LBL-30616
ESG-129

# Application of the Yoshida-Ruth Techniques to Implicit Integration, Multi-Maps Explicit Integration and to Taylor Series Extraction

Étienne Forest and Johan Bengtsson
Exploratory Studies Group
Lawrence Berkeley Laboratory[1]
University of California
Berkeley, Ca, 94720

Michael F. Reusch
Grumman Aerospace Corporation
Corporate Research Center
4 Independence Way, Princeton, NJ,08540

## Abstract

The full power of Yoshida's technique is exploited to produce an arbitrary order implicit symplectic integrator and multi-map explicit integrator. This implicit integrator uses a characteristic function involving the force term alone. Also we point out the usefulness of the plain Ruth algorithm in computing Taylor series map using the techniques first introduced by Berz in his "COSY-INFINITY" code.

---

[1] This work is supported by the U.S. Department of Energy under Contract No. DE-AC03-76SF00098

## 1. Introduction

The derivation of explicit symplectic integrators has followed a remarkable path since it was first introduced by R. Ruth [1] in 1983. After Ruth initial derivation for Hamiltonians of the form

$$H= A(\mathbf{p})+V(\mathbf{q}) \tag{1.1}$$

Forest[2] and Neri [3] rederived the Ruth's integrator using Lie Methods. These methods simplified the derivation to the point that Forest was able to get a $6^{th}$ order integrator[4]. More importantly however, it revealed the generality of Ruth's integrator: if H is reducible into two exactly solvable parts $H_1$ and $H_2$ then the integrator of Ruth can be used [2,4]. In addition, the result applies to any Lie group. Therefore one gained far more than just a compact derivation.

In this paper, we want to point out that a similar outcome emerges from carefully looking at Yoshida's elegant derivation[5] of Ruth's integrator. In section 2 , we extend Yoshida's assumptions to encompass a wider class of systems. In section 3, we point out the existence of an arbitrary order implicit integrator involving the force alone, which is a direct consequence of Yoshida's work. In section 4, we describe the multi-maps explicit integrator in the light of Yoshida's work. In the last sections , we apply the older Forest-Ruth point of view to the problem of Taylor series production by Hamiltonian exponentiation. Section 5 contains a description of this technique which was first introduced by Berz. In sections 6 and 7, we apply explicit integration to problems where this technique is only approximate.

## 2. General Rephrasing of Yoshida's Method

Consider a time independent Hamiltonian H , its Lie operator :-H: and it associated symplectic map $M(\tau)$ which results from integrating the equation of motion for a time $\tau$.

$$dM(t)/dt = M(t)\ {:}{-H}{:} \qquad \Rightarrow M(\tau) = \exp(\tau{:}{-H}{:}) \tag{2.1}$$

Let us assume that by some method, we find a symplectic approximation $T_{2n}(\tau)$ of $M(\tau)$, which contains no even powers of $\tau$ in the Lie exponent, or equivalently $T_{2n}(\tau)T_{2n}(\tau)^{-1} = \mathrm{I}$ :

$$T_{2n} = M(\tau) + O(\tau^{2n+1}) = \exp(\tau{:}{-H}{:} + \tau^{2n+1} R(\tau^{2n})) \tag{2.2}$$

Yoshida's prescription is to construct a 2n+2 integrator as follows:

$$T_{2n+2}(\tau) = T_{2n}(z_0\tau)\, T_{2n}(z_1\tau)\, T_{2n}(z_0\tau) \tag{2.3}$$

Using (2.2) , quoting Yoshida , one gets:

$$z_0 = -\frac{2^{1/(2n+1)}}{2-2^{1/(2n+1)}} \qquad z_1 = \frac{1}{2-2^{1/(2n+1)}} \tag{2.4}$$

In addition, Yoshida derived a $6^{th}$ and $8^{th}$ order integrator using the second order approximate map $T_2$.

In his paper, Yoshida gave the impression that his results are applicable only to a Hamiltonian of the form

$$H = H_1 + H_2 , \tag{2.5}$$

as in the Forest-Neri generalization of Ruth's method. In fact, a careful reading of Yoshida's paper reveals the remarkable generality of all his integrators. We exploit this feature in the next section.

## 3. Arbitrary Order Implicit Integrator with only the Force Term

In some complex problems, the explicit integrator of Ruth cannot be used: one cannot split the Hamiltonian into two solvable parts. For these type of problems, one can write a generating function which approximates $M(\tau)$:

$$M(\tau) \equiv \mathbf{q}\cdot\mathbf{p}^{\mathbf{f}} + \tau\, H(\mathbf{q}, \mathbf{p}^{\mathbf{f}}) + O(\tau^2) \tag{3.1}$$

or,

$$M(\tau) \equiv \mathbf{q}\cdot\mathbf{p^f} + \tau\, H(\mathbf{q}, \mathbf{p^f}) - \frac{\tau^2}{2}\frac{\partial H}{\partial \mathbf{q}}\cdot\frac{\partial H}{\partial \mathbf{p}} + O(\tau^3) \tag{3.2}$$

and so on. The general case involves higher and higher derivatives of H [6]. This can now be avoided by using Yoshida's techniques.

By constructing a second order approximation $T_2$ of the form (2.2), we can use directly Yoshida's formulae. This approximation is famous and originally due to Poincaré:

$$\mathbf{q^f} = \mathbf{q} + \tau \frac{\partial H}{\partial \mathbf{x}_2}\left(\frac{\mathbf{q}+\mathbf{q^f}}{2}, \frac{\mathbf{p}+\mathbf{p^f}}{2}\right), \qquad \mathbf{p^f} = \mathbf{p} - \tau \frac{\partial H}{\partial \mathbf{x}_1}\left(\frac{\mathbf{q}+\mathbf{q^f}}{2}, \frac{\mathbf{p}+\mathbf{p^f}}{2}\right). \tag{3.3}$$

Here, $\mathbf{x}_1$ and $\mathbf{x}_2$ refer to the arguments **q** and **p** of the original Hamiltonian H.

Because of the symmetry between initial and final variables in (3.3) under time reversal, this map has all the properties needed in the construction of the Yoshida integrator. Hence formula (2.3) is directly applicable as well as all the other formulae in Yoshida's paper. Such integrators are constructed from (3.3) by repeated applications of the formula with $z_n\tau$ appropriately substituted for $\tau$.

Recently, in an internal report, one of the authors[7] built a fourth order integrator using (3.3) and got equation (2.4) with n=1. However, lacking the insight provided by Yoshida's paper, he did not see the connection to the old Ruth integrator.

Finally, by extending phase space (see section 6) and applying (3.3), we see that the time dependent case is obtained by evaluating (3.3) in the middle of a given time step.

$$q^f = q + \tau \frac{\partial H}{\partial x_2}\left(\frac{q+q^f}{2}, \frac{p+p^f}{2}, t+\frac{\tau}{2}\right), \qquad p^f = p - \tau \frac{\partial H}{\partial x_1}\left(\frac{q+q^f}{2}, \frac{p+p^f}{2}, t+\frac{\tau}{2}\right). \quad (3.4)$$

## 4. Multi-Map Explicit Integrators

In the reference 2, section 5.4, Forest and Ruth point out the a symmetrized product of exact solutions is always quadratic. In fact, it has no terms of even powers in $\tau$. Therefore if the Hamiltonian can be split into N exactly solvable parts a high order explicit integrator of the Yoshida type can be built following equation (2.3). The map $T_2$ will have the following form:

$$H = H_1 + H_2 + \ldots H_N$$

$$N_i = \exp( :- H_i:)$$

$$T_2 = N_1\left(\frac{\tau}{2}\right) N_2\left(\frac{\tau}{2}\right) \ldots N_N(\tau) \ldots N_2\left(\frac{\tau}{2}\right) N_1\left(\frac{\tau}{2}\right). \quad (4.1)$$

This trivial result may be very useful for certain Hamiltonians.

In the remaining sections, we switch our attention to the computation of Taylor series maps.

## 5. Automatic Differentiation Integrators

In recent years Berz has been promoting a new approach to compute Taylor series maps[8]. Whenever it is appropriate to use such maps as the main ingredient of tracking, simulation and analysis (we will not get into this debate here), Berz has proposed the following scheme to get the Taylor series to order $N_0$:

Under the following assumptions :

1) time independent H (usually a length variable in beam dynamics)

2) H sends the origin of phase space into itself

i.e. $H = \sum_{n=2}^{\infty} H_n$, where the $H_n$ are homogeneous polynomials in $(\mathbf{q},\mathbf{p})$, (5.1)

one can get the Taylor series map to order $N_0$ by expanding the operator $\exp(:-\tau H:)$ and letting it act on the phase space variables $(\mathbf{q},\mathbf{p})$ :

$$(\mathbf{q}^f,\mathbf{p}^f) \equiv \lim_{M\to\infty} \sum_{k=0}^{M} \frac{\left(:-\tau \sum_{n=2}^{N_0+1} H_n:\right)^k}{k!} (\mathbf{q},\mathbf{p}) + \ldots O\left(|(\mathbf{q},\mathbf{p})|^{N_0+1}\right) \qquad (5.2)$$

On a computer, the coefficients of the Taylor series converge rapidly and only a few Poisson brackets are needed. This approach is extremely useful as the spread of software using this technique indicates[9,10,11]. But what if assumptions 1 or 2 are relaxed? Then one must integrate the Taylor series and again, the Ruth algorithm fits the technique like a glove.

We now show to apply the Ruth-Yoshida technique to improve the accuracy of the Taylor series when assumption 1) is relaxed.

## 6. Time-dependent Exponentiation

The trick used is well-known. We extend the dimensionality of phase space:

$$(\mathbf{q},\mathbf{p}) \quad \text{goes to} \quad (\mathbf{q},\mathbf{p},t,p_t) \tag{6.1}$$

$$H \quad \text{goes to} \quad K = H + p_t \tag{6.2}$$

In the Taylor series integrator context of the previous section, the series generated by $\exp(:-\tau H:)$ and $\exp(:-\tau p_t:)$ are exactly solvable. Hence the Hamiltonian can be split into two exactly solvable parts. Therefore the formulae of Ruth-Yoshida[5] or Forest[4] are directly applicable. We start with the general form of a two map integrator acting on $(\mathbf{q},\mathbf{p},t,p_t)$:

$$\exp(:-\tau K:)(\mathbf{q},\mathbf{p},t,p_t) \approx \left\{\prod_{j=1}^{N} \exp(:-\tau^1{}_j H:)\ \exp(:-\tau^2{}_j\, p_t:)\right\}(\mathbf{q},\mathbf{p},t,p_t)$$

$$\text{where,}\quad \sum\tau^1{}_j = \tau \ \text{and}\ \sum\tau^2{}_j = \tau \qquad (6.3)$$

By inserting a sequence of identity maps, we can move all the time translations inside the function H:

$$\left\{\prod_{j=1}^{N} \exp(:-\tau^1{}_j H:)\ \exp(:-\tau^2{}_j\, p_t:)\right\} = \left\{\prod_{j=1}^{N} \exp(:-\tau^1{}_j H(t+\delta_j):)\right\}\exp(:-\tau\, p_t:)$$

$$\text{where}\qquad \delta_j = t + \tau^2{}_1 + \ldots.\tau^2{}_{j-1} \qquad (6.4)$$

When acting on $(\mathbf{q},\mathbf{p},t)$, the results is just:

$$\exp(:-\tau H:)(\mathbf{q},\mathbf{p},t) \approx \left(\prod_{j=1}^{N} \exp(:-\tau^1{}_j H(t+\delta_j):)\ (\mathbf{q},\mathbf{p})\ ,\ t+\tau\right) \qquad (6.5)$$

In this new expression all the quantities are evaluated in the original non-extended phase space.

## 7. Non Zero Reference Orbit

Finally, one may be interested in systems where the reference orbit is not the origin of phase space. Let us examine the time independent case first. Obviously, the Taylor series is given by equation (5.2). However, the coefficients of the various monomials are not computed exactly. More specifically, for an arbitrary Hamiltonian, the coefficient of a monomial of degree k in (**q**,**p**) will have an error of order $\tau^{N_0+1-k}$. Clearly, the zeroth order monomial is the orbit itself and it will be known to order $\tau^{N_0+1}$. For high values of the maximum order $N_0$, one gets very accurate results for the low order monomials and therefore there is little value in trying to modify the straight forward exponentiation of equation (5.2)[2]. However, for low order calculations, it may be desirable to use a Ruth-Yoshida integrator of an order comparable to $N_0$.

The derivation of the procedure starts with the assumption that we know the zeroth order orbit. Let us denote it by $\mathbf{r}(t)=(\mathbf{q}(t),\mathbf{p}(t))$. Then the Hamiltonian generating motion around $\mathbf{r}(t)$ is given by:

$$H_{\mathbf{r}} = H(\mathbf{x}+\mathbf{r}) - \mathbf{x}\cdot\nabla H\Big|_{\mathbf{r}} \tag{7.1}$$

Unfortunately, $H_{\mathbf{r}}$ is time dependent and the function $\mathbf{r}(t)$ is an

[2]Time independent polynomial Hamiltonians of order less than $N_0$ are exactly computed by regular exponentiation.

unknown function of time. Temporarily, ignoring this last glitch, we can apply to (7.1) the results of section 6. In fact, we simply re-copy equation (6.5):

$$\exp(:-\tau K:)(\mathbf{q},\mathbf{p},t) \approx \left( \prod_{j=1}^{N} \exp(:-\tau^1{}_j H_{\mathbf{r}}(t+\delta_j):)\ (\mathbf{q},\mathbf{p})\ ,\ t+\tau \right) \tag{7.2}$$

here ,

$$H_{\mathbf{r}}(t+\delta_j) = H(\mathbf{x}+\mathbf{r}(t+\delta_j)) - \mathbf{x}\cdot\nabla H \Big|_{\mathbf{r}(t+\delta_j)} \tag{7.3}$$

We are left with the problem of computing $\mathbf{r}(t+\delta_j)$ with an accuracy comparable with the method of integration. This can be done with equation (5.2): one simply extracts the zeroth order of the map. Also we can use a standard integration method.

Finally, it is clear from the form of equation (7.3) that the assumptions 1 and 2 of section 5 can be relaxed simultaneously and still a Ruth-Yoshida integrator can be constructed.

Acknowledgements

We would like to thank the Exploratory Studies Group leader Dr. Swapan Chattopadhyay for his support of theoretical pursuits. We also thank Prof. John Cary who encouraged us to find a connection between explicit and implicit integration.

References


[1] R.D. Ruth ,IEEE Trans. Nucl. Sci. NS-30 (1983) 2669

[2] E. Forest and R.D. Ruth, Physica D 43 (1990) 105

[3] F. Neri, Department of Physics, University of Maryland, preprint (1988)

[4] E. Forest, J. Comp. Phys. , accepted for publication (1991)

[5] H. Yoshida, Phys. Letter A, 150, (1990) 262

[6] P.J. Channel and C. Scovel , Los Alamos National Laboratory preprint LA-UR-88-1828 (1988)

[7] M.F. Reusch, Grumman Aerospace Corporation, Space Electronics Division Preprint TPP-SED-04-91, (1990)

[8] M. Berz, Part. Accel., 24, (1989) 109

[9] M. Berz, LBL preprint LBL-28881, COSY-INFINITY Reference Manual.

[10] F. Neri and J. Van Zeijts have developed a code "TLIE" which uses the methods of section 5. (Private communication)

[11] J. Bengtsson, LBL preprint LSAP-116. This preprint describes an alternative route to produce a "COSY-INFINITY" type code. It uses a professionally written PASCAL compiler/interpreter and the old Differential Algebra Package of Berz (See [8,9]) and is therefore compatible with all the software developed to do perturbative calculations such as normal form algorithms. (See E. Forest, M. Berz and J. Irwin, Part. Accel., 24, (1989) 91)