Relations among Lie Formal Series and Construction of Symplectic Integrators *

P.-V. Koseleff

Aleph et Géode
Centre de Mathématiques, École Polytechnique
91128 Palaiseau
e-mail : koseleff@polytechnique.fr

Abstract. Symplectic integrators are numerical integration schemes for hamiltonian systems. The integration step is an explicit symplectic map. 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 possible solutions for integrators of low order.

1 Introduction

Lie series and Lie transformations have found many applications, particularly in celestial mechanics (see [3]) or in hamiltonian perturbation theory (see for example [2, 4, 6]). These techniques have the advantage of providing explicit approximating systems that are also hamiltonian.

In hamiltonian mechanics, it is often important to know the time evolution mapping, that is to say the position of the solution after a certain given time. In celestial mechanics, long integrations have mostly used high order multistep integration methods. A disadvantage of such methods is that the error in position grows quadratically in time or linearly with symmetric integrators.

For very long time integration, there has been recently a development of numerical methods preserving the symplectic structure (see for example [7, 14, 15, 16]), 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 give some general methods to manipulate formal Lie series and Lie algebra automorphisms. We recall some theorems related to exponential

* Published in AAECC'10 proceedings, Lecture Notes in Computer Science, **673**, 1993

identities and give explicit methods to compute them. They make use the Lyndon basis, which is particularly adapted to this problem.

In section **3.**, we recall first some definitions of the Hamilton formalism. Then we show how the algorithms described in section **2.** provide symplectic integrators. The idea of such constructions originates in Forest & Ruth ([7]) or more recently Yoshida ([16]). Our approach in this paper is to combine the use of proper Lie transforms and exponentials. This avoids many unnecessary direct calculations of exponential indentities. At the end we propose some improvement in the case when the Hamiltonian is seperated into kinetic and potential energies.

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

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

In this paper 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. X^* is totally ordered with the lexicographic order.

$M(X)$ is the free magma generated by X. Having defined $M_1(X)$ as X, we define $M_n(X)$ by induction on n:

$$M_n(X) = \bigcup_{p+q=n} M_p \times M_q \quad \text{and} \quad M(X) = \bigcup_{n\geq 1} M_n(X). \tag{1}$$

$\mathcal{A}_R(X)$ 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:

$$[a,[b,c]] + [b,[c,a]] + [c,[a,b]] = 0. \tag{2}$$

$L_R(X)$ 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, 9, 10]):

$$\sum_{d|n} d \dim L_d(X) = q^n. \tag{3}$$

2.2 Formal Lie series

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

$$\tilde{L}(X) = \prod_{n \geq 0} \tilde{L}_n(X) \quad \text{and} \quad \tilde{\mathcal{A}}(X) = \prod_{n \geq 0} \tilde{\mathcal{A}}_n(X). \tag{4}$$

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

$$[x, y] = \sum_{n \geq 0} \sum_{p+q=n} [x_p, y_q]. \tag{5}$$

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

$$\begin{array}{rlrl} \exp : \tilde{\mathcal{A}}(X)^+ & \to 1 + \tilde{\mathcal{A}}(X)^+ & \log : 1 + \tilde{\mathcal{A}}(X)^+ & \to \tilde{\mathcal{A}}(X)^+ \\ x & \mapsto \sum_{n \geq 0} \dfrac{x^n}{n!} & x & \mapsto -\sum_{n \geq 1} \dfrac{(1-x)^n}{n!}. \end{array} \tag{6}$$

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*

$$\log\left[\exp(x)\exp(y)\right] \in \tilde{L}(X)^+. \tag{7}$$

More precisely, we have the following

Lemma 2. *Given $x, y \in \tilde{L}(X)^+$, we have*

— $\exp(x)\exp(y) = \exp(z)$ *where* $z \in \tilde{L}(X)^+$,
— $z = z_p + z_q + \sum_{n \geq p+q} z_n$ *and* $z_p + z_q = x_p + y_q$,
— $z_m \in \tilde{L}_m(x_p, \ldots, x_m, y_q, \ldots, y_m)$ *for* $m \geq p + q$.

Using the preceding lemmas we deduce (see [12]) the

Proposition 3 (Factored product expansion). *Given $k \in \tilde{L}(X)^+$, there is a unique series $g \in \tilde{L}(X)^+$ such that*

$$\exp(\textstyle\sum_{n\geq 1} k_n) = \cdots \exp(g_n) \cdots \exp(g_1). \tag{8}$$

The above proposition is proved by induction, constructing $g \in \tilde{L}(X)$ and $k^{(p)} \in \prod_{n>p} \tilde{L}_n(X)$ such that, for each $p \geq 1$,

$$\exp(k) = \exp(k^{(p)}) \exp(g_p) \cdots \exp(g_1). \tag{9}$$

2.3 Lie series automorphisms

We denote for x in $\tilde{L}(X)$ by $L(x)$ or L_x, the Lie operator $L_x y = [x, y]$. From the Jacobi identity (2) we have $[L_x, L_y] = L_{[x,y]}$, in which $[,]$ denotes the commutator. 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

$$T L_f T^{-1} = L_{Tf}. \tag{10}$$

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

$$\exp(L_x) y = \sum_{i\geq 0} \frac{L_x^i}{i!} y. \tag{11}$$

From the Jacobi identity (2), we have by induction on $k \geq 0$, for any $f, g, h \in \tilde{L}(X)^+$

$$L_f^k [g, h] = \sum_{i=0}^{k} \binom{k}{i} \left[L_f^i g, L_f^{k-i} h \right].$$

We therefore deduce that

$$\begin{aligned} \exp(L_f)[g, h] &= \sum_{n\geq 0} \frac{1}{n!} \sum_{p=0}^{n} \binom{n}{p} \left[L_f^p g, L_f^{n-p} h \right] \\ &= \sum_{p+q\geq 0} \tfrac{1}{p+q!} \tfrac{p+q!}{p!q!} \left[L_f^p g, L_f^q h \right] = [\exp(L_f) g, \exp(L_f) h]. \end{aligned} \tag{12}$$

Thus, for each $x \in \tilde{L}(X)$, $\exp(L_x)$ is a Lie algebra automorphism. 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. Using (10) and $\frac{d}{dt}\exp(tL_x) = L_x \exp(tL_x)$, we obtain the following identity:

$$\frac{d}{dt}\exp(tL_x)\exp(tL_y) = L\left[x + \exp(tL_x)y\right]\exp(tL_x)\exp(tL_y). \qquad (13)$$

The map $S(t) = \exp(tL_x)\exp(tL_y) \in \mathbf{G}$ is the solution of (13). For a given z, the solution of $\frac{d}{dt}S = L_z S$ is not necessarily $\exp(tL_z)$ as z may depend on t, but is known as the inverse Lie transformation associated to $\int_t z dt$. For $w = \sum_{n\geq 1} t^n w_n$, T_w and T_w^{-1} are the solution ([3]) of

$$\frac{d}{dt}T_w = -T_w L_{\frac{dw}{dt}} \quad \text{and} \quad \frac{d}{dt}T^{-1}w = L_{\frac{dw}{dt}} T_t^{-1}. \qquad (14)$$

For $g \in \tilde{L}(X)$, we have (see [2, 3]) $G = \sum_{n\geq 0} G_n = T_w^{-1} g$ where

$$G_0 = g_0, \quad G_{0,n} = g_n, \quad G_{p,q} = \sum_{k=1}^{p} \tfrac{k}{p}[w_k, G_{p-k,q}], \quad G_n = \sum_{p=0}^{n} G_{p,n-p}. \quad (15)$$

The Dragt-Finn transform. There is another transformation that plays an important role in the Lie transformations theory that is called the Dragt-Finn transform and is an infinite product of exponential maps (see [4]).

Given $g = \sum_{n\geq 1} g_n$, we define M_g and M_g^{-1} as

$$M_g = \exp(-L_{g_1})\cdots\exp(-L_{g_n})\cdots \quad \text{and} \quad M_g^{-1} = \cdots\exp(L_{g_n})\cdots\exp(L_{g_1}) \quad (16)$$

Using proposition 3, we express the exponential of a Lie operator as a Dragt-Finn transform.

2.4 Relations between the exponential and the Lie transform.

The three above transformations are totally defined by generating series which satisfy the following :

Proposition 4. *Given $w, k, g \in \tilde{L}(X)^+$, there exist*

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

We first prove the third part of the above proposition.
Given $M_g^{-1}(t) = \cdots\exp(t^n L_{g_n})\cdots\exp(tL_{g_1})$, we have using (10)

$$\begin{aligned}\frac{d}{dt}M_g &= \sum_{n\geq 1}\left[e^{-tL_{g_3}}\cdots e^{-t^{n-1}L_{g_{n-1}}}\right]\left[\frac{d}{dt}\left[e^{-t^n L_{g_n}}\right]\right]\left[e^{-t^{n+1}L_{g_{n+1}}}\cdots\right]\\ &= \sum_{n\geq 1}\left[e^{-tL_{g_3}}\cdots e^{-t^{n-1}L_{g_{n-1}}}\right]\left[-nt^{n-1}L_{g_n}e^{-t^n L_{g_n}}\right]\left[e^{-t^{n+1}L_{g_{n+1}}}\cdots\right]\end{aligned}$$

$$
\begin{aligned}
&= M_g \sum_{n\geq 1} M_g^{-1} \left[e^{-tL_{g_3}} \cdots e^{-t^{n-1}L_{g_{n-1}}}\right] \left[-nt^{n-1}L_{g_n}\right] \left[e^{-t^n L_{g_n}} \cdots\right] \\
&= M_g \sum_{n\geq 1} \left[\cdots e^{t^n L_{g_n}}\right] \left[-nt^{n-1}L_{g_n}\right] \left[e^{-t^n L_{g_n}} \cdots\right] \\
&= M_g L \left[\sum_{n\geq 1} -nt^{n-1} \left[\cdots e^{t^n L_{g_n}}\right] g_n\right]. \qquad (17)
\end{aligned}
$$

On the other hand, from (14), we have $\frac{d}{dt}T_w = -T_w L_{\frac{dw}{dt}}$. With the initial conditions $T_w(0) = M_g(0) = Id$, we deduce that $T_w = M_g$ iff

$$
\frac{dw}{dt} = \sum_{n\geq 1} t^{n-1} \left[\sum_{k=1}^{n} k \sum_{\substack{(k+1)m_{k+1}+\cdots \\ +(n-k)m_{n-k}=n-k}} \frac{L_{g_{n-k}}^{m_{n-k}} \cdots L_{g_{k+1}}^{m_{k+1}}}{m_{k+1}! \cdots m_{n-k}!} g_k\right], \qquad (18)
$$

or equivalently

$$
w_n = \sum_{k=1}^{n} \frac{k}{n} \sum_{\substack{(k+1)m_{k+1}+\cdots \\ +(n-k)m_{n-k}=n-k}} \frac{L_{g_{n-k}}^{m_{n-k}} \cdots L_{g_{k+1}}^{m_{k+1}}}{m_{k+1}! \cdots m_{n-k}!} g_k = g_n + G_n \qquad (19)
$$

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

Using the proposition 3, one proves the existence of $g = \sum_{n\geq 1} g_n$ such that

$$
\exp(\textstyle\sum_{n\geq 1} L_{k_n}) = \cdots \exp(L_{g_n}) \cdots \exp(L_{g_1}), \qquad (20)
$$

in which $g_n = k_n + K_n$ and $K_n \in L_{\mathbb{Q}}(k_1, \ldots, k_{n-1})$. Combining (19) and (20) we deduce (4).

⋆⋆⋆

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 from (13).

2.5 Computing the relations.

In order to compute the relations between the generating series we try to solve at each order

$$
\exp(L_k)a = T_w^{-1}a. \qquad (21)
$$

We first have the following lemma resulting from the expansion of the exponential or the Lie transform (15)

Lemma 5. *Let* $T = \exp(L_k)$ *(resp.* $T = T_w^{-1}$*) and* $A = \sum_n A_n = Ta$*, then for each* $n \geq 0$*,* $A_n = -[a, k_n] + K_n$ *(resp.* $A_n = -[a, w_n] + W_n$*) in which* $K_n \in L(a, k_1, \dots k_{n-1})$ *(resp.* $W_n \in L(a, w_1, \dots w_{n-1})$*).*

In order to compute the relations, we need a basis of the free Lie algebra $L(X)$. We propose here the use of the Lyndon basis that has many useful properties.

Basis of the free Lie Algebra. Given $w = uv$ a word of X^*, we will say that u and v are left factor and right factor respectively. For any $u, v \in X^*$, uv and vu are said conjugate and therefore X^* is divided in conjugate classes. The minimal element of each conjugate class is called a Lyndon word. The set $\mathbf{L}$ of Lyndon words satisfies many properties like (see [10])

Lemma 6. $w \in \mathbf{L}$ *iff there exist* $u < v \in \mathbf{L}$ *such that* $w = uv$*.*

Unfortunately a Lyndon word may be decomposed in many ways. For example $aabb = a.abb = aab.b$. For $l < m$ and $lm \in \mathbf{L}$, we call $\sigma(lm) = (l, m)$ the standard factorization of lm when $|m|$ is maximal. Therefore, we define a one-to-one correspondence between $\mathbf{L}$ and the Lyndon brackets $\mathcal{L} \subset M(X)$. We define

- $\Lambda : \mathbf{L} \to \mathcal{L} \subset M(X)$ by: $\Lambda(a) = a$ if $a \in X$ otherwise $\Lambda(lm) = (\Lambda(l), \Lambda(m))$ if $\sigma(lm) = (l, m)$.
- $\delta : M(X) \to X^*$ as the canonical application of unparenthesing.

Denoting $\mathcal{L} \cap M_n(X)$ by $\mathcal{L}_n(X)$, we have (see [10]) the following

Theorem 7. $\mathcal{L}_n(X)$ *is a basis of* $L_n(X)$*.*

Construction of the basis. One of the main properties is that (see [10])

Lemma 8. *if* $u < v \in \mathcal{L}$ *then* $[u, v] \in \mathcal{L}$ *iff* $|u| = 1$ *or* $u = [u_1, u_2] < v \leq u_2$*.*

One can now built the Lyndon basis as follows:

$$\begin{aligned}
\mathcal{L}_1(X) &= X, \\
\mathcal{L}_2(X) &= \{[x, y]; x < y \in \mathcal{L}_1\}, \\
\mathcal{L}_n(X) &= \bigcup_{x \in \mathcal{L}_1(X)} \{[x, y]; y \in \mathcal{L}_{n-1}(X), x < y\} \qquad (22) \\
& \bigcup \bigcup_{p=2}^{n} \bigcup_{x \in \mathcal{L}_p(X)} \{[x, y]; y \in \mathcal{L}_{n-p}(X), [x_1, x_2] = x < y \leq x_2\}. \qquad (23)
\end{aligned}$$

If $\mathcal{L}_1$ is well sorted then the $\bigcup$ in (23) are disjoint and the results are sorted. The knowledge of the basis is actually not very useful to work in the free Lie algebra except in some specific cases that will occur in the last section.

Decomposition onto the basis. We give here an algorithm for writing a Lie polynomial in terms of Lyndon brackets. This algorithm (see [10]) is also a proof that the Lyndon brackets generate the free Lie algebra.

Given two polynomials that are linear combinations of Lyndon brackets $p = \sum_i \alpha_i p_i$ and $q = \sum_i \beta_i q_i$, we have $p * q = \sum_{i,j} \alpha_i \beta_j \mathtt{mult}(p_i, q_j)$ in which $\mathtt{mult}(a, b)$ denotes the decomposition of $[a, b]$ onto the Lyndon basis. The point is to know how to multiply two Lyndon brackets. We will use the algorithm proposed by Perrin [10]. Implementations have been realized by Petitot [11] and myself more recently.

if $u = v$ **then** $\mathtt{mult}(u, v) := 0$
else if $v < u$ **then** $\mathtt{mult}(u, v) := -\mathtt{mult}(v, u)$
if $|u| = 1$ **then** $\mathtt{mult}(u, v) := 1.[u, v]$
else $u = [u_1, u_2]$ **if** $v \leq u_2$ **then** $\mathtt{mult}(u, v) := 1.[u, v]$
else $\mathtt{mult}(u, v) := 1.u_1 * \mathtt{mult}(u_2, v) + \mathtt{mult}(u_1, v) * 1.u_2$.

2.6 Solving triangular systems

We deduce from the lemma 8 the following useful

Lemma 9. *Let $X = \{a\} \bigcup X_1$ where $a < b$ for each $b \in X_1$. Then for each $x = \sum_i \alpha_i x_i \in L(X_1)$, the decomposition of $[a, x]$ onto the Lyndon basis of $\mathcal{L}(X)$ is $[a, x] = \sum_i \alpha_i [a, x_i]$.*

This lemma shows that the injective mapping

$$\mathcal{L}(X_1) \to \mathcal{L}(\{a\} \bigcup X_1) \tag{24}$$

$$x \mapsto (a, x) \tag{25}$$

may be extended to $L_a : L(X_1) \to L(\{a\} \bigcup X_1)$. This property is specific to the Lyndon basis.

⋆⋆⋆

With this lemma, (21) becomes a triangular system in form

$$\begin{cases} [a, k_1] = [a, w_1] \\ [a, k_2] + K_2 = [a, w_2] + W_2 \\ \vdots \; \vdots \; \vdots \\ [a, k_n] + K_n = [a, w_n] + W_n \end{cases}, \tag{26}$$

in which $K_i - W_i \in L_{\mathbb{Q}}(a, k_1, \cdots, k_{i-1}, w_1, \cdots, w_{i-1})$. This system can be solved by successive evaluations of the k_i's (resp. w_i's) using the the factorization lemma 9. The relation (19) cannot be generated using equation (21) and the Hall basis.

⋆⋆⋆

This method may be used in order to express any $T \in \mathbf{G}$ as an exponential or as the inverse of a Lie transform. Let $A = Ta = \sum_{n\geq 0} A_n$. We formally compute for example $E = \exp(L_k)a = \sum_{n\geq 0} E_n \in \tilde{L}(a, k_1, \ldots, k_n, \ldots)$. We therefore obtain the following triangular system

$$\begin{cases} A_0 = E_0 = a \\ A_1 = E_1 = -[a, k_1] \\ A_2 = E_2 = -[a, k_2] + R_2 \\ \quad\vdots \quad\;\; \vdots \quad\;\; \vdots \\ A_n = E_n = -[a, k_1] + R_n \end{cases} \tag{27}$$

that may be solved by the factorization lemma (9) as the system is consistent.

This method can also be applied for the computing of any relation between generating series in $\mathbf{G}$ like the Baker-Campbell-Hausdorff formula. For example we found at the order 6

$$\begin{aligned} \log[\exp x \exp y] = {} & x + y - \tfrac{1}{2}\,[x,\, y] + \tfrac{1}{12}\,[x,\, [x,\, y]] + \tfrac{1}{12}\,[[x,\, y],\, y] \\ & - \tfrac{1}{24}\,[x,\, [[x,\, y],\, y]] - \tfrac{1}{720}\,[x,\, [x,\, [x,\, [x,\, y]]]] + \tfrac{1}{180}\,[x,\, [x,\, [[x,\, y],\, y]]] \\ & + \tfrac{1}{180}\,[x,\, [[[x,\, y],\, y],\, y]] + \tfrac{1}{120}\,[[x,\, y],\, [[x,\, y],\, y]] + \tfrac{1}{360}\,[[x,\, [x,\, y]],\, [x,\, y]] \\ & - \tfrac{1}{720}\,[[[[x,\, y],\, y],\, y],\, y] + \tfrac{1}{1440}\,[x,\, [x,\, [x,\, [[x,\, y],\, y]]]] \\ & - \tfrac{1}{360}\,[x,\, [x,\, [[[x,\, y],\, y],\, y]]] - \tfrac{1}{240}\,[x,\, [[x,\, y],\, [[x,\, y],\, y]]] \\ & - \tfrac{1}{720}\,[x,\, [[x,\, [x,\, y]],\, [x,\, y]]] + \tfrac{1}{1440}\,[x,\, [[[[x,\, y],\, y],\, y],\, y]] \end{aligned}$$

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 Hamiltonian formalism

An hamiltonian system is the given of a phase space E which can be identified to $\mathbb{R}^{2n}$, a set of variables

$$(q, p) = (q_1, \ldots, q_n, p_1, \ldots, p_n) = (z_1, \ldots, z_{2n}), \tag{28}$$

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

$$\dot{p}_i = -\frac{\partial h}{\partial q_i}, \dot{q}_i = \frac{\partial h}{\partial p_i}, \quad 1 \leq i \leq n, \tag{29}$$

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

$$\{f, g\} = \sum_{i=1}^{n} \frac{\partial f}{\partial p_i}\frac{\partial g}{\partial q_i} - \frac{\partial g}{\partial p_i}\frac{\partial f}{\partial q_i} \tag{30}$$

that turns the set of smooth functions on E onto a Lie algebra, (29) becomes

$$\dot{z}_i = \{z_i, h\} = -L_h z_i, \quad 1 \leq i \leq 2n, \tag{31}$$

and for any function f on the phase space we get

$$\dot{f} = \tfrac{\partial f}{\partial t} + \{f, h\} = -L_h f + \tfrac{\partial f}{\partial t} \tag{32}$$

along the trajectories. In particular, if h is not time-dependent, it is a first integral of the system.

From the Jacobi identity (2), we deduce that $[L_f, L_g] = L_{\{f,g\}}$, where $[,]$ denotes the commutator.

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 $TL_fT^{-1} = L_{Tf}$.

3.1 Time-evolution mapping

A canonical transformation appearing in hamiltonian mechanics is the time-evolution mapping $S_h(t) : z \mapsto z(t)$. From (31), $S_h(t)$ is the solution of the differential equation

$$\frac{d}{dt}S_h(t) = -S_h(t)L_h, S_h(0) = Id. \tag{33}$$

If h is not time-dependent we have $S_h(t) = e^{-tL_h}$ and a formal solution of (31) is given by its Taylor series, called Lie series

$$z(t) = \sum_{n\geq 0} t^n \frac{L_h^n}{n!} z. \tag{34}$$

For example, if $h = \frac{\omega}{2}(p^2 + q^2)$, then

$$S_h(t) = \begin{pmatrix} \cos(\omega t) & -\sin(\omega t) \\ \sin(\omega t) & \cos(\omega t) \end{pmatrix}.$$

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 and from proposition (4), there exists $k = \sum_{n\geq 0} t^n k_n$ such that $S_h(t) = e^{-tL_k}$. Furthermore, we have an algorithm to compute k. k is an invariant function of the system but is not the Hamiltonian governing the system.

3.2 Discrete integration

h is not necessarly as simple as above and it may be quit hard to calculate $S_h(t)$ so we try to calculate truncated Lie series or approximating solutions by discrete integration.

The Euler scheme to integrate (29) on the path τ is the mapping

$$\begin{pmatrix} q \\ p \end{pmatrix} \to \begin{pmatrix} q_\tau \\ p_\tau \end{pmatrix} = \begin{pmatrix} q \\ p \end{pmatrix} + \tau \begin{pmatrix} \frac{\partial h}{\partial p} \\ -\frac{\partial h}{\partial q} \end{pmatrix} \tag{35}$$

which is generally not symplectic. When $h = \frac{\omega}{2}(p^2 + q^2)$ we obtain the mapping

$$\begin{pmatrix} p_\tau \\ q_\tau \end{pmatrix} = \begin{pmatrix} 1 & -\omega\tau \\ \omega\tau & 1 \end{pmatrix} \begin{pmatrix} p \\ q \end{pmatrix} \tag{36}$$

which is not symplectic since its determinant equals $1 + \omega^2\tau^2$. Furthermore at each step τ, the energy grows by a factor $1 + \omega^2\tau^2$. As the total energy is a first integral for the hamiltonian system, it is obvious that the difference between the exact solution and the discrete solution (36) grows secularly. Moreover the product $S(t)$ of the two symplectic transformations

$$\begin{cases} p \longrightarrow p - \tau \dfrac{\partial H}{\partial q} \\ q \longrightarrow q \end{cases} \quad \text{and} \quad \begin{cases} p \longrightarrow p \\ p \longrightarrow p + \tau \dfrac{\partial H}{\partial p} \end{cases} . \tag{37}$$

is symplectic. With $h = \frac{\omega}{2}\left(p^2 + q^2\right)$, the previous operator becomes

$$S(\tau) = \begin{pmatrix} 1 - \omega^2\tau^2 & \omega\tau \\ -\omega\tau & 1 \end{pmatrix}. \tag{38}$$

3.3 Symplectic schemes

The case when $h = T(p) + V(q)$ is a sum of a kinetic energy and a potential plays an important role. Let us denote by $S_T(t) = e^{-tL_T}$ and $S_V(t) = e^{-tL_V}$ the time-evolution mappings associated to T and V respectively. As $\{V, p\}$ depends on q and $\{T, q\}$ depends on p, we have

$$S_T(t)p = p, S_T(t)q = q + t\frac{\partial T}{\partial p}, S_V(t)p = p - t\frac{\partial V}{\partial q}, S_V(t)q = q. \tag{39}$$

On the other hand, we have through the Baker-Campbell-Hausdorff formula

$$S(t) = S_T(t)S_V(t) = e^{-t(L_T+L_V)+\frac{t^2}{2}L_{\{T,V\}}+o(t^2)} = S_h(t) + o(t) \tag{40}$$

that is to say $S(t)$ is a linear symplectic map close to the time evolution mapping.

The main idea is to construct for given n and k, $S^{(n)}(t) = S_h(t) + o(t^k)$ as

$$S^{(n)}(t) = S_T(c_1 t)S_V(d_1 t) \cdots S_T(c_n t)S_V(d_n t). \tag{41}$$

For a given integration step, we then obtain a series of transformations

$$q^0 = q, p^0 = p, p^{i+1} = p^i - d_i \frac{\partial V}{\partial q}(q^i), q^{i+1} = q^i + c_i \frac{\partial T}{\partial p}(p^{i+1}) \tag{42}$$

and $p_\tau = p^n, q_\tau = q^n$ are computed after n evaluations of $\frac{\partial T}{\partial p}$ and $\frac{\partial V}{\partial q}$.

3.4 Symplectic Integrators

Let us consider an Hamiltonian $H = A + B$, the two maps $S_A(t) = e^{-tL_A}$ 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

$$S_A(c_1 t) S_B(d_1 t) \cdots S_A(c_n t) S_B(d_n t) = e^{-tL_H} + o(t^k). \tag{43}$$

Direct method: This can be reformulated, looking for $c_1, \ldots, c_n, d_1, \ldots d_n$, such that

$$S_A(c_1 t) S_B(d_1 t) \cdots S_A(c_n t) S_B(d_n t) z = e^{-tL_H} z + o(t^k). \tag{44}$$

At each order p, let us consider $\tilde{L}_p(z, A, B)$, in which $|z|_* = 0$, $|A|_* = |B|_* = 1$. The part of order t^p of the left hand side of (43) belongs to the subspace of $\tilde{L}_{p+1}(z, A, B)$ generated by the Lie monomials in which z appears once. The dimension of this subspace is 2^p.

Invariant function: The problem (43) is equivalent to the finding of an invariant function $K(t) = H + o(t^{k-1})$ such that

$$S_A(c_1 t) S_B(d_1 t) \cdots S_A(c_n t) S_B(d_n t) = e^{-tK}. \tag{45}$$

Using the Baker-Campbell-Hausdorff formula, one express $K = \sum_{n \geq 0} t^n K_{n+1}$ onto $\tilde{L}(A, B)$, in which $|A|_* = |B|_* = 1$. K_p belongs to $\tilde{L}_p(A, B)$ which dimension is given by Witt's formula.

Perturbed Hamiltonian: The problem (43) is also equivalent to the finding of an Hamiltonian $W(t) = H + o(t^{k-1})$ such that

$$S_A(c_1 t) S_B(d_1 t) \cdots S_A(c_n t) S_B(d_n t) = S_W. \tag{46}$$

Using (13) and (14), one can express $W(t) = \sum_{n \geq 0} t^n W_{n+1}$ in $\tilde{L}(A, B)$. With this method, there is no need to calculate any exponential identity. We have to bear in mind that $S_W(t) = T_{\tilde{W}}$ in which $\frac{d\tilde{W}}{dt} = W$.

⋆⋆⋆

Using the third method, one gets the four first symplectic integrators.

- For $k = 1$ one has two linear equations and a solution is $c_1 = d_1 = 1$
- For $k = 2$ the solution is reached for $n = 2$ and $c_1 = c_2 = \frac{1}{2}, d_1 = 1$. We thus obtain the second-order symplectic integrator $S_2 = S_A(\frac{t}{2}) S_B(t) S_A(\frac{t}{2})$.

– For $k = 3$, we get after reduction

$$d_2 + 2c_1 = 1, d_1 - 2c_1 = 0, c_3 + c_1 = \frac{1}{2}, c_2 = \frac{1}{2}, c_1^2 - \frac{1}{2}c_1 + \frac{1}{12} = 0. \quad (47)$$

We thus have 2 complex solutions involving 5 factors. A real solution with 6 factors is for example (see also [7])

$$c_1 = -c_2 = \frac{2}{3}, d_3 = \frac{1}{24}, d_2 = -\frac{3}{4}, d_1 = -\frac{7}{24}, c_3 = 1. \quad (48)$$

– For $k = 4$, we get after reduction by some Gröbner package implemented in Axiom

$$\begin{cases} d_3 + 288\ c_1^4 - 312\ c_1^3 + 96\ c_1^2 - 14\ c_1 + \frac{1}{2} = 0 \\ d_2 - 288\ c_1^4 + 312\ c_1^3 - 96\ c_1^2 + 16\ c_1 - \frac{3}{2} = 0 \\ d_1 - 2\ c_1 = 0 \\ c_4 + 144\ c_1^4 - 156\ c_1^3 + 48\ c_1^2 - 7\ c_1 + \frac{1}{4} = 0 \\ c_3 + c_1 - \frac{1}{2} = 0 \\ c_2 - 144\ c_1^4 + 156\ c_1^3 - 48\ c_1^2 + 7\ c_1 - \frac{3}{4} = 0 \\ c_1^5 - \frac{5}{4}\ c_1^4 + \frac{13}{24}\ c_1^3 - \frac{1}{8}\ c_1^2 + \frac{1}{64}\ c_1 - \frac{1}{1152} = 0 \end{cases} . \quad (49)$$

The last polynomial is factorized over $\mathbb{Q}$ in $(c_1^2 - \frac{1}{4}\ c_1 + \frac{1}{24})(c_1^3 - c_1^2 + \frac{1}{4}\ c_1 - \frac{1}{48})$. Taking c_1 as one of the complex roots of $c_1^2 - \frac{1}{4}\ c_1 + \frac{1}{24} = 0$, one finds

$$d_3 + 2\ c_1 = \frac{1}{2}, d_2 = \frac{1}{2}, d_1 = 2\ c_1, c_4 + c_1 = \frac{1}{4}, c_3 + c_1 = \frac{1}{2}, c_2 - c_1 = \frac{1}{4} \quad (50)$$

or equivalently

$$c_4 = \bar{c_1}, c_3 = \bar{c_2} = \frac{1}{2} - c_1, d_3 = \bar{d_1} = 2\bar{c_1}, d_2 = \frac{1}{2}. \quad (51)$$

Taking c_1 as root of $c_1^3 - c_1^2 + \frac{1}{4}\ c_1 - \frac{1}{48} = 0$, for example $c_1 = \frac{1}{2(\sqrt[3]{2}-1)}$, one gets

$$d_3 = d_1 = 2c_1, d_2 = 1 - 4c_1, c_4 = c_1, c_2 = c_3 = \frac{1}{2} - c_1. \quad (52)$$

We found all the solutions for this integrator. The 3 above were already known.

– This method cannot be applied for $k = 6$ as the set of equations is too big. There is no integrator with less than 13 factors, as tested with the Macaulay package.

The real valued integrators for $k = 2$ or 4 are reversible, that means $S(-t) = S^{-1}(t)$.

3.5 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 10 ([13]). *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 built 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 should find a sixth-order integrator as a product of 19 operators.

⋆⋆⋆

One can try to find directly reversible integrators looking for

$$S_R^{(n)}(t)=S_A(c_nt)S_B(d_nt)\cdots S_A(c_1t)S_B(d_nt)S_A(c_0t)S_B(d_1t)S_A(c_1t)\cdots S_B(d_nt)S_A(c_nt)$$

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 (4)

Lemma 11. *If $S_R^{(n)}=e^{-tL_K}=T_{tW}$ with $h=K+o(t^{2k-2})=W+o(t^{2k-2})$, then $W=h+o(t^{2k-1})$.*

As $S_R^{(n)}$ is reversible, $K(t)=A+B+\sum_{n\geq k}t^{2n}K_{2n+1}$. From the proposition (4), we have $W(t)=A+B+\sum_{n\geq 2k-1}t^nW_{n+1}$ in which $2kW_{2k}=K_{2k}+R_{2k}$ and $R_{2k}\in\tilde{L}_{\mathbb{Q}[c_0,\ldots,c_n,d_1,\ldots,d_n]}\{K_1,\ldots,K_{2k-1}\}$. As $K_2=K_3=\cdots=K_{2k}=0$, we deduce that $W_{2k}=0$.

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 $\mathbb{Q}$.

⋆⋆⋆

Another solution has been proposed by Yoshida [16] consisting in the finding of reversible integrators as reversible product of second-order integrators S_2. We look for

$$S^{(n)}(t) = S_2(c_n t) \cdots S_2(c_1 t) S_2(c_0 t) S_2(c_1 t) \cdots S_2(c_n t) = e^{-tL_{K^{(n)}}}. \qquad (53)$$

Since S_2 is reversible we have $S_2(t) = \exp(-tL_k)$ where

$$K = K_1 + t^2 K_3 + t^4 K_5 + t^6 K_7 + t^8 K_9 + o(t^{10}). \qquad (54)$$

We work now on the free Lie algebra on the alphabet $X = \{K_1, K_3, K_5, K_7, K_9\}$ in which $|K_i|_* = i$. We therefore have

$$K^{(0)} = c_0 K_1 + t^2 c_0^3 K_3 + t^4 c_0^5 K_5 + t^6 c_0^7 K_7 + t^8 c_0^9 K_9 + o(t^{10}). \qquad (55)$$

Bearing in mind that $K^{(n)}$ has only odd terms and belongs to $\tilde{L}(X)$, we will compute:

— the Lyndon basis of $L_{2n+1}(X)$ denoted by $K_{1,1}, K_{3,1}, \ldots, K_{5,1}, \ldots, K_{7,1}, \ldots, K_{9,1}, \ldots$

— $\log\left[S_2(xt) e^{-tL_{\tilde{H}}} S_2(xt)\right]$ at a given order k in which $\tilde{H} = \sum_{i,j} a_{i,j} K_{i,j}$ is generic.

- For $k = 4$, we find the real valued reversible integrator previously found by the direct method or using the lemma (10).
- 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. Thus, we find 36 complex integrators and 3 real valued. All the solutions are reached with this method as there is at most 39 solutions.
- For $k = 8$, Yoshida ([16]) 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.

3.6 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 can therefore hope to find symplectic integrators of order 4 or 6 with 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 like above

$$e^{-tL_{V_1}} p = p - t\frac{\partial V_1}{\partial q} \quad \text{and} \quad e^{-tL_{V_1}} q = q. \tag{56}$$

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

$$S_{c_n,z_n}(t)S_T(d_nt)\cdots S_{c_1,z_1}(t)S_T(d_0t)S_{c_1,z_1}(t)\cdots S_T(d_nt)S_{c_n,z_n}(t) \tag{57}$$

or

$$S_T(d_nt)S_{c_n,z_n}(t)\cdots S_T(d_1t)S_{c_0,z_0}(t)S_T(d_1t)\cdots S_{c_n,z_n}(t)S_T(d_nt) \tag{58}$$

With this method we found an integrator of order 4 as a product of 5 factors and an integrator of order 6 as product of 9 factors.

– For the fourth-order integrator, we find as general solution

$$z_1 + \tfrac{1}{2}\, z_0 + \tfrac{1}{48} = 0, d_1 - \tfrac{1}{2} = 0, c_0 - \tfrac{2}{3} = 0, c_1 - \tfrac{1}{6} = 0 \tag{59}$$

and we can take $z_1 = 0$, $z_0 = -\frac{1}{24}$, $d_1 = \frac{1}{2}, c_0 = \frac{2}{3}, c_1 = \frac{1}{6}$.

– For the sixth-order integrator, we find

$$\begin{gathered} z_2 = 0, z_1 - \tfrac{15}{16}\, c_2^2 + \tfrac{1}{4}\, c_2 - \tfrac{1}{96} = 0, z_0 - \tfrac{3}{8}\, c_2^2 - \tfrac{1}{4}\, c_2 + \tfrac{1}{48} = 0, \\ d_2 + 3\, c_2 - \tfrac{1}{2} = 0, d_1 - 3\, c_2 = 0, c_0 - 30\, c_2^2 + 12\, c_2 - 1 = 0, \\ c_1 + 15\, c_2^2 - 5\, c_2 = 0, c_2^3 - \tfrac{1}{2}\, c_2^2 + \tfrac{1}{18}\, c_2 - \tfrac{1}{540} = 0 \end{gathered}$$

Moreover the evaluation of $\frac{\partial V_1}{\partial q}$ requires 2 evaluations so the above integrators require in fact 6 evaluations and 12 evaluations at each step respectively, which is an improvement with respect to the integrators found in the general case.

⋆⋆⋆

In table 1., we give for each order and each method, the number of polynomial equations to solve, the number of operators involved in the integrators and the number of solutions. For the first column, D means *using the direct method (44)*, L means *using the Lie transformations or the exponential (46) or (45)*, RL means *looking for reversible integrators using Lie transformations (lemma (11))*, S_2 means *looking for reversible products of operators* S_2. In the column

	Polynomials				Operators			Solutions		
			Reversible			Reversible			Reversible	
Order	D	L	RL	S_2	L	RL	S_2	L	RL	S_2
1	2	2	2		1			1		
2	4	1		1	3	3	3	1		
3	8	2	4		5			3		
					6			∞		
4	16	3		1	7	7	7	5-1	3-1	3-1
5	32	6	6		11?			46?		
6	64	9		2	≥ 13	15	15		39	39-3
7	128	18	18							
8	256	30		4			31			?-5
9	512	56	56							
10	1024	99		8						

Table 1. — Symplectic Integrators —

"solutions", when two numbers appear, the first one is the number of solutions and the second one the number of real solutions.

For example, in the row corresponding to the order 4, the set of algebraic equalities contains 30 polynomials (sum in the column) with the method D, 8 polynomials with the method L, 6 polynomials with the method RL and 2 polynomials with the method S_2. In the same row, one finds solutions that give integrators of order 4 as product of 7 operators. One finds 5 solutions with the method L (1 real solution), and 3 with the other methods. In the row corresponding to the order 3, there are 3 integrators as product of 5 operators but none is real valued and there is an infinity of real valued integrators as product of 6 single operators.

4 Conclusion

We showed in this paper that there are exactly 5 fourth-order symplectic integrators involving 7 operators. Three of them are known (see [7, 16]). We showed, that there are exactly 39 reversible sixth-order symplectic integrators involving 15 operators. All of them are reversible products of second-order integrators. Three of them were known ([16]). In ([16]), Yoshida has found 5 eight-order integrators involving 31 operators: here we proved that there are not reversible products of 5 fourth-order integrators.

We have shown why the Lyndon basis is particularly adapted for computing the relations between Lie transforms and exponentials. We also found integrators in the case when $h = T(p) + V(q)$ and $T(p)$ is a quadratic form in p.

Bibliography

[1] Bourbaki, N.: Groupes et algèbres de Lie, Éléments de Mathématiques,

Hermann, Paris, 1972.

[2] Cary, J.R.: Lie Transform Perturbation Theory for Hamiltonian Systems, in Physics Reports, North-Holland Publishing Company **79-2** (1981), 129–159.

[3] Deprit, A.: Canonical transformations depending on a small parameter, Cel. Mech. **1** (1969), 12–30.

[4] Dragt, A. J., Finn, J. M.: Lie Series and invariant functions for analytic symplectic maps, J. Math. Physic **17** (1976), 2215–2227.

[5] Dragt, A. J., Healy, L. M.: Concatenation of Lie Algebraic Maps, in Lie Methods in Optics II, Lec. Notes in Physics **352** (1988).

[6] Finn, J. M.: Lie Series: a Perspective, Local and Global Methods of nonlinear Dynamics, Lec Notes in Physics **252** (1984), 63–86.

[7] Forest, E., Ruth, D.: Fourth-Order Symplectic Integration, Physica D **43** (1990), 105–117.

[8] Koseleff, P.-V., Thèse de troisième cycle, École Polytechnique, (to appear).

[9] Michel, J.: Bases des Algèbres de Lie Libres, Étude des coefficients de la formule de Campbell-Hausdorff, Thèse, Orsay, 1974.

[10] Perrin, D.: Factorization of free monoids, in Lothaire M., Combinatorics On Words, Chap. 5, Addison-Wesley (1983).

[11] Petitot, M.: Algèbre non commutative en Scratchpad : application au problème de la réalisation minimale analytique, Thèse, Université de Lille I, 1991.

[12] Steinberg, S.: Lie Series, Lie Transformations, and their Applications, in Lie Methods in Optics, Lec. Notes in Physics **250** (1985).

[13] Suzuki M.: Fractal Decomposition of Exponential Operators with Applications to Many-Body Theories and Monte Carlo Simulations, Ph. Letters A **146** (1990), 319–323.

[14] Wisdom J., Holman, M.: Symplectic Maps for the N-Body Problem, The Astr. J. **102(4)** (1991), 1528–1538.

[15] Yoshida, H.: Conserved Quantities of Symplectic Integrators for Hamiltonian Systems, Physica D (1990).

[16] Yoshida, H.: Construction Of Higher Order Symplectic Integrators, Ph. Letters A **150,** (1990), 262–268.

This article was processed using the LaTeX macro package with LLNCS style