Exhaustive Search of Symplectic Integrators using Computer Algebra ⋆

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Abstract. We find symplectic integrators using universal exponential identities or relations among formal Lie series. We give here general methods to compute such identities in a free Lie algebra. We recover by these methods all the previously known symplectic integrators and some new ones. We list all minimal solutions for integrators of low order. We give some improvement in the case when the Hamiltonian is in form $T(p) + V(q)$. We give also all reversible fourth-order symplectic integrators for the planetary hamiltonian expressed in canonical heliocentric coordinates.

1 Introduction

For very long time integration, there has been recently a development of numerical methods preserving the symplectic structure (see for example [7, 18, 19, 20]), which seem to be more efficient with respect to the computational cost.

Symplectic integrators may be seen as the time evolution mapping of a slightly perturbed Hamiltonian, that is to say as a Lie transformation that can be represented either by an exponential, a product of increasing order single exponentials or a proper Lie transformation. Constructing explicit high order symplectic integrators requires the manipulation of formal identities like exponential identities.

In section **2.**, we remind first some definitions of the Hamilton formalism. In section **3.**, we give some general methods to manipulate formal Lie series and Lie algebra automorphisms. We remind some theorems related to exponential identities and give explicit methods to compute them. They make use the Lyndon basis, which is particularly adapted to this problem. Most of this material has been published already in [9] but is not necessarily known by the reader.

In section **4.**, we show how the algorithms described in section **3.** provide symplectic integrators. The idea of such constructions originates in Forest & Ruth ([7]) or more recently Yoshida ([20]). Our approach in this paper is to

⋆ Published in *Integration Algorithms and Classical Mechanics*, Fields Institut communications, **10**, pp. 103-120, 1996

combine the use of proper Lie transforms and exponentials. This avoids many unnecessary direct calculations of exponential identities. At the end we propose some improvement in the case when the Hamiltonian is separated into kinetic and potential energies. We give also some fourth-order integrator for the planetary Hamiltonian and show that they are minimals.

All the algorithms described in the present paper have been implemented using Axiom (NAG) running on IBM-RS/6000-550.

Between the preparation of this paper and its publication, many papers have been published on the subject and specially [13].

1.1 Symplectic Integrators

Given a phase space E which can be identified to $\mathbb{R}^{2n}$, a set of variables

$$(q, p) = (q_1, \ldots, q_n, p_1, \ldots, p_n) = (z_1, \ldots, z_{2n}), \tag{1}$$

and an Hamiltonian $h = h(p, q, t)$, we consider the system of differential equations

$$\dot{p}_i = -\frac{\partial h}{\partial q_i}, \dot{q}_i = \frac{\partial h}{\partial p_i}, \quad 1 \leq i \leq n, \tag{2}$$

where $\dot{z} = \frac{dz}{dt}$ denotes the total time derivative. Introducing the Poisson bracket

$$\{f, g\} = \sum_{i=1}^{n} \frac{\partial f}{\partial p_i}\frac{\partial g}{\partial q_i} - \frac{\partial g}{\partial p_i}\frac{\partial f}{\partial q_i} \tag{3}$$

that turns the set of smooth functions on E onto a Lie algebra, (2) becomes

$$\dot{z}_i = \{z_i, h\} = -L_h z_i, \quad 1 \leq i \leq 2n. \tag{4}$$

A transformation on the phase space E is said canonical if it preserves the Poisson brackets. Such transformations are also called symplectic as their Jacobians belong to the symplectic group. One extends the canonical transformations on the functions on the phase space by $Tf(z) = f(T(z))$. Canonical transformations act on the Lie algebra of the Lie operators by $TL_fT^{-1} = L_{Tf}$. Here $L_f : g \mapsto \{f, g\}$. The set of L_f is a Lie algebra with $[Lf, L_g] = L_{\{f,g\}}$.

The time-evolution mapping $S_h(t) : z \mapsto z(t)$ is a canonical transformation. From (4), $S_h(t)$ is the solution of the differential equation

$$\frac{d}{dt}S_h(t) = -S_h(t)L_h, S_h(0) = \mathbb{1}. \tag{5}$$

If h is not time-dependent we have $S_h(t) = e^{-tL_h}$ and a formal solution of (4) is given by its Taylor series, called Lie series

$$z(t) = \sum_{n \geq 0} (-t)^n \frac{L_h^n}{n!} z. \tag{6}$$

If h is time-dependent, say for example $h = \sum_{n\geq 0} t^n h_n$, then $S_h(t)z$ may be written as a Lie series. If

$$Z = S_h(t)z = \sum_{n\geq 0} t^n Z_n,$$

we get from (4)

$$Z_0 = z, \quad Z_n = -\sum_{p=1}^{n} \tfrac{1}{n} L_{h_p} Z_{n-p}.$$

More generally, see ([3]), $S_h(t)$ is a series of operators $\sum_{n\geq 0} t^n (S_h)_n$ where

$$(S_h)_0 = 1\!\!1, (S_h)_n = -\sum_{p=1}^{n} \tfrac{1}{n} L_{h_p} (S_h)_{n-p}.$$

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Let us consider an Hamiltonian $h = A + B$, the two time-evolution mappings $S_A(t) = e^{-tL_A}$ and $S_B(t) = e^{-tL_B}$, and a given integer k, one seeks a minimal set of coefficients $c_1, \ldots, c_n, d_1, \ldots d_n$, such that

$$S^{(n)}(t) = S_A(c_1 t) S_B(d_1 t) \cdots S_A(c_n t) S_B(d_n t) = e^{-tL_h} + o(t^k). \tag{7}$$

$S^{(n)}(t)$ is a canonical transformation as composition of canonical transformations. The above expression may be considered as an equality between truncated Lie series. The aim of our paper is to show how one can solve this general problem considering the equation (7) as an universal identity between formal transformations on Lie algebra.

2 Lie algebraic formalism

In hamiltonian mechanics, the use of Lie methods or Lie transformations is efficient when it becomes easy to manipulate Lie polynomials and to express exponential identities like the Baker-Campbell-Hausdorff formula. Our aim in this section is to give general methods for the computation of such identities.

These identities are universal Lie algebraic identities, that is to say they do not depend on the Lie algebra we work in or the Lie bracket we use. We work in free Lie algebras and with formal Lie series, neglecting all the convergence problems that can appear with analytical functions for example.

We will use the Lyndon basis for the formal computations but all the identities can be later evaluated in any Lie algebra.

2.1 Definitions

X will denote an alphabet, that is to say an ordered set (possibly endless). R is a ring which contains the rational numbers $\mathbb{Q}$. X^* is the free monoid generated by X and is totally ordered with the lexicographic order. $M(X)$ is the free magma generated by X. It contains X and is equipped with a composition law : $(x, y) \mapsto (x, y)$.

$\mathcal{A}(X, R)$ is the associative algebra, that is to say the R-algebra of X^*.

A Lie algebra is an algebra in which the multiplication law $[,]$ is bilinear, alternate and satisfies the Jacobi identity:

$$[a, [b, c]] + [b, [c, a]] + [c, [a, b]] = 0. \tag{8}$$

$L(X, R)$ or $L(X)$ is the free Lie algebra on X. It is defined as the quotient of the R-algebra of $M(X)$ by the ideal generated by the elements (u, u) and $(u, (v, w)) + (v, (w, u)) + (w, (u, v))$.

An element of $M(X)$ considered as element of $L(X)$ will be called a Lie monomial. $L_n(X)$ is the free module generated by those of length n. Thus $L(X)$ is graded by the length denoted by $|x|$ for $x \in M(X)$. If $|X| = q < \infty$ we have Witt's formula (see [1, 14, 15]):

$$\sum_{d|n} d \dim L_d(X) = q^n. \tag{9}$$

Given a weighted alphabet X in which each letter a has an integer weight $||a||$, we take the weight as graduation for $L(X)$ which is defined as the unique extension of the weight in X. We denote by $\tilde{L}_n(X)$ (resp. $\tilde{\mathcal{A}}_n(X)$) the submodule of $L(X)$ (resp. $\mathcal{A}(X)$) spanned by the elements of weight n.

2.2 Formal Lie series

We define the formal Lie series $\tilde{L}(X)$ and $\tilde{\mathcal{A}}(X)$ as

$$\tilde{L}(X) = \prod_{n \geq 0} \tilde{L}_n(X) \quad \text{and} \quad \tilde{\mathcal{A}}(X) = \prod_{n \geq 0} \tilde{\mathcal{A}}_n(X). \tag{10}$$

We will write $x \in \tilde{L}(X)$ as a series $\sum_{n \geq 0} x_n$. $\tilde{L}(X)$ is a complete Lie algebra with the Lie bracket

$$([x, y])_n = \sum_{p+q=n} [x_p, y_q]. \tag{11}$$

Denoting by $\tilde{L}(X)^+$ (resp. $\tilde{\mathcal{A}}(X)^+$) the ideal of $\tilde{L}(X)$ (resp. $\tilde{\mathcal{A}}(X)$) generated by the elements of positive weight, we can define the exponential and the logarithm as

$$\begin{array}{ll} \exp : \tilde{\mathcal{A}}(X)^+ \to 1 + \tilde{\mathcal{A}}(X)^+ & \log : 1 + \tilde{\mathcal{A}}(X)^+ \to \tilde{\mathcal{A}}(X)^+ \\ \qquad x \mapsto \sum_{n \geq 0} \dfrac{x^n}{n!} & \qquad x \mapsto -\sum_{n \geq 1} \dfrac{(1-x)^n}{n}. \end{array} \tag{12}$$

They are mutually reciprocal functions and we have (see [1, Ch. II, §5]) the

Theorem 1 (Campbell-Hausdorff). *If* $x, y \in \tilde{L}(X)^+$ *then*

$$\log\left[\exp(x)\exp(y)\right] \in \tilde{L}(X)^+. \tag{13}$$

Using the preceding lemma we deduce (see [4, 16]) the

Proposition 2 (Factored product expansion). *Given* $k \in \tilde{L}(X)^+$*, there is a unique series* $g \in \tilde{L}(X)^+$ *such that*

$$\exp(\textstyle\sum_{n\geq 1} k_n) = \cdots \exp(g_n) \cdots \exp(g_1). \tag{14}$$

2.3 Lie series automorphisms

For x in $\tilde{L}(X)$ we denote the Lie operator $L_x y = [x, y]$ by $L(x)$ or L_x. From the Jacobi identity (8) we have $[L_x, L_y] = L_x L_y - L_y L_x = L_{[x,y]}$. The set of L_x is a Lie algebra that we call the adjoint Lie algebra. For any Lie series automorphisms T, we have by definition $[Tf, Tg] = T[f, g]$. The Lie series automorphisms act on the adjoint Lie algebra by

$$T L_f T^{-1} = L_{Tf}. \tag{15}$$

Let us give now some example of Lie transformations that play an important role in hamiltonian mechanics.

The exponential. Given $x \in \tilde{L}(X)^+$, we consider $\exp(L_x)$ defined as

$$\exp(L_x) y = \sum_{i\geq 0} \frac{L_x^i}{i!} y. \tag{16}$$

From the Campbell-Hausdorff theorem (1), the set of all $\exp(L_x)$ is a group $\mathbf{G}$ that we will call the Lie transformations group.

The Lie transform. For $w = \sum_{n\geq 1} t^n w_n$, we denote by T_w and T_w^{-1} the solution ([3]) of

$$\frac{d}{dt} T_w = -T_w L_{\frac{dw}{dt}} \quad \text{and} \quad \frac{d}{dt} T_w^{-1} = L_{\frac{dw}{dt}} T_t^{-1}. \tag{17}$$

With the notation of (5), we have $T_w^{-1} = S_{\frac{dw}{dt}}$. For $g \in \tilde{L}(X)$, we have (see [2, 3]) $T_w^{-1} g = \sum_{n\geq 0} G_n$ where

$$G_0 = g_0, \quad G_{0,n} = g_n, \quad G_{p,q} = \sum_{k=1}^{p} \tfrac{k}{p}[w_k, G_{p-k,q}], \quad G_n = \sum_{p=0}^{n} G_{p,n-p}. \tag{18}$$

We call this transformation the Deprit transform. The composite T of two Lie transforms T_u and T_v satisfies

$$\frac{dT}{dt} = \frac{dT_u}{dt}T_v + T_u\frac{dT_v}{dt} = -T_uL_{\frac{du}{dt}}T_v - T_uT_vL_{\frac{dv}{dt}} \tag{19}$$

$$= -T\left(T_v^{-1}L_{\frac{du}{dt}}T_v + L_{\frac{dv}{dt}}\right) \tag{20}$$

$$= -TL_{T_v^{-1}\frac{du}{dt}+\frac{dv}{dt}}\cdot \tag{21}$$

So $T = T_w$ where $\dfrac{dw}{dt} = T_v^{-1}\dfrac{du}{dt} + \dfrac{dv}{dt}$.

The Dragt-Finn transform. The Dragt-Finn transform is the infinite product of exponential maps (see [4]). Given $g = \sum_{n\geq 1} g_n$, we define M_g and M_g^{-1} as

$$M_g = \exp(-L_{g_1})\cdots\exp(-L_{g_n})\cdots, \quad M_g^{-1} = \cdots\exp(L_{g_n})\cdots\exp(L_{g_1}). \tag{22}$$

Note that this transformation will be used in this paper as a technical support for proving relations between Lie series.

2.4 Relations between transformations

The three above transformations are totally defined by generating series and are connected by the following

Proposition 3 ([8]). *Given $w, k, g \in \tilde{L}(X)^+$, there exist*

— $k' \in \tilde{L}(X)^+$ *with* $k'_n - w_n \in L(w_1, \dots w_{n-1})$ *such that* $\exp(L_{k'}) = T_w^{-1}$,
— $g' \in \tilde{L}(X)^+$ *with* $g'_n - k_n \in L(k_1, \dots k_{n-1})$ *such that* $M_{g'}^{-1} = \exp(L_k)$,
— $w' \in \tilde{L}(X)^+$ *with* $w'_n - g_n \in L(g_1, \dots g_{n-1})$ *such that* $T_{w'}^{-1} = M_g^{-1}$.

The third part of the above proposition has been already proved by Finn ([6]), but not in terms of Lie polynomials. One proves (see [8, 10]) that $T_w = M_g$ if and only if

$$\frac{dw}{dt} = \sum_{n\geq 1} t^{n-1}\left[\sum_{k=1}^{n} k \sum_{\substack{(k+1)m_{k+1}+\cdots\\+(n-k)m_{n-k}=n-k}} \frac{L_{g_{n-k}}^{m_{n-k}}\cdots L_{g_{k+1}}^{m_{k+1}}}{m_{k+1}!\cdots m_{n-k}!}g_k\right], \tag{23}$$

or equivalently

$$w_n = \sum_{k=1}^{n}\frac{k}{n}\sum_{\substack{(k+1)m_{k+1}+\cdots\\+(n-k)m_{n-k}=n-k}} \frac{L_{g_{n-k}}^{m_{n-k}}\cdots L_{g_{k+1}}^{m_{k+1}}}{m_{k+1}!\cdots m_{n-k}!}g_k = g_n + G_n \tag{24}$$

in which $G_n \in L(g_1, \dots, g_{n-1})$.

Using the proposition (2), one proves the existence of $g = \sum_{n\geq 1} g_n$ such that

$$\exp(\textstyle\sum_{n\geq 1} L_{k_n}) = \cdots \exp(L_{g_n}) \cdots \exp(L_{g_1}), \tag{25}$$

in which $g_n = k_n + K_n$ and $K_n \in L(k_1, \ldots, k_{n-1})$. Combining (24) and (25) we deduce proposition 3.

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We deduce in passing that any Lie transformation $T \in \mathbf{G}$ may be expressed as an exponential of a Lie operator or as an infinite product of single exponentials or as a proper Lie transform. The use of a representation depends deeply on the result we look for. For example, if we have to compose transformations, it is much easier to consider Lie transforms because their product is a Lie transform whose generating function appears easily.

Explicit relations up to any given order may be easily computed, using the Lyndon basis. For example, given $w = \sum_{n\geq 1} w_n$, we have at the order 6 $\exp(L_k) = T_w^{-1}$ in which

$$\begin{aligned} k = {} & w_1 + w_2 + w_3 - \tfrac{1}{6}\,[w_1,\, w_2] + w_4 - \tfrac{1}{4}\,[w_1,\, w_3] + w_5 - \tfrac{3}{10}\,[w_1,\, w_4] \\ & - \tfrac{1}{10}\,[w_2,\, w_3] + \tfrac{1}{120}\,[w_1,\, [w_1,\, w_3]] + \tfrac{1}{60}\,[[w_1,\, w_2],\, w_2] \\ & + \tfrac{1}{360}\,[w_1,\, [w_1,\, [w_1,\, w_2]]] + w_6 - \tfrac{1}{3}\,[w_1,\, w_5] - \tfrac{1}{6}\,[w_2,\, w_4] \\ & + \tfrac{1}{60}\,[w_1,\, [w_1,\, w_4]] + \tfrac{1}{30}\,[w_1,\, [w_2,\, w_3]] + \tfrac{1}{24}\,[[w_1,\, w_3],\, w_2] \\ & + \tfrac{1}{240}\,[w_1,\, [w_1,\, [w_1,\, w_3]]] - \tfrac{1}{180}\,[w_1,\, [[w_1,\, w_2],\, w_2]] \end{aligned}$$

3 Search of symplectic integrators

Let $h = A + B$ be an Hamiltonian. For given integers n and k, one looks for a set $c_1, \ldots, c_n, d_1, \ldots d_n$, such that

$$S^{(n)}(t) = S_A(c_1 t) S_B(d_1 t) \cdots S_A(c_n t) S_B(d_n t) = S_h(t) + o(t^k). \tag{26}$$

Let $R = \mathbb{Q}[c_1, \ldots, c_n, d_1, \ldots, d_n]$, $\tilde{L}_p(\{A, B\})$ be the submodule of $\tilde{L}(\{A, B\})$ spanned by elements of weight p, where $||A|| = ||B|| = 1$. Using the Witt formula (9), the dimension l_p of $\tilde{L}_p(\{A, B\})$ satisfies $\sum_{d|n} d l_d = 2^n$.

Let $\tilde{L}_p\{z, A, B\}$ be the submodule of $\tilde{L}(\{z, A, B\})$, spanned by those of weight p, in which the partial commutative degree in z is 1 (here $||z|| = 0$). Using the Lyndon basis, one proves directly that the dimension of $\tilde{L}_p\{z, A, B\}$ is 2^p.

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In order to solve equation (26), we have to express exponential identities first. We first prove the algebraic equalities obtained by representing the integrators in several ways.

Proposition 4. *Let us consider the following problems:*

1. *Having expressed* $S^{(n)}(t)$ *as* $\exp(-\sum_{p\geq 1} t^p L_{K_p})$*, solve* $K_1 = A+B, K_2 = \cdots = K_k = 0$,
2. *Having expressed* $S^{(n)}(t)$ *as* $\exp(-tL_{G_1})\cdots\exp(-t^p L_{G_p})\cdots$*, solve* $G_1 = A+B, G_2 = \cdots = G_k = 0$,
3. *Having expressed* $S^{(n)}(t)$ *as* $T_{(tW_1+\cdots+t^p W_p+\cdots)}$*, solve* $W_1 = A+B, W_2 = \cdots = W_k = 0$.
4. *Having expressed* $Z = S^{(n)}(t)z$*, solve* $Z_0 = (\exp(-tL_{A+B})z)_0, \ldots, Z_k = (\exp(-tL_{A+B})z)_k$.

The solutions of these four problems are the zeroes of the same polynomial ideal.

Denoting the Lyndon basis $\mathcal{L}_p(\{A,B\})$ by $(x_{p,1},\ldots,x_{p,l_p})$, we have

$$K_p = \sum_{i=1}^{l_p} K_{p,i}x_{p,i}, G_p = \sum_{i=1}^{l_p} G_{p,i}x_{p,i}, W_p = \sum_{i=1}^{l_p} W_{p,i}x_{p,i}. \tag{27}$$

For the first three methods, the solutions are the zeroes of the ideals

$$\begin{aligned} \mathcal{I}_K^{(k)} &= (K_{1,1}-1, K_{1,2}-1) + (K_{i,j}; 2\leq i\leq k, 1\leq j\leq l_i),\\ \mathcal{I}_G^{(k)} &= (G_{1,1}-1, G_{1,2}-1) + (G_{i,j}; 2\leq i\leq k, 1\leq j\leq l_i),\\ \mathcal{I}_W^{(k)} &= (W_{1,1}-1, W_{1,2}-1) + (W_{i,j}; 2\leq i\leq k, 1\leq j\leq l_i). \end{aligned} \tag{28}$$

We have to bear in mind that S_W is the Deprit transform associated to $\int_0^t W(u)\,du$. We therefore get the relations due to the proposition 3:

$$\begin{aligned} K_p &= \tfrac{1}{p}W_p + R_p^W, \quad R_p^W \in L_p(W_1,\ldots,W_{p-1}),\\ \tfrac{1}{p}W_p &= G_p + R_p^G, \quad R_p^G \in L_p(G_1,\ldots,G_{p-1}),\\ G_p &= K_p + R_p^K, \quad R_p^K \in L_p(K_1,\ldots,K_{p-1}). \end{aligned} \tag{29}$$

We first have $K_1 = G_1 = W_1$. For $p > 1$, each R_p^W may be expressed in the Lyndon basis $\mathcal{L}_p(\{A,B\})$ and the coefficients are polynomials. Each monomial contains a $W_{i,j}$ where $i > 1$ and thus belongs to $\mathcal{I}_W^{(k)}$. We therefore deduce that $\mathcal{I}_K^{(k)} \subset \mathcal{I}_W^{(k)}$. On the same way, we deduce $\mathcal{I}_W^{(k)} \subset \mathcal{I}_G^{(k)}$ and $\mathcal{I}_G^{(k)} \subset \mathcal{I}_K^{(k)}$.

We thus have $\mathcal{I}_K^{(k)} = \mathcal{I}_W^{(k)} = \mathcal{I}_G^{(k)}$.

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Z_p belongs to $\tilde{L}_p\{z,A,B\}$ which basis is denoted by $z_{p,1},\ldots,z_{p,2^p}$. If $Z_p = \sum_{q=1}^{2^p} Z_{p,q}z_{p,q}$ and $(\exp(-tL_{A+B})z)_p = \sum_{q=1}^{2^p} a_{p,q}z_{p,q}$, the solutions of **4.** are the zeroes of

$$\mathcal{I}_Z^{(k)} = (Z_{i,j} - a_{i,j}, 1\leq i\leq k, 1\leq j\leq 2^i) \tag{30}$$

From $S^{(n)}(t)z - \exp(-tL_{A+B})z = \left(S^{(n)}(t) - \exp(-tL_{A+B})\right)z = o(t^k)$, we deduce for $p = 1$

$$Z_1 - \{z, A+B\} = -(L_{G_1} - L_{A+B})z = \{z, G_1 - (A+B)\} = 0, \tag{31}$$

that is, onto the basis $([z,A],[z,B])$,

$$Z_{1,1} - 1 = G_{1,1} - 1 = 0, \quad Z_{1,2} - 1 = G_{1,2} - 1 = 0. \tag{32}$$

For $1 < p \leq k$, we have

$$\begin{aligned}
Z_p - \tfrac{(-1)^p}{p!} L^p_{A+B} z &= \left[\sum_{m_1+\cdots+pm_p=p} (-1)^{m_1+\cdots+m_p} \frac{L^{m_1}_{G_1}\cdots L^{m_p}_{G_p}}{m_p!\cdots m_1!} - (-1)^p \frac{L^p_{A+B}}{p!} \right] z \\
&= \tfrac{(-1)^p}{p!} \left(L^p_{G_1} - L^p_{A+B}\right) z - L_{G_p} z + \qquad (33) \\
&\qquad \sum_{\substack{m_1+\cdots+(p-1)m_{p-1}=p \\ m_1<p}} (-1)^{m_1+\cdots+m_{p-1}} \frac{L^{m_1}_{G_1}\cdots L^{m_{p-1}}_{G_{p-1}}}{m_p!\cdots m_1!} z \qquad (34) \\
&= 0. \qquad (35)
\end{aligned}$$

$L^p_{G_1} - L^p_{A+B}$ may be written as

$$\sum_{k_1+\cdots+k_p+l_1+\cdots+l_p=p} \left(G^{k_1+\cdots+k_p}_{1,1} G^{l_1+\cdots+l_p}_{1,2} - 1 \right) L^{k_1}_A L^{l_1}_B \cdots L^{k_p}_A L^{l_p}_B. \tag{36}$$

A coefficient of (36) may be expressed as

$$G^k_{1,1} G^l_{1,2} - 1 = (G^k_{1,1} - 1) G^l_{1,2} + (G^l_{1,2} - 1) \in (G_{1,1} - 1, G_{1,2} - 1). \tag{37}$$

Each $L^{k_1}_A L^{l_1}_B \cdots L^{k_p}_A L^{l_p}_B$ is a sum of $z_{p,q}$ so any coefficient in $(L^p_{G_1} - L^p_{A+B})z$ belongs to $(G_{1,1}-1, G_{1,2}-1) \subset \mathcal{I}^{(p)}_G$. Other terms in (33) and (34) have coefficients in $(G_{2,1}, \ldots, G_{p,1}, \ldots G_{p,l_p}) \subset \mathcal{I}^{(p)}_G$. We thus deduce that $\mathcal{I}_Z(p) \subset \mathcal{I}^p_G$.

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Suppose we have for each $m < p$, $\mathcal{I}^{(m)}_Z = \mathcal{I}^{(m)}_G$. At the order p, from (35), we deduce also that

$$\begin{aligned}
-L_{G_p} z = \overbrace{Z_p - \tfrac{(-1)^p}{p!} L^p_{A+B} z}^{(I)} - \overbrace{\tfrac{(-1)^p}{p!} \left(L^p_{G_1} - L^p_{A+B}\right) z}^{(II)} - \\
\underbrace{\sum_{m_1+\cdots+m_{p-1}=p, m_1<n} (-1)^{m_1+\cdots+m_{p-1}} \frac{L^{m_1}_{G_1}\cdots L^{m_{p-1}}_{G_{p-1}}}{m_p!\cdots m_1!} z}_{(III)}.
\end{aligned} \tag{38}$$

Each term on the r.h.s. of the above equation, has a decomposition onto the Lyndon basis $z_{p,q}$. Coefficients of (I) belong to $\mathcal{I}_Z^{(p)}$, coefficients of (II) and (III) belong to $(G_{1,1}-1, G_{1,2}-1) \subset \mathcal{I}_G^{(p-1)} \subset \mathcal{I}_Z^{(p-1)} \subset \mathcal{I}_Z^{(p)}$.

We deduce that the coefficients of the $L_{G_p}z$ decomposition onto the $z_{p,q}$ belong to $\mathcal{I}_Z^{(p)}$. As solution of (38), the coefficients of G_p onto the $x_{p,q}$ belong to $\mathcal{I}_Z^{(p)}$ We thus have $\mathcal{I}_G^{(p)} \subset \mathcal{I}_Z^{(p)}$ and eventually $\mathcal{I}_G^{(p)} = \mathcal{I}_Z^{(p)}$.

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In order to obtain symplectic integrators, we can use one of these methods which are algebraically equivalent. We will not use the Dragt-Finn representation as its mathematical interpretation in terms of invariants is not clear. Nevertheless, composition of Factored Product transformations is widely used in optics ([5]).

Direct method. The problem (26) may be solved, looking for all z

$$S^{(n)}(t)z = S_A(c_1t)S_B(d_1t)\cdots S_A(c_nt)S_B(d_nt)z = S_h(t)z + o(t^k). \qquad (39)$$

At each order p, we obtain a system of 2^p polynomial equations.

Invariant function. Problem (39) may be solved by expressing $S^{(n)}$ as an exponential and looking for $c_1, \ldots, c_n, d_1, \ldots d_n$ such that

$$S^{(n)}(t) = S_A(c_1t)S_B(d_1t)\cdots S_A(c_nt)S_B(d_nt) = e^{-tL_K} \qquad (40)$$

with $K = h + o(t^{k-1})$. K is not the Hamiltonian governing the system given by $S^{(n)}$, but an invariant function. At each order p, there is l_p polynomial equations to solve. In order to get these, we have to compute some Baker-Campbell-Hausdorff formulas.

Perturbed Hamiltonian. One can also express $S^{(n)}(t)$ as a Lie transform

$$S_A(c_1t)S_B(d_1t)\cdots S_A(c_nt)S_B(d_nt) = S_W \qquad (41)$$

where $W = h + o(t^{k-1})$. The condition is obtained by writing

$$\frac{d}{dt}S_W = -S_W L_W = -S_h L_h + o(t^{k-1}). \qquad (42)$$

W is the Hamiltonian governing the system which time-evolution mapping is $S^{(n)}$. At each order p, there is the same number of equations as previously but that avoids many unnecessary direct calculations of Baker-Campbell-Hausdorff formulas.

3.1 First integrators

For a given order k, and for a given method (see table 1) one seeks a minimal n such that $S^{(n)}(t)$ is a kth-order symplectic integrator. One looks for the zeroes of a polynomial ideal. We use here algebraic methods like Gröbner basis that we compute using AXIOM (when possible) or MACAULAY that works in a ring $\mathbb{Z}/p\mathbb{Z}$ and gives some precious results.

For low orders, these methods furnish symplectic integrators. All the following results have been obtained with algorithms on Lie series and have been implemented t in AXIOM ([8]). We then obtain the polynomials that define the variety we look at. For low orders, these can be described ([9]).

• The solution for $k = 1$ is given by $c_1 = d_1 = 1$ and

$$S_1(t) = S^{(2)}(t) = S_A(t)S_B(t). \tag{43}$$

• The solution for $k = 2$ is given by

$$S_2(t) = S^{(3)}(t) = S_A(\tfrac{t}{2})S_B(t)S_A(\tfrac{t}{2}) = S_1(t)S_1^{-1}(-t). \tag{44}$$

This approximant is reversible, that is to say satisfies $S_2^{-1}(t) = S_2(-t)$.

• Solutions for $k = 3$ are

$$\begin{aligned} S_3(t) &= S_A(ct)S_B(ct)S_B(ct)S_A(ct)S_A(\bar{c}t)S_B(\bar{c}t)S_B(\bar{c}t)S_A(\bar{c}t) \\ &= S_2(ct)S_2(\bar{c}t) \end{aligned} \tag{45}$$

where $c^2 - \frac{1}{2}\ c + \frac{1}{12} = 0$.

• When $k = 4$, we find two sets of solutions and 5 solutions. The corresponding integrators have 7 factors. If $c^3 - 2c^2 + c = \frac{1}{6}$, we get

$$S_4(t) = S_2(ct)S_2((1-2c)t)S_2(ct). \tag{46}$$

These solutions are known and have been given also by Yoshida ([20]).

If c is a root of $c^2 - \frac{1}{2}c + \frac{1}{6} = 0$, we get two other solutions:

$$S_4(t) = S_2(ct)S_2((c+\bar{c})t)S_2(\bar{c}t). \tag{47}$$

• For $k = 5$, one gets exactly 46 solutions as product of 5 approximants S_2.

• For $k = 6$, an exhaustive list is still unknown. If we add the condition of being reversible, we get at most 39 solutions, working in $\mathbb{Z}/31991\mathbb{Z}$. All integrators are products of second-order integrators. The real valued integrators for $k = 2$ or 4 are reversible, that means $S(-t) = S^{-1}(t)$.

3.2 Reversible Integrators

Representing a reversible integrator $S(t)$ by an exponential $\exp(-tL_K)$, we deduce that $K(t) = K(-t)$. Looking for reversible integrators, we can deduce from the Campbell-Hausdorff formula the

Lemma 5 ([17]). *If $S_{2k}(t)$ is a reversible symplectic integrator of order $2k$, then*

$$S(t) = S_{2k}\left(\frac{1}{2-\sqrt[2k+1]{2}}t\right) S_{2k}\left(-\frac{\sqrt[2k+1]{2}}{2-\sqrt[2k+1]{2}}t\right) S_{2k}\left(\frac{1}{2-\sqrt[2k+1]{2}}t\right)$$

is a reversible symplectic integrator of order $2k+2$.

This lemma allows us to build reversible symplectic integrators of order $2k$ as products of $2.3^{k-1}+1$ single operators S_A or S_B. With this method we find a 19-factor sixth-order integrator.

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One can try to find directly reversible integrators looking for reversible products

$$S_R^{(n)}(t) = S_A(c_n t)S_B(d_n t)\cdots S_A(c_1 t)S_B(d_1 t)S_A(c_0 t)S_B(d_1 t)S_A(c_1 t)\cdots S_B(d_n t)S_A(c_n t).$$

Denoting by $S^{(n)}(t)$ the operator

$$S_A(c_n t)S_B(d_n t)\cdots S_A(c_1 t)S_B(d_1 t)S_A(\tfrac{c_0}{2}t), \tag{48}$$

we obtain $S_R^{(n)}$ as $S^{(n)}(t){S^{(n)}}^{-1}(-t)$ that we can express as an exponential or a Lie transform. Representing $S_R^{(n)}$ as an exponential e^{-tL_K} has the advantage that $K(t) = K(-t)$. Moreover we have the following lemma resulting from proposition 3:

Lemma 6. *Let $\mathcal{I}_W^{(k)} = (W_{1,1}-1, W_{1,2}-1, W_{2,1}, \ldots, W_{k,1}, \ldots, W_{k,l_k})$, be the polynomial ideal defining the solutions of $S_r^{(n)}(t) = S_{W(t)} = S_h + o(t^k)$. For each $2p \le k$, we have*

$$\{W_{2p,1}, \ldots, W_{2p,l_{2p}}\} \subset \mathcal{I}_W^{(2p-1)} \quad \textit{so} \quad \mathcal{I}_W^{(2p)} = \mathcal{I}_W^{(2p-1)}. \tag{49}$$

Using proposition 4, we get for each $1 \le 2p \le k$,

$$\mathcal{I}_K^{(p)} = \mathcal{I}_W^{(p)} = (K_{1,1}-1, K_{1,2}-1, K_{2,1}, \ldots, K_{p,1}, K_{p,l_p}) \tag{50}$$

where the $K_{i,j}$ are the coefficient of K satisfying $\exp(-tK(t)) = S_r^{(n)}$. As S_W is reversible, we have $K_{2p} = 0$, for each p, that is $\mathcal{I}_K^{(2p)} = \mathcal{I}_K^{(2p-1)}$ and $\mathcal{I}_W^{(2p)} = \mathcal{I}_W^{(2p-1)}$.

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This lemma proves that there is no need to consider odd terms of the Hamiltonian obtained with reversible integrators.

• For $k = 4$, one finds 3 reversible integrators obtained with the direct method.

• For $k = 6$, one proves that there is no solutions for $n < 8$. For $n = 8$, one sees, using the Hilbert function implemented in MACAULAY, that the variety of solutions in $\mathbb{Z}/p\mathbb{Z}$ ($p = 31991$) is constituted of 39 points. There is at most 39 algebraic solutions over $\mathbb{Q}$.

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Another solution has been proposed by Yoshida [20] consisting in the finding of reversible integrators as reversible product of second-order integrators S_2. We look for

$$S^{(n)}(t) = S_2(c_n t) \cdots S_2(c_1 t) S_2(c_0 t) S_2(c_1 t) \cdots S_2(c_n t) = e^{-tL_{K^{(n)}}}. \qquad (51)$$

• For $k = 4$, we find the real valued reversible integrator previously found by the direct method or using the lemma (5).

• For $k = 6$, we have four equations with four unknowns $c_0, \ldots, c_3$. The solution is obtained after eliminations with

$$\begin{aligned} P_0(c_0) = {} & c_0^{39} + 4\, c_0^{38} - 18\, c_0^{37} - \tfrac{232}{3}\, c_0^{36} + \tfrac{6469}{45}\, c_0^{35} + \tfrac{8108}{15}\, c_0^{34} - \tfrac{82144}{135}\, c_0^{33} - \\ & \tfrac{239008}{135}\, c_0^{32} + \tfrac{870652}{675}\, c_0^{31} + \tfrac{5898416}{2025}\, c_0^{30} - \tfrac{618824}{675}\, c_0^{29} - \tfrac{5158016}{2025}\, c_0^{28} + \\ & \tfrac{2525372}{30375}\, c_0^{27} + \tfrac{32135888}{30375}\, c_0^{26} - \tfrac{1377776}{10125}\, c_0^{25} - \tfrac{33361568}{91125}\, c_0^{24} + \tfrac{536566}{10125}\, c_0^{23} + \\ & \tfrac{35651416}{455625}\, c_0^{22} - \tfrac{19660868}{1366875}\, c_0^{21} - \tfrac{8051504}{455625}\, c_0^{20} + \tfrac{5636474}{1366875}\, c_0^{19} + \tfrac{11313208}{4100625}\, c_0^{18} - \\ & \tfrac{17674448}{20503125}\, c_0^{17} - \tfrac{8733536}{20503125}\, c_0^{16} + \tfrac{1302268}{6834375}\, c_0^{15} + \tfrac{87632}{2460375}\, c_0^{14} - \tfrac{624184}{20503125}\, c_0^{13} + \\ & \tfrac{288448}{922640625}\, c_0^{12} + \tfrac{3333844}{922640625}\, c_0^{11} - \tfrac{716752}{922640625}\, c_0^{10} - \tfrac{127664}{553584375}\, c_0^{9} + \tfrac{143264}{922640625}\, c_0^{8} - \\ & \tfrac{136499}{4613203125}\, c_0^{7} - \tfrac{19996}{8303765625}\, c_0^{6} + \tfrac{117142}{41518828125}\, c_0^{5} - \tfrac{33848}{41518828125}\, c_0^{4} + \\ & \tfrac{17431}{124556484375}\, c_0^{3} - \tfrac{9668}{622782421875}\, c_0^{2} + \tfrac{656}{622782421875}\, c_0 - \tfrac{64}{1868347265625} = 0, \end{aligned}$$

and $c_1 = P_1(c_0), c_2 = P_2(c_0), c_3 = P_3(c_0)$ where P_1, P_2, P_3 are polynomials of degree 38. P_0 is irreducible over $\mathbb{Q}$ and has only three real roots. All the solutions are reached with this method as there is at most 39 solutions.

• For $k = 8$, Yoshida ([20]) has found 5 real valued integrators using numerical methods. These integrators involve 31 single integrators S_A or S_B. We proved, using standard basis computed with Macaulay, that these integrators are not products of 5 fourth-order symplectic integrators.

3.3 Special cases

Most of the times, when $h = T(p) + V(q)$, the kinetic energy is just a quadratic form in p. That means that $\{T, V\}$ is of degree one in p, $\{\{T, V\}, V\}$ depends only on q and $\{\{\{T,V\},V\},V\}=0$. We may find symplectic integrators of order 4 or 6 involving less terms.

Unfortunately, there is no integrator of order 4 using less than 7 terms.

As $\{\{T,V\},V\}$ depends only on q, $V_1=\alpha V+t^2\beta\{\{T,V\},V\}$ depends only on q and t for any α,β and we have

$$e^{-tL_{V_1}}p=p-t\frac{\partial V_1}{\partial q} \quad \text{and} \quad e^{-tL_{V_1}}q=q. \tag{52}$$

Denoting $e^{-t(\alpha L_V+\beta t^2 L_{\{\{T,V\},V\}})}$ by $S_{\alpha,\beta}(t)$ we look now for integrators $S^{(n)}$ as product of

$$S_{c_n,z_n}(t)S_T(d_nt)\cdots S_{c_1,z_1}(t)S_T(d_0t)S_{c_1,z_1}(t)\cdots S_T(d_nt)S_{c_n,z_n}(t) \tag{53}$$

or

$$S_T(d_nt)S_{c_n,z_n}(t)\cdots S_T(d_1t)S_{c_0,z_0}(t)S_T(d_1t)\cdots S_{c_n,z_n}(t)S_T(d_nt) \tag{54}$$

With this method we found a 5-factor fourth-order integrator and an 9-factor sixth-order integrator (see [9]).

3.4 Decomposition into more terms

One can generalize the search of symplectic integrators to the case of 3 operators (see for example Suzuki [17]).

In this part, we show how to find minimal symplectic integrators in the case when $h=A_1+A_2+A_3$, using the algorithms previously described. Such integrators can be useful for planetary problems written in the canonical heliocentric variables of Poincaré (see [12]).

We will give an exhaustive list for orders 1, 2 and 4. It is clear that any permutation on A_1,A_2,A_3 will also give an integrator.

The first-order integrator is

$$S_1(t)=S_{A_1}(t)S_{A_2}(t)S_{A_3}(t). \tag{55}$$

• From $S_2(t)=S_{A_2}(\frac{t}{2})S_{A_3}(t)S_{A_2}(\frac{t}{2})$, we deduce an second-order integrator for $A_1+(A_2+A_3)$:

$$\begin{aligned} S_2(t) &= S_{A_1}(\tfrac{t}{2})S_{A_2}(\tfrac{t}{2})S_{A_3}(t)S_{A_2}(\tfrac{t}{2})S_{A_1}(\tfrac{t}{2}). \\ &= S_1(\tfrac{t}{2})S_1^{-1}(-\tfrac{t}{2}) \end{aligned} \tag{56}$$

• Looking for reversible fourth-order integrators, we could deduce from the 7-factor fourth-order integrator S_4 for A_1+A_3, that

$$S_{A_3}(d_2t)S_4(c_1t)S_{A_3}(d_1t)S_4(c_0t)S_{A_3}(d_1t)S_4(c_1t)S_{A_3}(d_2t) \tag{57}$$

is a 25-factor fourth-order integrator for $h=(A_1+A_2)+A_3$.

Using the lemma 5, one obtains a 13-factor fourth-order symplectic integrator as a product of 3 reversible second-order integrators:

$$S_{A_1}(\tfrac{a}{2}t)S_{A_2}(\tfrac{a}{2}t)S_{A_3}(at)S_{A_2}(\tfrac{a}{2}t)S_{A_1}(\tfrac{a+b}{2}t)S_{A_2}(\tfrac{b}{2}t)S_{A_3}(bt)S_{A_2}(\tfrac{b}{2}t)$$
$$S_{A_1}(\tfrac{a+b}{2}t)S_{A_2}(\tfrac{a}{2}t)S_{A_3}(at)S_{A_2}(\tfrac{a}{2}t)S_{A_1}(\tfrac{a}{2}t). \qquad (58)$$

where $a = \frac{1}{2-\sqrt[3]{2}}, b = -\frac{\sqrt[3]{2}}{2-\sqrt[3]{2}}$.

Let us prove now that these integrators are minimal regards to the number of factors. For a given order k, a kth-order integrator is an operator of length m:

$$S^{(m)}(t) = S_{A_1}(x_1t)S_{A_2}(x_2t)S_{A_3}(x_3t)\cdots S_{A_m}(x_mt), \qquad (59)$$

where $i-1 = m \bmod 3$. A p-factor kth-order integrator is a sequence $(x_1,\ldots,x_m)$ in which $x_1x_m \neq 0$ and $m-p$ of the x_i's are equals to zero. In such a sequence, there is no 2 consecutive zeroes, otherwise its length would be $m-2$. For the integrator (56), we have

$$x_1 = \tfrac{1}{2}, x_2 = \tfrac{1}{2}, x_3 = 1, x_4 = 0, x_5 = \tfrac{1}{2}, x_6 = 0, x_7 = \tfrac{1}{2}.$$

For given m and k the set of sequence $(x_1,\ldots,x_m)$ satisfying

$$S_{A_1}(x_1t)S_{A_2}(x_2t)S_{A_3}(x_3t)\cdots S_{A_m}(x_mt) = S_h(t) + o(t^k), \qquad (60)$$

is an algebraic variety. For a given order k, let us denote by M_k the minimal integer such that each minimal kth-order integrator (up to a permutation of (A_1, A_2, A_3)) may be written as $S^{(m)}$ where $m \leq M_k$. Each kth-order integrator (up to a permutation of A_1, A_2, A_3) will be a sequence that is solution of

$$S^{(m)}(x_1,\ldots,x_m) = S_{A_1}(x_1t)\cdots S_{A_m}(x_mt) = S_{A_1+A_2+A_3}(t) + o(t^k), \qquad (61)$$

with $m \leq M_k$.

The second-order example shows that $M_2 \geq 7$. Let S_2 be any 5-factor second-order integrator. Its length is at most 9. If its length is 9 then we have $x_2 = x_4 = x_6 = x_8 = 0$. By transposing A_2 and A_3, the sequence $(x_1, x_3, x_5, x_7, x_9)$ gives also a 5-factor integrator.

If its length is 8, then there are 3 zeroes in the subsequence $x_2,\ldots,x_7$, because $x_1x_8 \neq 0$. There is only two possibilities: $x_2 = x_4 = x_6 = 0$ or $x_3 = x_5 = x_7 = 0$. In the first case, by transposing A_2 and A_3, the sequence $(x_1, x_3, x_5, x_7, 0, x_8)$ gives a 6-factor integrator. In the second case, the same transposition gives also a 5-factor integrator with the sequence $(x_1, 0, x_2, x_4, x_6, x_8)$. It proves that any 5-factor operator (e.g. second-order integrator) (up to permutations) has a length less than 7.

- There is no 5-factor second-order integrator of length 5.
- Looking for integrators of length 6, one finds

$$S_2(t) = S_{A_1}(ct)S_{A_2}(ct)S_{A_3}(ct)S_{A_1}(\bar{c}t)S_{A_2}(\bar{c}t)S_{A_3}(\bar{c}t) = S_1(ct)S_1(\bar{c}t) \qquad (62)$$

where c is a complex root of $c^2 - c + \frac{1}{2}$.

• Looking for all possible solution involving 7 variables, we have $x_1x_7 \neq 0$ so for a 5-factor integrator we must have $x_2x_3x_5x_6 = 0$. We thus find

$$x_1 = x_7 = \frac{1}{2}, x_4 = 0, (x_2 - \frac{1}{2})x_2 = 0, x_2 = x_3 - \frac{1}{2} = \frac{1}{2} - x_6 = 1 - x_5. \quad (63)$$

If $x_2 = 0$ or $x_2 = 1$, we find the integrator (56). That proves that any minimal real second-order integrator has 5 factors and length 7.

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Let S be a 7-factor operator. One can suppose that the 2 first factors are S_{A_1} and S_{A_2}. Let m be its length and express S as

$$S(t) = S_{A_1}(x_1t)S_{A_2}(x_2t)S_{A_3}(x_3t)\cdots S_{A_m}(x_mt) \quad (64)$$

in which $x_1x_2x_m \neq 0$. The subsequence $(x_2, \ldots x_{m-1})$ has a length $m-2$ and corresponds to a 5-factor operator. We thus deduce that $m-2 \leq 8$ because x_{m-1} could be zero. So any 7-factor operator may be written as an operator of length $m \leq 10$.

Suppose now that S has length 10 and that $x_1x_2x_{10} \neq 0$. There are 3 zeroes in the subsequence $x_3, \ldots, x_9$ and there are not consecutive. The only solutions are

$a)$ $x_3 = x_5 = x_7 = 0$, $b)$ $x_3 = x_5 = x_8 = 0$, $c)$ $x_3 = x_5 = x_9 = 0$,
$d)$ $x_3 = x_6 = x_8 = 0$, $e)$ $x_3 = x_6 = x_9 = 0$, $f)$ $x_3 = x_7 = x_9 = 0$,
$g)$ $x_4 = x_6 = x_8 = 0$, $h)$ $x_4 = x_6 = x_9 = 0$, $i)$ $x_4 = x_7 = x_9 = 0$,
$j)$ $x_5 = x_7 = x_9 = 0$.

Let us suppose that $S(t)S^{-1}(-t)$ is a reversible fourth-order integrator. If we suppose now that $A_1 = 0$, then $S(t)S^{-1}(t)$ is still a fourth-order integrator for $A_2 + A_3$. It implies that we must have at least 2 factors S_{A_2} and 2 factors S_{A_3} in S. So the only cases to consider are $a), g), j)$.

In the first case, suppose that $A_2 = 0$, then we obtain

$$S'(t) = S_{A_1}((x_1 + x_4)t)S_{A_3}((x_6 + x_9)t)S_{A_1}(x_{10}t).$$

In the second case, suppose that $A_3 = 0$, then we get

$$S'(t) = S_{A_1}(x_1t)S_{A_2}((x_2 + x_5)t)S_{A_1}((x_7 + x_{10})t).$$

In the third case, suppose that $A_1 = 0$, then we obtain

$$S'(t) = S_{A_2}(x_2t)S_{A_3}((x_3 + x_6)t)S_{A_2}(x_8t).$$

One of those case would imply that there is 5-factor fourth-order integrator which is impossible.

It shows that any minimal reversible fourth-order integrator S_4 may be found by looking for a 7 factor operator $S(t)$ of maximal length 9, such that $S_4 = S(t)S^{-1}(-t)$.

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If we look for all possible reversible 13 factor fourth-order integrators we get a zero dimensional algebraic variety of degree 12 and c_0 satisfies

$$(c_0^9 - 2\ c_0^8 + c_0^7 + \tfrac{2}{3}\ c_0^6 - c_0^5 + \tfrac{2}{3}\ c_0^3 - \tfrac{5}{9}\ c_0^2 + \tfrac{2}{9}\ c_0 - \tfrac{1}{27})(c_0^3 + c_0^2 - c_0 + \tfrac{1}{3}) = 0.$$

We therefore get 2 sets of solutions:

$$\begin{aligned}
&c_0 = 2e_1 = 2d_1,\\
&c_1 = e_2 = d_2 = 27\ c_0^8 - \tfrac{81}{2}\ c_0^7 + \tfrac{9}{2}\ c_0^6 + \tfrac{45}{2}\ c_0^5 - 15\ c_0^4 - 9\ c_0^3 + \tfrac{27}{2}\ c_0^2 - \tfrac{15}{2}\ c_0 + 2,\\
&c_2 = d_3 = e_3 = -c_1 - \tfrac{1}{2}c_0 - \tfrac{1}{2},\\
&c_0^9 - 2\ c_0^8 + c_0^7 + \tfrac{2}{3}\ c_0^6 - c_0^5 + \tfrac{2}{3}\ c_0^3 - \tfrac{5}{9}\ c_0^2 + \tfrac{2}{9}\ c_0 - \tfrac{1}{27} = 0.
\end{aligned}$$

and

$$\begin{aligned}
&c_1 = e_2 = 0,\\
&d_2 = d_3 = e_3 = \tfrac{1}{2}c_2 = -\tfrac{1}{4}\ c_0 + \tfrac{1}{4},\\
&d_1 = \tfrac{1}{2}c_0,\\
&e_1 = \tfrac{1}{4}c_0 + \tfrac{1}{4},\\
&c_0^3 + c_0^2 - c_0 + \tfrac{1}{3} = 0.
\end{aligned}$$

The first set gives 17-factor integrators while the second set gives 13-factor integrators as product of four S_{A_1}, six S_{A_2} and three S_{A_3}. As we can exchange A_1, A_2 and A_3, we shall take for A_2 the part for which the time-evolution mapping has the lowest cost.

3.5 Planetary Hamiltonian

Wisdom and Holman ([18]) have used a symplectic integrator for their integrations of the solar system which allowed them to use a longer step size. They used an expression of the Planetary Hamiltonian in term of Jacobi coordinates for which the Hamiltonian is splitted in two parts. Here we prefer to use the canonical heliocentric variables of Poincaré which provides a more elegant and symmetrical formulation of the hamiltonian ([12]), which is then expressed in three integrable parts : H_0, T_1, U_1.

H_0 corresponds to the sum of n disjoint Keplerian problems. T_1 is the perturbation depending only on the actions and U_1 depends only on the positions. We are thus led to search for symplectic integrators for Hamiltonians which decompose in three integrable parts $H = A + B + C$.

Let us consider O the center of mass of $n+1$ bodies of masses $m_0, \ldots, m_n$ in gravitational interaction. Let u_i be the coordinates with respect to O and and $\Delta_{i,j} = \|u_i - u_j\|$, the Hamiltonian becomes

$$H = T + U = \tfrac{1}{2} \sum_{i=0}^{n} m_i \left\|\dot{u}_i\right\|^2 - G \sum_{0 \le i < j \le n} \tfrac{m_i m_j}{\Delta_{i,j}}. \tag{65}$$

Let $\tilde{u}_i = m_i \dot{u}_i$, we obtain in canonical coordinates

$$T = \tfrac{1}{2} \sum_{i=0}^{n} \frac{\|\tilde{u}_i\|}{m_i}. \tag{66}$$

Let us consider now the heliocentric coordinates: $r_0 = u_0, r_i = u_i - u_0$. In order to have canonical variables, we take

$$\tilde{r}_0 = \sum_{i=0}^{n} u_i = 0, \tilde{r}_i = \tilde{u}_i, \quad 1 \le i \le n \tag{67}$$

or

$$\tilde{u}_0 = -\sum_{i=1}^{n} \tilde{r}_i, \tilde{u}_i = \tilde{r}_i, \quad 1 \le i \le n. \tag{68}$$

The kinetic energy becomes

$$T = \tfrac{1}{2} \sum_{i=1}^{n} \frac{\|\tilde{r}_i\|^2}{m_i} + \tfrac{1}{2} \frac{\left\|\sum_{i=1}^{n} \tilde{r}_i\right\|^2}{m_0} \tag{69}$$

$$= \tfrac{1}{2} \sum_{i=1}^{n} \|\tilde{r}_i\|^2 \left[\tfrac{1}{m_i} + \tfrac{1}{m_0}\right] + \sum_{0<i<j} \frac{\tilde{r}_i . \tilde{r}_j}{m_0} \tag{70}$$

and

$$U = -G \sum_{i=1}^{n} \frac{m_0 m_i}{r_i} - G \sum_{0<i<j \le n} \frac{m_i m_j}{\Delta_{i,j}}. \tag{71}$$

One can write $H = H_0 + H_1$ with $H_0 = T_0 + U_0$, $H_1 = T_1 + U_1$ where H_0 is the Hamiltonian of n disjoint two body problems: the planet of mass $\frac{m_0 m_i}{m_0 + m_i}$ around the sun of mass $m_0 + m_i$. H_1 may be considered as an interactive perturbation. We thus have

$$T_0 = \tfrac{1}{2} \sum_{i=1}^{n} \|\tilde{r}_i\|^2 \left[\tfrac{1}{m_i} + \tfrac{1}{m_0}\right], U_0 = -G \sum_{i=1}^{n} \frac{m_0 m_i}{r_i} \tag{72}$$

$$T_1 = \sum_{0<i<j} \frac{\tilde{r}_i . \tilde{r}_j}{m_0}, U_1 = -G \sum_{0<i<j \le n} \frac{m_i m_j}{\Delta_{i,j}}. \tag{73}$$

H_1 is particularly simple as the kinetic energy and the potential energy depend on coordinates and momenta respectively.

Writing $H = H_0 + T_1 + U_1$ where T_1 is very easy to integrate, we can try to use the integrator defined in (57). That is what we will do in a near future at the Bureau des Longitudes.

4 Conclusion

We showed in this paper that there are exactly 5 7-factor fourth-order symplectic integrators. Three of them are known (see [7, 20]). There are exactly 46 11-factor fifth-order symplectic We showed, that there are exactly 39 15-factor reversible sixth-order symplectic integrators. All of them are reversible products of second-order integrators. Three of them were known ([20]). In the case when $h = A+B+C$, we show that minimal second-order integrator have length 5 and reversible fourth-order integrator have length 13.

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