A fourth-order diagonally implicit Runge-Kutta-Nyström method with dispersion of high order

N. Senu, M. Suleiman, F. Ismail, and M. Othman

Abstract—A new diagonally implicit Runge-Kutta-Nyström (RKN) method is developed for the integration of initial-value problems for second-order ordinary differential equations possessing oscillatory solutions. This method is more accurate when compared with current methods of similar type for the numerical integration of second-order ordinary differential equations with periodic solutions, using constant step size.

Keywords—Runge-Kutta-Nyström methods; Diagonally implicit; Phase-lag; Oscillatory solutions.

I. INTRODUCTION

This paper deals with numerical method for second-order ODEs, in which the derivative does not appear explicitly,

\[ y'' = f(x, y), \quad y(x_0) = y_0, \quad y'(x_0) = y'_0 \]  

(1)

for which it is known in advance that their solution is oscillating. Such problems often arise in different areas of engineering and applied sciences such as celestial mechanics, quantum mechanics, elastodynamics, theoretical physics and electronics. An s-stage Runge-Kutta-Nyström (RKN) method for the numerical integration of the IVP is given by

\[
\begin{align*}
    y_{n+1} &= y_n + h y'_n + h^2 \sum_{j=1}^{s} b_j k_j \\
    y'_{n+1} &= y'_n + h \sum_{j=1}^{s} b_j k_j
\end{align*}
\]

(2)

where

\[
\begin{bmatrix}
    c_1 \\
    \vdots \\
    c_s
\end{bmatrix}
\]

The RKN parameters \( a_i, b_j, b'_j \) and \( c_j \) are assumed to be real and \( s \) is the number of stages of the method. Introduce the \( s \)-dimensional vectors \( c, b \) and \( s \times s \) matrix \( A \), where

\[
\begin{align*}
    c &= [c_1, c_2, \ldots, c_s]' \quad b = [b_1, b_2, \ldots, b_s]' \\
    b' &= [b'_1, b'_2, \ldots, b'_s]'
\end{align*}
\]

\[
A = [a_i] \text{ respectively.}
\]

RKN methods can be divided into two broad classes: explicit \((a_\beta = 0, k \geq j)\) and implicit \((a_\beta = 0, k < j)\). The latter contains the class of diagonally implicit RKN (DIRKN) methods for which all the entries in the diagonal of \( A \) are equal. The RKN method above can be expressed in Butcher notation by the table of coefficients

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

Generally problems of the form (1) which have periodic solutions can be divided into two classes. The first class consists of problems for which the solution period is known a priori. The second class consists of problems for which the solution period is initially unknown. Several numerical methods of various types have been proposed for the integration of both classes of problems. See Stiefel and Bettis [3], van der Houwen and Sommeijer [12], Gautschi [16] and others.

When solving (1) numerically, attention has to be given to the algebraic order of the method used, since this is the main criterion for achieving high accuracy. Therefore, it is desirable to have a lower stage RKN method with maximal order. This will lessen the computational cost. If it is initially known that the solution of (1) is of periodic nature then it is essential to consider phase-lag (or dispersion) and amplification (or dissipation). These are actually two types of truncation errors. The first is the angle between the true and the approximated solution, while the second is the distance from a standard cyclic solution. In this paper we will derive a new diagonally implicit RKN method with three-stage fourth-order with dispersion of high order.

A number of numerical methods for this class of problems of the explicit and implicit type have been extensively developed. For example, van der Houwen and Sommeijer [12],...
Simos, Dimas and Sideridis, [15], and Senu, Suleiman and Ismail [18] have developed explicit RKN methods of algebraic order up to five with dispersion of high order for solving oscillatory problems. For implicit RKN methods, see for example van der Houwen and Sommeijer [13], Sharp, Fine and Burrage [14] and Imoni, Otunta and Ramamohan [17].

In this paper a dispersion relation is imposed and together with algebraic conditions to be solved explicitly. In the following section the construction of the new three-stage fourth-order diagonally implicit RKN method is described. Its coefficients are given using the Butcher tableau notation. Finally, numerical tests on second order differential equation problems possessing an oscillatory solutions are performed.

II. ANALYSIS OF PHASE-LAG

In this section we shall discuss the analysis of phase-lag for RKN method. The first analysis of phase-lag was carried out by Bursa and Nigro [10]. Then followed by Gladwell and Thomas [5] for the linear multistep method, and for explicit and implicit Runge-Kutta(-Nystrom) methods by van der Houwen and Sommeijer [12], [13]. The phase analysis can be divided in two parts; inhomogeneous and homogeneous components. Following van der Houwen and Sommeijer [12], inhomogeneous phase error is constant in time, meanwhile the homogeneous phase errors are accumulated as \( n \) increases. Thus, from that point of view we will confine our analysis to the phase-lag of homogeneous component only.

The phase-lag analysis of the method (2) is investigated using the homogeneous test equation

\[
y^* = (i\lambda)^2 y(t).
\]

Alternatively the method (2) can be written as

\[
y_{n+1} = y_n + hy_n + h^2 \sum_{i=1}^s b_i f(t_n + c_i h, Y_i)
\]

where

\[
Y_i = y_n + c_i h y_n + h^2 \sum_{j=1}^s a_{ij} f(t_n + c_j h, Y_j).
\]

By applying the general method (2) to the test equation (1) we obtain the following recursive relation as shown by Papageorgiou, Famelis and Tsitouras [4]

\[
\begin{bmatrix} y_{n+1} \\ h y_{n+1} \end{bmatrix} = D \begin{bmatrix} y_n \\ h y_n \end{bmatrix}, \quad z = \lambda h,
\]

\[
D(H) = \begin{bmatrix} 1 - H b^T (I + HA)^{1-e} & 1 - H b^T (I + HA)^{-1} e \\ -H b^T (I + HA)^{-1} e & 1 - H b^T (I + HA)^{1-e} \end{bmatrix} (I + HA)^{1-e}
\]

where \( H = z^2, e = (1\cdots1)^T, c = (c_1, \cdots, c_s)^T \). Here \( D(H) \) is the stability matrix of the RKN method and its characteristic polynomial

\[
\xi^2 - \text{tr}(D(z^2))\xi + \det(D(z^2)) = 0,
\]

is the stability polynomial of the RKN method. Solving difference system (5), the computed solution is given by

\[
y_n = 2 | \rho |^{z-\phi} \text{cos}(\alpha + \rho) \text{cos}(\chi + nz).
\]

The exact solution of (1) is given by

\[
y(t_n) = 2 | \sigma | \text{cos}(\chi + nz).
\]

Eq. (6) and (7) led us to the following definition.

**Definition 1.** (Phase-lag). Apply the RKN method (2) to (1). Then we define the phase-lag \( \varphi(z) = z - \phi \). If \( \varphi(z) = \mathcal{O}(z^{-1}) \), then the RKN method is said to have phase-lag order \( q \). Additionally, the quantity \( \alpha(z) = 1 - | \rho | \) is called amplification error. If \( \alpha(z) = \mathcal{O}(z^{-1}) \), then the RKN method is said to have dissipation order \( r \).

Let us denote

\[
R(z^2) = \text{trace}(D) \quad \text{and} \quad S(z^2) = \det(D).
\]

From Definition 1, it follows that

\[
\varphi(z) = z - \text{cos}^{-1} \left( \frac{R(z^2)}{2S(z^2)} \right), \quad | \rho | = S(z^2).
\]

Let us denote \( R(z^2) \) and \( S(z^2) \) in the following form

\[
R(z^2) = \frac{2 + \alpha z^2 + \cdots + \alpha_s z^{2s}}{(1 + \lambda z^2)^r},
\]

\[
S(z^2) = \frac{1 + \beta z^2 + \cdots + \beta_s z^{2s}}{(1 + \lambda z^2)^r},
\]

where \( \lambda = 2i \) is diagonal element in the Butcher tableau. Here the necessary condition for the fourth-order accurate diagonally implicit RKN method (2) to have hase-lag order six in terms of \( \alpha_i \) and \( \beta_i \) is given by

\[
\alpha_5 - \beta_5 = 8\lambda^6 - 12\lambda^4 + \frac{\lambda^2}{2} - \frac{1}{360}.
\]

Notice that the fourth-order method is already dispersive order four and dissipative order five. Furthermore dispersive order is even and dissipative order is odd.
III. CONTRACTION OF THE METHOD

In the following we shall derive a three-stage fourth-order accurate diagonally implicit RKN method with dispersive order six, by taking into account the dispersion relation in section II. The RKN parameters must satisfy the following algebraic conditions to find fourth-order accuracy as given in Hairer and Wanner [2].

\[
\sum b_j = \frac{1}{2}, \quad \sum b_j c_j = \frac{1}{2}
\]

\[
\sum b_j c_j = \frac{1}{6}, \quad \frac{1}{2} \sum b_j^2 c_j^2 = \frac{1}{6}
\]

\[
\frac{1}{2} \sum b_j c_j^2 = \frac{1}{24}, \quad \frac{1}{6} \sum b_j^2 c_j = \frac{1}{24}
\]

For most methods the \( c_j \) need to satisfy

\[
\frac{1}{2} c_j^2 = \sum a_{ij} (i = 1, \ldots, s).
\]

In Sharp, Fine and Burrague [14] stated that fourth-order method with dispersive order eight do not exist. Therefore, the method of algebraic order four \( (p = 4) \) with dispersive order six \( (q = 6) \) and dissipative order five \( (r = 5) \) is now considered. From algebraic conditions \((11)-(15)\), it formed eleven equations with thirteen unknowns to be solved. We let \( b_1 = 0 \) and \( \lambda \) be a free parameter. Therefore the following solution of one-parameter family is obtain

\[
a_{21} = -2 \lambda^2 + \frac{1}{6} \sqrt{3} \frac{1}{12},
\]

\[
a_{31} = \frac{288 \lambda^3 - 24 \lambda - 72 \lambda^2 - 24 \lambda^2 \sqrt{3} + 3 - \sqrt{3} + 12 \lambda \sqrt{3}}{12(12 \lambda - 3 + \sqrt{3})},
\]

\[
a_{32} = \frac{-1 + 96 \lambda^2 - 8 \lambda - 24 \lambda^2}{2(12 \lambda^2 - 3 + \sqrt{3})}, b_1 = 0, b_2 = \frac{1}{4}, c_1 = \frac{1}{4}, b_3 = \frac{1}{4}, c_2 = \frac{1}{4}.
\]

\[
B'_0 = 0, b'_0 = \frac{1}{2}, b'_1 = \frac{1}{2}, c'_1 = 2 \lambda, c'_2 = \frac{1}{6}, c'_3 = \frac{1}{2} + \frac{\sqrt{3}}{6}.
\]

From the above solution, we are going to derive a method with dispersion of order six. The six order dispersion relation \((10)\) need to be satisfied and this can be written in terms of RKN parameters which corresponds to the above family of solution yields the following equation

\[
(2880 \lambda^4 \sqrt{3} + (960 - 1440 \lambda) \lambda^3 + 120 - 40 \sqrt{3}) \lambda^2 + (120 \sqrt{3} - 192) \lambda - 11 \sqrt{3} + 18)/240(12 \lambda - 3 + \sqrt{3}) = 0,
\]

and solving for \( \lambda \) yields

\[-0.1015757589, 0.09374433416, 0.2097189023 and 0.1056624327.\]

The first two values will give us a nonempty stability interval while the others will produce the methods with empty stability interval. Taking the first two values of \( \lambda \), give us two fourth-order diagonally implicit RKN methods with dispersive order six.

For \( \lambda = -0.1015757589 \), the following method will be produced. This method will be denoted by DIRKN3(4,6)NEW (see Table I).

<table>
<thead>
<tr>
<th>Method</th>
<th>( q )</th>
<th>( d )</th>
<th>( | r^{(s)} |_2 )</th>
<th>( | r^{(t)} |_2 )</th>
</tr>
</thead>
<tbody>
<tr>
<td>DIRKN3(4,6)NEW</td>
<td>6</td>
<td>1.19 × 10^{-4}</td>
<td>1.88 × 10^{-7}</td>
<td>1.70 × 10^{-7}</td>
</tr>
<tr>
<td>DIRKN3(4,4)IMONI</td>
<td>4</td>
<td>-</td>
<td>3.75 × 10^{-7}</td>
<td>3.22 × 10^{-7}</td>
</tr>
<tr>
<td>DIRKN3(4,4)HS</td>
<td>4</td>
<td>1.43 × 10^{-7}</td>
<td>6.35 × 10^{-10}</td>
<td>1.59 × 10^{-10}</td>
</tr>
<tr>
<td>DIRKN3(4,6)SHARP</td>
<td>6</td>
<td>1.02 × 10^{-1}</td>
<td>1.85 × 10^{-8}</td>
<td>6.26 × 10^{-8}</td>
</tr>
</tbody>
</table>

Table II compares the properties of our method with the methods derived by van der Houwen and Sommeijer [20], Sharp, Fine and Burrage [14] and Imoni, Otunta and Ramamohan [17].
IV. PROBLEM TESTED

In this section we use our method to solve homogeneous and inhomogeneous problems whose exact solution consists of a rapidly or/and a slowly oscillating function. For purposes of illustration, we will compare our results with those derived by using three methods; DIRKN three-stage fourth-order derived by van der Houwen and Sommeijer [20] and Imoni, Otunta and Ramamohan [17], and three-stage fourth-order dispersive order six derived by Sharp, Fine and Burrage [14].

\[ \frac{d^2 y(t)}{dt^2} = -100y(t), \quad y(0) = 1, \quad y'(0) = -2 \]

Exact solution \( y(t) = -\frac{1}{10}\sin(10t) + \cos(10t) \)

**Problem 2**

\[ \frac{d^2 y(t)}{dt^2} = -y(t) + t, \quad y(0) = 1, \quad y'(0) = 2 \]

Exact solution \( y(t) = \sin(t) + \cos(t) + t \)

Source: Allen and Wing [19]

**Problem 3 (Inhomogeneous system)**

\[ \frac{d^2 y_1(t)}{dt^2} = -v^2 y_1(x) + v^2 f(t) + f'(t), \quad y_1(0) = a + f(0), \quad y_1'(0) = f'(0), \]

\[ \frac{d^2 y_2(t)}{dt^2} = -v^2 y_2(t) + v^2 f(t) + f'(t), \quad y_2(0) = f(0), \quad y_2'(0) = va + f'(0), \]

Exact solution is \( y_1(t) = a \cos(vt) + f(t), \quad y_2(t) = a \sin(vt) + f(t), \quad f(t) \) is chosen to be \( e^{-0.003t} \) and parameters \( v \) and \( a \) are 20 and 0.1 respectively.

Source: Lambert and Watson [7]

**Problem 4 (An almost Periodic Orbit problem)**

\[ \frac{d^2 y_1(t)}{dt^2} + y_1(t) = 0.001\cos(t), \quad y_1(0) = 1, \quad y_1'(0) = 0 \]

\[ \frac{d^2 y_2(t)}{dt^2} + y_2(t) = 0.001\sin(t), \quad y_2(0) = 0, \quad y_2'(0) = 0.99995 \]

Exact solution \( y_1(t) = \cos(t) + 0.0005\sin(t), \quad y_2(t) = \sin(t) - 0.0005\cos(t) \)

Source: Stiefel and Bettis [3]

The following notations are used in Table III-VI:

- **DIRKN(3,6)NEW**: A three-stage fourth-order dispersive order six method with 'small' dissipation constant and principal local truncation errors derived in this paper.
- **DIRKN(3,4)IMONI**: A three-stage fourth-order derived by Imoni, Otunta and Ramamohan [17].
- **DIRKN(3,4)HS**: A three-stage fourth-order dispersive order four derived by van der Houwen and Sommeijer [20].
- **DIRKN(3,6)SHARP**: A three-stage fourth-order dispersive order six as in Sharp, Fine and Burrage [14].

V. NUMERICAL RESULTS

The results for the four problems above are tabulated in Tables III-VI. One measure of the accuracy of a method is to examine the \( \text{Emax}(T) \), the maximum error which is defined by

\[ \text{Emax}(T) = \max \| y(t_n) - y_n \| \]

where \( t_n = t_0 + nh, \quad n = 1, 2, ..., \frac{T-t_0}{h} \).

Tables III-V show the absolute maximum error for **DIRKN(3,6)NEW**, **DIRKN(3,4)IMONI**, **DIRKN(3,4)HS** and **DIRKN(3,6)SHARP** methods when solving Problems 1-4 with three different step values. From numerical results in Table III-V, we observed that the new method is more accurate compared with **DIRKN(3,4)IMONI** and **DIRKN(3,4)HS** methods which do not relate to the dispersion order of the method. Also the new method is more accurate compared with **DIRKN(3,6)SHARP** method although the dispersion order is the same but the dissipation constant for our method is smaller than the **DIRKN(3,6)SHARP** method (see Table II).

### TABLE III

<table>
<thead>
<tr>
<th>h</th>
<th>Method</th>
<th>T=100</th>
<th>T=1000</th>
<th>T=4000</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.0025</td>
<td><strong>DIRKN(3,6)NEW</strong></td>
<td>6.648037(-10)</td>
<td>1.043226(-7)</td>
<td>7.728272(-7)</td>
</tr>
<tr>
<td>0.005</td>
<td><strong>DIRKN(3,4)IMONI</strong></td>
<td>1.564618(-2)</td>
<td>1.462288(-1)</td>
<td>4.706900(-1)</td>
</tr>
<tr>
<td>0.005</td>
<td><strong>DIRKN(3,4)HS</strong></td>
<td>1.256190(-7)</td>
<td>1.368907(-6)</td>
<td>5.831462(-6)</td>
</tr>
<tr>
<td>0.005</td>
<td><strong>DIRKN(3,6)SHARP</strong></td>
<td>3.015030(-3)</td>
<td>3.022988(-2)</td>
<td>1.212070(-2)</td>
</tr>
<tr>
<td>0.01</td>
<td><strong>DIRKN(3,6)NEW</strong></td>
<td>1.274632(-7)</td>
<td>1.264149(-6)</td>
<td>5.038593(-6)</td>
</tr>
<tr>
<td>0.01</td>
<td><strong>DIRKN(3,4)IMONI</strong></td>
<td>5.968009(-2)</td>
<td>4.622395(-1)</td>
<td>5.831462(-1)</td>
</tr>
<tr>
<td>0.01</td>
<td><strong>DIRKN(3,4)HS</strong></td>
<td>6.697730(-7)</td>
<td>6.696616(-6)</td>
<td>2.733871(-5)</td>
</tr>
<tr>
<td>0.01</td>
<td><strong>DIRKN(3,6)SHARP</strong></td>
<td>2.556924(-6)</td>
<td>2.562414(-5)</td>
<td>1.025522(-4)</td>
</tr>
<tr>
<td>0.0025</td>
<td><strong>DIRKN(3,6)NEW</strong></td>
<td>1.404280(-9)</td>
<td>1.281645(-8)</td>
<td>5.298188(-8)</td>
</tr>
<tr>
<td>0.005</td>
<td><strong>DIRKN(3,4)IMONI</strong></td>
<td>2.012136(-2)</td>
<td>1.848016(-1)</td>
<td>5.632254(-1)</td>
</tr>
<tr>
<td>0.005</td>
<td><strong>DIRKN(3,4)HS</strong></td>
<td>6.697730(-7)</td>
<td>6.696616(-6)</td>
<td>2.733871(-5)</td>
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<tr>
<td>0.005</td>
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<td>1.025522(-4)</td>
</tr>
</tbody>
</table>
In this paper we have derived diagonally implicit three-stage fourth-order and dispersive order six with 'small' dissipation constant and principal local truncation errors. We have also performed various numerical tests. From the results tabulated in Table III-VI, we conclude that the new method is more accurate for integrating second-order equations possessing an oscillatory solution when compared to the current DIRKN methods derived by van der Houwen and Sommeijer [20], Sharp, Fine and Burrage [14] and Imoni, Onuta and Ramamohan [17].

VI. CONCLUSION

Notation : 1.234567(-4) means 1.234567 × 10^{-4}

REFERENCES