

# A Three-Stage Multiderivative Explicit Runge-Kutta Method

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## ABSTRACT

In recent years, the derivation of Runge-Kutta methods with higher derivatives has been on the increase. In this paper, we present a new class of three stage Runge-Kutta method with first and second derivatives. The consistency and stability of the method is analyzed. Numerical examples with excellent results are shown to verify the accuracy of the proposed method compared with some existing methods.

**Keywords:** Multiderivative; Autonomous; Runge-Kutta; Stability; Convergence; Initial Value Problems

## 1. Introduction

The derivation of Runge-Kutta schemes involving higher derivatives is now on the increase. Traditionally, given an initial value problem (IVP), classical explicit Runge-Kutta methods are derived with the intention of performing multiple evaluations of  $f(y)$  in each internal stage for a given accuracy. Recently, Akanbi [1,2] derived multi-derivative explicit Runge-Kutta method involving up to second derivative. Goeken and Johnson [3] also derived explicit Runge-Kutta schemes of stages up to four with the first derivative of  $f(y)$ . However, the new scheme is derived with the notion of incorporating higher order derivatives of  $f(y)$  up to the second derivative. The cost of internal stage evaluations is reduced greatly and there is an appreciable improvement on the attainable order of accuracy of the method.

## 2. Derivation of the Proposed Scheme

The general form of a single step method for solving the Initial Value Problem (IVP)

$$y'(x) = f(x, y), y(x_0) = y_0 \quad (1)$$

is defined as

$$y_{n+1} = y_n + h\Phi_T(x_n, y_n; h) \quad (2)$$

where  $\Phi_T(x_n, y_n; h)$  is obtained using the Taylor's series expansion of an arbitrary function:

$$\Phi_T(x_n, y_n; h) = \sum_{r=0}^{\infty} \frac{h^r}{(r+1)!} \left( \frac{\partial}{\partial x} + f \frac{\partial}{\partial y} \right)^r f(x, y) \quad (3)$$

and for the autonomous case of (1), in which  $y' = f(y)$ ,  $\Phi_T(x_n, y_n; h)$  becomes

$$\Phi_T(y_n; h) = \sum_{r=0}^{\infty} \frac{h^r}{(r+1)!} \left( f \frac{\partial}{\partial y} \right)^r f(y) \quad (4)$$

The proposed scheme of this paper is of the form

$$y_{n+1} = y_n + h\Phi_{3sMEREK}(x_n, y_n; h) \quad (5)$$

where

$$\Phi_{3sMEREK}(x_n, y_n; h) = (d_1 k_1 + d_2 k_2 + d_3 k_3) \quad (6)$$

$$k_1 = f(y_n)$$

$$k_2 = f\left(y_n + hb_{21}k_1 + c_{21}fh^2f_y + \frac{1}{2}c_{22}h^3(f^2f_{yy} + ff_y^2)\right)$$

$$k_3 = f\left(y_n + hb_{31}k_1 + hb_{32}k_2 + c_{31}fh^2f_y + \frac{1}{2}c_{32}h^3(f^2f_{yy} + ff_y^2)\right)$$

Expanding  $k_2$  and  $k_3$  in Taylor's series and substituting the result into (5), the coefficients of the powers of  $h$  are then compared with that of (3) to obtain the following system of equations:

$$d_1 + d_2 + d_3 = 1$$

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$$b_{21}d_2 + b_{31}d_3 + b_{32}d_3 = \frac{1}{2}$$

$$c_{21}d_2 + (b_{21}b_{32} + c_{31})d_3 = \frac{1}{6}$$

$$\frac{1}{2}b_{21}^2d_2 + \frac{1}{2}(b_{31} + b_{32})^2d_3 = \frac{1}{6}$$

$$\frac{c_{22}d_2}{2} + \left( b_{32}c_{21} + \frac{c_{32}}{2} \right) d_3 = \frac{1}{24}$$

$$b_{21}c_{21}d_2 + \frac{c_{22}d_2}{2} + \left( \frac{1}{2}b_{21}^2b_{32} + b_{21}b_{32}(b_{31} + b_{32}) + b_{31}c_{31} + b_{32}c_{31} + \frac{c_{32}}{2} \right) d_3 = \frac{1}{6}$$

$$\frac{1}{6}b_{21}^3d_2 + \frac{1}{6}(b_{31} + b_{32})^3d_3 = \frac{1}{24}$$

$$\frac{1}{2}b_{32}c_{22}d_3 = \frac{1}{120}$$

$$\frac{1}{2}c_{21}^2d_2 + \frac{1}{2}b_{21}c_{22}d_2 + \left( \frac{1}{2}b_{21}^2b_{32}^2 + b_{21}b_{32}c_{21} + b_{32}(b_{31} + b_{32})c_{21} + \frac{b_{32}c_{22}}{2} + b_{21}b_{32}c_{31} + \frac{c_{31}^2}{2} + \frac{1}{2}(b_{31} + b_{32})c_{32} \right) d_3 = \frac{11}{120}$$

$$\frac{1}{2}b_{21}c_{22}d_2 + \left( \frac{1}{2}b_{21}^2b_{32}(b_{31} + b_{32}) + \frac{1}{2}(b_{31} + b_{32})c_{32} \right) d_3 = \frac{1}{30}$$

Solving the above system of equations, we have the set of solutions in **Table 1**.

The above solution set gives rise to a family of 3-stage multi-derivative explicit Runge-Kutta schemes. The proposed scheme denoted by 3sMERK above is thus given by

$$y_{n+1} = y_n + \frac{h}{6}(k_1 + k_2 + 4k_3)$$

$$k_2 = f \left( y_n + hk_1 + \frac{2}{5}h^2ff_y + \frac{1}{10}h^3(f^2f_{yy} + ff_y^2) \right)$$

$$k_3 = f \left( y_n + \frac{3}{8}hk_1 + \frac{1}{8}hk_2 + \frac{1}{40}h^2ff_y - \frac{1}{80}h^3(f^2f_{yy} + ff_y^2) \right)$$

### 3. Convergence and Stability of the Method

#### 3.1. Existence and Uniqueness of Solution

The properties of the incremental function  $\Phi_{3sMERK}(x_n, y_n; h)$  of the newly derived scheme are in general, very crucial to its stability and convergence characteristics [1,4-8].

**Theorem 3.1.**

Let  $f(x, y)$ , where  $f: \square \times \square^n \rightarrow \square^n$ , be defined and continuous for all  $(x, y)$  in the region  $\mathcal{D}$  defined by

$\mathcal{D} = \{a \leq x \leq b; -\infty \leq y \leq \infty\}$ , where  $a, b$  are finite, and let there exist a constant  $L$  such that

$$\|f(x, y) - f(x, \hat{y})\| \leq L\|y - \hat{y}\| \tag{7}$$

holds every  $(x, y), (x, \hat{y}) \in \mathcal{D}$ , then for any  $\xi \in \square^n$ , there exist a unique solution  $y(x)$  of the problem (1), where  $y(x)$  is continuous and differentiable for all  $(x, y) \in \mathcal{D}$ .

The requirement (7) is known as the Lipschitz's condition, and the constant  $L$  is a Lipschitz's constants [6, 7,9-11]. We shall assume that the hypothesis of this theorem is satisfied by the IVP (1). The following lemma will be useful for establishing the aforementioned characteristics.

**Lemma 3.2.**

Let  $\{\delta_i, i = 0(1)n\}$  be a set of real numbers. If there exist finite constants  $\Gamma$  and  $\Pi$  such that

$$|\delta_{i+1}| \leq \Gamma|\delta_i| + \Pi, i = 0(1)n-1, \tag{8}$$

then

$$|\delta_i| \leq \frac{\Gamma^i - 1}{\Gamma - 1} \Pi + \Gamma^i |\delta_0|, \Gamma \neq 1. \tag{9}$$

**Proof.** When  $i = 0$ , (9) is satisfied identically as  $|\delta_0| \leq |\delta_0|$ .

Suppose (9) holds whenever  $i = j$  so that

$$|\delta_j| \leq \frac{\Gamma^j - 1}{\Gamma - 1} \Pi + \Gamma^j |\delta_0| \tag{10}$$

Then, from (8)  $i = j$  implies that

$$|\delta_{j+1}| \leq \Gamma |\delta_j| + \Pi. \tag{11}$$

On substituting (10) into (11), we have

$$|\delta_{j+1}| \leq \frac{\Gamma^{j+1} - 1}{\Gamma - 1} \Pi + \Gamma^{j+1} |\delta_0|. \tag{12}$$

Hence, (9) holds for all  $i \geq 0$ . □

#### 3.2. Accuracy and Stability

Usually, during the implementation of a computational scheme, errors are generated. The magnitude of the error determines how accurate and stable a scheme is. For instance, if the magnitude of the error is sufficiently small, the computational results would be accurate. However, if the magnitude of the error becomes so large, it can make the method unstable. The sources of error for these schemes and their principal error functions are discussed in Butcher [5,6], Fatunla [7] and Lambert [9, 10]. The following theorem guarantees the stability of the 3sMERK methods.

**Theorem 3.3.**

Suppose the IVP (1) satisfies the hypotheses of Theorem 3.1, then the new 3sMERK algorithm is stable.

**Table 1. Examples of three-stage MERK methods.**

Parameter	Method <sub>1</sub>	Method <sub>2</sub>	Method <sub>3</sub>	3sMERK
$d_1$	$\frac{169}{816}$	$\frac{1}{6}$	$\frac{1}{9}$	$\frac{1}{9}$
$d_2$	$\frac{5488}{7089}$	$\frac{1}{36}(16+\sqrt{6})$	$\frac{1}{36}(16-\sqrt{6})$	$\frac{1}{6}$
$d_3$	$\frac{125}{6672}$	$\frac{1}{36}(16-\sqrt{6})$	$\frac{1}{36}(16+\sqrt{6})$	$\frac{2}{3}$
$b_{21}$	$\frac{17}{28}$	$\frac{1}{10}(6-\sqrt{6})$	$\frac{1}{10}(6+\sqrt{6})$	1
$b_{31}$	$\frac{91976}{10625}$	$\frac{3(-402-197\sqrt{6})}{1250}$	$\frac{3(-402+197\sqrt{6})}{1250}$	$\frac{3}{8}$
$b_{32}$	$\frac{108976}{10625}$	$\frac{2}{625}(489+179\sqrt{6})$	$\frac{2}{625}(489-179\sqrt{6})$	$\frac{1}{8}$
$c_{21}$	$\frac{289}{1568}$	$\frac{3}{100}(7-2\sqrt{6})$	$\frac{3}{100}(7+2\sqrt{6})$	$\frac{2}{5}$
$c_{22}$	$\frac{17}{196}$	$\frac{1}{500}(54-19\sqrt{6})$	$\frac{1}{500}(54+19\sqrt{6})$	$\frac{1}{5}$
$c_{31}$	$\frac{3092}{625}$	$\frac{3(-321-106\sqrt{6})}{2500}$	$\frac{3(-321+106\sqrt{6})}{2500}$	$\frac{1}{40}$
$c_{32}$	$\frac{1823}{625}$	$\frac{-342-37\sqrt{6}}{2500}$	$\frac{-342+37\sqrt{6}}{2500}$	$\frac{1}{40}$

**Proof.** Let  $y_n$  and  $z_n$  be two sets of solutions generated recursively by the 3sMERK method with the initial condition  $y(x_0) = x_0, z(x_0) = z_0, |y_0 - z_0| = \delta_0$ , and

$$\delta_n = |y_n - z_n|, n \geq 0 \tag{13}$$

$$y_{n+1} = y_n + h\Phi_{3sMERK}(x_n, y_n; h) \tag{14}$$

$$z_{n+1} = z_n + h\Phi_{3sMERK}(x_n, z_n; h) \tag{15}$$

It implies that

$$y_{n+1} - z_{n+1} = y_n + z_n + h(\Phi_{3sMERK}(x_n, y_n; h) - \Phi_{3sMERK}(x_n, z_n; h))$$

Applying triangle inequality and (13), we have

$$|\delta_{n+1}| \leq (1 + h\mathcal{L})|\delta_n|, n \geq 0$$

If we assume  $\Gamma = 1 + h\mathcal{L}$ , and  $\Pi = 0$ , then Lemma 3.2 implies that  $|\delta_n| \leq K|\delta_0|$ , where  $K = e^{\mathcal{L}(b-a)} < \alpha$ . This implies the stability of the 3sMERK scheme.  $\square$

### 4. Numerical Experiments

The proposed 3sMERK scheme (6) is applied to the two IVPs below and the results obtained are compared with the standard 3-stage methods of Runge-Kutta (Heun's)

[7,9,10] and that of Goeken and Johnson [3] stated in (16) and (17) respectively.

#### 4.1. Heun's Scheme

$$\left. \begin{aligned} y_{n+1} &= y_n + \frac{h}{4}(K_1 + 3K_3) \\ K_1 &= f(y_n), \\ K_2 &= f\left(y_n + \frac{h}{3}K_1\right), \\ K_3 &= f\left(y_n + \frac{2h}{3}K_2\right). \end{aligned} \right\} \tag{16}$$

#### 4.2. Goeken's Scheme

$$\left. \begin{aligned} y_{n+1} &= y_n + \frac{h}{6}(K_1 + K_2 + 4K_3), \\ K_1 &= f(y_n), \\ K_2 &= f\left(y_n + hK_1 + \frac{1}{2}h^2f_y(y_n)K_1\right), \\ K_3 &= f\left(y_n + \frac{h}{8}(3K_1 + K_2)\right). \end{aligned} \right\} \tag{17}$$

**Table 2. The absolute values of error of  $y(x)$  in Problem 1 using the proposed scheme and other methods,  $h = 0.001; 0.005; 0.025; 0.125$ .**

$h$	$x$	Heun's Method	Goeken's Method	Proposed 3sMERK
0.001	1.00E-01	4.5286E-05	6.6613E-16	1.1102E-16
	2.00E-01	8.1951E-05	2.2204E-15	9.9920E-16
	3.00E-01	1.1123E-04	2.7756E-15	8.8818E-16
	4.00E-01	1.3418E-04	3.3307E-15	9.9920E-16
	5.00E-01	1.5177E-04	3.5527E-15	7.7716E-16
	6.00E-01	1.6478E-04	4.4409E-15	1.3323E-15
	7.00E-01	1.7395E-04	4.8295E-15	1.4433E-15
	8.00E-01	1.7988E-04	4.4964E-15	1.1102E-15
	9.00E-01	1.8310E-04	4.3854E-15	9.9920E-16
	1.00E+00	1.8408E-04	4.2188E-15	8.3267E-16
0.005	1.00E-01	2.2732E-04	4.7329E-13	5.5511E-16
	2.00E-01	4.1132E-04	8.5643E-13	8.8818E-16
	3.00E-01	5.5819E-04	1.1623E-12	6.6613E-16
	4.00E-01	6.7335E-04	1.4025E-12	6.6613E-16
	5.00E-01	7.6149E-04	1.5862E-12	8.8818E-16
	6.00E-01	8.2673E-04	1.7224E-12	9.9920E-16
	7.00E-01	8.7262E-04	1.8180E-12	1.2212E-15
	8.00E-01	9.0226E-04	1.8802E-12	1.3323E-15
	9.00E-01	9.1834E-04	1.9141E-12	1.2212E-15
	1.00E+00	9.2316E-04	1.9243E-12	1.3878E-15
0.025	1.00E-01	1.1592E-03	3.0075E-10	1.2540E-12
	2.00E-01	2.0964E-03	5.4425E-10	2.2693E-12
	3.00E-01	2.8435E-03	7.3869E-10	3.0799E-12
	4.00E-01	3.4284E-03	8.9119E-10	3.7157E-12
	5.00E-01	3.8752E-03	1.0080E-09	4.2024E-12
	6.00E-01	4.2050E-03	1.0945E-09	4.5631E-12
	7.00E-01	4.4361E-03	1.1554E-09	4.8169E-12
	8.00E-01	4.5845E-03	1.1948E-09	4.9812E-12
	9.00E-01	4.6637E-03	1.2162E-09	5.0706E-12
	1.00E+00	4.6858E-03	1.2227E-09	5.0978E-12
0.125	5.00E-01	2.1221E-02	6.8484E-07	1.4309E-08
	1.00E+00	2.5292E-02	8.3075E-07	1.7358E-08

**Table 3. The absolute values of error of  $y(x)$  in Problem 2 using the proposed scheme and other methods,  $h = 0.001; 0.005; 0.025; 0.125$ .**

h	x	Heun's Method	Goeken's Method	Proposed 3sMERK
0.001	1.00E-01	6.0487E-07	8.8818E-16	8.8818E-16
	2.00E-01	1.2336E-06	2.2204E-16	2.2204E-16
	3.00E-01	1.8867E-06	4.4409E-16	4.4409E-16
	4.00E-01	2.5647E-06	8.8818E-16	8.8818E-16
	5.00E-01	3.2680E-06	1.3323E-15	1.3323E-15
	6.00E-01	3.9972E-06	1.5543E-15	1.3323E-15
	7.00E-01	4.7527E-06	1.5543E-15	1.3323E-15
	8.00E-01	5.5351E-06	2.4425E-15	2.2204E-15
	9.00E-01	6.3447E-06	1.5543E-15	1.3323E-15
	1.00E+00	7.1821E-06	2.4425E-15	2.2204E-15
0.005	1.00E-01	3.0216E-06	4.4409E-16	0.0000E+00
	2.00E-01	6.1625E-06	8.8818E-16	2.2204E-16
	3.00E-01	9.4251E-06	1.5543E-15	4.4409E-16
	4.00E-01	1.2812E-05	1.9984E-15	6.6613E-16
	5.00E-01	1.6325E-05	2.2204E-15	8.8818E-16
	6.00E-01	1.9968E-05	2.4425E-15	8.8818E-16
	7.00E-01	2.3743E-05	2.6645E-15	6.6613E-16
	8.00E-01	2.7651E-05	2.8866E-15	4.4409E-16
	9.00E-01	3.1696E-05	3.1086E-15	2.2204E-16
	1.00E+00	3.5879E-05	3.5527E-15	2.2204E-16
0.025	1.00E-01	1.5040E-05	1.9607E-13	0.0000E+00
	2.00E-01	3.0674E-05	3.9857E-13	2.2204E-16
	3.00E-01	4.6914E-05	6.0796E-13	4.4409E-16
	4.00E-01	6.3773E-05	8.2401E-13	4.4409E-16
	5.00E-01	8.1263E-05	1.0476E-12	4.4409E-16
	6.00E-01	9.9397E-05	1.2779E-12	6.6613E-16
	7.00E-01	1.1819E-04	1.5152E-12	6.6613E-16
	8.00E-01	1.3764E-04	1.7601E-12	1.1102E-15
	9.00E-01	1.5778E-04	2.0122E-12	1.1102E-15
	1.00E+00	1.7860E-04	2.2717E-12	1.3323E-15
0.125	5.00E-01	3.9725E-04	6.4241E-10	1.4915E-12
	1.00E+00	8.7330E-04	1.3932E-09	3.0043E-12

### 4.3. Problem 1

Consider the IVP

$$y' = -y, y(0) = 1 \quad (18)$$

with the theoretical solution  $y = e^{-x}$ .

### 4.4. Problem 2

Consider the IVP

$$y' = \frac{y}{4} - \frac{y^2}{80}, y(0) = 1 \quad (19)$$

with the theoretical solution

$$y = \frac{20}{1 + 19e^{-\frac{x}{4}}}.$$

## 5. Conclusions

The results generated by the proposed scheme in this paper when applied to the problems above, evidently proved the extent of accuracy of the scheme. **Tables 2** and **3** above show the absolute error associated with the schemes for the test problems with the variation of the step length. The computations above clearly show the accuracy of the method. The standard Heun's (third order) method grows faster in error than the method of Goeken and the newly derived scheme. However, 3sMERK performed best among the three methods.

Based on the two problems solved above, it follows that the scheme is quite efficient. We therefore conclude that the 3sMERK method proposed is reliable, stable and with high accuracy.

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