Diagonally Implicit Runge-Kutta Nystrom General Method Order Five for Solving Second Order IVPs

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Abstract: - A diagonally implicit Runge-Kutta-Nystróm General (SDIRKNG) method of fifth order with an explicit first stage for the integration of second-order IVPs is presented. A standard set of test problems are tested upon and the numerical results are compared when the same set of test problems are reduced to first-order system and solved using existing fifth order singly diagonally implicit Runge-Kutta method. The time taken to solve each problem over all the stepsizes are also compared. The results suggest the superiority of the new method.

Key-Words: - Diagonally implicit, Runge-Kutta-Nystróm, Second-order IVPs.

1 Introduction

Many physical problems can be formulated in the form of ordinary differential equations. These differential equations can be classified as boundary value problem and initial value problems. Work on boundary value problem can be seen in Gordeziani et. al [1]. Systems of second order ordinary differential equations arise in many physical problems, such as celestial mechanics, astrophysics, electronics and molecular dynamics. The general form of the second order ordinary differential equation can be written as follows

$$y'' = f(x, y, y'), \quad x_0 \le x \le x_n, \tag{1}$$

with the given initial conditions

$$y(x_0) = y_0, \; y'(x_0) = y'_0,$$

where $y \in \Re^n$, and $f : \Re \times \Re^n \times \Re^n \to \Re^n$. The function f is assumed to have derivative of arbitrary order everywhere in $\Re$. Using Runge-Kutta (RK) type of methods equation (1) can be solved using two general techniques, the first one is to transform (1) to first-order problem and then use any RK method. Many classes of RK methods have been developed, these include the method constructed by Ismail et. al [2], Din et. al [3], Verner [4] and fifth order singly diagonally implicit Runge-Kutta (SDIRK) method due to Cooper and Sayfy [5] which can be found in Hairer and Wanner [6]. The second technique is to solve (1) directly using Runge-Kutta-Nystróm General (RKNG) method. This method generates approximations y_{n+1} and y'_{n+1}, to $y(x_{n+1})$ and $y'(x_{n+1})$ respectively, for n=0,1,…, according to

$$\left.\begin{aligned} y_{n+1} &= y_n + hy'_n + h^2\sum_{i=1}^{q} b_i k_i, \\ y'_{n+1} &= y'_n + h\sum_{i=1}^{q} b'_i k_i, \end{aligned}\right\} \tag{2}$$

where q is the number of stages, $h = x_{n+1} - x_n$, and

$$k_i = f(x_n + c_i h, y_n + c_i h y'_n + h^2\sum_{j=1}^{i} a_{ij} k_j, y'_n + \sum_{j=1}^{i} a'_{ij} k_j)$$

$i = 1, \dots, q.$

We refer to (2) as generalized Runge-Kutta-Nystróm method. Unlike their close relatives, the Runge-Kutta-Nystróm formulas for the special second order initial value problem $y'' = f(x, y)$, the

RKNG schemes have been infrequently investigated. Zurmühl [7] presented a pair of fourth order formulas requiring four stages whose c, a' and b' coincided with the tableau of parameters for the classical Runge-Kutta method for first-order ordinary differential equations. Ansorge and Tornig [8] performed a stability analysis of the classical RKNG using a scalar second-order differential equations with constant real coefficients. In determining the stability region of the method, technique used to solve the stability polynomial can also be obtained from Muresan [9]. Further improvements in fourth order, four stage RKNG methods, have been reported by Chawla and Sharma [10]. A number of explicit RKNG schemes, having orders five, six and seven, have been proposed by Fehlberg [11] and Fine [12]. In this paper we are going to derive fifth order singly diagonally implicit Runge-Kutta Nystrom method with an explicit first stage and use it to solve system of second order IVPs.

2 Derivation of the Method

Generally, RKNG method can be written as follows

$$y_{n+1} = y_n + hy'_n + h^2\sum_{i=1}^{q} b_i k_i ,$$

$$y'_{n+1} = y'_n + h\sum_{i=1}^{q} b'_i k_i ,$$

$$k_i = f(x_n + c_i h, y_n + hc_i y'_n + h^2\sum_{j=1}^{i} a_{ij}k_j , y'_n + h\sum_{j=1}^{i} a'_{ij}k_j)$$

$$i = 1,\ldots,q \qquad (3)$$

or it can be written in an extended Butcher tableau as

$$\begin{array}{c|ccc|ccc} c_1 & a_{11} & & & a'_{11} & & \\ \vdots & \vdots & \ddots & & \vdots & \ddots & \\ c_q & a_{q1} & \ldots & a_{qq} & a'_{q1} & \ldots & a'_{qq} \\ \hline & b_1 & \ldots & b_q & b'_1 & \ldots & b'_q \end{array}$$

where the coefficients $a_{ij}, a'_{ij}, b_i, b'_i$ determine the method and the parameters are required to satisfy the following equations

$$\frac{1}{2}c_i^2 = \sum_{j=1}^{i} a_{ij} \;,\; (i = 1,\ldots,q) , \qquad (4)$$

and $$c_i = \sum_{j=1}^{i} a'_{ij} \;,\; (i = 1,\ldots,q) . \qquad (5)$$

Based on the work of Hairer and Wanner [13], Fine [12] listed the order conditions of RKNG method up to order six.

Here, we listed all the order conditions related to y' up to order five in Table 1. And all the order conditions up to order five related to y are given in Table 2.

TABLE I

ORDER CONDITIONS UP TO ORDER FIVE FOR y'

$\sum_i b'_i = 1$ (1.1)	$\sum_{ij} b'_i c_i a_{ij} c_j = \frac{1}{30}$ (1.12) *
$\sum_i b'_i c_i = \frac{1}{2}$ (1.2)	$\sum_{ij} b'_i c_i a'_{ij} c_j^2 = \frac{1}{15}$ (1.13)
$\sum_i b'_i c_i^2 = \frac{1}{3}$ (1.3)	$\sum_{ijk} b'_i c_i a'_{ij} a'_{jk} c_k = \frac{1}{30}$ (1.14)
$\sum_{ij} b'_i a'_{ij} c_j = \frac{1}{6}$ (1.4)	$\sum_{ij} b'_i a_{ij} c_j^2 = \frac{1}{60}$ (1.15) *
$\sum_i b'_i c_i^3 = \frac{1}{4}$ (1.5)	$\sum_{ijk} b'_i a_{ij} a'_{jk} c_k = \frac{1}{120}$ (1.16) *
$\sum_{ij} b'_i c_i a'_{ij} c_j = \frac{1}{8}$ (1.6)	$\sum_{ij} b'_i (a'_{ij} c_j)^2 = \frac{1}{20}$ (1.17)

$\sum_{ij} b'_i a'_{ij} c_j^2 = \frac{1}{12}$ (1.7)	$\sum_{ij} b'_i a'_{ij} c_j^3 = \frac{1}{20}$ (1.18)
$\sum_{ijk} b'_i a'_{ij} a'_{jk} c_k = \frac{1}{24}$ (1.8)	$\sum_{ijk} b'_i a'_{ij} c_j a'_{jk} c_k = \frac{1}{40}$ (1.19)
$\sum_{ij} b'_i a_{ij} c_j = \frac{1}{24}$ (1.9)*	$\sum_{ijk} b'_i a'_{ij} a_{jk} c_k = \frac{1}{120}$ (1.20)*
$\sum_{i} b'_i c_i^4 = \frac{1}{5}$ (1.10)	$\sum_{ijk} b'_i a'_{ij} a'_{jk} c_k^2 = \frac{1}{60}$ (1.21)
$\sum_{ij} b'_i c_i^2 a'_{ij} c_j = \frac{1}{10}$ (1.11)	$\sum_{ijkl} b'_i a'_{ij} a_{jk} a'_{kl} c_l = \frac{1}{120}$ (1.22)

TABLE 2

ORDER CONDITIONS UP TO ORDER FIVE FOR y

$\sum_{i} b_i = \frac{1}{2}$ (2.1)	$\sum b_i c_i a'_{ij} c_j = \frac{1}{40}$ (2.6)
$\sum_{i} b_i c_i = \frac{1}{6}$ (2.2)	$\sum b_i a'_{ij} c_j^2 = \frac{1}{60}$ (2.7)
$\sum_{i} b_i c_i^2 = \frac{1}{12}$ (2.3)	$\sum b_i a'_{ij} a'_{jk} c_k = \frac{1}{120}$ (2.8)
$\sum b_i a'_{ij} c_j = \frac{1}{24}$ (2.4)	$\sum b_i a_{ij} c_j = \frac{1}{120}$ (2.9) **
$\sum_{i} b_i c_i^3 = \frac{1}{20}$ (2.5)	

Now we need to list down the order conditions which depend on c, b' and a' only and this set is called set S1 or set belongs to y', it consists of all equations in

Table 1 except those denoted by (*).

The second set of equations which depend on c, b and a' or we called it set S2 which belongs to y. It consists of all equations in Table 2 except those denoted by (**).

Finally all equations denoted by * and ** from Table 1 and 2 belong to the set of equations S3 which belong to both y and y'.

There are 17 equations in S1, 8 equations in S2 and 6 equations in S3, a total number of 31 equations.

Now look at set S1 and use the simplifying assumption

$$\sum_{ij} a'_{ij} c_j = \frac{c_i^2}{2} \qquad (6)$$

Certain order equations can be removed as follows:

1. $\sum_{ij} b'_i a'_{ij} c_j = \frac{1}{6}$ (1.4) , $\sum_{i} b'_i c_i^2 = \frac{1}{3}$, (1.2)

$\sum b'_i \left(\sum a'_{ij} c_j - \frac{c_i^2}{2} \right) = 0$, keep (1.2) and

remove (1.4)

2. $\sum_{ij} b'_i c_i a'_{ij} c_j = \frac{1}{8}$ (1.6) , $\sum_{i} b'_i c_i^3 = \frac{1}{4}$, (1.5)

$\sum b'_i c_i \left(\sum a'_{ij} c_j - \frac{c_i^2}{2} \right) = 0$, remove (1.6) and

keep (1.5)

3. $\sum b'_i a'_{ij} a'_{jk} c_k = \frac{1}{24}$ (1.8), $\sum b'_i a'_{ij} c_j^2 = \frac{1}{12}$ (1.7)

$\sum b'_i a'_{ij} c_i \left(\sum a'_{jk} c_k - \frac{c_j^2}{2} \right) = 0$, remove (1.8)

and keep (1.7)

4. $\sum b'_i c_i^2 a'_{ij} c_j = \frac{1}{10}$, (1.11), $\sum b'_i c_i^4 = \frac{1}{5}$ (1.10)

$$\sum b_i' c_i^2 \left(\sum a_{ij}' c_j - \frac{c_i^2}{2} \right) = 0$$, remove (1.11), keep (1.10)

5. $\sum b_i' c_i a_{ij}' a_{jk}' c_k = \frac{1}{30}$ (1.14),

$\sum b_i' c_i a_{ij}' c_j^2 = \frac{1}{15}$ (1.13)

$$\sum b_i' c_i a_{ij}' \left(\sum a_{jk}' c_k - \frac{c_j^2}{2} \right) = 0$$, remove (1.14) and keep (1.13)

6. $\sum b_i' (a_{ij}' c_j)^2 = \frac{1}{20}$ (1.17), $\sum b_i' c_i^2 a_{ij}' c_j = \frac{1}{10}$ (1.11)

$$\sum b_i' a_{ij}' c_j \left(\sum a_{jk}' c_k - \frac{c_j^2}{2} \right) = 0$$, remove (1.17) and keep (1.11)

7. $\sum b_i' a_{ij}' c_j a_{jk}' c_k = \frac{1}{40}$, (1.19), $\sum b_i' a_{ij}' c_j^3 = \frac{1}{20}$, (1.18)

$$\sum b_i' a_{ij}' c_j \left(\sum a_{jk}' c_k - \frac{c_j^2}{2} \right) = 0$$, remove (1.19) and keep (1.18)

8. $\sum b_i' a_{ij}' a_{jk} a_{kl}' c_l = \frac{1}{120}$, (1.22),

$\sum b_i' a_{ij}' a_{jk}' c_k^2 = \frac{1}{60}$, (1.21)

$$\sum b_i' a_{ij}' a_{jk}' \left(\sum a_{kl}' c_l - \frac{c_k^2}{2} \right) = 0,$$ remove (1.22) keep (1.21).

Now use the simplifying assumption

$$\sum_{ij} a_{ij}' c_j^2 = \frac{c_i^3}{3} , \qquad (7)$$

9. $\sum b_i' a_{ij}' c_j^2 = \frac{1}{12}$, (1.7), $\sum_i b_i' c_i^3 = \frac{1}{4}$, (1.5)

$$\sum b_i' \left(\sum a_{ij}' c_j^2 - \frac{c_i^3}{3} \right)$$, remove (1.7) keep (1.5)

10. $\sum b_i' c_i a_{ij}' c_j^2 = \frac{1}{15}$, (1.13), $\sum_i b_i' c_i^4 = \frac{1}{5}$, (1.10)

$$\sum b_i' c_i \left(\sum a_{ij}' c_j^2 - \frac{c_i^3}{3} \right)$$, remove (1.13) keep (1.10)

11. $\sum b_i' a_{ij}' a_{jk}' c_k^2 = \frac{1}{60}$ (1.21), $\sum_{ij} b_i' a_{ij}' c_j^3 = \frac{1}{20}$ (1.18)

$$\sum b_i' a_{ij}' \left(\sum a_{jk}' c_k^2 - \frac{c_j^3}{3} \right)$$, remove (1.21) keep (1.18)

Thus equations needed to be satisfied for set S1 are (1.1), (1.2), (1.3), (1.5), (1.10) and (1.18) provided the simplifying assumptions are satisfied for $i = 1, 2, \cdots, q$.

Now look at S2, we can still use the same simplifying assumption

Using (6) we have

12. $\sum_{ij} b_i a_{ij}' c_j = \frac{1}{24}$ (2.2.4), $\sum_i b_i c_i^2 = \frac{1}{12}$ (2.3)

$$\sum b_i \left(\sum a_{ij}' c_j - \frac{c_i^2}{2} \right) = 0$$, remove (2.4) keep (2.3)

13. $\sum b_i c_i a'_{ij} c_j = \frac{1}{40}$ (2.6) , $\sum_i b_i c_i^3 = \frac{1}{20}$ (2.5)

$\sum b_i c_i \left(\sum a'_{ij} c_j - \frac{c_i^2}{2} \right) = 0$, remove (2.6) keep (2.5)

14. $\sum b_i a'_{ij} a'_{jk} c_k = \frac{1}{120}$ (2.8),

$\sum b_i a'_{ij} c_j^2 = \frac{1}{60}$,(2.7)

$\sum b_i a'_{ij} \left(\sum a'_{jk} c_k - \frac{c_j^2}{2} \right) = 0$ remove (2.8),

keep (2.7)

Using assumption (7) we have

15. $\sum b_i a'_{ij} c_j^2 = \frac{1}{60}$ (2.7), $\sum_i b_i c_i^3 = \frac{1}{20}$, (2.5)

$\sum b_i \left(\sum a'_{ij} c_j^2 - \frac{c_i^3}{3} \right) = 0$, remove (2.7),

keep (2.5).

Thus for S2, equations to be satisfied are (2.1), (2.2), (2.3) and (2.5).

Now look at S3, which consists of equations (1.9), (1.12), (1.15), (1.16), (1.20) and (2.9), use the simplifying assumption

$$\sum a_{ij} c_j - \frac{c_i^3}{6} = 0 \quad (8)$$

16. $\sum_{ij} b'_i a_{ij} c_j = \frac{1}{24}$ (1.9), $\sum_i b'_i c_i^3 = \frac{1}{4}$ (1.5)

$\sum b'_i \left(\sum a_{ij} c_j - \frac{c_i^3}{6} \right) = 0$, remove (1.9),

keep (1.5) .

17. $\sum_{ijk} b'_i a_{ij} a'_{jk} c_k = \frac{1}{120}$, (1.16),

$\sum_{ij} b'_i a_{ij} c_j^2 = \frac{1}{60}$, (1.15)

$\sum b'_i a_{ij} \left(\sum a'_{jk} c_k - \frac{c_j^2}{2} \right) = 0$, using simplifying assumption (6) remove (1.16), keep (1.15).

18. $\sum_{ij} b'_i c_i a_{ij} c_j = \frac{1}{30}$ (1.12), $\sum_i b'_i c_i^4 = \frac{1}{5}$ (1.10)

$\sum b'_i c_i \left(\sum a_{ij} c_j - \frac{c_i^3}{6} \right) = 0$, remove (1.12)

19. $\sum_{ijk} b'_i a'_{ij} a_{jk} c_k = \frac{1}{120}$ (1.20),

$\sum_{ij} b'_i a'_{ij} c_j^3 = \frac{1}{20}$, (1.18)

$\sum b'_i a'_{ij} \left(\sum a_{jk} c_k - \frac{c_j^3}{6} \right) = 0$, remove (1.20) ,

20. $\sum b_i a_{ij} c_j = \frac{1}{120}$ (2.9), $\sum_i b_i c_i^3 = \frac{1}{20}$ (2.5)

$\sum b_i \left(\sum a_{ij} c_j - \frac{c_i^3}{6} \right) = 0$, remove (2.9).

The only equations needed to be satisfied for this set are (1.15) and simplifying assumption (8)

Now look at simplifying assumptions (6) and (7).

For $i = 1$ we have

$$a'_{11} c_1 = \frac{c_1^2}{2} \; a'_{11} {c_1}^2 = \frac{c_1^3}{3} \Rightarrow c_1 = a_{11} = 0$$

$$a'_{22} c_2 = \frac{c_2^2}{2} \Rightarrow c_2 = 2a'_{22} = 2\gamma, \quad (9)$$

(γ is the diagonal element a'_{ii} for $i>1$)

$$a'_{22}c_2^2 = \frac{c_2^3}{2} \Rightarrow c_2 = 3\gamma$$

thus it is not true and (7) cannot be satisfied for $i=2$ thus we need to have

$$b'_2 = 0, \quad \sum b'_2 c_2 = 0, \quad \sum b'_i a'_{i2} = 0 \qquad (10)$$

From S2 since we are also using (7) we need to have (from no 15). $b_2 = 0$

and (6) are satisfied for i =1,2,3,4,5 and (7) are satisfied for i =1,2,3,4,5. From set S1 other equations needed to be satisfied are

(1.1), (1.2), (1.3), (1.5), (1.10) and (1.18)

From S3 and simplifying assumption (8),

it is satisfied for for i =1 since $c_1 = 0$

$$a_{22}c_2 = \frac{c_2^3}{6} \Rightarrow c_2^2 = 6\beta \qquad (11)$$

(β is the diagonal element of a_{ii} for $i>1$

From (9) and (10) we obtained

$$c_2^2 = 6\beta = (2\gamma)^2 \Rightarrow \beta = 2\frac{\gamma^2}{3}$$

and (8) are satisfied for $i = 1,2,3,4$

The following are the steps taken to obtain the coefficients of the fifth order RKNG method

Step 1: set $\gamma = 0.125$, from (9) we have $c_2 = 2\gamma = 0.25$.

Step 2: From (6) and (7) for $i=3$, solve for a'_{32} and c_3,

Step 3: From (6) and (7) for $i=4$, solve for a'_{42} and a'_{43} ,

using the values of $c_4 = 0.5$ and c_3 obtained in step 2.

Step 4: Set $c_5 = 0.75$ and $c_6 = 0.9$, from (1.1), (1.2), (1.3) , (1.5) , (1.10) solve for $b'_i = 1,3,4,5,6$

Step 5: Set $a'_{52} = 0.1$, use (6) and (7) for $i=5$, solve for a'_{53} *and* a'_{54}.

Step 6: From equations (10), (1.18), (6) and (7) for $i=6$, solve for $a'_{62}, a'_{63}, a'_{64}$ *and* a'_{65}

Step 7; From equations (6), (7), (8) and taking

$\sum b_i a'_{i2} = 0$,we can solve

for b_1, b_3, b_4, b_5 and b_6

Step 8: Using (8) for *i*= 3 and the value of β solve for a_{32}.

Step 9: Set $a_{42} = 0.2$, solve for a_{43} using (8) for *i*=4.

Step10: Setting $a_{54} = 0.1, \quad a_{64} = 0.08, a_{65} = 0.0125$

solve for a_{52}, a_{62} and a_{63} from (8) (i =5,6) and (1.15).

The coefficients of fifth order SDIRKNG method with an explicit first stage obtained are as follows:

$c_1 = 0$
$c_2 = 0.25$
$c_3 = 0.1584936491$

$c_4 = 0.5$

$c_5 = 0.75$

$c_6 = 0.9$
$a'_{11} = 0$
$a'_{22} = 0.125$
$a'_{32} = -0.0290063509$
$a'_{33} = 0.125$

$a'_{42} = 0.022329099254$
$a'_{43} = 0.359116756473$
$a'_{44} = 0.125$

$a'_{52} = 0.1$
$a'_{53} = 0.317542648004$
$a'_{54} = 0.224340139456$
$a'_{55} = 0.125$
$a'_{62} = -0.038642219058$

$a'_{63} = 0.0689709691963$
$a'_{64} = 0.6079139921497$
$a'_{65} = -0.016970535867$
$a'_{66} = 0.125$

$b'_1 = 0.0436530665024$
$b'_2 = 0.0$
$b'_3 = 0.2632661857157$
$b'_4 = 0.3839745961478$
$b'_5 = 0.0793923533556$
$b'_6 = 0.2297137982784$

$a_{22} = 0.010416666667$
$a_{32} = -0.00394963671$
$a_{33} = 0.010416666667$

$a_{42} = 0.2$
$a_{43} = -02168856619609$
$a_{44} = 0.010416666667$
$a_{52} = 0183012701700$
$a_{53} = 0.05$
$a_{54} = 0.1$
$a_{55} = 0.010416666667$
$a_{62} = -0.022392583874$
$a_{63} = 0.4312358656237$
$a_{64} = 0.08$
$a_{65} = 0.0125$
$a_{55} = 0.010416666667$

$b_1 = 0.039272128476$
$b_2 = 0.0$
$b_3 = 0.231411318713$
$b_4 = 0.178263195251$
$b_5 = 0.033934514049$
$b_6 = 0.017118843508$

where the values of a_{i1} and a'_{i1} for (i=1(1)6) are

given by $a_{i1} = \frac{1}{2}c_i^2 - \sum_{j=2}^{i} a_{ij}$, and $a'_{i1} = c_i - \sum_{j=2}^{i} a_{ij}$.

3 Numerical Results

The following are some of the problems used to validate the new method.

Problem 3.1

$$y''_1 = -y'_2, \qquad y_1(0) = 0, \; y'_1(0) = \frac{1}{1-e^{-1}},$$

$$y''_2 = -y'_1, \; y_2(0) = 1, \quad y'_2(0) = \frac{1}{1-e^{-1}},$$

$0 \le x \le 10$

Solution: $y_1(x) = \frac{1-e^{-x}}{1-e^{-1}}$, $y_2(x) = \frac{2-e^{-1}-e^{-x}}{1-e^{-1}}$.

Source: Edwards Jr and Penny [14].

Problem 3.2

$$y''_1 = -4x^2 y_1 + \frac{2y'_1}{r_1 r_2}, \qquad x \ge x_0,$$

$$y''_2 = -4x^2 y_2 + \frac{2y'_2}{r_1 r_2}, \quad x \ge x_0,$$

$\sqrt{0.5\pi} \le x \le 10$

$$y_1(x_0) = 0, \quad y_2(x_0) = 1, \quad y'_1(x_0) = -(2\pi)^{\frac{1}{2}},$$

$y_2'(x_0) = 0$,

$r_1 = \sqrt{y_1'^2 + y_2'^2}$ and $r_2 = \sqrt{y_1^2 + y_2^2}$

Solution: $y_1(x) = \cos(x^2)$, $y_2(x) = \sin(x^2)$.

Source: Sharp and Fine [15].

Problem 3.3

$$y'' + 8y' + ky = 0, \quad 0 \le x \le 10$$

$$y(0) = 1, \qquad y'(0) = -12, \qquad k = 16.$$

Solution: $y(x) = (1 - 8x)e^{-4x}$.

Source:www.faculty.valencia.cc.fi.us/pfernandz/des/chapter5.pdf (20.9.2006).

Problem 3.4

$$y'' + 100y = \sin(y)$$
$$y(0) = 0, \quad y'(0) = 1, \quad 0 \le x \le 20\pi$$

There is no true solution but the value at 20π is 0.000392823991.

Source: Chawla and Rao [16]

Problem 3.5

$$y_1'' = -y_2' + \cos(x), \quad y_1(0) = -1, \quad y_1'(0) = -1$$
$$y_2'' = y_1 + \sin(x), \quad y_2(0) = 1, \quad y_2'(0) = 0$$

$$0 \le x \le 4\pi$$

Solutions:

$$y_1(x) = -\cos(x) - \sin(x), \quad y_2(x) = \cos(x)$$

The results obtained from the new method which was derived in section 2 are compared with the results when the same problems are solved using SDIRK method of order five and five stage due to Cooper and Sayfy [5]. In the SDIRK method the indirect approach is used to solve the problems by transforming them into a first-order differential equation of doubled dimension by considering the vector (y, y') as the new variables, Since the method is implicit we do three iterations for the first k and two iterations for the subsequent k.

The time taken for solving the problems numerically over $h = 1\text{x}10^{-r}$ where $r = 1,2,3,4,5$ is also given in figure 1.

The numerical results are given in Tables 3-7. The notations used are as follows:

MTHD: Method used.

H~ The size of the step.

FCN ~ the number of functions evaluations.

STEP ~ the number of steps.

ERR ~ $\max_i |y(t_i) - y_{t_i}|$, (absolute value of the true solution minus the computed solution at the mesh point i).

Methods used are:

RKNG 5: SDIRKNG method of order five and six stages which was derived in this paper.

RK 5: The SDIRK method order five and five stages due to Cooper and Sayfy [5], and

0.1234(-10) means 0.1234 X (10^{-10}).

TABLE 3: NUMERICAL RESULTS FOR PROBLEM 3.1

MTHD	H	FCN	STEP	ERR
RKNG 5 RK 5	0.1	1100 1100	100 100	1.2716(-5) 3.9274(-5)
RKNG 5 RK 5	0.01	11000 11000	1000 1000	1.2397(-8) 3.6935(-8)
RKNG 5 RK 5	0.001	110000 110000	10000 10000	1.2401(-11) 3.6709(-11)
RKNG 5 RK 5	0.0001	1100000 1100000	100000 100000	1.88064(-13) 1.9214(-13)

TABLE 4: NUMERICAL RESULTS FOR PROBLEM 3.2

MTHD	H	FCN	STEP	ERR
RKNG 5 RK 5	0.1	957 957	87 87	0.1342 19.9744
RKNG 5 RK 5	0.01	9614 9614	874 874	1.42700(-6) 0.3250
RKNG 5 RK 5	0.001	96206 96206	8746 8746	2.3520(-10) 3.26279(-4)
RKNG 5 RK 5	0.0001	962126 962126	87466 87466	2.2957(-10) 3.2608(-7)

TABLE5: NUMERICAL RESULTS FOR PROBLEM 3.3

MTHD	H	FCN	STEP	ERR
RKNG 5 RK 5	0.1	1100 1100	100 100	3.8330(-3) 7.5216(-2)
RKNG 5 RK 5	0.01	11000 11000	1000 1000	3.1762(-6) 5.6381(-5)
RKNG 5 RK 5	0.001	110000 110000	10000 10000	3.1140(-9) 5.4728(-8)
RKNG 5 RK 5	0.0001	1100000 1100000	100000 100000	3.1301(-12) 5.4712(-11)

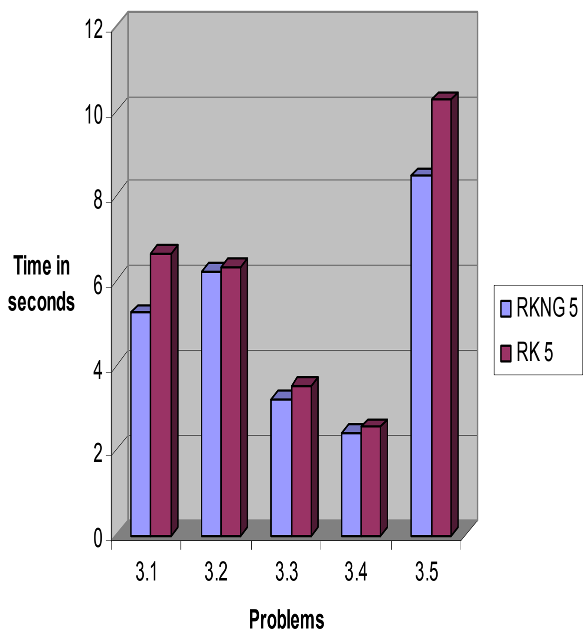
TABLE6: NUMERICAL RESULTS FOR PROBLEM 3.4

MTHD	H	FCN	STEP	ERR
RKNG 5 RK 5	0.1	6908 6908	628 628	2.2160(-2) 3.9282(-4)
RKNG 5 RK 5	0.01	69113 69113	6283 6283	1.8528(-3) 1.5255(-3)
RKNG 5 RK 5	0.001	691141 691141	62831 62831	8.5040(-4) 8.52981(-4)
RKNG 5 RK 5	0.0001	6911498 6911498	628318 628318	5.3071(-5) 5.3071(-5)

TABLE7: NUMERICAL RESULTS FOR PROBLEM 3.5

MTHD	H	FCN	STEP	ERR
RKNG 5 RK 5	0.1	1375 1375	125 125	3.1147(-5) 7.6378(-2)
RKNG 5 RK 5	0.01	13816 13816	1256 1256	4.2094(-9) 7.9699(-5)
RKNG 5 RK 5	0.001	138226 138226	12566 12566	2.0216(-11) 8.0015(-8)
RKNG 5 RK 5	0.0001	1382293 1382293	125663 125663	2.3747(-10) 2.1853(-10)

Figure 3.1: Total time taken to solve the problems



4 Conclusion

For most of the problems tested, we can conclude that solving the general second order equations directly using the fifth order RKNG method produced smaller error compared to reduction to first order systems. From the number of function evaluations we can say that though the RKNG method is six stages but the first stage is explicit thus no iteration is needed to evaluate the first *k*, hence the method is effectively contain five stages which is comparable to the SDIRK method.

In terms of time taken to solve the problems over all the stepsizes, RKNG 5 required slightly less time compared to RK 5, and we believed that if the problems consist of larger system of equations then the total time gained will be more apparent.

Thus, the method RKNG 5 for the solving the second order IVPs directly is more efficient than the RK 5 method.

References:

[1] D. G. Gordeziani, H. V. Meladze ad T.D. Davitashvili. On One Generalization of Boundary Value Problem for Ordinary Differential Equations on Graphs in the Three-dimensional Space, *WSEAS Transaction on Mathematics*, vol 8, no 8, 2009: 457-466.

[2] F. Ismail, N. I. Che Jawias, M. Suleiman and A. Jaafar, Solving Linear Ordinary Differential Equations using Singly Diagonally Implicit Runge-Kutta fifth order five stage method. *WSEAS Transaction on Mathematics,* vol 8, no 8, 2009: 393-402.

[3] U. K. S. Din, F. Ismail, M. Suleiman and M. Othman, *Applied Mathematics,* New York: Springer 2009.

[4] J. H. Verner , Explicit Runge-Kutta methods with estimates of the local truncation error. *SIAM J. Numer. Anal.* 1978, 15(4), 67-75.

[5] J. G. Cooper J. G. andA. Sayfy , Semiexplicit A-stable Runge-Kutta methods. *Math of Comp.*, 1979 vol 33, pp. 541-556.

[6] E. Hairer, E. and G. Wanner, *Solving Ordinary Differential Equations II, stiff and Differential Algebraic Problems*, Berlin:Springer-Verlag. 1991.

[7] R. Zurmül, Runge-Kutta-Verfahren zur numerischen Integration von Differentialgleichungen *n*-ter Ordnung. *ZAMM* 28 , 1948: 173-182.

[8] R. Ansorge, and W. Tornig, Zur Stabilität des Nyströmischen Verfahrens. *ZAMM* 40: 1960, : 568-578.

[9] C. A. Muresan, The Polynomial Roots Repartition and Minimum Roots Separation, *WSEAS Transaction on Mathematics*, vol 8, no7, 2008: 515-527.

[10] M. M. Chawla, and S. R. Sharma. Families of direct fourth-order methods for the numerical solution of general second-order initial value problems. *ZAMM 60* 1980*:* 469-475.

[10] E. Fehlberg, . Classical seventh-, sixth-, and fifth-order Runge-Kutta-Nystróm formulas with stepsize control for general second-order differential equations. *NASA Technical Report R*-432 1974.

[12] J. M. Fine, Low Order Practical Runge-Kutta-Nystróm Methods. *Computing by Springer-Verlag* 1987*,* 38: 281-297.

[13] E. Hairer, E. and G. Wanner. A theory for Nystróm methods, *Numer. Math.* 25 1976: 383-400.

[14] Edwards Jr, C. H. and Penny, D. E. (1993). *Elementary Differential Equations with Boundary Value Problem*. Prentice-Hall, Englewood Cliffs, New Jersey.

[15] Sharp, P. W. and Fine, J. M. (1992). Some Nystróm pairs for the general second-order initial-value problem. *Journal of Comut. And Appl. Math.,* 42: 279-291.

[16] Chawla M.M and Rao P. S. (1985). High-accuracy P-stable methods for $y'' = f(t, y)$, *IMA J. Numer Anal.* (5) 215-220.