High order symplectic integrators for perturbed Hamiltonian systems

Jacques Laskar and Philippe Robutel
Astronomie et Systèmes Dynamiques,
IMC-CNRS UMR8028,
77 Av Denfert-Rochereau, 75014 Paris

submitted, April 27, 2000; *revised,* November, 21, 2000

Abstract. A family of symplectic integrators adapted for the integration of perturbed Hamiltonian systems of the form $H = A + \varepsilon B$ was given in (McLachlan, 1995). We give here a constructive proof that for all integer p, such integrator exists, with only positive steps, and with a remainder of order $O(\tau^p\varepsilon+\tau^2\varepsilon^2)$, where τ is the stepsize of the integrator. Moreover, we compute the analytical expressions of the leading terms of the remainders at all orders. We show also that for a large class of systems, a corrector step can be performed such that the remainder becomes $O(\tau^p\varepsilon + \tau^4\varepsilon^2)$. The performances of these integrators are compared for the simple pendulum and the planetary 3-Body problem of Sun-Jupiter-Saturn.

Keywords: symplectic integrators, Hamiltonian systems, planetary motion, Lie algebra

1. Introduction

Symplectic integrators, due to their good stability properties are now currently used for long time integrations of the Solar System, starting with the work of Wisdom and Holman (1991). Despite some improvement resulting from a good choice of initial conditions (Saha and Tremaine, 1992) or the addition of a corrector to the output of the numerical integration (Wisdom *et al.*, 1996), it is surprising that the integration method which is currently used in most computations (see Duncan *et al.*, 1998) is the celebrated 'leapfrog' method of order 2 (Ruth, 1983). A reason for this choice is probably due to the fact that the methods of higher order which have been found by Forest and Ruth (1990) or Yoshida (1990) do not present very good stability properties for large stepsize, due to the presence of negative steps.

In the present work, we consider perturbed Hamiltonians on the form $H = A+\varepsilon B$ were both A and B are integrable. For such Hamiltonians, (McLachan, 1995) proposed a family of of symplectic integrators with positive steps, but the generality of his demonstration, made on a simple example is not obvious. In the present work, we use a constructive approach to demonstrate the existence at all orders of this family of symplectic integrators. Moreover, our explicit derivation allows us to compute the first terms of the remainders at all orders and to derive, for a large class of systems, a new set of symplectic integrators with a corrector step which improves even more the precision of the integrators (sections 9–10). These two families improve the precision of the integration by several orders of magnitude with respect to the commonly used leapfrog method, and present good stability properties at large stepsizes.

2. Lie formalism

According to Yoshida, (1990), the search of symplectic integrators using Lie formalism was introduced by Neri (1988). Since then, it was largely developed by Yoshida (1990), Suzuki (1991, 1992), Koseleff (1993, 1996), and Mclachlan (1995, 1998). Let $H(p,q)$ be an Hamiltonian defined on $\mathbb{R}^n \times \mathbb{T}^n$, where (p,q) are the actions and angle-like variables. Hamilton equations are

$$\frac{dp_j}{dt} = -\frac{\partial H}{\partial q_j} \; ; \quad \frac{dq_j}{dt} = \frac{\partial H}{\partial p_j} \tag{1}$$

and the Poisson bracket of f, g is defined on $\mathbb{R}^n \times \mathbb{T}^n$ by

$$\{f,g\} = \sum_j \frac{\partial f}{\partial p_j}\frac{\partial g}{\partial q_j} - \frac{\partial f}{\partial q_j}\frac{\partial g}{\partial p_j} \tag{2}$$

If we denote $x = (p,q)$, we obtain

$$\frac{dx}{dt} = \{H, x\} = L_H x \ . \tag{3}$$

where L_H is the differential operator defined by $L_\chi \ f = \{\chi, f\}$. The solution $x(t)$ of (3) with $x(0) = x_0$ is obtained formally as

$$x(t) = \sum_{n\geq 0} \frac{t^n}{n!} L_H^n \, x_0 = \mathrm{e}^{tL_H} \, x_0 \ . \tag{4}$$

A symplectic scheme for integrating (3) from t to $t+\tau$ consists of approximating in a symplectic way the operator $\mathrm{e}^{\tau L_H}$. Indeed, as $H = A + \varepsilon B$, the Campbell-Baker-Hausdorff (CBH) theorem ensures that

$$\mathrm{e}^{\tau L_H} = \mathrm{e}^{\tau L_A} \mathrm{e}^{\tau L_{\varepsilon B}} + o(\tau) \ . \tag{5}$$

The operator $S_1 = \mathrm{e}^{\tau L_A} \mathrm{e}^{\tau L_{\varepsilon B}}$ thus provides the simplest symplectic scheme for such Hamiltonians. This can be generalized with a combination of several steps involving successively A and εB in order to obtain integrators of higher orders. A general integrator with n steps will be

$$S_n = \mathrm{e}^{c_1 \tau L_A} \mathrm{e}^{d_1 \tau L_{\varepsilon B}} \ldots \mathrm{e}^{c_n \tau L_A} \mathrm{e}^{d_n \tau L_{\varepsilon B}} \tag{6}$$

where the constants (c_i, d_i) will be chosen in order to improve the order of the integrator. Such integrators are very easy to implement on a computer, as they consist in the sequence of operators (6), where $\mathrm{e}^{c\tau L_A}$ and $\mathrm{e}^{d\tau L_{\varepsilon B}}$ are exact integrations over $c\tau$ and $d\tau$ of the integrable Hamiltonians A and B. Using CBH theorem, and the linearity of the Lie

derivative, we are ensured of the existence of a formal series

$$\begin{aligned} K &= k_{1,1}A + \varepsilon k_{1,2}B + \tau\varepsilon k_{2,1}\{A,B\} \\ &+\tau^2\varepsilon k_{3,1}\{A,\{A,B\}\} + \tau^2\varepsilon^2 k_{3,2}\{\{A,B\},B\} \\ &+\tau^3\varepsilon k_{4,1}\{A,\{A,\{A,B\}\}\} + \tau^3\varepsilon^2 k_{4,2}\{A,\{\{A,B\},B\}\} \\ &+\tau^3\varepsilon^3 k_{4,3}\{\{\{A,B\},B\},B\} + O(\tau^4) \end{aligned} \tag{7}$$

where the coefficients $k_{i,j}$ are polynomials of total degree i in the variables (c_m, d_n), with rational coefficients, such that

$$S_n(\tau) = \mathrm{e}^{c_1\tau L_A}\mathrm{e}^{d_1\tau L_{\varepsilon B}}\cdots\mathrm{e}^{c_n\tau L_A}\mathrm{e}^{d_n\tau L_{\varepsilon B}} = \mathrm{e}^{\tau L_K} \tag{8}$$

It should be noted that in order to define these expressions in an unambigous way, one needs to decompose the Poisson brackets involving A and B over a basis of canonical elements of the free Lie algebra $\mathcal{L}(A,B)$ generated by A and B and the Poisson bracket $\{\,,\,\}$. Following Koseleff (1993), this is done here by using the Lyndon basis. The scheme $S_n(\tau)$ integrates in an exact manner the formal Hamiltonian K. A symplectic integrator for $H = A + \varepsilon B$ will be obtained at order p if $K = A + \varepsilon B + O(\tau^p)$. In the most general way, this will be achieved by solving the algebraic equations

$$\begin{aligned} k_{1,1} = 1\ ; \qquad k_{1,2} = 1\ ; \\ k_{i,j} = 0 \qquad \text{for} \qquad (i \le p)\,. \end{aligned} \tag{9}$$

In particular, we have $k_{1,1} = c_1 + c_2 + \cdots c_n = 1$, $k_{1,2} = d_1 + d_2 + \cdots d_n = 1$, for $p \ge 1$.

3. Symmetric integrators

We will now restrict ourselves to symmetric integrators, that is integrators $S_n(\tau)$ such that $S_n(\tau)^{-1} = S_n(-\tau)$. We will have

$$-\tau L_{K(\tau)} = -\tau L_{K(-\tau)} \tag{10}$$

thus $K(-\tau) = K(\tau)$, and the formal Hamiltonian $K(\tau)$ is even. As we distinguish A and εB, we will have several classes $\mathcal{SABA}_k$ and $\mathcal{SBAB}_k$ of symmetric symplectic operators defined by their prototypes

$$\begin{aligned} \mathcal{SABA}_{2n} &: \mathrm{e}^{c_1\tau L_A}\mathrm{e}^{d_1\tau L_{\varepsilon B}}\cdots\mathrm{e}^{d_n\tau L_{\varepsilon B}}\mathrm{e}^{c_{n+1}\tau L_A}\mathrm{e}^{d_n\tau L_{\varepsilon B}}\cdots\mathrm{e}^{d_1\tau L_{\varepsilon B}}\mathrm{e}^{c_1\tau L_A} \\ \mathcal{SABA}_{2n+1} &: \mathrm{e}^{c_1\tau L_A}\mathrm{e}^{d_1\tau L_{\varepsilon B}}\cdots\mathrm{e}^{c_{n+1}\tau L_A}\mathrm{e}^{d_{n+1}\tau L_{\varepsilon B}}\mathrm{e}^{c_{n+1}\tau L_A}\cdots\mathrm{e}^{d_1\tau L_{\varepsilon B}}\mathrm{e}^{c_1\tau L_A} \\ \mathcal{SBAB}_{2n-1} &: \mathrm{e}^{d_1\tau L_{\varepsilon B}}\mathrm{e}^{c_2\tau L_A}\mathrm{e}^{d_2\tau L_{\varepsilon B}}\cdots\mathrm{e}^{d_n\tau L_{\varepsilon B}}\mathrm{e}^{c_{n+1}\tau L_A}\mathrm{e}^{d_n\tau L_{\varepsilon B}}\cdots\mathrm{e}^{c_2\tau L_A}\mathrm{e}^{d_1\tau L_{\varepsilon B}} \\ \mathcal{SBAB}_{2n} &: \mathrm{e}^{d_1\tau L_{\varepsilon B}}\mathrm{e}^{c_2\tau L_A}\cdots\mathrm{e}^{c_{n+1}\tau L_A}\mathrm{e}^{d_{n+1}\tau L_{\varepsilon B}}\mathrm{e}^{c_{n+1}\tau L_A}\cdots\mathrm{e}^{c_2\tau L_A}\mathrm{e}^{d_1\tau L_{\varepsilon B}} \end{aligned} \tag{11}$$

The index of the integrator is the total number of evaluations of A and B which are necessary for each step. With these notations, the classical leapfrog integrator can be considered as $SBAB_1 = \mathrm{e}^{\frac{\tau}{2}L_{\varepsilon B}}\mathrm{e}^{\tau L_A}\mathrm{e}^{\frac{\tau}{2}L_{\varepsilon B}} \in \mathcal{SBAB}_1$ or as $SABA_1 = \mathrm{e}^{\frac{\tau}{2}L_A}\mathrm{e}^{\tau L_{\varepsilon B}}\mathrm{e}^{\frac{\tau}{2}L_A} \in \mathcal{SABA}_1$. In both cases, the integrator is of order 2 and the formal Hamiltonian is $K = A + \varepsilon B + O(\tau^2\varepsilon)$. The fourth order solution found by Forest and Ruth (1990) or in an other way by Yoshida (1990) is either of the form $\mathcal{SABA}_3$ or $\mathcal{SBAB}_3$ that is, for $\mathcal{SBAB}_3$

$$SFRA_3 = \mathrm{e}^{d_1\tau L_{\varepsilon B}}\mathrm{e}^{c_2\tau L_A}\mathrm{e}^{d_2\tau L_{\varepsilon B}}\mathrm{e}^{c_3\tau L_A}\mathrm{e}^{d_2\tau L_{\varepsilon B}}\mathrm{e}^{c_2\tau L_A}\mathrm{e}^{d_1\tau L_{\varepsilon B}} \tag{12}$$

with

$$\begin{cases} c_3 + 2c_2 = 1 \\ d_1 + d_2 = 1/2 \\ 1/12 - 1/2\, c_2 + 1/2\, c_2^2 + c_2\, d_1 - c_2^2\, d_1 = 0; \\ -1/24 + 1/4\, c_2 - c_2\, d_1 + c_2\, d_1^2 = 0 \end{cases} \tag{13}$$

This system has a single real solution with approximate values $d_1 \approx 0.6756$, $c_2 \approx 1.3512$, $d_2 \approx -0.1756$, $c_3 \approx -1.7024$. The problem with this integrator is that due to the presence of negative time steps, the absolute value of the time steps remains high, and for large stepsizes, at an equivalent cost, the leapfrog integrators become more effective. In fact, Suzuki (1991) has demonstrated that it is not possible to obtain integrators of order $p > 2$ with only positive steps. The problem of the negative stepsize can nevertheless be overcome.

4. Integrators for perturbed Hamiltonian

In the previous sections, we have not yet taken into account the existence of the small parameter ε. Indeed, the terms of second order of K (7) are $\tau^2\varepsilon k_{3,1}\{A,\{A,B\}\}$ and $\tau^2\varepsilon^2 k_{3,2}\{\{A,B\},B\}$ which are respectively of order $\tau^2\varepsilon$ and $\tau^2\varepsilon^2$. One can thus try to cancel only the largest term, that is $k_{3,1} = 0$. This can be done using

$$\mathcal{SABA}_2 : \mathrm{e}^{c_1\tau L_A}\mathrm{e}^{d_1\tau L_{\varepsilon B}}\mathrm{e}^{c_2\tau L_A}\mathrm{e}^{d_1\tau L_{\varepsilon B}}\mathrm{e}^{c_1\tau L_A} \tag{14}$$

or

$$\mathcal{SBAB}_2 : \mathrm{e}^{d_1\tau L_{\varepsilon B}}\mathrm{e}^{c_2\tau L_A}\mathrm{e}^{d_2\tau L_{\varepsilon B}}\mathrm{e}^{c_1\tau L_A}\mathrm{e}^{d_1\tau L_{\varepsilon B}}. \tag{15}$$

With the type $\mathcal{SABA}_2$, one obtains $d_1 = \frac{1}{2}$, $c_2 = 1 - 2c_1$ and

$$\begin{aligned} K_{\mathcal{SABA}_2} = A + \varepsilon B &+ \tau^2\varepsilon\left(\frac{1}{12} - \frac{1}{2}c_1 + \frac{1}{2}c_1^2\right)\{A,\{A,B\}\} \\ &+ \tau^2\varepsilon^2\left(-\frac{1}{24} + \frac{1}{4}c_1\right)\{\{A,B\},B\} + O(\tau^4\varepsilon) \end{aligned} \tag{16}$$

As we search for only positive stepsize, we find a unique solution for cancelling the term in $\varepsilon\tau^2$, that is

$$c_2 = \frac{1}{\sqrt{3}}\,; \quad c_1 = \frac{1}{2}\left(1 - \frac{1}{\sqrt{3}}\right)\,; \quad d_1 = \frac{1}{2}\,; \tag{17}$$

with these coefficients, we obtain $K_{\mathcal{SABA}_2} = A + \varepsilon B + O(\tau^4\varepsilon + \tau^2\varepsilon^2)$. In a similar way, we obtain the solution for $\mathcal{SBAB}_2$

$$d_2 = \frac{2}{3}\,; \quad d_1 = \frac{1}{6}\,; \quad c_2 = \frac{1}{2}\,; \tag{18}$$

and as previously $K_{\mathcal{SBAB}_2} = A + \varepsilon B + O(\tau^4\varepsilon + \tau^2\varepsilon^2)$. Quite surprisingly, this latest integrator which is in most cases much more precise than the leapfrog integrator ($\mathcal{SBAB}_1$) at the same cost (see section 8), does not seem to have been used so far.

5. Higher orders

It becomes then tempting to iterate this process at higher order. We will not try to remove the term of order $\tau^2\varepsilon^2$, which is not the most important for large stepsize when ε is small. We will search for solutions S_n of the form $\mathcal{SABA}_n$ or $\mathcal{SBAB}_n$ for which the associated Hamiltonian K_{S_n} verifies

$$K_{S_n} = A + \varepsilon B + O(\tau^{2n}\varepsilon + \tau^2\varepsilon^2) \tag{19}$$

For this, we need to cancel at all order $p < 2n$ the coefficient $k_{p,1}$ of the single term of order $\tau^p\varepsilon$ in the Lyndon decomposition of K_{S_n}

$$\tau^p\varepsilon k_{p,1}\{A,\{A,\{A,\ldots\{A,B\}\}\}\ldots\} \tag{20}$$

We thus need to compute the part of K_{S_n} which is of degree ≤ 1 in B. We will use some results on calculus on free Lie algebra for which the reader should refer to (Bourbaki, 1972). We will call $\mathcal{L}(U,V)$ the free Lie algebra generated by U and V, endowed with its canonical associative structure. We will also use the symbol $\equiv$ for the equality in $\mathcal{L}(U,V)$ modulo terms of degree ≥ 2 in V. We have the two lemmas (Bourbaki, 1972)

LEMMA 1.

$$\mathrm{e}^U\, V\, \mathrm{e}^{-U} = \mathrm{e}^{ad(U)}\, V \tag{21}$$

where the exponential of X is formally defined as $\exp(X) = \sum_{n=0}^{+\infty} X^n/n!$, and where the adjoint operator ad is defined as $ad(X).Y = [X,Y]$.

LEMMA 2.

$$\mathrm{e}^{U+V} \equiv \mathrm{e}^U + \mathrm{e}^U \left(\frac{1-\mathrm{e}^{-ad(U)}}{ad(U)}\right) V\ . \tag{22}$$

The next result is a generalisation of a classical expansion at degree 1 in V of the Campbell-Baker-Hausdorff formula.

PROPOSITION 1. *Let $\gamma \in \mathbb{R}$. Then there exists $W \in \mathcal{L}(U,V)$ such that*

$$\mathrm{e}^{\gamma U}\mathrm{e}^{V}\mathrm{e}^{(1-\gamma)U} = \mathrm{e}^{W} \tag{23}$$

with

$$W \equiv U + \frac{ad(U)\mathrm{e}^{\gamma\, ad(U)}}{\mathrm{e}^{ad(U)}-1}\,V \tag{24}$$

that is

$$W \equiv U + \sum_{p=0}^{+\infty} \frac{B_p(\gamma)}{p!} ad(U)^p\, V \tag{25}$$

and where $B_n(x)$ are the Bernoulli polynomial defined as

$$\frac{t\,\mathrm{e}^{tx}}{\mathrm{e}^{t}-1} = \sum_{n=0}^{+\infty} B_n(x)\frac{t^n}{n!} \tag{26}$$

Indeed, the existence of $W \in \mathcal{L}(U,V)$ satisfying the above relation is given by the CBH theorem, on the other hand, we have

$$\mathrm{e}^{\gamma U}\mathrm{e}^{V}\mathrm{e}^{(1-\gamma)U} \equiv \mathrm{e}^{U} + \mathrm{e}^{U}\,\mathrm{e}^{(\gamma-1)U} V \mathrm{e}^{(1-\gamma)U} \tag{27}$$

and from lemma 1, this is also equal to

$$\mathrm{e}^{U} + \mathrm{e}^{U}\,\mathrm{e}^{(\gamma-1)ad(U)} V\ . \tag{28}$$

As for $V = 0$, we have $W = U$, we can set $W \equiv U + W_1$, where W_1 is of degree 1 in V, and from lemma 2

$$\mathrm{e}^{W} \equiv \mathrm{e}^{U} + \mathrm{e}^{U}\left(\frac{1-\mathrm{e}^{-ad(U)}}{ad(U)}\right) W_1 \tag{29}$$

thus

$$W_1 = \frac{ad(U)\mathrm{e}^{(\gamma-1)ad(U)}}{1-\mathrm{e}^{-ad(U)}}\,V \tag{30}$$

which ends the proof. For $\gamma = 1$, we recover the CBH results. This result is then easily generalized to the case of multiple products.

PROPOSITION 2. *Let $c_1, \ldots c_n, d_1, \ldots, d_n \in \mathbb{R}$, such that $\sum_{i=1}^{n} c_i = 1$. Then there exists $W \in \mathcal{L}(U,V)$ such that*

$$\mathrm{e}^{c_1 U}\mathrm{e}^{d_1 V}\mathrm{e}^{c_2 U}\mathrm{e}^{d_2 V}\ldots\mathrm{e}^{c_n U}\mathrm{e}^{d_n V} = \mathrm{e}^{W} \tag{31}$$

with

$$W \equiv U + \sum_{k=1}^{n} d_k \frac{ad(U)\mathrm{e}^{\gamma_k\, ad(U)}}{\mathrm{e}^{ad(U)}-1}\,V \tag{32}$$

that is

$$W \equiv U + \sum_{p=0}^{+\infty} \left(\sum_{k=1}^{n} d_k \, \frac{B_p(\gamma_k)}{p!} \right) ad(U)^p \, V \tag{33}$$

with $\gamma_k = c_1 + \ldots + c_k$.

This is staightforward as soon as we remark that

$$\mathrm{e}^{c_1 U} \mathrm{e}^{d_1 V} \mathrm{e}^{c_2 U} \mathrm{e}^{d_2 V} \ldots \mathrm{e}^{c_n U} \mathrm{e}^{d_n V} \equiv \sum_{k=1}^{n} d_k \mathrm{e}^{\gamma_k U} \, V \mathrm{e}^{(1-\gamma_k) U} + \mathrm{e}^{U} \tag{34}$$

Remark : As $B_0(x) = 1$, if $\sum_{k=1}^{n} d_k = 1$, we have

$$W \equiv U + V + \sum_{p=1}^{+\infty} \left(\sum_{k=1}^{n} d_k \, \frac{B_p(\gamma_k)}{p!} \right) ad(U)^p \, V \ . \tag{35}$$

6. Computation of the coeffcients

Proposition 2 , applied with $U = \tau L_A$ and $V = \tau \varepsilon L_B$, gives directly the algebraic equations which could then be solved for obtaining integrators of arbitrary order for perturbed systems. The problem is thus reduced to the search for coeffcients γ_k, d_k such that

$$\sum_{k=1}^{n} d_k \, g(\gamma_k, t) = 1 + o(t^N) \tag{36}$$

for N as high as possible with

$$g(x,t) = \frac{t \, \mathrm{e}^{x\,t}}{\mathrm{e}^{t} - 1} \ . \tag{37}$$

That is, with $\sum_{k=1}^{n} c_k = 1$, we will have to solve an algebraic system of equations of the form

$$\begin{aligned} &\sum_{k=1}^{n} d_k \, B_0(\gamma_k) = \sum_{k=1}^{n} d_k = 1 \\ &\sum_{k=1}^{n} d_k \, B_p(\gamma_k) = 0 \quad \text{for } 0 < p \leq N \ . \end{aligned} \tag{38}$$

It should be noted that all the integrators $\mathcal{SABA}_n$ and $\mathcal{SBAB}_n$ can be written on the general form (31) by taking $d_n = 0$ or $c_1 = 0$ in (31). Moreover, if we search for symmetric integrators, all the relations in (38) will be automatically fullfilled for odd values of p.

In this case, we just have to consider even values of p, for which we give the Bernoulli polynomials up to $p = 10$.

$$\begin{aligned}
B_0(x) &= 1 \\
B_2(x) &= \frac{1}{6} - x + x^2 \\
B_4(x) &= -\frac{1}{30} + x^2 - 2\,x^3 + x^4 \\
B_6(x) &= \frac{1}{42} - \frac{x^2}{2} + \frac{5\,x^4}{2} - 3\,x^5 + x^6 \\
B_8(x) &= -\frac{1}{30} + \frac{2\,x^2}{3} - \frac{7\,x^4}{3} + \frac{14\,x^6}{3} - 4\,x^7 + x^8 \\
B_{10}(x) &= \frac{5}{66} - \frac{3\,x^2}{2} + 5\,x^4 - 7\,x^6 + \frac{15\,x^8}{2} - 5\,x^9 + x^{10}
\end{aligned} \tag{39}$$

For example, the first integrators $SABA_2 = \mathrm{e}^{c_1 U}\mathrm{e}^{d_1 V}\mathrm{e}^{c_2 U}\mathrm{e}^{d_1 V}\mathrm{e}^{c_1 U}$ will be obtained by solving the set of equations

$$\begin{aligned}
2c_1 + c_2 &= 1 \\
2d_1 &= 1 \\
d_1 B_2(\gamma_1) + d_1 B_2(\gamma_2) &= 0
\end{aligned} \tag{40}$$

with $\gamma_1 = c_1, \gamma_2 = c_1 + c_2$, thus $\gamma_2 = 1 - \gamma_1$. As $g(1-x,t) = g(x,-t)$, we have for all p

$$B_p(1-x) = (-1)^p B_p(x) \tag{41}$$

and the previous system reduces to

$$d_1 = 1/2 \qquad c_2 = 1 - 2c_1 \qquad B_2(c_1) = 0 \tag{42}$$

and we recover the previous results. For $SABA_3 = \mathrm{e}^{c_1 U}\mathrm{e}^{d_1 V}\mathrm{e}^{c_2 U}\mathrm{e}^{d_2 V}\mathrm{e}^{c_2 U}\mathrm{e}^{d_1 V}\mathrm{e}^{c_1 U}$ we have

$$\begin{aligned}
c_1 + c_2 &= 1/2 \\
d_2 + 2d_1 &= 1 \\
d_1 B_2(\gamma_1) + d_2 B_2(\gamma_2) + d_1 B_2(\gamma_3) &= 0 \\
d_1 B_4(\gamma_1) + d_2 B_4(\gamma_2) + d_1 B_4(\gamma_3) &= 0
\end{aligned} \tag{43}$$

with $\gamma_1 = c_1$, $\gamma_2 = c_1 + c_2 = 1/2$, and $\gamma_3 = c_1 + c_2 + c_2 = 1 - c_1$. We have thus $B_2(\gamma_2) = -1/12, B_4(\gamma_2) = 7/240, B_2(\gamma_3) = B_2(c_1), B_4(\gamma_3) = B_4(c_1)$. We are thus left with

$$\begin{aligned}
c_2 &= 1/2 - c_1 \\
d_2 &= 1 - 2d_1 \\
d_1 B_2(c_1) - (1 - 2d_1)/24 &= 0 \\
d_1 B_4(c_1) + 7(1 - 2d_1)/480 &= 0
\end{aligned} \tag{44}$$

The resolution of this system is made easily and provide a single solution for which all the coefficients c_i, d_i are positive

$$c_1 = \frac{5 - \sqrt{15}}{10}; \quad c_2 = \frac{\sqrt{15}}{10}; \quad d_1 = \frac{5}{18}; \quad d_2 = \frac{4}{9} \tag{45}$$

This can be continued at all orders, but algebraic equations becomes more complicated as the order increases. The symplectic integrators up to order 10 are listed in Table I.

7. McLachlan solution

While we were writing a first version of this work, we realized that McLachlan (1995) had already found all the previous integrators. The paper of McLachlan is obviously not well-known to astronomers, otherwise they would have used at least the integrators $\mathcal{SABA}_2, \mathcal{SBAB}_2, \mathcal{SABA}_3$ and $\mathcal{SBAB}_3$ which have very good properties[1]. McLachlan just makes the computations on a very simple one degree of freedom example of the form $H(p,q) = p - F(q)$ for which the integration of the equations reduces to a simple integral $p(t) = \int_0^t F'(q)dq$ while the symplectic scheme is of the form of a sum $\tilde{p}(t) = \sum_i d_i F'(\gamma_i)$. This reduces the search of these symplectic integrators to the search of weights and nodes in an integral formula. He then claims that this is representative of the most general case. Although this may be true, the argument is not as straightforward as the constructive method which is presented here. On the other hand, the argument of McLachlan can be adapted here to complete the present proof and to provide the expression for the coefficients of these symplectic integrators at any order. Indeed, if we observe that

$$\frac{\mathrm{e}^t - 1}{t} = \int_0^1 \mathrm{e}^{xt} dx \ , \tag{46}$$

and that $(\mathrm{e}^t - 1)/t = O(1)$, the problem of finding d_k, γ_k verifying (36) is equivalent to the search of weights d_k and nodes γ_k such that

$$\sum_{k=1}^{n} d_k \, \mathrm{e}^{\gamma_k \, t} = \int_0^1 \mathrm{e}^{xt} dx + o(t^N) \tag{47}$$

The solution of this problem is known classically as the Gauss integration formula. The values of γ_k are given by $\gamma_k = (1 + x_k)/2$ where x_k are the roots of the degree n Legendre polynomial $P_n(x)$. The associated weights d_k are all positive and are given by

$$d_k = \frac{1}{(1 - x_k^2) \left(P_n'(x_k)\right)^2} \tag{48}$$

More precisely, if we consider an integrator of type

$$\mathcal{SABA}_n : \mathrm{e}^{c_1 U} \mathrm{e}^{d_1 V} \mathrm{e}^{c_2 U} \mathrm{e}^{d_2 V} \ldots \mathrm{e}^{c_n U} \mathrm{e}^{d_n V} \mathrm{e}^{c_{n+1} U} \ , \tag{49}$$

without any assumption of symmetry, we will have, in the above formula $d_{n+1} = 0$, thus, for $k = 1, \ldots, n$, the coefficients $\gamma_k = (1 + x_k)/2$ where x_k are the roots of $P_n(x)$. All x_k are

[1] The first integrators of the family ($\mathcal{SABA}_2, \mathcal{SBAB}_2, \mathcal{SABA}_3$ and $\mathcal{SBAB}_3$) have been also recently reported by Chambers and Murison (2000). The integrator $\mathcal{SBAB}_2$ is mentioned in the book of E. Forest (1998).

in the interval $[-1,1]$. We will thus have $\gamma_k \in [0,1]$. If we put the γ_k in ascending order, the values of the coefficients $c_k = \gamma_{k+1} - \gamma_k$ are all positive and $c_{n+1} = 1 - \gamma_n$. Moreover, the roots of the Legendre polynomial are symmetric with respect to zero. The γ_k are thus symmetric with respect to $1/2$ and so will be the c_k and d_k. The symplectic integrator is thus symmetric, and this hypothesis was not necessary. This is not the case for Lie algebra symbolic computation, where the assumption that the integrator is symmetric decreases in a large amount the number of the variables. For an integrator of type

$$\mathcal{SBAB}_n : \mathrm{e}^{d_1 V}\mathrm{e}^{c_2 U}\mathrm{e}^{d_2 V}\ldots\mathrm{e}^{c_n U}\mathrm{e}^{d_n V}\mathrm{e}^{c_{n+1} U}\mathrm{e}^{d_{n+1} V} \ , \tag{50}$$

we need to set $\gamma_1 = c_1 = 0$ in formula (47), which means that in the integration formula, one node is fixed to an extremity of the interval $[0,1]$. On the other hand, we have $\gamma_{n+1} = \sum_{i=1}^{n+1} c_i = 1$. The problem is thus to find nodes and weights for a Gauss formula with fixed nodes at the boundary of the interval of integration. The solution is given by the Gauss-Lobatto formulas (Abramovitz and Stegund, 1965). For $k = 2,\ldots,n$, we have $\gamma_k = (1+x_k)/2$ where x_k are the $n-1$ roots of $P_n'(x)$, and

$$d_1 = d_{n+1} = \frac{1}{n(n+1)}; \quad d_k = \frac{1}{n(n+1)(P_n(x_k))^2}; \quad \text{for} \quad k = 2,\ldots,n \ . \tag{51}$$

As previously, the integrators are symmetrical. These relations thus allow us to obtain in a straightforward manner symplectic integrators for perturbed systems at any order without the need to solve algebraic equations which are difficult to handle at large orders. Moreover, it provides a demonstration that this solutions exists at any order, with positive coefficients c_k, d_k.

8. Numerical examples

In this section, we will test the efficiency of the family of integrators $\mathcal{SABA}_n$ and $\mathcal{SBAB}_n$ on a simple pendulum example and on a planetary problem. For the simple pendulum

$$H = \frac{p^2}{2} + \varepsilon\cos q \tag{52}$$

we apply directly the previous computations with $A = p^2/2$ and $\varepsilon B = \varepsilon\cos q$. For each value of the stepsize τ, we have measured the maximum difference between the energy at the origin and the computed energy along the trajectories, over a time $T = 25000$. This comparison is performed for $\varepsilon = 0.1$ and $\varepsilon = 0.001$ (Fig. 1). For $\mathcal{SABA}_n$ or $\mathcal{SBAB}_n$, the logarithm of differences are plotted versus $\log(\tau')$, where $\tau' = \tau/n$. In such a way, as n is the number of evaluations of $\exp(c\tau L_A)$ and $\exp(d\tau L_B)$ for the given integrator, the integrators are compared at constant cost. As expected, for sufficiently small stepsize, the residuals behave as $\tau^2\varepsilon^2$ for $n \geq 2$, and as $\tau^2\varepsilon$ for the leapfrog integrator ($n = 1$). It is also clear that for small stepsize, nothing is really gained by increasing the order of the integrator (n), beyond $n = 2$.

For large stepsize, this is not true, as the term $\tau^{n+2}\varepsilon$ or $\tau^{n+3}\varepsilon$ (see next section) is still dominant, and we observe an increase of the slope with the order of the integrator, until unstabilities appear, probably due to the divergence of the remainders (it should be reminded that if a stepsize of 1 is used for $\mathcal{SABA}_1$, a stepsize of n is used for $\mathcal{SABA}_n$). In most cases, $n = 3$ or $n = 4$ seems to be the best choices.

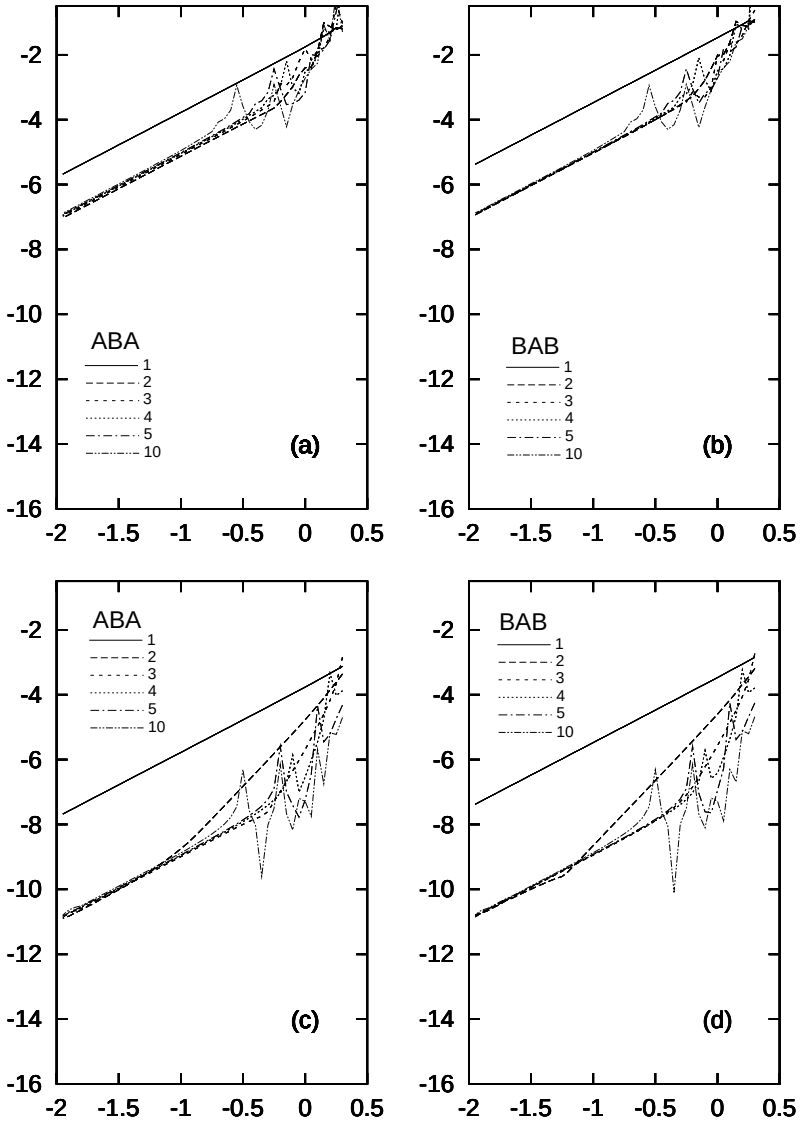

Figure 1. Fig.1–6. Logarithm of relative energy error plotted versus $\log(\tau')$, where $\tau' = \tau/n$, τ the stepsize, and n is the index of the method (and the curve) for the various symplectic integrators of the family $\mathcal{SABA}_n$ and $\mathcal{SBAB}_n$. Fig. 1. Simple pendulum with $\varepsilon = 0.1$ (a-b) and $\varepsilon = 0.001$ (c-d).

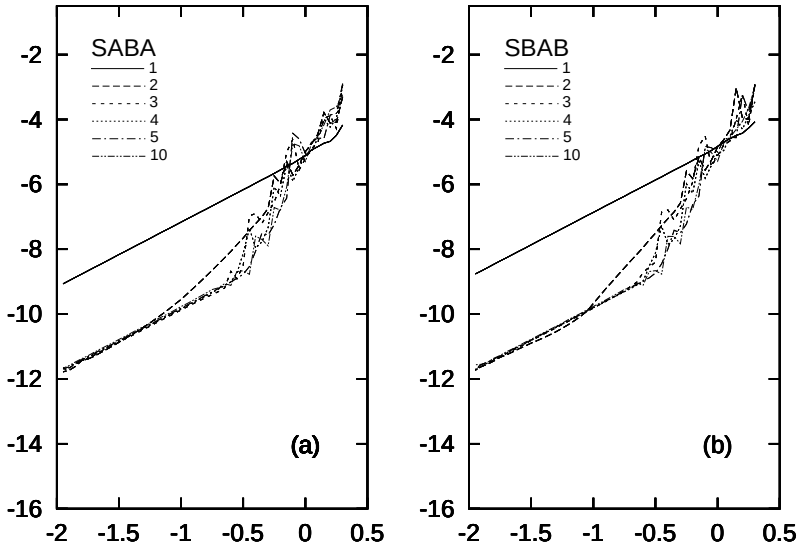

Figure 2. Relative energy error versus stepsize for the Sun-Jupiter-Saturn problem in Jacobi coordinates for the family of integrators $\mathcal{SABA}_n$ and $\mathcal{SBAB}_n$.

In the case of the planetary N-Body problem, the situation is more complicated. The Hamiltonian is split in an integrable Keplerian part, A, and a perturbation, B, corresponding to the mutual gravitational interaction of the planets. The Keplerian part is integrated in elliptical coordinates, while the perturbation (which is essentially a sum of inverses of the mutual distances of the planets) is integrated in rectangular cartesian coordinates (Wisdom and Holman, 1991).

There are several possible choice of coordinates for this decomposition. The initial choice of Wisdom and Holman, (1991), was to use Jacobi coordinates. In this case, B is integrable, as it depends only on the positions q. In Poincaré heliocentric coordinates (see Laskar, 1990, Laskar and Robutel, 1995), the expressions are simpler, but the perturbation B needs to be split in two terms $B = B_1(p) + B_2(q)$ which depends only on the momentum p, or on the positions q. As the methods which are presented here depend only on the linear part (in L_B) of the integrator, they can be adapted in a straightforward manner to this case, by substituting in their expresions $\exp L_{B_1} \exp L_{B_2}$ or $\exp L_{B_2} \exp L_{B_1}$ to $\exp L_B$. In doing so one needs to be sure that the final symplectic scheme is still symmetric, which will ensure that no term of order 2 will appear in the decomposition of the corresponding formal Hamiltonian K in equation (7). The use of these coordinates for symplectic integrators was first proposed by Koseleff (1993, 1996) and Touma and Wisdom (1994).

In the present case, we will use Jacobi coordinates, as this choice will be motivated by the next sections which require that B depends only on q. In Jacobi coordinates, we did the computation for the Sun-Jupiter-Saturn system over 25000 years (Fig. 2), and obtained very similar results as for the simple pendulum with $\varepsilon = 0.001$. This is understandable

as this is of the order of the ratio of perturbation due to the mutual interaction of the planets over the potential of the Sun. It can be clearly seen that for all $n \geq 2$, these integrators outperformed by several orders of magnitude the precision of the leapfrog integrator, except for very large stepsizes. The best choices being again $n = 3$ or $n = 4$. In all figures, it is very obvious that the $\tau^2\varepsilon^2$ term is the main limiting factor. We will now make an explicit computation of this term and present a strategy to get rid of it.

9. Computation of the remainders

We compute here the remainders of the symplectic integrators $\mathcal{SABA}_n$ and $\mathcal{SBAB}_n$. By switching the roles of U and V in (31), we obtain easily

PROPOSITION 3. *Let $c_1, \ldots c_n, d_1, \ldots, d_n \in \mathbb{R}$, such that $\sum_{i=1}^n c_i = \sum_{i=1}^n d_i = 1$. Then there exists $W \in \mathcal{L}(U, V)$ such that*

$$\mathrm{e}^{c_1 U}\mathrm{e}^{d_1 V}\mathrm{e}^{c_2 U}\mathrm{e}^{d_2 V}\ldots\mathrm{e}^{c_n U}\mathrm{e}^{d_n V} = \mathrm{e}^{W} \tag{53}$$

with

$$\begin{aligned} W \tilde{\equiv} U + V &+ \sum_{p=1}^{+\infty}\left(\sum_{k=1}^{n} d_k \frac{B_p(\gamma_k)}{p!}\right) ad(U)^p V \\ &+ \sum_{p=1}^{+\infty}\left(\sum_{k=1}^{n} c_k \frac{B_p(\delta_{k-1})}{p!}\right) ad(V)^p U \end{aligned} \tag{54}$$

with $\delta_0 = 0, \delta_k = d_1 + \ldots + d_k$, and where $\tilde{\equiv}$ is the equivalence modulo terms of degree ≥ 2 in U and V in $\mathcal{L}(U, V)$.

If we apply this result to compute the largest term in the remainder of the previous symplectic integrators, we obtain for each integrator

$$\begin{aligned} W = A + B &+ \left(\sum_{k=1}^{n} c_k \frac{B_2(\delta_{k-1})}{2}\right) \{\{A, B\}, B\}\tau^2\varepsilon^2 \\ &+ \left(\sum_{k=1}^{n} d_k \frac{B_p(\gamma_k)}{p!}\right) L_A^{2p} B \tau^{2p}\varepsilon + O(\tau^4\varepsilon^2 + \tau^{2p+2}\varepsilon) \end{aligned} \tag{55}$$

We can be more specific for the two classes of integrators $\mathcal{SABA}_n$ and $\mathcal{SBAB}_n$ by taking into account the fact that these integrators are reversible. In this case, each integrator of the classes $\mathcal{SABA}_{2n}$, $\mathcal{SABA}_{2n+1}$, $\mathcal{SBAB}_{2n}$, $\mathcal{SBAB}_{2n+1}$, with $\sum_{i=1}^n c_i = \sum_{i=1}^n d_i = 1$, is the time-$\tau$ evolution of the flow of the Hamiltonian W, with the following remainders :
– $\mathcal{SABA}_{2n}$: we have $2n + 1$ steps with $d_{2n+1} = 0$ and, for $p = 0, \ldots, n$

$$\left\{\begin{array}{lll} c_{n+1+p} & = c_{n+1-p}\ ; & \gamma_{n+p} = 1 - \gamma_{n+1-p}\ ; \\ d_{n+p} & = d_{n+1-p}\ ; & \delta_{n+p} = 1 - \delta_{n-p}\ ; \end{array}\right. \tag{56}$$

which gives, after reduction of the symmetries, and $d_n = 1/2 - \delta_{n-1}$, $c_{n+1} = 1 - 2\gamma_n$

$$\begin{aligned} W = A + \varepsilon B + \left(\frac{c_{n+1}}{2} B_2(1/2) + \sum_{k=1}^{n} c_k B_2(\delta_{k-1}) \right) \{\{A,B\},B\} \tau^2 \varepsilon^2 \\ + \left(2 \sum_{k=1}^{n} d_k B_{2n+2}(\gamma_k) \right) \frac{L_A^{2n+2}}{(2n+2)!} B \tau^{2n+2} \varepsilon + O(\tau^4 \varepsilon^2 + \tau^{2n+4} \varepsilon) \end{aligned} \tag{57}$$

– $\mathcal{SABA}_{2n+1}$: We have $2n+2$ steps, with $d_{2n+2} = 0$, $d_{n+1} = 1 - 2\delta_n$, $c_{n+1} = 1/2 - \gamma_n$, and, for $p = 0, \ldots, n$

$$\left\{ \begin{array}{ll} c_{n+1+p} = c_{n+2-p} \ ; & \gamma_{n+1+p} = 1 - \gamma_{n+1-p} \ ; \\ d_{n+1+p} = d_{n+1-p} \ ; & \delta_{n+p} \quad = 1 - \delta_{n+1-p} \ ; \end{array} \right. \tag{58}$$

which gives, after reduction of the symmetries

$$\begin{aligned} W = A + \varepsilon B + \left(\sum_{k=1}^{n+1} c_k B_2(\delta_{k-1}) \right) \{\{A,B\},B\} \tau^2 \varepsilon^2 \\ + \left(d_{n+1} \, B_{2n+4}(1/2) + 2 \sum_{k=1}^{n} d_k \, B_{2n+4}(\gamma_k) \right) \frac{L_A^{2n+4}}{(2n+4)!} B \tau^{2n+4} \varepsilon \\ + O(\tau^4 \varepsilon^2 + \tau^{2n+6} \varepsilon) \end{aligned} \tag{59}$$

– $\mathcal{SBAB}_{2n}$: This case is easily obtained by setting $c_1 = 0$ in $\mathcal{SABA}_{2n+1}$. We obtain for the new Hamiltonian

$$\begin{aligned} W = A + \varepsilon B + \left(\sum_{k=2}^{n+1} c_k B_2(\delta_{k-1}) \right) \{\{A,B\},B\} \tau^2 \varepsilon^2 \\ + \left(d_{n+1} \, B_{2n+2}(1/2) + 2 \sum_{k=1}^{n} d_k \, B_{2n+2}(\gamma_k) \right) \frac{L_A^{2n+2}}{(2n+2)!} B \tau^{2n+2} \varepsilon \\ + O(\tau^4 \varepsilon^2 + \tau^{2n+4} \varepsilon) \end{aligned} \tag{60}$$

– $\mathcal{SBAB}_{2n+1}$: This case is easily obtained by setting $c_1 = 0$ in $\mathcal{SABA}_{2n+2}$.

$$\begin{aligned} W = A + \varepsilon B + \left(\frac{c_{n+2}}{2} B_2(1/2) + \sum_{k=2}^{n+1} c_k B_2(\delta_{k-1}) \right) \{\{A,B\},B\} \tau^2 \varepsilon^2 \\ + \left(2 \sum_{k=1}^{n+1} d_k B_{2n+4}(\gamma_k) \right) \frac{L_A^{2n+4}}{(2n+4)!} B \tau^{2n+4} \varepsilon + O(\tau^4 \varepsilon^2 + \tau^{2n+6} \varepsilon) \end{aligned} \tag{61}$$

10. Correctors

The integrators $\mathcal{SABA}_n$ and $\mathcal{SBAB}_n$ have very good properties for small values of the parameter ε. Their numerical properties were studied in section 8. We have seen that the main limiting factor is the term in $\{\{A,B\},B\}$, which order is $\tau^2\varepsilon^2$. It would be of course very nice to get rid also of this term, but the result of Suzuki (1991) tells us that it is not possible to get rid simultaneously of the two terms $\{\{A,B\},B\}$ and $\{A,\{A,B\}\}$ with integrators having only positive values for the c_i, d_i constants. It is not forbidden to have negative values for some of the constants, but as $\sum c_i = \sum d_i = 1$, having only positive constants ensures that the values of the constants becomes smaller as the order of the integrator increases. This prevents explosion of the coefficients of the remainders which are polynomial in the c_i, d_i.

In order to get rid of the $\{\{A,B\},B\}$ term, one can use an alternate strategy, which is possible when A is quadratic in the actions p, and B depends only on the positions q (this is in particular the case for the pendulum Hamiltonian, or for the N-Body problem when expressed in Jacobi coordinates). In this case, $\{\{A,B\},B\}$ depends only on q and is thus integrable. It is then possible to compute it, and to add an additional step to the integrator $\mathcal{S}$ of the form

$$\mathcal{S}_C = \mathrm{e}^{-\tau^3\varepsilon^2 \frac{c}{2} L_{\{\{A,B\},B\}}} \mathcal{S} \mathrm{e}^{-\tau^3\varepsilon^2 \frac{c}{2} L_{\{\{A,B\},B\}}} \tag{62}$$

where c is the coefficient of $\{\{A,B\},B\}$ in W (Eq. 57–61). The new corrected integrator $\mathcal{S}_C$ is still symmetric, and thus additional terms will appear only at order τ^4. The values of the coefficients c used in the correctors up to order 10 are listed in Table II. For some of the lowest orders, algebraic formulas can be given, but they become very rapidly cumbersome, and a better accuracy will be obtained by using the decimal value which is given here with 40 digits. The plots of the residuals for these new integrators are presented in the case of the pendulum with $\varepsilon = 0.1$ and $\varepsilon = 0.001$ (Fig.3-4), and the Sun-Jupiter-Saturn problem in Jacobi coordinates (Fig. 5). As we attain now the limitation due to round-off errors, computations were performed also in quadruple precision. It is clear that now the slope of the residuals corresponds to the τ^4 terms and that we got rid of the $\tau^2\varepsilon^2$ term[2].

11. Composition of integrators

The corrector method of section 10 provide a family of integrators $\mathcal{SABA}_{Cn}$, $\mathcal{SBAB}_{Cn}$ of order 4 in τ and higher order in ε with remainders $O(\tau^4\varepsilon^2) + O(\tau^k\varepsilon)$ with $k = n+2$ for n even, and $k = n+3$ for n odd. These integrators have very good numerical properties, but

[2] Correctors of the form $\mathrm{e}^{C}\mathcal{S}\mathrm{e}^{-C}$ were also introduced in (Wisdom *et al.*, 1996). In this case, the composition rules allow to compute the corrector step only when an output is needed, but the stability of such a procedure, especially when the solution is chaotic is not clear. In (Wisdom *et al.*, 1996), the proposed corrector is in general not integrable and constructed to remove the $\varepsilon\tau^n$ terms, while in the present case, the $\varepsilon\tau^n$ terms are already removed by the construction of the symplectic integrators $\mathcal{SABA}_n, \mathcal{SBAB}_n$, and the corrector step is an integrable additional step which is used to remove the remaining $\varepsilon^2\tau^2$ term.

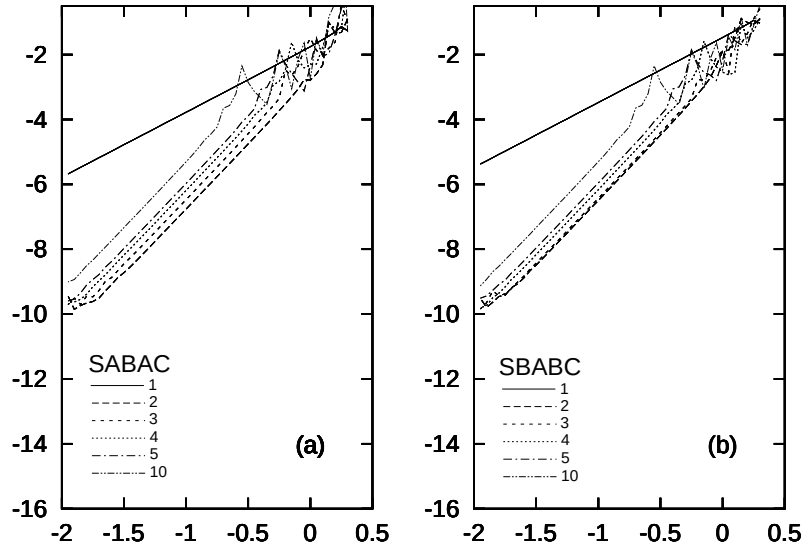

Figure 3. Relative energy error versus stepsize for the simple pendulum with $\varepsilon = 0.1$ for $\mathcal{SABA}_n$ and $\mathcal{SBAB}_n$ with correctors.

it is still possible to improve them by using the composition method of Yoshida (1990). Indeed, if $\mathcal{S}(\tau)$ is an integrator of order $2k$, then it is possible to find c such that

$$\mathcal{S}(\tau)\mathcal{S}(c\tau)\mathcal{S}(\tau) \tag{63}$$

is an integrator of order $2k+2$. Indeed, the symmetry of the integrator ensures that there are no terms in τ^{2k+1} in the remainders, and a straightforward computation gives the condition of cancellation of the terms in τ^{2k}

$$c^{2k+1} + 2 = 0 \tag{64}$$

that is $c = -2^{\frac{1}{2k+1}}$. It should be noted that as c is close to -1, the cost of this composition scheme, which we will denote $\mathcal{S}^2$, is roughly 3 times more expensive than the initial integrator $\mathcal{S}$. Practically, we do one step forward, one step backward, and then one step forward again. Nevertheless, if one generalises this sheme to a composition $\mathcal{S}^{2m}$ defined as

$$\mathcal{S}^{2m}(\tau) = \mathcal{S}^m(\tau)\mathcal{S}(c\tau)\mathcal{S}^m(\tau) \tag{65}$$

the condition (64) gives $c = -(2m)^{\frac{1}{2k+1}}$. Usually c is still not very large, and the additionnal backward step becomes negligeable for large values of m. Unfortunately, as one would expect, when m increases, the size of the remainders also increases and when we analyse the precision versus cost, it appears that we gain only for small values of m (Fig. 6). These integrators are still interesting, especially when one searches for high accuracy, which means small step size.

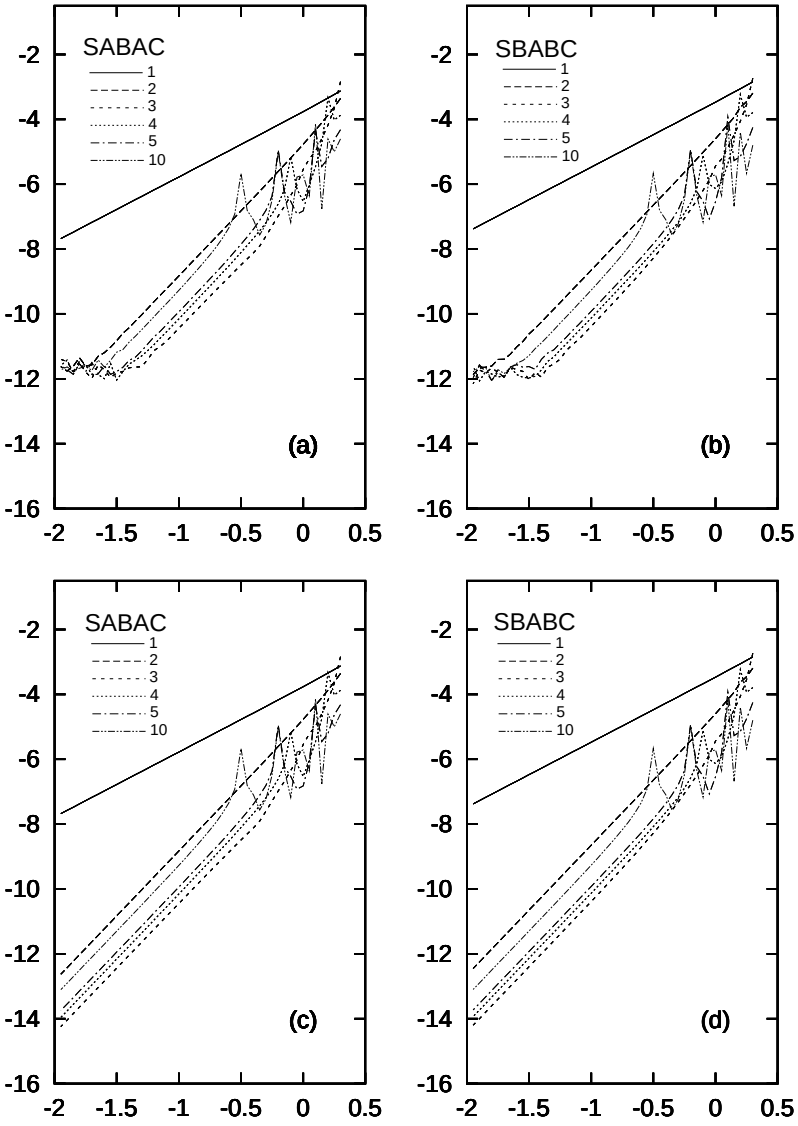

Figure 4. Relative energy error versus stepsize for the simple pendulum with $\varepsilon = 0.001$ for $\mathcal{SABA}_n$ and $\mathcal{SBAB}_n$ with correctors in double (a-b) and quadruple (c-d) precision.

12. Miscellanous remarks

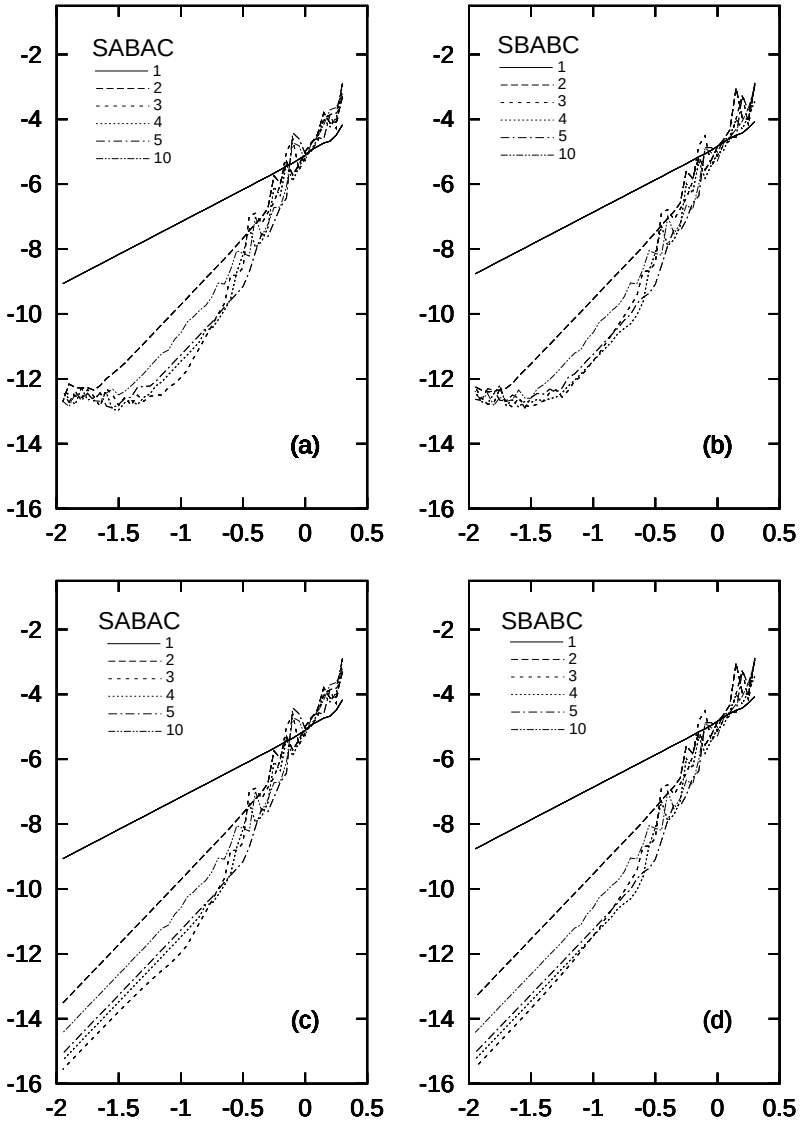

Figure 5. Relative energy error versus stepsize for the Sun-Jupiter-Saturn problem in Jacobi coordinates for $\mathcal{SABA}_n$ and $\mathcal{SBAB}_n$ with correctors in double (a-b) and quadruple (c-d) precision.

12.1. Integrals

The following result is obtained immediately:

PROPOSITION 4. *Let $H = A + B$. If F is an integral of H and F commutes with A ($\{A, F\} = 0$), then F is a true integral of the symplectic integration of H by any of the integrators constructed above.*

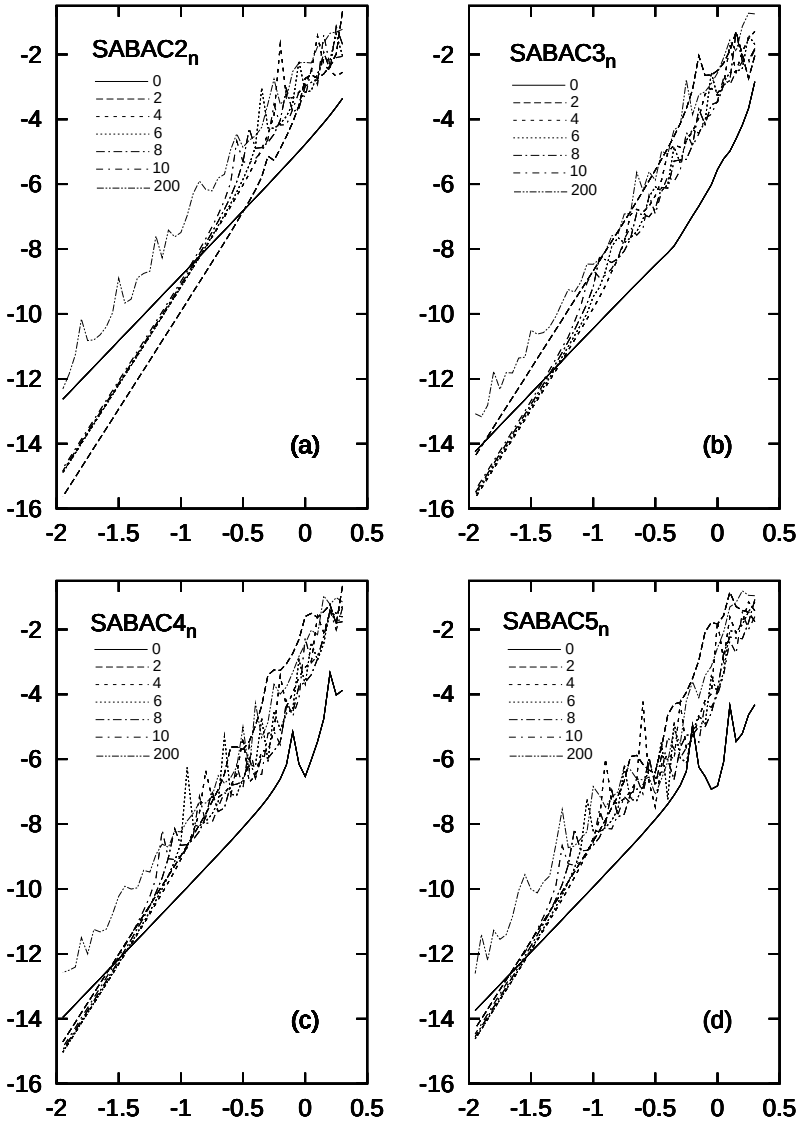

Figure 6. Relative energy error versus stepsize for the simple pendulum with $\varepsilon = 0.001$ for the composition of $\mathcal{SABA}_n$ and $\mathcal{SBAB}_n$ for $n = 2$ (a), $n = 3$ (b), $n = 4$ (c), and $n = 5$ (d). The index of the curve corresponds to the number of iterates $2m$ in the composition method (Eq.65).

Indeed, as $\{A, F\} = 0$, and $\{H, F\} = 0$, we have $\{B, F\} = 0$, and thus F commutes with any element of the free Lie algebra $\mathcal{L}(A, B)$. Thus, if the integrator $\mathcal{S}(\tau)$ is defined by $\mathcal{S}(\tau) = \mathrm{e}^{\tau L_W}$ where $W \in \mathcal{L}(A, B)$, we have $\{W, F\} = 0$. In particular, in Jacobi or heliocentric coordinates, the angular momentum depends only on the action variables and thus commutes with the Hamiltonian of the Keplerian unperturbed problem. The

angular momentum is thus an exact integral of the symplectic integration of the N-body problem. In constrast, the initial Hamiltonian is only an approximate integral (at order $O(\tau^p\varepsilon^2)+O(\tau^k\varepsilon)$). This feature can be used to check for the accumulation of errors in the integration.

12.2. Non Hamiltonian systems

In fact, the present results apply to general first order differential equations, and not only for Hamiltonian systems. Indeed, the only properties which are used are formal properties of the Lie algebra of the Lie derivatives along the vector fields defined by A and B. If a differential system of order 1 can be written on the form

$$\dot{X} = (L_A + L_B)X \tag{66}$$

where L_A and L_B are differential operators, for which the two systems $\dot{X} = L_A X$ and $\dot{X} = L_B X$ are integrable, then the symplectic integrators defined above will apply in the same way. Even more, if F is an integral of the system (66) such that $L_A F = 0$ and $L_B F = 0$, then F is also an integral for the symplectic integrator.

12.3. $H = A + B_1 + B_2$

It happens very often that the perturbation is not integrable, but can be splitted in two parts $B = B_1 + B_2$ which are integrable separately (this is the case in Poincaré heliocentric coordinates). As was already stated, the integrators $\mathcal{SABA}_n$ and $\mathcal{SBAB}_n$ can be used provided some small modifications, but it will not be possible to use the correctors as defined in section 10.

13. Conclusions

We have presented here a new and constructive proof for the existence at all orders of the families of symplectic integrators $\mathcal{SABA}_n$ and $\mathcal{SBAB}_n$, which were first described by McLachlan (1995). We have also obtained the expressions of the leading terms of the remainders for all n. These integrators are particularly adapted to perturbed Hamiltonian systems of the form $H = A+\varepsilon B$, where A and B are integrable separately, and in particular for planetary N-body problems.

Moreover, when A is quadratic in the actions p and B depends only on the positions q, the new family of integrators $\mathcal{SABA}_{Cn}$ and $\mathcal{SBAB}_{Cn}$ given in section 10 provide integration scheme which is of order 4 in τ, and has a remainder of the order of $O(\tau^4\varepsilon^2 + \tau^p\varepsilon)$, where $p = n + 2$ or $p = n + 3$. For practical use, it seems that the integrators for $n = 3$ or $n = 4$ are the most efficients. Although they require additional computations for the corrector, the corrected integrators $\mathcal{SABA}_{Cn}$ and $\mathcal{SBAB}_{Cn}$ will beat the simple integrators $\mathcal{SABA}_n$ and $\mathcal{SBAB}_n$ in many occasions, but unless one searches for very high accuracy with small stepsize, composition as described in section 11 is usually not very useful.

All the integrators which are presented here have only positive stepsize, except for the corrector. It should still be investigated whether some integrators of order 4 with negative stepsize could be useful.

References

Abramovitz, M., Stegund, I.:1965, 'Handbook of Mathematical functions', Dover, New York.

Bourbaki, N: 1972, 'Groupes et algèbres de Lie, Eléments de Mathématiques', Hermann, Paris.

Chambers, J., Murison, M.A.: 2000, 'Pseudo-high-order symplectic integrators', *Astron. J.*, **119**, 425–433.

Channell, P.J., Neri, F.R.: 1996, 'An introduction to symplectic integrators', Integration algorithms and classical mechanics (Toronto, ON, 1993), *Fields Inst. Commun.*, **10**, Amer. Math. Soc., Providence, RI, 45–58.

Duncan, M., Levison, H., Lee, M.H.: 1998, 'A multiple time step symplectic algorithm for integrating close encounters', *Astron. J.*, **116**, 2067–2077.

Forest, E., Ruth, R.D.: 1990, 'Fourth-order symplectic integration', *Phys. D*, **43(1)**, 105–117.

Forest, E.: 1992, 'Sixth-order Lie group integrators', *J. Comput. Phys.*, **99**, no. 2, 209–213.

Forest, E.: 1998, 'Beam Dynamics. A new attitude and framework', Harwood Academic Publishers.

Koseleff, P.-V.: 1993, 'Relations among Lie formal series and construction of symplectic integrators', in *Applied algebra, algebraic algorithms and error-correcting codes* (San Juan, PR, 1993), Lecture Notes in Comput. Sci., 673, Springer, Berlin, 213–230.

Koseleff, P.-V.: 1996, 'Exhaustive search of symplectic integrators using computer algebra', in Integration algorithms and classical mechanics (Toronto, ON, 1993), *Fields Inst. Commun.*, **10**, Amer. Math. Soc., Providence, RI, 103–119.

Laskar, J.: 1990, 'Systèmes de variables et éléments', *in Les Méthodes Modernes de la Mécanique Céleste*, D. Benest, C. Froeschlé eds. (Goutelas, 1989), Editions Frontières.

Laskar, J., Robutel, P.: 1995, 'Stability of the planetary three-body problem. I Expansion of the Planetrary Hamiltonian', *Celest. Mech.*, **62**, 193–217.

McLachlan, R.I.: 1995, 'Composition methods in the presence of small parameters', *BIT*, **35**, no. 2, 258–268.

McLachlan, R.I., Quispel, G.R.W., Turner, G.S.: 1998, 'Numerical integrators that preserve symmetries and reversing symmetries', *SIAM J. Numer. Anal.*, **35**,no. 2, 586–599

Neri, F.: 1988, 'Lie algebras and canonical integration', Dept. of Physics, University of Maryland, preprint.

Ruth, R.: 1983, 'A canonical integration technique', IEEE Transactions on Nuclear Science, **30**, 2669–2671.

Touma, J., Wisdom, J.: 1994, 'Lie-Poisson integrators for rigid body dynamics in the Solar System', *Astron. J.* **107**, 1189–1202.

Saha, P., Tremaine, S.: 1992, 'Symplectic integrators for Solar System dynamics', *Astron. J.* **104**, 1633–1640.

Suzuki, M.: 1991, 'General theory of fractal path integrals with applications to many-body theories and statistical physics', *J. Math. Phys.*, **32(2)**, 400–407.

Suzuki, M.: 1992, 'General theory of higher-order decomposition of exponential operators and symplectic integrators', *Phys. Lett. A*, **165**, no. 5-6, 387–395.

Wisdom, J., Holman, M.: 1991, 'Symplectic Maps for the N-Body Problem', *Astron. J.*, **102(4)**, 1528–1538.

Wisdom, J., Holman, M., Touma, J.: 1996, 'Symplectic correctors', Integration algorithms and classical mechanics (Toronto, ON, 1993), Fields Inst. Commun., 10, Amer. Math. Soc., Providence, RI, 217–244.

Yoshida, H.: 1990, 'Construction of higher order symplectic integrators', *Phys. Lett. A*, **150**, no. 5-7, 262–268.

Acknowledgements

We thank A. Albouy, A. Chenciner, D. Sauzin for very useful discussions, and F. Joutel for his help in the implementation of the integrators. Although it does not appear in the final work, the development of these integrators was largely facilitated by the use of LIE_TRIP, an algebraic manipulator for Lie algebra, which was developped with the unvaluable help of M. Gastineau.

Table I. Coefficients of the integrators $\mathcal{SABA}_n$ and $\mathcal{SBAB}_n$ up to $n = 10$.

		$SABA_1$	
c_1	$1/2$	d_1	1
		$SABA_2$	
c_1	$1/2 - \sqrt{3}/6$	d_1	$1/2$
c_2	$\sqrt{3}/3$		
		$SABA_3$	
c_1	$1/2 - \sqrt{15}/10$	d_1	$5/18$
c_2	$\sqrt{15}/10$	d_2	$4/9$
		$SABA_4$	
c_1	$1/2 - \sqrt{525 + 70\sqrt{30}}/70$	d_1	$1/4 - \sqrt{30}/72$
c_2	$\left(\sqrt{525 + 70\sqrt{30}} - \sqrt{525 - 70\sqrt{30}}\right)/70$	d_2	$1/4 + \sqrt{30}/72$
c_3	$\sqrt{525 - 70\sqrt{30}}/35$		
		$SABA_5$	
c_1	$1/2 - (\sqrt{490 + 42\sqrt{105}} + \sqrt{490 - 42\sqrt{105}})/84$	d_1	$(322 - 13\sqrt{70})/1800$
c_2	$\sqrt{490 - 42\sqrt{105}}/42$	d_2	$(322 + 13\sqrt{70})/1800$
c_3	$(\sqrt{490 + 42\sqrt{105}} - \sqrt{490 - 42\sqrt{105}})/84$	d_3	$64/225$
		$SABA_6$	
c_1	$0.033765242898423986093849222753002695$	d_1	$0.085622246189585172520148071086366447$
c_2	$0.135630063868443757075450979737044631$	d_2	$0.180380786524069303784916756918858056$
c_3	$0.211295100191533802515448936669596706$	d_3	$0.233956967286345523694935171994775497$
c_4	$0.238619186083196908630501721680711935$		
		$SABA_7$	
c_1	$0.025446043828620737736905157976074369$	d_1	$0.064742483084434846635305716339541009$
c_2	$0.103788363371682042331162455383531428$	d_2	$0.139852695744638333950733885711889791$
c_3	$0.167843017110998636478629180601913472$	d_3	$0.190915025252559472475184887744487567$
c_4	$0.202922575688698583453303206038480732$	d_4	$256/1225$
		$SABA_8$	
c_1	$0.019855071751231884158219565715263505$	d_1	$0.050614268145188129576265677154981095$
c_2	$0.081811689541954746046003466046821277$	d_2	$0.111190517226687235272177997213120442$
c_3	$0.135567033748648876886907443643292044$	d_3	$0.156853322938943643668981100993300657$
c_4	$0.171048883710339590439131453414531184$	d_4	$0.181341891689180991482575224638597 81$
c_5	$0.183434642495649804939476142360183981$		
		$SABA_9$	
c_1	$0.015919880246186955082211898548163565$	d_1	$0.040637194180787205985946079055261825$
c_2	$0.066064566090495147768073207416968997$	d_2	$0.090324080347428702029236015621456405$
c_3	$0.111329837313022698495363874364130346$	d_3	$0.130305348201467731159371434709316425$
c_4	$0.144559004648390734135082012349068788$	d_4	$0.156173538520001420034315203292221833$
c_5	$0.162126711701904464519269007321668304$	d_5	$16384/99225$
		$SABA_{10}$	
c_1	$0.013046735741414139961017993957773973$	d_1	$0.033335672154344068796784404946665896$
c_2	$0.054421580914093604672933661830479502$	d_2	$0.074725674575290296572888169828848666$
c_3	$0.092826899194980052248884661654309736$	d_3	$0.109543181257991021997767467114081596$
c_4	$0.123007087084888607717530710974544707$	d_4	$0.134633359654998177545613460784734677$
c_5	$0.142260527573807989957219971018032089$	d_5	$0.147762112357376435086946497325669165$
c_6	$0.148874338981631210884826001129719985$		

Table I.

	$SBAB_1$		
c_2	1	d_1	$1/2$
	$SBAB_2$		
c_2	$1/2$	d_1 d_2	$1/6$ $2/3$
	$SBAB_3$		
c_2 c_3	$1/2-\sqrt{5}/10$ $\sqrt{5}/5$	d_1 d_2	$1/12$ $5/12$
	$SBAB_4$		
c_2 c_3	$1/2-\sqrt{3/7}/2$ $\sqrt{3/7}/2$	d_1 d_2 d_3	$1/20$ $49/180$ $16/45$
	$SBAB_5$		
c_2 c_3 c_4	$1/2-\sqrt{3+6/\sqrt{7}}/6$ $(\sqrt{3+6/\sqrt{7}}-\sqrt{3-6/\sqrt{7}})/6$ $\sqrt{1/3-2/3\sqrt{7}}$	d_1 d_2 d_3	$1/30$ $(14-\sqrt{7})/60$ $(14+\sqrt{7})/60$
	$SBAB_6$		
c_2 c_3 c_4	$1/2-\sqrt{(15+2\sqrt{15})/33}/2$ $\sqrt{5/22-\sqrt{5/33}/2}$ $\sqrt{5/44-\sqrt{5/3}/22}$	d_1 d_2 d_3 d_4	$1/42$ $31/175-\sqrt{3/5}/20$ $31/175+\sqrt{3/5}/20$ $128/525$
	$SBAB_7$		
c_2	$0.064129925745196692331277119389668281$	d_1	$1/56$
c_3	$0.140019983538232156596467514911355124$	d_2	$0.105352113571753019691496032887878162$
c_4	$0.191200481765331716687926735526300967$	d_3	$0.170561346241752182382120338553874086$
c_5	$0.209299217902478868768657260345351255$	d_4	$0.206229397329351940783526485701104895$
	$SBAB_8$		
		d_1	$1/72$
c_2	$0.050121002294269921343827377790831021$	d_2	$0.082747680780402762523169860014604153$
c_3	$0.111285857950361201933229908663497754$	d_3	$0.137269356250080867640352809289686363$
c_4	$0.157034407842279797367566679191341619$	d_4	$0.173214255486523172557565766069859144$
c_5	$0.181558731913089079355376034354329607$	d_5	$2048/11025$
	$SBAB_9$		
c_2	$0.040233045916770593085533669588830933$	d_1	$1/90$
c_3	$0.090380021530476869412913242981253705$	d_2	$0.066652995425535055563113585377696449$
c_4	$0.130424457647530289670965541064286364$	d_3	$0.112444671031563226059728910865523921$
c_5	$0.156322996072028735517477663386542232$	d_4	$0.146021341839841878937791128687221946$
c_6	$0.165278957666387024626219765958173533$	d_5	$0.163769880591948728328255263958446572$
	$SBAB_{10}$		
		d_1	$1/110$
c_2	$0.032999284795970432833862931950308183$	d_2	$0.054806136633497432230701724790175355$
c_3	$0.074758978372457357854928159995462766$	d_3	$0.093584940890152602054070760949717460$
c_4	$0.109624073333469706075726923315353220$	d_4	$0.124024052132014157020042433210936377$
c_5	$0.134738595704632807519526226959347078$	d_5	$0.143439562389504044339611201665767616$
c_6	$0.147879067793469695715955757779528754$	d_6	$32768/218295$

Table II. Coefficients for the correctors up to order 10 for $\mathcal{SABA}_n$ and $\mathcal{SBAB}_n$

n	$c_{\mathcal{SABA}_n}$	$c_{\mathcal{SBAB}_n}$
1	$1/12$	$-1/24$
2	$(2-\sqrt{3})/24$	$1/72$
3	$(54-13\sqrt{15})/648$	$(13-5\sqrt{5})/288$
4	0.00339677504820860133153215778349214 4	$(3861-791\sqrt{21})/64800$
5	0.00227054312141926481943495505003913 0	0.00238148667295363418747038623218145 3
6	0.00162445984162428252145225851246360 8	0.00168134651209190632656369321529643 4
7	0.00121964391276041847257921182233164 5	0.00125176561603940000307251610025119 1
8	0.00094930817774560223479217750353505 4	0.00096879796807368857165468420846298 2
9	0.00075984602286043664635819667417681 5	0.00077234902399995207822768681026032 3
10	0.00062193433148616642649704984535864 6	0.00063032004416316784079863876266511 2