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Implicit third derivative Runge-Kutta-Nyström method with trigonometric coefficients

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Abstract The paper presents a trigonometrically-fitted implicit third derivative Runge-Kutta-Nystöm method (TTRKNM) whose coefficients depend on the frequency and stepsize for periodic initial value problems. The TTRKNM is a pair of methods which is obtained from its continuous version and applied to produce simultaneous approximations to the solution and its first derivative at each point in the interval of interest. A discussion of the stability property of the method is given. Numerical experiments are performed to demonstrate the accuracy and efficiency of the method.

Keywords Third derivative · Runge-Kutta-Nystöm method · Oscillatory initial value problems · Trigonometrically-fitted

Mathematics Subject Classification (2010) 65L05 · 65L06

1 Introduction

Although Second Order Differential Equations (DEs) can always be transformed into an equivalent first order system, second order DEs naturally arise in several areas of application, such celestial mechanics, circuit theory, control theory, chemical kinetics, astrophysics, and biology. Therefore, it is imperative to seek numerical techniques that can solve them directly. Initial value problems (IVPs) in which the first

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derivative does not appear explicitly are an important subclass of second order DEs; a vast number of which does not posses theoretical solutions. Thus, several numerical techniques for directly solving this subclass of IVPs has been proposed (see Lambert and Watson [20], Twizell and Khaliq [27], Ananthakrishnaiah [2], Simos [24], Hairer [11], Nörsett, and Wanner [10], Van der Houwen and Sommeijer [28], and Tsitouras [26]). In the case of direct solution for the general second order IVPs in which the first derivative does appear explicitly, fewer methods have been proposed (see Vigo-Aguiar and Ramos [29], Chawla and Sharma [4], Jator, [16], Mahmoud and Osman [18], and Awoyemi [3]). It turns out that some of these IVPs possess solutions with special properties that may be known in advance, taking advantage of when designing numerical methods.

A reasonable amount of attention has been focused on developing methods that take advantage of the special properties of the solution that may known in advance (see Coleman and Ixaru [6], Simos [23], Vanden et al. [30], Vigo-Aguiar et al. [33], Franco [9], Fang et al. [7], Nguyen et al. [21], Wua and Tian [34], Ramos and Vigo-Aguiar [31], Franco and Gomez [8], Kalogiratou [12], and Ozawa [22]). Nevertheless, most of these methods are restricted to solving special second order IVPs in step-by-step fashion.

In this paper, we propose a TTRKNM whose coefficients are functions of the frequency and the stepsize, which takes advantage of the special properties of the solution. For instance, when the frequency or a reasonable estimate of it is known in advance, the method performs better than the polynomial based methods. Moreover, the TTRKNM is applied as a pair of methods that simultaneously produce approximations to the solution and its first derivative at each point in the interval of interest (see Jator et al. [17] and Ngwane and Jator [19]). In this way, the method performs better than its predictor-corrector implementation as demonstrated in Section 5.2.

This paper is organized as follows. In Section 2, we derive the TTRKNM. The error and stability analysis of the TTRKNM are discussed in Section 3 and in Section 4 the implementation of the method is discussed. Numerical examples are given in Section 5 to show the accuracy and efficiency of the TTRKNM. Finally, we give some concluding remarks in Section 6.

2 Derivation of the TTRKNM

Consider the general second order IVP

$$y'' = f(x, y, y'), \quad y(x_0) = y_0, \; y'(x_0) = y'_0, \; x_0 \le x \le x_N, \tag{1}$$

where $f : \Re \times \Re^{2s} \to \Re^s$, $N > 0$ is an integer, and s is the dimension of the system. However, we assume the scalar form of (1) in the derivation process, since the proposed method can be applied to the system (1) by obvious notational modifications.

In what follows, we defined the TTRKNM as a pair of methods for the numerical integration of (1) by

$$y_{n+1} = y_n + hy'_n + h^2 \sum_{j=0}^{1} \beta_j f_{n+j} + h^3 \sum_{j=0}^{1} \gamma_j g_{n+j}, \tag{2}$$

$$hy'_{n+1} = hy'_n + h^2 \sum_{j=0}^{1} \beta'_j f_{n+j} + h^3 \sum_{j=0}^{1} \gamma'_j g_{n+j}, \tag{3}$$

where β_j, and γ_j, $j = 0, 1$ are continuous coefficients. We assume that y_{n+j} is the numerical approximation to the analytical solution $y(x_{n+j})$, y'_{n+j} is an approximation to $y'(x_{n+j})$,

$$f_{n+j} = f(x_{n+j}, y_{n+j}, y'_{n+j}), \quad g_{n+j} = g(x_{n+j}, y_{n+j}, y'_{n+j}),$$

$$g_{n+j} = \frac{df(x,\ y(x),\ y'(x))}{dx}|(_{x_{n+j},\ y_{n+j},\ y'_{n+j}}), \quad j = 0, 1.$$

In order to derive (2) and (3), we initially seek a continuous local approximation $U(x)$ on the interval $[x_n, x_{n+1}]$ of the form

$$U(x) = \alpha_0(x) y_n + \delta_0(x) hy'_n + h^2 \sum_{j=0}^{1} \beta_j(x) f_{n+j} + h^3 \sum_{j=0}^{1} \gamma_j(x) g_{n+j} \tag{4}$$

whose first derivative is given by

$$U'(x) = \frac{d}{dx} U(x) \tag{5}$$

where $\alpha_0(x)$, $\delta_0(x)$, $\beta_j(x)$, and $\gamma_j(x)$, $j = 0, 1$ are continuous coefficients. We assume that $y_{n+j} = U(x_n + jh)$ is the numerical approximation to the analytical solution $y(x_{n+j})$, $y'_{n+j} = U'(x_n + jh)$ is an approximation to $y'(x_{n+j})$, $f_{n+j} = U''(x_n + jh)$ is an approximation to $y''(x_{n+j})$, and $g_{n+j} = U'''(x_n + jh)$ is an approximation to $y'''(x_{n+j})$, $j = 0, 1$.

The construction of the continuous method (4) with(5) as a consequence is given in the following theorem:

Theorem 2.1 *Let* $P_j(x) = x^j, j = 0, \ldots, 3$, $P_4 = \sin(wx)$, $P_5 = \cos(wx)$ *be basis functions and* $V = (y_n, y'_n, f_n, f_{n+1}, g_n, g_{n+1})^T$ *a vector, where* T *is the transpose. Consider the matrices* W *defined as*

$$W = \begin{pmatrix} P_0(x_n) & \cdots & P_5(x_n) \\ P'_0(x_n) & \cdots & P'_5(x_n) \\ P''_0(x_n) & \cdots & P''_5(x_n) \\ P''_0(x_{n+1}) & \cdots & P''_5(x_{n+1}) \\ P'''_0(x_n) & \cdots & P'''_5(x_n) \\ P'''_0(x_{n+1}) & \cdots & P'''_5(x_{n+1}) \end{pmatrix}$$

and W_j obtained by replacing the j^{th} column of W by the vector V, and let the following conditions be satisfied

$$U\left(x_n\right)=y_n, \quad U'\left(x_n\right)=y_n' \tag{6}$$

$$U''\left(x_{n+j}\right)=f_{n+j}, \quad U'''\left(x_{n+j}\right)=g_{n+j}, j=0,1, \tag{7}$$

then, the continuous representations (4) and (5) are equivalent to the following:

$$U(x)=\sum_{j=0}^{5}\frac{\det(W_j)}{\det(W)}P_j(x), \tag{8}$$

$$U'(x)=\frac{d}{dx}\left(\sum_{j=0}^{5}\frac{\det(W_j)}{\det(W)}P_j(x)\right), \tag{9}$$

Proof The proof follows the approach given in Jator [16] with slight notational modifications. We begin the proof by requiring that the method (4) be defined by the assumed basis functions

$$\begin{cases} \alpha_0(x)=\sum_{i=0}^{5}\alpha_{i+1,0}P_i(x),\ \delta_0(x)=\sum_{i=0}^{5}h\delta_{i+1,0}P_i(x), \\ h^2\beta_j(x)=\sum_{i=0}^{5}h^2\beta_{i+1,j}P_i(x), \quad h^3\gamma_j(x)=\sum_{i=0}^{5}h^3\gamma_{i+1,j}P_i(x),\ j=0,1, \end{cases} \tag{10}$$

where $\alpha_{i+1,0},\ h\delta_{i+1,0},\ h^2\beta_{i+1,j}$, and $h^3\gamma_{i+1,j}$, are coefficients to be determined.

Substituting (10) into (4) we have

$$\begin{aligned} U(x) &= \sum_{i=0}^{5}\alpha_{i+1,0}P_i(x)y_n+\sum_{i=0}^{5}h\delta_{i+1,0}P_i(x)y_n' \\ &+\sum_{j=0}^{1}\sum_{i=0}^{5}h^2\beta_{i+1,j}P_i(x)f_{n+j}+\sum_{j=0}^{1}\sum_{i=0}^{5}h^3\gamma_{i+1,j}P_i(x)g_{n+j}, \end{aligned}$$

which is simplified to

$$\begin{aligned} U(x) &= \sum_{i=0}^{5}\{\alpha_{i+1,0}P_i(x)y_n+h\delta_{i+1,0}P_i(x)y_n'+\sum_{j=0}^{1}h^2\beta_{i+1,j}P_i(x)f_{n+j} \\ &+\sum_{j=0}^{1}h^3\gamma_{i+1,j}P_i(x)g_{n+j}\}, \end{aligned}$$

and expressed as

$$U(x)=\sum_{i=0}^{5}\ell_iP_i(x), \tag{11}$$

where

$$\begin{aligned} \ell_i &= \alpha_{i+1,0}P_i(x)y_n+h\delta_{i+1,0}P_i(x)y_n'+\sum_{j=0}^{1}h^2\beta_{i+1,j}P_i(x)f_{n+j} \\ &+\sum_{j=0}^{1}h^3\gamma_{i+1,j}P_i(x)g_{n+j}. \end{aligned}$$

By imposing conditions (6) and (7) on (11), we obtain a system of six equations, which can be expressed as

$$WL=V,$$

where $L = (\ell_0, \ell_1, \ldots, \ell_5)^T$ is a vector of six undetermined coefficients.

We then proceed to determining the elements of L via Cramer's Rule. Thus,

$$\ell_j = \frac{\det(W_j)}{\det(W)}, \, j = 0, 1, \ldots, 5,$$

where W_j is obtained by replacing the j^{th} column of W by V. In order to obtain our continuous approximation, we use the newly found elements of L to rewrite (11) as

$$U(x) = \sum_{j=0}^{5} \frac{\det(W_j)}{\det(W)} P_j(x),$$

whose first derivative is given by

$$U'(x) = \frac{d}{dx}\left(\sum_{j=0}^{5} \frac{\det(W_j)}{\det(W)} P_j(x)\right).$$

The proof is complete. □

The methods (2) and (3) are specified by evaluating (8) and (9) at $x = x_{n+1}$. That is, $y_{n+1} = U(x_n + h)$ and $y'_{n+1} = U'(x_n + h)$ yield methods (2) and (3) whose coefficients and their corresponding Taylor series equivalence are given as follows:

$$\begin{cases} \beta_{1,0} = \frac{(6u\cos(u/2)+2u^3\cos(u/2)-12\sin(u/2)-3u^2\sin(u/2))}{6u^2(u\cos(u/2)-2\sin(u/2))} \\ \quad = \frac{7}{20} + \frac{u^2}{8400} + \frac{u^4}{756000} + \frac{37u^6}{2328480000} + \frac{59u^8}{302702400000} + \frac{2753u^{10}}{1144215072000000} + \ldots, \\ \beta_{1,1} = \frac{(-6u\cos(u/2)+u^3\cos(u/2)+12\sin(u/2)-3u^2\sin(u/2))}{6u^2(u\cos(u/2)-2\sin(u/2))} \\ \quad = \frac{3}{20} - \frac{u^2}{8400} - \frac{u^4}{756000} - \frac{37u^6}{2328480000} - \frac{59u^8}{302702400000} - \frac{2753u^{10}}{1144215072000000} + \ldots, \\ \gamma_{1,0} = \frac{(-12u\csc(u/2)-u^3\csc(u/2)+12u\cos(u)\csc(u/2)-2u^3\cos(u)\csc(u/2)+9u^2\csc(u/2)\sin(u))}{12u^3(u\cos(u/2)-2\sin(u/2))} \\ \quad = \frac{1}{20} + \frac{19u^2}{25200} + \frac{13u^4}{756000} + \frac{109u^6}{258720000} + \frac{28703u^8}{2724321600000} + \frac{303689u^{10}}{1144215072000000} + \ldots, \\ \gamma_{1,1} = \frac{(2u^3\csc(u/2)+u^3\cos(u)\csc(u/2)-3u^2\csc(u/2)Sin(u))}{12u^3(u\cos(u/2)-2\sin(u/2))} \\ \quad = -\frac{1}{30} - \frac{u^2}{1575} - \frac{u^4}{63000} - \frac{59u^6}{145530000} - \frac{7043u^8}{681080400000} - \frac{12539u^{10}}{47675628000000} + \ldots, \end{cases} \tag{12}$$

$$
\begin{cases}
\beta'_{1,0} = \frac{(3u^3\cos(u/2)-6u^2\sin(u/2))}{6u^2(u\cos(u/2)-2\sin(u/2))} \\
\quad = \frac{1}{2} \\
\beta'_{1,1} = \frac{(3u^3\cos(u/2)-6u^2\sin(u/2))}{6u^2(u\cos(u/2)-2\sin(u/2))} \\
\quad = \frac{1}{2} \\
\gamma'_{1,0} = \frac{(-12u\csc(u/2)-3u^3\csc(u/2)+12u\cos(u)\csc(u/2)-3u^3\cos(u)\csc(u/2)+12u^2\csc(u/2)\sin(u))}{12u^3(u\cos(u/2)-2\sin(u/2))} \\
\quad = \frac{1}{12} + \frac{u^2}{720} + \frac{u^4}{30240} + \frac{u^6}{1209600} + \frac{u^8}{47900160} + \frac{691u^{10}}{1307674368000} + \ldots, \\
\gamma'_{1,1} = \frac{(12u\csc(u/2)+3u^3\csc(u/2)-12u\cos(u)\csc(u/2)+3u^3\cos(u)\csc(u/2)-12u^2\csc(u/2)\sin(u))}{12u^3(u\cos(u/2)-2\sin(u/2))} \\
\quad = -\frac{1}{12} - \frac{u^2}{720} - \frac{u^4}{30240} - \frac{u^6}{1209600} - \frac{u^8}{47900160} - \frac{691u^{10}}{1307674368000} + \ldots,
\end{cases}
\tag{13}
$$

where $u = wh$ and w is the frequency.

Remark 2.2 We note that when $u \to 0$ the trigonometric coefficients given by (10) and (11) are vulnerable to heavy cancelations and hence the coefficients of the corresponding Taylor series expansion must be used (see Simos [16]).

3 Error analysis and stability

3.1 Local truncation error

We define the local truncation errors (LTEs) of (2) and (3) specified by the coefficients (12) and (13) as

$$
\aleph_1[y(x_n); h] = y(x_n + h) - y_n - hy'_n - h^2 \sum_{j=0}^{1} \beta_j y''(x_n + jh) - h^3 \sum_{j=0}^{1} \gamma_j y'''(x_n + jh),
$$

$$
\aleph_2[y(x_n); h] = hy'(x_n + h) - hy'_n - h^2 \sum_{j=0}^{1} \beta'_j y''(x_n + jh) - h^3 \sum_{j=0}^{1} \gamma'_j y'''(x_n + jh).
$$

Assuming that $y(x)$ is sufficiently differentiable, we can expand the terms in $\aleph_1$ and $\aleph_2$ as a Taylor series about the point x_n to obtain the expressions for the LTEs as

$$
\aleph_1[y(x_n); h] = \frac{h^6}{1440}(w^2 y^{(4)}(x_n) + y^{(6)}(x_n)) + O(h^7). \tag{14}
$$

$$
\aleph_2[y(x_n); h] = \frac{h^6}{720}(w^2 y^{(4)}(x_n) + y^{(6)}(x_n)) + O(h^7). \tag{15}
$$

Remark 3.1 The TTRKNM reduces to a polynomial based method as $u \to 0$.

3.2 Stability

The methods (2) and (3) specified by the coefficients (10) and (11) are combined to give the TTRKNM, which is expressed as

$$A^{(0)}Y_{\mu} = A^{(1)}Y_{\mu-1} + h^2(B^{(1)}F_{\mu-1} + B^{(0)}F_{\mu}), \tag{16}$$

where $Y_{\mu},\ F_{\mu},\ Y_{\mu-1},\ F_{\mu-1},\ \mu = 1,\dots,N,\ n = 1,2,\dots,N$ are given as $Y_{\mu} = (y_{n+1}, hy'_{n+1})^T$, $F_{\mu} = (f_{n+1}, hg_{n+1})^T$, $Y_{\mu-1} = (y_n, hy'_n)^T$, $F_{\mu-1} = (f_n, hg_n)^T$, $A^{(i)}$, $B^{(i)}$, $i = 0, 1$ are 2×2 matrices whose entries are given by the coefficients of the methods (2) and (3).

The linear-stability of the TTRKNM is discussed by applying the method to the test equation $y'' = -\lambda^2 y$, where λ is a real constant (see [6]). Letting $\Upsilon = \lambda h$, it is easily shown as in [5] that the application of (16) to the test equation yields

$$Y_{\mu} = M(\Upsilon^2; u)Y_{\mu-1}\ ,\ M(\Upsilon^2; u) := (A^{(0)} + \Upsilon^2 B^{(0)})^{-1}(A^{(1)} - \Upsilon^2 B^{(1)}), \tag{17}$$

where the matrix $M(\Upsilon^2; u)$ is the amplification matrix which determines the stability of the method. In the spirit of [5], the eigenvalues of $M(\Upsilon^2; u)$ are the roots of the characteristics equation

$$\rho^2 - 2\Gamma(\Upsilon^2; u)\rho + \Theta(\Upsilon^2; u) = 0, \tag{18}$$

where $\Gamma(\Upsilon^2; u) = \frac{1}{2}\ trace\ M(\Upsilon^2; u)$ and $\Theta(\Upsilon^2; u) = det\ M(\Upsilon^2; u)$ are rational functions.

Definition 3.2 A region of stability is a region in the $q - u$ plane, throughout which $|\rho(\Upsilon^2; u)| \leq 1$, where $|\rho(\Upsilon^2; u)|$ is the spectral radius of $M(\Upsilon^2; u)$ (see [6]).

We note that the periodicity condition is given by $\Theta(\Upsilon^2; u) = 1$, in which case, $\Gamma(\Upsilon^2; u)$ is the stability function and (18) becomes

$$\rho^2 - 2\Gamma(\Upsilon^2; u)\rho + 1 = 0. \tag{19}$$

Definition 3.3 Let $\Gamma(\Upsilon^2; u)$ be the stability function, we then define the interval of periodicity as the largest interval $(0, h_0)$ such that $|\Gamma(\Upsilon^2; u)| < 1$ for all steplengths $h\epsilon(0, h_0)$. Suppose h_0 is finite, and $|\Gamma(\Upsilon^2; u)| < 1$ also holds for $h\epsilon(\eta_1, \eta_2)$, for $\eta_1 > h_0$, then, (η_1, η_2) is the secondary interval of periodicity (see [5]).

Remark 3.4 It is observed that in the $q - u$ plane the TTRKNM is stable for $q \ \epsilon\ [0, 55.59]$ and $u \ \epsilon\ [-\pi, \pi]$ (see Fig.1). The stability region is also confirmed numerically as demonstrated in Table 5. However, the TTRKNM has a primary interval of periodicity for $q \ \epsilon\ (0, 9.87)$ and a secondary interval of periodicity for $q \ \epsilon\ ([0, 55.59)$ for $u \ \epsilon\ [-2.6, 2.6]$.

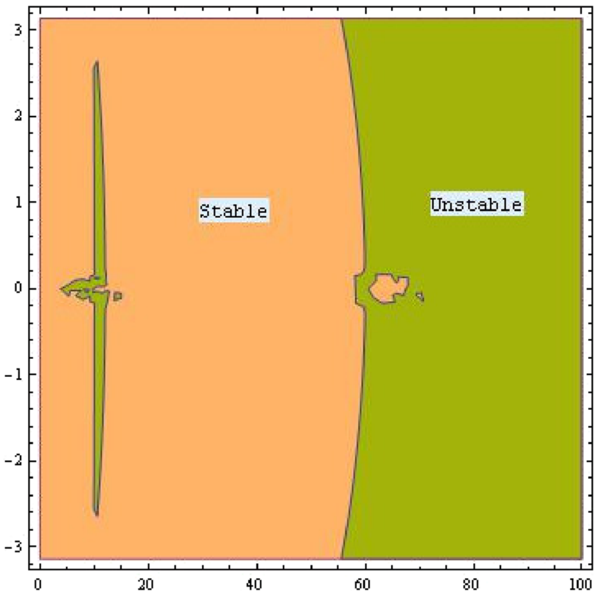

Fig. 1 The stability region for the TTRKNM plotted in the (q, u)-plane

4 Implementation of the TTRKNM

4.1 Block approach

The TTRKNM was implemented in a block-by-block fashion using a code written in Mathematica 9.0 enhanced by the feature $NSolve[\ \ ]$ for linear problems, while nonlinear problems were solved by the Newton's method enhanced by the feature $FindRoot[\ ]$ (see Keiper and Gear [13]). It is vital to note that Mathematica can symbolically compute derivatives, hence the entries of the Jacobian matrix which involve the partial derivatives of both f and g are automatically generated. In particular, the TTRKNM (14) is applied to (1) on the range of interest as follows:

- Choose $N,\ h = (b-a)/N$; using (14), $n = 1,\ \mu = 1$, the values of $(y_1, y_1')^T$ are simultaneously obtained over the sub-interval $[x_0, x_1]$, as y_0 and y_0' are known from the IVP (1).
- For $n = 2,\ \mu = 2$, the values of $(y_2, y_2')^T$ are simultaneously obtained over the sub-interval $[x_1, x_2]$, as y_1 and y_1' are known from the previous block.
- The process is continued for $n = 3, \ldots, N$ and $\mu = 3, \ldots, N$ to obtain the numerical solution to (1) on sub-intervals $[x_2, x_3], \ldots, [x_{N-1}, x_N]$.

4.2 Predictor-corrector approach

The TTRKNM was also implemented in a predictor-corrector mode in which on the partition Γ_N, an approximation is obtained at x_{n+1} only after an approximation at

x_n has been computed, where $\digamma_N : a = x_0 < x_1 < \ldots < x_N = b, \quad x_{n+1} = x_n + h, n = 0, \ldots, N-1$. In order to facilitate this implementation, we use the explicit versions of (2) and (3) as predictors, which are defined as follows:

$$\begin{cases} y_{n+1} = y_n + hy'_n + \frac{1-\cos(hw)}{w^2}(u) f_n + \frac{hw-Sin[hw]}{w^3} g_n, \\ hy'_{n+1} = hy'_n + \frac{h\sin(hw)}{w}(u) f_n + \frac{h-h\cos(hw))}{w^2} g_n. \end{cases} \tag{20}$$

5 Numerical examples

In this section, we have tested the TTRKNM on some numerical examples using a constant stepsize to illustrate its accuracy and efficiency. In particular, we have demonstrated the superiority of the block form by implementing the TTRKNM both in the block-mode and predictor-corrector mode. We have included a test problem which is traditionally used in the literature to discuss stability to validate the fact that the TTRKNM has a moderately large stability region. We have calculated the absolute error of the approximate solution as $Err = |y(x_N) - y_N|$. It is worth noting that the number of function evaluations (NFEs) per step involved in implementing the TTRKNM in block-mode is two, while its predictor-corrector mode implementation requires four function evaluations per step due to the introduction of the predictor as discussed in Section 5.2.

Example 5.1 We consider the following inhomogeneous IVP by Simos [23].

$$y'' = -100y + 99\sin(x), \ \ y(0) = 1, \ \ y'(0) = 11, \ \ x \in [0, 1000]$$

where the analytic solution is given by

$$\text{Exact} : y(x) = \cos(10x) + \sin(10x) + \sin(x).$$

The exponentially-fitted method in Simos [23] is of fourth order and hence comparable to the fourth order TTRKNM. It is obvious from Table 1 that TTRKNM is more

Table 1 Results, with $\omega = 10$, for Example 5.1

TTRKNM			Simos [23]	
N	Err	NFEs	Err	NFEs
1000	5.4×10^{-4}	2002	1.4×10^{-1}	8000
2000	1.9×10^{-4}	4002	3.5×10^{-2}	16000
4000	5.4×10^{-6}	8002	1.1×10^{-3}	32000
8000	3.0×10^{-7}	16002	8.4×10^{-5}	64000
16000	1.8×10^{-8}	32002	5.5×10^{-6}	128000
32000	5.2×10^{-10}	64002	3.5×10^{-7}	256000

Table 2 Results, with $\omega = 1.01$, for Example 5.2

TTRKNM		Simos		Ixaru et al.	
N	Err	N	Err	N	Err
150	3.6×10^{-3}	150	–	150	–
300	1.3×10^{-6}	300	1.7×10^{-3}	300	1.1×10^{-3}
600	2.4×10^{-6}	600	1.9×10^{-4}	600	5.4×10^{-5}
1200	1.7×10^{-7}	1200	1.4×10^{-5}	1200	1.9×10^{-6}
2400	1.1×10^{-8}	2400	8.7×10^{-7}	2400	6.2×10^{-8}

accurate and requires fewer NFEs than the method in [23]. Hence, for this example, TTRKNM is superior in terms accuracy and efficiency.

Example 5.2 We consider the nonlinear Duffing equation which was also solved by Simos [23] and Ixaru and Vanden Berghe [15].

$$y'' + y + y^3 = B\cos(\Omega x),\ \ y(0) = C_0,\ \ y'(0) = 0.$$

The analytic solution is given by

$$\text{Exact}: y(x) = C_1\cos(\Omega x) + C_2\cos(3\Omega x) + C_3\cos(5\Omega x) + C_4\cos(7\Omega x),$$

where $\Omega = 1.01$, $B = 0.002$, $C_0 = 0.200426728069$, $C_1 = 0.200179477536$, $C_2 = 0.246946143 \times 10^{-3}$, $C_3 = 0.304016 \times 10^{-6}$, $C_4 = 0.374 \times 10^{-9}$. We choose $\omega = 1.01$

We compare the end-point global errors for TTRKNM with the fourth order methods in Simos [23] and Ixaru et al. [15]. It is obvious from Table 2 that the errors produced by TTRKNM are smaller than those given in Simos [23] and Ixaru et al. [15]. Hence, for this example, the TTRKNM is superior in terms of accuracy.

Table 3 Results, with $\omega = 1,\ e = 0.005$, for Example 5.3

TTRKNM		FESDIRK4(3)		ESDIRK4(3)	
N	Err	N	Err	N	Err
150	4.1×10^{-3}	170	2.866×10^{-1}	277	2.153×10^{0}
200	1.2×10^{-3}	225	7.846×10^{-3}	496	1.494×10^{-1}
300	6.2×10^{-5}	381	1.399×10^{-3}	884	9.359×10^{-3}
600	2.7×10^{-7}	680	1.690×10^{-4}	1573	6.200×10^{-4}
800	2.7×10^{-8}	1207	1.846×10^{-5}	2796	4.416×10^{-5}
1600	1.1×10^{-10}	2144	1.938×10^{-6}	4970	3.412×10^{-6}
2400	4.3×10^{-12}	3806	1.993×10^{-7}	8833	2.848×10^{-7}
3200	4.3×10^{-15}	6762	2.021×10^{-8}	15706	2.530×10^{-8}

Table 4 Results, with $\omega = 4$, for Example 5.4

TIRK3		RADAU5		EFRK43		TTRKNM	
NFEs	Err	NFEs	Err	NFEs	Err	NFEs	Err
907	2.5×10^{-4}	853	2.2×10^{-4}	2057	3.7×10^{-4}	804	6.6×10^{-5}
1288	6.6×10^{-6}	1208	4.4×10^{-4}	1715	3.0×10^{-4}	1204	1.3×10^{-5}
1682	7.0×10^{-6}	1639	6.0×10^{-6}	3079	2.7×10^{-5}	1604	4.1×10^{-6}

Example 5.3 Consider the given two-body problem which was solved by Ozawa [22].

$$y_1'' = -\frac{y_1}{r^3},\ y_2'' = -\frac{y_2}{r^3},\ r = \sqrt{y_1^2 + y_2^2},$$

$$y_1(0) = 1 - e,\ y_1'(0) = 0,\ y_2(0) = 0,\ y_2'(0) = \sqrt{\frac{1+e}{1-e}},\ x\epsilon[0, 50\pi],$$

where $e,\ 0 \le e < 1$ is an eccentricity. The exact solution of this problem is

$$\text{Exact}: y_1(x) = \cos(k) - e,\ y_2(x) = \sqrt{1-e^2}\sin(k),$$

where k is the solution of the Kepler's equation $k = x + e\sin(k)$. We choose $\omega = 1$.

In Table 3, we compare the results obtained using the TTRKNM to those obtained via the explicit singly diagonally implicit Runge-Kutta (ESDIRK) and the functionally fitted ESDIRK (FESDIRK) methods given in Ozawa [22]. It is obvious from Table 3 that the TTRKNM performs better than those in Ozawa [22] in terms of accuracy.

Example 5.4 We consider the nonlinear system of second order IVP (see [21])

$$y_1'' = (y_1 - y_2)^3 + 6368y_1 - 6384y_2 + 42\cos(10x), \quad y_1(0) = 0.5,\ y_1'(0) = 0,$$

$$y_1'' = -(y_1 - y_2)^3 + 12768y_1 - 12784y_2 + 42\cos(10x), \quad y_2(0) = 0.5,\ y_2'(0) = 0,\ x\epsilon[0, 10],$$

with exact solution $y_1(x) = y_2(x) = \cos(4x) - \cos(4x)/2$.

Table 5 Results, with $\omega = 1$, for Example 5.5

$N = 203(q \in [0, 59.88])$		$N = 202(q \ni [0, 59.88])$
x	Err	Err
5.0	5.0×10^{-13}	2.0×10^{-12}
10.0	5.7×10^{-12}	3.1×10^{-11}
15.0	2.5×10^{-12}	5.3×10^{-9}
20.0	8.3×10^{-12}	7.4×10^{-7}
25.0	9.8×10^{-12}	1.2×10^{-4}
30.0	5.5×10^{-12}	1.7×10^{-2}

Table 6 Results, with $\omega = 1$, for Example 5.6

RK4			TTRKNM	
N	NFEs	Err	NFEs	Err
8	64	5.7×10^{-4}	9	1.4×10^{-4}
16	128	2.2×10^{-4}	17	1.7×10^{-5}
32	256	1.8×10^{-5}	33	1.2×10^{-6}
64	512	1.3×10^{-6}	65	7.9×10^{-8}
128	1024	8.4×10^{-8}	129	5.0×10^{-9}

This problem was chosen to demonstrate the performance of the TTRKNM on a nonlinear system. The accuracy and efficiency of the TTRKNM are measured by the end-point global errors for the y-component and the corresponding NFEs used. The results obtained using the TTRKNM are displayed in Table 4 and compare with those given in [21]. It is seen from Table 4 that TTRKNM performs generally better than those in [21] in terms of accuracy and efficiency.

Example 5.5 We consider the stiff second order IVP (see [1])

$$y_1'' = (\varepsilon - 2)y_1 + (2\varepsilon - 2)y_2, \quad y_2'' = (1 - \varepsilon)y_1 + (1 - 2\varepsilon)y_2,$$

$$y_1(0) = 2,\ y_1'(0) = 0, \quad y_2(0) = -1,\ y_2'(0) = 0\ ,\ \varepsilon = 2500,\ x\epsilon\ [0, 10\pi].$$

$y_1(x) = 2\cos x, \quad y_2(x) = -\cos x$, where ε is an arbitrary parameter and $w = 1$.

This problem was chosen to justify the stability of the TTRKNM. The method is stable when $q \in [0, 59.88]$ and $u \in [-\pi, \pi]$. In Table 5, we give the absolute errors at selected values of x, which indicate that choosing $N = 203$, the method is stable since for this value of N, $q \in [0, 59.88]$. However, for $N = 202$, $q \ni [0, 59.88]$, hence the method becomes unstable.

5.1 Problems where y' appears explicitly.

In this subsection, we show that the TTRKNM is applicable to problems where y' appears explicitly.

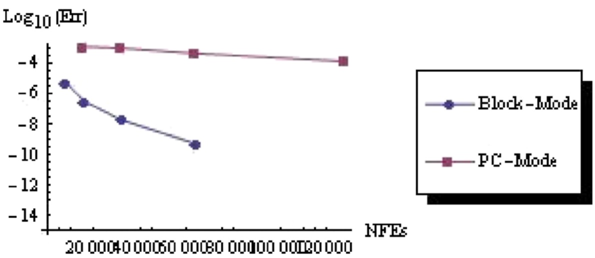

Fig. 2 Efficiency curves for Example 5.1

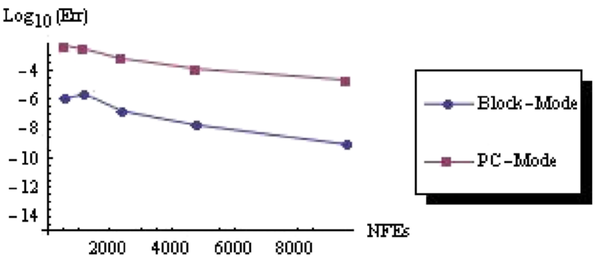

Fig. 3 Efficiency curves for Example 5.2

Example 5.6 We consider the given Bessel's IVP solved on [1, 8] (see Vigo-Aguiar and Ramos[33]).

$$x^2y'' + xy' + (x^2 - 0.25)y = 0, \quad y(1) = \sqrt{\frac{2}{\pi}}\sin 1 \simeq 0.6713967071418031,$$

$$y'(1) = (2\cos 1 - \sin 1)/\sqrt{2\pi} \simeq 0.0954005144474746.$$

$$\text{Exact} : y(x) = J_{1/2}(x) = \sqrt{\frac{2}{\pi x}}\sin x$$

The theoretical solution at $x = 8$ is $y(8) = \sqrt{\frac{2}{8\pi}}\sin(8) \simeq 0.2790927891080 58969$ and we choose $w = 1$.

This problem was chosen to demonstrate the performance of the TTRKNM on a general second order IVP with variable coefficients. It was solved using the fourth-order Runge-Kutta method (RK4) and TTRKNM. We have chosen to compare these methods because their orders are the same. It is obvious from Table 6 that TTRKNM performs better than the RK4 method in terms of accuracy (smaller errors) and is more efficient (smaller NFEs).

5.2 Block versus predictor-corrector implementations

In order to demonstrate the superiority of the Block implementation of the TTRKNM over its predictor-corrector implementation, we have used the two techniques to solve

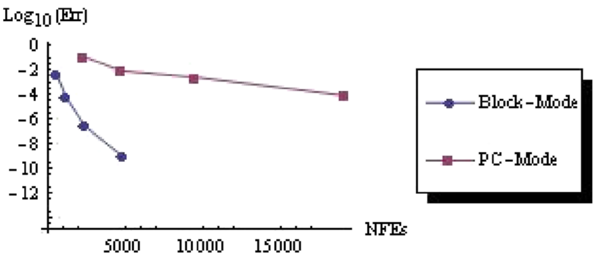

Fig. 4 Efficiency curves for Example 5.3

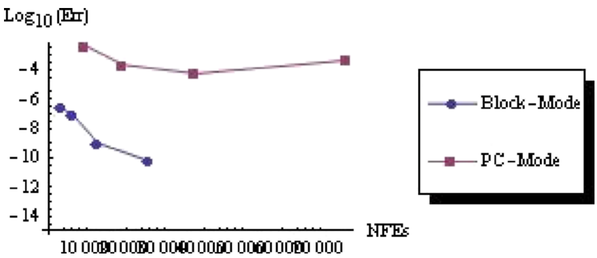

Fig. 5 Efficiency curves for Example 5.4

examples 5.1, 5.2, 5.3, 5.4, 5.6 and the results are displayed in Figs. 2, 3, 4, 5, 6. We note that example 5.5 is excluded since it is primarily included in the examples to demonstrated the stability of the TTRKNM.

It is noticed from Figs. 2–6 that the block-implementation (Block-Mode) of the TTRKNM is superior to its implementation in the predictor-corrector mode (PC-Mode).

5.3 TTRKNM versus fourth-order standard Runge-Kutta-Nystöm method (N4) given in Sommeijer [25]

In this subsection, the TTRKNM is compared to N4 given in [25], since the two methods are of the same order and use two function evaluations per step. It is observed the TTRKNM is more accurate than N4. The details of the numerical results are in given in Tables 7,8, 9,10, 11.

Example 5.7 We consider the following IVP taken from [25].

$$y'' + 25y + 100\cos(5x), \quad y(0) = 1, \quad y'(0) = 5, \quad x \in [0, 10]$$

where the analytic solution is given by

$$\text{Exact}: y(x) = \cos(5x) + \sin(5x) + 10x\sin(5x).$$

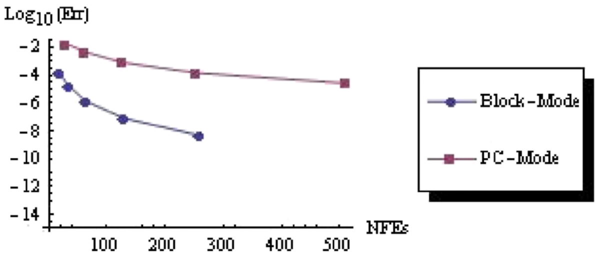

Fig. 6 Efficiency curves for Example 5.6

Table 7 Results, with $\omega = 5$, for Example 5.7

	TTRKNM			N4
N	Err	NFEs	Err	NFEs
200	1.4×10^{-4}	402	1.1×10^{-1}	400
400	8.9×10^{-6}	802	1.3×10^{-2}	800
800	5.6×10^{-7}	1602	1.5×10^{-3}	1600
1600	1.8×10^{-8}	3202	1.9×10^{-4}	3200
3200	2.1×10^{-9}	6402	2.3×10^{-5}	6400

Table 8 Results, with $\omega = 10$, for Example 5.1

	TTRKNM				N4
N	Err	NFEs	N	Err	NFEs
1000	5.4×10^{-4}	2002	8000	1.3×10^{0}	16000
2000	1.9×10^{-4}	4002	16000	1.3×10^{0}	32000
4000	5.4×10^{-6}	8002	32000	1.3×10^{0}	64000
8000	3.0×10^{-7}	16002	64000	9.0×10^{-1}	128000
16000	1.8×10^{-8}	32002	128000	4.1×10^{-2}	256000
32000	5.2×10^{-10}	64002	256000	5.2×10^{-3}	512000

Table 9 Results, with $\omega = 1.01$, for Example 5.2

TTRKNM		N4	
N	Err	N	Err
150	3.6×10^{-3}	600	5.9×10^{-2}
300	1.3×10^{-6}	1200	8.0×10^{-3}
600	2.4×10^{-6}	2400	1.0×10^{-3}
1200	1.7×10^{-7}	4800	1.3×10^{-4}
2400	1.1×10^{-8}	9600	1.6×10^{-5}

Table 10 Results, with $\omega = 1,\ e = 0.005$, for Example 5.3

TTRKNM		N4	
N	Err	N	Err
200	1.2×10^{-3}	800	1.4×10^{0}
300	6.2×10^{-5}	1600	1.2×10^{-1}
600	2.7×10^{-7}	3200	1.2×10^{-3}
800	2.7×10^{-8}	6400	2.1×10^{-4}
1600	1.1×10^{-10}	12800	6.8×10^{-5}
2400	4.3×10^{-12}	25600	1.8×10^{-5}
3200	4.3×10^{-15}	51200	4.6×10^{-6}

Table 11 Results, with $\omega = 4$, for Example 5.4

N4		TTRKNM	
NFEs	Err	NFEs	Err
1200	2.5×10^{-1}	804	6.6×10^{-5}
1600	1.4×10^{-4}	1204	1.3×10^{-5}
2400	4.1×10^{-5}	1604	4.1×10^{-6}

5.4 Estimating the frequency

A classical procedure for estimating the frequency is not available, however, some techniques for estimating the frequency are given in [14, 32]. A preliminary testing indicates that a good estimate of the frequency can be obtained by demanding that $LTE(2) = 0$, and solving for the frequency. In particular, solve for ω given that

$$\frac{h^6}{1440}(w^2 y^{(4)}(x_n) + y^{(6)}(x_n)) = 0,$$

$$\frac{h^6}{1440} D^4(w^2 + D^2)y = 0,$$

where $y^{(j)} = \frac{d^j y}{dx^j}$, $j = 4, 6$ are j^{th} derivative, $D = \frac{d}{dx}$ is a differential operator, and w is assumed to be a constant. We estimate the frequency by imposing that

$$(w^2 + D^2)y = 0, \tag{21}$$

and solving for w at $x = x_n$. We implemented this procedure on example 4.2 and obtained $w = 10$ which is in agreement with the known frequency. Hence, this procedure is interesting and will be the subject of our future research.

6 Conclusions

We have proposed a TTRKNM which is self-starting, accurate, and efficient. It is implemented without the use of predictors and has a moderately large region of stability. Details of the numerical results are displayed in Tables 1–5. The superiority of the block implementation over its predictor-corrector implementation is demonstrated computationally as given in Figs. 2–6. Our future research will be focused on developing methods equipped with a strategy for estimating unknown frequencies.

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