A TENTH ORDER SYMPLECTIC RUNGE KUTTA NYSTRÖM METHOD.

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Abstract. A tenth order explicit symmetric and in consequence symplectic Runge Kutta Nyström method is presented here. We derive the order conditions needed and solve them for the parameters of the method. Numerical results indicate the superiority of the new method compared to the other high order symplectic methods appeared in the literature until now.

Keywords : Runge-Kutta-Nyström methods, Hamiltonian problems, symplectic methods.

1. Introduction.

The initial value problem

$$y'' = f(t, y), \ y(t_0) = y_0, \ y'(t_0) = y_0', \ t \in [t_0, t_{\text{end}}] \tag{1}$$

where $f : \mathbb{R} \times \mathbb{R}^m \to \mathbb{R}^m$, and $y_0, y_0' \in \mathbb{R}^m$, is usually approximated at a discrete set of points (t_n, y_n, y_n') by an explicit s-stage Runge-Kutta-Nyström (RKN) method of order p. The form of this method is

$$\begin{aligned}
f_i &= f(t_n + c_i h_n, y_n + c_i h_n y_n' + h_n^2 \sum_{j=1}^{i-1} a_{ij} f_j), \quad i = 1, 2, \cdots, s \\
y_{n+1} &= y_n + h_n y_n' + h_n^2 \sum_{i=1}^{s} b_i f_i, \\
y_{n+1}' &= y_n' + h_n \sum_{i=1}^{s} b_i' f_i,
\end{aligned}$$

with $h_n = t_{n+1} - t_n$. The coefficients of a RKN method can be presented using matrices in the Butcher tableau [1],

$$\begin{array}{c|c}
c & A \\
\hline
 & b \\
 & b'
\end{array}$$

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where $A \in R^{s\times s}$, $b^{\mathrm{T}}, b'^{\mathrm{T}}, c \in R^{s}$.

If f in (1) is the gradient of a scalar potential $-V = -V(y)$ and if we set $p = \dot{y}$, $q = y$, then (1) can be rewritten as

$$\frac{dp^J}{dt} = -\frac{\vartheta V}{\vartheta q^J}, \quad \frac{dq^J}{dt} = p^J, \quad 1 \le J \le m$$

This is the separable Hamiltonian system of ordinary differential equations

$$\frac{dp^J}{dt} = -\frac{\vartheta H}{\vartheta q^J}, \quad \frac{dq^J}{dt} = \frac{\vartheta H}{\vartheta p^J}, \quad 1 \le J \le m$$

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

A RKN method is said to be canonical or symplectic if it preserves the symplectic structure of the space of variables (p, q). Suris [11] showed that an RKN method is symplectic if

$$b_i = b_i'(1 - c_i) \quad i = 1, 2, \ldots, s \tag{2}$$

and

$$b_i'(b_j - a_{ij}) = b_j'(b_i - a_{ji}), \quad 1 \le i, j \le s. \tag{3}$$

Assumptions (2) and (3) are too restrictive since they actually determine matrix A according to the formula $a_{ij} = b_j'(c_i - c_j)$. Another interesting result is that, if the method is explicit and symmetric then it is symplectic [9]. An RKN is symmetric when

$$c_i = 1 - c_{s+1-i}, \quad b_i' = b_{s+1-i}', \quad i = 1, 2, \ldots, s.$$

So only few coefficients remain to be determined, in order to solve the equations of conditions (order conditions) and derive a symmetric RKN method.

2. The order conditions and the new method.

The general form of an s-stages symplectic integrator is given by [7],

$$q_{i+1} = q_0 + \gamma_i h \frac{\partial T}{\partial p}(p_0), \; p_{i+1} = p_0 - d_i h \frac{\partial V}{\partial p}(q_0), \; i = 1, 2, \ldots, s-1 \tag{4}$$

with q_0 and p_0 the initial values and q_s and p_s the numerical solution at $t_n + h$. The transformation from q_0, p_0 to q_s, p_s is symplectic.

Yoshida in [15], suggested that when $s = 2r + 1$ and setting $d_{2r+2} = 0$, $d_1 = d_{2r+1} = w_r$, $d_2 = d_{2r} = w_{r-1}, \cdots$, $d_r = d_{r+2} = w_1$, $d_{r+1} = w_0 = 1 - 2\sum\limits_{i=1}^{r} w_i$ and $\gamma_1 = \gamma_{2r+2} = \frac{1}{2}w_r$, $\gamma_2 = \gamma_{2r+1} = \frac{1}{2}(w_r + w_{r-1}), \cdots$, $\gamma_{r+1} = \gamma_{r+2} = \frac{1}{2}(w_1 + w_0)$, then we may get the equivalent s-stage RKN method:

Table 1: Order conditions.

3rd order	$b'C^2e = \frac{1}{3}$.
5th order	$b'C^4e = \frac{1}{5},\ b'CAc = \frac{1}{30}$.
7th order	$b'C^6e = \frac{1}{7},\ b'C^3Ac = \frac{1}{42},\ b'C^2AC^2e = \frac{1}{84},\ b'CA^2c = \frac{1}{840}$.
9th order	$b'C^8e = \frac{1}{9},\ b'C^3AC^3e = \frac{1}{180},\ b'C^2AC^4e = \frac{1}{270},\ b'CAC^5e = \frac{1}{378},$
	$b'CA^3c = \frac{1}{45360},\ b'C^2ACAc = \frac{1}{1620},\ b'CAC^2Ac = \frac{1}{2268},$
	$b'C^3A^2c = \frac{1}{1080},\ b'C^2A^2C^2e = \frac{1}{3240}$.
11th order	$b'C^{10}e = \frac{1}{11}, b'C^7Ac = \frac{1}{66}, b'C^6AC^2e = \frac{1}{220}, b'C^5AC^3e = \frac{1}{220},$
	$b'C^4AC^4e = \frac{1}{330}, b'C^2\left((AC^2e).(AC^2e)\right) = b'C^2\left(AC^2e\right)^2 = \frac{1}{1584},$
	$b'C\left(Ac\right)^3 = \frac{1}{2376}, b'\left(A^2c\right)^2 = \frac{1}{158400}, b'\left((AC^2e).(A^2C^2e)\right) = \frac{1}{47520},$
	$b'\left(AC^3e\right)^2 = \frac{1}{4400}, b'C\left(AC^2e\right).\left(AC^3e\right) = \frac{1}{2640}, b'C^2\left(Ac\right).\left(AC^3e\right) = \frac{1}{1320},$
	$b'C^3\left(Ac\right).\left(AC^2e\right) = \frac{1}{792}b'C^4\left(Ac\right)^2 = \frac{1}{396}, b'\left(Ac\right).\left(AC^5e\right) = \frac{1}{2772},$
	$b'C\left(Ac\right).\left(AC^4e\right) = \frac{1}{1980}, b'\left(AC^4e\right).\left(AC^2e\right) = \frac{1}{3960},$
	$b'\left(A^2c\right).\left(AC^3e\right) = \frac{1}{26400}, b'C^2\left(Ac\right).\left(A^2c\right) = \frac{1}{7920},$
	$b'C\left(Ac\right).\left(A^2C^2e\right) = \frac{1}{23760}, b'C\left(Ac\right).\left(ACAc\right) = \frac{1}{11880}.$
	$b'C\left(AC^2e\right).\left(A^2c\right) = \frac{1}{15840}, b'\left(Ac\right)^2.\left(AC^2e\right) = \frac{1}{4752}.$

In the table above we substitute $C = \mathrm{diag}(c)$, $e = [1,1,...,1]^T \in R^s$ while the dot (.) represents a component by component multiplication. So if $u, v, w \in R^s$, then $u = v.w \Rightarrow u_i = v_i w_i,\ i = 1, 2, \cdots, s$.

$$c = \begin{bmatrix} \frac{1}{2}w_r \\ \frac{1}{2}w_{r-1} + w_r \\ \vdots \\ \frac{1}{2}w_1 + \sum\limits_{i=2}^{r} w_i \\ 1/2 \\ 1 - c_r \\ \vdots \\ 1 - c_2 \\ 1 - c_1 \end{bmatrix}, \quad (b')^{\mathrm{T}} = \begin{bmatrix} w_r \\ w_{r-1} \\ \vdots \\ w_1 \\ 1 - 2\sum\limits_{i=1}^{r} w_i \\ w_1 \\ \vdots \\ w_{r-1} \\ w_r \end{bmatrix}.$$

Actually this is a composition method, consisting of r repetitions of Leap Frog method using the proper step $w_i h$. Under these assumptions the even order equations vanish and the finally the order conditions to be solved are given in table 1. As a consequence p can be only an even number.

These equations remain independent when using the fact that the equations with symmetric left hand sides of the form $b'\phi_1 A\phi_2$ and $b'\phi_2 A\phi_1$ are equivalent for any subtree ϕ_1, ϕ_2 [6]. Additionally, we may drop the equations including[1] Ae, and we can also drop their equivalent equations. For example from the twenty equations of seventh order [3], only four remain to be satisfied. We observe that $b'C^3Ac = \frac{1}{42}$ drops $b'CAC^3e = \frac{1}{140}$, $b'CA^2c = \frac{1}{840}$ drops $b'(Ac).(Ac) = \frac{1}{252}$ while the self-symmetric $b'C^2AC^2e = \frac{1}{84}$ drops nothing. Equations like $b'(Ae)^2 - \frac{1}{20} = b'\left(\frac{1}{2}C^2e - \frac{1}{8}b'^2\right)^2 - \frac{1}{20} = \frac{1}{4}b'C^4e - \frac{1}{8}(b'^{\,3}).C^2e + \frac{1}{64}b'^{\,5} - \frac{1}{20} = \frac{1}{4}\times\frac{1}{5} - 0 + 0 - \frac{1}{20} = 0,$[2] are automatically satisfied. The order conditions $b'C^4Ae = \frac{1}{14}$ or $b'CACAe = \frac{1}{280}$ are also dropped because of Ae, while equations like $b'AC^4e = \frac{1}{210}$ is dropped since it is symmetric to $b'C^4Ae = \frac{1}{14}$.

Such methods behave the same as if we had used the assumptions (3) and $Ae = \frac{1}{2}C^2e$ together, [3]. The enumeration of equations follows from Theorem 3.2 in [3]. So for $m_3'^* = 1$, $m_5'^* = 2$, $m_7'^* = 4$, $m_9'^* = 9$, $m_{11}'^* = 23$, $m_{13}'^* = 63$, and $m_{15}'^* = 182$. According to this enumeration the stages s_i for obtaining i-th order are, $s_4 = 3 = 2m_3'^* + 1$, $s_6 = 7 = 2\left(m_3'^* + m_5'^*\right) + 1$, $s_8 = 15$, $s_{10} = 33$, $s_{12} = 79$, $s_{14} = 205$, $s_{16} = 569$.

In order to construct a 10th order method, 16 equations of condition need to be solved. This means that we require 16 variables $w_1, w_2, \ldots, w_{16}$ and $2\times 16 + 1 = 33$ stages. This is a very difficult task for someone to accomplish but we manage to get some solutions. One of these solutions is given in Table 2 in 45-digits of accuracy. The high precision of the coefficients is obligatory since the method is expected to perform in quadruple arithmetic for long intervals.

It can be verified that the method of table 2 satisfies all 288 order conditions of a 10th order RKN method needed when $Ae \neq \frac{1}{2}C^2e$ (see 3rd column of Table 1 in [3]). It also satisfies the order conditions concerning b automatically from (2).

3. Numerical results

We choose the Kepler problem to perform our tests. Its potential is $V(q) = -1/\|q\|$. As initial conditions we have $p^1 = 0$, $p^2 = \sqrt{\frac{1+e}{1-e}}$, $q^1 = 1-e$, $q^2 = 0$. The eccentricity is chosen to be $e = 1/2$. For our choice the solution is 2π periodic. The errors were measured in the absolute maximum norm of $\mathbb{R}^4$, at the endpoints 10π, 100π and 1000π. The methods tested were divided in two groups. The former group contains the symplectic methods:

(i) The 33 stages, 10th order method NEW10 appeared in the previous section. We integrated this method using the step sizes $2\pi/31$, $\pi/31$ and $2\pi/93$.

(ii) A 31stages, 10th order method S10 given by Suzuki, [13]. Its coefficients are presented in table 3. We tried here the stepsizes $2\pi/33$, $\pi/33$ and $2\pi/99$.

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[1] $Ae = \frac{1}{2}C^2e - \frac{1}{8}b'^2$

[2] $b'^{\,i}.e = 0$ for $i = 3, 5, \ldots, p-1$, [12].

Table 2: Solution of 10th order.

$$w_1 = 0.02690013604768968151437422144441685467297755661$$
$$w_2 = 0.939801567135683337900037741418097674632505563$$
$$w_3 = -0.00803583920385358749646880826318191806393661063$$
$$w_4 = -0.866485197373761372803661767454208401679117010$$
$$w_5 = 0.102311291119359873107856328506713154132814244 9$$
$$w_6 = -0.197077215139308010137601846510549195866052508 5$$
$$w_7 = 0.617877713318069357335731125307019691019646679$$
$$w_8 = 0.190727289600012100160590383689119827044143601 2$$
$$w_9 = 0.207260502885248255938295463000262077796906037 7$$
$$w_{10} = -0.395006197760920667393122535979679328161187572$$
$$w_{11} = -0.582423447311644594710573905438945739845940956$$
$$w_{12} = 0.742673314357319863476853599632017373530365297$$
$$w_{13} = 0.164337549520467291015144024408044321057050157 9$$
$$w_{14} = -0.615116639060545182658778437156157368647972997$$
$$w_{15} = 0.201750414036764035058286163337901348171217248 8$$
$$w_{16} = 0.452387172243467206175886586074233539323363950 45$$

Table 3: Coefficients of 10th order method of Suzuki.

$$w_1 = .2511533095387726982616883$$
$$w_2 = -.6369257308162692976516439$$
$$w_3 = .7477954563227205558861854$$
$$w_4 = .1154223875364780004665333$$
$$w_5 = .7341233481533524507511856$$
$$w_6 = -.8878678069874644807057962$$
$$w_7 = -.6512663158972613330899293$$
$$w_8 = .5311659336578173351561816$$
$$w_9 = .1307499863921240887409958$$
$$w_{10} = .8950269744648292197242156$$
$$w_{11} = -.4500114055934121490287758$$
$$w_{12} = .2150000213788581353291374$$
$$w_{13} = -.5198079779534024447151808$$
$$w_{14} = -.8002447419481216045467065$$
$$w_{15} = .6122193440386721474677501$$
$$w_0 = 1 - 2 \sum_{i=1}^{15} w_i = .4269344354246134148889169$$

Table 4: NEW10, Suzuki10 and Calvo Sanz-Serna8

end point	function evaluations	NEW10	S10	C-SS8
10π	5115	$1.0 \cdot 10^{-5}$	$2.0 \cdot 10^{-4}$	$4.7 \cdot 10^{-6}$
	10230	$1.1 \cdot 10^{-8}$	$1.0 \cdot 10^{-6}$	$2.3 \cdot 10^{-8}$
	15345	$1.9 \cdot 10^{-10}$	$4.1 \cdot 10^{-8}$	$9.1 \cdot 10^{-10}$
100π	51150	$1.0 \cdot 10^{-4}$	$2.0 \cdot 10^{-3}$	$4.7 \cdot 10^{-5}$
	102300	$1.1 \cdot 10^{-7}$	$1.0 \cdot 10^{-5}$	$2.3 \cdot 10^{-7}$
	153450	$1.8 \cdot 10^{-9}$	$4.1 \cdot 10^{-7}$	$9.0 \cdot 10^{-9}$
1000π	511500	$1.0 \cdot 10^{-3}$	$2.0 \cdot 10^{-2}$	$4.7 \cdot 10^{-4}$
	1023000	$1.1 \cdot 10^{-6}$	$1.0 \cdot 10^{-4}$	$2.3 \cdot 10^{-6}$
	1534500	$1.8 \cdot 10^{-8}$	$4.1 \cdot 10^{-6}$	$9.0 \cdot 10^{-8}$

Global errors observed at $10\pi, 100\pi$ and 1000π, for the three symplectic methods under consideration.

(iii) The 26stages, 24 evaluations per step, 8th order symplectic formula C-SS8, [3]. We tried the stepsizes $2\pi/42.6$, $\pi/85.2$ and $2\pi/127.9$.

The methods were implemented according to (4). The steplengths used, are chosen so the total number of function evaluations for the methods are equal. The stepsizes are chosen to be constant during the integration since variable steps destroy symplectiness [4]. The errors at various end points were notified at table 4.

Interpreting the results we observe a nice linear in time, growth of the error. This is a significant characteristic of symplectic methods since this growth is quadratic for conventional methods [4]. So, when we integrate the problem up to $10^9\pi$ with NEW10 using stepsize $2\pi/93$, we spend $1.5345 \cdot 10^{12}$ function evaluations expecting an error about $1.8 \cdot 10^{-2}$. We also observe that the new 10th order method achieves better accuracies. But the remarkable result is that Suzuki 10th order method does not justify its order. When doubling or tripling the step using a pth order method then the error has to be 2^p or 3^p times greater respectively. This fact holds for NEW10 and C-SS8 but not for S10. Actually, S10 justifies an eighth order of accuracy.

The latter group contains three common RKN pairs.

(i) PT86, the RKN pair of orders eight and six presented in [10].

(ii) DEP86, the RKN pair of orders eight and six presented in [5],

(iii) DEP12(10), the RKN pair of orders twelve and ten presented in [5].

These pairs were run for tolerances $10^{-12}, 10^{-13}, \cdots, 10^{-24}$, in quadruple precision, using variable step-size implementation according to the guidelines given in [14]. For reasons of comparison to table 4 we estimated the errors that might be generated at the same costs. This estimation was done by linear interpolation on the decimal digits of accuracy achieved by each pair.

From Table 5 we observe an advantage of PT86 over DEP86 for about half decimal

Table 5: PT86, DEP86 and DEP12(10)

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end point	function evaluations	PT86	DEP86	DEP12(10)
	5115	$7.6 \cdot 10^{-14}$	$1.2 \cdot 10^{-13}$	$1.7 \cdot 10^{-18}$
10π	10230	$8.6 \cdot 10^{-17}$	$1.4 \cdot 10^{-15}$	$7.3 \cdot 10^{-23}$
	15345	$8.1 \cdot 10^{-18}$	$7.4 \cdot 10^{-17}$	$2.9 \cdot 10^{-24}$
	51150	$1.9 \cdot 10^{-11}$	$7.4 \cdot 10^{-11}$	$7.4 \cdot 10^{-17}$
100π	102300	$3.4 \cdot 10^{-14}$	$1.3 \cdot 10^{-13}$	$7.7 \cdot 10^{-20}$
	153450	$8.2 \cdot 10^{-16}$	$2.9 \cdot 10^{-15}$	$3.3 \cdot 10^{-22}$
	511500	$2.0 \cdot 10^{-9}$	$8.2 \cdot 10^{-9}$	$2.2 \cdot 10^{-14}$
1000π	1023000	$3.9 \cdot 10^{-12}$	$1.6 \cdot 10^{-11}$	$8.6 \cdot 10^{-18}$
	1534500	$9.6 \cdot 10^{-14}$	$4.0 \cdot 10^{-13}$	$3.9 \cdot 10^{-20}$

Global errors estimated at 10π, 100π and 1000π, for the three RKN pairs under consideration.

digit. On the other hand both 8th order RKN pairs reveal higher accuracy than NEW10 for about $5-6$ decimal digits. There is a possibility of comparable results if we integrate 8(6) pairs up to $10^9\pi$, as well. Then at a cost of $1.5345 \cdot 10^{12}$ function evaluations mentioned before we will normally observe only $1-2$ digits of accuracy. As a conjecture NEW10 outperforms conventional eighth order nonsymplectic variable steplength integrators when using very small stepsizes at extremely long integrations. The pair DEP12(10) is far more efficient than all the other methods. There is no possibility to compete it with a 10th order symplectic method since decreasing the step-size we simply increase the difference of accuracy in favor of DEP12(10). Finally twelfth order symplectic methods require too many stages per step, and there is a doubt if such methods are able to cover the efficiency superiority of DEP12(10).

4. Discussion.

A new 10th order symplectic Runge-Kutta-Nyström method at a cost of 33 stages per step is presented for first time in this article. Numerical results show its advantage when high accuracy is requested, compared to lower order methods of this category. According to the discussion in [2] there is a possibility to throw away one of the last four equations of ninth order in table 1. Then the number of the remaining equations coincides with the number reported by McLachlan [8] and Suzuki [12]. In these papers it seems to be a contradiction in the number of the equations needed for constructing higher order methods, but both agree that 31 stages are required for a 10th order method. According to McLachlan $s_{10} = 31$, $s_{12} = 67$, $s_{14} = 147$, $s_{16} = 326$, while according to Suzuki $s_{14} = 135$, $s_{16} = 277$. Suzuki lists the equations up to 11th order in [12]. Later he solved them correctly in order to derive some 31 stage 10th order methods [13]. Unfortunately, these methods are only of 8th order of accuracy according to our RKN-type implementation, since they fail to solve six of the nine equations of order nine, given in Table 1. So, the relevant theory needs reconsideration. Perhaps $s_{10} = 31$ or $s_{12} < 79$ holds after a careful interpretation of the results in [2], but the true conditions seem to differ than those given in [12].

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