Available online at www.isr-publications.com/jmcs
J. Math. Computer Sci. 16 (2016), 205–210
Research Article

Online: ISSN 2008-949x
Journal of Mathematics and Computer Science
Journal Homepage: www.tjmcs.com - www.isr-publications.com/jmcs

An optimized explicit TDRK method for solving oscillatory problems

Yong Wang[a], Min Sun[b,*], Hongchun Sun[a]

[a]School of Business, Linyi University, Linyi, Shandong, 276005, P. R. China.

[b]School of Mathematics and Statistics, Zaozhuang University, Zaozhuang 277160, P. R. China.

Abstract

In this paper, a new optimized explicit two-derivative Runge-Kutta (TDRK) method with frequency-depending coefficients is proposed, which is derived by nullifying the dispersion, the dissipation, and the first derivative of the dispersion. The new method has algebraic order four and is dispersive of order five and dissipative of order four. In addition, the phase analysis of the new method is also presented. Numerical experiments are reported to show the efficiency of the new method.

Keywords: Two-derivative Runge-Kutta method, phase fitting, oscillatory problem.
2010 MSC: 65L05, 65L06.

1. Introduction

In this paper, we are concerned with efficient integrations of the following system of first-order ordinary differential equations (ODEs):

$$y' = f(x, y), \quad y(x_0) = y_0, \tag{1.1}$$

where $y \in \mathcal{R}^N$, and $f : \mathcal{R} \times \mathcal{R}^N \to \mathcal{R}^N$ is a smooth function. Such problems arise in different fileds such as astrophysics, celestial mechanics and molecular physics and so forth.

Many efficient numerical methods have been developed for the numerical solution of problem (1.1), among which, Runge-Kutta (RK) type methods are favorable, because the initial values that are available are sufficient for them to run. In fact, during the last four decades, many efficient RK type methods are designed, such as the exponentially-fitted RK method in [4, 5], the optimized RK method in [6], the phase-fitted RK method in [7], etc. Quite recently, Chan, et al. [2] presented a new type RK method, that is the Two-Derivative Runge-Kutta (TDRK) method, which incorporates the second order derivative in the scheme. Compared with the classical RK type methods, the most prominent characteristic of the TDRK

*Corresponding author
Email addresses: wangyongshandong@sina.com (Yong Wang), ziyouxiaodou@163.com (Min Sun), sunhongchun@lyu.edu.cn (Hongchun Sun)

Received 2016-01-28

method is that it can reach higher order with the same number of stages. In fact, the TDRK method has received the attention of many researchers, and many TDRK methods have been designed. For example, Zhang, et al. [9] firstly extended the idea of trigonometrical fitting to TDRK methods, and proposed a trigonometrically fitted fifth-order TDRK method. Then, Fang, et al. [3] further studied the trigonometrical fitting TDRK (TFTDRK) method and proposed four TFTDRK methods of order four or five. Similarly, in [8], Yang, et al. developed an exponentially fitted TDRK, and applied it to the resonant-state problem of the Woods Saxon potential with fixed step-size and the Lennard-Jones potential with variable step-size. The numerical results in [3, 8, 9] indicate that these new TDRK methods are quite efficient when compared with some famous RK methods in the literature.

Very recently, Anastassi, et al. [1] designed an optimized RK method with zero phase-lag and its derivatives, which is tested to by very efficient for the radial Schrödinger equation. In this paper, we intend to propose a new TDRK method based on the idea of [1]. The rest of the paper is organized as follows. In Section 2, we introduce some necessary definitions for designing the new method. The coefficients of the new optimized TDRK method are presented in Section 3. Section 4 studies the phase property of our new optimized method, and some numerical experiments are given in Section 5. Finally, Section 6 is devoted to some conclusive remarks.

2. The explicit TDRK method

By [2], we can define a modified explicit TDRK method as follows:

$$\begin{cases} Y_i = y_n + c_i h f(x_n, y_n) + h^2 \sum_{j=1}^{i-1} a_{ij} g(x_n + c_j h, Y_j), i = 2, \dots, s, \\ y_{n+1} = y_n + h\beta f(x_n, y_n) + h^2 \sum_{i=1}^{s} b_i g(x_n + c_i h, Y_i), \end{cases} \tag{2.1}$$

where $g(x, y) = y''(x, y) := \frac{\partial f(x,y)}{\partial x} + \frac{\partial f(x,y)}{\partial y} f(x, y)$, and $a_{ij}, b_i, c_i (1 \le j < i \le s)$ and β are some real constants. Obviously, the coefficients of the above iterative scheme can be expressed by the following Butcher tableau:

$$\begin{array}{c|cccc} 0 & 0 & & & \\ c_2 & a_{12} & 0 & & \\ \vdots & \vdots & \vdots & \vdots & \\ c_s & a_{s1} & \cdots & a_{s,s-1} & \\ \hline \beta & b_1 & \cdots & b_{s-1} & b_s \end{array}$$

It is clear that the above TDRK reduces to a traditional TDRK in [2] if $\beta = 1$.

Now we present the phase properties of the above TDRK method following the line of traditional RK method. By applying the explicit TDRK method (2.1) to the following linear scalar equation:

$$y' = \mathrm{i}\omega y, \quad \mathrm{i}^2 = -1, \tag{2.2}$$

in which $\omega > 0$ is an estimate of the principle frequency of the studied problem, we obtain

$$y_{n+1} = M(v) y_n, \quad v = \omega h. \tag{2.3}$$

Here $M(v)$ is called the stability function.

Definition 2.1 ([3]). For the explicit TDRK method (2.1) with stability function $M(v)$, the following quantities are called the *phase-lag* (or *dispersion*) and the *amplification factor error* (or *dissipation error*), respectively:

$$P(v) = v - \arg(M(v)), \quad D(v) = 1 - |M(v)|.$$

In addition, the method is said to be dispersive of order q and dissipative of order p if

$$P(v) = \mathcal{O}(v^{q+1}), \quad D(v) = \mathcal{O}(v^{p+1}).$$

If $P(v) = 0$ and $D(v) = 0$, the method is called *phase fitted* (*zero dispersive*) and *amplification fitted* (*zero dissipative*), respectively.

Denoting $M(v) = U(v) + \mathrm{i}V(v)$ with $U(v)$ and $V(v)$ the real and imaginary parts of $M(v)$, we can derive

$$U(v) = 1 - v^2 b^\top (I + v^2 A)^{-1} e, \quad V(v) = v(1 - v^2 b^\top (I + v^2 A)^{-1} c),$$

where $e = (1, 1, \ldots, 1)^\top \in \mathcal{R}^{s\times 1}$. Thus, we get

$$P(v) = v - \arctan \frac{V(v)}{U(v)}), \quad D(v) = 1 - \sqrt{U(v)^2 + V(v)^2}. \tag{2.4}$$

Then, we can rewrite the functions $U(v)$ an $V(v)$ in the following expand form:

$$\begin{aligned} U(v) &= 1 - r_1 v^2 + r_2 v^4 - r_3 v^6 + \ldots + (-1)^s r_s v^{2s}, \\ V(v) &= v\beta - q_1 v^3 + q_2 v^5 - q_3 v^7 + \ldots + (-1)^s q_s v^{2s+1}, \end{aligned}$$

where the coefficients $r_i, q_i (i = 1, 2, \ldots, s)$ are defined by the above TDRK parameters b and A.

3. The new optimized explicit TDRK method

For simplicity, we consider the two-stage TDRK method given by the Butcher tableau:

$$\begin{array}{c|cc} 0 & 0 & 0 \\ \frac{1}{2} & \frac{1}{8} & 0 \\ \hline \\ \beta(v) & b_1(v) & b_2(v) \end{array}$$

In which, $\beta(v), b_1(v), b_2(v)$ are some real even functions of $v = h\omega$. Obviously, if we set $\{\beta(v), b_1(v), b_2(v)\} = \{1, \frac{1}{6}, \frac{1}{3}\}$, that is the constant coefficients, a classical fourth-order TDRK method in [2] is recovered. In the following, considering that the solution to the problem (1.1) is often oscillatory, we shall derive some frequency-depending coefficients by optimizing the dispersion and dissipation error properties. Motivated by the ideas in [3, 9], by a simple computation, we get the dispersion, the first derivative of dispersion, and the dissipation error of the TDRK method (2.1), which depend on $\beta(v), b_1(v), b_2(v)$ as follows:

$$\begin{cases} P(v) = \tan(v) - \dfrac{M}{N}, \\ D(v) = 1 - \sqrt{M^2 + N^2}, \\ DP(v) = \sec^2(v) - \dfrac{M'N - MN'}{N^2}, \end{cases} \tag{3.1}$$

in which

$$\begin{aligned} M &= \beta(v)v - \frac{1}{2} b_2(v) v^3, \\ N &= 1 - (b_1(v) + b_2(v))v^2 + \frac{1}{8} b_2(v) v^4. \end{aligned}$$

Setting the system of equations in (3.1) equals to zero and solving it yields

$$\begin{aligned} \beta(v) =& \frac{2\sin(v)\cos(v) + (\sin(v))^2 v + 4\sin(v) - 2v}{v(4\cos(v) + \sin(v)v)}, \\ b_1(v) =& (-1/2 - 8\cos(v)v - 4\sin(v)v^2 + 8\sin(v)\cos(v) + 16\sin(v) \\ & - 3\sin(v)v^2\cos(v) - v^3 + 8(\sin(v))^2 v)/(v^3(4\cos(v) + \sin(v)v)), \\ b_2(v) =& -4\frac{\sin(v)\cos(v) + v - 2\sin(v)}{v^3(4\cos(v) + \sin(v)v)}. \end{aligned} \tag{3.2}$$

In some cases, the following Taylor series expansions of (3.2) must be used

$$\begin{aligned}
\beta(v) &= 1 - \frac{1}{120}v^4 + \frac{1}{560}v^6 + \frac{1}{30240}v^8 + \cdots, \\
b_1(v) &= \frac{1}{6} + \frac{1}{30}v^2 - \frac{17}{2520}v^4 + \frac{149}{362880}v^6 - \frac{1027}{15966720}v^8 + \cdots, \\
b_2(v) &= \frac{1}{3} - \frac{1}{30}v^2 + \frac{1}{252}v^4 + \frac{11}{181440}v^6 + \frac{2881}{39916800}v^8 + \cdots.
\end{aligned}$$

Now we are going to check the algebraic order conditions given by [3] for the new optimized method. Second algebraic order:

$$\sum_{i=1}^{2} b_i(v) = \frac{1}{2} - \frac{1}{360}v^4 + \frac{19}{40320}v^6 + \frac{19}{2419200}v^8 + \cdots = \frac{1}{2} + \mathcal{O}(v^4).$$

Third algebraic order:

$$\sum_{i=1}^{2} b_i(v)c_i = \frac{1}{6} - \frac{1}{60}v^2 + \frac{1}{504}v^4 + \frac{11}{362880}v^6 + \frac{2881}{79833600}v^8 + \cdots = \frac{1}{6} + \mathcal{O}(v^2).$$

Fourth algebraic order:

$$\sum_{i=1}^{2} b_i(v)c_i^2 = \frac{1}{12} - \frac{1}{120}v^2 + \frac{1}{1008}v^4 + \frac{11}{725760}v^6 + \frac{2881}{159667200}v^8 + \cdots = \frac{1}{12} + \mathcal{O}(v^2).$$

Therefore, our new proposed method is of order four. By a simple computation, we get the local truncation error of the above method:

$$L.T.E. = \frac{h^5}{17280}(2880y^{(5)} + 144f + 288y'' + 120g_2y^{(3)}) + \mathcal{O}(h^6).$$

4. Analysis of phase properties

Definition 4.1. For the TDRK with stability function $M(\mathrm{i}\theta, v)$, the following two quantities

$$\tilde{P}(\theta, v) = \theta - \arg(M(\mathrm{i}\theta, v)), \quad \tilde{D}(\theta, v) = 1 - |M(\mathrm{i}\theta, v)|$$

are called the phase-lag (dispersion) and amplification factor error (dissipation), respectively. If

$$\tilde{P}(\theta, v) = c_\phi \theta^{q+1} + \mathcal{O}(\theta^{q+3}), \quad \tilde{D}(\theta, v) = c_d \theta^{p+1} + \mathcal{O}(\theta^{p+3}),$$

then the corresponding TDRK is said to be of a phase lag order q and dissipation order p, respectively.

Setting $r = v/\theta = \omega/\lambda$, in which λ denotes the real frequency of the studied fist-order differential equation and ω is the corresponding fitting frequency, we can deduce the phase lag and the dissipation error of the optimized explicit TDRK method derived in the above section:

$$\begin{aligned}
\tilde{P}(\theta, r\theta) &= \frac{(1-r^2)^2}{120}\theta^5 + \mathcal{O}(\theta^7), \\
\tilde{D}(\theta, r\theta) &= \frac{(r^2-1)(4r^2-5)}{720}\theta^6 + \mathcal{O}(\theta^8).
\end{aligned}$$

Thus, the new optimized explicit TDRK has a phase-lag of order four and a dissipation of order five.

5. Numerical results

In this section, we shall compare the new method with some existing highly efficient integrators in the scientific literature, which are listed as follows:

(i) MTDRKA: The first modified TDRK method derived by Fang et al in [3].

(ii) MTDRKB: The second modified TDRK method derived by Fang et al in [3].

(iii) NETDRK: The new explicit TDRK method derived in Section 3.

Problem 5.1. Consider the following inhomogeneous equation

$$y'' + 100y = 99\sin(x), \quad y(0) = 1, y'(0) = 11,$$

which has the following exact solution:

$$y(x) = \cos(10x) + \sin(10x) + \sin(x).$$

Here, we choose $\omega = 10$ and solve the problem numerically on the interval [0, 100]. We list the end-point global error in Table 1, in which h denotes the step-size.

Table 1: Comparison of the end-point global errors

h	MTDRKA	MTDRKB	NETDRK
$1/2^8$	1.7745×10^{-7}	3.5285×10^{-7}	1.8245×10^{-9}
$1/2^9$	5.5992×10^{-9}	1.1082×10^{-8}	1.1370×10^{-10}
$1/2^{10}$	1.7850×10^{-10}	3.4981×10^{-10}	7.0784×10^{-12}

Problem 5.2. Consider the following linear periodic problem:

$$y'' + 10000y = (10000 - 4x^2)\cos(x^2) - 2\sin(x^2), \quad y(0) = 1, y'(0) = 100,$$

which has exact solution:

$$y(x) = \sin(100x) + \cos(x^2).$$

Here we take $\omega = 100$, and the numerical results given in Table 2 are derived with the constant step-size $h = 2^{-9-i}, i = 1, 2, 3, 4$ on the interval [0, 100].

Table 2: Comparison of the end-point global errors

h	MTDRKA	MTDRKB	NETDRK
$1/2^{10}$	1.7×10^{-3}	1.6×10^{-3}	1.7×10^{-3}
$1/2^{11}$	8.4215×10^{-4}	8.3939×10^{-4}	8.4172×10^{-4}
$1/2^{12}$	4.1945×10^{-4}	4.1939×10^{-4}	4.1946×10^{-4}
$1/2^{13}$	2.0936×10^{-4}	2.0936×10^{-4}	2.0936×10^{-4}

The results in Tables 1-2 indicate that our method is comparable to the other two methods.

6. Conclusion

In this paper, a new optimized explicit two-derivative Runge-Kutta method is proposed, which nullifies the dispersion, the dissipation, and the first derivative of the dispersion, and its local truncation error is also given. Some numerical experiments are presented at the end.

Acknowledgments

This work is supported by the Shandong Province Natural Science Foundation (ZR2010AL005) and the Applied Mathematics Enhancement Program of Linyi University.

References

[1] Z. A. Anastassi, T. E. Simos, *An optimized Runge-Kutta method for the solution of orbital problems,* J. Comput. Appl. Math., **175** (2005), 1–9. 1

[2] R. P. K. Chan, A. Y. J. Tasi, *On explicit two-derivative Runge-Kutta methods,* Numer. Algorithms, **53** (2010), 171–194. 1, 2, 2, 3

[3] Y. Fang, X. You, *New optimized two-derivative Runge-Kutta type methods for solving the radial Schrödinger equation,* J. Math. Chem., **52** (2014), 240–254. 1, 2.1, 3, 3, 5

[4] T. E. Simos, *An exponentially-fitted Runge-Kutta method for the numerical integration of initial-value problems with periodic or oscillating solutions,* Comput. Phys. Comm., **115** (1998), 1–8. 1

[5] T. E. Simos, *Exponentially and trigonometrically fitted methods for the solution of the Schrödinger equation,* Acta Appl. Math., **110** (2010), 1331–1352. 1

[6] T. E. Simos, *A two-step method with vanished phase-lag and its first two derivatives for the numerical solution of the Schrödinger equation,* J. Math. Chem., **49** (2011), 2486–2518. 1

[7] T. E. Simos, J. V. Aguiar, *A modified phase-fitted Runge-Kutta method for the numerical solution of the Schrödinger equation,* J. Math. Chem., **30** (2001), 121–131. 1

[8] Y. Yang, K. Wu, Y. Fang, *Exponentially fitted TDRK pairs for the Schrödinger equation,* J. Math. Chem., **53** (2015), 1470–1487. 1

[9] Y. Zhang, H. Che, Y. Fang, X. You, *A new trigonometrically fitted two-derivative Runge-Kutta method for the numerical solution of the Schrödinger equation and related problems,* J. Appl. Math., **2013** (2013), 9 pages. 1, 3