). Observe that with only three B evaluations in a symmetric kernel we get a (7, 6, 4) method, whereas with one additional evaluation a (7, 6, 5, 4) scheme is attained in the general case. It is worth noting that a (7, 6, 4) method with a *BAB*-type composition has also been constructed, whereas no (7, 6, 5, 4) scheme with *ABA*-type composition exists with real coefficients.

When the unperturbed part of the Hamiltonian (1) is quadratic in the momenta and $H_1 = H_1(\mathbf{q})$ we obtain, by following the same approach, the (6, 4) and (7, 6, 5) schemes collected in Table V, with effective order four and five, respectively. Both methods are given with and without using the modified perturbation $C_{\alpha,\beta}$. In the first case only one $C_{\alpha,\beta}$ evaluation is needed for attaining a (6, 4) scheme and two of them in a non-symmetric kernel of a (7, 6, 5) method. It is also worth noticing that the (6, 4, 3) integrator given in Table IV is now a (6, 4) scheme. The (7, 6, 5, 4) integrator on its side is, as a matter of fact, a (7, 6) scheme because the symmetric kernel used satisfies directly the sixth order conditions [2].

At this point we should add some comments on the convenience of using modified perturbations. One has to weigh the pros and cons. The main advantage is

TABLE IV

Coefficients, stability limit h^* and errors of the new processing methods for near-integrable Hamiltonian systems the effective error is given by $E_f = mE_r^{1/s_n}$

(6, 4, 3)	$a_1 = \frac{1}{2}\left(1+\sqrt{1+\frac{2}{\sqrt{3}}}\right)$	$b_1 = \frac{1}{2}\left(1-\sqrt{1+\frac{2}{\sqrt{3}}}\right)$
(NS-2,4)	$z_1 = 0$	$y_1 = -1/2$
	$z_2 = -0.4842296798457861$	$y_2 = -0.071444491827245766$
	$z_3 = 0.3104400973059574$	$y_3 = 0.5119423407689261$
	$z_4 = 0.9112603236884162$	$y_4 = -0.2256471548948410$
	$h^* = 2\sqrt{3}$	
	$E_r^{1/3} = 0.2464$	
(7, 6, 4)	$a_1 = 0.5600879810924619$	$b_1 = 1.5171479707207228$
(ABA-3,6)	$z_1 = -0.3346222298730800$	$y_1 = -1.621810118086801$
	$z_2 = 1.097567990732164$	$y_2 = 0.0061709468110142$
	$z_3 = -1.038088746096783$	$y_3 = 0.8348493592472594$
	$z_4 = 0.6234776317921379$	$y_4 = -0.0511253369989315$
	$z_5 = -1.102753206303191$	$y_5 = 0.5633782670698199$
	$z_6 = -0.0141183222088869$	$y_6 = -1/2$
	$h^* = 2.3221$	
	$E_r^{1/4} = 0.3801$	
(7, 6, 5, 4)	$a_1 = -0.6659279171311354$	$b_1 = 0.0962499147414666$
		$b_2 = -0.0649951074268679$
(BAB-4,6)	$z_1 = -0.5682049251492933$	$y_1 = 0.2005780724079215$
	$z_2 = 0.2817876004745961$	$y_2 = -0.3923456667727871$
	$z_3 = 0.7168960305523042$	$y_3 = -0.9517071967056039$
	$z_4 = 0.4332386614652446$	$y_4 = -0.0443156930081850$
	$z_5 = -0.3552157340165512$	$y_5 = 0.7361124293734198$
	$z_6 = -0.5825683076056897$	$y_6 = 0.3776113804258454$
	$h^* = 3.1477$	
	$E_r^{1/4} = 0.1845$	

that with more parameters in each exponential we have more flexibility to obtain higher order methods. On the other hand, one has to consider the increase of the computational cost. If we denote by τ_i the CPU time needed to evaluate $\exp(hL_{H_i})$, $i = 0, 1$, by τ_c the CPU time needed to perform the change of coordinates for the flows of H_0 and H_1 to be exactly computable, and by τ_I the CPU time needed for computing $\exp(hL_{C_{\alpha,\beta}})$, then the total CPU time increases by a factor $r(\tau_0 + \tau_I + 2\tau_c)/(m(\tau_0 + \tau_1 + 2\tau_c))$, where m and r stand for the number of H_1 and $C_{\alpha,\beta}$ evaluations, respectively. Observe that in the splitting (1) of the

TABLE V

Coefficients, stability limit h^* and errors of the new processing methods for a Hamiltonian $H = H_0(\mathbf{q}, \mathbf{p}) + \varepsilon H_1(\mathbf{q})$ with H_0 quadratic in $\mathbf{p}$

(6, 4)	$c_1 = 1/24$	
(ABA-1,5)	$z_1 = 0$	$y_1 = -0.1659120515409654$
with $(C_{\alpha,\beta})$	$z_2 = -0.9125829692505096$	$y_2 = -0.1237659000825160$
	$z_3 = -0.3605243318856133$	$y_3 = 0.0250397323738759$
	$z_4 = 0.7354063037876117$	$y_4 = 0.2269372219010943$
	$z_5 = 1/2$	$y_5 = 0$
	$h^* = 2\sqrt{3}$	
	$E_r^{1/4} = 0.1770$	
(6, 4)	$a_1 = -1/10$	$b_1 = \frac{1}{2} - \sqrt{\frac{133}{132}}$
(NS-2,4)	$z_1 = 0$	$y_1 = -0.1677635606904907$
no $(C_{\alpha,\beta})$	$z_2 = -0.8166530657446426$	$y_2 = -0.6620928448641953$
	$z_3 = -0.2644713063762618$	$y_3 = 0.1030583772761163$
	$z_4 = 0.3962246110336624$	$y_4 = 0.6922763403734603$
	$h^* = 2\sqrt{3}$	
	$E_r^{1/4} = 0.1891$	
(7, 6, 5)	$a_1 = -1/2$	$b_1 = \frac{45+\sqrt{1785}}{90}$
(NS-2,5)	$c_1 = \frac{33915+915\sqrt{1785}}{1285200}$	$c_2 = \frac{33915-915\sqrt{1785}}{1285200}$
with $(C_{\alpha,\beta})$	$z_1 = 0$	$y_1 = -0.1351128250649565$
	$z_2 = -0.8727464748693424$	$y_2 = 0.3712122429685866$
	$z_3 = -0.0934121328200023$	$y_3 = -0.2025522965297111$
	$z_4 = 0.4938054631210707$	$y_4 = -0.7782649705100380$
	$z_5 = -0.7876465915203159$	$y_5 = 0$
	$w_1 = w_5 = 0$	$w_2 = 0.0375959002450306$
	$w_3 = -0.0288760437687322$	$w_4 = -0.0024000778613867$
	$h^* = 3.0171$	
	$E_r^{1/5} = 0.2130$	
(7, 6, 5)	$a_1 = 1.158378661341834$	$b_1 = -1/2$
(NS-3,6)	$a_2 = -1.269999100723601$	$b_2 = 0.00226820843284365$
no $(C_{\alpha,\beta})$	$z_1 = -1.306469822900446$	$y_1 = 0.5502936143904913$
	$z_2 = -0.3604623184177194$	$y_2 = 0.0412470329584325 5$
	$z_3 = 0.3004052627685708$	$y_3 = -0.5571928644135203$
	$z_4 = 1.149353532702771$	$y_4 = -0.5401379261370885$
	$z_5 = -0.9412099358386227$	$y_5 = -0.9868225091585909$
	$z_6 = 0.00122059292248524$	$y_6 = 1$
	$h^* = 2.7517$	
	$E_r^{1/5} = 0.2422$	

Hamiltonian it is not true in general that $\tau_0 \ll \tau_1$ and/or $\tau_c \ll \tau_1$, as is usually the case in the more conventional splitting in kinetic and potential energy terms.

Before concluding this section some remarks concerning the stability of the new methods are also in order. Here we consider the stability of the processing methods applied to the harmonic oscillator $H(q, p) = H_0 + H_1 = p^2/2 + q^2/2$, ($\varepsilon = 1$), but, as shown in [15], the results are valid for any problem in which H_0 and H_1, when linearized about some state, are simultaneously diagonalizable.

When a processed method is applied to the integration of the harmonic oscillator the matrices M_{K} and $M_{\mathcal{H}}$ corresponding to the kernel and the whole method, respectively, are related through a similarity transformation

$$M_{\mathcal{H}} = M_{\mathrm{P}}^{-1} M_{\mathrm{K}} M_{\mathrm{P}},$$

where M_{P} is the symplectic matrix associated with the processor. Thus $M_{\mathcal{H}}$ and M_{K} have the same eigenvalues and therefore, the same stability properties.

In Tables IV and V we include the stability limits h^* attained by the different methods. These values are not optimal, in the sense that, in principle, one can construct specific methods with larger stability intervals with the same number of function evaluations [15], but in any case they are such that the resulting schemes do not require very severe restrictions concerning the time step used for integration.

4. Numerical Examples

In this section we test the new symplectic integrators on simple Hamiltonian systems and compare their performance with some of the best unprocessed symplectic algorithms we have found in the recent literature.

EXAMPLE 1. First we consider the time-dependent harmonic oscillator given by

$$H = \tfrac{1}{2}(p^2 + q^2) + \varepsilon \cos(wt)\, \tfrac{1}{2} p^2 q^2 \tag{15}$$

with $H_0 = (1/2)(p^2 + q^2)$ and $H_1 = \cos(wt)\, p^2 q^2/2$. We take $w = 2\pi$ and determine the trajectory with initial condition $q_0 = 0$, $p_0 = 1$ for 50 periods of H_0. Then we compare the mean error in the position during the last period.

Figure 1 shows, in a log–log scale, this error as a function of the number of e^B evaluations for $\varepsilon = 0.05$. Solid lines correspond to high efficient symplectic schemes taken from the literature for this class of problems: the symmetric sixth-order composition for separable Hamiltonian systems with nine stages given in [12] (denoted by m6), the $(8, 4)$ *BAB*-type method obtained by McLachlan in [13] (m84) and the processed method $(8, 2)$ specifically designed by McLachlan for near-integrable Hamiltonians [14] (p. 82). Dashed lines denoted by p643, p764 and p7654 correspond to the new processing methods whose coefficients are collected in Table IV.

We observe that m84 and p643 behave as fourth order schemes, whereas p764 and p7654 perform as sixth order methods. The reason for this behaviour lies in

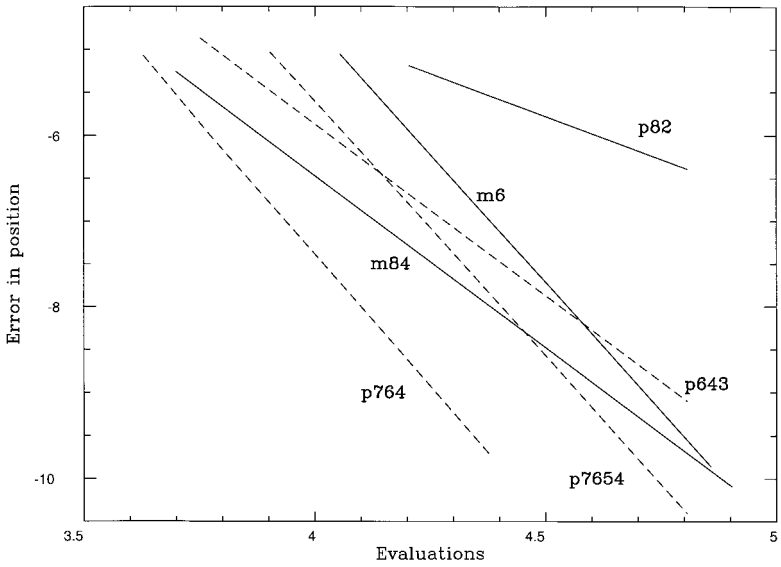

Figure 1. Average distance between exact and numerical q-trajectories vs. number of B evaluations for the Hamiltonian (15) with $\varepsilon = 0.05$. Solid lines correspond to symplectic integrators taken from the literature for near-integrable Hamiltonians and dashed lines stand for the new symplectic schemes with processing.

the fact that, for this example, the dominant term of the error is proportional to ε^2 and thus the accuracy greatly improves when the value of ε decreases.

Other values of ε in the range $0.005 \leqslant \varepsilon \leqslant 0.1$ have been explored with essentially similar relative results, the only difference being a global shift of the curves by an amount which is proportional to ε^2.

On the other hand, the effective sixth order processed method given in [2] for general Hamiltonians of the form $H = \mathcal{A} + \mathcal{B}$ is about one order of magnitude more efficient than m6 for this example.

Here it is clear the superiority of the new processed method $(7, 6, 4)$ designed specifically for near-integrable systems. We should mention that a purely theoretical comparison based on the effective error defined in the previous section shows that p643 ($E_f = 0.4928$) reveals more efficient than p764 ($E_f = 1.1404$) and p7654 ($E_f = 0.7380$), against what this example shows. The reason for this behaviour could lie in the fact that, in this case, the dominant term of the error is proportional to ε^2.

EXAMPLE 2. In order to illustrate the performance of the processing schemes collected in Table V, we consider the perturbed Kepler Hamiltonian

$$H = \frac{1}{2}(p_x^2 + p_y^2) - \frac{1}{r} - \frac{\varepsilon}{2r^3}\left(1 - \alpha\frac{3x^2}{r^2}\right) \tag{16}$$

with $r = \sqrt{x^2 + y^2}$. This Hamiltonian describes in first approximation the dynamics of a satellite moving into the gravitational field produced by a slightly oblate spheric planet. The motion takes place in a plane containing the symmetry axis of the planet when $\alpha = 1$, whereas $\alpha = 0$ corresponds to a plane perpendicular to that axis [16].

We split the perturbed Hamiltonian (16) as $H = H_0 + \varepsilon H_1$, with

$$H_0 = \frac{1}{2}(p_x^2 + p_y^2) - \frac{1}{r}, \qquad H_1 = -\frac{1}{2r^3}\left(1 - \alpha\frac{3x^2}{r^2}\right)$$

and it is readily verified that

$$\{H_0, \{H_0, \{H_0, H_1\}\}\} = 0.$$

We take $\varepsilon = 0.001$, which approximately corresponds to a satellite moving under the influence of the Earth [7] and initial conditions $x = 1 - e$, $y = 0$, $p_x = 0$, $p_y = \sqrt{(1+e)/(1-e)}$, with $e = 0.8$. These initial conditions would produce an orbit with eccentricity e in the unperturbed Kepler problem. Notice that for the Hamiltonian (16) the effect of the perturbation depends obviously of the value of ε, but also of the orbit being perturbed. The trajectory considered here with $e = 0.8$ is not a particularly favourable one.

We determine numerically the trajectory for $\alpha = 1$ up to the final time $t_f = 50 \times 2\pi$ and compute the mean error in energy and position (measured as the Euclidean norm in $\mathbb{R}^4$) achieved by each method. Observe that in the first case the results will be largely independent of t_f because the error in energy does not increase secularly for symplectic integrators.

Here we can apply methods which incorporate modified perturbations $e^{-h\varepsilon C_{b,c}}$ into the algorithm. Then the following map has to be evaluated:

$$e^{-h\varepsilon C_{b,c}} p_x = p_x + h\varepsilon\left(b\frac{A}{r^7} - h^2\varepsilon c\frac{C}{(r^7)^2}\right)x,$$

$$e^{-h\varepsilon C_{b,c}} p_y = p_y + h\varepsilon\left(b\frac{B}{r^7} - h^2\varepsilon c\frac{D}{(r^7)^2}\right)y, \tag{17}$$

where $A = (3/2)(\alpha(3x^2 - 2y^2) - r^2)$, $B = (3/2)(\alpha 5x^2 - r^2)$, $C = 9(2r^4 + 3\alpha r^2(y^2 - 4x^2) + \alpha^2(18x^4 + x^2y^2 - 2y^4))$ and $D = 9(2r^4 - 15\alpha r^2x^2 + 5\alpha^2x^2(5x^2 + 2y^2))$. Notice that the increment in the computational cost with respect to the evaluation of $e^{-h\varepsilon bB}$ (which corresponds to $c = 0$) is only due to a few very simple additional operations. In other words, using the notation introduced in the previous section, $\tau_1 \lesssim \tau_I$.

If the Keplerian part of the Hamiltonian is solved in action-angle coordinates, then two changes of variables are needed and the CPU time of the integration method per step due to the use of modified perturbation increases by a factor $\Delta\tau = (\tau_0 + \tau_I + 2\tau_c)/(\tau_0 + \tau_1 + 2\tau_c)$. In this case $\tau_0 \sim \tau_1$ and the most expensive part of

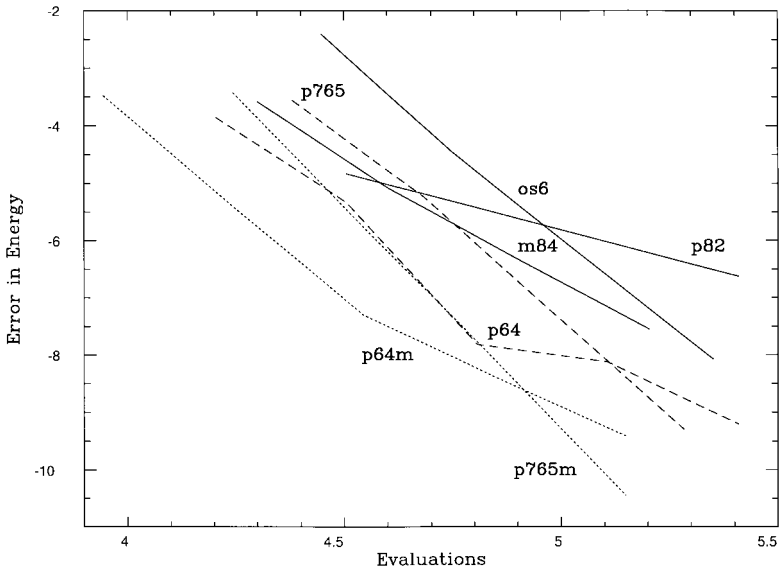

Figure 2. Relative error in energy vs. number of B evaluations for the perturbed Kepler Hamiltonian (16) with $\varepsilon = 0.001$ and $\alpha = 1$. Dashed lines correspond to the $(6, 4)$ and $(7, 6, 5)$ processing methods of Table V, whereas dotted lines stand for the same class of methods incorporating modified perturbations.

the process is the change of variables, so that $\tau_0 + 2\tau_c$ is significantly greater than τ_1 and τ_I, whereas τ_1 is only slightly smaller than τ_I. Alternatively, we have integrated H_0 in Cartesian coordinates using the f and g Gauss functions [4, 25], and solving Kepler equation by Newton iteration method. Then $\Delta\tau = (\tau_0 + \tau_I)/(\tau_0 + \tau_1)$, but now τ_0 is considerably greater than τ_1 and τ_I. In our numerical experiments we have found always $1.05 < \Delta\tau < 1.10$ depending on the value of the time step h and the number of iterations required by the Newton method. This estimate remains also valid in the first case. To be conservative, the 10% value has been used in drawing the figures we present.

Figures 2 and 3 show the mean error in energy and position, respectively, as functions of the number of e^B evaluations. Solid lines correspond to: (a) the most efficient seven-stage sixth-order symmetric Runge–Kutta–Nyström (RKN) method given in [19] (os6) applied to (16) considered as $H = H_0 + \varepsilon H_1$, (b) the near-integrable scheme m84 and (c) the processed method p82 given by McLachlan [14]. Dashed lines denoted by p64 and p765 correspond to the $(6, 4)$ and $(7, 6, 5)$ processing methods given in Table V without modified perturbations, whereas dotted lines labelled as p64m and p765m stand for the same class of methods incorporating $e^{-h\varepsilon C_{b,c}}$ evaluations.

From the figure it is clear the higher performance of our new processing methods with respect to both the standard symplectic integrators considered and other processed methods designed for near-integrable Hamiltonian systems. This im-

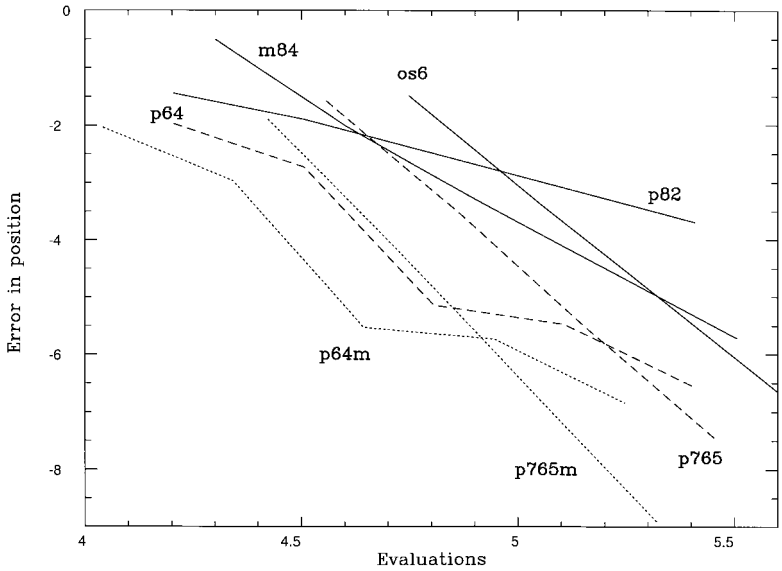

Figure 3. Error in position (measured as the Euclidean norm in $\mathbb{R}^4$) vs. number of B evaluations for the second example. Lines are coded as in Figure 2.

provement is particularly noticeable when the modified perturbation $C_{b,c}$ is incorporated into the schemes.

The next step should be to consider a kernel involving three evaluations of the modified perturbation $C_{b,c}$ and then to design a specific processor for the near-integrable case. In fact, such a kernel has been already presented in [2], where a sixth order RKN processed method was proposed. This integrator, when applied to the Hamiltonian of Equation (16), behaves essentially as a $(7, 6)$ scheme, thus providing results which are very similar to those given by p765m, unless ε is much smaller.

These examples show that with non-symmetric kernels involving two B evaluations it is possible to build $(6, 4, 3)$ and $(6, 4)$ methods which are more efficient than the corresponding $(8, 2)$ schemes constructed from a symmetric kernel with the same number of evaluations.

It should be also stressed that our new processing methods not involving modified perturbations show better efficiency than other standard integrators for this example.

5. Conclusions

We have derived new high-order symplectic integration algorithms for small perturbations of exactly solvable Hamiltonian systems. The schemes, referred to as processing methods, are defined by the composition $e^P e^{-hK} e^{-P}$, in which each exponential is an explicitly exactly computable composition of symplectic map-

pings. In order to obtain efficient methods, (a) we have considered the minimum number of stages in e^{-hK} so that the kernel conditions have real solutions, and (b) we have applied an optimization procedure to the election of the processor.

The methods of effective order four and five thus constructed work well in practice even for values of the perturbation parameter not so small. Following this treatment it is possible in principle to build higher order schemes and/or incorporate into them more correct terms in εh^n. These new methods have proven to be competitive with more traditional symplectic schemes and even with the processing methods appearing in the recent literature for near-integrable Hamiltonian systems.

To properly appreciate the performance of the new methods proposed in this paper one should compare their results with the ones obtained with other non-perturbative splitting (e.g., $H(\mathbf{p}, \mathbf{q}) = T(\mathbf{p}) + V(\mathbf{q})$). As a general trend we have found that the last mentioned methods are not very sensitive to the effect of the perturbation, while the new ones introduced here improve significantly when the perturbation diminishes. It could then be very interesting to implement them to carry out the numerical integration of different problems arising in Dynamical Astronomy.

Acknowledgments

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Appendix

As stated in the text we denote by $\left\{E_{n,i}\right\}_{i=1}^{c(n)}$ a basis of $L^n(A, B)$. In this work we have taken:

$n = 1$	$E_{1,1} = A, \quad E_{1,2} = B$
$n = 2$	$E_{2,1} = [A, B]$
$n = 3$	$E_{3,1} = [A, A, B], \quad E_{3,2} = [B, A, B]$
$n = 4$	$E_{4,1} = [A, A, A, B], \quad E_{4,2} = [B, A, A, B], \quad E_{4,3} = [B, B, B, A]$
$n = 5$	$E_{5,1} = \left[A, E_{4,1}\right], \quad E_{5,2} = \left[B, E_{4,1}\right], \quad E_{5,3} = -\left[A, E_{4,2}\right]$
	$E_{5,4} = \left[B, E_{4,2}\right], \quad E_{5,5} = \left[A, E_{4,3}\right], \quad E_{5,6} = \left[B, E_{4,3}\right]$
$n = 6$	$E_{6,1} = \left[A, E_{5,1}\right], \quad E_{6,2} = \left[B, E_{5,1}\right], \quad E_{6,3} = \left[A, E_{5,2}\right]$
	$E_{6,4} = \left[A, E_{5,4}\right], \quad E_{6,5} = \left[B, E_{5,2}\right], \quad E_{6,6} = \left[A, E_{5,5}\right]$
	$E_{6,7} = \left[B, E_{5,5}\right], \quad E_{6,8} = \left[A, E_{5,6}\right], \quad E_{6,9} = \left[B, E_{5,6}\right]$
$n = 7$	$E_{7,2j-1} = \left[A, E_{6,j}\right], \quad E_{7,2j} = \left[B, E_{6,j}\right], \quad j = 1, \ldots, 9$

For a general $H = \mathcal{A} + \mathcal{B}$, $A \equiv L_{\mathcal{A}}$, $B \equiv L_{\mathcal{B}}$ and the corresponding $f_{i,j}$ coefficients of Equation (4) are given in terms of polynomial relations involving $k_{i,j}$ and $p_{i,j}$. In particular, $f_{1,1} = f_{1,2} = 1$ for consistency, and

$$\begin{aligned} f_{2,1} &= k_{2,1} - p_{1,2} + p_{1,1}, \\ f_{3,1} &= k_{3,1} - p_{2,1} + k_{2,1}p_{1,1} - \tfrac{1}{2}p_{1,1}(p_{1,2} - p_{1,1}), \\ f_{3,2} &= k_{3,2} - p_{2,1} + k_{2,1}p_{1,2} - \tfrac{1}{2}p_{1,2}(p_{1,2} - p_{1,1}). \end{aligned} \tag{18}$$

The second order condition $f_{2,1} = 0$ gives $p_{1,2} - p_{1,1} = k_{2,1}$. To obtain a third order processed method we must impose, in addition, $f_{3,1} = f_{3,2} = 0$. The first equation leads to

$$p_{2,1} = k_{3,1} + k_{2,1}p_{1,1} - \tfrac{1}{2}p_{1,1}k_{2,1}.$$

Then after substitution in $f_{3,2}$, we get

$$f_{3,2} = k_{3,2} - k_{3,1} + \tfrac{1}{2}k_{2,1}^2 \equiv -N_{3,1},$$

which shows that $f_{3,2}$ depends only on the kernel coefficients. In this way we obtain one condition to be satisfied by the kernel. This procedure can be carried out at higher orders, thus obtaining the explicit form of the conditions collected in the following table, where only the starred entries hold if $[B, B, B, A] = 0$:

Order 3	$(*)$	$N_{3,1} \equiv k_{3,1} - k_{3,2} - \frac{1}{2}k_{2,1}^2 = 0$
Order 4		$N_{4,1} \equiv k_{4,3} + k_{4,2} - k_{4,1} + \frac{1}{6}k_{2,1}^3 = 0$
Order 5	$(*)$	$N_{5,1} \equiv k_{5,2} - k_{5,1} + k_{4,1}k_{2,1} - \frac{1}{2}k_{3,1}^2 = 0$
	$(*)$	$N_{5,2} \equiv k_{5,3} + k_{5,4} + k_{4,2}k_{2,1} - k_{3,2}k_{3,1} = 0$
		$N_{5,3} \equiv k_{5,5} - k_{5,6} - k_{4,3}k_{2,1} - \frac{1}{2}k_{3,2}^2 = 0$
Order 6	$(*)$	$N_{6,1} \equiv 5(k_{6,1} - k_{6,2}) - 3(k_{6,3} - k_{6,5}) + 2k_{4,1}k_{3,1} -$
		$-(k_{5,3} - 3k_{5,2} + 5k_{5,1})k_{2,1} - k_{4,2}k_{3,1} + \frac{3}{2}k_{4,1}k_{2,1}^2 - k_{3,1}^2k_{2,1} = 0$
		$N_{6,2} \equiv 5(k_{6,9} - k_{6,8}) - 3(k_{6,7} - k_{6,6} + \frac{1}{3}k_{6,4}) - 2k_{4,3}k_{3,2} +$
		$+(k_{5,4} - 3k_{5,5} + 5k_{5,6})k_{2,1} - k_{4,2}k_{3,2} + \frac{3}{2}k_{4,3}k_{2,1}^2 + k_{3,2}^2k_{2,1} = 0$
		$N_{6,3} \equiv k_{6,1} - k_{6,2} - k_{6,3} + k_{6,4} + k_{6,5} - k_{6,6} + k_{6,7} + k_{6,8} -$
		$-k_{6,9} - \left(k_{5,3} + k_{5,4} - k_{5,2} - k_{5,5}\right)k_{2,1} + \frac{1}{30}k_{2,1}^5 = 0$

In the following table we indicate explicitly which coefficients have to be simultaneously cancelled to obtain the previous kernel conditions in a given order n, $n = 3, \ldots, 6$. By extending the previous analysis it can be shown that the $f_{i,j} = 0$, $i = 3, 4, 5$, conditions in each row are all but one automatically satisfied by the processor coefficients, the remaining one being proportional to the corresponding kernel condition.

At sixth order all except three coefficients $f_{6,i}$ can be annihilated by the processor, whereas the remaining ones (for instance $f_{6,5}$, $f_{6,8}$ and $f_{6,9}$) are linear combinations of $N_{6,1}$, $N_{6,2}$ and $N_{6,3}$. Then, in principle, a processor for schemes (7,6,4) and (7,6,5,4) could be designed in such a way that $f_{6,1} = f_{6,2} = f_{6,3} = f_{6,4} = f_{6,6} = f_{6,7} = 0$, and thus, provided the kernel is symmetric (which implies $N_{6,1} = N_{6,2} = N_{6,3} = 0$), all sixth order conditions are satisfied. These new methods could be advantageous for problems where the error coefficients $f_{7,2}$ and $f_{7,3}$ are much smaller than $f_{6,5}$, $f_{6,6}$, $f_{6,7}$, $f_{6,8}$ and $f_{6,9}$.

Order 3	$\varepsilon f_{3,1} = \varepsilon^2 f_{3,2} = 0$	$\Rightarrow$	$N_{3,1} = 0$
Order 4	$\varepsilon f_{4,1} = \varepsilon^2 f_{4,2} = \varepsilon^3 f_{4,3} = 0$	$\Rightarrow$	$N_{4,1} = 0$
Order 5	$\varepsilon f_{5,1} = \varepsilon^2 f_{5,2} = 0$	$\Rightarrow$	$N_{5,1} = 0$
	$\varepsilon^2 f_{5,3} = \varepsilon^3 f_{5,4} = 0$	$\Rightarrow$	$N_{5,2} = 0$
	$\varepsilon^3 f_{5,5} = \varepsilon^4 f_{5,6} = 0$	$\Rightarrow$	$N_{5,3} = 0$
Order 6	$\varepsilon f_{6,1} = \varepsilon^2 f_{6,2} = \varepsilon^2 f_{6,3} = \varepsilon^3 f_{6,5} = 0$	$\Rightarrow$	$N_{6,1} = 0$
	$\varepsilon^3 f_{6,4} = \varepsilon^3 f_{6,6} = \varepsilon^4 f_{6,7} = \varepsilon^4 f_{6,8} = \varepsilon^5 f_{6,9} = 0$	$\Rightarrow$	$N_{6,2} = 0$
	$\varepsilon f_{6,1} = \varepsilon^2 f_{6,2} = \cdots = \varepsilon^5 f_{6,9} = 0$	$\Rightarrow$	$N_{6,3} = 0$

References

1. Blanes, S.: *Estudio de la evolución de sistemas dinámicos clásicos y cuánticos utilizando métodos algebraicos*, Ph. D. Thesis. Universitat de València, 1998.
2. Blanes, S., Casas, F. and Ros, J.: 'Symplectic integrators with processing: a general study', *SIAM J. Sci. Comput* **21** (1999), 711–727.
3. Butcher, J.: 'The effective order of Runge–Kutta methods', in: *Conference on the numerical solution of differential equations.* Lecture Notes in Math., Vol. 109, Springer, Berlin, 1969, 133–139.
4. Danby, J. M. A.: *Fundamentals of Celestial Mechanics*, Willmann-Bell, Richmond, 1988.
5. Gladman, B., Duncan, M. and Candy, J.: 'Symplectic integrators for long-term integrations in Celestial Mechanics', *Celest. Mech. & Dyn. Astr.* **52** (1991), 221–240.
6. Kinoshita, H. Yoshida, H. and Nakai, H.: 'Symplectic integrators and their application to Dynamical Astronomy', *Celest. Mech. & Dyn. Astr.* **50** (1991), 59–71.
7. Kirchgraber, U.: 'An ODE-solver based on the method of averaging', *Numer. Math.* **53** (1988), 621–652.
8. Koseleff, P.-V.: *Formal Calculus for Lie Methods in Hamiltonian Mechanics*. Ph.D. Thesis, Lawrence Berkeley Laboratory, 1994.
9. Liao, X.: 'Symplectic integrator for general near-integrable Hamiltonian system', *Celest. Mech. & Dyn. Astr.* **66** (1997), 243–253.
10. López-Marcos, M. A., Sanz-Serna, J. M. and Skeel, R. D.: 'Cheap enhancement of symplectic integrators', in: D. F. Griffiths and G. A. Watson (eds), *Numerical Analysis 1995*, Longman Harlow (Essen), 1996, pp. 107–122.
11. Magnus, W., Karrass, A. and Solitar, D.: *Combinatorial Group Theory*, 2nd revised edition, Dover, New York, 1976.

12. McLachlan, R. I.: 'On the numerical integration of ordinary differential equations by symmetric composition methods', *SIAM J. Sci. Comput.* **16** (1995), 151–168.
13. McLachlan, R. I.: Composition methods in the presence of small parameters, *BIT* **35** (1995), 258–268.
14. McLachlan, R. I.: 'More on symplectic correctors', In: J. E. Marsden, G. W. Patrick, and W. F. Shadwick (eds) *Integration Algorithms and Classical Mechanics*, American Mathematical Society, Providence, R.I., 1996, pp. 141–149.
15. McLachlan, R. I. and Gray, S. K.: 'Optimal stability polynomials for splitting methods, with application to the time-dependent Schrödinger equation', *Appl. Numer. Math.* **25** (1997), 275–286.
16. Meirovich, L.: *Methods of Analytical Dynamics*, McGraw-Hill, New York, 1988.
17. Michel, P. and Valsecchi, G. B.: 'Numerical experiments on the efficiency of second-order mixed-variable symplectic integrators for n-body problems', *Celest. Mech. & Dyn. Astr.* **65** (1997), 355–371.
18. Mikkola, S.: 'Practical symplectic methods with time transformation for the few-body problem', *Celest. Mech. & Dyn. Astr.* **67** (1997), 145–165.
19. Okunbor, D. I. and Skeel, R. D.: 'Canonical Runge–Kutta–Nyström methods of orders five and six', *J. Comp. Appl. Math.* **51** (1994), 375–382.
20. Rowlands, G.: 'A numerical algorithm for Hamiltonian systems', *J. Comput. Phys.* **97** (1991), 235–239.
21. Saha, P. and Tremaine, S.: 'Symplectic integrators for solar system dynamics', *Astron. J.* **104** (1992), 1633–1640.
22. Sanz-Serna, J. M. and Calvo, M. P.: *Numerical Hamiltonian Problems*, Chapman & Hall, London, 1994.
23. Suzuki, M.: 'Improved Trotter-like formula', *Phys. Lett. A* **180** (1993), 232–234.
24. Varadarajan, V. S.: *Lie Groups, Lie Algebras and Their Representations*, Springer-Verlag, New York, 1984.
25. Wisdom, J. and Holman, M.: 'Symplectic maps for the N-body problem', *Astron. J.* **102** (1991), 1528–1538.
26. Wisdom, J., Holman, M. and Touma, J.: 'Symplectic correctors', in: J. E. Marsden,, G. W. Patrick, and W. F. Shadwick, (eds) *Integration Algorithms and Classical Mechanics*, American Mathematical Society, Providence, R.I., 1996, pp. 217–244.
27. Yoshida, H.: 'Construction of higher order symplectic integrators', *Phys. Lett. A* **150** (1990), 262–268.
28. Yoshida, H.: 'Recent progress in the theory and application of symplectic integrators', *Celest. Mech. & Dyn. Astr.* **56** (1993), 27–43.