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EXTRAPOLATION OF SYMPLECTIC INTEGRATORS

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Abstract

We build high order numerical methods for solving differential equations by applying extrapolation techniques to a Symplectic Integrator of order $2n$. We show that, in general, the qualitative properties are preserved at least up to order $4n+1$. This new procedure produces much more efficient methods than those obtained using the Yoshida composition technique.

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1 Introduction

In recent years the importance of preserving geometric properties of the exact solution when numerically solving a system of differential equations has been repeatedly emphasized.

The aim of Geometric Integration is to provide such a type of numerical algorithms, the so-called Geometric Integrators (GI). When qualitative properties are at issue GI have proved to be superior to general purpose methods [6]. But, if high precision is desired, the most efficient methods are, in general, those based on extrapolation techniques (ET).

In ET one starts with a basic low order integration method which is applied with different time steps h. Then, by an appropriate combination of the results, one obtains a new method which approximates the exact solution to a higher order with essentially no additional cost. Richardson's process of deferred approach to the limit $h \to 0$ is a clear and classical example.

The question naturally arises of what happens when the basic method used in extrapolation is a geometric integrator. As a first approach to this problem we apply conventional extrapolation to improve the efficiency of the method. We find that exact preservation of geometric properties of the solution of a differential system is lost.

In spite of this situation, however, it is the aim of this paper to show that, if we start with a GI of order n and extrapolate it to a higher order n', the new method will still preserve geometric properties up to at least order $2n+1$ and in any case to an order higher than n'. So, the undesired effects of non-geometric schemes will still finally show up but their appearence will be considerably delayed and the errors they originate can be made of the same order of the round-off errors for sufficiently high n.

In the literature a common way to obtain higher order geometric integrators is to use Yoshida's composition method [9]. This technique is very important from the theoretical point of view but produce, in general, computationally costly algorithms. For this reason it is worthwhile to look for other strategies. We will see how the use of ET originates much more efficient methods than those obtained using the Yoshida idea while effectively preserving the qualitative features of the solution. They may constitute then a valid alternative.

2 Extrapolation with a basic symplectic method

To be definite we consider symplecticity as the geometric property to be preserved and so from now on we restrict ourselves to the classical Hamiltonian dynamics setting.

Given a Hamiltonian function $H(\mathbf{q}, \mathbf{p})$, the time evolution of the corresponding dynamical system is obtained by evaluating the action of the operator

$$\mathcal{M}(t) = e^{tL_H} \tag{1}$$

on the initial conditions. Here L_H is the Lie operator associated with H, which acts on an arbitrary function $f(\mathbf{q}, \mathbf{p})$ according to the rule $L_H f = \{f, H\}$, where

$\{f, H\}$ stands for the Poisson bracket. Very often it is possible to split

$$L_H \equiv \mathbf{X} = \mathbf{X}_1 + \cdots + \mathbf{X}_s, \tag{2}$$

where the action of $e^{t\mathbf{X}_i}$, $i = 1, \ldots, s$, can be exactly computed. Then a usual procedure to evaluate the action of $\mathcal{M}(t)$ is to approximate it by a composition of the flows $e^{t\mathbf{X}_i}$. For instance, the symmetric composition

$$\Phi_2(h) = e^{\frac{h}{2}\mathbf{X}_1} \cdots e^{\frac{h}{2}\mathbf{X}_{s-1}} e^{h\mathbf{X}_s} e^{\frac{h}{2}\mathbf{X}_{s-1}} \cdots e^{\frac{h}{2}\mathbf{X}_1} \tag{3}$$

produces a second order symplectic integration method for a time step h: $e^{h\mathbf{X}} - \Phi_2(h) = O(h^3)$. In general, if $\Phi_{2n}(h)$ is a symmetric $2n$-th order method, then

$$\Phi_{2n+2}(h) = \Phi_{2n}(z_1 h)\Phi_{2n}(z_0 h)\Phi_{2n}(z_1 h), \tag{4}$$

with $z_1 = 1/(2 - 2^{\frac{1}{2n+1}})$ and $z_0 = 1 - 2z_1$, is a symplectic method of order $2n + 2$. This technique for constructing symplectic integrators of arbitrarily high orders was proposed independently by Yoshida [9, 10] and Suzuki [7], its main drawback being the high number of evaluations needed. Observe also that $z_1 > 1$ and then $z_0 < -1$, so that application of scheme (4) requires two steps forward and one backward. When $\mathbf{X} = \mathbf{X}_1 + \mathbf{X}_2$ other specific symplectic methods have been designed which are much more efficient than schemes (4), particularly when $\mathbf{X}_2 \ll \mathbf{X}_1$ in some sense [2] or in the Runge-Kutta-Nyström case [3].

Symmetric symplectic integrators are very efficient and in addition their dependence on h is particularly amenable to extrapolation. Let then Φ_{2n} be such a method of order $2n$ for the Hamiltonian vector field (2). Then, for one time step h, it is true that

$$\Phi_{2n}(h) = \exp\left[h\left(\mathbf{X} + h^{2n}\mathbf{N}(h)\right)\right], \tag{5}$$

where $\mathbf{N}(h) = \sum_{i=0}^{\infty} h^{2i}\mathbf{N}_{2i}$, and $\mathbf{N}_{2i}$ are operators belonging to the free Lie algebra $L(\mathbf{X}_1, \ldots, \mathbf{X}_s)$ generated by $\mathbf{X}_j$, $j = 1, \ldots, s$. This can be considered as the vector space spanned by $\mathbf{X}_j$ and all their independent nested Lie brackets.

If the time step is divided in k substeps and the method is applied k times, then

$$\Phi_{2n}^{(k)}(h) \equiv \left(\Phi_{2n}\left(\frac{h}{k}\right)\right)^k = \exp\left[h\left(\mathbf{X} + \left(\frac{h}{k}\right)^{2n}\mathbf{N}\left(\frac{h}{k}\right)\right)\right]. \tag{6}$$

Taking different values of k we obtain different approximate solutions after one step. In this paper we limit ourselves to polynomic extrapolation techniques which consider a linear combination of the approximate solutions achieved with the basic method Φ_{2n},

$$\Psi(h) = \sum_{i=1}^{m} \alpha_i \Phi_{2n}^{(k_i)}(h) \tag{7}$$

and fix the m integers k_i and determine the coefficients α_i so as to eliminate the lowest order terms and thus obtain a higher order integrator. The basic method being symplectic, we can state the following theorem.

Theorem 1 *If the basic $2n$-th order method Φ_{2n} is symmetric and symplectic, then by applying polynomic extrapolation it is possible to construct integration methods of order $2(n+l)$, $l=1,\dots,n$, which are symplectic up to order $4n+1$.*

Proof. We can use the Baker-Campbell-Hausdorff and Zassenhaus formulae [8] for writing the extropolation method $\Psi(h)$ of eq. (7) in the symmetric form

$$\Psi(h) = e^{\frac{h}{2}\mathbf{X}}\mathbf{Y}e^{\frac{h}{2}\mathbf{X}}, \tag{8}$$

where

$$\mathbf{Y} = \sum_{i=1}^{m} \alpha_i e^{h^{2n+1}\mathbf{W}_i}, \qquad \mathbf{W}_i = \frac{1}{k_i^{2n}}\mathbf{R}\left(\frac{h}{k_i}\right)$$

and $\mathbf{R}(h/k_i) = \sum_{j=0}^{\infty}(h/k_i)^{2j}\mathbf{R}_{2j}$, with $\mathbf{R}_{2j} \in L(\mathbf{X}_1,\dots,\mathbf{X}_s)$. Now a Taylor expansion leads to

$$\mathbf{Y} = G_0\mathbf{I} + h^{2n+1}\sum_{j=0}^{\infty} h^{2j}G_{2n+2j}\mathbf{R}_{2j} + \frac{1}{2}h^{4n+2}\sum_{j=0}^{\infty} h^{2j}G_{4n+2j}\mathbf{S}_{2j} + \cdots$$

where

$$G_s = \sum_{i=1}^{m}\frac{\alpha_i}{k_i^s}, \qquad \mathbf{S}_{2s} = \sum_{i=0}^{s}\mathbf{R}_{2i}\mathbf{R}_{2s-2i}, \qquad s = 0,1,2,\dots .$$

We then have a method of order $2(n+l)$, $l=1,\dots,n$, if $G_0 = 1$ and $G_{2n+2j} = 0$ for $j = 0,1,\dots,l-1$. This can be accomplished if $m = l+1$ and the coefficients α_i satisfy the linear system of equations

$$\begin{pmatrix} 1 & 1 & \cdots & 1 \\ \frac{1}{k_1^{2n}} & \frac{1}{k_2^{2n}} & \cdots & \frac{1}{k_m^{2n}} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{1}{k_1^{2n+2m-4}} & \frac{1}{k_2^{2n+2m-4}} & \cdots & \frac{1}{k_m^{2n+2m-4}} \end{pmatrix} \begin{Bmatrix} \alpha_1 \\ \alpha_2 \\ \vdots \\ \alpha_m \end{Bmatrix} = \begin{Bmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{Bmatrix}.$$

Thus

$$\mathbf{Y} = \mathbf{I} + h^{2(n+l)+1}\mathbf{Z} + \frac{1}{2}h^{4n+2}\sum_{j=0}^{\infty} h^{2j}G_{4n+2j}\mathbf{S}_{2j} + \cdots \tag{9}$$

with

$$\mathbf{Z} = \sum_{j=0}^{\infty} h^{2j}G_{2(n+l+j)}\mathbf{R}_{2(l+j)} \tag{10}$$

containing only operators in the Lie algebra $L(\mathbf{X}_1,\dots,\mathbf{X}_s)$, so that it is possible to write

$$\begin{aligned} \mathbf{Y} &= e^{h^{2(n+l)+1}\mathbf{Z}} + \frac{1}{2}h^{4n+2}\big(G_{4n}\mathbf{S}_0 + h^2G_{4n+2}\mathbf{S}_2 + \cdots + \\ &\quad h^{4l}(G_{4n+4l}\mathbf{S}_{4l} - G_{2n+2l}^2\mathbf{R}_{2l}^2) + O(h^{4l+2})\big) + \mathbf{r}(h) \end{aligned} \tag{11}$$

where $\mathbf{r}(h) = O(h^{6n+3})$. It is clear that $\mathbf{Y} = e^{h^{2(n+l)+1}\mathbf{Z}} + O(h^{4n+2})$ and the resulting method Ψ is of order $2(n+l)$ and preserves the symplectic character of the evolution up to order $4n+1$. $\square$

According to this result, if the basic method is order four, six or eight, then the symplectic character is preserved up to order h^9, h^{13} or h^{17}, respectively. In the later case, for values of h sufficiently small, the method will be symplectic up to round-off error.

We emphasize the use of this theorem to obtain methods of order $2(n+l)$, $l = 1, 2$, which behave in practice as symplectic schemes with better efficiency than other strictly symplectic algorithms. In fact, it is possible to build methods of these orders which preserve the symplectic property up to order higher than $4n+1$ (in practice, $4n+3$ or $4n+5$) simply by canceling G_{4n+2r} for $r = 0, 1, \ldots$. We could rise even more the order of preservation of symplecticity but then the order of consistency of the method increases and efficiency could be lost.

In Table 1 we list the linear equations to be solved, besides the condition $G_0 = 1$, in order to obtain different methods by extrapolation techniques. We denote by $\Psi_{i,j}^{(s)}$ a method of order $i = 2(n+l)$, $l = 1, \ldots, n$, which is symplectic up to order $s = 4n + 1 + 2r$, $r = 0, 1, \ldots, r_{\max}$, obtained by extrapolating a basic symplectic method of order $j = 2n$. A detailed analysis of eq. (11) shows that $r_{\max} = 2l - 1$ if n and l are such that $4l < 2n + 1$.

In particular, for constructing a method $\Psi_{6,4}^{(13)}$ we must solve the equations $G_0 = 1$, $G_4 = 0$ (6-th order conditions: $l = 1$) and $G_8 = G_{10} = 0$ to achieve preservation of the symplectic character up to order 13 ($r = 2$), whereas the method $\Psi_{12,8}^{(17)}$ requires solving the 12-th order conditions $G_0 = 1$, $G_8 = G_{10} = 0$ ($l = 2$, $r = 0$). In this way we end up with

$$\begin{aligned}
\Psi_{6,4}^{(13)} &= \frac{1}{3912975}\left(4194304\ \Phi_4^{(8)} - 282624\ \Phi_4^{(4)} + 1296\ \Phi_4^{(2)} + \Phi_4\right) \\
\Psi_{12,8}^{(17)} &= \frac{1}{260865}\left(262144\ \Phi_8^{(4)} - 1280\ \Phi_8^{(2)} + \Phi_8\right).
\end{aligned} \tag{12}$$

The Table suggests that it is convenient in practice to take $l = 1$ or 2 and basic methods of high order (six or eight) to obtain extrapolation schemes effectively symplectic up to round-off error. In this way, the particular sequence of k_i values chosen for extrapolation is not relevant.

For the sake of illustration of the results obtained, we consider next the harmonic oscillator Hamiltonian

$$H = T(p) + V(q) = \frac{1}{2}p^2 + \frac{1}{2}q^2.$$

Let $M_X(h)$ denote the exact matrix evolution associated with $X = H$, T and V, i.e., $(q(h), p(h))^T = M_X(h)(q(0), p(0))^T$. Then

$$M_H(h) = \begin{pmatrix} \cos(h) & \sin(h) \\ -\sin(h) & \cos(h) \end{pmatrix}, \quad M_T(h) = \begin{pmatrix} 1 & h \\ 0 & 1 \end{pmatrix}, \quad M_V(h) = \begin{pmatrix} 1 & 0 \\ -h & 1 \end{pmatrix}.$$

We consider as basic methods the following 4-th and 6-th order symplectic

n	l	Method	Equations	r	$r_{\max}$
1	1	$\Psi_{4,2}^{(5)}$	$G_2 = 0$	0	0
2	1	$\Psi_{6,4}^{(9)}$	$G_4 = 0$	0	2
		$\Psi_{6,4}^{(11)}$	$G_8 = 0$	1	
		$\Psi_{6,4}^{(13)}$	$G_{10} = 0$	2	
3	1	$\Psi_{8,6}^{(13)}$	$G_6 = 0$	0	2
		$\Psi_{8,6}^{(15)}$	$G_{12} = 0$	1	
		$\Psi_{8,6}^{(17)}$	$G_{14} = 0$	2	
3	2	$\Psi_{10,6}^{(13)}$	$G_6 = G_8 = 0$	0	4
		$\Psi_{10,6}^{(17)}$	$G_{12} = G_{14} = 0$	2	
		$\Psi_{10,6}^{(21)}$	$G_{16} = G_{18} = 0$	4	
4	1	$\Psi_{10,8}^{(17)}$	$G_8 = 0$	0	2
		$\Psi_{10,8}^{(19)}$	$G_{16} = 0$	1	
		$\Psi_{10,8}^{(21)}$	$G_{18} = 0$	2	
4	2	$\Psi_{12,8}^{(17)}$	$G_8 = G_{10} = 0$	0	4
		$\Psi_{12,8}^{(21)}$	$G_{16} = G_{18} = 0$	2	

Table 1: *Extrapolation methods $\Psi_{i,j}^{(s)}$ of order i built from symplectic j-th order schemes and equations needed to solve. The number of substeps required is $m = l + 1$ and the methods preserve symplecticity up to order $s = 4n + 1 + 2r$. Here $r_{\max}$ denotes the maximum value of r a method of order $2(n + l)$ can attain.*

symmetric schemes built by Yoshida [9]:

$$\begin{aligned} \Phi_4(h) &= \Phi_2(x_1h)\Phi_2(x_0h)\Phi_2(x_1h) \\ \Phi_6(h) &= \Phi_2(w_1h)\Phi_2(w_2h)\Phi_2(w_3h)\Phi_2(w_4h)\Phi_2(w_3h)\Phi_2(w_2h)\Phi_2(w_1h) \end{aligned} \tag{13}$$

where $\Phi_2(h) = M_T(h/2)M_V(h)M_T(h/2)$ is the well known leapfrog method and

$$\begin{array}{ll} x_1 = \frac{1}{2-2^{1/3}} & x_0 = 1 - 2x_1 \\ w_1 = 0.78451361047755726382 & w_2 = 0.23557321335935813368 \\ w_3 = -1.17767998417887100695 & w_4 = 1 - 2(w_1 + w_2 + w_3). \end{array}$$

In Table 2 we collect the main term in the truncation error for several methods obtained by extrapolation from these basic methods. We check the preservation of the symplectic character of the approximate evolution matrix simply by computing its determinant (a 2×2 matrix A is symplectic iff $\det(A) = 1$). As we can observe, these results are in complete agreement with the above deduced theoretical estimates.

3 Comparison with composition methods

As a criterion to estimate the error of a $2(n + l)$-th order method obtained from a symplectic basic scheme $\Phi_{2n}(h)$ we may introduce the quantity $E_f =$

i,j,s	$\Psi_{i,j}^{(s)}$	$\Psi_{i,j}^{(s)}(h) - M_H(h)$	$\det\left(\Psi_{i,j}^{(s)}(h)\right)$
$6,4,9$	$\frac{1}{15}\left(16\Phi_4^{(2)} - \Phi_4\right)$	$\begin{pmatrix} 0 & -8.6\times 10^{-4} \\ -2.0\times 10^{-3} & 0 \end{pmatrix} h^7$	$1+1.8\times 10^{-4}h^{10}$
$6,4,11$	$\frac{1}{3825}\left(4096\Phi_4^{(4)} - 272\Phi_4^{(2)} + \Phi_4\right)$	$\begin{pmatrix} 0 & -1.0\times 10^{-5} \\ -2.3\times 10^{-5} & 0 \end{pmatrix} h^7$	$1+1.3\times 10^{-7}h^{12}$
$8,6,13$	$\frac{1}{2^6-1}\left(2^6\Phi_6^{(2)} - \Phi_6\right)$	$\begin{pmatrix} 0 & 6.4\times 10^{-6} \\ 8.6\times 10^{-6} & 0 \end{pmatrix} h^9$	$1+1.6\times 10^{-7}h^{14}$

Table 2: *Error and degree of symplecticity for different $\Psi_{i,j}^{(s)}$ methods obtained by extrapolating the basic symplectic integrator Φ_j.*

$p\,\varepsilon\,\|\mathbf{R}_{2l}\|^{\frac{1}{2(n+l)}}$, where p counts the number of times the basic method is applied, ε measures the error of the method and $\|\cdot\|$ denotes some norm of the main error term at order $2(n+l)+1$. In this section we make some comments on the relative merits of composition and extrapolation methods with respect to p and ε.

The number of evaluations needed to increase by $2l$ the order of the basic symmetric method $\Phi_{2n}(h)$ by applying eq. (4) is $p=3^l$. Instead, with extrapolation with the sequence $k_i = 2^{i-1}$, $i=1,\dots,l+1$, this number is $p=\sum_{i=1}^{l+1} 2^{i-1} = 2^{l+1}-1$, which grows more slowly with l.

In order to analyze the behaviour of ε in both types of techniques, let us consider again $\Phi_{2n}(h)$ as given by eq. (5). Then the Yoshida composition (4) leads to:

$$S_{2n+2}(h) = \exp\left(h\mathbf{X} + h^{2n+3}\left(y_{2n+3}\mathbf{N}_2 + v_{2n+3}[\mathbf{X},[\mathbf{X},\mathbf{N}_0]]\right) + O(h^{2n+5})\right),$$

with $y_{2n+3} = 2(x^2-1)/(x-2)$, $x=2^{1/2n+1}$, and $v_{2n+3} < y_{2n+3}$. Here $[A,B]$ denotes the usual Lie bracket.

On the other hand, with extrapolation we obtain:

$$\Psi_{2n+2,2n}^{(4n+1)} = \frac{1}{2^n-1}\left(2^n\Phi_{2n}^{(2)} - \Phi_{2n}\right) = \exp\left(h\mathbf{X} + h^{2n+3}e_{2n+3}\mathbf{N}_2 + O(h^{2n+5})\right) + O(h^{4n+1}),$$

with $e_{2n+3} = \dfrac{-3}{4(2^{2n}-1)}$.

A first estimate shows that $\left|\dfrac{y_{2n+3}}{e_{2n+3}}\right| \sim 2^{2n}$, which indicates how greater is the error in the Yoshida scheme. If we apply twice the composition to obtain a method of order $2n+4$ then the quotient of errors will be $\left|\dfrac{y_{2n+5}}{e_{2n+5}}\right| \sim 2^{2n}2^{2n+2} = 2^{4n+2}$. In the next section we will see that this is perfectly in accordance with the results in the numerical examples.

4 Numerical Examples

We test numerically, in a non-trivial problem, the new methods based on the extrapolation technique in comparison with standard high-order symplectic integrators. In particular, we compare with the integration methods obtained by applying Yoshida's technique, eq. (4), and study to what extent the symplectic character is kept in the numerical approximation.

In our experiments we consider the Kepler Hamiltonian

$$H(\mathbf{q},\mathbf{p}) = \frac{1}{2}\left(p_x^2+p_y^2\right) - \frac{1}{\sqrt{q_x^2+q_y^2}},$$

which is a standard test bench for symplectic integrators, with initial conditions $p_x = 0$, $p_y = \sqrt{\frac{1+e}{1-e}}$, $q_x = 1-e$, $q_y = 0$, and eccentricity $e = 0.5$. These correspond to an orbit of period 2π and energy $-1/2$.

Figures 1(a) and 1(b) show, in a log-log scale, the average error in energy as a function of time obtained along $2^{15} = 32768$ periods with different sixth-order schemes constructed from the fourth-order symplectic method Φ_4 of eq. (13): dotted lines correspond to the Yoshida technique, dash-dotted lines stand for the extrapolation method $\Psi_{6,4}^{(9)}$ given in Table 2 and solid lines correspond to $\Psi_{6,4}^{(13)}$, given in eq. (12). The step size h is chosen in such a way that all methods require 900 (Fig. 1(a)) and 3600 (Fig. 1(b)) evaluations of the potential per period, respectively.

In Figure 1(a), due to the big step used, the linear growth in the energy error appears after a small number of periods for the extrapolation method. Nevertheless, when h is four times smaller (Fig. 1(b)) it is considerably delayed for $\Psi_{6,4}^{(9)}$ and much more for $\Psi_{6,4}^{(13)}$, which is effectively symplectic in the whole time interval considered. In fact, we can easily estimate this delay: if we write the dominant terms in the error of a method $\Psi_{i,j}^{(s)}$ as $Ah^i + Bh^s$, then the linear growth appears when $|B/A|\, h^{s-i} \simeq 1$. When h is divided by a factor β the undesired effects are delayed by a time of the order β^{s-i}. In our case $\beta = 4$, $i = 6$, and $s = 9$ or 13 so $\Psi_{6,4}^{(13)}$ will be more efficient than Yoshida's method during 10-20 millions of periods (without considering round-off errors) while being effectively symplectic for approximately one million periods. Observe in passing that the error in Yoshida's method is approximately 2^4 times greater, as predicted in the previous section.

Figure 1(c) shows the average error in energy and Figure 1(d) in position (as the Euclidean norm in $\mathbb{R}^4$) obtained by two 12-th order methods constructed by applying Yoshida's technique ($\Phi_{12,8}$, dotted lines) and extrapolation ($\Psi_{12,8}^{(17)}$, dash-dotted lines) to the 17 stages symmetric symplectic eighth-order method ($SS, m = 17$) designed by McLachlan [4], Φ_8. The step size chosen is $h = \frac{2\pi}{20}$ for both methods, so that $\Phi_{12,8}$ requires nine evaluations of Φ_8 per step, whereas only seven are needed for $\Psi_{12,8}^{(17)}$. From the Figure we see that $\Psi_{12,8}^{(17)}$ provides results which are four orders of magnitude more accurate than $\Phi_{12,8}$ while still effectively preserving the symplectic character of the evolution. Again this is in agreement with the estimate (2^{18}) of the previous section when the different number of evaluations is taken into account. The 14-th order schemes built from Φ_8 give still much better results.

In order to compare the efficiency of the new extrapolation methods, we show in Figure 2 the average error in energy against the number of potential evaluations obtained after 500 periods with different symplectic 8-th order integrators recently appeared in the literature:

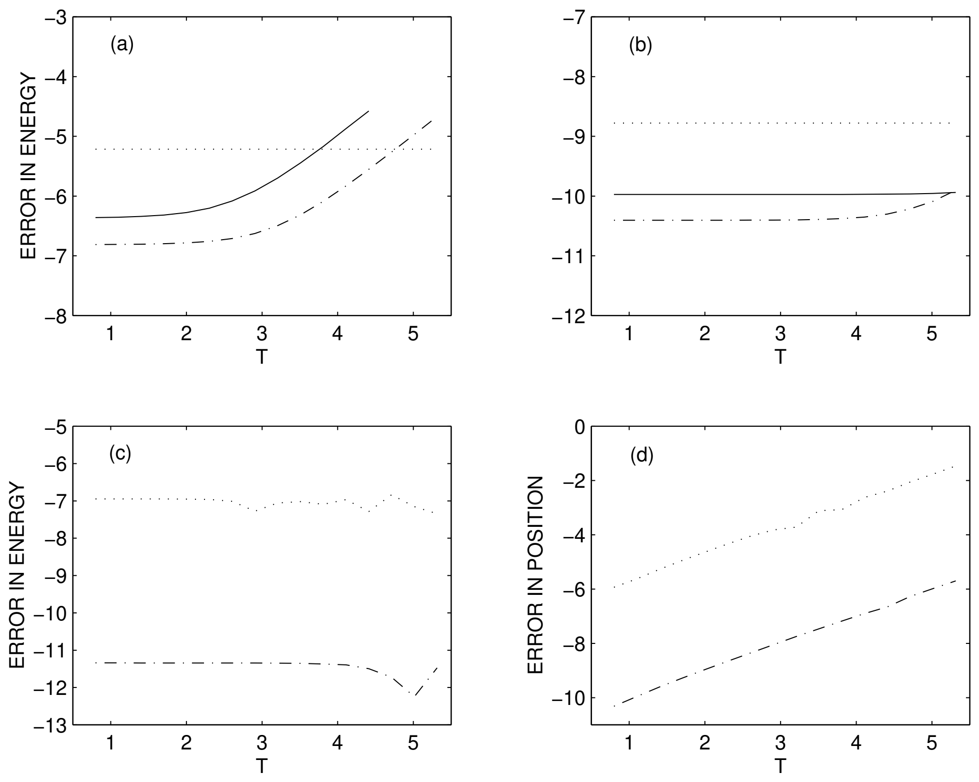

Figure 1: **(a)** and **(b)**: Average error in energy vs. time for the Kepler problem obtained with the extrapolation methods $\Psi_{6,4}^{(9)}$ (dash-dotted lines), $\Psi_{6,4}^{(13)}$ (solid lines) and the 6-th order integrator built by applying Yoshida's technique to the basic symplectic method Φ_4 of eq. (13). In **(b)** the step size h es four times smaller than in **(a)**. **(c)** and **(d)**: Average error in energy (**(c)**) and position (**(d)**) obtained by the extrapolation method $\Psi_{12,8}^{(17)}$ (dash-dotted lines) and the 12-th order integrator built by applying Yoshida's technique to a basic 8-th order symplectic method.

- Yos8: The best 15 stages method given by Yoshida [9];
- CSS8: The 24 stages method given by Calvo and Sanz-Serna [6];
- McL8: The 17 stages method given by McLachlan [4];
- pm8: The 5 stages method using modified functions given in [3].

These well established methods are compared with $\Psi_{8,6}^{(13)}$ (ex6-8 in the figure) obtained using the nine stages sixth-order symmetric symplectic method $(SS, m = 9)$ of McLachlan [4] as the basic method. We observe that, when high precision is considered, the efficiency of ex6-8 is very similar to that of CSS8. We clearly notice how the ET can produce, in a very simple form, highly efficient methods when applied to good basic methods.

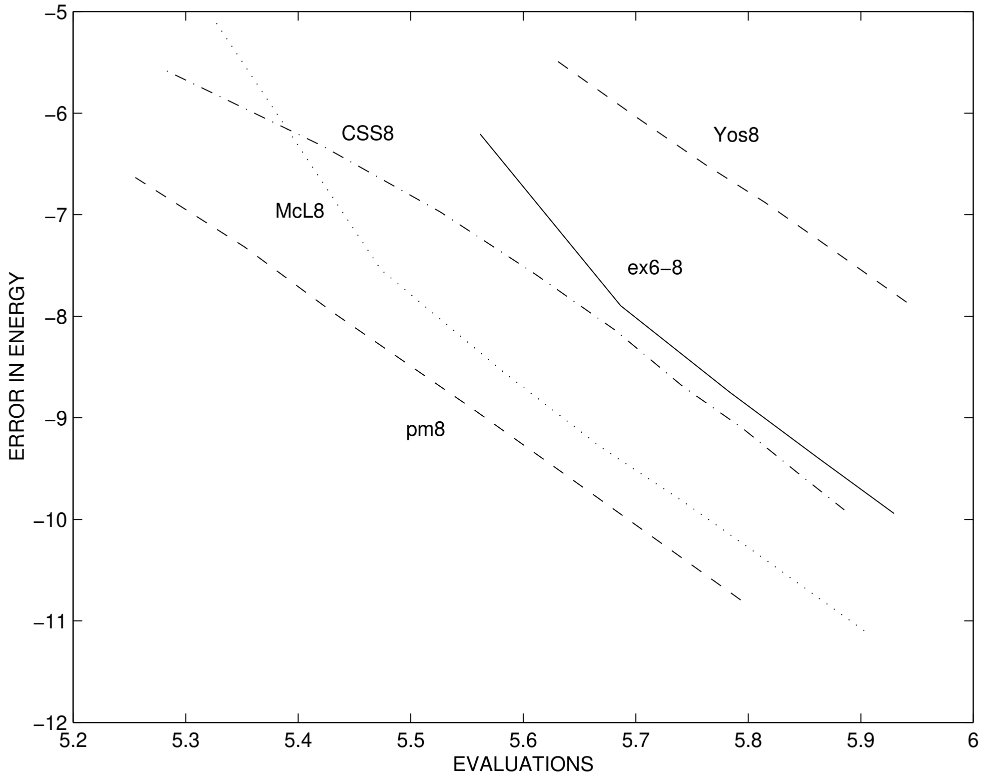

Figure 2: Average error in energy vs. number of potential evaluations for the Kepler problem obtained with the new extrapolation method $\Psi_{8,6}^{(13)}$ (ex6-8) in comparison with other 8-th order strictly symplectic integrators.

5 Final comments

In the last years there has been a dramatic growth of the literature on symplectic integration of Hamiltonian dynamical systems, especially concerning the characterization of existing numerical methods which preserve symplecticity and also on the construction of new classes of symplectic methods. With respect to one-step methods, it has been shown that the family of Runge-Kutta and Runge-Kutta-Nyström shemess are symplectic if their coefficients satisfy certain well known relations [6], whereas there is no universal criterion for symplecticity of multistep methods, although this is an active field of research [5]. By pursuing a similar goal we address in this paper the question of the preservation of symplecticity by extrapolation methods obtained from a basic $2n$-th order symplectic scheme. In general, the answer given by Theorem 1 is that, although the resulting method is not symplectic, it preserves symplecticity up to order $4n+1$ and even to higher order.

In this paper the purpose was not to construct an scheme with variable step size and arbitrarily high order from a basic second order method, but to start with a high order symplectic method (six or eight) and build efficient integration algorithms of order eight, ten or twelve which behave in practice as symplectic integrators. This is at variance with the ordinary use of extrapolation methods in solving ordinary differential equations.

In fact, we have shown, both theoretically and in numerical experiments, that by applying the polynomic extrapolation idea, it is possible to build integration methods which are more efficient than those obtained by employing Yoshida's composition technique without losing in practice the nice properties of symplectic methods. Even more, the efficiency of our simple 8-th order scheme $\Psi_{8,6}^{(13)}$ is analogous to other standard symplectic integrators.

Recently, the construction of explicit Runge-Kutta methods of order p which mimic symplectic ones as far as the error propagation is concerned, has been afforded by Aubry and Chartier [1]. They call such a p-th order method pseudo-symplectic of order $q > p$ (in practice, $q = 2p$) if it preserves the symplectic form to within $O(h^q)$-terms. In [1] some second and third-order methods of pseudo-symplectiness order four and six have been explicitly obtained, but the construction of higher order schemes in this framework is cumbersome.

In this paper we have shown how to use polinomic extrapolation to obtain p-th order pseudo-symplectic explicit methods of pseudo-symplectiness order $q > n$, with p as high as desired, simply by solving a system of linear equations. We have given methods even with $q = 2p + 1$, although schemes with lower values of q behave as strictly symplectic ones over long integration intervals when high order basic methods are considered.

In this work we have used as the basic method for extrapolation an explicit symmetric symplectic integrator. It is clear, however, that the same procedure can also be applied with a basic implicit method. In fact, implicit integration schemes require the solution of several systems of nonlinear equations per step, and this is a serious drawback for achieving high order methods. In this case, the use of ET could be particularly efficient. If one starts the integration with the substeps h/k_m, $k_m = 2^{m-1}$, one finds two advantages: *i)* the nonlinear equations are solved with few iterations and *ii)* we have approximate solutions in 2^{m-1} intermediate points. These approximate solutions can be used in order to speed up considerably the other $2^{m-1}-1$ substeps corresponding to the other k_i.

Extrapolation methods are also especially amenable for integrating irreversible systems. As is well known, for this type of systems, numerical integration methods with non-negative coefficients are commonly used. It is interesting then that the extrapolation methods introduced in this paper ensure this characteristic provided the basic method fulfills it.

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References

[1] A. Aubry and P. Chartier, *Pseudo-symplectic Runge-Kutta methods*, BIT **38** (1998), 439-461; *A note on pseudo-symplectic Runge-Kutta methods*, BIT **38** (1998), 802-806.

[2] S. Blanes, F. Casas and J. Ros, *Processing integration for near-integrable Hamiltonian systems*, submitted to Celes. Mech. Dyn. Astron.

[3] S. Blanes, F. Casas and J. Ros, *High-order Runge-Kutta-Nyström methods with processing*, submitted.

[4] R.I. McLachlan, *On the numerical integration of ordinary differential equations by symmetric composition methods*, SIAM J. Sci. Comput., **16** (1995), 151-168.

[5] R.I. McLachlan and C. Scovel, *A survey of open problems in symplectic integration*, in: Integration Algorithms and Classical Mechanics, J.E. Marsden, G.W. Patrick, and W.F. Shadwick, eds., American Mathematical Society, Providence, R.I., 1996, 151-180.

[6] J.M. Sanz-Serna and M.P. Calvo, *Numerical Hamiltonian Problems,* Chapman & Hall, London, 1994.

[7] M. Suzuki, *Fractal decomposition of exponential operators with application to many-body theories and Monte Carlo simulations*, Phys. Lett. A, **146** (1990), 319-323.

[8] R.M. Wilcox, *Exponential operators and parameter differentiation in Quantum Physics*, J. Math. Phys., **8** (1967), 962-982.

[9] H. Yoshida, *Construction of higher order symplectic integrators*, Phys. Lett. A, **150** (1990), 262-268.

[10] H. Yoshida, *Recent progress in the theory and application of symplectic integrators*, Celes. Mech. Dyn. Astron., **56** (1993), 27-43.