

A Modified Runge-Kutta-Nyström Method by using Phase Lag Properties for the Numerical Solution of Orbital Problems

Dimitris F. Papadopoulos¹ and T.E. Simos^{2,3}

¹ Dept. Business Admin., Faculty of Management and Economy, Technological Educational Institute of Patras, Greece

² Department of Mathematics, College of Sciences, King Saud University, Riyadh, KSA

³ Laboratory of Computational Sciences, Faculty of Sciences and Technology, University of Peloponnese, Greece

Received: 24 Apr. 2012; Revised 21 Jul. 2012; Accepted 18 Oct. 2012

Published online: 1 Mar. 2013

Abstract: In this paper, a new modified Runge-Kutta-Nyström method of third algebraic order is developed. The new modified RKN method has phase-lag and amplification error of order infinity, also the first derivative of the phase lag is of order infinity. Numerical results indicate that the new method presented in this paper, is much more efficient than other methods of the same algebraic order, for the numerical integration of orbital problems.

Keywords: Runge-Kutta-Nyström methods, Orbital problems, Phase-fitted, Amplification-fitted, derivatives, initial value problems, oscillating solution

1. Introduction

Much research has been done on the second order periodic initial and boundary value problems with oscillating and/or periodic solutions the recent years (see [13] - [28] and references therein).

Last decades many researchers developed optimized methods based on the phase lag properties ([1] - [10]). Moreover, the very last years a new methodology has been developed which is basing the optimization of a method to the nullification of the phase lag and its derivative ([4],[6],[7],[8],[9],[10]). This new methodology was applied on the multistep methods [4].

In the present paper, an effort is being made to combine for first time in literature the nullification of phase lag, amplification error and phase lag's derivative. The new modified Runge-Kutta-Nyström that is being constructed, contains three additional variable coefficients (in comparison with the classical RKN method), which depend on $z = wh$, where w is the dominant frequency of the problem and h is the step length of integration. In order to evaluate the above coefficients, the new method combines the

nullification of phase-lag, amplification factor and phase-lag's derivative.

The new modified RKN method that obtained, will be used for the numerical solution of some well-known orbital problems.

2. The modified Runge-Kutta-Nyström method

In this section we present the general form of the new modified method, which can be used for the numerical integration of second order ordinary differential equations with the following form

$$\frac{d^2 y(t)}{dt^2} = f(t, y(t)) \quad (1)$$

The general form of the new modified RKN method is given below

$$y_n = y_{n-1} + hy'_{n-1} + h^2 \sum_{i=1}^m b_i f(t_{n-1} + c_i h, f_i),$$

* Corresponding author: e-mail: tsimos.conf@gmail.com

$$y_n = y'_{n-1}G + h \sum_{i=1}^m b'_i f(t_{n-1} + c_i h, f_i), \quad (2)$$

where

$$f_i = y_{n-1} + hc_i y'_{n-1} + h^2 \sum_{j=1}^{i-1} \alpha_{ij} f(t_{n-1} + c_j h, f_j) \quad (3)$$

$$i = 1, \dots, m$$

As it is obvious, for $G = 1$, the classical Runge Kutta Nyström method is obtained. In the present paper and based on the requirement of the development of the new method, value G is a variable and depends on z (which is the product of the frequency w and the step-size h). In section (4) we will present a development of a three-stage modified Runge-Kutta-Nyström method of third algebraic order.

3. Phase-lag analysis of the modified Runge-Kutta-Nyström method

For the development of the new modified method we compare the exact and the numerical solution of the following test equation

$$\frac{d^2 y(t)}{dt^2} = (iw)^2 y(t) \implies y''(t) = -w^2 y(t), \quad w \in R \quad (4)$$

In the test equation (4) we apply the modified RKN method (2) and we are led to the numerical solution

$$\begin{bmatrix} y_n \\ hy'_n \end{bmatrix} = D^n \begin{bmatrix} y_0 \\ hy'_0 \end{bmatrix}, \quad D = \begin{bmatrix} A(z^2) & B(z^2) \\ \dot{A}(z^2) & \dot{B}(z^2) \end{bmatrix}, \quad (5)$$

where $z = wh$ and A, B, \dot{A}, \dot{B} are polynomials in z^2 , completely determined by the parameters of the method (2).

The eigenvalues of the amplification matrix $D(z^2)$ are the roots of the characteristic equation

$$r^2 - \text{tr}(D(z^2))r + \det(D(z^2)) = 0 \quad (6)$$

In phase analysis one compares the phases of $\exp(iz)$ with the phases of the roots of the characteristic equation (6). The following definition is originally formulated by van der Houwen and Sommeijer [1].

Definition 1 (Phase-lag). Apply the RKN method (2) to the general method (4). Then we define the phase-lag $\Phi(z) = z - \arccos(\text{tr}(D)/2\sqrt{\det(D)})$. If $\Phi(z) = O(z^{q+1})$, then the RKN method is said to have phase-lag order q . In addition, the quantity $a(z) = 1 - \sqrt{\det(D)}$ is called amplification error.

where $z = wh$. From definition 1 it follows that

$$\Phi(z) = z - \arccos\left(\frac{R(z^2)}{2\sqrt{Q(z^2)}}\right),$$

$$a(z) = 1 - \sqrt{Q(z^2)}. \quad (7)$$

If at a point z , $a(z) = 0$, then the Runge Kutta Nyström method has zero dissipation at this point.

According to the definition 1 we have the following theorem.

0			
1/2	1/8		
1	0	1/2	
	1/6	2/6	0
	1/6	b'_2	b'_3

Table 1 third-stage explicit Runge-Kutta-Nyström method

Theorem 1 If we have phase-lag of order infinity and at a point z , $a(z) = 0$ then,

$$\left. \begin{array}{l} z - \arccos\left(\frac{R(z^2)}{2\sqrt{Q(z^2)}}\right) = 0 \\ 1 - \sqrt{Q(z^2)} = 0 \end{array} \right\} \implies \begin{array}{l} R(z^2) = 2\cos(z) \\ Q(z^2) = 1 \end{array}$$

for more details see ([5])

Lemma 1 For the derivation of a RKN method with nullification of phase lag, amplification error and phase lag's derivative, we must satisfy the conditions:

$$\begin{array}{l} R(z^2) = 2\cos(z), \\ Q(z^2) = 1, \\ R'(z^2) = -2\sin(z) \end{array} \quad (8)$$

4. Construction of the new modified RKN method

In this section we demonstrate the procedure for the derivation of the new modified RKN method, which is a three-stage explicit Runge-Kutta-Nyström method of third algebraic order. From equations 2 and 4, the three-stage explicit modified RKN method can be written in the following form:

$$\begin{array}{l} y_n = y_{n-1} + hy'_{n-1} + h^2(b_1 f_1 + b_2 f_2 + b_3 f_3), \\ y'_n = y'_{n-1}G + h(b'_1 f_1 + b'_2 f_2 + b'_3 f_3), \end{array} \quad (9)$$

where

$$\begin{array}{l} f_1 = f(t_{n-1}, y_{n-1}), \\ f_2 = f(t_{n-1} + c_2 h, y_{n-1} + c_2 h y'_{n-1} + h^2 a_{21} f_1), \\ f_3 = f(t_{n-1} + c_3 h, y_{n-1} + c_3 h y'_{n-1} \\ \quad + h^2(a_{31} f_1 + a_{32} f_2)), \end{array} \quad (10)$$

At this point we consider the third-stage explicit RKN method which is presented by the Butcher tableau 1.

From the Butcher tableau 1, equation 9 is transformed as follows:

$$\begin{array}{l} y_n = y_{n-1} + hy'_{n-1} + h^2\left(\frac{1}{6}f_1 + \frac{2}{6}f_2\right), \\ y'_n = y'_{n-1}G + h\left(\frac{1}{6}f_1 + b'_2 f_2 + b'_3 f_3\right), \end{array} \quad (11)$$

where

$$\begin{aligned}
 f_1 &= f(t_{n-1}, y_{n-1}), \\
 f_2 &= f(t_{n-1} + \frac{1}{2}h, y_{n-1} + \frac{1}{2}hy'_{n-1} + \frac{1}{8}h^2 f_1), \\
 f_3 &= f(t_{n-1} + h, y_{n-1} + hy'_{n-1} + \frac{1}{2}h^2 f_2),
 \end{aligned}
 \tag{12}$$

In order to obtain the expressions of the coefficients b'_2 , b'_3 and G , we apply numerical method 11 to the test equation 4, and thus we compute the polynomials A, \dot{A}, B, \dot{B} in terms of the modified Runge-Kutta-Nyström parameters. From these polynomials we obtain the expressions of $R(z^2)$ and $Q(z^2)$. Then, according to Lemma 1 we solve the system of four equations ($R(z^2) = 2\cos(z)$, $Q(z^2) = 1$, $R'(z^2) = -2\sin(z)$) and thus we obtain the expressions of the coefficients which are fully depended from the product of the step-length h and the frequency w .

$$b'_2 = -1/3 (384 z^3 \sin(z) - 54 z^6 - 960 z^2 + 304 z^4 + 1152 z^2 \cos(z) + 3 z^8 - 84 z^5 \sin(z) + 6 z^7 \sin(z) + 24 z^6 \cos(z) - 336 z^4 \cos(z) - 576 z \sin(z) + 1152 - 1152 \cos(z)) / (z^2 (88 z^2 - 96 - 18 z^4 + z^6))$$

$$b'_3 = -1/6 (1152 z \sin(z) + 56 z^4 - 1152 + 96 z^2 + 1152 \cos(z) - 16 z^6 - 336 z^3 \sin(z) + 24 z^5 \sin(z) + z^8 + 48 z^4 \cos(z) - 576 z^2 \cos(z)) / (z^2 (88 z^2 - 96 - 18 z^4 + z^6))$$

$$G = -1/12 (-1152 + 480 z^2 - 120 z^4 - 4 z^6 + 2304 \cos(z) + 1152 z \sin(z) - 480 z^3 \sin(z) + 48 z^5 \sin(z) + 144 z^4 \cos(z) - 1536 z^2 \cos(z) + z^8) / (88 z^2 - 96 - 18 z^4 + z^6)$$

For small values of x the following Taylor series expansions are used

$$b'_2 = \frac{2}{3} - \frac{1}{240} z^4 - \frac{29}{20160} z^6 - \frac{2753}{1814400} z^8 - \frac{57221}{53222400} z^{10} - \frac{41764193}{58118860800} z^{12}$$

$$b'_3 = \frac{1}{6} + \frac{1}{96} z^4 + \frac{11}{1920} z^6 + \frac{731}{201600} z^8 + \frac{68237}{29030400} z^{10} + \frac{41163389}{26824089600} z^{12}$$

$$G = 1 + \frac{1}{180} z^6 + \frac{11}{4480} z^8 + \frac{10411}{7257600} z^{10} + \frac{108551}{119750400} z^{12} + \frac{68305253}{116237721600} z^{14}$$

5. Numerical illustrations

In this section we will apply our method to three well known orbital problems. We are going to compare our results with other methods designed for solving second order ordinary differential equations. The methods used in the comparison have been denoted by:

- MRKN3: The new third-order MRKN method with three stages, derived in Section 4.
- RKN3: The classical third-order RKN method with three

stages from which we were using the coefficients .

- PL6RKN3: The third-order RKN method with phase lag of order six and zero amplification error of *van der Houwen and Sommeijer [1]*.
- EFRKN3: The fourth-order exponential fitted RKN method with three stages, of *J.M. Franco [2]* .

One way to measure the efficiency of the method is to compute the accuracy in the decimal digits, that is $-\log_{10}$ (maximum error through the integration intervals) versus the computational effort measured by the \log_{10} (number of function evaluations required). The problems are tested in the interval $[0, 1000]$.

Problem 1.(Orbit problem by Stiefel and Bettis [12])

$$\begin{aligned}
 y'' &= -y(t) + \epsilon \exp(it), \quad y(t) \in C \\
 y(0) &= 1, \quad y'(0) = (1 - \frac{1}{2}\epsilon)i,
 \end{aligned}$$

where $\epsilon = 0.001$

The analytical solution is

$$y(t) = \cos(t) + \frac{1}{2}\epsilon t \sin(t) + i[\sin(t) - \frac{1}{2}\epsilon t \cos(t)]$$

Problem 2.(Orbit problem by Franco and Palacios [11])

$$\begin{aligned}
 y'' &= -y(t) + \epsilon \exp(i\psi t), \\
 y(0) &= 1, \quad y'(0) = i,
 \end{aligned}$$

where $\epsilon = 0.001$ and $\psi = 0.01$

The analytical solution $y(t) = y_1(t) + iy_2(t)$ is given by:

$$\begin{aligned}
 y_1(t) &= \frac{1 - \epsilon - \psi^2}{1 - \psi^2} \cos(t) + \frac{\epsilon}{1 - \psi^2} \cos(\psi t), \\
 y_2(t) &= \frac{1 - \epsilon\psi - \psi^2}{1 - \psi^2} \sin(t) + \frac{\epsilon}{1 - \psi^2} \sin(\psi t)
 \end{aligned}$$

Problem 3.(Two-Body problem)

$$y''_1 = -\frac{y_1}{r^3}, \quad y''_2 = -\frac{y_2}{r^3}$$

where $r = \sqrt{y_1^2 + y_2^2}$,

$$y_1(0) = 1, \quad y'_1(0) = 0, \quad y_2(0) = 0, \quad y'_2(0) = 1.$$

The analytical solution is

$$y_1(t) = \cos(t) \text{ and } y_2(t) = \sin(t)$$

In the figures we display the efficiency curves, that is the accuracy versus the computational cost measured by the number of function evaluations required by each method.

Numerical results indicate that the new method derived in section 4 is much more accurate than the other methods.

More specifically the new method (MRKN3) is more accurate from the classical (RKN3) one by one decimal digit for the two-body problem and by three decimals for the rest two problems. Also the new RKN method remains more accurate than the PL6RKN3 by two decimals in all cases. Finally the new method has achieved better accuracy from the EFRKN4 method by two decimals for the two body problem and by three decimals for the rest two problems.

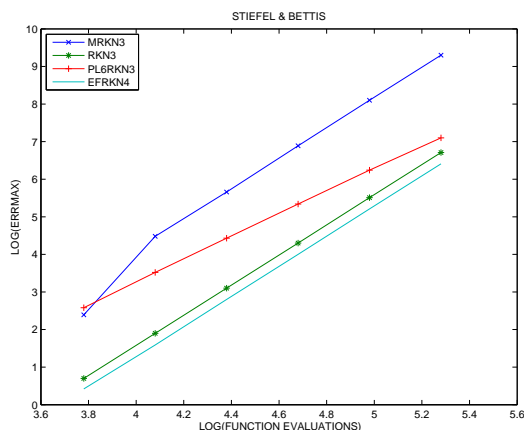


Figure 1 Efficiency for the Stiefel and Bettis Problem

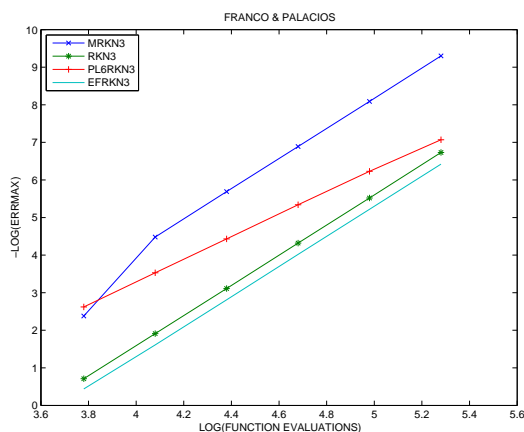


Figure 2 Efficiency for the Franco and Palacios Problem

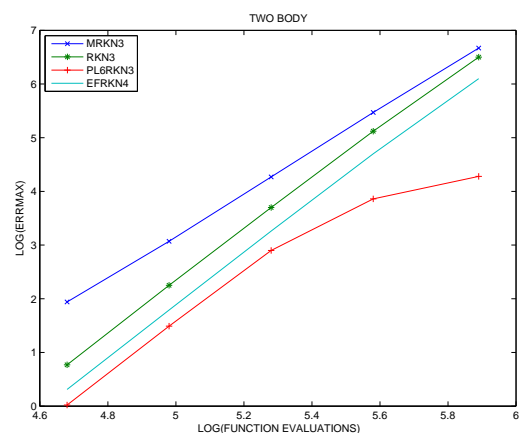


Figure 3 Efficiency for the Two Body Problem

6. Conclusions

The new modified RKN method, developed in this paper is much more efficient than all the other methods that take place, in any case. The new method remained more efficient for all the problems and in some cases was more accurate than the other methods up to three decimals.

References

- [1] P.J. van der Houwen, B.P. Sommeijer, Explicit Runge-Kutta-Nyström methods with reduced phase errors for computing oscillating solutions, *SIAM J. Numer. Anal.* 24 (1987) 595-617.
- [2] J.M. Franco, Exponentially fitted explicit Runge-Kutta-Nyström methods, *Journal of Computational and Applied Mathematics* 167 (2004) 1-19.
- [3] T. E. Simos, Jesu's Vigo Aguiar, A modified Runge-Kutta method with phase-lag of order infinity for the numerical solution of the Schrödinger equation and related problems, *Comput. Chem.* 25 (2001) 275-281.
- [4] T. E. Simos, A new Numerov-type method for the numerical solution of the Schrödinger equation, *J. Math. Chem.* 46 (2009) 9811007.
- [5] D.F. Papadopoulos, Z.A. Anastassi, T.E. Simos, A modified phase-fitted and amplification-fitted Runge-Kutta-Nyström method for the numerical solution of the radial Schrödinger equation, *J. Mol. Model.*, 16 (2010) 1339-1346.
- [6] D.F. Papadopoulos, T.E. Simos, A New Methodology for the Construction of Optimized Runge-Kutta-Nyström Methods, *J. of Modern Physics C*, 22 (2011) 623-634.
- [7] Ibraheem Alolyan and T.E. Simos, High algebraic order methods with vanished phase-lag and its first derivative for the numerical solution of the Schrödinger equation, *J. Math. Chem.* 48 (2010) 925-958.
- [8] Ibraheem Alolyan and T.E. Simos, A family of ten-step methods with vanished phase-lag and its first derivative for the numerical solution of the Schrödinger equation, *J. Math. Chem.* 49 (2011) 1843-1888.
- [9] Konguetsof A, A hybrid method with phase-lag and derivatives equal to zero for the numerical integration of the Schrödinger equation, *J. Math. Chem.* 49 (2011) 1330-1356.
- [10] A. A. Kosti, Z. A. Anastassi and T. E. Simos, An optimized explicit Runge-Kutta method with increased phase-lag order for the numerical solution of the Schrödinger equation and related problems, *J. Math. Chem.* 47 (2010) 315-330.
- [11] J.M. Franco and M. Palacios, High-order P-stable multistep methods, *Journal of Computational and Applied Mathematics*, 30(1) (1990) 110
- [12] E. Stiefel and D. G. Bettis, Stabilization of Cowell's method, *Numerische Mathematik*, 13(2) (1969) 154-175
- [13] A. Konguetsof and T.E. Simos, A generator of hybrid symmetric four-step methods for the numerical solution of the Schrödinger equation, *Journal of Computational and Applied Mathematics* 158(1) 93-106(2003)
- [14] Z. Kalogiratou, T. Monovasilis and T.E. Simos, Symplectic integrators for the numerical solution of the Schrödinger equation, *Journal of Computational and Applied Mathematics* 158(1) 83-92(2003)

- [15] Z. Kalogiratou and T.E. Simos, Newton-Cotes formulae for long-time integration, *Journal of Computational and Applied Mathematics* 158(1) 75-82(2003)
- [16] G. Psihoyios and T.E. Simos, Trigonometrically fitted predictor-corrector methods for IVPs with oscillating solutions, *Journal of Computational and Applied Mathematics* 158(1) 135-144(2003)
- [17] T.E. Simos, I.T. Famelis and C. Tsitouras, Zero dissipative, explicit Numerov-type methods for second order IVPs with oscillating solutions, *Num. Algor.* 34(1) 27-40(2003)
- [18] T.E. Simos, Dissipative trigonometrically-fitted methods for linear second-order IVPs with oscillating solution, *Appl. Math. Lett.* 17(5) 601-607(2004)
- [19] K. Tselios and T.E. Simos, Runge-Kutta methods with minimal dispersion and dissipation for problems arising from computational acoustics, *Journal of Computational and Applied Mathematics* Volume: 175(1) 173-181(2005)
- [20] D.P. Sakas and T.E. Simos, Multiderivative methods of eighth algebraic order with minimal phase-lag for the numerical solution of the radial Schrödinger equation, *Journal of Computational and Applied Mathematics* 175(1) 161-172(2005)
- [21] G. Psihoyios and T.E. Simos, A fourth algebraic order trigonometrically fitted predictor-corrector scheme for IVPs with oscillating solutions, *Journal of Computational and Applied Mathematics* 175(1) 137-147(2005)
- [22] Z. A. Anastassi and T.E. Simos, An optimized Runge-Kutta method for the solution of orbital problems, *Journal of Computational and Applied Mathematics* 175(1) 1-9(2005)
- [23] T.E. Simos, Closed Newton-Cotes trigonometrically-fitted formulae of high order for long-time integration of orbital problems, *Appl. Math. Lett.* 22 (10) 1616-1621(2009)
- [24] S. Stavroyiannis and T.E. Simos, Optimization as a function of the phase-lag order of nonlinear explicit two-step P-stable method for linear periodic IVPs, *Appl. Num. Math.* 59(10) 2467-2474(2009)
- [25] T.E. Simos, Exponentially and Trigonometrically Fitted Methods for the Solution of the Schrödinger Equation, *Acta Appl. Math.* 110(3) 1331-1352(2010)
- [26] T. E. Simos, New Stable Closed Newton-Cotes Trigonometrically Fitted Formulae for Long-Time Integration, *Abstract and Applied Analysis*, Volume 2012, Article ID 182536, 15 pages, 2012 doi:10.1155/2012/182536
- [27] T.E. Simos, Optimizing a Hybrid Two-Step Method for the Numerical Solution of the Schrödinger Equation and Related Problems with Respect to Phase-Lag, *Journal of Applied Mathematics*, Volume 2012, Article ID 420387, 17 pages, doi:10.1155/2012/420387, 2012
- [28] Z.A. Anastassi and T.E. Simos, A parametric symmetric linear four-step method for the efficient integration of the Schrödinger equation and related oscillatory problems, *Journal of Computational and Applied Mathematics* 236 38803889(2012)



Dimitris F. Papadopoulos

is presently employed as an Assistant Professor at Technological Educational Institute of Patras (Greece). He obtained his PhD from University of Peloponnese (GR) in 2010. His research area is numerical analysis and applied mathematics. He has published 12 (twelve) research articles in reputed in-

ternational journals and conferences of mathematical science.



Theodore E. Simos

is a Visiting Professor within the Distinguished Scientists Fellowship Program at the Department of Mathematics, College of Sciences, King Saud University, P. O. Box 2455, Riyadh 11451, Saudi Arabia and Professor at the Laboratory of Computational Sciences of the Department of Computer Science and Tech-

nology, Faculty of Sciences and Technology, University of Peloponnese, GR-221 00 Tripolis, Greece. He holds a Ph.D. on Numerical Analysis (1990) from the Department of Mathematics of the National Technical University of Athens, Greece. He is Highly Cited Researcher in Mathematics, Active Member of the European Academy of Sciences and Arts, Active Member of the European Academy of Sciences and Corresponding Member of European Academy of Sciences, Arts and Letters. He is Editor-in-Chief of three scientific journals and editor of more than 25 scientific journals. He is reviewer in several other scientific journals and conferences. His research interests are in numerical analysis and specifically in numerical solution of differential equations, scientific computing and optimization. He is the author of over 400 peer-reviewed publications and he has more than 2000 citations (excluding self-citations).