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SYMPLECTIC INTEGRATION WITH PROCESSING: A GENERAL STUDY*

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Abstract. The number of conditions to be satisfied by the operators K and P in symplectic integrators with processing, given by $e^P e^{-hK} e^{-P}$, is determined for a Hamiltonian of the form $H = \mathcal{A} + \mathcal{B}$. The conditions for K are explicitly written up to order six and used to obtain more efficient methods with fewer evaluations per step than other symplectic integrators. Special cases in which the number of conditions for the kernel is drastically reduced are also studied. It is shown that the kernel completely determines the optimal method one can obtain by processing.

Key words. initial value problems, symplectic integrators, processing technique, Hamiltonian systems

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1. Introduction.

During the last few years the search for symplectic integrators has met with good success. As is well known, these are methods designed to solve Hamiltonian equations in classical mechanics numerically, while at the same time preserving the symplectic character of time evolution. For many problems this has proved to be essential, and it is important to look for the most efficient methods of this type [23]. All that is discussed in this paper referring to classical mechanics rests exclusively on the Lie algebraic structure of the theory. Therefore it also applies to, among other fields, quantum mechanics, with only the obvious replacement of Poisson brackets by operator commutators, symplectic transformations by unitary operators, etc.

The problem of the time evolution of a classical system with Hamiltonian $H(\mathbf{q}, \mathbf{p})$ is basically reduced to evaluating the action of the operator

$$\mathcal{M}(t, t_0) = e^{-(t-t_0)L_H}, \tag{1}$$

where t is the evolution parameter which we take to be the time, t_0 is the initial instant (henceforth, $t_0 = 0$), and L_H is the Lie operator associated with H. It acts on an arbitrary analytic function $f(\mathbf{q}, \mathbf{p})$ according to the rule $L_H f = \{H, f\}$, where $\{H, f\}$ stands for the Poisson bracket. Often, it is possible to separate

$$L_H = A + B, \tag{2}$$

where the action of e^{-tA} and e^{-tB} can be exactly evaluated. This parallels the separation $H = \mathcal{A} + \mathcal{B}$ and $A \equiv L_{\mathcal{A}}$, $B \equiv L_{\mathcal{B}}$. In most of the cases, but not all, $\mathcal{A}$ and $\mathcal{B}$ correspond, respectively, to the kinetic energy depending only on the momentum variables $\mathbf{p}$ and the potential energy, a function of the $\mathbf{q}$ coordinates.

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These Hamiltonians are sometimes said to be separable. This terminology should not be confused with Stäckel separability in a Hamilton–Jacobi equation which ensures integrability of the Hamiltonian system.

One usual procedure to evaluate the action of the operator (1) is to approximate it by a product of exponentials of simpler elements of the Lie algebra which we know how to apply exactly (or at least up to a desired order). This is the idea behind composition methods, which have been extensively studied by using either the Baker–Campbell–Hausdorff (BCH) formula [10, 12, 14, 18, 24, 29] or, alternatively, the rooted trees techniques [7, 20, 21].

Recently, a new modification has been proposed: the so called processing method. This technique as a tool to improve the efficiency of Runge–Kutta methods can be traced back to the work of Butcher [5] as early as 1969 and has more recently been incorporated into the context of symplectic integrators by Rowlands [22], Wisdom, Holman, and Touma [28], and McLachlan [17]. In order to reduce the number of evaluations per time step $h = t/N$ in the integration process, a composition given by

$$e^{-h\mathcal{H}(h)} \equiv e^{P} e^{-hK} e^{-P} \tag{3}$$

is considered. After N steps we see that $e^{-tL_H} \cong e^{-t\mathcal{H}(h)} = e^{P}\left(e^{-hK}\right)^{N} e^{-P}$. At first we apply e^{P}, then e^{-hK} acts once per step, and e^{-P} will be evaluated only when output is desired. This fact makes it especially interesting to look for an expression of e^{-hK} as simple as possible and let e^{P} help in attaining the desired order of approximation. Usually e^{-hK} is called the kernel or basic method and e^{P} the corrector or processor. Observe that the exactly symplectic character of the integration scheme is preserved.

When this idea has been applied to slightly perturbed systems or to Hamiltonians with quadratic kinetic energy, it resulted in very efficient integration methods being produced [2, 13, 14, 17, 22, 28]. Nevertheless, in the general case, some doubts about the usefulness of the processing method have been cast [17, 25]. The situation, then, calls for a general study of the problem in order to know whether and when it is worthwhile to use the processing technique.

This is the task undertaken in the present paper. In particular, we obtain the number of conditions to be satisfied by the kernel of a symplectic processing method of any order and construct explicitly these conditions up to order six [8]. Once a permissible kernel has been fixed we analyze the optimization of the processor in order to get more efficient symplectic schemes. Our main result in this respect is that the minimum error which can be achieved by the whole method is solely determined by the kernel [3]. The analysis is carried out by employing exclusively Lie algebraic techniques.

The preceding study allows us to construct fourth-, fifth- and sixth-order symplectic integrators which require fewer evaluations per step than most of the usual methods while producing more efficient algorithms. This is so both for $H = \mathcal{A} + \mathcal{B}$ and Hamiltonians with quadratic kinetic energy.

The main results of the paper are contained in sections 2 and 4. Explicit symplectic integrators are built in section 3 which are then tested in practice on two numerical examples in section 5. Finally the main conclusions are collected in section 6.

2. Analysis of the processing methods.

2.1. Notation and general setting. Let $L(A, B)$ be the free Lie algebra generated by A and B. In what follows 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 $[L_1, L_2, \ldots, L_s] \equiv [L_1, [L_2, \ldots, L_s]]$. Let $L^m(A,B)$ be the subspace of $L(A,B)$ generated by the independent brackets of order m. We call $c(m)$ its dimension, its first 8 values being 2, 1, 2, 3, 6, 9, 18, 30 (see [15]) 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.

The two basic ingredients of an integrator with processing are the processor e^P and the kernel e^{-hK}. From a practical point of view it is generally not necessary to use an exactly symplectic processor because its effects are not propagated by the numerical integrator [14]. Nevertheless in this work we take as processors the strictly symplectic composition

$$e^P = \prod_i^s e^{hz_iA}\ e^{hy_iB} \tag{4}$$

characterized by the number s of B evaluations. As far as the kernel is concerned, we use two types of compositions:

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

$$e^{-hK} = \prod_{i=1}^m e^{-hb_iB}\ e^{-ha_iA}. \tag{5}$$

(ii) *Symmetric* kernel, referred to as S-m:

— m odd: $\left(2\sum_{i=1}^r a_i = b_r + 2\sum_{i=1}^{r-1} b_i = 1, \quad r = \frac{m+1}{2}\right)$,

$$e^{-hK} = e^{-ha_1A}e^{-hb_1B}\cdots e^{-ha_rA}\ e^{-hb_rB}\ e^{-ha_rA}\cdots e^{-hb_1B}e^{-ha_1A}; \tag{6}$$

— m even: $\left(2\sum_{i=1}^r a_i = b_{r+1} + 2\sum_{i=1}^r b_i = 1, \quad r = \frac{m}{2}\right)$,

$$e^{-hK} = e^{-hb_1B}\cdots e^{-ha_rA}\ e^{-hb_{r+1}B}\ e^{-ha_rA}\cdots e^{-hb_1B}. \tag{7}$$

By repeated application of the BCH formula the kernel and processor generators K and P in $L(A,B)$ can be written as a power series in h:

$$K = \sum_{i=1}^\infty \left\{ h^{i-1} \sum_{j=1}^{c(i)} k_{i,j}E_{i,j} \right\}, \qquad P = \sum_{i=1}^\infty \left\{ h^i \sum_{j=1}^{c(i)} p_{i,j}E_{i,j} \right\}. \tag{8}$$

The consistency conditions $k_{1,1} = k_{1,2} = 1$ originate from the constraints on the a_i and b_i coefficients given in (5)–(7).

The basic equation (3) of the processing method will lead us to

$$\begin{aligned} \mathcal{H}(h) &= \exp(\operatorname{ad} P)\, K = K + [P,K] + \frac{1}{2}[P,P,K] + \cdots \\ &= \sum_{i=1}^\infty \left\{ h^{i-1} \sum_{j=1}^{c(i)} f_{i,j}E_{i,j} \right\} = f_{1,1}A + f_{1,2}B \\ &\quad + hf_{2,1}[A,B] + h^2\{f_{3,1}[A,A,B] + f_{3,2}[B,A,B]\} + \cdots, \end{aligned} \tag{9}$$

where ad P stands for the adjoint operator of P [26]. If equations (8) are used, the $f_{i,j}$ coefficients are given in terms of polynomial relations involving $k_{i,j}$ and $p_{i,j}$ with

the structure

$$f_{i,j} = k_{i,j} + \sum_{s=1}^{c(i-1)} \alpha_{j,s} p_{i-1,s} + \sum_{l=1}^{i-1} \sum_{m=1}^{c(l)} k_{l,m} \sum_r \tau_r \prod_{q,s} (p_{q,s})^{n_{q,s}^{(r)}}, \tag{10}$$

where we have, for later convenience, explicitly separated in $[P,K]$ the contributions from $[P, A+B]$. Here $\alpha_{j,s}$ and τ_r are numerical coefficients and the condition

$$l + \sum_{q,s} q\ n_{q,s}^{(r)} = i \tag{11}$$

has to be satisfied for $1 \le l \le i-1$ and all r values appearing in (10). Furthermore, $f_{1,1} = f_{1,2} = 1$.

Specific integration nth-order methods are obtained by requiring the $f_{i,j}$ to vanish up to $i = n$, which amounts to approximating e^{-hL_H} by $e^{-h\mathcal{H}(h)}$ to the desired order n:

$$\mathcal{H}(h) = L_H + h^n \sum_{j=1}^{c(n+1)} f_{n+1,j} E_{n+1,j} + \mathcal{O}(h^{n+1}), \tag{12}$$

where $f_{n+1,j}$ already take into account the solution of the cancellation of the previous coefficients. As a criterion to estimate the error of a method the following quantity is usually introduced:

$$E_r = \sqrt{\sum_{j=1}^{c(n+1)} |f_{n+1,j}|^2}. \tag{13}$$

To include somehow the computational cost of the algorithm one defines the effective error as $E_f \equiv m E_r^{1/n}$, where m is the number of B evaluations per time step. Observe, however, that the numerical value of E_r depends on the vector basis used in the Lie algebra.

2.2. The general case of $H = A + B$ Hamiltonians. The equations $f_{i,j} = 0$, $i \le n$, cannot be solved for an arbitrary kernel using only the processor coefficients. There are restrictions on the permissible form of K. The following theorem, which parallels the one for Runge–Kutta methods obtained by Butcher and Sanz-Serna [6], fixes the number of these conditions for a processing method.

THEOREM 1. *The number $k(n)$ of necessary conditions to be satisfied by the kernel generator K of a nth-order symplectic integrator with processing for $n \ge 2$ is*

$$k(n) = c(n) - 1. \tag{14}$$

To prove this statement we observe that by (9) to obtain a method of order n we only have to consider terms in P until order $n-1$. The number of $p_{i,j}$ coefficients involved is then $\sum_{i=1}^{n-1} c(i)$, while the number of $k_{i,j}$ which appear coincides with the number of $f_{i,j}$ to be cancelled and is $\sum_{i=2}^{n} c(i)$. We proceed by induction: for $n = 2$ the only condition $f_{2,1} = 0$ simply forces $k_{2,1} - p_{1,2} + p_{1,1} = 0$ and any $k_{2,1}$ will do. Thus $k(2) = 0$. Suppose $k(n)$ has been determined; then to go to order $n+1$ we increase the number of $f_{i,j}$ to be cancelled by $c(n+1)$, but we have only $c(n)$ extra

TABLE 1

Conditions to be satisfied by the kernel up to order 6 for a Hamiltonian $H = \mathcal{A} + \mathcal{B}$. If $[B, B, B, A] = 0$, only the starred conditions survive.

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

$p_{i,j}$ coefficients to do the job. More specifically, (10) can be written as

$$f_{n+1,j} = k_{n+1,j} + \sum_{s=1}^{c(n)} \alpha_{j,s} p_{n,s} + G_j(k_{2,1}, \ldots, k_{n,c(n)}), \qquad j = 1, \ldots, c(n+1), \tag{15}$$

where G_j are polynomials in which the $p_{i,j}$, $i \le n-1$, have been eliminated in favor of the $k_{i,j}$ coefficients. To eliminate the $p_{n,s}$ coefficients from the system $f_{n+1,j} = 0$, the rank of the $c(n+1) \times c(n)$ matrix α with elements $\alpha_{j,r}$ should be $c(n)$. But this is indeed the case because, in the free Lie algebra generated by A and B, one can always obtain a basis for the $c(n+1)$ dimensional subspace which includes the elements $[A, E_{n,i}]$, $i = 1, \ldots, c(n)$. This guarantees that α has a lower triangular submatrix in $c(n)$ dimensions with no zero elements in the main diagonal and then has rank $c(n)$. So we conclude $k(n+1) = k(n) + c(n+1) - c(n)$. The telescopic character of this recurrence allows one to write down its solution as $k(n) = k(2) + c(n) - c(2)$, which is (14) because $c(2) = 1$. For $n = 3, \ldots, 8$ this gives $k(n) = 1,\ 2,\ 5,\ 8,\ 17,\ 29$.

Table 1 collects the explicit form of these conditions up to the sixth order using the basis given in the appendix.

The meaning of Theorem 1 should be clear: it states the number of *necessary* conditions to be satisfied by the kernel coefficients $k_{i,j}$. For each solution of these equations one still has to solve for a_i, b_i in the kernel composition. The theorem by no means ensures that real solutions exist for these coefficients. In some cases, then, one can be forced to take more complicated forms for $\exp(-hK)$ than originally guessed.

Once a kernel with real coefficients satisfying the system of $k(n)$ equations is proposed, we still must fix the corrector to ensure $f_{i,j} = 0$ for $i \le n$. If we denote by $p(n)$ the number of equations to be solved for the processor coefficients, we have $k(n) + p(n) = \sum_{i=2}^{n} c(i)$. Taking into account the previous result, we have $p(2) = 1$ and

$$p(n) = 1 + \sum_{i=2}^{n-1} c(i), \qquad n > 2, \tag{16}$$

which for $n = 3, 4, 5, 6, 7$ gives $p(n) = 2, 4, 7, 13, 21$.

Before presenting some examples of integration methods built along these lines we discuss the simplifications we get in two particular cases: when a more elaborated but symmetric kernel is considered, and when the terms $\mathcal{A}$ and $\mathcal{B}$ of the Hamiltonian have some special properties. A particular simplifying analysis could also be made for slightly perturbed Hamiltonians, $\mathcal{H} = \mathcal{A} + \epsilon\mathcal{B}$, with $\epsilon \ll 1$ [2, 17, 19, 27, 28].

2.3. The case of symmetric kernels. Let us now take a symmetric kernel, (6) or (7). It can be proved that in this case the expansion (8) has

$$k_{2n,i} = 0, \qquad i = 1, 2, \ldots, c(2n). \tag{17}$$

In particular, when the condition $f_{2,1} = 0$ for a second-order method is imposed, this leads to $p_{1,1} = p_{1,2}$ and we are free to choose, for example, $p_{1,1} = p_{1,2} = 0$. With this choice we can specify further the operator P in the processor as follows.

THEOREM 2. *The expansion coefficients for the P operator of the processor of an nth-order symplectic integrator with symmetric kernel must satisfy*

$$p_{2m-1,i} = 0, \qquad i = 1, 2, \ldots, c(2m-1), \qquad m = 2, \ldots, \left[\tfrac{n}{2}\right], \tag{18}$$

provided we choose $p_{1,1} = p_{1,2} = 0$. Here $[x]$ stands for the integer part of x.

The proof proceeds by induction: we have taken $p_{1,1} = p_{1,2} = 0$ and let us assume $p_{2u-1,i} = 0$ for $u < r$. The coefficients $p_{2r-1,i}$ will appear in $f_{m,l}$ for $m \geq 2r$. In (10) for $i = 2r$ and symmetric kernel only odd values of l will contribute to the last sum on the right. But then $\sum_{q,s} q n_{q,s}^{(r)} = 2r - l =$odd and at least one factor $p_{q,s}$ with odd q must appear which makes zero the whole contribution. So finally we are left with

$$f_{2r,j} = \sum_{s=1}^{c(i-1)} \alpha_{j,s} p_{2r-1,s}$$

for $r < \left[\frac{n}{2}\right]$, $j = 1, \ldots, c(2r)$. When conditions $f_{2r,j} = 0$ are imposed to have a symplectic integrator of the required order we get a homogeneous system of $c(2r)$ equations with $c(2r-1)$ unknowns which certainly has the solution $p_{2r-1,l} = 0$. □

The announced simplification for symplectic integrators with symmetric kernels follows from the next theorem.

THEOREM 3. *The number $k(2n)$ of necessary conditions to be satisfied by the kernel generator K of an even order symplectic integrator with processing and a symmetric kernel for $n \geq 2$ satisfies*

$$k(2n) = k(2n-1).$$

To prove this result let us observe that the conditions on the kernel coefficients are independent of the specific form taken for the P operator. Then we can choose without loss of generality $p_{2r+1,i} = 0$, $i = 1, \ldots, c(2r+1)$, for all r. When this is used with a symmetric kernel then only even powers of h will appear in $\mathcal{H}$ in (9). This means that $f_{2r,i}$ vanish identically for $i = 1, \ldots, c(2r)$, and so these coefficients will not count when looking for conditions on the kernel coefficients.

As a consequence of this theorem the number of conditions for the k_{ij} coefficients in a symplectic integrator with symmetric kernel is

$$k(2r+1) = 1 + \sum_{s=2}^{r} \{c(2s+1) - c(2s)\},$$
$$k(2r+2) = k(2r+1),$$

TABLE 2

Conditions to be satisfied by a symmetric kernel up to order 6 for a Hamiltonian $H = \mathcal{A} + \mathcal{B}$. If $[B, B, B, A] = 0$, only the starred conditions survive.

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

which gives $1, 1, 4, 4, 13, 13$ for orders $3, \ldots, 8$. Table 2 collects the only conditions from Table 1 which survive for symmetric kernels.

These results, together with Theorem 2, give extremely simple conditions for the processor coefficients. The only nonzero values are, for methods up to sixth order,

$$p_{2,1} = k_{3,1}, \quad p_{4,1} = k_{5,1}, \quad p_{4,2} = k_{5,4} - \frac{1}{2}k_{3,1}^2, \quad p_{4,3} = k_{5,6}. \tag{19}$$

As is well known [23], a general nonsymmetric scheme can be composed with its backward form to yield a method of at least the same accuracy but requiring one fewer evaluation of the action of each of the two parts of the operator and thus reducing the effective error. If this symmetrization procedure is applied only to the kernel, a new analysis of the processor and kernel conditions could be necessary.

2.4. Hamiltonians with quadratic kinetic energy. There are cases in which, besides e^{-hA} and e^{-hB}, we can also evaluate exactly the action of $e^{-hC_{b,c}}$ with $C_{b,c} = bB + h^2 c[B, A, B]$, b and c being free parameters. This is the case for instance when we deal with nonrelativistic Hamiltonians and A and B are the Lie operators associated, respectively, with the kinetic and potential energy. $C_{b,c}$ is usually referred to as modified potential. Then one can replace in the kernel and processor compositions all e^{-hbB} factors by the more general ones $e^{-hC_{b,c}}$, which allows us to introduce two parameters with only one exponential.

In these cases the actual number $d(n)$ of independent commutators involving n operators one can build with A and B satisfies, for $n > 3$, $d(n) < c(n)$. For example, let C_i denote either A or B operators, and let us assign to C_i an index r_i with values -1 and 1, respectively. Then one can see that $[C_1, C_2, \ldots, C_n]$ will vanish identically as soon as, starting from the right, the sum of r_i adds up to 2. In particular, $[B, B, B, A] = 0$ and the eight first values of $d(n)$ are in principle 2, 1, 2, 2, 4, 5, 10, 15, while the number of conditions for the kernel is considerably reduced: $k(i) = 1, 1, 3, 4, 9, 14$ for $i = 3, \ldots, 8$. Notice that in this particular case Theorem 1 still holds with $d(n)$ replacing $c(n)$, and the starred entries in Table 1 give the equations to be satisfied by the kernel coefficients up to order 6 for this type of Hamiltonian. Furthermore, if a symmetric kernel is used then $k(i) = 1, 1, 3, 3, 8, 8$ for $i = 3, \ldots, 8$. These reductions for the kernel have a counterpart in the processor structure: in (16) one has also to substitute $c(i)$ with $d(i)$ which for $n = 4, 5, 6, 7$ gives $p(n) = 4, 6, 10, 15$.

3. New symplectic integrators with processing. We apply now the analysis of the previous section to the construction of new and efficient symplectic integration algorithms with processing, both in the general $H = \mathcal{A} + \mathcal{B}$ case and when $[B, B, B, A] = 0$ (Runge–Kutta–Nyström or RKN case, for short). For comparison with other well-established efficient symplectic integrators we also report their error

calculated, obviously, in the same basis used in this work. Further details can be found in [1].

In order to present our new methods in as concise a form as possible we designate a method of order n by the label

$$(n : \text{X-}m, s)$$

in which m and s have been introduced in (4)–(7), and X=NS, S, NSRKN, SRKN indicate the nonsymmetric or symmetric character of the kernel both in the general and the RKN case. In the last instance the replacements $y_i B \to C_{y_i,v_i}$, $b_i B \to C_{b_i,c_i}$ have to be made in P and K and the criterion for estimating the computational effort required has to be reformulated. It turns out, however, that for a number of problems the evaluation of $C_{b,c}$ can be done at the cost of at most two independent B evaluations and typically even cheaper because of reuse of certain calculations in the computer [14].

Table 3 below collects the coefficients (with the last a_i and b_i omitted) and effective errors of our new methods. We also include, in parentheses, the effective errors of those unprocessed symplectic algorithms with the best efficiency at each order existing in the literature.

3.1. The general case of $H = A + B$ Hamiltonians.

Fourth order. The shortest symmetric kernel we can use is of the form (6) with $m = 3$. One free parameter is still present for optimization because only the first equation in Table 2 has to be satisfied. For the processor there are $p(4) = 4$ equations to solve. A choice which ensures the existence of real solutions is to take (4) with $s = 3$. The effective error of the best method we found with this processor [1] is $E_f = 0.7959$. Observe that this kernel has the same structure, and then the same computational cost, as the well-known fourth-order method used in [29] with $E_f = 1.3352$. This clearly shows the great improvement one obtains when processing is implemented.

Fifth order. The kernel has to satisfy the five first equations in Table 1, so we propose a composition of eight exponentials and six parameters, i.e., an NS-4 kernel. Again there is a free parameter for optimization purposes. For the processor we have $p(5) = 7$ equations to be satisfied and we consider (4) with $s = 4$. After solving all the equations and searching the solutions that give the minimum error we get the method (5:NS-4,4) given in Table 3.

Sixth order. Again it is advantageous to consider a symmetric kernel, so that only the four equations in Table 2 have to be satisfied. On the other hand we have fourteen equations to be solved for determining the processor. Thus we propose the composition (6:S-5,7). In Table 3 we present the best method we were able to find. The effective error $E_f = 1.8880$ has to be compared with $E_f = 2.1351$ achieved by the symmetric method given by McLachlan [18] with nine evaluations of B.

3.2. Hamiltonians with quadratic kinetic energy.

Fourth order. The simplest symmetric composition that satisfies the single condition for the kernel at this order is

$$e^{-hK} = e^{-\frac{1}{2}hA} e^{-hC_{1,1/24}} e^{-\frac{1}{2}hA}, \tag{20}$$

which has been studied in detail in [2, 13, 14, 22]. For determining the processor it is necessary to solve four equations, so that one possible choice for the method is (4:SRKN-1,2).

TABLE 3
Coefficients and effective errors of the new symplectic integrators with processing.

	$a_1 = -3.068877096032787$	$b_1 = -0.0188$
Order 5	$a_2 = 0.069136863057925$	$b_2 = 0.228020026949214$
	$a_3 = 2.132236793077397$	$b_3 = -0.274397602327546$
(5:NS-4,4)	$z_1 = 0$	$y_1 = -0.831482178617918$
(—)	$z_2 = -0.058741792287332$	$y_2 = 0.869497654626095$
$E_f = 1.4573$	$z_3 = -0.155682248638743$	$y_3 = -0.694638307539625$
	$z_4 = -1.739396727797721$	$y_4 = 0.003491184157440$
	$a_1 = -\frac{2}{5}$	$b_1 = \frac{42+\sqrt{1389}}{84}$
	$c_1 = \frac{26391+868\sqrt{1389}}{933408}$	$c_2 = \frac{26391-868\sqrt{1389}}{933408}$
(5:NSRKN-2,2)	$z_1 = -0.2598277426708327$	$y_1 = -0.6249287013618940$
$(E_f = 0.9840)$	$z_2 = -0.8789034357785656$	$y_2 = 0.0087247119259793$
$E_f \in (0.4577, 0.9154)$	$v_1 = -0.0156990164295207$	$v_2 = -0.0008843356433671$
	$a_1 = 0.528734306841523$	$b_1 = 2.223125692756331$
	$a_2 = -0.227224814678775$	$b_2 = 0.047256775178394$
Order 6	$z_1 = 0.520443768753836$	$y_1 = 0.113599703192743$
	$z_2 = -0.112258504451409$	$y_2 = -0.194068392832917$
(6:S-5,7)	$z_3 = -0.973494161013953$	$y_3 = -0.033895302345452$
$(E_f = 2.1351)$	$z_4 = 0.362347738903427$	$y_4 = 0.303351445876588$
$E_f = 1.8880$	$z_5 = 0.212540146576188$	$y_5 = 0.700101572328687$
	$z_6 = -0.018738314192914$	$y_6 = -1.946137373022707$
	$z_7 = -\sum_{i=1}^{6} z_i$	$y_7 = -\sum_{i=1}^{6} y_i$
	$a_1 = -0.0682610383918630$	$b_1 = 0.2621129352517028$
	$c_1 = 0$	$c_2 = 0.0164011128160783$
	$z_1 = 0.1$	$y_1 = 0.2537166197209512$
	$z_2 = -0.4023008059870294$	$y_2 = 0.0128486628306805$
(6:SRKN-3,5)	$z_3 = -2(z_1 + z_2)$	$y_3 = -y_2$
$(E_f = 1.0345)$	$z_4 = z_2$	$y_4 = -y_1$
$E_f \in (0.7203, 0.9603)$	$z_5 = z_1$	$y_5 = 0$
	$v_1 = -0.0415641538822374$	$v_2 = -0.0098385717021198$
	$v_3 = 0.0108739542111000$	$v_4 = 0.0361124178022208$
	$v_5 = 0$	

With this prescription we get two sets of real solutions for the coefficients in closed form. More specifically, if we denote $s \equiv (1/6)\sqrt{3 + 2\sqrt{3}}$, then

$$\begin{array}{lll} y_1 = \mp\sqrt{3}s, & v_1 = \pm s/24, & z_1 = \pm(1 - \sqrt{3})s, \\ y_2 = 0, & v_2 = 0, & z_2 = \mp s, \end{array} \tag{21}$$

and the effective error is $E_f = 0.2736\ m$.

Fifth order. The kernel must satisfy the first three starred conditions in Table 1. This can be done by the composition NSRKN-2 which in principle could also serve for a sixth-order method, but in this case no real solutions exist. With respect to the processor, $p(5) = 6$ equations must be solved. Thus we propose a (5:NSRKN-2,2) composition and obtain the method given in Table 3. The effective error $E_f \in (0.4577, 0.9154)$, depending on the weight we give to the $C_{b,c}$ evaluations, which is favorably compared with the value 0.9840 obtained by the scheme proposed in [16], with six evaluations of B per step.

Sixth order. With a symmetric kernel only the three starred conditions in Table 2 have to be fulfilled. We consider the composition (6:SRKN-3,5) and the solution we have found is collected in Table 3. The effective error $E_f \in (0.7202, 0.9603)$, in contrast with the value 1.0345 achieved by the best symmetric RKN scheme with $m = 7$ designed by Okunbor and Skeel [21].

4. Optimal processing.

4.1. General considerations. The effective error E_f was defined in section 2.1 as a measure of the efficiency of a symplectic integrator. From the examples of the previous section we see that equations $N_{i,j} = 0$, $i \leq n$, of section 2 are far from uniquely fixing all the coefficients characterizing a method. In this section we systematically study an optimization procedure in order to get for a given kernel the most efficient methods of a prescribed order n. We prove that the kernel itself determines the minimum effective error one can achieve by processing [3]. Even more, this minimum error can be written directly in terms of the functions $N_{n+1,j}$ which would appear in the conditions for the kernel at order $n+1$.

From (13) and (15), the coefficients $p_{n,s}$ which minimize E_r are

$$\mathbf{p}_{(n)} = -\beta^{-1}\alpha^T \left(\mathbf{k}_{(n+1)} + \mathbf{G}(k_{2,1}, \ldots, k_{n,c(n)})\right), \tag{22}$$

where the vector notation

$$\begin{aligned} \mathbf{p}_{(n)} &= (p_{n,1}, \ldots, p_{n,c(n)}), \\ \mathbf{k}_{(n+1)} &= (k_{n+1,1}, \ldots, k_{n+1,c(n+1)}), \\ \mathbf{G} &= (G_1, \ldots, G_{c(n+1)}) \end{aligned} \tag{23}$$

has been used and $\beta = \alpha^T\alpha$. When solution (22) is substituted in (15) we get for the optimal nth-order method

$$\mathbf{f}^{op}_{(n+1)} = (I - \alpha\beta^{-1}\alpha^T)\left(\mathbf{k}_{(n+1)} + \mathbf{G}\right) \tag{24}$$

with $\mathbf{f}^{op}_{(n+1)} \equiv (f^{op}_{n+1,1}, \ldots, f^{op}_{n+1,c(n+1)})$.

It is interesting to remark that, from this equation, the minimum error is entirely determined by the kernel, as we anticipated. We can prove the following theorem.

THEOREM 4. *The coefficients $f^{op}_{n+1,j}$ can be written as a linear combination of the functions $N_{n+1,j}$ which determine the conditions for the kernel at order $n+1$:*

$$f^{op}_{n+1,j} = \sum_{s=1}^{c(n+1)-c(n)} \gamma_{js} N_{n+1,s}, \qquad j = 1, \ldots, c(n+1). \tag{25}$$

We prove this statement for $n = 3$ using the basis given in the appendix. From (24) we can write

$$f^{op}_{4,j} = \mu_{j,3}\ k_{4,3} + \mu_{j,2}\ k_{4,2} + \mu_{j,1}\ k_{4,1} + F(\ k_{2,1},\ k_{3,1}),$$

where condition $N_{3,1} = 0$ has been used to eliminate $k_{3,2}$, F is a polynomial expression, and $\mu_{j,k}$ are numerical coefficients. Taking $N_{4,1}$ from Table 1 we have

$$f^{op}_{4,j} = \mu_{j,3}\ N_{4,1} + Q(\ k_{2,1},\ k_{3,1},\ k_{4,1},\ k_{4,2}),$$

where Q is another polynomial expression. Up to this point $k_{4,j}$ are still completely free parameters. Suppose now we impose the fourth-order kernel condition $N_{4,1} = 0$ and use it to express one of the $k_{4,j}$, say, $k_{4,3}$, in terms of the set $\{k_{2,1},\ k_{3,1},\ k_{4,1},\ k_{4,2}\}$. Then with $\mathbf{p}_{(n)}$ given by (22) we would build a fourth-order method. But this means $f^{op}_{4,j} = 0$. As this has to be true for any choice of

TABLE 4
Optimal coefficients for processing methods up to order 6.

$n=3$	$f^{op}_{4,3}=f^{op}_{4,2}=-f^{op}_{4,1}=\frac{1}{3}N_{4,1}$
$n=4$	$f^{op}_{5,2}=-f^{op}_{5,1}=\frac{1}{2}N_{5,1};\ f^{op}_{5,3}=f^{op}_{5,4}=\frac{1}{2}N_{5,2};\ f^{op}_{5,5}=-f^{op}_{5,6}=\frac{1}{2}N_{5,3}$
$n=5$	$f^{op}_{6,1}=-f^{op}_{6,2}=\frac{1}{1772}\,(227N_{6,1}-99N_{6,2}-411N_{6,3})$ $f^{op}_{6,3}=-f^{op}_{6,5}=\frac{1}{1772}\,(83N_{6,1}-165N_{6,2}-285N_{6,3})$ $f^{op}_{6,4}=\frac{1}{443}\,(52N_{6,1}+50N_{6,2}+221N_{6,3})$ $f^{op}_{6,7}=-f^{op}_{6,6}=\frac{1}{886}\,(-76N_{6,1}+39N_{6,2}+323N_{6,3})$ $f^{op}_{6,9}=-f^{op}_{6,8}=\frac{1}{443}\,(-28N_{6,1}+61N_{6,2}+119N_{6,3})$
$n=6$	$\lvert f^{op}_{7,2j-1}\rvert=\lvert f^{op}_{7,2j}\rvert=\frac{1}{2}\lvert N_{7,j}\rvert \qquad j=1,\ldots,9$

$\{k_{2,1},\ k_{3,1},\ k_{4,1},\ k_{4,2}\}$, we must conclude that $Q(\ k_{2,1},\ k_{3,1},\ k_{4,1},\ k_{4,2})=0$ identically and then $f^{op}_{4,j}=\mu_{j,3}\ N_{4,1}$ which, with $\gamma_{j,1}=\mu_{j,3}$, is (25) we wanted to prove.

The generalization to higher orders is straightforward and basis independent. In the optimized nth order, one has to consider the conditions for the kernel to order $n+1$, $(N_{n+1,s},\ s=1,\ldots,c(n+1)-c(n))$. From these expressions we choose the same number of independent $k_{n+1,j}$ coefficients and repeat the process carried out for the third order.

Observe that the coefficients γ_{js} in (25) can be obtained from the linear term of (24), i.e., from the $c(n+1)\times c(n+1)$ matrix

$$M^{op}\equiv I-\alpha\beta^{-1}\alpha^{T}.$$

Table 4 collects the results for Hamiltonians of the general type $H=\mathcal{A}+\mathcal{B}$ up to order $n=6$.

Notice that case $n=6$ involves $N_{7,j}$ which are not given in Table 1. They have been obtained in the form $N_{7,j}=k_{7,2j}-k_{7,2j-1}+G(k)$, where $G(k)$ is a polynomial expression of $k_{i,j}$ with $i<7$, using the codes of [11].

For the RKN case there is a trivial simplification in third, fourth, and sixth orders. For fifth order we have

$$f^{op}_{6,1}=-f^{op}_{6,2}=\frac{5}{68}N_{6,1};\quad f^{op}_{6,3}=-f^{op}_{6,5}=\frac{-3}{68}N_{6,1};\quad f^{op}_{6,4}=0. \tag{26}$$

4.2. Fourth-order examples. We present here some optimized methods as an illustration of the procedure just discussed. Our strategy for method building will be similar to the one used in section 3, except that now the processor has to be chosen so as to minimize the error. For this to be the case $p^{op}(n)\equiv p(n+1)$ equations have to be satisfied by processor coefficients.

The general case of $H=\mathcal{A}+\mathcal{B}$ Hamiltonians.

(i)*Method* I. We have considered the symmetric kernel S-3 and found the optimal method for $b_1=-0.175$, with effective error $E_f=0.5653$. For the processor, in principle, we have to solve eight equations, but to have a real solution we take a composition (4:S-3,5). One possible set of solutions for the optimized method is given in Table 5.

(ii)*Method* II. To get still better results we have also considered a (4:S-4,4) method. Now, we have two parameters for minimizing the error. We have found different sets of solutions with similar minimum values. One of them is $b_1=0.24$, $b_2=-0.1$ which gives effective error $E_f=0.4041$, improving the corresponding of the previous scheme. The corresponding coefficients can be read from Table 5.

TABLE 5
Coefficients and effective errors of the new optimized fourth-order processing methods.

Order 4	$a_1 = \frac{\sqrt{1646169}-147}{1680}$	$b_1 = -\frac{7}{40}$
	$z_1 = -1.450228208075020$	$y_1 = -0.026109696957887$
(4:S-3,5)	$z_2 = 0.470250210499111$	$y_2 = 0.066841578109894$
$(E_f = 0.6227)$	$z_3 = 1.480280303520878$	$y_3 = 2.989840731091553$
$E_f = 0.5653$	$z_4 = -(z_1 + z_2 + z_3 + z_5)$	$y_4 = -(y_1 + y_2 + y_3)$
	$z_5 = -\frac{1}{2}$	$y_5 = 0$
	$a_1 = \frac{57+\sqrt{18069}}{300}$	$b_1 = \frac{6}{25}$
		$b_2 = -\frac{1}{10}$
	$z_1 = -0.1171835753202670$	$y_1 = -0.5903105192555323$
(4:S-4,4)	$z_2 = 0.8785444960116207$	$y_2 = 0.00137327945651155115$
$(E_f = 0.6227)$	$z_3 = -0.8972532123604465$	$y_3 = 0.3958521503201655$
$E_f = 0.4041$	$z_4 = -(z_1 + z_2 + z_3)$	$y_4 = -(y_1 + y_2 + y_3)$
	$c_1 = \frac{1}{24}$	
	$z_1 = 0$	$y_1 = -0.1859353996846055$
(4:SRKN-1,4)	$z_2 = -0.8749306155955435$	$y_2 = -0.0731969797858114$
$(E_f = 0.4764)$	$z_3 = 0.2371066801510219$	$y_3 = 0.1576624269298081$
$E_f \in (0.1624, 0.3248)$	$z_4 = 0.5363539829039128$	$y_4 = 0$
	$v_i = 0 \quad i = 1, 2, 3, 4$	
	$a_1 = -\frac{1}{10}$	$b_1 = \frac{1}{2} - \sqrt{\frac{133}{132}}$
	$c_1 = c_2 = 0$	
(4:NSRKN-2,4)	$z_1 = 0$	$y_1 = 0.1937696215758170$
$(E_f = 0.4764)$	$z_2 = 0.5349755290809216$	$y_2 = 0.9311511462564267$
$E_f = 0.3467$	$z_3 = -0.3086327690445878$	$y_3 = -0.1053624334726687$
	$z_4 = 0.1428375011411086$	$y_4 = 0$
	$v_i = 0 \quad i = 1, 2, 3, 4$	

These errors should be compared with the value 0.6227 obtained by the best of the symmetric symplectic methods built by McLachlan in [18] (S, $m = 5$).

Hamiltonians with quadratic kinetic energy.

(i) *Kernels with modified potentials.* Let us consider the kernel given by (20), which gives $N_{5,1} = N_{5,2} = 1/1440$ and $E_r = 1/1440$, while the effective error is $E_f \in (0.1624, 0.3248)$. Once completed with the processor we get the (4:SRKN-1,4) method given in Table 5. The resulting scheme is essentially as effective as the method designed in [14] with the S-2 kernel and $c_1 = 0$.

(ii) *Kernels without modified potentials.* It might be useful also to have available some RKN symplectic processed methods which do not consider modified potentials in the composition. As an example we give in Table 5 a (4:NSRKN-2,4) method which has $E_f = 0.3467$. It improves the best of the RKN symplectic methods without modified potentials, built by Calvo and Sanz-Serna in [7] with $E_f = 0.4764$.

5. Numerical examples. We illustrate the practical performance of some of the above processing methods and error calculations with some brief examples. As usual we check the degree of exactness in the preservation of the energy and the pointwise accuracy in the determination of the trajectory.

Example 1. The one-dimensional generalized harmonic oscillator is perhaps one of the simplest examples of a Hamiltonian system that can be separated, in different ways, into two nontrivial pieces, $H = \mathcal{A} + \mathcal{B}$, with the flows corresponding to $\mathcal{A}$ and to $\mathcal{B}$ explicitly and exactly computable. In addition, the exact time evolution of H is also at hand, so comparison with the approximate solution obtained by the different

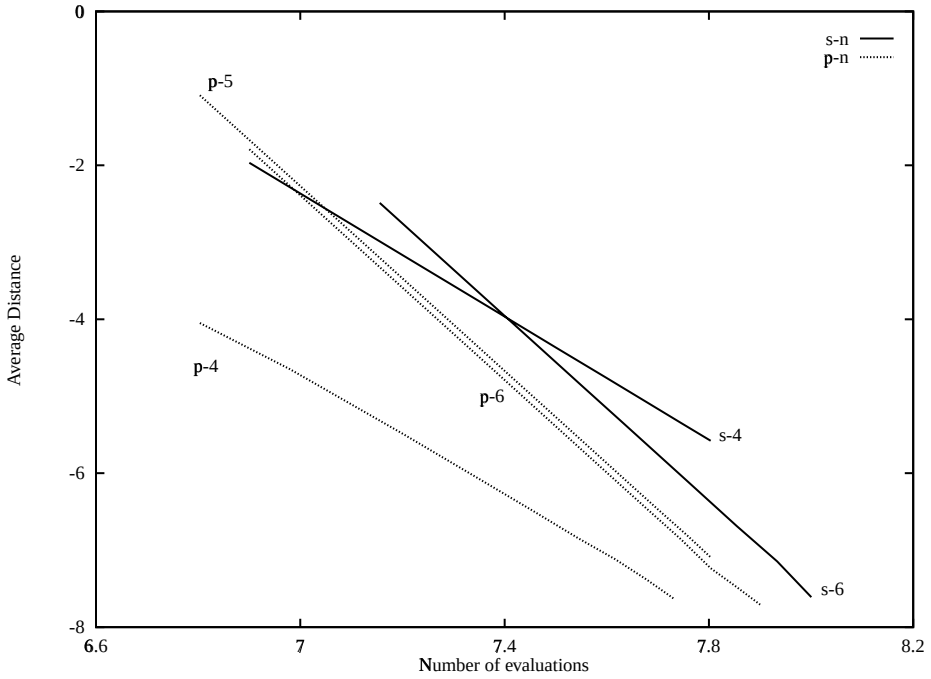

FIG. 1. *Average distance between exact and numerical trajectories vs. number of B evaluations for the generalized harmonic oscillator with $\lambda = 0.9$. Solid lines denoted by* s-n *correspond to standard (unprocessed) symplectic integrators of order n and dashed lines stand for the new nth-order symplectic schemes with processing* (p-n)*, respectively.*

numerical algorithms is possible.

If we take

$$\mathcal{A} = \frac{1}{2}(p^2 + q^2), \qquad \mathcal{B} = \lambda(pq + q^2), \tag{27}$$

then all the elements $E_{i,j}$ of our basis are nonvanishing and thus we test our methods in a nontrivial case. We choose $\lambda = 0.9$ and determine numerically the periodic trajectory with initial conditions $q_0 = p_0 = 1$ (energy $E = 2.8$) for a large number of periods (39,741) and compute the mean error in the Euclidean distance in phase space between the exact and the approximate solutions.

Figure 1 shows this average distance in terms of the number of evaluations of B. Solid lines denoted by s-n correspond to the fourth- (S, $m = 5$) and sixth- (SS, $m = 9$) order symmetric methods given by McLachlan [18] (effective errors given in Table 3), whereas dashed lines p-n stand for processing schemes (4:S-4,4), (5:NS-4,4), and (6:S-5,7) of Tables 3 and 5. It is worth noting the superiority of the processing algorithms over the standard symplectic compositions. The processing method (5:NS-4,4) performs as a sixth-order integrator due to the influence on the global error of higher order terms for the time steps used. On the other hand, the optimized fourth-order processing scheme works significantly better even than the other processing methods considered for this example. This outstanding improvement encourages the construction of optimized higher order methods by following a similar procedure.

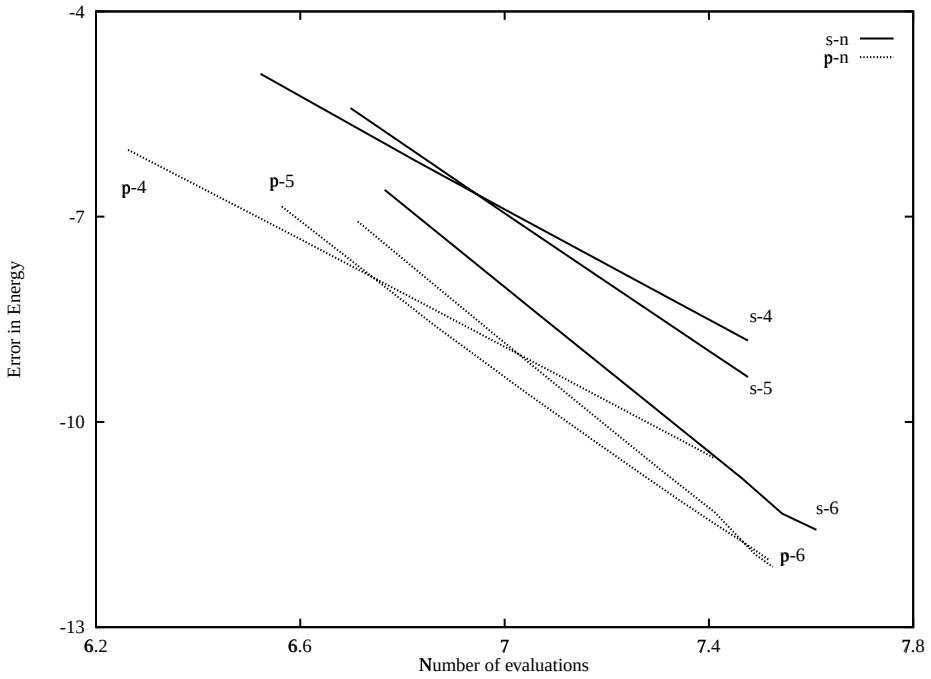

FIG. 2. *Relative error in energy vs. number of B evaluations for the Hénon-Heiles Hamiltonian with $E = 0.1$. For this example one evaluation of $C_{b,c}$ is approximately equivalent to 1.1 evaluations of B. The codes are similar to those used in Figure 1.*

Example 2. Next we consider the well-known Hénon–Heiles Hamiltonian [9]

$$H(\mathbf{q},\mathbf{p}) = \frac{1}{2}(p_1^2 + p_2^2) + \frac{1}{2}(q_1^2 + q_2^2) + q_1^2 q_2 - \frac{1}{3}q_2^3 \tag{28}$$

with energy $E = 0.1$ and integrate the trajectory with initial conditions ($q_1 = 0$, $q_2 = -0.36$, $p_1 > 0$, $p_2 = 0.12$) up to a final time $t_f = 2.95 \times 10^5$. The mean relative errors in the energy are shown in Figure 2 as a function of the number of B evaluations. This number is determined by considering that, on average, 1 evaluation of $C_{b,c}$ is approximately equivalent to 1.1 evaluations of B [2]. The processing methods considered are the (5:NSRKN-2,2) and (6:SRKN-3,5), together with the optimized (4:SRKN-1,4) schemes.

Observe the large advantage of the new processing schemes over the standard RKN symplectic integrators whose effective errors are given in Tables 3 and 5. This improvement is particularly noticeable for our optimized fourth-order method. Concerning the fifth-order processing algorithm, it behaves as a sixth-order method for $h > 0.03$ because seventh-order terms $f_{7,j}$ dominate the leading error terms $f_{6,j}$ (at least by a factor 2).

Figure 3 displays the same results as Figure 2 but now considers the more conservative estimation that one $C_{b,c}$ evaluation is equivalent to at most two independent B evaluations. Even in this case the processing methods perform better than the standard ones. The results attained by the optimized fourth-order schemes with and without modified potential (not shown in the figure) are very similar in this situation.

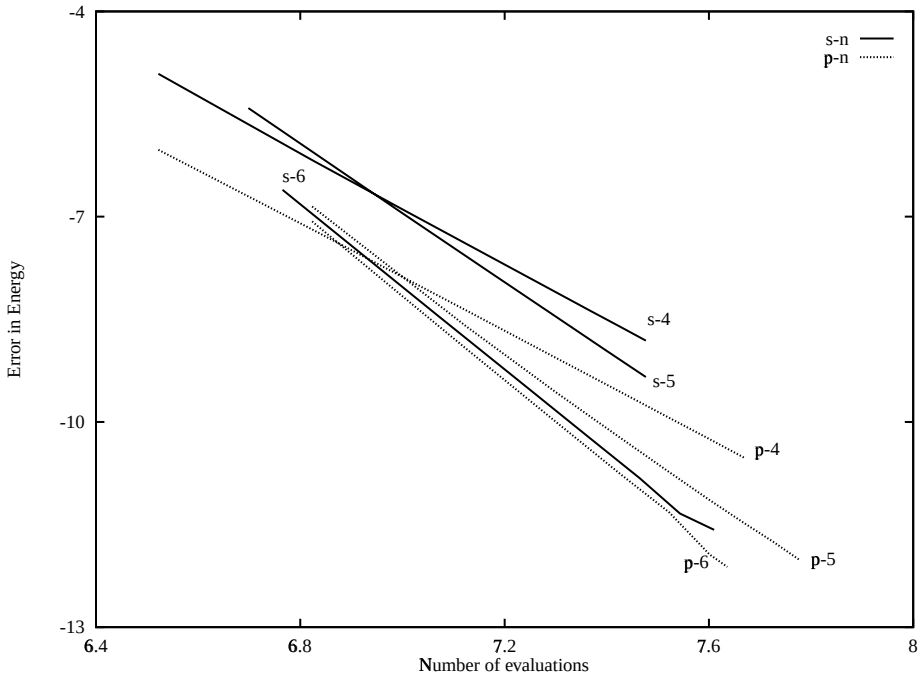

FIG. 3. *Same as Figure 2 if we consider that one evaluation of $C_{b,c}$ is equivalent to two independent B evaluations.*

6. Conclusions. In this paper we have analyzed the processing technique to obtain symplectic integrators for Hamiltonians which can be split into two exactly solvable parts, $H = \mathcal{A} + \mathcal{B}$. We have determined the number of equations to be satisfied by a kernel to build an algorithm of order n. These conditions have been explicitly written up to sixth order. When symmetric kernels are used or when $\mathcal{A}$ and $\mathcal{B}$ satisfy specific algebraic relations the number of conditions is lowered. Our results are summarized in the following table:

Kernel	$n=3$	$n=4$	$n=5$	$n=6$	$n=7$	$n=8$
General	1	2	5	8	17	29
Symmetric	1	1	4	4	13	13
RKN	1	1	3	4	9	14
RKN, symm.	1	1	3	3	8	8

Following this approach we have presented actual realizations of several symplectic integrators up to sixth order which have better efficiency than alternative symplectic methods found in recent literature. It is important to observe that in general this improvement is obtained by the reduction in the number of evaluations of the kernel operator.

We have also presented an optimization procedure which leads directly to the minimum error one can get in terms of the kernel coefficients. This fact can give further momentum to the construction of higher order optimized integrators with processing [4].

In order to give further evidence for these conclusions two Hamiltonian systems have been treated by our methods as test-bench. The comparison with other ap-

proaches confirms the better performance of our processed integrators, as theoretically expected.

Appendix. Lie algebra elements.

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

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

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