Two-step RKN Direct Method for Special Second-order Initial and Boundary Value Problems

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Abstract—**In this study, a class of direct numerical integrators for solving special second-order ordinary differential equations (ODEs) is proposed and studied. The method is multistage and multistep in nature. This class of integrators is called "two-step Runge-Kutta-Nyström", denoted by TSRKN. The direct approach to higher-order ODEs is desirable to avoid tedious computational work caused by converting the higher-order ODEs into the system of first-order equations. The order conditions for the TSRKN are derived using Taylors series expansion and according to the order conditions, a three-stage TSRKN method which is convergent of order four is constructed. The convergence analysis of the method is discussed and the performance of the newly derived method is compared with existing methods. The numerical results show the superiority of the TSRKN method in terms of number of function evaluations and demonstrate that the TSRKN can also be used to solve linear second-order boundary value problems (BVPs) since Runge-Kutta-Nyström (RKN) approach is practically used to only solve higher-order initial value problems (IVPs) directly.**

Index Terms—**Two-step method, Runge-Kutta-Nyström method, Two-point boundary value problem, Initial value problem, Convergence.**

I. Introduction

Differential equations are able to describe the dynamics of several complex systems and problems in mathematics, which can be classified into the initial and boundary value problems. Boundary value problem (BVP) differs from initial value problem (IVP) in that the boundary conditions are specified at more than one point and in that solutions of the differential equation over an interval, satisfying the boundary conditions at the endpoints, are required ([1], p.1). These problems can be found in various science and engineering domains and applications including fluid dynamics and chemical reactions, elastic beams, spread of diseases, etc. (see [2], [3], and [4], p.7 - p.27).

This study is concerned with finding an approximate solution to the special second-order ordinary differential equation (ODE) of the form

$$\frac{d^2u}{dt^2} = f(t,u), \quad t \in [o,d], \tag{1}$$

with initial conditions:

$$u(o) = \sigma_1, \quad u'(o) = \sigma_2. \tag{2}$$

or boundary conditions:

$$u(o) = \sigma_1, \quad u'(d) = \varpi, \tag{3}$$

$$u'(o) = \sigma_2, \quad u'(d) = \varpi. \tag{4}$$

Where $u(t) \in R^d$, $f : [o,d] \times R^d \to R^d$ is a continuous function which does not contain the first derivative. The proofs of existence and uniqueness of solutions to BVPs and IVPs are possible ([5], [3]), but sometimes it is difficult to provide proof for majority of ODEs. This is due to certain conditions, whether in terms of differential equations or boundary conditions and for this reason, they remain unproven. Finding analytical solutions to some ODEs considers one of the difficulties faced by the researchers, due to the scarcity of analytical methods since most of the ODEs encountered were difficult, with either complicated boundary conditions or complicated differential equations ([6], [7], [8], [9]). For such cases, recourse must be made to numerical methods.

Commonly, researchers solve the second-order ODEs (1) numerically by using direct approaches, for example, Runge-Kutta-Nyström (RKN) methods and special linear multistep (LMS) methods (see [10]). RKN approach introduced by Nyström [11] in now widely applied in many areas. Numerous forms of RKN methods have been introduced and studied in recent decades, such as trigonometrically or exponentially fitted methods for solving high oscillatory problems ([12], [13]), implicit methods [14] for numerical solution of stiff ordinary differential equations, and symmetric and symplectic methods for Hamiltonian systems ([10], [15]). LMS methods [10] are known to be more efficient in solving ODE (1), unlike RKN methods which require more function evaluations to achieve the same order. However, the former often suffers from instability [16] and it required more costly subroutines to come out with starting values which lead to complicated computation and longer time. Some researchers studied and proposed new methods that combine the advantages of linear multistep methods and RKN methods. One of these researchers is Coleman who presented a new class of two-step hybrid methods, and proved the effectiveness of the proposed methods through the numerical experiments [17]. Recently, two-step and four-step hybrid methods have been studied by Franco [18] and Li et al. [16] respectively. Although the efficiency of these methods have been proven, unfortunately, they do not contain

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y'_n-values in their formulas. In many fields of applied science, it is very important to calculate the y'_n-values. For example, in mechanics, this calculation is needed to find the velocity. Thus, in this study, we are motivated to propose a class of two-step RKN method since RKN's formulation makes full use of the information transferred from y'_n-value, considers as a self-starting method and it's cheaper to implement. The paper is organized as follows: we present the construction of a class of RKN method in Sections II and III. Analysis on the method's order, consistency, and stability is conducted in Section IV. To check the method's validity and effectiveness, some tested problems will be examined in Section V. Finally, we conclude findings from this study in Section VI.

II. Derivation of the TSRKN Method

Definition 1. The general η-stage two-step Runge-Kutta-Nyström (TSRKN) method for the differential equation (1) is defined as:

$$\begin{cases} u_{n+2} = u_n + 2\,h\,u'_n + h^2 \sum_{i=1}^{\eta} \bar{v}_i \kappa_n^i, \\ u'_{n+2} = u'_n + h \sum_{i=1}^{\eta} v_i \kappa_n^i, \\ \kappa_n^i = f(t_n + c_i\,h, u_n + c_i h u'_n + h^2 \sum_{j=1}^{i} a_{ij} \kappa_n^j, \end{cases} \tag{5}$$

where $c_i, \bar{v}_i, v_i, a_{ij}$ for $i = 1, 2, \ldots, \eta$ and $j = 1, 2, \ldots, \eta$ are the parameters of the TSRKN method which are supposed to be real. When $a_{ij} = 0$ for $i \le j$, the method is said to be explicit and it can be given by the tableaux as follows (see Table I).

TABLE I
η-stage TSRKN Method

c_1	a_{11}		$\ldots$		$a_{1\eta}$
$\vdots$	$\vdots$		$\ddots$		$\vdots$
c_η	$a_{\eta 1}$		$\ldots$		$a_{\eta\,\eta}$
	$\bar{v}_1$	$\bar{v}_2$	$\ldots$	$\bar{v}_{\eta-1}$	$\bar{v}_\eta$
	v_1	v_2	$\ldots$	$v_{\eta-1}$	v_η

To determine the method's (5) coefficients, we expand the TSRKN method expressions by using the Taylor series expansion. This expansion is equated to the Taylor series expansion of the true solution. The direct expansion of the truncation error is used to derive the order conditions for the TSRKN method. This idea is introduced by Dormand [19] which is based on the derivation of order conditions for the Runge-Kutta method.

The TSRKN form (5) can be expressed as

$$u_{n+2} = u_n + 2\,h\,\Theta(t_n, u_n, h), \tag{6}$$
$$u'_{n+2} = u'_n + h\,\Theta'(t_n, u_n, h), \tag{7}$$

where

$$\Theta(t_n, u_n, h) = u'_n + h\sum_{i=1}^{\eta} \bar{v}_i \kappa_n^i,$$
$$\Theta'(t_n, u_n, h) = \sum_{i=1}^{\eta} v_i \kappa_n^i, \tag{8}$$

are the increment functions and κ_n^i is given in method (5). If Λ is the Taylor series increment function, then the local truncation errors (LTE) of the solution and the local truncation errors (LTE$'$) of the derivative can be gained by substituting the exact solution $u(t)$ of ODE (1) into the TSRKN increment function. This gives

$$\begin{aligned} LTE_{n+1} &= h\,[\Theta - \Lambda], \\ LTE'_{n+1} &= h\,[\Theta' - \Lambda']. \end{aligned} \tag{9}$$

It is best to give these expressions in terms of elementary differentials, then, the Taylor series increment can be written as:

$$\begin{aligned} \Lambda &= 2u'_n + \frac{2^2}{2} h F_1^{(2)} + \frac{2^3}{6} h^2 F_1^{(3)} + \frac{2^4}{24} h^3 F_1^{(4)} \\ &+ \frac{2^5}{120} h^4 (F_1^{(5)} + F_2^{(5)}) + O(h^5), \\ \Lambda' &= 2F_1^{(2)} + \frac{2^2}{2} h F_1^{(3)} + \frac{2^3}{6} h^2 F_1^{(4)} + \frac{2^4}{24} h^3 (F_1^{(5)} + F_2^{(5)}) \\ &+ O(h^4), \end{aligned} \tag{10}$$

where

$$\begin{aligned} F_1^{(2)} &= f, \\ F_1^{(3)} &= f_t + f_u u', \\ F_1^{(4)} &= f_{tt} + 2u' f_{tu} + (u')^2 f_{uu} + f f_u. \end{aligned} \tag{11}$$

Substituting (11) into (8), the increment function Θ and Θ' for an η-stage TSRKN formula becomes

$$\begin{aligned} \sum_{i=1}^{\eta} \bar{v}_i \kappa_n^i &= \sum_{i=1}^{\eta} \bar{v}_i F_1^{(2)} + h \sum_{i=1}^{\eta} \bar{v}_i c_i F_1^{(3)} + \frac{1}{2} h^2 \sum_{i=1}^{\eta} \bar{v}_i c_i^2 F_1^{(4)} \\ &+ O(h^3), \\ \sum_{i=1}^{\eta} v_i \kappa_n^i &= \sum_{i=1}^{\eta} v_i F_1^{(2)} + h \sum_{i=1}^{\eta} v_i c_i F_1^{(3)} + \frac{1}{2} h^2 \sum_{i=1}^{\eta} v_i c_i^2 F_1^{(4)} \\ &+ O(h^3). \end{aligned} \tag{12}$$

Using (8) and (10), the LTE can be written as

$$\begin{aligned} LTE_{n+1} &= h^2 \Big[\sum_{i=1}^{\eta} \bar{v}_i \kappa_n^i - \Big(\frac{2^2}{2} F_1^{(2)} + \frac{2^3}{6} h F_1^{(3)} \\ &+ \frac{2^4}{24} h^2 F_1^{(4)} + \ldots \Big) \Big], \\ LTE'_{n+1} &= h \Big[\sum_{i=1}^{\eta} v_i \kappa_n^i - \Big(2F_1^{(2)} + \frac{2^2}{2} h F_1^{(3)} \\ &+ \frac{2^3}{6} h^2 F_1^{(4)} + \ldots \Big) \Big]. \end{aligned} \tag{13}$$

By substituting (12) into (13) and using MAPLE software to expand it as a Taylor expansion (as introduced by [20]), the order conditions for η-stage TSRKN method of order five are obtained as shown in Table II.

All indexes are from 1 to η. For higher-order TSRKN methods, we can use the simplifying assumption below that reduces the number of equations to be solved:

$$\frac{1}{2} c_i^2 = \sum_{j=1}^{\eta} a_{ij}, \quad i = 1, \ldots, \eta \tag{14}$$

TABLE II
THE ORDER CONDITIONS FOR η-STAGE TSRKN METHOD

Order	Conditions
The order conditions for u_{n+2}	
2	$\sum \bar{v}_i = 2$
3	$\sum \bar{v}_i c_i = \frac{4}{3}$
4	$\frac{1}{2}\sum \bar{v}_i c_i^2 = \frac{2}{3}$
5	$\frac{1}{6}\sum \bar{v}_i c_i^3 = \frac{8}{15}, \quad \sum \bar{v}_i a_{ij} c_j = \frac{8}{15}$
The order conditions for u'_{n+2}	
Order	Conditions
1	$\sum v_i = 2$
2	$\sum v_i c_i = 2$
3	$\frac{1}{2}\sum v_i c_i^2 = \frac{4}{3}$
4	$\frac{1}{6}\sum v_i c_i^3 = \frac{2}{3}, \quad \sum v_i a_{ij} c_j = \frac{2}{3}$
5	$\frac{1}{24}\sum v_i c_i^4 = \frac{8}{15}, \quad \frac{1}{4}\sum v_i c_i a_{ij} c_j = \frac{8}{15}, \quad \frac{1}{2}\sum v_i a_{ij} c_j^2 = \frac{8}{15}$

III. CONSTRUCTION OF EXPLICIT 3-STAGE TSRKN METHOD

Definition 2. The method is said to have order p if p is the largest positive integer such that

$$u(t+2\,h) - u(t+h) - 2\,h\Theta(t;u(t);h) = O(h^{p+1}) \quad (15)$$

where $u(t)$ is the analytical solution as in Dormand [19].
For the derivation of the three-stage TSRKN method of order four, solving simultaneously the algebraic conditions for u_{n+2} and u'_{n+2} up to fourth-order together with the simplifying assumption in Eq. (14), and by imposing c_3 as a free parameter, then the following unique solution will be obtained

$$a_{2,1} = \tfrac{32}{121},\ a_{3,1} = \tfrac{3111}{16000},\ a_{3,2} = \tfrac{20009}{16000},\ \bar{v}_1 = \tfrac{47}{102},$$

$$\bar{v}_3 = \tfrac{400}{1819},\ \bar{v}_2 = \tfrac{847}{642},\ c_2 = \tfrac{8}{11},\ v_1 = \tfrac{47}{204},\ v_2 = \tfrac{1331}{1284},$$

$$v_3 = \tfrac{4000}{5457}.$$

The global error of the fifth-order conditions is defined as follows:

$$\parallel \tau_g^{(5)} \parallel_2 = \sqrt{\sum_{i=1}^{n'_{p+1}} (\tau_i'^{(5)})^2 + \sum_{i=1}^{n_{p+1}} (\tau_i^{(5)})^2}, \quad (16)$$

where $\tau'^{(5)}$ and $\tau^{(5)}$ are the local truncation error terms of the TSRKN method for u'_{n+2} and u_{n+2} respectively and $\tau_g^{(5)}$ is the global truncation error. Based on the free parameter c_3 we get the global truncation error term of fifth-order condition for u_{n+2} and u'_{n+2} as follows:

$$\begin{aligned}\parallel \tau_g^{(5)} \parallel_2 &= \frac{1}{300135}\,(48400000000\,{c_3}^8 + 4356000000\,{c_3}^6 \\ &- 1652062720000\,{c_3}^4 - 106670784000\,{c_3}^3 \\ &+ 40036008100\,{c_3}^2 - 256230451840\,c_3 \\ &+ 15201198248233)^{\frac{1}{2}}.\end{aligned}$$

From empirical experiment, $c_3 = \frac{17}{10}$ provides the accurate method with $\parallel \tau_g^{(5)} \parallel_2 = 6.697279576$, then, the parameters shown by the following Table are the three-stage fourth-order two-step explicit RKN method which is referred to as TSRKN3s4 (see Table III).

TABLE III
THE TSRKN3S4 METHOD

0	0	0	0
$\frac{8}{11}$	$\frac{32}{121}$	0	0
$\frac{17}{10}$	$\frac{3111}{16000}$	$\frac{20009}{16000}$	0
	$\frac{47}{102}$	$\frac{847}{642}$	$\frac{400}{1819}$
	$\frac{47}{204}$	$\frac{1331}{1284}$	$\frac{4000}{5457}$

IV. ANALYSIS OF THE METHOD

This section discusses the convergence, consistency, and stability of the suggested TSRKN method.

A. Consistency

Definition 3. For the multi-step method to be consistent, its order p must be greater than or equal to 1 (see [21]).

Therefore, the derived method is consistent because its order is fourth ($p = 4 \geq 1$).

B. Stability

Definition 4. The multi-step method is said to be zero stable if no root $\zeta_i, i = 1,2$ of the first characteristic polynomial $\chi(\zeta)$ has a modulus greater than one (see [21]).

Rewrite Eq. (5) in matrix form as below:

$$\begin{bmatrix}1 & 0\\0 & 1\end{bmatrix}\begin{bmatrix}u_{n+2}\\hu'_{n+2}\end{bmatrix} = \begin{bmatrix}1 & 2\\0 & 1\end{bmatrix}\begin{bmatrix}u_n\\hu'_n\end{bmatrix},$$

where $I = \begin{bmatrix}1 & 0\\0 & 1\end{bmatrix}$ is the identity matrix coefficient of u_{n+2} and hu'_{n+2}

and $A = \begin{bmatrix}1 & 2\\0 & 1\end{bmatrix}$ is matrix coefficient of u_n and $h\,u'_n$, respectively.

Then, the first characteristic polynomial of TSRKN method is

$$\chi(\zeta) = det[I\zeta - A] = det\begin{vmatrix}\zeta - 1 & 2\\0 & \zeta - 1\end{vmatrix}.$$

$$0 = (\zeta - 1)^2, \quad \zeta = 1, 1. \quad (17)$$

According to Definition 4 and Eq. (17), the TSRKN method is zero stable.

Now, to analyze the linear stability property of the numerical method, we apply method (5) to the following test equation (the same idea implemented in [16]).

$$u'' = -\lambda^2 u, \qquad \lambda > 0. \tag{18}$$

The stability polynomial obtained is as follows:

$$\begin{aligned}\Phi(\xi, H) &= \xi^2 - \left(\frac{4}{55}\,H^3 + \frac{4}{3}\,H^2 + 4\,H + 2\right)\xi \\ &+ \frac{38}{495}\,H^3 + 1.\end{aligned}$$

Where $H = -(\lambda h)^2$, TSRKN3s4 possesses the interval of absolute stability (-2.48,0). From the stability interval, the biggest value of h can be found which can be taken by the method to keep it always stable.

C. Convergence

Definition 5. The method is said to be convergent if it is consistent and zero stable [21].

Since the proposed method has achieved the conditions of consistency and zero stability, this means that the TSRKN3s4 method is convergent.

V. Numerical Experiments

To evaluate the performance of the new TSRKN3s4 method, we are going to use it to solve a set of special second-order ODEs chosen from the scientific literature, and compare the results with existing methods considered in the paper. In the numerical comparisons, we use the maximum error and number of function evaluations criteria.

We use the abbreviations below in our numerical results.

- **TSRKN3s4:** Three-stage two-step RKN method of order four derived in this study.
- **RKN3s4H:** Three-stage RKN direct method of order four given in [22].
- **RKN3s4G:** Three-stage fourth-order RKN method derived by [23].
- **QBSM:** Fourth-order Quintic B-spline collocation method given in [24].
- **PSM:** Quartic spline method given in [25].
- **QSM:** Quadratic spline method given in [26].
- **CSM:** Cubic spline method given in [26].
- **NSM:** Non-polynomial spline method given in [26].
- **3BVP:** Direct three-point block one-step method given in [27].
- **F.N:** The number of function evaluations.
- **Steps:** Number of steps taken.
- **MAXE:** The maximum error recorded in a given interval of the solution.

A. Boundary Value Problems

In this subsection, we use the linear shooting technique together with the TSRKN method for the approximate solution of BVPs.

1) Implementation of the Method: The implementation for solving the Eq. (1) with the mentioned boundary conditions is basically the same with slight differences which can be seen as shown below:
The Eq. (1) with the boundary condition (3) will be replaced into two initial value problems which are as follows:

$$\begin{aligned}&\psi'' = q(t)\,\psi + r(t), \quad \psi(o) = \sigma_1, \quad \psi'(o) = 0,\\ &\bar{\psi}'' = q(t)\,\bar{\psi}, \quad \bar{\psi}(o) = 0, \quad \bar{\psi}'(o) = 1.\end{aligned} \tag{19}$$

Then, by performing the linear combination between these two IVPs in Eq. (19), the linear shooting method will be obtained as follows:

$$\bar{\psi}(t) = \psi(t) + C\,\bar{\psi}(t), \quad \text{where} \quad C = \frac{\varpi - \psi'(d)}{\bar{\psi}'(d)}. \tag{20}$$

The same procedure will be used for solving the Eq. (1) with the boundary condition (4) with slight modifications in terms of the initial conditions and linear shooting method. First, the Eq. (1) with the boundary condition (4) will be replaced into two IVPs with their initial conditions as shown in Eq. (21):

$$\begin{aligned}&\psi'' = q(t)\,\psi + r(t), \quad \psi(o) = 0, \quad \psi'(o) = \sigma_2,\\ &\bar{\psi}'' = q(t)\,\bar{\psi}, \quad \bar{\psi}(o) = 1, \quad \bar{\psi}'(o) = 0.\end{aligned} \tag{21}$$

Then, by performing the linear combination between these two IVPs in Eq. (21), the linear shooting method will be obtained as follows:

$$u(t) = \psi(t) + C\,\bar{\psi}(t), \quad \text{where} \quad C = \frac{\varpi - \psi'(d)}{\bar{\psi}'(d)}. \tag{22}$$

2) Algorithm of Shooting Technique via TSRKN Method:
INPUT: σ_1, σ_2, ϖ boundary conditions; o, d endpoints; N number of subintervals.
OUTPUT: approximations $\varphi_{1,i}$ to $u(t_i)$; $\varphi_{2,i}$ to $u'(t_i)$ for each $i = 0, 1, ..., N$.
Step 1: Set $h = (d - o)/2\,N$;
(For boundary condition (3)), set

$$\begin{aligned}\psi_{1,0} &= \sigma_1;\\ \psi_{2,0} &= 0;\\ \bar{\psi}_{1,0} &= 0;\\ \bar{\psi}_{2,0} &= 1.\end{aligned}$$

(For boundary condition (4)), set

$$\begin{aligned}\psi_{1,0} &= 0;\\ \psi_{2,0} &= \sigma_2;\\ \bar{\psi}_{1,0} &= 1;\\ \bar{\psi}_{2,0} &= 0.\end{aligned}$$

Step 2: For $i = 0, \ldots, N-1$ do Step 3 and Step 4.
(TSRKN method is used in Step 3 and Step 4.)
Step 3: Set $t = o + 2\,ih$.
Step 4: Set

$\kappa^1 = f_1(t,\, \psi_{1,i})$;
$\kappa^i = f_1(t + c_i\,h, \psi_{1,i} + c_i\,h\,\psi_{2,i} + h^2 \sum_{j=1}^{i-1} a_{ij}\,\kappa^j)$;
$\psi_{1,i+2} = \psi_{1,i} + 2\,h\,\psi_{2,i} + h^2 \sum_{i=1}^{\eta} \bar{v}_i\,\kappa^i$;
$\psi_{2,i+2} = \psi_{2,i} + h \sum_{i=1}^{\eta} v_i\,\kappa^i$;

$\bar{\kappa^1} = f_2(t,\, \bar{\psi}_{1,i})$;
$\bar{\kappa^i} = f_2(t + c_i\,h, \bar{\psi}_{1,i} + c_i\,h\,\bar{\psi}_{2,i} + h^2 \sum_{j=1}^{i-1} a_{ij}\,\bar{\kappa^j})$;

$\bar{\psi}_{1,i+2} = \bar{\psi}_{1,i} + 2\,h\,\bar{\psi}_{2,i} + h^2\,\sum_{i=1}^{\eta} \bar{v}_i\,\bar{\kappa^i}$;
$\bar{\psi}_{2,i+2} = \bar{\psi}_{2,i} + h\,\sum_{i=1}^{\eta} v_i\,\bar{\kappa^i}$;
Step 5: (For boundary condition (3)), set

$$\begin{gathered}\varphi_{1,0} = \sigma_1\ ; \\ \varphi_{2,0} = \frac{(\varpi - \psi_{2,N})}{\bar{\psi}_{2,N}}\ ; \\ \text{OUTPUT } (o, \varphi_{1,0}, \varphi_{2,0}).\end{gathered}$$

(For boundary condition (4)), set

$$\begin{gathered}\varphi_{1,0} = \sigma_2\ ; \\ \varphi_{2,0} = \frac{(\varpi - \psi_{2,N})}{\bar{\psi}_{2,N}}\ ; \\ \text{OUTPUT } (o, \varphi_{1,0}, \varphi_{2,0}).\end{gathered}$$

Step 6: For $i = 1, \dots, N$ set

$$\begin{gathered}\Omega 1 = \psi_{1,i} + \varphi_{2,0}\,\bar{\psi}_{1,i}; \\ \Omega 2 = \psi_{2,i} + \varphi_{2,0}\,\bar{\psi}_{2,i}; \\ t = a + 2\,ih; \\ \text{OUTPUT } (t, \Omega 1, \Omega 2).\end{gathered}$$

Step 7: Stop (the process is complete).

Problem 1:
Consider a thin rod of length L which temperature at $x = 0$ is fixed to t_0 while the other endpoint $x = L$ is thermally isolated. Assume that the rod has a cross-section with constant area equal to A and that the perimeter of A is p. The temperature u of the rod at a generic point $x \in (0, L)$ is governed by the following BVP

$$\begin{aligned} -\delta\,A\,u'' + \gamma p\,u &= 0, \quad 0 \le x \le L, \\ u(0) &= u_0, \quad u'(L) = 0, \end{aligned}$$

where δ is the thermal conductivity and γ denotes the convective transfer coefficient. The exact solution of the problem is the (smooth) function

$$u(x) = u_0\,\frac{\cosh(\mu(L-x))}{\cosh(\mu L)},$$

where $\mu = \sqrt{\frac{\gamma p}{\delta A}}$, and assume that the rod's length is $L = 100\,cm$ and that the rod has a circular cross-section of radius $2\,cm$ (and thus, $A = 4\pi cm^2$, $p = 4\pi cm$). Also set $u_0 = 10^\circ\,C$, $\gamma = 2$ and $\delta = 200$.
Source: [28] p.558.

Problem 2: Consider the Reaction-Diffusion application problem
$u'' - 10^{-2}\,u = 0, \quad t \in [0, 1],$
$u(0) = 1, \quad u'(1) = 0.$
Exact solution: $u(t) = \frac{\cosh\sqrt{10^{-2}}\,(1-t)}{\cosh\sqrt{10^{-2}}}$.
Source: [1] p.68.

Problem 3: Consider the linear BVP
$u'' = -u - 1, \quad t \in [0, 1],$
$u'(0) = -u'(1) = \frac{1-\cos(1)}{\sin(1)}.$
Exact solution: $u(t) = \cos(t) + \frac{1-\cos(1)}{\sin(1)}\sin(t) - 1$.
Source: [24].

Problem 4: Consider the linear BVP
$u'' = -tu + (3 - t - t^2 + t^3)\sin(t) + 4t\cos(t), \quad t \in [0, 1],$
$u'(0) = -1, \quad u'(1) = 2\sin(1).$
Exact solution: $u(t) = (t^2 - 1)\sin(t)$.
Source: [25].

B. Initial Value Problems

Problem 5: Consider the two coupled oscillators with different frequencies

$$\begin{cases} u_1'' + u_1 = 2\epsilon u_1 u_2, \quad u_1(0) = 1, \quad u_1'(0) = 0, \\ u_2'' + 2u_2 = \epsilon u_1^2 + 4\epsilon u_2^3, \quad u_2(0) = 1, \quad u_2'(0) = 0. \end{cases}$$

Source: [16].
Where $\epsilon = 10^{-3}$, $0 \le t \le 10$, and the problem is solved with the step sizes $h = 4/(3.2^j)$, $j = 1, 2, 3, 4$ for each method.

Problem 6: Consider a nonlinear wave equation, studied by Jiyong et al. [16]

$$\begin{cases} \frac{\partial^2 u}{\partial t^2} - \frac{\partial^2 u}{\partial x^2} = u^5 - u^3 - 10u, \quad 0 < x < 1, \quad t > 0, \\ u(0,t) = u(1,t) = 0, \quad u(x,0) = \frac{x(1-x)}{100}, \quad u_t(x,0) = 0. \end{cases}$$

This problem is transferred to the ODEs system in time, by using symmetric differences of second-order

$$\begin{cases} \frac{d^2 u_i}{dt^2} - \frac{u_{i+1} - 2u_i + u_{i-1}}{\Delta x^2} = u_i^5 - u_i^3 - 10u_i, \quad 0 < t < t_{end}, \\ u_i(0) = \frac{x_i(1-x_i)}{100}, \quad u_i'(0) = 0, \quad i = 1, \dots, N-1, \end{cases}$$

where $\Delta x = 1/N$ is the spatial mesh step and $x_i = i\Delta x$. This semi-discrete oscillatory system has the form

$$\begin{cases} \frac{d^2 U}{dt^2} + MU = F(t, U), \quad 0 < t < t_{end}. \\ U(0) = \left(\frac{x_1(1-x_1)}{100}, \dots, \frac{x_{N-1}(1-x_{N-1})}{100}\right)^T, \quad U'(0) = 0, \end{cases}$$

where $U(t) = (u_1(t), \dots, u_{N-1}(t))^T$ with $u_i(t) \approx u(x_i, t)$, $i = 1, \dots, N-1$,

$$M = \frac{1}{\Delta x^2}\begin{pmatrix} 2 & -1 & & & \\ -1 & 2 & -1 & & \\ & \ddots & \ddots & \ddots & \\ & & -1 & 2 & -1 \\ & & & -1 & 2 \end{pmatrix}$$

and $F(t, U) = \left(u_1^5 - u_1^3 - 10u_1, \dots, u_{N-1}^5 - u_{N-1}^3 - 10u_{N-1}\right)^T$.
The system is integrated with $N = 20$, in the interval [0, 10] and the step sizes $h = 4/(3.30.j)$, $j = 1, 2, 3, 4$ for each method.

The numerical solution to IVPs 5 and 6 (that have no exact solution) is found by taking the approximate solution obtained by the conventional 3-stage fourth-order RKN3s4G method with small step size h as the exact solution (the idea from [16]).

For comparison purposes, Tables IV, V, VI, VIII, X, and XI summarized the numerical results obtained from the TSRKN3s4, one-step RKN3s4H and RKN3s4G direct methods. These three methods have the same behavior, order and number of stages. In addition, all the numerical results in Tables IV, V, VI, and VIII were computed using the same shooting strategy as explained in Section V.

In solving BVPs, it is observed in Table IV at $h = \frac{1}{16}$, $h = \frac{1}{64}$, and $h = \frac{1}{128}$, the accuracy of RKN3s4H and RKN3s4G is comparable and slightly better than TSRKN3s4. Whereas at $h = \frac{1}{32}$, TSRKN3s4 and RKN3s4H have the same maximum error but RKN3s4G provides better accuracy. In solving Problem 2, at step size $\frac{1}{16}$ and $\frac{1}{32}$, RKN3s4H

TABLE IV
NUMERICAL RESULTS FOR PROBLEM 1 FOR TSRKN3S4, RKN3S4H, AND RKN3S4G METHODS

h	Methods	F.N	Steps	MAXE
$\frac{1}{16}$	TSRKN3s4	48	8	2.020450902 (-2)
	RKN3s4H	96	16	2.380008876 (-3)
	RKN3s4G	96	16	1.114941947 (-3)
$\frac{1}{32}$	TSRKN3s4	96	16	9.999666680 (-4)
	RKN3s4H	192	32	1.296792552 (-4)
	RKN3s4G	192	32	6.268651822 (-5)
$\frac{1}{64}$	TSRKN3s4	192	32	5.659636107 (-5)
	RKN3s4H	384	64	7.451809623 (-6)
	RKN3s4G	384	64	3.662572766 (-6)
$\frac{1}{128}$	TSRKN3s4	384	64	3.318097021 (-6)
	RKN3s4H	768	128	4.471133135 (-7)
	RKN3s4G	768	128	2.216358665 (-7)

TABLE V
NUMERICAL RESULTS FOR PROBLEM 2 FOR TSRKN3S4, RKN3S4H, AND RKN3S4G METHODS

h	Methods	F.N	Steps	MAXE
$\frac{1}{16}$	TSRKN3s4	48	8	3.794742298 (-13)
	RKN3s4H	96	16	4.873879078 (-14)
	RKN3s4G	96	16	2.375877273 (-14)
$\frac{1}{32}$	TSRKN3s4	96	16	2.298161661 (-14)
	RKN3s4H	192	32	3.330669074 (-15)
	RKN3s4G	192	32	1.887379142 (-15)
$\frac{1}{64}$	TSRKN3s4	192	32	1.110223025 (-15)
	RKN3s4H	384	64	1.110223025 (-15)
	RKN3s4G	384	64	1.776356839 (-15)
$\frac{1}{128}$	TSRKN3s4	384	64	6.661338148 (-16)
	RKN3s4H	768	128	8.881784197 (-16)
	RKN3s4G	768	128	3.774758284 (-15)

TABLE VI
NUMERICAL RESULTS FOR PROBLEM 3 FOR TSRKN3S4, RKN3S4H, AND RKN3S4G METHODS.

h	Methods	F.N	Steps	MAXE
$\frac{1}{16}$	TSRKN3s4	48	8	2.350150965 (-8)
	RKN3s4H	96	16	4.091090203 (-8)
	RKN3s4G	96	16	1.506375799 (-7)
$\frac{1}{32}$	TSRKN3s4	96	16	1.519599350 (-9)
	RKN3s4H	192	32	2.553082024 (-9)
	RKN3s4G	192	32	9.436514931 (-9)
$\frac{1}{64}$	TSRKN3s4	192	32	9.641782303 (-11)
	RKN3s4H	384	64	1.595078514 (-10)
	RKN3s4G	384	64	5.901376558 (-10)
$\frac{1}{128}$	TSRKN3s4	384	64	6.068997735 (-12)
	RKN3s4H	768	128	9.968748049 (-12)
	RKN3s4G	768	128	5.901376558 (-11)

and RKN3s4G obtained comparable maximum error which is slightly less than TSRKN3s4 maximum error. At $h = \frac{1}{64}$, all methods recorded similar accuracy. TSRKN3s4 and RKN3s4H obtained the same accuracy that is slightly better than RKN3s4G at $h = \frac{1}{128}$ as represented in Table V. TSRKN3s4 and RKN3s4H achieved the same maximum error at $h = \frac{1}{16}$ and $h = \frac{1}{128}$, which is smallest compared to RKN3s4G. All methods obtained comparable maximum error at $h = \frac{1}{32}$. Besides that, TSRKN3s4 has less one-decimal accuracy than other methods for solving Problem 3 with $h = \frac{1}{64}$ as displayed in Table VI. By observing the numerical results of Table VIII, it is clearly visible that the accuracy of the three methods is almost identical.

In the case of IVPs, two nonlinear problems that have

TABLE VII
COMPARISON OF THE MAXE FOR PROBLEM 3.

Method	h			
	$\frac{1}{16}$	$\frac{1}{32}$	$\frac{1}{64}$	$\frac{1}{128}$
TSRKN3s4	2.350 (-8)	1.519 (-9)	9.641 (-11)	6.068 (-12)
QBSM [24]	2.319 (-8)	1.449 (-9)	9.061 (-11)	5.544 (-12)
PSM [25]	4.528 (-7)	8.423 (-9)	2.211 (-10)	6.408 (-12)
QSM [26]	1.931 (-4)	4.832 (-5)	1.208 (-5)	3.021 (-6)
CSM [26]	1.781 (-4)	4.452 (-5)	1.113 (-5)	2.783 (-6)
NSM [26]	2.160 (-5)	2.677 (-6)	3.331 (-7)	4.154 (-8)

TABLE VIII
NUMERICAL RESULTS FOR PROBLEM 4 FOR TSRKN3S4, RKN3S4H, AND RKN3S4G METHODS.

h	Methods	F.N	Steps	MAXE
$\frac{1}{16}$	TSRKN3s4	48	8	6.710818591 (-7)
	RKN3s4H	96	16	5.697312339 (-7)
	RKN3s4G	96	16	9.807928810 (-7)
$\frac{1}{32}$	TSRKN3s4	96	16	3.974903434 (-8)
	RKN3s4H	192	32	3.519391428 (-8)
	RKN3s4G	192	32	6.049207924 (-8)
$\frac{1}{64}$	TSRKN3s4	192	32	2.414114173 (-9)
	RKN3s4H	384	64	2.185738451 (-9)
	RKN3s4G	384	64	3.753443530 (-9)
$\frac{1}{128}$	TSRKN3s4	384	64	1.486646731 (-10)
	RKN3s4H	768	128	1.361587692 (-10)
	RKN3s4G	768	128	2.337059626 (-10)

TABLE IX
COMPARISON OF THE MAXE FOR PROBLEM 4.

Method	h			
	$\frac{1}{16}$	$\frac{1}{32}$	$\frac{1}{64}$	$\frac{1}{128}$
TSRKN3s4	6.710 (-7)	3.974 (-8)	2.414 (-9)	1.486 (-10)
3BVP [27]	3.49 (-6)	1.87 (-7)	1.28 (-8)	7.76 (-10)
PSM [25]	5.045 (-6)	1.625 (-7)	5.577 (-9)	1.892 (-10)
QSM [26]	3.081 (-3)	7.704 (-4)	1.926 (-4)	4.799 (-5)
CSM [26]	2.883 (-3)	7.207 (-4)	1.802 (-4)	4.504 (-5)
NSM [26]	3.241 (-4)	3.988 (-5)	4.944 (-6)	6.155 (-7)

TABLE X
NUMERICAL RESULTS FOR PROBLEM 5 FOR TSRKN3S4, RKN3S4H, AND RKN3S4G METHODS.

$h = 4/(3.2^j)$	Methods	F.N	Steps	MAXE
$j = 1$	TSRKN3s4	24	7	2.85 (-3)
	RKN3s4H	45	15	1.24 (-3)
	RKN3s4G	45	15	8.13 (-4)
$j = 2$	TSRKN3s4	45	15	7.74 (-4)
	RKN3s4H	135	30	1.47 (-4)
	RKN3s4G	135	30	7.80 (-5)
$j = 3$	TSRKN3s4	90	30	7.20 (-5)
	RKN3s4H	315	60	1.10 (-5)
	RKN3s4G	315	60	5.00 (-6)
$j = 4$	TSRKN3s4	180	60	5.00 (-6)
	RKN3s4H	672	120	4.23 (-2)
	RKN3s4G	672	120	4.23 (-2)

TABLE XI
NUMERICAL RESULTS FOR PROBLEM 6 FOR TSRKN3S4, RKN3S4H, AND RKN3S4G METHODS.

$h = 4/(3.30.j)$	Methods	F.N	Steps	MAXE
$j = 1$	TSRKN3s4	339	112	8.13 (-4)
	RKN3s4H	675	225	7.07 (-4)
	RKN3s4G	675	225	2.27 (-4)
$j = 2$	TSRKN3s4	675	225	5.81 (-4)
	RKN3s4H	2025	450	7.11 (-4)
	RKN3s4G	2025	450	1.07 (-4)
$j = 3$	TSRKN3s4	1014	337	6.02 (-4)
	RKN3s4H	4050	675	7.13 (-4)
	RKN3s4G	4050	675	6.90 (-5)
$j = 4$	TSRKN3s4	1350	450	5.40 (-4)
	RKN3s4H	6750	900	7.14 (-4)
	RKN3s4G	6750	900	5.10 (-5)

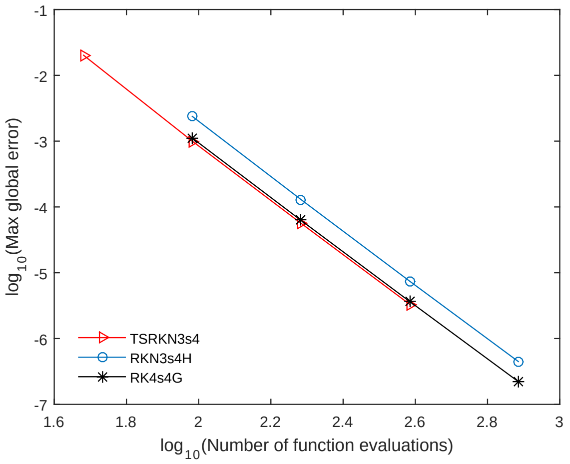

Fig. 1. The Efficiency Curve for Problem 1 with $h = \frac{1}{2^i}, i = 4, \ldots, 7$.

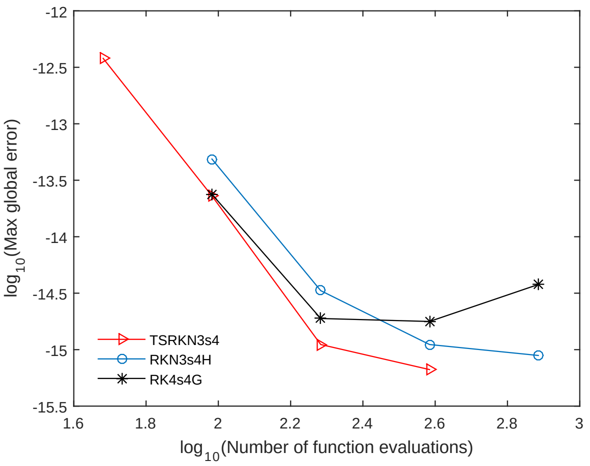

Fig. 2. The Efficiency Curve for Problem 2 with $h = \frac{1}{2^i}, i = 4, \ldots, 7$.

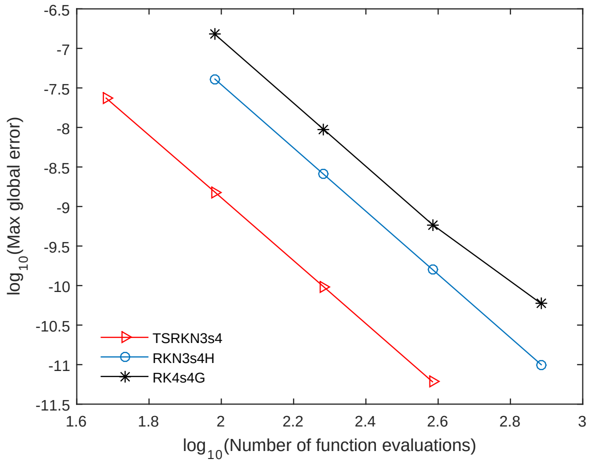

Fig. 3. The Efficiency Curve for Problem 3 with $h = \frac{1}{2^i}, i = 3, \ldots, 7$.

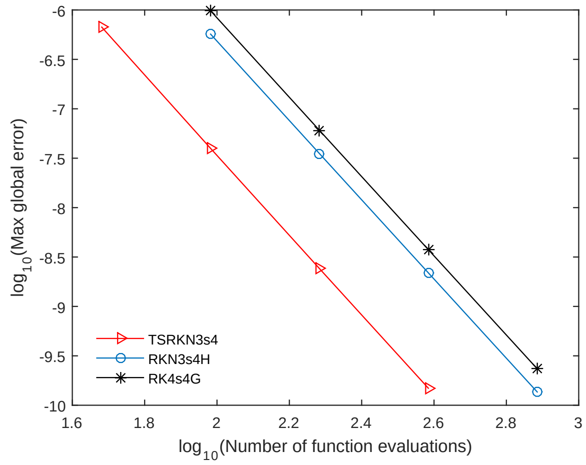

Fig. 4. The Efficiency Curve for Problem 4 with $h = \frac{1}{2^i}, i = 3, \ldots, 7$.

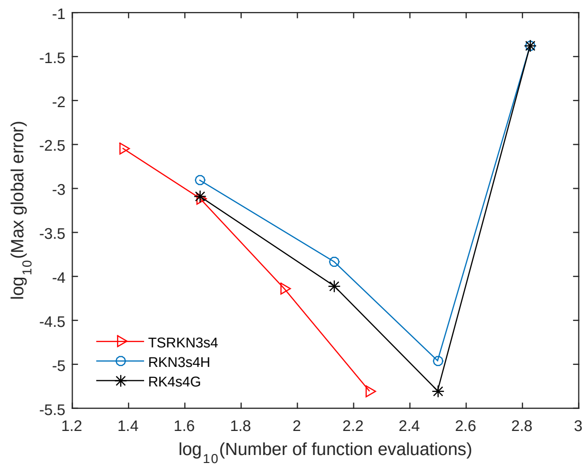

Fig. 5. The Efficiency Curve for Problem 5 with $h = 4/(3.2^j), j = 1, \ldots, 4$.

no exact solution were considered. Tables X and XI show that the proposed method agrees with the RKN3s4H and RKN3s4G methods in terms of maximum error, and this can be seen through the comparable results. Nevertheless, Tables IV, V, VI, VIII, X, and XI demonstrate the superiority of TSRKN3s4 compared to other one-step methods in terms of less number of function evaluations and less number of steps taken (about 50% less). This is due to the TSRKN3s4 method that converges rapidly because the step size taken is bigger (i.e., two steps forward) than the step size used in the one-step method.

It should be noted that all the previous one-step RKN methods are used to solve IVPs in scientific literature and

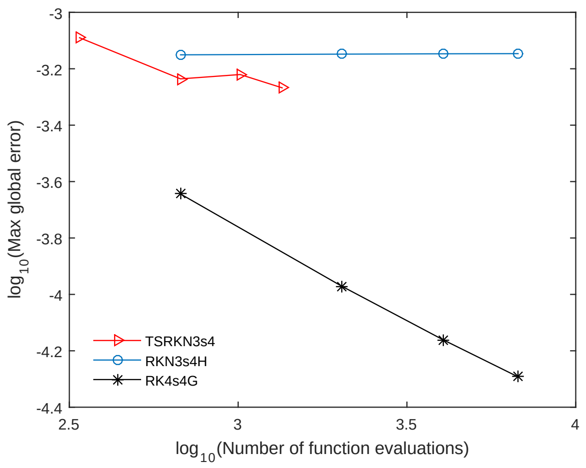

Fig. 6. The Efficiency Curve for Problem 6 with $h = 4/(3.30.j), j = 1, \ldots, 4$.

in order to verify whether the new method is able to solve BVPs or not, a comparison was made using the direct block one-step and spline methods were used to solve this type of problem. Taking into consideration that the direct block, spline, and two-step Runge-Kutta-Nyström methods have different behaviors. As depicted in Table VII, at $h = 1/16$ and $h = 1/64$, the accuracy of TSRKN3s4 and QBSM are comparable. However, TSRKN3s4 obtained better accuracy than PSM, QSM, CSM, and NSM methods. This reflects that TSRKN3s4 achieved the smallest magnitude of error when compared the numerical outputs with the actual solution. At $h = 1/32$ and $h = 1/128$, TSRKN3s4 dominated the QSM, CSM, and NSM methods in terms of accuracy, while the maximum error of TSRKN3s4 is comparable with QBSM and PSM. Table IX demonstrates that TSRKN3s4 obtained superiority in terms of accuracy compared to the other methods at all step sizes, except for $h = 1/64$, where the accuracy of TSRKN3s4 is comparable with PSM, and for $h = 1/128$, where TSRKN3s4 has the same maximum error as PSM and 3BVP methods.

Figures 1-6 represents the efficiency and accuracy of the methods by plotting the graph of the logarithm of the maximum global error against the logarithm number of function evaluations. From the graphs, the TSRKN3s4 method has a lesser number of function evaluations compared to other existing RKN methods. However, the results for Problems 5 and 6 given in Figures 5 and 6 show that TSRKN3s4 method can also be efficiently used to solve problems without exact solutions.

As a concluding remark, the proposed two-step RKN method is a better alternative to existing one-step RKN methods for solving special second-order ODEs because the proposed method manages to give less function call and less number of steps, thus improving the overall efficiency of the method.

VI. Conclusion

In this research, the order conditions of the TSRKN method up to order five were derived. Based on these order conditions, we obtained the three-stage TSRKN method of order four. The results show that the TSRKN method is better compared to one-step RKN methods in terms of number of function evaluations per step. In addition, results shown in Table VII and Table IX are more promising compared to the direct three-point block and spline methods in terms of accuracy. Overall, we can conclude that the two-step RKN approach can be an alternative method to solve special second-order IVPs and BVPs directly.

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