Jewel Journal of Scientific Research (JJSR) 3(1): 158- 164, 2015
©Federal University, Kashere-Nigeria (ISSN: 2384 - 6267)
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Third order extended Runge-Kutta Nyström methods for the solution of special second order differential equations

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Abstract: Explicit extended Runge-Kutta Nyström type method is constructed for the numerical integration of special second order system of differential equations of the form $y'' = f(x, y)$. Additional parameters are introduced into classical Runge-Kutta Nyström method in such a way that the first derivative of $f(x, y)$ might be required for the integration. Results from numerical experiments reveal the superiority of the new method over several methods in the scientific literature.

Keywords: Experiment, explicit, global error, integration, stability.

Introduction

In this paper we present a new family of Runge-Kutta Nyström methods that are capable of integrating special second order initial value problems of the form

$$y'' = f(x, y), y(x_0) = y_0, y'(x_0) = y'_0, \quad (1)$$

The specialty associated to this type of equation is the fact that $f(x, y)$ does not depend on y' explicitly. This type of equation can be used to model problems arising in different fields of science and engineering, for instance, area of quantum mechanics, electronics, quantum chemistry, astrophysics, and celestial mechanics.

One of the easiest numerical ways of integrating (1) is by transforming it into a system of first order equations and apply any suitable method for solving first order equations, e.g Runge-Kutta or linear multi-step method. However, it will be computationally economical if a method that can directly integrate (1) is designed. This attempt has been made by several authors (Sommeijer, 1987; Domand, 1996; Al-khasawneh, 2007; Senu, 2009; 2010; Rabiei, 2012) and this type of method is referred to as Runge-Kutta Nyström (RKN) method. There are several Runge-Kutta Nyström methods in the scientific literature today. It is worth knowing that classical RKN method evolved from the modification of classical RK method. As a result, any successful modification done to RK method is capable of producing a modified RKN method (Wu, 2006).

One of the modified RK methods with desirable numerical behaviors in the literature is extended RK methods. These types of methods were introduced by Goeken and Johnson (Johnson, 2000). Further work on these methods can be seen in (Wu, 2006). In line with this, we propose a family of extended Runge-Kutta Nyström methods of the form

$$y_{n+1} = y_n + hy'_n + h^2 \sum_{i=1}^{m} (b_i k_{i1} + hc_i k_{i2}), \quad (2a)$$

$$y'_{n+1} = y'_n + h \sum_{i=1}^{m} (b'_i k_{i1} + hc'_i k_{i2}), \quad (2b)$$

$$k_{i1} = f(x_n + \hat{c}_i h, y_n + h\hat{c}_i y'_n + h^2 \sum_{s=1}^{i-1} a_{is} k_{s1}), \quad (2c)$$

$$k_{i2} = G(x_n + \hat{c}_i h, y_n + h\hat{c}_i y'_n + h^2 \sum_{s=1}^{i-1} a_{is} k_{s1}). \quad (2d)$$

We assume $a_{is}, b_i, b'_i, c_i, c'_i$ and $\hat{c}_i$ are real and m might be greater or equal to the number of stages of the method. Suppose **b**, **b′**, **c**, **c′** and $\hat{\mathbf{c}}$ are m-dimensional vectors and **A** an $m \times m$ matrix, where **b** = $[b_1, b_2, ..., b_m]^T$, **b′** = $[b'_1, b'_2, ..., b'_m]^T$, **c** $= [c_1, c_2, ..., c_m]^T$, **c′** $= [c'_1, c'_2, ..., c'_m]^T$, $\hat{c} = [\hat{c}_1, \hat{c}_2, ..., \hat{c}_m]^T$ and **A** = $[a_{is}]$. With these, the general form of the method is summarized as follows

$\hat{c}$	**A**
	b^T
	c^T
	b'^T
	c'^T

The remaining part of the paper is organized as follows: in section 2, the third order extended Runge-Kutta Nyström method with three function calls per step is derived. Stability analysis of the method is presented in section 3. In section 4, we present numerical experiments to demonstrate the effectiveness of the proposed method. Finally, conclusions are drawn based on the performance of the new method in section 5.

Extended Runge-Kutta Nyström method of order three

The general form of third order method when we consider $m = 3$ in (2) is

$$y_{n+1} = y_n + hy'_n + h^2[b_1k_{11} + b_2k_{21} + b_3k_{31} + h(c_1k_{12} + c_2k_{22} + c_3k_{32})], \quad (3a)$$

$$y'_{n+1} = y'_n + h[b'_1k_{11} + b'_2k_{21} + b'_3k_{31} + h(c'_1k_{12} + c'_2k_{22} + c'_3k_{32})], \quad (3b)$$

$$\left.\begin{aligned} k_{11} &= f(x_n, y_n), \\ k_{12} &= G(x_n, y_n), \end{aligned}\right\} \quad (3c)$$

$$\left.\begin{aligned} k_{21} &= f(x_n + \hat{c}_2 h, y_n + h\hat{c}_2 y'_n + h^2 a_{21} k_{11}), \\ k_{22} &= G(x_n + \hat{c}_2 h, y_n + h\hat{c}_2 y'_n + h^2 a_{21} k_{11}), \end{aligned}\right\} \quad (3d)$$

$$\left.\begin{aligned} k_{31} &= f(x_n + \hat{c}_3 h, y_n + h\hat{c}_3 y'_n + h^2(a_{31}k_{11} + a_{32}k_{21})), \\ k_{32} &= G(x_n + \hat{c}_3 h, y_n + h\hat{c}_3 y'_n + h^2(a_{31}k_{11} + a_{32}k_{21})). \end{aligned}\right\} \quad (3e)$$

Our task at this juncture is to specify the third order method by deriving its coefficients. This can be accomplished by employing the Taylor series expansions of (3) and comparing the terms of h, h^2, h^3 with that of the exact solution of $y'' = f(x, y)$. We obtained the following set of equations as a result of the comparison,

$$b_1 + b_2 + b_3 = \frac{1}{2}, \quad b_2\hat{c}_2 + b_3\hat{c}_3 + c_1 + c_2 + c_3 = \frac{1}{6}$$

$$b'_2\hat{c}_2 + b'_3\hat{c}_3 + c'_1 + c'_2 + c'_3 = \frac{1}{2}$$

$$b_2\hat{c}_2^2 + b_3\hat{c}_3^2 + c_2\hat{c}_2 + c_3\hat{c}_3 = \frac{1}{12}$$

$$\tfrac{1}{2}b'_2\hat{c}_2^2 + \tfrac{1}{2}b'_3\hat{c}_3^2 + c'_2\hat{c}_2 + c'_3\hat{c}_3 = \frac{1}{6}$$

$$c_1 + c_2 + c_3 = 0, \quad c'_1 + c'_2 + c'_3 = 0$$

$$c_2\hat{c}_2 + c_3\hat{c}_3 = 0, \quad c'_2\hat{c}_2 + c'_3\hat{c}_3 = 0$$

which form the order conditions of the method. Where $f(x, y) = f$, $G(x, y) = f_x + ff_y$ and the row sum condition of RKN method, $\frac{1}{2}\hat{c}_i = \sum a_{is}$, is assumed to hold. The order conditions of third order method consist of ten equations to be solved in fourteen unknown parameters. Consequently, we have four free parameters. Let $\hat{c}_2, \hat{c}_3, c_3$ and c_3' be chosen as the free parameters, the remaining parameters are given in terms of the free parameters as follows:

$$b_1 = \frac{1}{12}\frac{-2\hat{c}_2 + 6\hat{c}_2\hat{c}_3 - 2\hat{c}_3 + 1}{\hat{c}_2\hat{c}_3},$$

$$b_2 = -\frac{1}{12}\frac{2\hat{c}_3 - 1}{12\hat{c}_2(\hat{c}_2 - \hat{c}_3)},$$

$$b_3 = \frac{1}{12}\frac{2\hat{c}_3 - 1}{12\hat{c}_3(\hat{c}_2 - \hat{c}_3)},$$

$$b_1' = \frac{1}{6}\frac{-3\hat{c}_2 + 6\hat{c}_2\hat{c}_3 - 3\hat{c}_3 + 2}{\hat{c}_2\hat{c}_3}$$

$$b_2' = -\frac{1}{6}\frac{3\hat{c}_2 - 2}{\hat{c}_2(\hat{c}_2 - \hat{c}_3)},$$

$$b_3' = -\frac{1}{6}\frac{3\hat{c}_2 - 2}{\hat{c}_3(\hat{c}_2 - \hat{c}_3)},$$

$$c_1 = \frac{c_3(\hat{c}_2 - \hat{c}_3)}{\hat{c}_2},$$

$$c_2 = -\frac{\hat{c}_3 c_3}{\hat{c}_2},$$

$$c_1' = \frac{c_3'(\hat{c}_2 - \hat{c}_3)}{\hat{c}_2},$$

$$c_2' = \frac{c_3'\hat{c}_3}{\hat{c}_2}.$$

Where $\hat{c}_2 \neq \hat{c}_3, c_2' \neq 0, c_3' \neq 0$. The basis for choosing the free parameters will be to make the principal error norms as small as possible (Domand, 1996) and to have less function call per step of the integration. This will guarantee an accurate yet efficient method. The principal error norm is defined as the square root of sum of the squares of the principal error terms of the method (Domand, 1996). Hence, the choice of $\hat{c}_2 = \frac{1}{3}, \hat{c}_3 = \frac{3}{2}, c_3 = c_3' = 0.$ and an additional requirement $a_{32} = \frac{4}{3}$ gives the best coefficients of the 3-stage third order extended Runge-Kutta Nyström method with error norms of y and y' as $\varepsilon^4 = 7.86\times10^{-3}$ and $\varepsilon'^4 = 3.92\times10^{-2}$ respectively. The method is given in the tableau below.

Table1: Coefficients of the Method.

$\frac{1}{12}$	$\frac{1}{288}$			
$\frac{1}{2}$	$-\frac{121}{1192}$	$\frac{75}{298}$		
$\frac{4}{5}$	$-\frac{1201}{1192}$	$\frac{21894}{130375}$	$\frac{1}{7}$	
	$-\frac{1}{12}$	$\frac{72}{215}$	$\frac{1}{15}$	$\frac{25}{516}$
	0	0	0	
	$-\frac{7}{24}$	$\frac{144}{215}$	$\frac{8}{45}$	$\frac{1375}{3096}$
	0	0	0	

Stability Analysis

We study the stability properties of the extended Runge-Kutta Nyström method by considering the homogenous test equation $y'' = -\alpha^2 y$. (4)

Applying (2) to the test equation (4) yields

$$\begin{bmatrix} y_{n+1} \\ hy'_{n+1} \end{bmatrix} = R(z)\begin{bmatrix} y_n \\ hy'_n \end{bmatrix},$$

$$R(z) = \begin{bmatrix} r_{11}(z) r_{12}(z) \\ r_{21}(z) r_{22}(z) \end{bmatrix},$$

$$r_{11}(z) = \begin{bmatrix} 1 + zb^T(I - zA)^{-1} + \\ z^2 c^T(I + z(I - zA)^{-1}) \end{bmatrix} e, ,$$

$$r_{12}(z) = \begin{bmatrix} 1 + zb^T(I - zA)^{-1} + \\ z^2 c^T(I + z(I - zA)^{-1}) \end{bmatrix} \hat{c},$$

$$r_{21}(z) = \begin{bmatrix} 1 + zb'^T(\mathbf{I} - \mathbf{zA})^{-1} + \\ z^2 \mathbf{c}'^T(\mathbf{I} + \mathbf{z}(\mathbf{I} - \mathbf{zA})^{-1}) \end{bmatrix} \mathbf{e}, ,$$

$$r_{22}(z) = \begin{bmatrix} 1 + zb'^T(\mathbf{I} - \mathbf{zA})^{-1} + \\ z^2 c'^T(\mathbf{I} + \mathbf{z}(\mathbf{I} - \mathbf{zA})^{-1}) \end{bmatrix} \hat{c},$$

$z = -(\alpha h)^2$ and $\mathbf{e} = [1,1,1,...,1]^T$.

$R(z)$ is referred to stability matrix of the method. If r is the eigen value of $R(z)$, then characteristic equation associated with $R(z)$ is

$$r^2 = T(z)r + D(z) = 0 \quad (5)$$

Definition 3.1. *Interval* $(-z,0)$ *is referred to interval of absolute stability of the method if for all* $z \in (-z,0)$, $|r_{1,2}| < 1$, *where* $r_{1,2}$ *are the roots of (5).*

And the region bounded by the set of points for which $|r_{1,2}| = 1$ is referred to absolute stability region of RKN method, see (Al-khasawneh, 2007). Absolute stability region of the new method, which is comparable with the regions of existing methods, is given in section 4.

Numerical results:

In this section we evaluate how effective the proposed method in this paper is by solving some model problems in scientific literature. The results are compared with results of existing methods of its type in the literature. However, the following acronyms in this paper mean:

- **Maxero** $= |y_{n+1} - y(x_{n+1})|$: is maximum global error.
- **ERKN3:** third order method obtained in this paper.
- **VRKN3:** third order method proposed in (Senu, 2009).
- **DRK3:** third order Runge-Kutta method presented in (Domand, 1996).
- **ARKN 3:** third order method obtained in (Senu, 2010).

Problems 1-5 below are the test problems in this paper.

Problem 1: $y'' = -y, y(0) = 0, y'(0) = 1$, exact solution: $y(x) = \sin(x)$.

Problem 2:

$$y_1'' + y_1 = 0.001\cos(x), y_1(0) = 0, y_1'(0) = 0,$$

$$y_2'' + y_2 = 0.001\sin(x), y_2(0) = 0, y_2'(0) = 0.9995,$$

exact solution:
$$y_1(x) = \sin(x) + 0.0005\cos(x),$$
$$y_2(x) = \sin(x) - 0.0005\cos(x).$$

Problem 3:

$y'' = -y + x, y(0) = 1, y'(0) = 2,$ exact solution: $y(x) = \sin(x) + \cos(x) + x$.

Problem4 $y'' = -64y, y(0) = \frac{1}{4}, y'(0) = -\frac{1}{2}$,

exact solution:

$$y(x) = \frac{\sqrt{17}}{16}\sin(8x + t), t = \pi - \arctan(4).$$

Problem 5:

$$y'' = -v^2 y + (v^2 - 1)\sin(x), y(0) = 1, y'(0) = v + 1, v > 1,$$

exact solution:

$y(x) = \cos(vx) + \sin(vx) + \sin(x)$.

We solve the problems using h = *0.1*, *0.05*, *0.01*, *0.005* and *0.001*. And the interval considered for the cases is [0, 10].

Table 2: Comparison of maximum global error of third order RKN methods for problem1

H	Maxero			
	ERKN3	VRKN3	DRKN3	ARKN3
0.1	3.0×10^{-06}	1.5×10^{-05}	3.9×10^{-04}	7.8×10^{-05}
0.05	3.4×10^{-07}	3.7×10^{-06}	4.9×10^{-05}	1.0×10^{-05}
0.01	2.6×10^{-09}	1.5×10^{-07}	3.9×10^{-07}	8.2×10^{-08}
0.005	3.2×10^{-10}	3.7×10^{-08}	4.9×10^{-08}	1.0×10^{-08}
0.001	2.6×10^{-12}	1.5×10^{-09}	3.9×10^{-10}	8.2×10^{-11}

Table 3: Comparison of maximum global error of third order RKN methods for problem2

H	Maxero			
	ERKN3	VRKN3	DRKN3	ARKN3
0.1	3.3×10^{-06}	1.2×10^{-05}	3.9×10^{-04}	1.1×10^{-04}
0.05	3.8×10^{-07}	5.4×10^{-06}	4.9×10^{-05}	1.3×10^{-05}
0.01	3.0×10^{-09}	1.4×10^{-07}	3.9×10^{-07}	1.0×10^{-07}
0.005	3.7×10^{-10}	3.3×10^{-08}	4.9×10^{-08}	1.3×10^{-08}
0.001	3.9×10^{-12}	3.9×10^{-09}	3.9×10^{-10}	1.0×10^{-10}

Table 4: Comparison of maximum global error of third order RKN methods for problem3

H	Maxero			
	ERKN3	VRKN3	DRKN3	ARKN3
0.1	3.8×10^{-06}	3.5×10^{-05}	5.8×10^{-04}	1.2×10^{-04}
0.05	5.1×10^{-07}	6.9×10^{-06}	7.2×10^{-05}	1.4×10^{-05}
0.01	4.3×10^{-09}	2.1×10^{-07}	7.7×10^{-07}	1.6×10^{-07}
0.005	5.4×10^{-10}	5.3×10^{-08}	2.0×10^{-08}	1.4×10^{-08}
0.001	4.3×10^{-12}	2.0×10^{-09}	5.7×10^{-10}	1.1×10^{-10}

Table 5: Comparison of maximum global error of third order RKN methods for problem4

H	Maxero			
	ERKN3	VRKN3	DRKN3	ARKN3
0.1	1.2×10^{-02}	4.3×10^{-03}	$1.8 \times 10^{+01}$	1.2×10^{-01}
0.05	8.8×10^{-04}	8.2×10^{-04}	3.9×10^{-01}	1.5×10^{-02}
0.01	3.6×10^{-06}	2.3×10^{-05}	3.5×10^{-03}	1.3×10^{-05}
0.005	4.3×10^{-07}	5.5×10^{-06}	4.3×10^{-04}	1.4×10^{-08}
0.001	3.4×10^{-09}	2.1×10^{-07}	3.5×10^{-06}	1.0×10^{-07}

Table 6: Comparison of maximum global error of third order RKN methods for problem 5

H	Maxero			
	ERKN3	VRKN3	DRKN3	ARKN3
0.1	1.1×10^{-04}	2.4×10^{-04}	1.6×10^{-02}	2.1×10^{-03}
0.05	1.2×10^{-05}	5.1×10^{-05}	2.1×10^{-03}	2.5×10^{-04}
0.01	1.0×10^{-07}	1.7×10^{-06}	1.6×10^{-05}	2.0×10^{-06}
0.005	1.2×10^{-08}	4.2×10^{-07}	2.1×10^{-06}	2.5×10^{-07}
0.001	1.0×10^{-10}	1.6×10^{-08}	1.6×10^{-08}	2.0×10^{-09}

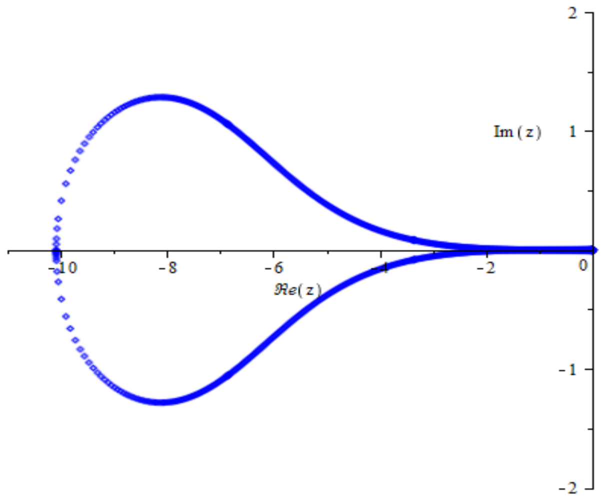

Figure 1: Stability region of ERKN3

Table 2-6 show the numerical accuracy of the new method and the existing methods for different constant step-sizes. The accuracy is measured in terms of maximum global error taken over the whole interval considered for the approximation. From the tables, we observe that the new third order method proposed in this paper has smaller maximum global errors when compared to the existing methods considered in this paper. This implies that the new method converges faster than the existing methods. The derivation as well as the implementation algorithms of the methods is coded using computer algebra package (MAPLE 16).

Conclusion

Extended Runge-Kutta Nyström methods of order three with three stages is derived in this paper. From the numerical results presented in section 4, we conclude that the new method is more promising than the existing methods considered in this paper.

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