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A Note on a Diagonally Implicit Runge-Kutta-Nyström Method

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It is shown that it is possible to obtain fourth-order accurate diagonally implicit Runge-Kutta-Nyström methods with only 2 stages. The scheme with the largest interval of periodicity, i.e. (0,12), is given. Furthermore, the requirement of *P*-stability decreases the order to 2.

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1. Introduction

For the numerical integration of the special second-order initial value problem

$$y'' = f(t,y), \quad y(t_0) = y_0, \quad y'(t_0) = y'_0 \,, \tag{1.1}$$

it is often advantageous applying a direct method for this type of differential equations, rather than rewriting (1.1) to its first-order form.

Therefore we consider general Runge-Kutta-Nyström methods which are of the form [5,6]

$$Y_{n,j} = y_n + c_j h y'_n + h^2 \sum_{l=1}^{m} a_{j,l} f(t_n + c_l h, Y_{n,l}) \;, \; j = 1,\dots,m \,, \tag{1.2a}$$

$$\begin{aligned} y_{n+1} &= y_n + h y'_n + h^2 \sum_{j=1}^{m} b_j f(t_n + c_j h, Y_{n,j}) \,, \\ y'_{n+1} &= y'_n + h \sum_{j=1}^{m} b'_j f(t_n + c_j h, Y_{n,j}) \,, \end{aligned} \tag{1.2b}$$

$$\tfrac{1}{2} c_j^2 = \sum_{l=1}^{m} a_{j,l} \,, \quad \forall j \,. \tag{1.2c}$$

Here h is the step size, $t_n = t_0 + nh$ and y_{n+1}, y'_{n+1} are approximations to the exact solution $y(t_{n+1})$ and $y'(t_{n+1})$. Since the computational complexity of this fully implicit scheme is a deterrent prospect, we confine our considerations to *diagonally* implicit (or semi-explicit [2]) methods, which result from (1.2) by setting $a_{j,l} = 0$ for $l > j$. These methods are much more attractive from a computational point of view, because now in each implicit relation in (1.2a) only one (unknown) $Y_{n,j}$ is involved. Furthermore, if we require $a_{j,j} = a (\neq 0)$ for all j, then the scheme allows for an efficient implementation because the decomposition of the matrix $I - ah^2 J_n$, $J_n = (\partial f / \partial y)|_{t_n}$ occurring in Newton-type methods can be used in all stages.

In the sequel these schemes are referred to as DIRKN methods; they are compactly represented by means of the Butcher array

$$\begin{array}{c|c} \mathbf{c} & A \\ \hline & \mathbf{b}^T \\ & \mathbf{b}'^T \end{array} \qquad A = \begin{bmatrix} a & & 0 \\ & \ddots & \\ a_{j,l}, & & \\ l<j & & a \end{bmatrix}$$

with obvious definition of $\mathbf{c}, \mathbf{b}$ and $\mathbf{b}'$.

In the case of *first-order* ODEs, this idea with respect to the choice of the A-matrix was introduced by NØRSETT [8] and, since then, extensively discussed in numerous papers (e.g. [1]). On the contrary, for *second-order* ODEs, this approach is rarely discussed in the literature; as a matter of fact, we are not aware of any such a paper.

In this note, we will derive a fourth-order, two-stage DIRKN method.

2. Stability

In studying the (linear) stability of DIRKN methods, we apply the scheme (1.2) to the scalar test equation

$$y'' = -\lambda^2 y \ , \qquad \lambda \in \mathbb{R} \ . \tag{2.1}$$

Setting $H = h\lambda$ and eliminating the intermediate results $Y_{n,j}$, the numerical solution satisfies [6]

$$\begin{bmatrix} y_{n+1} \\ hy'_{n+1} \end{bmatrix} = M(H^2) \begin{bmatrix} y_n \\ hy'_n \end{bmatrix}, \qquad M(H^2) = \begin{bmatrix} 1 - H^2 \mathbf{b}^T L^{-1} \mathbf{e} & 1 - H^2 \mathbf{b}^T L^{-1} \mathbf{c} \\ -H^2 \mathbf{b}'^T L^{-1} \mathbf{e} & 1 - H^2 \mathbf{b}'^T L^{-1} \mathbf{c} \end{bmatrix}, \tag{2.2}$$

where $L = I + H^2 A$ and $\mathbf{e} = (1, \cdots, 1)^T$.

Introducing the functions

$$S(H^2) = \text{Trace}\,(M) \quad \text{and} \quad P(H^2) = \text{Det}(M) \tag{2.3}$$

the characteristic equation corresponding to the difference equation (2.2) is of the form

$$\zeta^2 - S(H^2)\zeta + P(H^2) = 0 \ . \tag{2.4}$$

In this note we are particularly interested in DIRKN methods which are suitable for the integration of *periodic* initial value problems. Therefore, we introduce the following definitions (cf. [7]):

DEFINITION 1. An interval $(0, H_0^2)$ is called the interval of periodicity of the method (1.2) if the roots of (2.4) are complex conjugate and of modulus one.

DEFINITION 2. The method (1.2) is said to be P-stable if its interval of periodicity is $(0, \infty)$.

The feature of a nonempty interval of periodicity is important in integrating periodic solutions. It guarantees that for $H^2 \in (0, H_0^2)$ the numerical solution will not be damped (nor amplified); hence, the phenomenon of 'orbitally instability', as it was termed by STIEFEL and BETTIS [9] will not occur.

Obviously, if the method (1.2) has an interval of periodicity $(0, H_0^2)$ with $H_0^2 > 0$, then the product of the roots of (2.4) is equal to 1, for all $H^2 \in (0, H_0^2)$ (see Definition 1). Since, the term $P(H^2)$ in (2.4) equals the product of the roots of this quadratic, we have:

A necessary condition for the method (1.2) to possess a nonempty interval of periodicity in $P(H^2) \equiv 1$.

3. Construction of the method

In [5], Hairer derived m-stage methods of order $2m$. His starting point was the optimal (Gauss) methods [2] for first-order differential equations. The resulting methods are proved to be P-stable. However, they have a full A-matrix.

In this section we will study what is attainable within the class of two-stage DIRKN methods, possessing a nonempty interval of periodicity.

First we observe that, by virtue of the 'compatibility conditions' (1.2c), there are only six free parameters at our disposal. For fourth-order consistency, we have to satisfy eight conditions (see e.g.

[3]: three conditions for the y-component and five conditions for the y'-component. This seems to be overambitious, however there appears to exist a solution.

To simplify the analysis, we use a lemma due to Hairer [4]:

LEMMA: *Let*

$$b_j = b'_j(1-c_j) \quad , \qquad j = 1,...,m \, . \tag{3.1}$$

Then the order conditions for the y-component are a subset of the order conditions for the y'-component.
□

Now, in terms of the free parameters c_1, c_2, b'_1 and b'_2, the fourth-order conditions reduce to

$$b'_1 + b'_2 = 1 \; , \tag{3.2a}$$

$$b'_1 c_1 + b'_2 c_2 = 1/2 \; , \tag{3.2b}$$

$$b'_1 c_1^2 + b'_2 c_2^2 = 1/3 \; , \tag{3.2c}$$

$$b'_1 c_1^3 + b'_2 c_2^3 = 1/4 \; , \tag{3.2d}$$

$$b'_1 c_1^3 + b'_2 c_1 (c_2^2 + c_1 c_2 - c_1^2) = 1/12 \; . \tag{3.3}$$

The equations (3.2) are solved by

$$b'_1 = b'_2 = \frac{1}{2} \, , \quad c_1 = \frac{1}{2} \pm \frac{1}{6}\sqrt{3} \; , \quad c_2 = \frac{1}{2} \mp \sqrt{3} \; , \tag{3.4}$$

and it turns out that the remaining order condition (3.3) is satisfied by these values. Moreover, we found $P(H^2) \equiv 1$.

Now, the scheme is completely determined by (3.4), (3.1) and (1.2c).

Obviously, the periodicity condition requires $|S(H^2)| < 2$. It is easily verified that the first solution in (3.4), i.e. the one where superior signs are used, yields $H_0^2 = 12$, whereas the other solution, taking lower signs, results in $H_0^2 = 3 + 3\sqrt{3} \simeq 8.2$.

Hence, we are now able to formulate our final result: within the class of two-stage DIRKN methods it is possible to obtain fourth-order accuracy and the scheme with the largest interval of periodicity, i.e. $H_0^2 = 12$, is given by

$$\begin{array}{c|cc}
\frac{1}{2}+\frac{1}{6}\sqrt{3} & \frac{1}{6}+\frac{1}{12}\sqrt{3} & 0 \\[4pt]
\frac{1}{2}-\frac{1}{6}\sqrt{3} & -\frac{1}{6}\sqrt{3} & \frac{1}{6}+\frac{1}{12}\sqrt{3} \\[4pt]
\hline
 & \frac{1}{4}-\frac{1}{12}\sqrt{3}, & \frac{1}{4}+\frac{1}{12}\sqrt{3} \\[4pt]
 & \frac{1}{2} & \frac{1}{2}
\end{array} \tag{3.5}$$

Lastly, we state, without derivation, a few additional results:

(i) one may wonder whether it is possible to obtain P-stability within this class of two-stage DIRKN methods by decreasing the order from four to three. Here is the negative answer: There is no P-stable third-order two-stage DIRKN method. Moreover, the periodicity interval cannot be enlarged. It turned out that (3.5) possesses the optimal H_0^2-value for two-stage methods of (at least) order 3.

(ii) it should be observed that the c-values in (3.5) are the Gauss-Legendre quadrature points, which

are probably responsible for the relatively high order of this scheme. Therefore, it is natural to ask whether this choice is suitable in obtaining high-order DIRKN methods using more stages. We investigated the case $m=3$ and, once more, the answer is disappointing.
If we again impose condition (3.1), we have 8 additional conditions for order 6, and only 4 of them are fulfilled. However, the ones which are not satisfied, have extremely small error constants. Therefore, this method may be of interest because of its accurate behaviour and its relatively small extra costs (cf. the discussion in Section 1). This fourth-order three-stage method is given by

$$\begin{array}{c|ccc}
\frac{1}{2}-\frac{1}{10}\sqrt{15} & \frac{1}{5}-\frac{1}{20}\sqrt{15} & & \\
\frac{1}{2} & -\frac{3}{40}+\frac{1}{20}\sqrt{15} & \frac{1}{5}-\frac{1}{20}\sqrt{15} & \\
\frac{1}{2}+\frac{1}{10}\sqrt{15} & \frac{3}{25}+\frac{1}{50}\sqrt{15} & -\frac{3}{25}+\frac{2}{25}\sqrt{15} & \frac{1}{5}-\frac{1}{20}\sqrt{15} \\
\hline
 & \frac{5}{36}+\frac{1}{36}\sqrt{15} & \frac{2}{9} & \frac{5}{36}-\frac{1}{36}\sqrt{15} \\
 & \frac{5}{18} & \frac{4}{9} & \frac{5}{18}
\end{array} \qquad (3.6)$$

Finally, we remark that this scheme has an empty interval of periodicity. It is strongly stable (i.e. $|\zeta_i|<1$) for $H^2 \in (0,9.5) \cup (10.6,19.5)$ with $|\zeta(H^2)|<1.025$ for $H^2 \in (9.5,10.6)$ □

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