Relations among Lie Formal Series and Construction of Symplectic Integrators

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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 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 $L(X)$