Two Step Runge-Kutta-Nyström Methods for $y'' = f(x, y)$ and P–Stability

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Abstract. P-stability is an important requirement in the numerical integration of stiff oscillatory systems, but this desirable feature is not possessed by any class of numerical methods for $y'' = f(x, y)$. It is known, for example, that P–stable linear multistep methods have maximum order two and symmetric one step polynomial collocation methods can't be P-stable (Coleman 1992). In this note we show the existence of P-stable methods within a general class of two step Runge-Kutta-Nyström methods.

1 Introduction

Many physical problems arising from celestial mechanics, molecular dynamics, seismology and so on are modeled by Ordinary Differential Equations having periodic or oscillatory solutions of type

$$y''(t) = f(t, y(t)), \quad y(t_0) = y_0, \quad y'(t_0) = y'_0, \qquad y(t), f(t, y) \in R^n, \qquad (1)$$

Although it may be reduced into a first order system, the development of numerical methods for its direct integration seems more natural. Many linear multistep, hybrid and one step methods appeared in the literature: see for example [12, 4] for an extensive bibliography.

When the system is stiff some special stability properties are required, notably the P–stability. This concept was first introduced in [8], and it is of particular interest in the numerical treatment of periodic stiffness which is exhibited, for example, by Kramarz's system [7]. In this case two or more frequencies are involved, and the amplitude of the high frequency component is negligible or it is eliminated by the initial conditions. Then the choice of the step size is governed not only by accuracy demands, but also by stability requirements. P–stability ensures that the choice of the step size is independent of the values of frequencies, but it only depends on the desired accuracy [4, 10]. Moreover a necessary condition for a method to result P–stable is to be zero–dissipative. The property of nondissipativity is of primary interest in celestial mechanics for orbital computation, when it is desired that the computed orbits do not spiral inwards or outwards [12].

P.M.A. Sloot et al. (Eds.): ICCS 2002, LNCS 2331, pp. 459–466, 2002.

Only few numerical methods possess this desirable feature. It is worth mentioning that in the class of linear multistep methods for (1) P–stability can be reached only by methods of the second order and that the stability properties gradually deteriorate when the order increases. It is also known that symmetric one step polynomial collocation methods can't be P-stable [3], and no P–stable methods were found in the special class of two step collocation methods considered in [11].

We consider now a simple family of two step Runge–Kutta methods (TSRK) introduced in [6]:

$$\begin{aligned} y_{i+1} &= (1-\theta)y_i + \theta y_{i-1} + h\textstyle\sum_{j=1}^{m}(v_j f(x_{i-1}+c_j h, Y_{i-1}^j) + w_j f(x_i + c_j h, Y_i^j)), \\ Y_{i-1}^j &= y_{i-1} + h\textstyle\sum_{s=1}^{m} a_{js} f(x_{i-1}+c_s h, Y_{i-1}^s), \qquad j=1,\dots,m \\ Y_i^j &= y_i + h\textstyle\sum_{s=1}^{m} a_{js} f(x_i + c_s h, Y_i^s), \qquad j=1,\dots,m, \end{aligned} \tag{2}$$

for the not autonomous initial value problem

$$y'(t) = f(t, y(t)), \qquad y(t_0) = y_0, \tag{3}$$

where $f : \Re^q \rightarrow \Re^q$ is assumed to be sufficiently smooth. θ, v_j, w_j, a_{js}, b_{js}, $j, s, = 1, \dots, m$ are the coefficients of the methods.

It is known that the method is consistent if $\sum_{j=1}^{m}(v_j + w_j) = 1 + \theta$, and it is zero–stable if $-1 < \theta \leq 1$ [6].

The method (2) belongs to the class of General Linear Methods introduced by Butcher [1], with the aim of giving an unifying description of numerical methods for ODEs. (2) can be represented by the following Butcher's array:

$$\begin{array}{c|c} \mathbf{c} & \mathbf{A} \\ \hline \theta & \begin{array}{c} \mathbf{v}^T \\ \mathbf{w}^T \end{array} \end{array} = \begin{array}{c|cccc} c_1 & a_{11} & a_{12} & \cdots & a_{1m} \\ c_2 & a_{21} & a_{22} & \cdots & a_{2m} \\ \vdots & \vdots & \vdots & & \vdots \\ c_m & a_{m1} & a_{m2} & \cdots & a_{mm} \\ \hline \theta & \begin{array}{c} v_1 \\ w_1 \end{array} & \begin{array}{c} v_2 \\ w_2 \end{array} & \begin{array}{c} \cdots \\ \cdots \end{array} & \begin{array}{c} v_m \\ w_m \end{array} \end{array},$$

where $c_j = \sum_{j=1}^{m} a_{ij}$.

The reason of interest in this family lies in the fact that, advancing from x_i to x_{i+1} we only have to compute Y_i, because Y_{i-1} have already been evaluated in the previous step. Therefore the computational cost of the method depends on the matrix A, while the vector v adds extra degrees of freedom.

In this family A–stable methods exist [6], while no P–stable methods were found in [11] in the class of indirect collocation methods derived within family (2). We prove that P–stable methods, which are not collocation–based, can be constructed within the family (2) for the special second order ODEs (1).

2 Construction of the indirect method

To derive the method for the special second order system (1), from (2), following [5], we transform the system $y'' = f(x,y)$ into a first order differential equation of double dimension:

$$\begin{pmatrix} y \\ y' \end{pmatrix}' = \begin{pmatrix} y' \\ f(x,y) \end{pmatrix}, \qquad y(x_i) = y_i, \quad y'(x_i) = y'_i. \tag{3}$$

By making the interpretation

$$K_i^j = f(x_i + c_j h, Y_i^j),$$

which is usually done for Runge–Kutta methods, the following equivalent form of (2) is more convenient to our purpose:

$$\begin{aligned} y_{i+1} &= (1-\theta)y_i + \theta y_{i-1} + h\textstyle\sum_{j=1}^m (v_j K_{i-1}^j + w_j K_i^j), \\ K_{i-1}^j &= f(x_{i-1} + c_j h, y_{i-1} + h\textstyle\sum_{s=1}^m a_{js} K_{i-1}^s), \qquad j = 1,\dots,m, \\ K_i^j &= f(x_i + c_j h, y_i + h\textstyle\sum_{s=1}^m a_{js} K_i^s), \qquad j = 1,\dots,m, \end{aligned} \tag{4}$$

The application of the method (4) to the system (3) yields

$$\begin{aligned} K_{i-1}^j &= y'_{i-1} + h\textstyle\sum_{s=1}^m a_{js} K'^s_{i-1}, \\ K_i^j &= y'_i + h\textstyle\sum_{s=1}^m a_{js} K'^s_i, \\ K'^j_{i-1} &= f(x_{i-1} + c_j h, y_{i-1} + h\textstyle\sum_{s=1}^m a_{js} K_{i-1}^s), \\ K'^j_i &= f(x_i + c_j h, y_i + h\textstyle\sum_{s=1}^m a_{js} K_i^s), \\ y_{i+1} &= (1-\theta)y_i + \theta y_{i-1} + h\textstyle\sum_{j=1}^m (v_j K_{i-1}^j + w_j K_i^j), \\ y'_{i+1} &= (1-\theta)y'_i + \theta y'_{i-1} + h\textstyle\sum_{j=1}^m (v_j K'^j_{i-1} + w_j K'^j_i) \end{aligned} \tag{5}$$

If we insert the first two formulas of (5) into the others, we obtain

$$\begin{aligned} K'^j_{i-1} &= f(x_{i-1} + c_j h, y_{i-1} + h c_j y'_{i-1} + h^2 \textstyle\sum_{s=1}^m \bar{a}_{js} K'^s_{i-1}), \\ K'^j_i &= f(x_i + c_j h, y_i + h c_j y'_i + h^2 \textstyle\sum_{s=1}^m \bar{a}_{js} K'^s_i), \\ y_{i+1} &= (1-\theta)y_i + \theta y_{i-1} + h(\textstyle\sum_{j=1}^m v_j) y'_{i-1} + h(\textstyle\sum_{j=1}^m w_j) y'_i + \\ &\quad h^2 \left(\textstyle\sum_{s=1}^m (\bar{v}_s k'^s_{i-1} + \bar{w}_s K'^s_i)\right), \\ y'_{i+1} &= (1-\theta)y'_i + \theta y'_{i-1} + h\textstyle\sum_{s=1}^m (v_s K'^s_{i-1} + w_s K'^s_i) \end{aligned} \tag{6}$$

where

$$\bar{a}_{js} = \sum_k a_{jk} a_{ks}, \quad \bar{v}_s = \sum_k v_k a_{ks}, \quad \bar{w}_s = \sum_k w_k a_{ks}. \tag{7}$$

From (7), setting $\bar{\mathbf{A}} = \mathbf{A^2}$, $\bar{\mathbf{v}} = \mathbf{v^T A}$, $\bar{\mathbf{w}} = \mathbf{w^T A}$, the direct method (6) for the second order system (1) takes the following form

$$
\begin{aligned}
Y_{i-1}^j &= y_{i-1} + hc_j y'_{i-1} + h^2 \textstyle\sum_{s=1}^m \bar{a_{js}} f(x_{i-1} + c_s h, Y_{i-1}^s), \qquad j = 1, \ldots, m, \\
Y_i^j &= y_i + hc_j y'_i + h^2 \textstyle\sum_{s=1}^m \bar{a_{js}} f(x_i + c_s h, Y_i^s), \qquad j = 1, \ldots, m, \\
y_{i+1} &= (1-\theta) y_i + \theta y_{i-1} + h \textstyle\sum_{j=1}^m v_j y'_{i-1} + h \textstyle\sum_{j=1}^m w_j y'_i + \\
&\quad h^2 \textstyle\sum_{j=1}^m (\bar{v_j} f(x_{i-1} + c_j h, Y_{i-1}^j) + \bar{w_j} f(x_i + c_j h, Y_i^j)), \\
y'_{i+1} &= (1-\theta) y'_i + \theta y'_{i-1} + h \textstyle\sum_{j=1}^m (v_j f(x_{i-1} + c_j h, Y_{i-1}^j) + w_j f(x_i + c_j h, Y_i^j)).
\end{aligned} \tag{8}
$$

and it is represented by the Butcher array

$$
\begin{array}{c|c}
\mathbf{c} & \mathbf{A^2} \\
\hline
 & \mathbf{v^T A} \\
 & \mathbf{w^T A} \\
\theta & \mathbf{v} \\
 & \mathbf{w}
\end{array} \quad . \tag{9}
$$

Likewise to the one–step case, we call the method (8)–(9) two–step Runge–Kutta–Nyström (TSRKN) method.

3 Linear stability analysis

The homogeneous test equation for the linear stability analysis is

$$
y'' = -\omega^2 y, \quad \omega \in \mathbf{R} \tag{10}
$$

Following the analysis which has been performed in the one–step case (see [13]), the application of (8) to (10) yields the recursion

$$
\begin{aligned}
\mathbf{Y}_{i-1} &= \mathbf{N^{-1}}(y_{i-1}\mathbf{e} + hy'_{i-1}\mathbf{c}) \\
\mathbf{Y}_i &= \mathbf{N^{-1}}(y_i\mathbf{e} + hy'_i\mathbf{c}) \\
y_{i+1} &= (1-\theta)y_i + \theta y_{i-1} + h(\mathbf{v}^T\mathbf{e}\; y'_{i-1} + \mathbf{w}^T\mathbf{e}\; y'_i) - z^2(\bar{\mathbf{v}}^T\mathbf{Y_{i-1}} + \bar{\mathbf{w}}^T\mathbf{Y_i}) \\
hy'_{i+1} &= (1-\theta)hy'_i + \theta hy'_{i-1} - z^2(\mathbf{v}^T\mathbf{Y_{i-1}} + \mathbf{w}^T\mathbf{Y_i})
\end{aligned}
$$

where $z = \omega h, \quad \mathbf{e} = (1, \ldots, 1)^T, \quad N = I + z^2 A.$

Elimination of the auxiliary vectors $\mathbf{Y_{i-1}}$, $\mathbf{Y_i}$ yields

$$\begin{aligned} y_{i+1} &= (1-\theta)y_i + \theta y_{i-1} + h(\mathbf{v}^T\mathbf{e}\; y'_{i-1} + \mathbf{w}^T\mathbf{e}\; y'_i) - \\ &\quad z^2(\bar{\mathbf{v}}^T\mathbf{N^{-1}e}\; y_{i-1} + \bar{\mathbf{v}}^T\mathbf{N^{-1}c}\; hy'_{i-1} + \bar{\mathbf{w}}^T\mathbf{N^{-1}e}\; y_i + \bar{\mathbf{w}}^T\mathbf{N^{-1}c}\; hy'_i) \\ hy'_{i+1} &= (1-\theta)hy'_i + \theta hy'_{i-1} - z^2(\mathbf{v}^T\mathbf{N^{-1}e}\; y_{i-1} + \mathbf{v}^T\mathbf{N^{-1}c}\; hy'_{i-1} + \\ &\quad \mathbf{w}^T\mathbf{N^{-1}e}\; y_i + \mathbf{w}^T\mathbf{N^{-1}c}\; hy'_i). \end{aligned}$$

The resulting recursion is

$$\begin{pmatrix} y_i \\ y_{i+1} \\ h\, y'_i \\ h\, y'_{i+1} \end{pmatrix} = M(z^2) \begin{pmatrix} y_{i-1} \\ y_i \\ h\, y'_{i-1} \\ h\, y'_i \end{pmatrix}$$

with

$$M(z^2) = \begin{pmatrix} 0 & 1 & 0 & 0 \\ \theta - z^2\bar{\mathbf{v}}^T\mathbf{N^{-1}e} & 1-\theta- z^2\bar{\mathbf{w}}^T\mathbf{N^{-1}e} & \mathbf{v}^T\mathbf{e} - z^2\bar{\mathbf{v}}^T\mathbf{N^{-1}c} & \mathbf{w}^T\mathbf{e} - z^2\bar{\mathbf{w}}^T\mathbf{N^{-1}c} \\ 0 & 0 & 0 & 1 \\ -z^2\mathbf{v}^T\mathbf{N^{-1}e} & -z^2\mathbf{w}^T\mathbf{N^{-1}e} & \theta - z^2\mathbf{v}^T\mathbf{N^{-1}c} & 1-\theta- z^2\mathbf{w}^T\mathbf{N^{-1}c} \end{pmatrix}. \tag{11}$$

$M(z^2)$ in (11) is the *stability* or *amplification* matrix for the two–step RKN methods (8). The stability properties of the method depend on the eigenvalues of the amplification matrix, whose elements are rational functions of the parameters of the method. Then the stability properties depend on the roots of the stability polynomial

$$\pi(\lambda) = det(M(z^2) - \lambda I). \tag{12}$$

For the sake of completeness, we recall now the following two definitions.

Definition 1. $(0, H_0^2)$ *is the interval of periodicity for the two step RKN method if,* $\forall z^2 \in (0, H_0^2)$*, the roots of the stability polynomial* $\pi(\lambda)$ *satisfy:*

$$r_1 = e^{i\phi(z)}, \quad r_2 = e^{-i\phi(z)}, \quad |r_{3,4}| \le 1,$$

with $\phi(z)$ *real.*

Definition 2. *The two step RKN method is P–stable if its interval of periodicity is* $(0, +\infty)$*.*

For an A–stable method the eigenvalues of the amplification matrix are within the unit circle for all stepsizes and any choice of frequency in the test equations, and this ensures that the amplitude of the numerical solution of the test equation does not increase with time. If, what is more, there is no numerical dissipation, that is if the principal eigenvalues of the amplification matrix lie on the unit circle, then the method is P–stable [13].

4 One stage P-stable TSRKN method

Let us consider now the one stage TSRKN method (8) represented by the following Butcher array

c	a^2
	v a
	w a
θ	v
	w

(13)

The characteristic polynomial (12) of the method (13) is symmetric when, if λ is an eigenvalue of $M(z^2)$, then also $\frac{1}{\lambda}$ is an eigenvalue; in this case every stability interval is also an interval of periodicity. Therefore, to obtain a P–stable TSRKN method, it must be required that the characteristic polynomial (12) of the method is symmetric, and the periodicity interval is unlimited.

We can perform an analytical study of the inequalities representing the stability conditions for one stage two step RKN method (13). The TSRKN method (13) has order 1 if (see [6])

$$v + w = 1 + \theta, \quad -1 < \theta \leq 1.$$

The stability polynomial (12) of (13) can be written in the following way:

$$\pi(\lambda) = \lambda^4 + B(z^2)\lambda^3 + C(z^2)\lambda^2 + D(z^2)\lambda + E(z^2),$$

with

$$B(z^2) = \frac{(2a^2(\theta-1) + w(a+c))z^2 + 2(\theta-1)}{1+az^2},$$

$$C(z^2) = \frac{1 - 4\theta + \theta^2 + z^2(a^2 + a^2\theta^2 + (v-w)(a+c) + w^2 + \theta(a(w-4a) + cw))}{1+az^2},$$

$$D(z^2) = \frac{2(1-\theta)\theta + z^2(2a^2\theta(1-\theta) + v(\theta-1)(a+c) + w(2v - \theta(a+c)))}{1+az^2},$$

$$E(z^2) = \frac{\theta^2 + z^2(a^2\theta^2 - (a+c)\theta v + v^2)}{1+az^2}.$$

It is symmetric if and only if

$$E(z^2) \equiv 1, \qquad B(z^2) \equiv D(z^2).$$

The TSRKN method (13) has order 2 if the following conditions are satisfied [6]:

$$v + w = 1 + \theta, \qquad 2v(a-1) + 2wa = 1 - \theta. \tag{14}$$

If we ask now that $\pi(\lambda)$ is symmetric, then

$$E(z^2) \equiv 1 \quad \Longleftrightarrow \quad \theta^2 = 1,$$

from which $\theta = 1$ follows; indeed $\theta = -1$ violates the zero-stability of the method.

From (14), we must set

$$v = 2a, \qquad w = 2 - 2a.$$

Moreover $B(z^2) \equiv D(z^2)$ if and only if $c = a$ or $a = 1$.

We can choose a as free parameter and compute a value for it in such a way that the inequalities representing the stability conditions are satisfied (for example by using the Routh-Hurwutz criterion). In this way we conclude that the following method

$$\begin{array}{c|c}
a & a^2 \\
\hline
 & 2a^2 \\
 & 2a(1-a) \\
1 & 2a \\
 & 2(1-a)
\end{array} \;,$$

with $a > \dfrac{1}{2}$ is an order 2, one stage, P–stable two step RKN method.

5 Concluding remark.

In [11] we did not find any P–stable method in the class of indirect collocation two step RKN methods. The result obtained in this note encourage us to proceed in our investigation on two–step Runge–Kutta–Nyström methods. Indeed it is certainly possible to derive P–stable methods within this family, as we have just shown, and we are hopeful that it is also possible to obtain high order P–stable methods within the class of two–step RKN methods, if we do not consider indirect collocation based methods. To derive P–stable methods with an increased number of stages the usage of symbolic computation will be very useful, as already done successfully in [2] in the one–step case.

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