New Families of Symplectic Runge–Kutta–Nyström Integration Methods

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Abstract. We present new 6-th and 8-th order explicit symplectic Runge–Kutta–Nyström methods for Hamiltonian systems which are more efficient than other previously known algorithms. The methods use the processing technique and non-trivial flows associated with different elements of the Lie algebra involved in the problem. Both the processor and the kernel are compositions of explicitly computable maps.

1 Introduction

In Hamiltonian dynamics, a frequent special case occurs when the Hamiltonian function reads

$$H(\mathbf{q},\mathbf{p}) = \frac{1}{2}\mathbf{p}^T M^{-1}\mathbf{p} + V(\mathbf{q}) \ , \tag{1}$$

with M a constant, symmetric, invertible matrix. In this situation the equations of motion are

$$\dot{\mathbf{q}} = M^{-1}\mathbf{p} \ , \qquad \dot{\mathbf{p}} = -\nabla_{\mathbf{q}} V(\mathbf{q}) \tag{2}$$

or, after elimination of $\mathbf{p}$,

$$\ddot{\mathbf{q}} = -M^{-1}\nabla_{\mathbf{q}} V(\mathbf{q}) \ . \tag{3}$$

It is therefore natural to consider Runge–Kutta–Nyström (RKN) methods when the second order system (3) has to be solved numerically. These methods can be rendered symplectic, thus preserving qualitative features of the phase space of the original Hamiltonian dynamical system. In fact, a number of symplectic RKN schemes of order ≤ 4 have been designed during the last decade which outperform standard non-symplectic methods (see [9] for a review), and the recent literature has devoted much attention to the integration of (1) by means of efficient high-order symplectic algorithms [5,6,8,11]. The usual approach is to compose a number of times the exact flows corresponding to the kinetic and potential energy in (1) with appropriately chosen weights to achieve the desired order. More specifically, if A and B denote the Lie operators

$$A = M^{-1}\mathbf{p}\nabla_{\mathbf{q}} \ , \qquad B = -(\nabla_{\mathbf{q}} V)\nabla_{\mathbf{p}} \tag{4}$$

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associated with $\frac{1}{2}\mathbf{p}^T M^{-1}\mathbf{p}$ and $V(\mathbf{q})$, respectively [1], then the exact solution of (2) can be written as

$$\mathbf{z}(t) = e^{t(A+B)}\mathbf{z}(0) \equiv e^{t(A+B)}\mathbf{z}_0 \ ,$$

where $\mathbf{z} = (\mathbf{q}, \mathbf{p})^T$, and the evolution operator $e^{t(A+B)}$ for one time step $h = t/N$ is approximated by

$$e^{h(A+B)} \simeq e^{hH_\mathrm{a}} \equiv \prod_{i=1}^{s} e^{ha_i A} e^{hb_i B} \tag{5}$$

with

$$\begin{aligned} e^{haA}\mathbf{z}_0 &= (\mathbf{q}_0 + haM^{-1}\mathbf{p}_0,\ \mathbf{p}_0)^T \\ e^{hbB}\mathbf{z}_0 &= (\mathbf{q}_0,\ \mathbf{p}_0 - hb\nabla_{\mathbf{q}} V(\mathbf{q}_0))^T \ . \end{aligned} \tag{6}$$

Observe that the approximate solution $\mathbf{z}_\mathrm{a}(t) = e^{tH_\mathrm{a}}\mathbf{z}_0$ evolves in the Lie group whose Lie algebra $L(A, B)$ is generated by A and B with the usual Lie bracket of vector fields [1].

The coefficients a_i, b_i in (5) are determined by imposing that

$$H_\mathrm{a} = A + B + \mathcal{O}(h^n) \tag{7}$$

to obtain an n-th order symplectic integration method. This makes necessary to solve a system of polynomial equations, which can be extraordinarily involved even for moderate values of n, so that various symmetries are usually imposed in (5) to reduce the number of determining equations. For instance, if the composition is left-right symmetric then H_a does not contain odd powers of h, but then the number of flows to be composed increases. Although additional simplifications also take place due to the vanishing of the Lie bracket $[B, [B, [B, A]]]$ for the Hamiltonian (1), the question of the existence of high-order RKN symplectic integrators more efficient than standard schemes is still open.

Recently, the use of the processing technique has allowed to develop extremely efficient methods of orders 4 and 6 [2]. The idea is to consider the composition

$$e^{h\mathcal{H}(h)} = e^P e^{hK} e^{-P} \tag{8}$$

in order to reduce the number of evaluations: after N steps we have $e^{t(A+B)} \simeq e^{t\mathcal{H}(h)} = e^P (e^{hK})^N e^{-P}$. At first e^P (the processor) is applied, then e^{hK} (the kernel) acts once per step, and finally e^{-P} is evaluated only when output is needed. Both the kernel and the processor are taken as composition of flows corresponding to A and B, in a similar way to (5).

In this paper, by combining the processing technique with the use of non-trivial flows associated with different elements of $L(A, B)$ we obtain optimal 6-th order RKN methods more efficient than others previously known and some 8-th order symplectic schemes with less function evaluations per step. The analysis can also be easily extended to a more general class of second order differential equations.

2 Analysis and New Methods

In addition to A and B there are other elements in $L(A,B)$ whose flow is explicitly and exactly computable. In particular, the flow corresponding to the operators

$$V_{3,1} \equiv [B,[A,B]] \qquad V_{5,1} \equiv [B,[B,[A,[A,B]]]] \tag{9}$$
$$V_{7,1} \equiv [B,[A,[B,[B,[A,[A,B]]]]]] \qquad V_{7,2} \equiv [B,[B,[B,[A,[A,[A,B]]]]]]$$

has an expression similar to the second equation of (6) by replacing $\nabla_{\mathbf{q}} V$ with an appropriate function $\mathbf{g}(\mathbf{q})$ [3]. Therefore it is possible to evaluate exactly $\exp(hC_{b,c,d,e,f})$, with

$$C_{b,c,d,e,f} = bB + h^2 c\, V_{3,1} + h^4 d\, V_{5,1} + h^6 (eV_{7,1} + fV_{7,2}) \ , \tag{10}$$

b, c, d, e, and f being free parameters. We can then substitute some of the $e^{hb_i B}$ factors by the more general ones $e^{hC_{b_i,c_i,d_i,e_i,f_i}}$ both in the kernel and the processor in order to reduce the number of evaluations and thus improve the overall efficiency. The operator $C_{b,c,d,e,f}$ will be referred in the sequel as modified potential, and we simply write $C_{b,c}$ when $d = e = f = 0$.

By repeated application of the Baker-Campbell-Hausdorff formula [10] the kernel and processor generators K and P can be written as

$$K = A + B + \sum_{i=2}^{\infty} \left\{ h^{i-1} \sum_{j=1}^{d(i)} k_{i,j} E_{i,j} \right\}, \qquad P = \sum_{i=1}^{\infty} \left\{ h^{i} \sum_{j=1}^{d(i)} p_{i,j} E_{i,j} \right\}, \tag{11}$$

where $d(m)$ denote the dimension of the space spanned by brackets of order m of A and B (its first 8 values being 2,1,2,2,4,5,10,15) and $\{E_{m,j}\}_{j=1}^{d(m)}$ is a basis of this space. Therefore

$$\mathcal{H}(h) = e^P K e^{-P} = A + B + \sum_{i=2}^{\infty} \left\{ h^{i-1} \sum_{j=1}^{d(i)} f_{i,j} E_{i,j} \right\}, \tag{12}$$

where the $f_{i,j}$ coefficients are given in terms of polynomials involving $k_{i,j}$ and $p_{i,j}$ [2]. Specific n-th order integration methods require that $f_{i,j} = 0$ up to $i = n$, and these equations impose restrictions to the kernel: it must satisfy $k(n) = d(n) - 1$ independent conditions ($n \geq 2$) [2], and $k(2n) = k(2n-1)$ if it is a symmetric composition. The explicit form of these conditions and the coefficients $p_{i,j}$ of the processor P in terms of $k_{i,j}$ up to order 8 have been obtained in [3]. It has also been shown that the kernel completely determines the optimal method we can obtain by processing [2]. Here optimal means that the main term of the local truncation error attains a minimum.

As stated above, we take as processor of a RKN method the explicitly computable composition

$$e^P = \prod_{i=1}^{r} e^{hz_i A} e^{hy_i B} \ , \tag{13}$$

where the replacement $\exp(hy_iB) \longmapsto \exp(hC_{y_i,v_i,\ldots})$ can be done when necessary, and the number r of B (or C) evaluations is chosen to guarantee that the $\sum_{i=1}^{n-1} d(i)$ equations $p_{i,j} = p_{i,j}(z_k, y_k)$ have real solutions.

As far as the kernel is concerned, due to the different character of the operators A and B, two types of symmetric compositions have been analyzed:

(i) Type ABA: $\left(\sum_{i=1}^{s+1} a_i = \sum_{i=1}^{s} b_i = 1\right)$

$$e^{hK} = e^{ha_1A} e^{hb_1B} e^{ha_2A} \cdots e^{ha_sA} e^{hb_sB} e^{ha_{s+1}A} \tag{14}$$

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

(ii) Type BAB: $\left(\sum_{i=1}^{s} a_i = \sum_{i=1}^{s+1} b_i = 1\right)$

$$e^{hK} = e^{hb_1B} e^{ha_1A} e^{hb_2B} \cdots e^{hb_sB} e^{ha_sA} e^{hb_{s+1}B} \tag{15}$$

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

A systematic analysis of the 6-th order case has been afforded in [3], where a number of optimal processed methods with modified potentials and $s = 2, 3$ were obtained. There also some methods involving only A and B evaluations with $s = 4, 5, 6$ were also reported, with their corresponding truncation error. Here we have generalized the study to seven stages ($s = 7$). Now the three free parameters allow to find an extremely efficient 6-th order processed method: it has error coefficients which are approximately 50 times smaller than the corresponding to the most efficient 6-th order symplectic non-processed RKN method with $s = 7$ given in [8]. In Table 1 we collect the coefficients of this new processed method and also of the most efficient 6-th order algorithm we have found involving the modified potential $C_{b,c,0,e,f}$ in the kernel and $C_{y,v}$ in the processor.

A similar study can be carried out, in principle, for the 8-th order case, although now the number of possibilities (and solutions) increases appreciably with respect to $n = 6$, so that the analysis becomes extaordinarily intricate. Here we have considered kernels with $s = 4, 5$ involving modified potentials and $s = 9, 10, 11$ when only A and B evaluations are incorporated. Taking into account the well known fact that methods with small coefficients have been shown to be very efficient [6], we apply this strategy for locating possible kernels. The coefficients of two of them are given in Table 1, although many others are available.

On the other hand, the coefficients z_k, y_k in the processor (13) have to satisfy 26 equations, but this number can be reduced by taking different types of compositions. For instance, if the coefficients in $e^Q = \prod_i e^{hz_iA} e^{hy_iB}$ are determined in such a way that $Q(h) = \frac{1}{2}P(h) + O(h^7)$, then $e^{Q(h)} e^{Q(-h)} = e^{P(h)} + O(h^8)$ because $P(h)$ is an even function of h up to order h^8. Then, only 16 equations are involved. Here also the criterium we follow is to choose the smallest coefficients z_k, y_k of $e^{Q(h)}$.

Table 1. Coefficients of the new symplectic RKN integrators with processing

Order 6; Type BAB; $s = 7$; $r = 8$		
$b_1 = 0.115899400930169$	$b_2 = -1.21532440212000$	$b_3 = 1.45706208067905$
$a_1 = 0.244868573793901$	$a_2 = -0.00214552789272415$	$a_3 = 0.301340867944477$
$z_1 = -0.350316247513416$	$z_2 = 0.0744434640156453$	$z_3 = -0.0369370026731913$
$z_4 = -0.0597184197245884$	$z_5 = 0.404915108936223$	$z_6 = -0.180941427380936$
$z_7 = -0.0346188279494959$	$z_8 = -\sum_{i=1}^{7} z_i$	
$y_1 = 0.218575120792731$	$y_2 = -0.370670464937763$	$y_3 = 0.342037685653768$
$y_4 = -0.225359207496863$	$y_5 = 0.0878524557495559$	$y_6 = 0.195239165175742$
$y_7 = -0.155222704734044$	$y_8 = -\sum_{i=1}^{7} y_i$	

Order 6; Type ABA; $s = 3$; $r = 6$; Modified potential		
$a_1 = -0.0682610383918630$	$b_1 = 0.2621129352517028$	$c_1 = d_1 = e_1 = f_1 = 0$
	$c_2 = 0.0164011128160783$	$d_2 = 0$
	$e_2 = 1.86194612413481 \cdot 10^{-5}$	$f_2 = -6.3155794861591 \cdot 10^{-6}$
$z_1 = 0.1604630501234888$	$y_1 = -0.012334538446142270$	$v_1 = 0.013816178183636998$
$z_2 = -0.1222126706298830$	$y_2 = -0.6610294848488182$	$v_2 = -0.050288359617427786$
$z_3 = 0.1916801124727711$	$y_3 = -0.023112349678219939$	$v_3 = -0.013462400168471472$
$z_4 = 0.5630722377955035$	$y_4 = 1.81521815949959 \cdot 10^{-4}$	$v_4 = 6.03819193361427 \cdot 10^{-4}$
$z_5 = -0.7612758792358986$	$y_5 = 2.3768244683666757$	$v_5 = -0.01$
$z_6 = -\sum_{i=1}^{5} z_i$	$y_6 = -\sum_{i=1}^{5} y_i$	$v_6 = 0.01$

Order 8; Type BAB; $s = 11$; $r = 8$		
$b_1 = 0.03906544126305366$	$b_2 = 0.216015988434324$	$b_3 = -0.126717696299036$
$b_4 = -0.04128542496526060$	$b_5 = 0.04458478096712717$	
$a_1 = 0.142940453575212$	$a_2 = 0.309791505162032$	$a_3 = 0.301210185530089$
$a_4 = -0.005822573683400349$	$a_5 = -0.344741324170165$	
$z_1 = -0.0295940574778285$	$z_2 = 0.0102454583206065$	$z_3 = 0.168519324003820$
$z_4 = -0.577391651425342$	$z_5 = 0.0991834279391326$	$z_6 = 0.0203810695211463$
$z_7 = -0.106234446989598$	$z_8 = -\sum_{i=1}^{7} z_i$	
$y_1 = 0.175492972679660$	$y_2 = -0.372698829093994$	$y_3 = -0.00224032125918971$
$y_4 = 0.0926169248899539$	$y_5 = -0.201446308655374$	$y_6 = 0.216983390044259$
$y_7 = -0.0918456713646654$	$y_8 = -\sum_{i=1}^{7} y_i$	

Order 8; Type BAB; $s = 5$; $r = 7$; Modified potential		
$d_1 = 0.0001219127419188233$		
$e_1 = 5.741889879702246 \cdot 10^{-6}$	$f_1 = -2.271708973531348 \cdot 10^{-6}$	
$b_2 = -0.1945897221635392$	$c_2 = 5.222572249380952 \cdot 10^{-4}$	
$a_1 = 0.6954511641703808$	$a_2 = -0.05$	
$z_1 = 0$	$y_1 = 0.3644761259072299$	$v_1 = 0.016298916362212911$
$z_2 = -0.004624860718237988$	$y_2 = -0.2849544383272169$	$v_2 = -0.019769812343547362$
$z_3 = 0.3423219445639433$	$y_3 = 0.2023898776842639$	$v_3 = 0.004608026684270971$
$z_4 = 0.1760176996772205$	$y_4 = -0.2743578195701579$	$v_4 = 0$
$z_5 = 0.3625045293826689$	$y_5 = -4.75975395524748 \cdot 10^{-3}$	$v_5 = 0$
$z_6 = -0.2729727321466362$	$y_6 = 0.1455974775779454$	$v_6 = 0$
$z_7 = -\sum_{i=1}^{6} z_i$	$y_7 = -\sum_{i=1}^{6} y_i$	$v_7 = 0$

3 A Numerical Example

To test in practice the efficiency of these new symplectic methods, we compare them with other schemes of similar consistency on a specific example. For order 6, these are the most efficient seven stage method designed by Okunbor and Skeel, OS6 [8], and the non-symplectic variable step RKN method, DP6, obtained in [4]. Concerning the 8-th order, we compare with the symplectic integrator due to Yoshida [11] (Yos8, 15 function evaluations per step), the method obtained by

McLachlan [6] (McL8, 17 stages) and the optimized symmetric scheme designed by Calvo and Sanz-Serna [5] (CSS8, 24 evaluations).

The example we consider is the perturbed Kepler Hamiltonian

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

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 planet. The motion takes place in a plane containing the symmetry axis of the planet [7].

We take $\varepsilon = 0.001$, which approximately corresponds to a satellite moving under the influence of the Earth, and initial conditions $x = 1 - e$, $y = 0$, $p_x = 0$, $p_y = \sqrt{(1+e)/(1-e)}$, with $e = 0.5$. We integrate the trajectory up to the final time $t_f = 1000\pi$ and then compute the error in energy, which is represented (in a log-log scale) as a function of the number of B evaluations.

Obviously, the computational cost of evaluating the modified potential must be estimated. This has been done by running the same program repeatedly with different types of modified potential and only with the evaluation of B. We observe that, for this problem, an algorithm using $C_{b,c,d,e,f}$ is twice as expensive as the same algorithm involving B evaluations, and only a 20% more computationally costly when $C_{b,c}$ are involved. This is so due to the reuse of certain calculations in the modified potentials.

With this estimate, we present in Fig. 1(a) the results obtained with the 6-th order processed methods of Table 1, in comparison with DP6 and OS6, whereas the relative performance of the 8-th order symplectic schemes is shown in Fig. 1(b). Solid lines denoted by pm$k$ and pk, $k = 6, 8$, are obtained by the new methods with and without modified potentials, respectively.

It is worth noticing the great performance of the symplectic processed schemes of Table 1 with respect to other standard symplectic and non-symplectic algorithms. This is particularly notorious in the case of the 6-th order integrators, due to the fact that a full optimization strategy has been carried out in the construction process. In the case of order 8, the new methods are also more efficient than other previously known symplectic schemes, although only a partial optimization has been applied. In this sense, there is still room for further improvement.

Finally, we should mention that the results achieved by p8 are up to two orders of magnitude better than those provided by McL8 for other examples we have tested. These include the simple pendulum, the Gaussian and the Hénon-Heiles potentials.

4 Final Comments

Although in the preceding treatment we have been concerned only with Hamiltonian systems, it is clear that essentially similar considerations apply to second

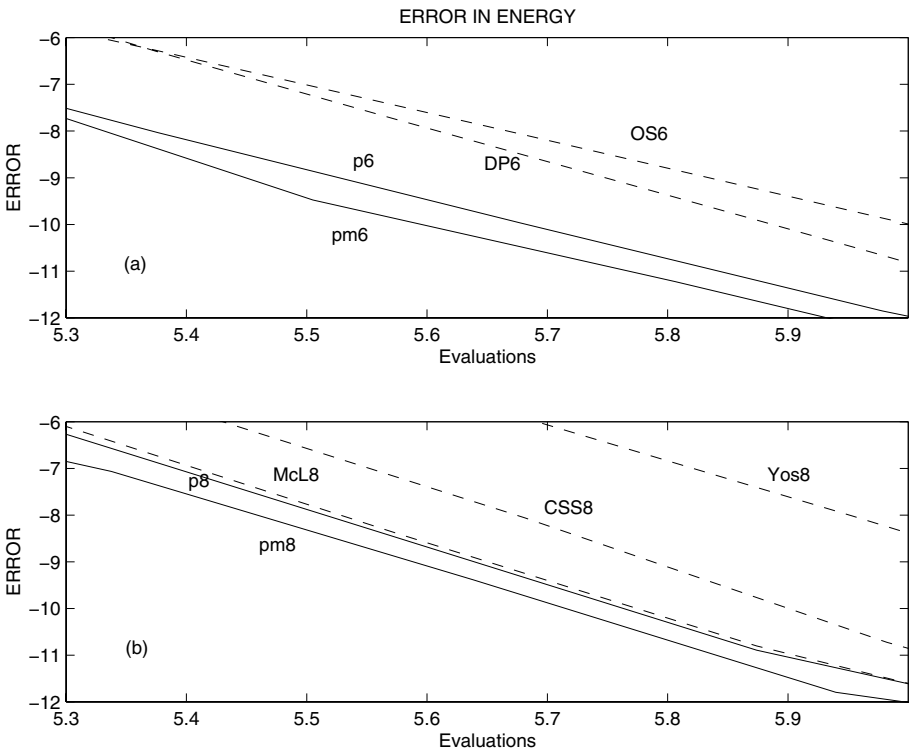

Fig. 1. Average errors in energy vs. number of evaluations for the sixth (a) and eighth (b) order processed symplectic RKN methods

order systems of ODE of the form

$$\ddot{\mathbf{x}} = \mathbf{f}(\mathbf{x}), \qquad \mathbf{x} \in \mathbb{R}^l, \qquad \mathbf{f} : \mathbb{R}^l \longrightarrow \mathbb{R}^l \tag{17}$$

when it is required that some qualitative or geometric property of (17) be preserved in the numerical discretization. In fact, introducing the new variables $\mathbf{z} = (\mathbf{x}, \mathbf{v})^T$, with $\mathbf{v} = \dot{\mathbf{x}}$, and the functions $\mathbf{f}_A = (\mathbf{v}, \mathbf{0})$, $\mathbf{f}_B = (\mathbf{0}, \mathbf{f}(\mathbf{x})) \in \mathbb{R}^{2l}$, we have

$$\dot{\mathbf{z}} = \mathbf{f}_A + \mathbf{f}_B, \tag{18}$$

with the systems $\dot{\mathbf{z}} = \mathbf{f}_A$ and $\dot{\mathbf{z}} = \mathbf{f}_B$ explicitly integrable in closed form. In this case the Lie operators A, B are given by

$$A = \mathbf{v} \cdot \nabla_{\mathbf{x}} \ , \qquad B = \mathbf{f}(\mathbf{x}) \cdot \nabla_{\mathbf{v}} \tag{19}$$

and the methods of Table 1 can be directly applied for carrying out the numerical integration. This is so even for the physically relevant class of time-dependent non-linear oscillators of the form

$$\ddot{\mathbf{x}} + \delta\, \dot{\mathbf{x}} + \mathbf{f}_1(\mathbf{x}) = \mathbf{f}_2(t) \ . \tag{20}$$

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References

1. V. I. Arnold, *Mathematical Methods of Classical Mechanics*, 2nd Ed., Springer, New York, 1989. 103
2. S. Blanes, F. Casas, and J. Ros, *Symplectic integrators with processing: a general study,* SIAM J. Sci. Comput., 21 (1999), pp. 711-727. 103, 104
3. S. Blanes, F. Casas, and J. Ros, *High–order Runge–Kutta–Nyström geometric methods with processing*, to appear. 104, 105
4. R. W. Brankin, I. Gladwell, J. R. Dormand, P. J. Prince, and W. L. Seward, *Algorithm 670. A Runge-Kutta-Nyström code*, ACM Trans. Math. Softw., 15 (1989), pp. 31-40. 106
5. M. P. Calvo and J. M. Sanz-Serna, *High-order symplectic Runge-Kutta-Nyström methods*, SIAM J. Sci. Comput., 14 (1993), pp. 1237-1252. 102, 107
6. R. I. McLachlan, *On the numerical integration of ordinary differential equations by symmetric composition methods*, SIAM J. Sci. Comput., 16 (1995), pp. 151-168. 102, 105, 107
7. L. Meirovich, *Methods of Analytical Dynamics*, McGraw-Hill, New York, 1988. 107
8. D. I. Okunbor and R. D. Skeel, *Canonical Runge-Kutta-Nyström methods of orders five and six*, J. Comp. Appl. Math., 51 (1994), pp. 375-382. 102, 105, 106
9. J. M. Sanz-Serna and M. P. Calvo, *Numerical Hamiltonian Problems,* Chapman & Hall, London, 1994. 102
10. V. S. Varadarajan, *Lie Groups, Lie Algebras, and Their Representations*, Springer-Verlag, New York, 1984. 104
11. H. Yoshida, *Construction of higher order symplectic integrators*, Phys. Lett. A, 150 (1990), pp. 262-269. 102, 106