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Sixth-Order Lie Group Integrators

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In this paper we present the coefficients of several sixth-order symplectic integrators of the type developed by R. Ruth. To get these results we fully exploit the connection with Lie groups. These integrators, as well as all the explicit integrators of Ruth, may be used in any equation where some sort of Lie bracket is preserved. In fact, if the Lie operator governing the equation of motion is separable into two solvable parts, the Ruth integrators can be used. © 1992 Academic Press, Inc.

1. INTRODUCTION

The purpose of this article is to provide a sixth-order explicit canonical integrator for Lie groups. Originally Ruth proposed a method to integrate the motion of a particle in Hamiltonians of the type [1]

$$H = A(\mathbf{p}) + V(\mathbf{x}), \tag{1}$$

where $\mathbf{x}$ and $\mathbf{p}$ are the canonically conjugate positions and momenta. Ruth was able to find a fourth-order integrator by solving eight very complicated equations numerically. Later, he found an analytic solution to the equations. This work remained unpublished and was known mostly in the accelerator community. Only the general method and a third-order integrator had been published [2].

Independently, Candy and Rozmus [3] rederived the fourth-order integrator of Ruth using the method proposed by Ruth. They cleaned up Ruth's approach substantially and obtained eight equations of a simpler appearance.

In the mean time, Neri and Forest [4] showed that the explicit integrator of Ruth has a greater realm of applicability than Ruth had realized. In fact, it could be used in any Lie group! In addition, the connection between Lie groups and Ruth's integrator provided an even simpler derivation of Ruth's fourth-order integrator. Forest was able to reduce Ruth's or Candy's eight equations to two simple equations easily reduceable to a single cubic equation [5].

In this paper, we will exploit the simplicity of the Lie "connection" to set up eight equations for the sixth-order explicit integrator. In Section 2, we review the connection with Lie groups and, in Section 3, the type of Hamiltonians suitable to Ruth's method. In Section 4, we introduce the idea of symmetrization. In Section 5, we derive a basis for the space of four-fold commutators which are needed in a sixth-order integrator. Using this we produce a numerical solution for the integrator. It should be said that an analytical solution probably does not exist because the equations are quintic. Finally, in Section 6, we discuss some very recent results[1] and derive some special purpose integrators for Hamiltonians of the form $\mathbf{p}^2/2 + V(\mathbf{x})$.

2. REVIEW OF THE LIE CONNECTION

It can be shown that Hamilton's equations generate symplectic maps. The equation for the map has a form similar to Schrödinger's equation for the unitary transformation in quantum mechanics [6],

$$\frac{d}{dt}\mathbf{M} = \mathbf{M} :-H(\mathbf{z}_0; t):, \tag{2}$$

where $:g(\mathbf{z}_0):$ is the Lie operator associated to the function $g(\mathbf{z}_0)$. The operator $:g(\mathbf{z}_0):$ is defined in terms of the Poisson bracket:

$$:g(\mathbf{z}_0): f(\mathbf{z}_0) = [g(\mathbf{z}_0), f(\mathbf{z}_0)] = \frac{\partial g}{\partial \mathbf{x}_0}\cdot\frac{\partial f}{\partial \mathbf{p}_0} - \frac{\partial g}{\partial \mathbf{p}_0}\cdot\frac{\partial f}{\partial \mathbf{x}_0}. \tag{3}$$

Here $\mathbf{z}_0 = (\mathbf{x}_0, \mathbf{p}_0)$ is a point in the initial phase space. From the nature of Eq. (2), one can see that $\mathbf{M}$, just like $:-H:$, operates on functions of $\mathbf{z}_0$. It propagates them forward in time according to the Hamiltonian $H(\mathbf{z}_0; t)$.

Because the time dependence can be removed formally by

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[1] Results obtained by Yoshida while this paper was being submitted.

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extending phase space, we will concentrate on time independent Hamiltonians [7]. For such systems, one can write a formal solution for $\mathbf{M}$,

$$\mathbf{M} = \exp(:-tH(\mathbf{z}_0):), \tag{4}$$

where $\mathbf{M}$ propagates any function for a time t.

In theory, we can get the position of the ray $\mathbf{z}_t$ at time t by using Eq. (4):

$$\begin{aligned} \mathbf{z}_t &= \exp(:-tH(\mathbf{z}_0):)\,\mathbf{z}_0 \\ &= \sum_{i=0}^{\infty} \frac{:-tH(\mathbf{z}_0):^i}{i!}\,\mathbf{z}_0. \end{aligned} \tag{5}$$

If we could sum up the series (5) to machine precision on a computer, it would be a symplectic integrator automatically, because it is the exact solution. Unfortunately, this is not always possible. However, if we look back at Eq. (1), we find that if the Hamiltonian has either the form $A(\mathbf{p})$ or $V(\mathbf{x})$, it is exactly solvable:

$$\begin{aligned} \mathbf{z}_t &= \exp(:-tV(\mathbf{x}_0):)\,\mathbf{z}_0 \\ &= \left(\mathbf{x}_0, \mathbf{p}_0 - t\frac{\partial}{\partial \mathbf{x}_0} V(\mathbf{x}_0)\right) \end{aligned} \tag{6a}$$

$$\begin{aligned} \mathbf{z}_t &= \exp(:-tA(\mathbf{p}_0):)\,\mathbf{z}_0 \\ &= \left(\mathbf{x}_0 + t\frac{\partial}{\partial \mathbf{p}_0} A(\mathbf{p}_0), \mathbf{p}_0\right). \end{aligned} \tag{6b}$$

This leads us to the Lie group generalization of Ruth's integrator. We review it in the next section.

3. THE TWO-MAPS INTEGRATOR

Consider a Hamiltonian H which can be split into two pieces H_1 and H_2 such that

$$\mathbf{z}_t = \mathbf{M}_i(t)\,\mathbf{z}_0 = \exp(:-tH_i(\mathbf{z}_0):)\,\mathbf{z}_0; \quad \text{for } i = 1, 2, \tag{7}$$

are known functions which can be evaluated to machine precision on a computer. This is the case of the Hamiltonian of Eq. (1) as we just pointed out in Section 2.

Now let us try to approximate the original map $\mathbf{M}(t)$ by a product involving the two maps $\mathbf{M}_1$ and $\mathbf{M}_2$:

$$\mathbf{M}(t) \approx \mathbf{M}(t;k) = \prod_{j=1}^{N} \mathbf{M}_1(t^1{}_j)\,\mathbf{M}_2(t^2{}_j) \tag{8}$$

by assumption, all the factors of $\mathbf{M}(t;k)$ are exactly solvable on a computer; hence the approximate map $\mathbf{M}(t;k)$ is symplectic. The fundamental question has two parts:

(i) Can we select the set $\{j=1, N \mid t^1{}_j, t^2{}_j\}$ such that $\|\mathbf{M}(t) - \mathbf{M}(t;k)\| = 0 + O(t^{k+1})$?

(ii) What is the minimal value of N (denoted N_k) which will allow us to obtain a kth-order integrator (i.e., $\|\mathbf{M}(t) - \mathbf{M}(t;k)\| = 0 + O(t^{k+1})$)?

Central to the answer of this question is the Campbell–Baker–Hausdorff theorem (CBH). According to the CBH theorem, Eq. (8) can be rewritten formally as

$$\mathbf{M}(t;k) = \prod_{j=1}^{N} \mathbf{M}_1(t^1{}_j)\,\mathbf{M}_2(t^2{}_j) = \exp(C) \tag{9a}$$

$$\begin{aligned} C = \sum_{i=1}^{2} \sum_{j=1}^{N} t^i{}_j :-H_i(\mathbf{z}_0): \\ + \text{multiple commutators of } :H_1: \text{ and } :H_2:. \end{aligned} \tag{9b}$$

The exact solution requires

$$C = -t(:H_1: + :H_2:). \tag{10}$$

This gives us a prescription for a first-order integrator:

$$\text{if } \sum_{j=1}^{N} t^i{}_j = t \quad \text{then} \quad C = -t(:H_1: + :H_2:) + \cdots + O(t^2). \tag{11}$$

We see immediately from (11) that the minimum N_1 is just 1. Therefore the simplest first-order canonical integrator is given by

$$\mathbf{M}(t;k=1) = \exp(-t:H_1:)\exp(-t:H_2:). \tag{12}$$

This simple integrator involves only the integrated sums in Eq. (11).

The quadratic integrator will involve double commutators. In general, because the exact solution for C does not contain any commutators, the kth integrator will require us to set all j-fold commutators from $j = k-1$ to $j = 1$ to zero.

4. SYMMETRIZED INTEGRATOR

To proceed further we need to find a basis for the multiple commutators of two arbitrary operators. With the help of a simple lemma, we will restrict ourselves to $(k-1)$-fold commutators where k is odd (i.e., commutators of k operators).

DEFINITION. A map is a symmetrized product of operators if the sequence of factors is the same when read from left to right or from right to left.

LEMMA. *Symmetrized products do not have odd-fold commutators when written as the exponential of a single operator C.*

Proof. We start by writing $\mathbf{M}$ as a symmetrized product involving an ordering parameter ε:

$$\mathbf{M} = \prod_{j=1}^{N} \exp(\varepsilon A_j) \prod_{j=N}^{1} \exp(\varepsilon A_j) = \exp(C(\varepsilon)). \quad (13)$$

Here the A_j's are some arbitrary operators. To prove the lemma, we compute the inverse of $\mathbf{M}$:

$$\begin{aligned}\mathbf{M}^{-1} &= \left\{\prod_{j=1}^{N} \exp(\varepsilon A_j) \prod_{j=N}^{1} \exp(\varepsilon A_j)\right\}^{-1} \\ &= \left\{\prod_{j=N}^{1} \exp(\varepsilon A_j)\right\}^{-1} \left\{\prod_{j=1}^{N} \exp(\varepsilon A_j)\right\}^{-1} \\ &= \prod_{j=1}^{N} \exp(-\varepsilon A_j) \prod_{j=N}^{1} \exp(-\varepsilon A_j). \end{aligned} \quad (14)$$

In Eq. (14), we obtain the inverses by reversing the ordering and using the well-known property

$$\exp(A_j)^{-1} = \exp(-A_j). \quad (15)$$

We notice from the last line in (14) that $\mathbf{M}(\varepsilon)^{-1} = \mathbf{M}(-\varepsilon) = \exp(C(-\varepsilon))$. However, property (15) implies that $\mathbf{M}(\varepsilon)^{-1} = \exp(-C(\varepsilon))$. These two equations force the relation

$$\begin{aligned} C(-\varepsilon) = -C(\varepsilon) &\Rightarrow C \text{ is odd in } \varepsilon \\ &\Rightarrow C \text{ contains only even-fold commutators.} \end{aligned} \quad (16)$$

This proves the lemma.

A simple application of the lemma is to use the first-order integrator of Eq. (12) to produce a second-order integrator by symmetrization:

$$\begin{aligned}\mathbf{M}(t; k=2) &= \exp\left(-\frac{t}{2} :H_1:\right) \\ &\times \exp(-t :H_2:) \exp\left(-\frac{t}{2} :H_1:\right). \end{aligned} \quad (17)$$

$\mathbf{M}(t; k=2)$ still obeys Eq. (9b) and is symmetrized thereby being truly quadratic.

5. A BASIS FOR THE TWO-FOLD AND FOUR-FOLD COMMUTATORS

Consider k arbitrary operators A_j; let us select one operator amongst them and without loss of generality we denote it by A_k. Then it can be shown that any sum C_k of $(k-1)$-fold commutators of the operators A_j can be expressed in terms of a class of "nested" commutators:

$$\begin{aligned} C_k = \sum_{j=1}^{(k-1)!} \alpha_{\pi_j} \{A_{\pi_{j(1)}}, \{A_{\pi_{j(2)}}, \\ \cdots \{A_{\pi_{j(k-1)}}, A_k\}\}\} \cdots \}\}\}\} \end{aligned} \quad (18a)$$

$\pi_j =$ the jth permutation of the

$(k-1)$ integers between 1 and $k-1$. (18b)

Assuming totally arbitrary operators, Eq. (18) tells us that we need $(k-1)!$ commutators to form a basis for the $(k-1)$-fold commutators. The proof of (18) is rather complex [8].

Equation (18) alone depicts a pretty gloomy prospect since it would imply that a sixth-order symmetrized integrator requires the zeroing of 26 commutators $(=2!+4!)$. This is not so because in our case the operators A_j's are not independent. Indeed, they are proportional to the two operators $:H_1:$ and $:H_2:$. This entails that many of the nests in (18) vanish or are related to one another. Table I gives the results for two-fold and four-fold commutators.

The results of Table I were found by brute force expansion of the nests involved. Notice that one half of Table I is obtainable from the other by symmetry. This table tells us that in addition to relation (11), a symmetrized ansatz for $\mathbf{M}(t; 6)$ will require at least eight free variables *unless* a hidden symmetry permits the accidental cancellation of more than one commutator at once (see Section 6). Here is our ansatz:

$$\begin{aligned}\mathbf{M}(t; 6) = {} & \mathbf{M}_1(\tfrac{1}{2}t - t^1{}_1 - t^1{}_2 - t^1{}_3 - t^1{}_4) \\ & \times \mathbf{M}_2(\tfrac{1}{2}t - t^2{}_1 - t^2{}_2 - t^2{}_3 - \tfrac{1}{2}t^2{}_4) \\ & \times \mathbf{M}_1(t^1{}_1)\, \mathbf{M}_2(t^2{}_1)\, \mathbf{M}_1(t^1{}_2) \\ & \times \mathbf{M}_2(t^2{}_2)\, \mathbf{M}_1(t^1{}_3)\, \mathbf{M}_2(t^2{}_3) \\ & \times \mathbf{M}_1(t^1{}_4)\, \mathbf{M}_2(t^2{}_4) \\ & \times \mathbf{M}_1(t^1{}_4)\, \mathbf{M}_2(t^2{}_3)\, \mathbf{M}_1(t^1{}_3) \\ & \times \mathbf{M}_2(t^2{}_2)\, \mathbf{M}_1(t^1{}_2)\, \mathbf{M}_2(t^2{}_1)\, \mathbf{M}_1(t^1{}_1) \\ & \times \mathbf{M}_2(\tfrac{1}{2}t - t^2{}_1 - t^2{}_2 - t^2{}_3 - \tfrac{1}{2}t^2{}_4) \\ & \times \mathbf{M}_1(\tfrac{1}{2}t - t^1{}_1 - t^1{}_2 - t^1{}_3 - t^1{}_4). \end{aligned} \quad (19)$$

TABLE I

Basis for the Even-fold Commutators of the Integrator

k	Commutators with an excess of H_1	Exchanging H_1 and H_2
3	$\{:H_1:, \{:H_1:, :H_2:\}\}$	$\{:H_2:, \{:H_2:, :H_1:\}\}$
	$\{:H_1:, \{:H_1:, \{:H_1:, \{:H_1:, :H_2:\}\}\}\}$	$\{:H_2:, \{:H_2:, \{:H_2:, \{:H_2:, :H_1:\}\}\}\}$
5	$\{:H_1:, \{:H_1:, \{:H_2:, \{:H_1:, :H_2:\}\}\}\}$	$\{:H_2:, \{:H_2:, \{:H_1:, \{:H_2:, :H_1:\}\}\}\}$
	$\{:H_2:, \{:H_1:, \{:H_1:, \{:H_1:, :H_2:\}\}\}\}$	$\{:H_1:, \{:H_2:, \{:H_2:, \{:H_2:, :H_1:\}\}\}\}$

This ansatz can be motivated by the following arguments:

(i) We need eight free parameters, these are the $\{j=1,4 \mid t^1{}_j, t^2{}_j\}$.

(ii) It must be symmetrized, hence, with the exception of $\mathbf{M}_2(t^2{}_4)$, all operators appear twice.

(iii) The operators $\mathbf{M}_1(\frac{1}{2}t - t^1{}_1 - t^1{}_2 - t^1{}_3 - t^1{}_4)$ and $\mathbf{M}_2(\frac{1}{2}t - t^2{}_1 - t^2{}_2 - t^2{}_3 - \frac{1}{2}t^2{}_4)$ are added to make sure that equation (11) is satisfied (i.e., the time step adds up correctly).

It would appear that a manipulator using the CBH formula would be needed to rewrite (19) in the form exp(C). Instead, we will solve the equation

$$\mathbf{M}(t;6) - \exp(-t(:H_1: + :H_2:)) = 0 + O(t^7). \tag{20}$$

On both sides we collect the coefficients of operators which are chosen so as to originate from the different commutators of Table I. Table II provides a possible choice. In Eq. (20), the coefficients of the operators of Table II are horrible polynomials in the set of variables $\{j=1,4 \mid t^1{}_j, t^2{}_j\}$. A program was written with the help of the differential algebra package of Berz [9] to evaluate these polynomials and their derivatives. A Monte Carlo procedure was used to locate the neighborhood of a solution. Finally, we zoomed in on the solution using a Newton search for extra digits. This is important to ensure that the error introduced by the integrator is truly scaling with the sixth power of the time step. The results are:

$$\begin{aligned}
t^1{}_1/t &= 1.24490030378348\ 10^{-1}\\
t^2{}_1/t &= -1.08371593275947\\
t^1{}_2/t &= -3.97593681977505\ 10^{-1}\\
t^2{}_2/t &= 2.88528568804383\ 10^{-1}\\
t^1{}_3/t &= 4.79518377447967\ 10^{-1}\\
t^2{}_3/t &= 6.70508186091578\ 10^{-1}\\
t^1{}_4/t &= -3.72762722606859\ 10^{-1}\\
t^2{}_4/t &= -1.41603363130538.
\end{aligned} \tag{21}$$

TABLE II

Operators Selected for the Computation of the Integrator

k	Operators with an excess of H_1	Exchanging H_1 and H_2
3	$:H_2::H_1::H_1:$	$:H_1::H_2::H_2:$
5	$:H_1::H_1::H_1::H_1::H_2:$	$:H_2::H_2::H_2::H_2::H_1:$
	$:H_2::H_1::H_1::H_1::H_2:$	$:H_1::H_2::H_2::H_2::H_1:$
	$:H_1::H_2::H_1::H_2::H_1:$	$:H_2::H_1::H_2::H_1::H_2:$

These results were checked on a simple one-dimensional nonlinear Hamiltonian and are probably accurate to at least 14 digits.

6. DO WE REALLY NEED EIGHT FREE PARAMETERS?

In this paper, we did not derived the Lie exponent C of Eq. (9a). In the mean time Yoshida, in a very elegant paper, using Lie methods and the CBH formula, has found three integrators requiring only six parameters ($t^1{}_4 = 0$ and $t^2{}_4 = 0$) and an eight-order integrator [10]. The author checked the results and obtained a few extra digits. Here are the results for completeness:

$$\begin{aligned}
t^1{}_1/t &= 5.1004341191845769875214540809\text{d}-01\\
t^2{}_1/t &= 2.3557321335935813368479318398\text{d}-01\\
t^1{}_2/t &= -4.7105338540975643663081124856\text{d}-01\\
t^2{}_2/t &= -1.1776799841788710069464156784\text{d}+00\\
t^1{}_3/t &= 6.8753168252520105968917024092\text{d}-02\\
t^2{}_3/t &= 6.5759316034195560944212486296\text{d}-01
\end{aligned} \tag{22a}$$

$$\begin{aligned}
t^1{}_1/t &= 7.2205442492378755356329149452\text{d}-01\\
t^2{}_1/t &= 4.2606818707920161960837141906\text{d}-03\\
t^1{}_2/t &= -1.0640122700653297522549548262\text{d}+00\\
t^2{}_2/t &= -2.1322852220014515207059933597\text{d}+00\\
t^1{}_3/t &= 1.2203376115315065322641369108\text{d}-01\\
t^2{}_3/t &= 1.1881763721538764135794103684\text{d}+00
\end{aligned} \tag{22b}$$

$$\begin{aligned}
t^1{}_1/t &= -3.4812637695304568885170257470\text{d}-01\\
t^2{}_1/t &= -2.1440353163053893106013017942\text{d}+00\\
t^1{}_2/t &= -1.0712532270105700201745169525\text{d}+00\\
t^2{}_2/t &= 1.5288622842492702522672398850\text{d}-03\\
t^1{}_3/t &= 1.1954883227639667425772711946\text{d}+00\\
t^2{}_3/t &= 1.1947238916218421074511378969\text{d}+00.
\end{aligned} \tag{22c}$$

In addition, it is possible to find special purpose integrators. For example, often the Hamiltonian has the form:

$$H = \mathbf{p}^2/2 + V(\mathbf{x}). \tag{23}$$

We immediatly notice that the following bracket vanishes:

$$[V(\mathbf{x}), [V(\mathbf{x}), \mathbf{p}^2/2]] = 0. \tag{24}$$

This implies that two commutators of Table II will vanish. Hence, we can look again for a six-parameter integrator. We have two choices: we can choose $H_1 = \mathbf{p}^2/2$ or $H_2 = \mathbf{p}^2/2$. Here are a few possible integrators: with $H_1 = \mathbf{p}^2/2$,

$$t^1{}_1/t = -5.97871616719574023100624801 35\text{d}-01$$

$$t^2{}_1/t = 1.31182410201052806203179945 47\text{d}-01$$

$$t^1{}_2/t = 5.88529064960644378531065908 74\text{d}-01$$

$$t^2{}_2/t = 9.21619775048851892922367184 31\text{d}-01$$

$$t^1{}_3/t = -4.34791370123196589652843918 39\text{d}-01$$

$$t^2{}_3/t = 1.34937885935668201726538452 35\text{d}-01$$

or

$$t^1{}_1/t = 5.17919466393391859400854091 19\text{d}-01$$

$$t^2{}_1/t = 1.82789540999773721170698496 39\text{d}-01$$

$$t^1{}_2/t = -1.32679625730344932298171440 23\text{d}+00$$

$$t^2{}_2/t = 8.62710114629165327368871743 15\text{d}-04$$

$$t^1{}_3/t = 9.08981366235931147737764095 48\text{d}-01$$

$$t^2{}_3/t = -5.86205145530487736049188577 56\text{d}-01;$$

with $H_2 = \mathbf{p}^2/2$,

$$t^1{}_1/t = 6.80668858912863516283977832 63\text{d}-01$$

$$t^2{}_1/t = 3.55757425910199292467350842 09\text{d}-01$$

$$t^1{}_2/t = 2.24235720535174808181095842 04\text{d}-01$$

$$t^2{}_2/t = -2.21421299623006195093033222 60\text{d}-01 \qquad (25)$$

$$t^1{}_3/t = -4.88237912781371657798407007 61\text{d}-01$$

$$t^2{}_3/t = -3.55372132699398763005513908 68\text{d}-02.$$

CONCLUSION

From the point of view of an accelerator physicist, sixth order is probably an upper limit, because we use the integrator for approximate modeling. In accelerator physics, one tries to reduce the number of time steps to a minimum while still preserving the topological properties that can be observed on a short time. Then the integrator is "let loose" for a large number of revolutions, usually past the domain of validity rigorously dictated by a study of error propagation. This must be done in systems where subtle but generic effects develop over a long time. These effects are often washed away by small violation of the symplectic character of the motion [11].

This is not necessarily the case in other fields. Indeed, Yoshida and others in celestial mechanics, remain very interested in high order integrators because they do more than just modeling. They are interested in the exact solution of the problem.

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7. See Ref. [5, Section 6].
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10. Yoshida's paper and preprint did not exist when our work was submitted. We recommend very strongly the reading of this paper. The reference is: H. Yoshida, *Phys. Lett. A* **150** (1990).
11. In Ref. [3], the authors provide a wealth of examples illustrating the qualitative differences between symplectic and non-symplectic integrators.