Title

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SIXTH-ORDER LIE GROUP INTEGRATORS*

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ABSTRACT

In this paper we present the coefficients of several 6th order symplectic integrator of the type developed by R. Ruth. To get these results we fully exploit the connection with Lie groups. This integrator, 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.

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1. Introduction

The purpose of this article is to provide a 6th 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 **x** and **p** are the canonically conjugate positions and momenta. Ruth was able to find a 4th 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 This work remained unpublished and was known mostly in the accelerator community.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 3rd order integrator had been published [2].

Independently, Candy and Rozmus [3] rederived the 4th 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 had 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 4th 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 6th 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 4-fold commutators which are needed in a 6th 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[2] 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:

$$:g(\mathbf{z_0}):\ f(\mathbf{z_0}) = [\ g(\mathbf{z_0}),\ f(\mathbf{z_0})\ ] = \frac{\partial g}{\partial \mathbf{x}_0} \circ \frac{\partial f}{\partial \mathbf{p}_0} - \frac{\partial g}{\partial \mathbf{p}_0} \circ \frac{\partial f}{\partial \mathbf{x}_0} \tag{3}$$

Here $\mathbf{z_0} = (\mathbf{x_0}, \mathbf{p_0})$ is a point in the initial phase space. From the nature of equation (2), one can see that $\mathbf{M}$, just like $: -H :$, operates on functions of

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

$\mathbf{z}_0$. It propagates them forward in time according to the Hamiltonian $H(\mathbf{z}_0\,;t)$.

Because the time dependence can be removed formally by extending phase space, we will concentrate on time independent Hamiltonians [7]. For such systems, one can write a formal solution for **M**:

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

where **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 equation (4):

$$\mathbf{z}_t = \exp(:-t\,H(\mathbf{z}_0):)\,\mathbf{z}_0 = \sum_{i=0}^{\infty} \frac{:-t\;H(\mathbf{z}_0):^{i}}{i!}\,\mathbf{z}_0 \tag{5}$$

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 equation (1), we find that if the Hamiltonian has either the form $A(\mathbf{p})$ or $V(\mathbf{x})$, it is exactly solvable:

$$\mathbf{z}_t = \exp(:-t\,V(\mathbf{x}_0):)\,\mathbf{z}_0 = (\,\mathbf{x}_0,\,\mathbf{p}_0 - t\frac{\partial}{\partial \mathbf{x}_0}V(\mathbf{x}_0)\,) \tag{6a}$$

$$\mathbf{z}_t = \exp(:-t\,A(\mathbf{p}_0):)\,\mathbf{z}_0 = (\,\mathbf{x}_0 + t\frac{\partial}{\partial \mathbf{p}_0}A(\mathbf{p}_0)\,,\,\mathbf{p}_0)\,. \qquad (6b)$$

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

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

are known functions which can be evaluated to machine precision on a computer. This is the case of the Hamiltonian of equation (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 $\mathbf{M}_2$:

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

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 get a k th 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, equation (8) can be rewritten formally as follows:

$$\mathbf{M}(t;k) = \prod_{j=1}^{N} \mathbf{M_1}(t^1{}_j)\ \mathbf{M_2}(t^2{}_j) = \exp(\ C\ ) \tag{9a}$$

$$C = \sum_{i=1}^{2} \sum_{j=1}^{N} t^i{}_j :\!-H_i(\mathbf{z_0})\!: + \text{multiple commutators of } :H_1: \text{ and } :H_2: \tag{9b}$$

The exact solution requires

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

This gives us a prescription for a first order integrator:

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

We see immediately from (11) that the minimum N_1 is just 1. Therefore the simplest 1st 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 equation (11).

The quadratic integrator will involve double commutators. In general, because the exact solution for C does not contain any commutators, the k^{th} 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 **M** as a symmetrized product involving an ordering parameter ε :

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

Here the A_j 's are some arbitrary operators. To prove the lemma, we compute the inverse of **M** :

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

In equation (14), we get the inverses by reversing the ordering and using the well known property:

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

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

$C(-\varepsilon)=-C(\varepsilon) \Rightarrow C$ is odd in $\varepsilon \Rightarrow C$ contains only even-fold commutators(16)

This proves the lemma.

A simple application of the lemma is to use the 1st order integrator of equation (12) to produce a second order integrator by symmetrization:

$$\mathbf{M}(t;k=2) = \exp(-\frac{t}{2}:H_1:)\exp(-t:H_2:)\exp(-\frac{t}{2}:H_1:) \tag{17}$$

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

5. A basis for the 2-fold and 4-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 :

$$C_k = \sum_{j=1}^{(k-1)!} \alpha_{\pi_j}\{A_{\pi_{j(1)}},\{A_{\pi_{j(2)}},\ldots\ldots\{A_{\pi_{j(k-1)}},A_k\}\}\}\ldots.\}\}\}\} \tag{18a}$$

π_j = the j^{th} permutation of the (k-1) integers between 1 and k-1. (18b)

Assuming totally arbitrary operators, equation (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 6^{th} 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. We now give the results for 2-fold and 4-fold commutators:

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

Table I : Basis for the even-fold commutators of the integrator

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 8 free variables **unless** a hidden symmetry permits the accidental cancellation of more than one commutator at once (see section 6). Here is our ansatz:

$$\begin{aligned}\mathbf{M}(t;6) = {} & \mathbf{M}_1\left(\tfrac{1}{2}t - t^{1}_{1} - t^{1}_{2} - t^{1}_{3} - t^{1}_{4}\right)\mathbf{M}_2\left(\tfrac{1}{2}t - t^{2}_{1} - t^{2}_{2} - t^{2}_{3} - \tfrac{1}{2}t^{2}_{4}\right) \\ & \mathbf{M}_1(t^{1}_{1})\mathbf{M}_2(t^{2}_{1})\mathbf{M}_1(t^{1}_{2})\mathbf{M}_2(t^{2}_{2})\mathbf{M}_1(t^{1}_{3})\mathbf{M}_2(t^{2}_{3})\mathbf{M}_1(t^{1}_{4}) \\ & \mathbf{M}_2(t^{2}_{4}) \\ & \mathbf{M}_1(t^{1}_{4})\mathbf{M}_2(t^{2}_{3})\mathbf{M}_1(t^{1}_{3})\mathbf{M}_2(t^{2}_{2})\mathbf{M}_1(t^{1}_{2})\mathbf{M}_2(t^{2}_{1})\mathbf{M}_1(t^{1}_{1}) \\ & \mathbf{M}_2\left(\tfrac{1}{2}t - t^{2}_{1} - t^{2}_{2} - t^{2}_{3} - \tfrac{1}{2}t^{2}_{4}\right)\mathbf{M}_1\left(\tfrac{1}{2}t - t^{1}_{1} - t^{1}_{2} - t^{1}_{3} - t^{1}_{4}\right) \qquad (19)\end{aligned}$$

This ansatz can be motivated by the following arguments:

i) We need 8 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 following equation:

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

On both side we collect the coefficients of operators which are chosen so as to originate from the different commutators of table 1 [9]. Table II provides a possible choice.

	Operators with an Excess of H 1	Exchanging H_1 and H_2
k=3	$:H_2::H_1::H_1:$	$:H_1::H_2::H_2:$
k=5	$:H_1::H_1::H_1::H_1::H_2:$	$:H_2::H_2::H_2::H_2::H_1:$
	$:H_2::H_1::H_1::H_1::H_2:$	$:H_1::H_2::H_2::H_2::H_1:$
	$:H_1::H_2::H_1::H_2::H_1:$	$:H_2::H_1::H_2::H_1::H_2:$

Table II . Operators selected for the computation of the integrator

In equation (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 zoommed on the solution using a Newton search for extra digits. This is important to insure that the error introduced by the integrator is truly scaling with the 6th power of the time step.

The results are:

$t^{1}{}_{1}/t = 1.24490030378348\ 10^{-1}$

$t^{2}{}_{1}/t=-1.08371593275947$

$t^{1}{}_{2}/t=-3.97593681977505\ 10^{-1}$

$t^{2}{}_{2}/t= 2.88528568804383\ 10^{-1}$

$t^{1}{}_{3}/t= 4.79518377447967\ 10^{-1}$

$t^{2}{}_{3}/t= 6.70508186091578\ 10^{-1}$

$t^{1}{}_{4}/t=-3.72762722606859\ 10^{-1}$

$t^{2}{}_{4}/t=-1.41603363130538$ (21)

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

6. Do we really need 8 free parameters ?

In this paper, we did not derived the Lie exponent C of equation (9a).

In the mean time Yoshida, in a very elegant paper, using Lie methods and the CBH formula, has found three integrators requiring only 6 parameters ($t^{1}{}_{4}=0$ and $t^{2}{}_{4}=0$) and an eight order integrator [10]. The author checked the results and got a few extra digits. Here are the results for completeness:

$t^{1}{}_{1}/t = 5.10043411918457698752145408\text{d-}01$

$t^{2}{}_{1}/t = 2.35573213359358133684793183\text{98d-}01$

$t^{1}{}_{2}/t = -4.71053385409756436630811248 56d-01$

$t^{2}{}_{2}/t = -1.17767998417887100694641567 84d+00$

$t^{1}{}_{3}/t = 6.87531682525201059689170240 92d-02$

$t^{2}{}_{3}/t = 6.57593160341955609442124862 96d-01$ (22a)

$t^{1}{}_{1}/t = 7.22054424923787553563291494 52d-01$

$t^{2}{}_{1}/t = 4.26068187079201619608371419 06d-03$

$t^{1}{}_{2}/t = -1.06401227006532975225495482 62d+00$

$t^{2}{}_{2}/t = -2.13228522200145152070599335 97d+00$

$t^{1}{}_{3}/t = 1.22033761153150653226413691 08d-01$

$t^{2}{}_{3}/t = 1.18817637215387641357941036 84d+00$ (22b)

$t^{1}{}_{1}/t = -3.48126376953045688851702574 70d-01$

$t^{2}{}_{1}/t = -2.14403531630538931060130179 42d+00$

$t^{1}{}_{2}/t = -1.07125322701057002017451695 25d+00$

$t^{2}{}_{2}/t = 1.52886228424927025226723988 50d-03$

$t^{1}{}_{3}/t = 1.19548832276396674257727119 46d+00$

$t^{2}{}_{3}/t = 1.19472389162184210745113789 69d+00$ (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 6 parameters 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 $H_1 = \mathbf{p}^2/2$

$t^1{}_1/t$ = -5.978716167195740231006248013 5d-01
$t^2{}_1/t$ = 1.311824102010528062031799454 7d-01
$t^1{}_2/t$ = 5.885290649606443785310659087 4d-01
$t^2{}_2/t$ = 9.216197750488518929223671843 1d-01
$t^1{}_3/t$ = -4.347913701231965896528439183 9d-01
$t^2{}_3/t$ = 1.349378859356682017265384523 5d-01

$t^1{}_1/t$ = 5.179194663933918594008540911 9d-01
$t^2{}_1/t$ = 1.827895409997737211706984963 9d-01
$t^1{}_2/t$ = -1.326796257303449322981714402 3d+00
$t^2{}_2/t$ = 8.627101146291653273688717431 5d-04
$t^1{}_3/t$ = 9.089813662359311477377640954 8d-01
$t^2{}_3/t$ = -5.862051455304877360491885775 6d-01

With $H_2 = \mathbf{p}^2/2$

$t^1{}_1/t$ = 6.806688589128635162839778326 3d-01
$t^2{}_1/t$ = 3.557574259101992924673508420 9d-01
$t^1{}_2/t$ = 2.242357205351748081810958420 4d-01
$t^2{}_2/t$ = -2.214212996230061950930332226 0d-01
$t^1{}_3/t$ = -4.882379127813716577984070076 1d-01
$t^2{}_3/t$ = -3.553721326993987630055139086 8d-02 (25)

Conclusion

From the point of view of an accelerator physicist, sixth order is probably an upper limit, because we use the integrator for approximate modelling. 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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5. E. Forest and R.D. Ruth, Physica **D**, 43, 105, (1990).

6. A.J. Dragt and E. Forest, J. Math. Phys., **24** , 2734(1983).

7. See reference 5, section 6.

8. See the appendix of reference 6.

9. The differential algebra package of Berz is a piece of software capable of performing automatic differentiation on a computer. For a description of the theory with special emphasis on accelerator physics see M. Berz, Part. Accel., **24**, 109 (1989).

10. Yoshida's paper and preprint did not exist when our work was submitted. We recommend very strongly the reading of his paper. The reference is: H. Yoshida, Physics Letters A, **150**, p.262. (Nov 1990)

11. In reference 3, the authors provide a wealth of examples illustrating the qualitative differences between symplectic and non-symplectic integrators.