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A NEW IMPROVED RUNGE-KUTTA FORMULA FOR DIRECTLY SOLVING $z''(t) = g(t, z, z')$

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Abstract: This paper deals with the derivation of an explicit two-stage third-order Improved Runge-Kutta Nyström (IRKNG) method for directly solving general second order ordinary differential equations (ODE). This method is two-step and the number of functions to be evaluated per step is less via comparsion to the existing RK methods. Numerical outcomes are offered to show the validity and competency of the newly IRKNG method as comparison with the general RKN and RK techniques.

AMS Subject Classification: 65L05, 65l06
Key Words: IRKNG method; Runge-Kutta Nyström method; second-order ordinary differential equations

1. Introduction

This paper is devoted to the construction of numerical method for solving general second order ordinary differential equations (ODEs) of the form

$$z'' = g(t, z, z'), \quad z(t_0) = z_0, \quad z'(t_0) = z'_0, \quad t \in [t_0, t_n]. \tag{1}$$

This problem often occurs in several fields of engineering and applied science,

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for instance, theoretical chemistry, circuit theory, biology, celestial mechanics, quantum physics, and control theory (see [1, 2, 3]).The conventional approach for solving problem (1) is to reduce to first order ODEs and thus use an appropriate method ([1, 4]). Otherwise, problem (1) has directly solved utilizing hybrid technique, Runge-Kutta Nyström (RKN) formula and two-step method. In the last decades, several authors have given a great attention on developing RKN methods (see [5, 6, 7, 8, 10, 11]).

Franco [9] constructed an explicit RKN formula for solving oscillatory problem $z'' + \omega^2 z = g(t, z, z')$, $\omega > 0$. You *et al.* [11] designed the extended RKN formulas to solve ODEs in form $z'' + Mz = g(z, z')$ and M is a frequency matrix of the problem. In this paper, we are going to construct an explicit Improved Runge-Kutta Nyström methods for solving problem (1), denoted as (IRKNG). The arrangement of the paper as: Construction of the IRKNG formula to solve (1) is given in Section 2. In Section 3, we derived the algebraic order conditions of IRKNG formula. Section 4 is devoted to construct explicit third order IRKNG method with two stage. In the later Section, test problems and numerical outcomes will be presented. Finally, Section 6 is devoted to conclusions.

2. The formulation of the newly IRKNG methods

Motivated by the Rabiei approach [13] to derive the algebraic order conditions for the IRKN formula, we extended the IRKN method to solve problem (1). The following form of IRKNG formula is taken for solving problem (1)

$$z_{n+1} = z_n + h\Big(b_1 g_1 - b_{-1} g_{-1} + \sum\nolimits_{i=2}^{s} b_i (g_i - g_{-i})\Big), \tag{2}$$

$$z'_{n+1} = z'_n + h\Big(b_1 u_1 - b_{-1} u_{-1} + \sum\nolimits_{i=2}^{s} b_i (u_i - u_{-i})\Big), \tag{3}$$

where

$$g_1 = z'_n, \quad g_{-1} = z'_{n-1}, \tag{4}$$

$$u_1 = u(t_n, z_n), \quad u_{-1} = u(t_{n-1}, z_{n-1}), \tag{5}$$

and for $2 \le i \le s$,

$$u_i = u\Big(t_n + c_i h, z_n + h\sum\nolimits_{k=1}^{i-1} a_{ik} g_k, z'_n + h\sum\nolimits_{j=1}^{i-1} a_{ij} u_j\Big), \tag{6}$$

$$u_{-i} = u\Big(t_{n-1} + c_i h, z_{n-1} + h\sum\nolimits_{k=1}^{i-1} a_{ik} g_{-k}, z'_{n-1} + h\sum\nolimits_{j=1}^{i-1} a_{ij} u_{-j}\Big), \tag{7}$$

$$g_i = z'_n + h\sum_{j=1}^{i-1} a_{ij}u_j, \tag{8}$$

$$g_{-i} = z'_{n-1} + h\sum_{j=1}^{i-1} a_{ij}u_{-j}. \tag{9}$$

Inserting (8) into (6) as well as (9) into (7), we get

$$\begin{aligned} u_i = u\Big(t_n + c_ih, z_n + h\sum_{k=1}^{i-1} a_{ik}\Big(z'_n + h\sum_{j=1}^{k-1} a_{kj}u_j\Big),& \\ z'_n + h\sum_{j=1}^{i-1} a_{ij}u_j\Big),& \qquad (10) \\ u_{-i} = u\Big(t_{n-1} + c_ih, z_{n-1} + h\sum_{k=1}^{i-1} a_{ik}\Big(z'_{n-1} + h\sum_{j=1}^{k-1} a_{kj}u_{-j}\Big),& \\ z'_{n-1} + h\sum_{j=1}^{i-1} a_{ij}u_{-j}\Big).& \qquad (11) \end{aligned}$$

By using the row condition $c_i = \sum_{j=1}^{i-1} a_{ij}$ for Runge-Kutta method and after some algebraic manipulation, equations (10) and (11) become

$$u_i = u\Big(t_n + c_ih, z_n + hc_iz'_n + h^2\sum_{j=1}^{i-1} \bar{a}_{ij}u_j, z'_n + h\sum_{j=1}^{i-1} a_{ij}u_j\Big), \tag{12}$$

$$\begin{aligned} u_{-i} = u\Big(t_{n-1} + c_ih, z_{n-1} + hc_iz'_{n-1} + h^2\sum_{j=1}^{i-1} \bar{a}_{ij}u_{-j},& \\ z'_{n-1} + h\sum_{j=1}^{i-1} a_{ij}u_{-j}\Big),& \qquad (13) \end{aligned}$$

where $\bar{a}_{ij} = \sum_{k=1}^{s} a_{ik}a_{kj}$, for $i = 2, 3, \dots, s$. $j = 1, 2, \dots,\ i-1$.

By inserting equations (4), (8) and (9) into equation (2), we obtain

$$\begin{aligned} z_{n+1} = z_n + h\Big(b_1 + \sum_{i=2}^{s} b_i\Big)z'_n - h\Big(b_{-1} + \sum_{i=2}^{s} b_i\Big)z'_{n-1}& \\ + h^2\sum_{i=2}^{s} b_i\sum_{j=1}^{i-1} a_{ij}\Big(u_j - u_{-j}\Big).& \qquad (14) \end{aligned}$$

Substituting the following algebraic order conditions given in [14] into equation (14)

$$b_1 - b_{-1} = 1,$$

$$b_{-1} + \sum_{i=2}^{s} b_i = \frac{1}{2},$$

we obtain

$$z_{n+1} = z_n + \frac{3}{2}hz'_n - \frac{1}{2}hz'_{n-1} + h^2\sum_{i=2}^{s} d_i(u_i - u_{-i}), \tag{15}$$

where $d_i = \sum_{j=1}^{s} b_i a_{ij}, i = 2, \ldots, s$. Replacing u_i with q_i and u_-i with q_{-i} in formulas (3) and (15), also replacing u_1 with q_1 and u_{-1} with q_{-1} in formula (5). Therefore, the general s-stage IRKNG method for solving (1) can be presented as follows:

$$z_{n+1} = z_n + \frac{3}{2}hz'_n - \frac{1}{2}hz'_{n-1} + h^2 \sum_{i=2}^{s} d_i(q_i - q_{-i}), \tag{16}$$

$$z'_{n+1} = z'_n + h\Big(b_1 q_1 - b_{-1} q_{-1} + \sum_{i=2}^{s} b_i(q_i - q_{-i})\Big), \tag{17}$$

where

$$q_1 = g(t_n, z_n), \tag{18}$$

$$q_{-1} = g(t_{n-1}, z_{n-1}), \tag{19}$$

$$q_i = g(t_n + c_i h, z_n + hc_i z'_n + h^2 \sum_{j=1}^{i-1} \bar{a}_{ij} q_j, \quad z'_n + h \sum_{j=1}^{i-1} a_{ij} q_j), \; i = 2, \ldots, s, \tag{20}$$

$$q_{-i} = g(t_{n-1} + c_i h, z_{n-1} + hc_i z'_{n-1} + h^2 \sum_{j=1}^{i-1} \bar{a}_{ij} q_{-j}, \quad z'_{n-1} + h \sum_{j=1}^{i-1} a_{ij} q_{-j}), \; i = 2, \ldots, s. \tag{21}$$

IRKNG method (16)-(21) is expressed using the following Butcher table (see Table 1).

$$\begin{array}{c|c|c} c & \bar{A} & A \\ \hline & b^T & d^T \end{array}$$

Table 1: The IRKNG Method

3. Order conditions for IRKNG method

Taylor series expansion is used to expand the IRKNG method (16)-(21) to get their parameters. After implementing some algebraic simplifications this extension equal to the real solution. Consequently, a nonlinear equations (called the order conditions) have found using Maple algebra package.

The Taylor series expansion of $z(t_n + h)$ and $z'(t_n + h)$ for the method order p are written respectively as follows:

$$z_{n+1} = z(t_n + h) = z(t_n) + hz'(t_n) + \frac{h^2}{2} z''(t_n) + \frac{h^3}{6} z'''(t_n) + \frac{h^4}{24} z^{(iv)}(t_n) + \ldots + O(h^{p+1}), \tag{22}$$

$$z'_{n+1} = z'(t_n + h) = z'(t_n) + hz''(t_n) + \frac{h^2}{2} z'''(t_n) + \frac{h^3}{6} z^{(iv)}(t_n) + \frac{h^4}{24} z^{(v)}(t_n) + \ldots + O(h^{p+1}). \tag{23}$$

Therefore, the algebraic order conditions of s-stage IRKNG formula up to fourth order can be given below.

For z:

$$\text{order three:} \quad \sum\nolimits_{i=2}^{s} d_i = \frac{5}{12}, \tag{24}$$

$$\text{order four:} \quad \sum\nolimits_{i=2}^{s} d_i c_i = \frac{1}{6}. \tag{25}$$

For z':

$$\text{order one:} \quad b_1 - b_{-1} = 1, \tag{26}$$

$$\text{order two:} \quad b_{-1} + \sum\nolimits_{i=2}^{s} b_i = \frac{1}{2}, \tag{27}$$

$$\text{order three:} \quad \sum\nolimits_{i=2}^{s} b_i c_i = \frac{5}{12}, \tag{28}$$

$$\sum\nolimits_{i=2}^{s} \sum\nolimits_{j=1}^{i-1} b_i a a_{ij} = \frac{5}{12}, \tag{29}$$

$$\text{order four:} \quad \sum\nolimits_{i=2}^{s} b_i c_i^2 = \frac{1}{3}, \tag{30}$$

$$\sum\nolimits_{i=3}^{s} \sum\nolimits_{j=2}^{i-1} b_i a a_{ij} c_j = \frac{1}{6}, \tag{31}$$

$$\sum\nolimits_{i=2}^{s} \sum\nolimits_{j=1}^{i-1} b_i a_{ij} = \frac{1}{6}, \tag{32}$$

$$\frac{1}{2} \sum\nolimits_{i=2}^{s} \sum\nolimits_{j=1}^{i-1} b_i a a_{ij}^2 + \sum\nolimits_{i=3}^{s} \sum\nolimits_{j=1}^{i-2} \sum\nolimits_{k=2}^{i-1} b_i a a_{ij} a a_{ik} = \frac{1}{6}, \tag{33}$$

$$\sum\nolimits_{i=2}^{s} \sum\nolimits_{j=1}^{i-1} b_i \, c_i \, a a_{ij} = \frac{1}{3}. \tag{34}$$

4. Construction of the newly IRKNG method

We proceed to derive two-stage IRKNG method of order three, denoted as IRKNG3. The following simplifying conditions are used

$$\sum_{j=1}^{s} aa_{ij} = c_i, \quad \sum_{j=1}^{s} a_{ij} = \frac{1}{2}c_i^2. \tag{35}$$

From (35) we have

$$aa_{21} = c_2, \quad a_{21} = \frac{1}{2}c_2^2. \tag{36}$$

The order conditions of IRKNG3 method must satisfy the following equations

$$d_2 = \frac{5}{12}, \tag{37}$$

$$b_1 - b_{-1} = 1, \tag{38}$$

$$b_{-1} + b_2 = \frac{1}{2}, \tag{39}$$

$$b_2 c_2 = \frac{5}{12}. \tag{40}$$

Solving equations (38) to (40) simultaneously yields a solution depend on c_2 as follows:

$$b_{-1} = \frac{6c_2 - 5}{12c_2}, \tag{41}$$

$$b_1 = \frac{18c_2 - 5}{12c_2}, \tag{42}$$

$$b_2 = \frac{5}{12c_2}. \tag{43}$$

The global truncation error for the fourth order IRKNG3 formula is given by

$$\|\tau_g^{(4)}\|_2 = \sqrt{\sum_{i=1}^{n_{p+1}} \left(\tau_i^{(4)}\right)^2 + \sum_{i=1}^{n_{p+1}} \left(\tau_i'^{(4)}\right)^2},$$

where $\tau^{(4)}$ and $\tau'^{(4)}$ are the truncation error of z and z', respectively. Hence, we have

$$\|\tau_g^{(4)}\|_2 = \frac{1}{24}\sqrt{225\, c_2^2 - 280\, c_2 + 96}. \tag{44}$$

By using the Minimize command in optimization package in Maple software, we obtain $c_2 = \frac{3}{5}$, which gives

$$
\begin{aligned}
\|\tau_g^{(4)}\|_2 &= 1.242259987499 \times 10^{-1}, \\
b_{-1} &= -\frac{7}{36}, \\
b_1 &= \frac{29}{36}, \\
b_2 &= \frac{25}{36}.
\end{aligned}
$$

Finally, the parameters of IRKNG method of two-stage third-order indicated by IRKNG3 can be written as follows (see Table 2).

$$
\begin{array}{c|cc|cc}
0 & 0 & & 0 & \\
\frac{3}{5} & \frac{9}{50} & 0 & \frac{3}{5} & 0 \\
\hline
-\frac{7}{36} & \frac{29}{36} & \frac{25}{36} & & \frac{5}{12}
\end{array}
$$

Table 2: The IRKNG3 Method

5. Problems tested

Some problems are solved to show the efficiency of IRKNG method in this section. We are comparing the numerical result with the currently RKN and RK formulas. In the comparison we have chosen the following methods:

- IRKNG3: the new two-stage IRKNG method of third-order constructed in this paper.
- RKN3C: the RKN method of third-order with three-stage given by Chawla et al. [6].
- RK3B: the RK method of third-order with three-stage given by Butcher [4].
- IRK3F: the third order IRK method with three-stage derived by Rabiei and Ismail [14].

Problem 1. ([16])

$$z'' = -\frac{1}{x}\,z' - \frac{(t^2 - 0.025)}{t^2}\,z,$$
$$z(1) = \sqrt{\frac{2}{\pi}}\,\sin(1) \simeq 0.6713967061418031,$$
$$z'(1) = (2\,\cos(1) - \sin(1))/\sqrt{2\pi} \simeq 0.0954005144474746.$$

The exact solution is

$$z(t) = J_{1/2}(t) = \sqrt{\frac{2}{\pi t}}\,\sin(t), \quad 1 \le t \le 6.$$

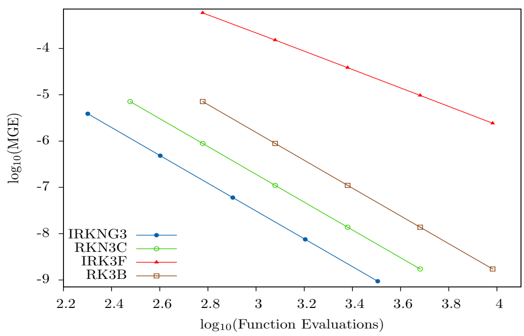

Figure 1: Effectiveness curves with $h = 0.05, 0.025, 0.0125,$ $0.00625, 0.003125$ for Problem 1

Problem 2. (Awoyemi [12])

$$z'' = \frac{(z')^2}{2z} - 2z,$$
$$z(\frac{\pi}{6}) = \frac{1}{4}, \quad z'(\frac{\pi}{6}) = \frac{\sqrt{3}}{2}, \, \pi = 3.14\ .$$

The exact solution is

$$z(t) = \sin^2(t), \quad 1 \le t \le 3.$$

Problem 3. ([15])

$$z'' = -\frac{8}{t}z' - tz + t^5 - t^4 + 44t^2 - 30t,$$

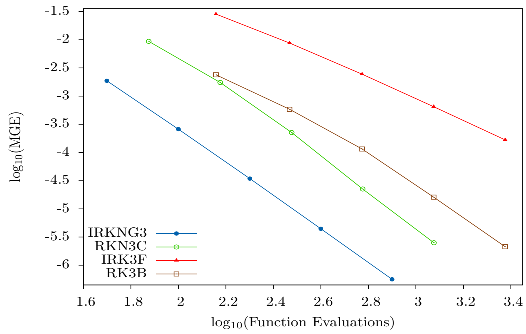

Figure 2: Effectiveness curves with $h = 0.1, 0.05, 0.025,$ $0.0125, 0.00625$ for Problem 2

$$z(1) = 0, \quad z'(1) = 1.$$

The exact solution is

$$z(t) = t^4 - t^3, \quad 1 \leq t \leq 10.$$

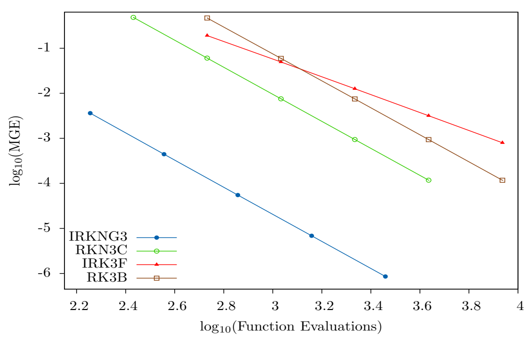

Figure 3: Effectiveness curves with $h = 0.1, 0.05, 0.025,$ $0.0125, 0.00625$ for Problem 3

Problem 4. (Franco [9])

$$z'' = -\omega^2 z - \delta z',$$
$$z(0) = 1, \quad z'(0) = -\delta/2.$$

The exact solution is

$$z(t) = \mathrm{e}^{-\delta t/2} \cos\left(\sqrt{\omega^2 - \delta^2/4}\right) t, \quad 0 \leq t \leq 20.$$

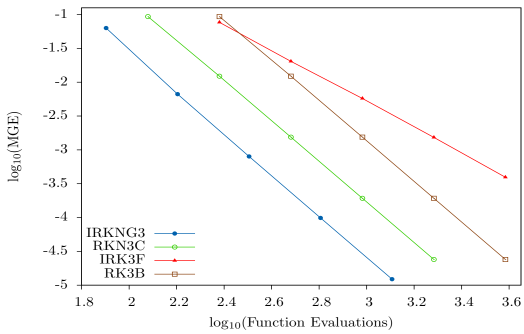

Figure 4: Effectiveness curves with $\omega = 1$, $\delta = 10^{-6}$, $h = 0.5, 0.25, 0.125, 0.0625, 0.03125$ for Problem 4

From Figures 1 to 4, we observed that IRKNG3 performs better efficiency than the existing RKN3C, RK3B and IRK3F methods of the same order.

6. Conclusion

A new third order two stage IRKNG3 method for direct solution of general second-order ODEs has constructed. The order conditions for IRKNG3 method are derived by using the approach of Taylor series expansion. From Numerical results given in all figures, we observed that the IRKNG3 method is better than the existing methods in terms of maximum error and number of function evaluations.

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