An adaptive optimized Runge-Kutta-Nyström method for second-order IVPs

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Abstract

This research paper is concerned with developing, analyzing, and implementing an adaptive optimized one-step block Nyström method for solving second-order initial value problems of ODEs and time-dependent partial differential equations. The new technique is developed through a collocation method with a new approach for selecting the collocation points. An embedding-like procedure is used to estimate the error of the proposed optimized method. The current approach has produced approximate solutions to real-world oscillatory, periodic and stiff application problems. The numerical experiments demonstrate that the introduced error estimation and stepsize control strategy presented in this manuscript has produced a good performance compared with some of the other existing numerical methods.

Keywords: Ordinary and time-dependent partial differential equations, optimized block Nyström method, variable stepsize formulation, error estimation and control, collocation method.

1. Introduction

Second-order ordinary differential equations (ODEs) are widely used to model real-world problems in engineering, control theory, physics, economics, physical and social sciences, etc. In this article, we consider problems of the form

$$\begin{aligned} y''(x) &= f(x, y(x), y'(x)), \\ & \quad y(a) = y_0,\ y'(a) = y'_0, x \in [a, b] \subset \mathbb{R}, y, f \in \mathbb{R}^d, \end{aligned} \tag{1}$$

where $a = x_0$ stands for the initial point, b, y_0, y'_0 are given, and f is assumed to be a continuous function that fulfils the Lipchitz's condition that guarantees the existence and uniqueness theorem in [1]. It is noteworthy to mention that a Vander Pol, Kepler's, Bessel, highly stiff oscillatory, simple harmonic and critically damped motion, and other similar problems can be written in the form of (1).

Many existing numerical methods for solving the class of problem in (1) have been analyzed; see for example [2] - [12]. Those strategies include Runge-Kutta type, linear multistep, Numerov-type, P-stable Obrechkoff, or collocation methods. One standard approach is to transform problem (1) to an equivalent system of first-order ODEs. Then the resulting system of equations is solved using suitable methods for first-order ODEs (see [13] and [14]).

In order to enhance the previously mentioned techniques, scholars like Kalogiratou et al. [15], Areo and Rufai ([16]), Ramos and Rufai [17], Amodio and Brugnano [18], and Ramos et al. [19] have derived and implemented block methods for solving the IVP (1) directly. The advantage of block methods over the Runge-Kutta type and predictor-corrector methods is that they can be less expensive regarding the number of functions evaluated and CPU time.

In this paper, we introduce a new optimized Runge-Kutta Nyström method (ORKNM) with an associated embedded method for error estimation, which makes it suitable for a variable stepsize implementation. The obtained adaptive form of the ORKNM is applied to solve directly problems defined in (1) and its special type in which the function f does not depend on $y'(x)$.

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2. Derivation of the method

Let $h > 0$ be the integration stepsize and $x_1 = x_0 + h$. Following the approach in [21], we assume that the exact solution of the IVP in (1) on $[x_0, x_1]$, is approximated by a polynomial $u(x_0 + sh)$, $s \in [0, 1]$ of degree seven, satisfying the collocation conditions $u''(x_0 + c_j h) = f_{c_j}$, where $c_0 = 0 < c_1 < c_2 < c_3 < c_4 < c_5 = 1$, $x_{c_j} = x_0 + c_j h$, $j = 1(1)4$, and $f_{c_j} = f(x_{c_j}, u(x_{c_j}), u'(x_{c_j}))$. In terms of the Lagrange basis polynomials $L_j(s)$ defined on the values $x_0 + c_j h$, $j = 0, \ldots, 5$, $u''(x_0 + sh)$ reads

$$u''(x_0 + sh) = \sum_{j=0}^{5} f_{c_j}\, L_j(s), \tag{2}$$

Integrating (2) once and twice, respectively, and exploiting the initial conditions in $s = 0$ leads to the following formulas

$$hy'(x_0 + sh) \simeq hu'(x_0 + sh) = hy'_0 + h^2 \sum_{j=0}^{5} \beta_j(s) f_{n+c_j}, \tag{3}$$

$$y(x_0 + sh) \simeq u(x_0 + sh) = y_0 + shy'_0 + h^2 \sum_{j=0}^{5} \alpha_j(s) f_{n+c_j}, \tag{4}$$

where $\alpha_j(s) = \int_0^s (s - r) L_j(r) dr$ and $\beta_j(s) = \int_0^s L_j(r) dr$. We then set $y_1 = u(x_0 + h)$, $y'_1 = u'(x_0 + h)$, and iterate the above procedure on subintervals $[x_n, x_{n+1}]$, $n = 0, 1, \ldots, N - 1$, of length h.
The proposed method is constructed by considering four intermediate points on $[x_0, x_1]$. A common procedure to increase the order of a collocation method is to choose the intermediate points in order to have a higher truncation error for the point x_1. Here instead of looking for the higher possible truncation error, we choose the intermediate points in order to rise by one the order of the local truncation error for $y(x_1)$, $y'(x_1)$ and $y(x_{c_3})$. For simplicity we fixed $c_2 = \frac{1}{2}$ and we look for the values of c_1, c_3, c_4. The truncation errors are obtained through the expansion in powers of h utilizing the Taylor series, resulting in

$$\begin{aligned}
\mathcal{L}[y(x_1), h] &= \frac{(-7c_1c_3c_4 + c_1 + c_3 + c_4 - 1)h^8 y^{(8)}(x_0)}{604800} + O(h^9),\\
\mathcal{L}[y(x_{c_3}), h] &= \frac{h^8 y^{(8)}(x_0)\, P_{c_3}}{604800} + O(h^9),\\
\mathcal{L}[y'(x_1), h] &= \frac{(-6 - 7c_3(-1 + c_4) + 7c_4 - 7c_1(-1 + c_3 + c_4))\, h^7 y^{(8)}(x_0)}{604800} + O(h^8).
\end{aligned} \tag{5}$$

with

$$P_{c_3} = c_3^4\Big(c_3\left(-5c_3^3 + (8c_4 + 12)\, c_3^2 - (21c_4 + 7)\, c_3 + 14c_4\right) + c_1\left(8c_3^3 - (14c_4 + 21)\, c_3^2 + (42c_4 + 14)\, c_3 - 35c_4\right)\Big).$$

Equating the principal terms in (5) to zero, we have

$$\begin{cases} -7c_1c_3c_4 + c_1 + c_3 + c_4 - 1 = 0\\ P_{c_3} = 0\\ -6 - 7c_3(-1 + c_4) + 7c_4 - 7c_1(-1 + c_3 + c_4) = 0\,. \end{cases} \tag{6}$$

The optimal coefficients derived by this procedure satisfying $0 < c_1 < c_3 < c_4 < 1$ are

$$c_1 = \frac{\left(7 - \sqrt{21}\right)}{14}, \quad c_3 = \frac{\left(7 + \sqrt{21}\right)}{14}, \quad c_4 = \frac{21 + 4\sqrt{21}}{42}.$$

Substituting the values of the coefficients and evaluating the formulas in (3) and (4) at $s = 1$, we get the approximations of $y(x_0 + h)$ and $y'(x_0 + h)$, given as follows

$$
\begin{aligned}
y_1 &= y_0 + hy'_0 + \frac{1}{360}h^2\left(18f_0 + 7\left(\sqrt{21}+7\right)f_{c_1} + 64f_{c_2} - 7\left(\sqrt{21}-7\right)f_{c_3}\right), \\
hy'_1 &= hy'_0 + \frac{1}{180}h^2\left(9f_0 + 49f_{c_1} + 64f_{c_2} + 49f_{c_3} + 9f_1\right).
\end{aligned} \tag{7}
$$

In order to implement the proposed optimized Runge-Kutta Nyström method in block form, some additional formulas must be considered. To do this, we take the values of $u(x_0 + sh)$ in (3) and $hu'(x_0 + sh)$ in (4) evaluated at the collocation points $s = c_1, c_2, c_3, c_4$. In this way, we obtain a total of ten formulas that form the proposed optimized block method.

3. Theoretical analysis

The obtained ORKNM can be formulated in matrix form as

$$
\bar{R}\, V_0 = h\,\bar{S}\; V'_0 + h^2\,\bar{T}\,F_0, \tag{8}
$$

with $\bar{R}, \bar{S}, \bar{T}$ constant matrices containing the coefficients of the ORKNM, given by;

$$
\bar{R} = \begin{pmatrix}
-1 & 1 & 0 & 0 & 0 & 0 \\
-1 & 0 & 1 & 0 & 0 & 0 \\
-1 & 0 & 0 & 1 & 0 & 0 \\
-1 & 0 & 0 & 0 & 1 & 0 \\
-1 & 0 & 0 & 0 & 0 & 1 \\
0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0
\end{pmatrix}; \qquad
\bar{S} = \begin{pmatrix}
\frac{1}{14}\left(7-\sqrt{21}\right) & 0 & 0 & 0 & 0 & 0 \\
\frac{1}{2} & 0 & 0 & 0 & 0 & 0 \\
\frac{1}{14}\left(\sqrt{21}+7\right) & 0 & 0 & 0 & 0 & 0 \\
\frac{1}{2}+\frac{2}{\sqrt{21}} & 0 & 0 & 0 & 0 & 0 \\
1 & 0 & 0 & 0 & 0 & 0 \\
1 & -1 & 0 & 0 & 0 & 0 \\
1 & 0 & -1 & 0 & 0 & 0 \\
1 & 0 & 0 & -1 & 0 & 0 \\
1 & 0 & 0 & 0 & -1 & 0 \\
1 & 0 & 0 & 0 & 0 & -1
\end{pmatrix}; \tag{9}
$$

$$
\bar{T} = \begin{pmatrix}
\frac{1111-171\sqrt{21}}{41160} & \frac{55}{6174} & \frac{2\left(419-98\sqrt{21}\right)}{15435} & \frac{1709-343\sqrt{21}}{17640} & -\frac{18}{1715} & \frac{12\sqrt{21}+41}{20580} \\
\frac{49}{1920} & \frac{7\left(8\sqrt{21}+35\right)}{5760} & \frac{1}{72} & -\frac{7\left(8\sqrt{21}-35\right)}{5760} & 0 & \frac{1}{1920} \\
\frac{171\sqrt{21}+919}{41160} & \frac{2401\sqrt{21}+11003}{123480} & \frac{2\left(98\sqrt{21}+449\right)}{15435} & \frac{1}{882} & \frac{18}{1715} & \frac{-12\sqrt{21}-55}{20580} \\
\frac{88612\sqrt{21}+426493}{17781120} & \frac{49\sqrt{\frac{7}{3}}}{720}+\frac{5545181}{53343360} & \frac{129361}{1666980}+\frac{16}{45\sqrt{21}} & \frac{7\sqrt{\frac{7}{3}}}{720}+\frac{112019}{7620480} & \frac{25}{24696} & \frac{-788\sqrt{21}-3607}{3556224} \\
\frac{1}{20} & \frac{7}{360}\left(\sqrt{21}+7\right) & \frac{8}{45} & \frac{1}{360}(-7)\left(\sqrt{21}-7\right) & 0 & 0 \\
\frac{41\sqrt{21}+189}{5880} & \frac{49}{360}-\frac{23}{840\sqrt{21}} & \frac{8}{45}-\frac{106}{105\sqrt{21}} & \frac{343-29\sqrt{21}}{2520} & -\frac{1}{35}\left(6\sqrt{\frac{3}{7}}\right) & \frac{1}{56}+\frac{41}{280\sqrt{21}} \\
\frac{1}{960}\left(81-8\sqrt{21}\right) & \frac{95\sqrt{21}+392}{2880} & \frac{\sqrt{\frac{7}{3}}}{48}+\frac{8}{45} & -\frac{7\left(25\sqrt{21}-56\right)}{2880} & \frac{3\sqrt{21}}{80} & \frac{1}{960}\left(-8\sqrt{21}-33\right) \\
\frac{23\sqrt{21}+189}{5880} & \frac{49}{360}+\frac{523}{840\sqrt{21}} & \frac{8}{45}+\frac{86}{105\sqrt{21}} & \frac{7}{360}\left(\sqrt{21}+7\right) & -\frac{1}{35}\left(6\sqrt{\frac{3}{7}}\right) & \frac{1}{56}+\frac{23}{280\sqrt{21}} \\
\frac{3368\sqrt{21}+48027}{1270080} & \frac{49}{360}+\frac{113269}{181440\sqrt{21}} & \frac{8}{45}+\frac{36871}{45360\sqrt{21}} & \frac{49}{360}+\frac{16717}{25920\sqrt{21}} & -\frac{65}{336\sqrt{21}} & \frac{737}{60480}+\frac{421}{7560\sqrt{21}} \\
\frac{1}{20} & \frac{49}{180} & \frac{16}{45} & \frac{49}{180} & 0 & \frac{1}{20}
\end{pmatrix}, \tag{10}
$$

and

$$V_0 = \left(y_0, y_{c_1}, y_{c_2}, y_{c_3}, y_{c_4}, y_1\right)^\top,$$
$$V_0' = \left(y_0', y_{c_1}', y_{c_2}', y_{c_3}', y_{c_4}', y_1'\right)^\top,$$
$$F_0 = \left(f_0, f_{c_1}, f_{c_2}, f_{c_3}, f_{c_4}, f_1\right)^\top.$$

We define the operator Γ related to the ORKNM in (8), assuming that $y(x)$ has enough derivatives, as

$$\Gamma[y(x); h] = \sum_{j\in I}\left[\Theta_j y\,(x+jh) - h\theta_j y'\,(x+jh) - h^2\vartheta_j y''\,(x+jh)\right], \tag{11}$$

where Θ_j, θ_j, and ϑ_j are respectively vector columns of $\bar{R}, \bar{S}$ and $\bar{T}$, and $I = \{0, c_1, c_2, c_3, c_4, 1\}$.
Expanding $y\,(x_0 + jh), y'\,(x_0 + jh)$ and $y''\,(x_0 + jh)$ in Taylor series about x_0 we have

$$\Gamma[y(x); h] = C_0 y(x) + C_1 h y'(x) + C_2 h^2 y''(x) + \cdots + C_q h^q y^q(x) + \ldots, \tag{12}$$

where

$$C_q = \frac{1}{q!}\left[\sum_{j\in I} j^q\Theta_j - q\sum_{j\in I} j^{q-1}\theta_j - q(q-1)\sum_{j\in I} j^{q-2}\vartheta_j\right], \tag{13}$$

and $q = 0, 1, 2, 3, 4, \ldots$. The order of the local truncation error is determined by the first non-null vector C_q.
We note that the resulting scheme is a Runge-Kutta Nyström method based on direct collocation. According to [21], if

$$y(x_1) - y_1 = O\left(h^{p_1+1}\right), \quad y'(x_1) - y_1' = O\left(h^{p_2+1}\right),$$

then the order of accuracy is defined as $p = \min\{p_1, p_2\}$.
By Theorem 3.2 of [21] we know that the method has global step point order of at least $p = 6$ and locally, the order of the y component is 7 and the order of the y' component is one lower. We have increased the global step point order with the special choice of the collocation points. Since Theorem 3.4 of [21] is satisfied with $p = s + q = 6 + 2 = 8$, then the ORKNM has global step point order $p = 8$.
By substituting the elements of the matrices defined in (9) and (10) we get the orders and LTEs for each of the formulas in (8), as given in Table 1.

Table 1: Order(p) and local truncation errors (LTEs) for the formulas in (8)

Formula	Order	local truncation errors
y_{c_1}	7	$-\frac{h^8 y^{(8)}(x_0)}{36303120} + O(h^9)$
y_{c_2}	7	$-\frac{h^8 y^{(8)}(x_0)}{30965760} + O(h^9)$
y_{c_3}	7	$\frac{\left(523\sqrt{21}+2401\right)h^9 y^{(9)}(x_0)}{853849382400} + O(h^{10})$
y_{c_4}	7	$-\frac{125 h^8 y^{(8)}(x_0)}{1204450394112} + O(h^9)$
y_1	8	$\frac{h^9 y^{(9)}(x_0)}{177811200} + O(h^{10})$
y_{c_1}'	6	$-\frac{11 h^7 y^{(8)}(x_0)}{8297856\sqrt{21}} + O(h^8)$
y_{c_2}'	6	$\frac{h^7 y^{(8)}(x_0)}{967680\sqrt{21}} + O(h^8)$
y_{c_3}'	6	$-\frac{h^7 y^{(8)}(x_0)}{41489280\sqrt{21}} + O(h^8)$
y_{c_4}'	6	$\frac{25 h^7 y^{(8)}(x_0)}{1792336896\sqrt{21}} + O(h^8)$
y_1'	8	$-\frac{h^9 y^{(10)}(x_0)}{1422489600} + O(h^{10})$

The stability properties of the method are studied by applying formula (8) to the following standard test equations

$$y''(x) = -\nu^2\, y(x), \quad \eta > 0, \tag{14}$$

$$y''(x) = -2\nu y'(x) - \nu^2 y(x), \quad \eta > 0, \tag{15}$$

where ν stands for a complex parameter and the above equations have bounded solutions that go to zero as x tends to infinity. Applying the ORKNM in (8) on (15) we have

$$P\begin{pmatrix} y_{c_1} \\ y_{c_2} \\ y_{c_3} \\ y_{c_4} \\ y_1 \\ y'_{c_1} \\ y'_{c_2} \\ y'_{c_3} \\ y'_{c_4} \\ y'_1 \end{pmatrix} = Q\begin{pmatrix} y_{c_1-1} \\ y_{c_2-1} \\ y_{c_3-1} \\ y_{c_4-1} \\ y_0 \\ y'_{c_1-1} \\ y'_{c_2-1} \\ y'_{c_3-1} \\ y'_{c_4-1} \\ y'_0 \end{pmatrix},$$

where P and Q are square matrices of dimension ten whose entries are obtained by the coefficients of the formulas given in (8). By letting $z = \nu h$, we study the stability of the proposed ORKNM through the eigenvalues of the amplification matrix ($M(z) = P^{-1}Q$). Figures 1 - 2 display the stability regions of the proposed ORKNM using the above test equations.

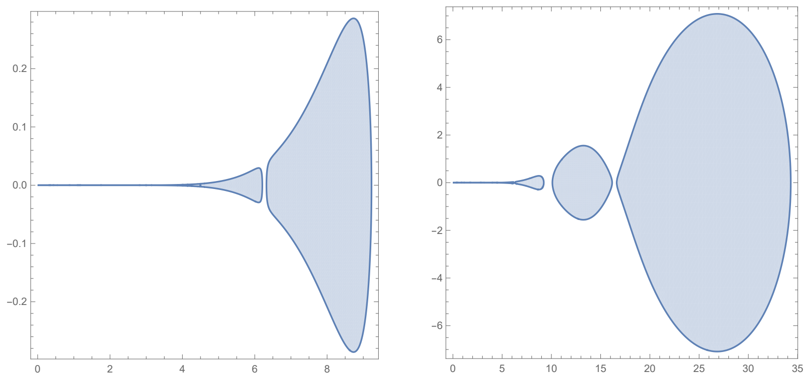

Figure 1: Stability region in the complex z-plane using (14).

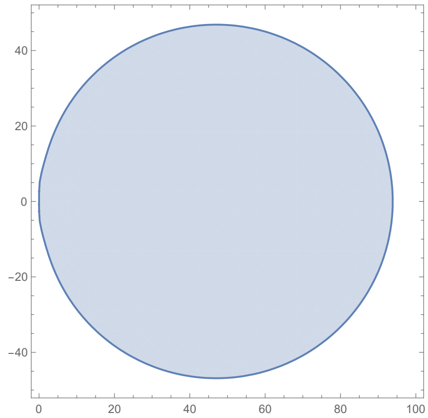

Figure 2: Stability region in the complex z-plane using (15).

4. Error estimation and mesh selection

From a practical point of view, it might be unreasonable to solve the IVP with a constant stepsize, especially when the true solution changes at very different rates in portions of the integration interval $[x_0, x_N]$. Thus, for the numerical method (8) to be reliable and, of course, efficient, it must be suitable for a variable stepsize (VSS) implementation. The approach of VSS is also known as adaptive since it adjusts the number and position of the steps utilized in the numerical solution to ensure that the truncation error is kept inside a predefined bound. To achieve a robust estimation of the local truncation error (LTE), we adopted a similar strategy as in Shampine, and Gordon [22].

The choice of a formula of a higher order that could be used for error estimation is not so simple. We use a strategy that requires two more function evaluations in this work. Following the procedure described in [25] but starting from the Hermite-Obreschkoff methods presented in [26], we use a central finite difference approach to get the coefficients for computing an approximation y^* to $y(x_1)$. The derivatives of the Hermite-Obreschkoff method of order 10 are approximated using a stencil of eight points with the previous computed function values f_{c_i}, $i = 0, \ldots, 5$ and two additional function evaluation at the points $c_6 = \frac{1}{2} - \frac{2}{\sqrt{21}}$ and $c_7 = \frac{3}{2} - \frac{2}{\sqrt{21}}$. The approximation of $y_{c_j}, y'_{c_j}, j = 6, 7$ needed for the evaluation of f are computed evaluating the collocation polynomial, requiring a linear combination of the function values. The following multistep formula of order $p = 9$ is then obtained

$$\begin{aligned} y_1^* \;=\; & y_0 + hy_0' + h^2\left(\frac{\left(2343 - 16\sqrt{21}\right)f_0}{51900} - \frac{\left(4\sqrt{21} + 21\right)f_1}{375} + \frac{\left(573\sqrt{21} + 3731\right)f_{c_1}}{29880}\right) \\ & + h^2\left(\frac{\left(2\sqrt{21} + 565\right)f_{c_2}}{3060} + \frac{\left(197 - 43\sqrt{21}\right)f_{c_3}}{1800}\right) \\ & + h^2\left(\frac{3\left(4\sqrt{21} + 21\right)f_{c_4}}{1000} + \frac{3f_{c_6}}{200} + \frac{3\left(30854\sqrt{21} + 141421\right)f_{c_7}}{30512875}\right), \end{aligned} \tag{16}$$

with local truncation error $LTE = \frac{4\sqrt{21}-63}{59744563200}h^{10}y^{(10)}(x_0) + O\left(h^{11}\right)$.

The obtained error estimate provides the basis for choosing the stepsize for the next step. The mesh selection is now made by computing an estimation of the relative mixed error as follows

$$EST = \frac{\left\|y_1^* - y_1\right\|}{\left(\frac{ATOL}{RTOL} + \left\|y_1\right\|\right)},$$

where y_1^* and y_1 are the values obtained by the formula in (16) and the method in (8), respectively, and ATOL and RTOL are the user's predefined tolerances. If EST $\leq$ RTOL, then we accept the results and take the next step as $h_{new} = 2 \times h_{old}$, that is, we double the stepsize to save the time and proceed the integration process with this h_{new} provided that $h_{min} \leq h_{new} \leq h_{max}$, where h_{min} and h_{max} are the minimum and maximum stepsizes allowed respectively. If EST > RTOL, then we reject the obtained results, decrease stepsize and repeat the calculations with the following new step

$$h_{new} = h_{old}\left(\frac{RTOL}{EST}\right)^{1/p}. \tag{17}$$

According to Stoer and Bulirsch [27], page 491, many researchers recommend the inclusion of a safety factor μ in (17) as follows:

$$h_{new} = \mu \times h_{old}\left(\frac{RTOL}{EST}\right)^{1/p}, \tag{18}$$

where $0 < \mu < 1$ is a suitable adjustment factor. In the numerical experiments section, we have used $\mu = 0.95$.

For comparison purposes, the implicit Lobatto III-A Runge-Kutta method of order eight has been implemented as an embedded Runge-Kutta method in variable stepsize mode. The following multistep formula of order ($p = 10$)

$$\begin{aligned} y_1^* &= y_0 + \frac{h\left(182475 f_0 + 2064384 f_{\frac{1}{4}} + 2064384 f_{\frac{3}{4}} + 2097152 f_{\frac{1}{8}} + 2097152 f_{\frac{7}{8}}\right)}{5953500} \\ &+ \frac{h\left(-2067261 f_{c_1} + 1400000 f_{c_2} - 2067261 f_{c_3} + 182475 f_1\right)}{5953500}, \end{aligned}$$

with the local truncation error $LTE = -\frac{17}{90128941056000} h^{11} y^{(11)}(x_0) + O\left(h^{12}\right)$ has been used to estimate the local error at each step and a similar strategy for mesh selection as given in (18) with $p = 10$ has also been utilized with the Runge-Kutta method.

5. Computational details

The new ORKNM is implemented in a step by step mode. We denote the obtained system from (8) as $\boldsymbol{F(y) = 0}$ where the unknowns are

$$\tilde{\mathbf{Y}} = (y_{c_1}, y'_{c_1}, y_{c_2}, y'_{c_2}, y_{c_3}, y'_{c_3}, y_{c_4}, y'_{c_4}, y_1, y'_1).$$

Since the ORKNM is an implicit scheme, we use a Modified Newton's method (MNM) to solve the obtained systems. The i-th iteration of the MNM is given by

$$\mathbf{J}_0^i\left(\tilde{\mathbf{Y}}^{\mathbf{i+1}} - \tilde{\mathbf{Y}}^{\mathbf{i}}\right) = -\mathbf{F}^i,$$

where $\mathbf{J}_0^i$ represents the frozen jacobian matrix of $\mathbf{F}$ at the starting value. The starting values to be used by MNM for solving the system on each iteration are taken as

$$y_{n+j} = y_n + (jh)y'_n + \frac{(jh)^2}{2} f_n, \quad y'_{n+j} = y'_n + (jh)f_n, \quad n = 0, 1, 2, \ldots, N-1, \; j = c_1, c_2, c_3, c_4, 1.$$

We can apply the ORKNM to solve systems of second-order IVPs by considering the following system of m equations:

$$\mathbf{y}'' = \mathbf{f}(x, \mathbf{y}^\top, \mathbf{y}'^\top), \quad \mathbf{y}(a) = \mathbf{y}_0, \quad \mathbf{y}'(a) = \dot{\mathbf{y}}_0, \qquad a = x_0 \le x \le b = x_0,$$

where $\mathbf{y} = (y_1, \ldots, y_d)^\top, \mathbf{y}' = (y'_1, \ldots, y'_d)^\top$,

$$\mathbf{f}(x, \mathbf{y}^\top, \mathbf{y}'^\top) = (f_1(x, \mathbf{y}^\top, \mathbf{y}'^T), \ldots, f_d(x, \mathbf{y}^\top, \mathbf{y}'^\top))^\top,$$

and $\mathbf{y}_0 = (y_{1,0}, \ldots, y_{d,0})^\top, \mathbf{y}'_0 = (\dot{y}_{1,0}, \ldots, \dot{y}_{d,0})^\top$. In the case of d-dimensional IVPs, we get the algebraic system of $10d$ equations, and we solved the obtained non-linear system using MNM, as in the scalar one-dimensional IVPs. The stopping criterion and the maximum number of iterations used while executing the MNM are $2 \times RTOL$ and 100, respectively.

6. Numerical Experiments

Here, we report the numerical performance of the proposed ORKNM on the class of second-order problems of the form (1). We note that the effectiveness and efficiency of the proposed strategy will rely on the VSS technique presented in section 4. The criteria utilized as a measure of the accuracy are the maximum absolute error (MAE) and the maximum relative error (MRE) on the integration interval, given respectively by the formulas

$$\begin{aligned} MAE &= \max_{j=0,\ldots,N} \left\| y(x_j) - y_j \right\|_\infty , \\ MRE &= \max_{j=0,\ldots,N} \left(\frac{\left\| y(x_j) - y_j \right\|}{\left(\frac{ATOL}{RTOL} + \left\| y(x_j) \right\| \right)} \right), \\ ROC &= -\log_2 \left(\frac{MAE_h}{MAE_{2h}} \right), \end{aligned}$$

where $y(x_j)$ is the exact solution, and y_j is the computed result at each point x_j of the discrete grid. The following abbreviations are utilized in Tables:

- ORKNM: The new optimized Runge-Kutta Nyström method developed in this paper.
- FM8P: The Falkner method of order eight (see [23]).
- FDM8P: The finite difference method of order eight (see [24, 28]).
- FDM9P-GFD: The finite difference method of order nine with generalized backward difference (see [24, 28]).
- FDM9P-GBD: The finite difference method of order nine with generalized forward difference (see [24, 28]).
- LOB-IIIA8P: The implicit Lobatto III-A Runge-Kutta method of order eight formulated in variable stepsize (see [29]).
- NS : Number of steps.
- MP : Mesh points.
- NRS : Number of rejected steps.
- NNI : Number of Newton iterations.
- NJAC : Number of Jacobian evaluations.
- ABE $y(x)$: Absolute error of the solution.
- ABE $y'(x)$: Absolute error of the first derivative solution.
- TNFE : Total number of function evaluations.
- h_{ini} : Initial stepsize.
- h_{min} : Minimum stepsize allowed.
- h_{max} : Maximum stepsize allowed.
- ATOL : Absolute Tolerance.
- RTOL : Relative Tolerance.
- CPU : Computational time in seconds.

6.1. *Numerical Experiment 1*

To determine the numerical rate of convergence of the proposed ORKNM, we first consider the following Bessel problem using fixed stepsize

$$x^2y''(x) + xy'(x) + (x^2 - 0.25)y(x) = 0\,, \qquad (19)$$
$$y(1) = \sqrt{\frac{2}{\pi}}\sin(1),\; y'(1) = \frac{2\cos(1) - \sin(1)}{\sqrt{2\pi}}, \quad 1 \leq x \leq 8,$$

whose exact solution is

$$y(x) = \sqrt{\frac{2}{\pi x}}\sin(x).$$

Table 2: MAEs and order of convergence for test Problem (19)

h	Method	*MAE*	*ROC*
$\frac{1}{10}$	ORKNM	1.88947×10^{-8}	
$\frac{1}{20}$	ORKNM	1.13901×10^{-10}	7.37
$\frac{1}{40}$	ORKNM	5.26579×10^{-13}	7.76
$\frac{1}{80}$	ORKNM	2.27596×10^{-15}	7.85

Table 3: Comparison of the numerical results for Problem (19) with $h_{ini} = 10^{-1}$

ATOL = RTOL	Method	NS	TFE	MP	MAE $y(x)$	MAE $y'(x)$
10^{-6}	ORKNM	6	48	49	5.75220×10^{-6}	2.68700×10^{-8}
	FM8P	65	74	66	4.58467×10^{-7}	6.34613×10^{-7}
10^{-7}	ORKNM	7	56	56	3.46870×10^{-7}	5.61510×10^{-9}
	FM8P	82	91	83	5.00841×10^{-8}	2.047023×10^{-7}
10^{-8}	ORKNM	8	64	63	5.64580×10^{-8}	2.89620×10^{-9}
	FM8P	97	106	98	6.93047×10^{-9}	9.26095×10^{-9}

In Table 2, we have included the numerical rate of convergence (ROC) to (19) which confirmed the order of convergence of the method.

In Table 3, we present the maximum absolute errors for the solution and its first-derivative solution obtained at the final point of the integration interval for (19). We observe that the error terms are similar, but the proposed ORKNM uses a small NS, which shows the good performance of the proposed method.

6.2. *Numerical Experiment 2*

Consider the non-linear homogeneous problem [24]

$$(y(x) + 1)y''(x) - 3(y'(x))^2 = 0\,, \qquad (20)$$
$$y(1) = 0,\; y'(1) = -\frac{1}{2}, \quad 1 \leq x \leq 10,$$

whose exact solution is

$$y(x) = \frac{1}{\sqrt{x}} - 1.$$

Table 4: Comparison of the numerical results on (20) with $h_{ini} = 8 \times 10^{-2}$

ATOL = RTOL	Method	NS	NRS	NNI	TFE	NJ	MP	MRE
10^{-6}	ORKNM	7	0	30	56	7	50	2.13206×10^{-7}
	FDM8P	6	0	68	49	40	68	9.56000×10^{-7}
	FDM9P-GFD	5	0	34	16	11	67	5.89000×10^{-7}
	FDM9P-GBD	5	0	34	16	11	67	5.74000×10^{-7}
10^{-7}	ORKNM	8	0	38	64	8	57	4.05649×10^{-8}
	FDM8P	7	0	77	54	44	79	1.24000×10^{-7}
	FDM9P-GFD	6	0	67	47	38	80	8.14000×10^{-8}
	FDM9P-GBD	6	0	67	47	38	80	7.57000×10^{-8}
10^{-8}	ORKNM	10	0	45	80	10	71	7.56256×10^{-9}
	FDM8P	9	0	102	71	58	101	1.98000×10^{-8}
	FDM9P-GFD	7	0	77	53	43	93	8.77000×10^{-9}
	FDM9P-GBD	7	0	77	53	43	93	8.18000×10^{-9}

Table 4 presents the comparison of maximum relative errors on the integration interval and the number of steps for different methods, evincing the good performance of the proposed ORKNM.

6.3. Numerical Experiment 3

Consider the Vander Pol problem that arises from electronics and illustrates the behaviour of non-linear vacuum tube circuits [30]

$$\begin{aligned} &y''(x) = \nu(1 - y(x)^2)y'(x) - y(x), \\ &y(0) = 2,\ y'(0) = 0, \quad 0 \leq x \leq 2000, \end{aligned} \tag{21}$$

whose exact solution is unknown.

Table 5: Comparison of the numerical results on (21) with $h_{ini} = 10^{-1}, \nu = 1000$

ATOL = RTOL	Method	NS	NRS	NNI	TFE	NJ	CPU	MRE
10^{-7}	ORKNM	317	94	1249	2536	411	2.57627	3.81286×10^{-9}
	LOB-IIIA8P	733	64	2004	5864	797	3.75841	3.16765×10^{-7}
10^{-8}	ORKNM	321	112	1280	2568	433	2.74884	2.50932×10^{-11}
	LOB-IIIA8P	754	73	2218	6032	827	4.12364	8.73680×10^{-8}
10^{-9}	ORKNM	345	115	1355	2760	460	2.97702	2.64965×10^{-13}
	LOB-IIIA8P	801	82	2633	6408	883	4.63263	3.17442×10^{-8}

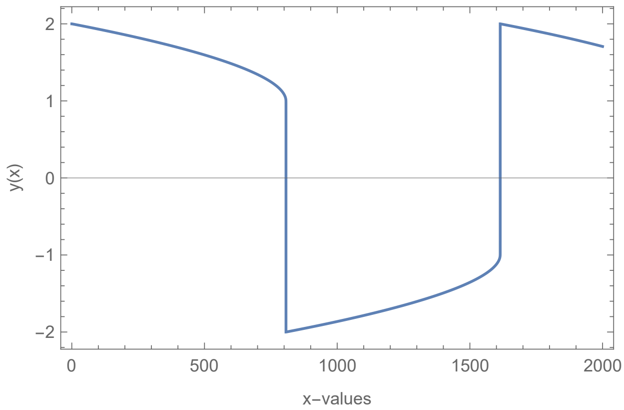

Figure 3: Discrete solution for (21) with ATOL = RTOL = 10^{-9}, $h_{ini} = 10^{-3}$.

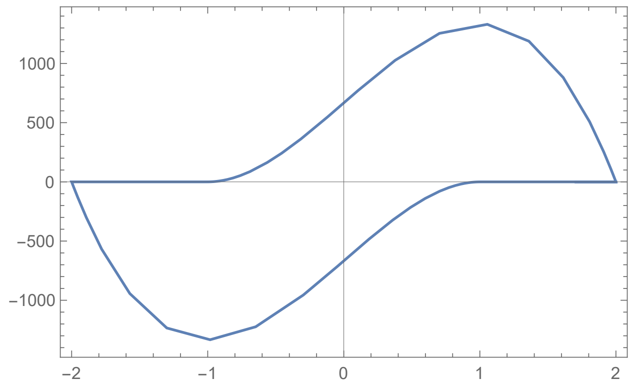

Figure 4: Limit cycle for the numerical experiment (21) with ATOL = RTOL = 10^{-9}, $h_{ini} = 10^{-3}$.

In order to compare the MRE for problem (21), the following reference solution at the final point $x_N = 2000$ given in [30] has been used,

$$y(x_N) = 1.706167732170469, \quad y'(x_N) = -0.0008928097010248125.$$

The comparison of the results for the proposed ORKNM and LOB-IIIA8P presented in Table 5 were obtained using $h_{min} = 10^{-9}$ and $h_{max} = 10$, respectively.

The data in Table 5 clearly show that the best performance corresponds to the ORKNM. In addition, these data are used to obtain the efficiency curves in Figure 3, which shows the good performance of the proposed method. The behavior of the approximate solution and the corresponding limit cycle are shown in Figures 4 and 5, respectively.

6.4. Numerical Experiment 4

In the fourth experiment, we solve the Kepler's problem (KP) [31]

$$y_1''(x) = -\frac{y_1(x)}{\left(y_1^2(x) + y_2^2(x)\right)^{\frac{3}{2}}}, \; y_1(0) = 1 - \epsilon, \; y_1'(0) = 0,$$

$$y_2''(x) = -\frac{y_2(x)}{\left(y_1^2(x) + y_2^2(x)\right)^{\frac{3}{2}}}, \; y_2(0) = 0, \; y_2'(0) = \sqrt{\frac{1+\epsilon}{1-\epsilon}}, \quad 0 \leq x \leq 20\pi. \tag{22}$$

The theoretical solution of the KP is

$$y_1(x) = \cos(v) - \epsilon, \; y_2(x) = \sqrt{1-\epsilon^2}\,\sin(v),$$

where v is the solution of the Kepler's equation, $v - \epsilon \sin(v) - x = 0$.

Table 6: Comparison of the numerical results on (22) with $h_{ini} = 10^{-2}, \epsilon = 0.9$

ATOL = RTOL	Method	NS	NRS	NNI	TFE	NJ	CPU	MRE
10^{-10}	ORKNM	470	223	2127	3760	693	6.93321	1.53986×10^{-4}
	LOB-IIIA8P	527	226	3195	4216	753	14.05239	5.83114×10^{-5}
10^{-12}	ORKNM	745	337	3247	59960	1082	10.50988	3.55175×10^{-6}
	LOB-IIIA8P	847	364	4939	6776	1211	22.40475	2.76875×10^{-6}
10^{-14}	ORKNM	1210	525	5206	9680	1735	17.01310	4.53147×10^{-9}
	LOB-IIIA8P	1380	566	8216	11040	1946	36.44788	9.28509×10^{-9}

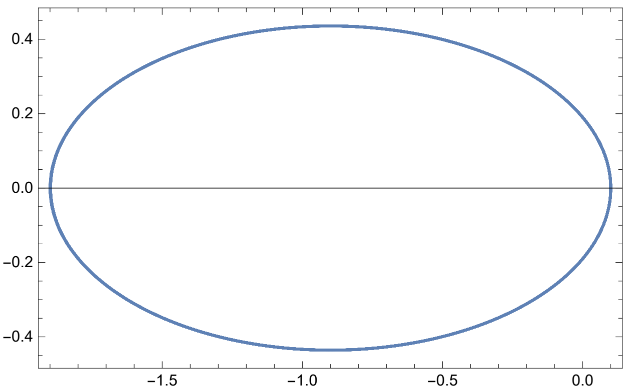

Figure 5: Discrete solutions for Problem (22) with ATOL = RTOL = 10^{-14}, $h_{ini} = 10^{-2}$.

The comparison of the results for the proposed ORKNM and LOB-IIIA8P presented in Table 6 were obtained using $h_{min} = 10^{-9}$ and $h_{max} = 5$, respectively.

The numerical results for the proposed ORKNM and LOB-IIIA8P reported in Table 6 were obtained taking $h_{min} = 10^{-12}$ and $h_{max} = 5$. Again, the MRE are similar, and the proposed ORKNM has smaller NS, CPU-times, NNI, TFE, and NJ, implying that the ORKNM is accurate for integrating the Kepler problem directly. The discrete solution in the phase plane is shown in Figure 6.

6.5. Numerical Experiment 5

Consider the time dependent semi-discretization of the problem given in [21]

$$\frac{\partial^2 y}{\partial t^2} = \frac{y^2}{(1 + 2x - 2x^2)} \frac{\partial^2 y}{\partial x^2} + y\left(4\cos^2(x) - 1\right), \quad (23)$$
$$0 \le t \le 2\pi, \quad 0 \le x \le 1,$$

with initial and Dirichlet boundary conditions so that the exact solution is

$$y(x, t) = (1 + 2x - 2x^2)\cos(x).$$

We solved (23) by discretizing the second-order spatial derivative, leaving the time variable continuous, and then applying the ORKNM, following a procedure as in the method of lines. The $\frac{\partial^2 y}{\partial x^2}$ in (23) is discretized by

$$\frac{\partial^2 y}{\partial x^2}(x_i, t) \simeq \frac{y(x_{i+1}, t) - 2y(x_i, t) + y(x_{i-1}, t)}{\delta x^2}, \quad (24)$$

where $\delta x = \dfrac{(x_{N+1} - x_0)}{N+1}$, N is the internal number of spatial nodes, $x_1 = x_0 + \delta x, \ldots, x_N = x_0 + N\delta x$, $x_{N+1} = x_0 + (N+1)\delta x$. Taking $N = 19$ and using (24) on the grid points $x_i = \frac{i}{20}$, $i = 1, \ldots, N$, we get $y_1, y_2, y_3, \ldots, y_N$ by solving the following system of differential equations after replacing $\frac{\partial^2 y}{\partial x^2}(x_i, t)$ in (24) into (23),

$$y_i'' = \frac{y_i^2}{1 + 2x_i - 2x_i^2} \frac{y_{i+1} - 2y_i + y_{i-1}}{\delta x^2} + y_i(4\cos^2(x) - 1), \; i = 1, \ldots, N. \tag{25}$$

Table 7: Comparison of the numerical results on (23) with $h_{ini} = 10^{-2}, N = 19$

ATOL = RTOL	Method	NS	NRS	NNI	TFE	NJ	CPU	MRE
10^{-2}	ORKNM	33	32	91	264	65	32.23438	3.6880×10^{-7}
	LOB-IIIA8P	65	16	171	520	81	77.82813	4.3822×10^{-8}
10^{-3}	ORKNM	69	69	248	552	138	74.68750	1.4969×10^{-9}
	LOB-IIIA8P	182	15	398	1456	197	201.28125	2.1512×10^{-10}
10^{-4}	ORKNM	147	149	583	1176	296	166.6410	1.3113×10^{-12}
	LOB-IIIA8P	556	13	1140	4448	569	571.45313	2.4563×10^{-12}

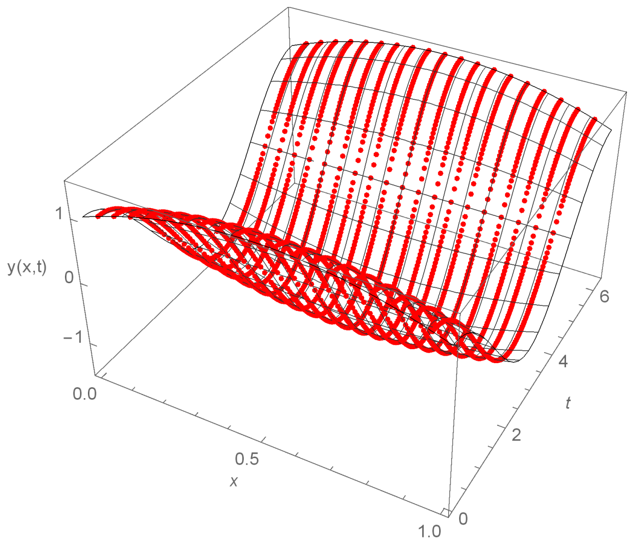

Figure 6: Exact and discrete solution (red points) for (21) with ATOL = RTOL = 10^{-4}, $h_{ini} = 10^{-2}$.

Table 7 presents the numerical results we obtained using $h_{min} = 10^{-4}$ and $h_{max} = 1$. Data in Table 7 and Figure 8 also ascertain the viability and effectiveness of the proposed ORKNM. Exact and approximate solution of the ORKNM for the (23) utilizing $h_{min} = 10^{-4}$ and $h_{max} = 1$ are plotted in Figure 9.

7. Conclusions

A new superconvergent collocation Runge Kutta Nyström method has been developed for the solution of second-order initial value problems. In particular, an accurate way to estimate the local truncation error allow us to implement an effective mesh selection strategy. The numerical results show that this method can be competitive with other existing numerical techniques.

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