

On the Rooted Tree and Component Analysis of an Explicit Fourth-Stage Fourth-Order Runge-Kutta Method

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Abstract

The object of this work is to concentrate on the $f(x,y)$ functional derivatives after using Taylor Series expansion to expand the fourth-stage fourth-order explicit Runge-Kutta method. Efforts will be made to vary the parameters with the aim of getting a fourth order formula that can improve results when implemented on initial-value problems. Efforts will also be made to represent the derived equations and their individual $f(x,y)$ functional derivatives on Butcher's rooted trees. This idea is derivable from general graphs and combinatorics.

Keywords: Rooted tree diagram, Components, explicit, $f(x,y)$ functional derivatives, Runge-Kutta Methods, Linear and non- linear equations, Taylor series, Graphs, Parameters, Initial-value Problems, Combinatorics

1.0 Introduction

The essence of this paper is to concentrate on the $f(x,y)$ functional derivatives after using Taylor Series to expand an explicit fourth- stage fourth- order Runge–Kutta method. The aim is to derive a fourth-stage fourth – order Runge-kutta formula that can improve performance. It also involves representing the derived equations and their individual $f(x,y)$ functional derivatives on Butcher's rooted trees. Scientific implementation of the formula on initial-value problems in ordinary differential equations of the form:

$y^1 = f(x, y), y(x_0) = y_0, a \leq x \leq b, h$ given, with a view to finding out its consistency and accuracy, is also carried out.

Explicit Runge – kutta (ERK) formulas are among the oldest and best – understood schemes in the numerical analysis tool kit. However, according to [1]; “despite the evolutions of a vast and comprehensive body of knowledge, ERK algorithms continue to be sources of active research”. The history of ERK methods began almost a century ago. Classic references are [2],[3] and [4]. According to [5], “the Runge –Kutta methods represent an important family of implicit and explicit iterative methods for approximation of ordinary differential equations in numerical analysis”.

Because of their elegance and simplicity, ERK methods are usually among the first to be taught in the ODE section of a numerical methods course. Thankfully, good quality introductory texts no longer dismiss “the Runge – kutta method” as a fixed step size implementation of the classic 4th order ERK formula. However, significant advancements in the state – of – the – art which post – date the work of [6], even in the fundamental area of deriving ERK formulas, tend to be ignored. According to [7], another side effect of the simple nature of the ERK formula is that a generation of non – experts have been tempted to write their own “quick and dirty” codes. It is widely acknowledged that “squeaky – clean” codes require a great deal of expertise and programming effort. A high – level discussion of some of the issues involved in ERK is found in [8]. Recent work on Runge-Kutta analysis can be found in [9 - 13]. More recent works are in [14 - 16].

The work of Butcher in [17,18,19,20,21] revealed much successes in the analysis of explicit Runge-Kutta methods and their transformation to rooted tree diagrams. This was because the continuation of the process of Taylor Series gives rise to very complicated formulas. It was therefore, advantages to use a graphical representation for a convenient analysis of the order of a Runge – kutta method; hence, the basic tree theory was introduced. A tree is a rooted graph which contains no circuits.

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The symbol T is used to represent the tree with only one vertex. All rooted trees can be represented using T and the operation [t₁, t₂, ..., t_m].

Hence, it is the differentials and equations derived that are represented on trees so as to enable us compare the order condition with their differentials for varying parameters.

References [22,23] pointed out that the Butcher group is the group of characters that had risen independently in their own work on rooted trees analysis in Runge – kutta methods for solving initial-value problems in ordinary differential equations.

Recent works on rooted tree analysis are found in [24 - 28].

Conclusively, despite the fact that good, reliable explicit Runge-Kutta formulas exist, there is still need for their transformation to rooted tree diagrams. Traditionally, Runge – kutta methods are all explicit, although recently, implicit Runge – kutta methods, which have improved weak stability characteristics have been considered. However, the transformation of implicit Runge-Kutta methods to rooted tree diagrams can also be explored.

2.0 Methods of Derivation

- i. From the general Runge-Kutta method, get a Fourth Stage-Fourth order method
- ii. Obtain the Taylor series expansion of k_i's about the point (x_n, y_n), i=2,3,4,
- iii. Carry out substitution to ensure that all the k_i's are in terms of k₁ only.
- iv. Insert the k_i's in terms of k₁ only into b₁k₁ + b₂k₂ + b₃k₃ + b₄k₄
- v. Separate all f(y) functional derivatives with their coefficients from all f(x,y) functional derivatives and their coefficients.
- vi. Discard all f(y) functional derivatives and their coefficients.
- vii. Equate the coefficients of all f(x,y) functional derivatives with the coefficients Taylor series expansion involving only f(x,y) functional derivatives of the form:

$$\phi(x, y, h) = f + \frac{h}{2!}f_x + \frac{h^2}{3!}(f_{xx} + 2ff_{xy} + f_xf_y) + \frac{h^3}{4!}(f_{xxx} + 3ff_{xxy} + 3f^2f_{xyy} + 3f_xf_{xy} + 5ff_yf_{xy} + 3ff_xf_{yy} + f_{xx}f_y + f_xf_y^2) \tag{1}$$

As a result, a set of linear/non-linear equations will be generated. Represent those equations and their f(x, y) functional derivatives on Butcher's rooted tree.

- viii. Vary the set of equations to derive a new fourth-stage fourth-order explicit Runge-Kutta formula.

3.0 Derivation of The Fourth – Order Fourth Stage ERK Method

According to Lambert (1991), the general R – Stage Runge – Kutta method is:

$$y_{n+1} = y_n + h\phi(x_n, y_n, h)$$

$$\phi(x_n, y_n, h) = \sum_{r=1}^R b_r k_r \quad k_1 = f(x, y)$$

$$k_r = f(x + hc_r, y + h \sum_{s=1}^{r-1} a_{rs}k_s), r = 2, 3, \dots, R \tag{2}$$

The formula is defined by the number of stages s, the nodes [c_r]_{r=1}^s, the internal weights [a_{rs}]_{s=1, r=2}^{r-1, s} and the external weights [b_r]_{r=1}^s.

From the above scheme, the fourth stage fourth – order method is:

$$y_{n+1} = y_n + h(b_1k_1 + b_2k_2 + b_3k_3 + b_4k_4) \quad k_1 = f(x_n, y_n)$$

$$k_2 = f(x_n + c_2, y_n + ha_{21}k_1)$$

$$k_3 = f(x_n + c_3h, y_n + h(a_{31}k_1 + a_{32}k_2))$$

$$k_4 = f(x_n + c_4h, y_n + h(a_{41}k_1 + a_{42}k_2 + a_{43}k_3)) \tag{3}$$

Using Taylor's series expansion for k_i's, we have:

$$k_1 = f(x_n, y_n)$$

$$k_2 = \sum_{r=0}^{\infty} \frac{1}{r!} (c_2h \frac{d}{dx} + ha_{21}k_1 \frac{d}{dy})^r f(x_n, y_n)$$

$$k_3 = \sum_{r=0}^{\infty} \frac{1}{r!} (c_3h \frac{d}{dx} + h(a_{31}k_1 + a_{32}k_2) \frac{d}{dy})^r f(x_n, y_n)$$

$$k_4 = \sum_{r=0}^{\infty} \frac{1}{r!} (c_4h \frac{d}{dx} + h(a_{41}k_1 + a_{42}k_2 + a_{43}k_3) \frac{d}{dy})^r f(x_n, y_n) \tag{4}$$

Hence, we have:

$$\begin{aligned}
 k_1 &= f \\
 k_2 &= f + (c_2hf_x + ha_{21}k_1f_y) + \frac{1}{2!}(c_2hf_x + ha_{21}k_1f_y)^2 \\
 &+ \frac{1}{3!}(c_2hf_x + ha_{21}k_1f_y)^3 + \frac{1}{4!}(c_2hf_x + ha_{21}k_1f_y)^4 + 0(h^5) \\
 k_3 &= f + (c_3hf_x + h(a_{31}k_1 + a_{32}k_2)f_y) + \frac{1}{2!}(c_3hf_x + h(a_{31}k_1 + a_{32}k_2)f_y)^2 \\
 &+ \frac{1}{3!}(c_3hf_x + h(a_{31}k_1 + a_{32}k_2)f_y)^3 + \frac{1}{4!}(c_3hf_x + h(a_{31}k_1 + a_{32}k_2)f_y)^4 + 0(h^5) \\
 k_4 &= f + (c_4hf_x + h(a_{41}k_1 + a_{42}k_2 + a_{43}k_3)f_y) + \frac{1}{2!}(c_4hf_x + h(a_{41}k_1 + a_{42}k_2 + a_{43}k_3)f_y)^2 \\
 &+ \frac{1}{3!}(c_4hf_x + h(a_{41}k_1 + a_{42}k_2 + a_{43}k_3)f_y)^3 \\
 &+ \frac{1}{4!}(c_4hf_x + h(a_{41}k_1 + a_{42}k_2 + a_{43}k_3)f_y)^4 + 0(h^5) \tag{5}
 \end{aligned}$$

Expanding fully and substituting the various k_i 's, $i = 2, 3, 4$ into their various positions in terms of k_1 only and collecting like terms, in terms of $f(x, y)$ functional derivatives only, and discarding everything that has to do with $f(y)$ functional derivatives, we have:

$$\begin{aligned}
 k_1 &= f \\
 k_2 &= f + hc_2f_x + \frac{h^2}{2!}c_2^2f_{xx} + h^2c_2a_{21}ff_{xy} + \frac{h^3}{3!}c_2^3f_{xxx} + \\
 &\frac{h^3}{2!}c_2^2a_{21}ff_{xxy} + \frac{h^3}{2!}c_2a_{21}^2f^2f_{xyy} + \frac{h^4}{4!}c_2^4f_{xxxx} + \\
 &\frac{h^4}{3!}c_2^3a_{21}ff_{xxyy} + \frac{h^4}{2!2!}c_2^2a_{21}^2f^2f_{xyyy} + \frac{h^4}{3!}c_2a_{21}^3f^3f_{xyyy} + 0(h^5) \\
 k_3 &= f + hc_3f_x \\
 &+ \frac{h^2}{2!}c_3^2f_{xx} + h^2c_3(a_{31} + a_{32})ff_{xy} + h^2c_2a_{32}f_xf_y + \frac{h^3}{3!}c_3^3f_{xxx} \\
 &+ \frac{h^3}{2!}c_3^2(a_{31} + a_{32})ff_{xxy} + \frac{h^3}{2!}c_3(a_{31}^2 + 2a_{31}a_{32} + a_{32}^2)f^2f_{xyy} \\
 &+ h^3c_2a_{32}(a_{31} + a_{32})ff_xf_y + h^3a_{21}a_{32}(c_2 + c_3)ff_yf_x + \frac{h^3}{2!}c_2^2a_{32}f_yf_{xx} \\
 &+ h^3c_2c_3a_{32}f_xf_{xy} + \frac{h^4}{4!}c_3^4f_{xxxx} + \frac{h^4}{3!}c_2^3a_{32}f_{xxx}f_y + \frac{h^4}{2!}c_2^2c_2a_{32}f_xf_{xxy} \\
 &+ \frac{h^4}{2!}a_{21}a_{32}(c_2^2 + c_3^2)ff_yf_{xy} + \frac{h^4}{3!}a_{21}a_{32}(2c_2a_{31} + 3c_2a_{21} + 6c_3a_{31})f^2f_yf_{xy} \\
 &+ \frac{h^4}{2!}c_3a_{32}c_2^2f_{xx}f_{xy} + \frac{h^4}{2!}c_2^2a_{32}(a_{31} + a_{32})ff_{xx}f_{yy} + \\
 &\frac{h^4}{2!}a_{21}a_{32}(2c_2a_{31} + 2c_2a_{32} + c_3a_{21})f^2f_{xy}f_{yy} + h^4c_3a_{32}c_2a_{21}ff_{xy}^2 + \frac{h^4}{2!}a_{32}^2c_2^2f_x^2f_{yy} \\
 &+ h^4a_{32}^2a_{21}c_2ff_xf_yf_{yy} + \frac{h^4}{2!}c_3c_2a_{32}(6a_{31} + 2a_{32})ff_xf_{xyy} \\
 &+ \frac{h^4}{2!}c_2a_{32}(a_{31}^2 + 2a_{31}a_{32} + a_{32}^2)f^2f_xf_{yyy} + \frac{h^4}{3!}c_3^3(a_{31} + a_{32})ff_{xxyy} \\
 &+ \frac{h^4}{2!2!}c_3^2(a_{31}^2 + 2a_{31}a_{32} + a_{32}^2)f^2f_{xyyy} + \frac{h^4}{3!}c_3(a_{31}^3 + 3a_{31}^2a_{32} + 3a_{31}a_{32}^2 + a_{32}^3)f^3f_{xyyy} + 0(h^5) \\
 k_4 &= f + hc_4f_x + h^2(c_4a_{42} + c_3a_{43})f_xf_y + \\
 &\frac{h^2}{2!}c_4^2f_{xx} + h^2c_4(a_{41} + a_{42} + a_{43})ff_{xy} + \frac{h^3}{2!}(c_2^2a_{42} + c_3^2a_{43})f_{xx}f_y + h^2(c_4a_{21}a_{42} + \\
 &c_3a_{31}a_{43} + c_3a_{32}a_{43})ff_{xy}f_y + h^3c_2a_{32}a_{43}f_xf_y^2 + h^3(c_2c_4a_{42} + c_3c_4a_{43})f_xf_{xy} \\
 &+ h^3c_2a_{32}a_{43}f_xf_y^2 + h^3(c_2c_4a_{42} + c_3c_4a_{43})f_xf_{xy} + h^3(c_2a_{21}a_{42} + c_4a_{31}a_{43} + \\
 &c_4a_{32}a_{43})ff_yf_{xy} + h^3(c_2a_{41}a_{42} + c_3a_{41}a_{43} + c_3a_{42}a_{43} + c_2a_{42}a_{43} + c_2a_{42}^2 +
 \end{aligned}$$

$$\begin{aligned}
 & c_3 a_{43}^2) f f_x f_{yy} + \frac{h^3}{3!} c_3^3 f_{xxx} + \frac{h^3}{2!} (c_4^2 a_{41} + c_4^2 a_{42} + c_4^2 a_{43}) f f_{xxy} + \frac{h^3}{2!} c_4 (a_{41}^2 + 2a_{41} a_{42} + \\
 & 2a_{41} a_{43} + a_{42}^2 + 2a_{42} a_{43} + a_{43}^2) f^2 f_{xyy} + \frac{h^4}{3!} (c_2^3 a_{42} + \\
 & c_3^3 a_{43}) f_{xxx} f_y + \frac{4}{3!} (3c_2^2 a_{21} a_{42} + c_3^2 a_{31} a_{43} + 3c_3^2 a_{32} a_{43} + 3c_4^2 a_{21} a_{42} + 3c_4^2 a_{31} a_{43} + \\
 & 3c_4^2 a_{32} a_{43}) f f_{xxy} f_y + \frac{h^4}{2!} (c_2 a_{21}^2 a_{42} + 2c_3 a_{31} a_{32} a_{43} + c_3 a_{31}^2 a_{43} + c_3 a_{32}^2 a_{43} + \\
 & 2c_4 a_{21} a_{41} a_{42} + 2c_4 a_{31} a_{41} a_{43} + 2c_4 a_{32} a_{41} a_{43} + 2c_4 a_{21} a_{42}^2 + 2c_4 a_{31} a_{42} a_{43} + \\
 & 2c_4 a_{32} a_{42} a_{43} + 2c_4 a_{21} a_{42} a_{43} + 2c_4 a_{31} a_{43}^2 + 2c_4 a_{32} a_{43}^2) f^2 f_y f_{xyy} + \\
 & \frac{h^4}{3!} (c_2^2 a_{32} a_{43}) f_{xx} f_y^2 + h^4 (c_2 a_{21} a_{32} a_{43} + c_3 a_{21} a_{32} a_{43} + c_4 a_{21} a_{32} a_{43}) f f_{xy} f_y^2 + \\
 & \frac{h^4}{2!} (2c_2 a_{31} a_{32} a_{43} + 2c_2 a_{32}^2 a_{43} + 2c_2 a_{32} a_{41} a_{43} + 2c_2 a_{32} a_{42} a_{43} + 2c_2 a_{31} a_{42} a_{43} + \\
 & 2c_2 a_{32} a_{42} a_{43} + 2c_3 a_{21} a_{42} a_{43} + 2c_2 a_{21} a_{42}^2 + c_2 a_{32} a_{43}^2 + c_3 a_{31} a_{43}^2 + c_3 a_{32} a_{43}^2 + \\
 & c_3 a_{31} a_{43}^2 + c_3 a_{32} a_{43}^2) f f_x f_y f_{yy} + h^4 (c_2 c_3 a_{32} a_{43} + c_2 c_4 a_{32} a_{43}) f_x f_y f_{xy} + \\
 & \frac{h^4}{2!} (c_2^2 c_4 a_{42} + c_3^2 c_4 a_{43}) f_{xx} f_{xy} + h^4 (c_2 c_4 a_{21} a_{42} + c_3 c_4 a_{31} a_{43} + c_3 c_4 a_{32} a_{43}) \\
 & f f_{xy}^2 + \frac{h^4}{2!} (c_4 a_{21}^2 a_{42} + c_4 a_{31}^2 a_{43} + 2c_4 a_{31} a_{32} a_{43} + c_4 a_{32}^2 a_{43} + 2c_2 a_{21} a_{41} a_{42} + \\
 & 2c_3 a_{31} a_{41} a_{43} + 2c_3 a_{32} a_{41} a_{43} + 2c_3 a_{31} a_{42} a_{43} + 2c_3 a_{32} a_{42} a_{43} + c_2 a_{21} a_{42}^2 + c_3 a_{31} a_{43}^2 + \\
 & c_3 a_{32} a_{43}^2) f^2 f_{xy} f_{yy} + \frac{h^4}{2!} (2c_2 c_3 a_{42} a_{43} + c_2^2 a_{42}^2 + c_3^2 a_{43}^2) f_x^2 f_{yy} + \frac{h^4}{2!} (c_2 c_4^2 a_{42} + \\
 & c_3 c_4^2 a_{43}) f_x f_{xxy} + h^4 (c_2 c_4 a_{41} a_{42} + c_3 c_4 a_{41} a_{43} + c_2 c_4 a_{42}^2 + c_3 c_4 a_{42} a_{43}) + \\
 & c_2 c_4 a_{42} a_{43} + c_3 c_4 a_{43}^2) f f_x f_{xyy} + \frac{h^4}{2!} (c_2 c_4^2 a_{42} + c_3 c_4^2 a_{43} + 2c_2 a_{41} a_{42}^2 + 2c_3 a_{41} a_{42} a_{43} + \\
 & 2c_2 a_{41} a_{42} a_{43} + c_3 c_4^2 a_{43} + 2c_2 c_4^2 a_{42} a_{43} + 2c_3 a_{41} a_{43}^2 + 2c_3 a_{42} a_{43}^2 + c_2 a_{42} a_{43}^2 + c_2 c_4^2 + \\
 & c_3 a_{43}^2) f^2 f_x f_{yyy} + \frac{h^4}{4!} c_4^4 f_{xxxx} + \frac{h^4}{3!} (c_4^3 a_{41} + c_4^3 a_{42} + c_4^3 a_{43}) f f_{xxx} + \frac{h^4}{2! 2!} c_4^2 (a_{41}^2 + \\
 & 2a_{41} a_{42} + 2a_{41} a_{43} + a_{42}^2 + 2a_{42} a_{43} + a_{43}^2) f^2 f_{xxy} + \frac{h^4}{3!} c_4 (a_{41}^3 + 3a_{41}^2 a_{42} + 3a_{41} a_{42} a_{43} + \\
 & 3a_{41} a_{42}^2 + 6a_{41} a_{42} a_{43} + 3a_{42}^2 a_{43} + 3a_{42} a_{43}^2 + a_{43}^3 + a_{43}^3) f^3 f_{xyy} + \frac{h^4}{2! 2!} (2c_2^2 a_{41} a_{42} + \\
 & 2c_2^2 a_{41} a_{43} + 2c_2^2 a_{42} a_{43} + c_2^2 a_{42}^2 + c_2^2 a_{43}^2) f f_{xx} f_{yy} + 0(h^5). \tag{6}
 \end{aligned}$$

Putting the k'_i ($f(x, y)$ functional derivatives only) into $y_{n+1} = y_n + h(b_1 k_1 + b_2 k_2 + b_3 k_3 + b_4 k_4)$ where $\phi(x, y, h) = b_1 k_1 + b_2 k_2 + b_3 k_3 + b_4 k_4$ and equating coefficients with the Taylor series expansion, we have the equations below:

$$b_1 + b_2 + b_3 + b_4 = 1 \tag{7}$$

$$b_2 c_2 + b_3 c_3 + b_4 c_4 = 1/2 \tag{8}$$

$$b_2 c_2^2 + b_3 c_3^2 + b_4 c_4^2 = 1/3 \tag{9}$$

$$b_2 c_2 a_{21} + b_3 c_3 (a_{31} + a_{32}) + b_4 c_4 (a_{41} + a_{42} + a_{43}) = \frac{1}{3} \tag{10}$$

$$b_3 c_2 a_{32} + b_4 (c_2 a_{42} + c_3 a_{43}) = \frac{1}{6} \tag{11}$$

$$b_2 c_2^3 + b_3 c_3^3 + b_4 c_4^3 = \frac{1}{4} \tag{12}$$

$$b_2 c_2^3 a_{21} + b_3 c_3^2 (a_{31} + a_{32}) + b_4 c_4^2 (a_{41} + a_{42} + a_{43}) = \frac{1}{4} \tag{13}$$

$$\begin{aligned}
 & b_2 c_2 a_{21}^2 + b_3 c_3 (a_{31}^2 + 2a_{21} a_{32} + a_{32}^2) + b_4 c_4 (a_{41}^2 + 2a_{41} a_{42} + \\
 & (a_{41}^2 + 2a_{41} a_{42} + 2a_{41} a_{43} + a_{42}^2 + 2a_{41} a_{43} + a_{43}^2)) = \frac{1}{4} \tag{14}
 \end{aligned}$$

$$b_3 c_2 a_{32} (a_{31} + a_{32}) + b_4 (c_2 a_{42} (a_{41} + a_{42} + a_{43}) + c_3 a_{43} (a_{41} + a_{42} + a_{43})) = 1/8 \tag{15}$$

$$\begin{aligned}
 & b_3 c_{21} a_{32} (c_2 + c_3) + b_4 (c_2 a_{21} a_{42} + c_3 a_{43} (a_{31} + a_{43}) + c_4 a_{21} a_{42} \\
 & + c_4 a_{43} (a_{31} + a_{32})) = \frac{5}{24} \tag{16}
 \end{aligned}$$









$$b_3 c_2^2 a_{32} + b_4 (c_2^2 a_{42} + c_3^2 a_{43}) = \frac{1}{12} \tag{17}$$

$$b_3 c_2 c_3 a_{32} + b_4 (c_2 c_4 a_{42} + c_3 c_4 a_{43}) = \frac{1}{8} \tag{18}$$

$$b_4 c_2 a_{32} a_{43} = \frac{1}{24} \tag{19}$$

Below is Table 1 Showing the above thirteen equations (equations 7 to 19), their $f(x,y)$ functional derivatives and rooted trees:

TABLE 1:

EQUATIONS	DERIVATIVES	R(T)	TREE	T	$\phi(t) = \frac{1}{r(t)}$
$b_1 + b_2 + b_3 + b_4 = 1$	f	1		t	$\sum_{i=1}^4 b_i = 1$
$b_2c_2 + b_3c_3 + b_4c_4 = 1/2$	f_x	2		[t]	$\sum_{i=2}^4 b_i c_i = 1/2$
$b_3a_{32}c_2 + b_4a_{42}c_2 + b_4a_{43}c_3 = 1/6$	f_{xy}	3		[₂ t] ₂	$\sum_{i=3,j=2}^{4,3} b_i a_{ij} c_j = 1/6$
$b_2c_2^2 + b_3c_3^2 + b_4c_4^2 = 1/3$	f_{xx}	3		[t ²]	$\sum_{i=2}^4 b_i c_i^2 = 1/3$
$b_2c_2^2 + b_3c_3^2 + b_4c_4^2 = 1/3$	f_{xy}				
$b_2c_2^3 + b_3c_3^3 + b_4c_4^3 = 1/4$	f_{xxx}	4		[t ³]	$\sum_{i=2}^4 b_i c_i^3 = 1/4$
$b_2c_2^3 + b_3c_3^3 + b_4c_4^3 = 1/4$	f_{xxy}				
$b_2c_2^3 + b_3c_3^3 + b_4c_4^3 = 1/4$	$f^2 f_{xy}$				
$b_4a_{43}a_{32}c_2 = 1/24$	$f_x f_y^2$	4		[3t] ₃	$\sum_{i=4,j=3,k=2}^{4,3,2} b_i a_{ij} a_{jk} c_k = 1/24$
$b_3a_{32}c_2^2 + b_4a_{42}c_2^2 + b_4a_{43}c_3^2 = 1/12$	$f_{xx}f_y$	4		[₂ t ²] ₂	$\sum_{i=3,j=2}^{4,3} b_i a_{ij} c_j^2 = 1/12$
$b_3a_{32}c_2^2 + b_4a_{42}c_2^2 + b_4a_{43}c_3^2 = 1/12$	$f_y f_{xy}$				
$b_3a_{32}c_2c_3 + b_4a_{42}c_2c_4 + b_4a_{43}c_3c_4 = 1/8$	$f f_{xy}$	4		{[t[t]]}	$\sum_{i=3,j=2}^{4,3} b_i c_i a_{ij} c_j = 1/8$
$b_3a_{32}c_2c_3 + b_4a_{42}c_2c_4 + b_4a_{43}c_3c_4 = 1/8$	$f_x f_{xy}$				
$b_3a_{32}c_2c_3 + b_4a_{42}c_2c_4 + b_4a_{43}c_3c_4 = 1/8$	$f_y f_{xy}$				

Hence, set $c_1 = 0, c_4 = 1, c_2 = 1/4, c_3 = 3/4$

(8) becomes $b_2 + 3b_3 + 4b_4 = 2$ (20)

(9) becomes $3b_2 + 27b_3 + 48b_4 = 16$ (21)

(12) becomes $b_2 + 27b_3 + 48b_4 = 16$ (22)

Solving (7), (20), (21) and (22), we have:

$b_1 = 1/18, b_2 = 4/9, b_3 = 4/9, b_4 = 1/18$

From (10), we have: $2a_{21} + 6(a_{31} + a_{32}) + (a_{41} + a_{42} + a_{43}) = 6$ (23)

From (11), we have: $8a_{32} + a_{42} + 3a_{43} = 12$ (24)

From (13), we have: $a_{21} + 9(a_{31} + a_{32}) + 2(a_{41} + a_{42} + a_{43}) = 9$ (25)

From (14), we have: $4a_{21}^2 + 12(a_{31} + a_{32})^2 + 2(a_{41} + a_{42} + a_{43})^2 = 9$ (26)

From (15), we have: $8a_{21}(a_{31} + a_{32}) + a_{42}(a_{41} + a_{42} + a_{43}) + 3a_{42}(a_{41} + a_{42} + a_{43}) = 9$ (27)

From (16), we have: $32a_{31}a_{32} + 5a_{21}a_{42} + 7a_{43}(a_{31} + a_{32}) = 15$ (28)

From (17), we have: $8a_{32} + a_{42} + 9a_{43} = 24$ (29)

From (18), we have: $6a_{32} + a_{42} + 3a_{43} = 9$ (30)

From (19), we have: $a_{32}a_{43} = 3$ (31)

Solving (24), (29) and (30), we have:

$a_{32} = \frac{3}{2}, a_{42} = -6, a_{43} = 2,$

Let $A = a_{21}, B = a_{31} + a_{32}, D = a_{41} + a_{42} + a_{43}$

Hence, (23) becomes: $2A + 6B + D = 6$ (32)

(25) becomes: $A + 9B + 2D = 9$ (33)

(26) becomes: $4A^2 + 12B^2 + 2D^2 = 9$ (34)

(27) becomes: $12B = 9$ (35)

(28) becomes: $18A + 14B = 15$ (36)

From (35) $B = 3/4$ (37)

Hence, (32) becomes: $2A + D = 3/2$ (38)

(33) becomes: $A + 2D = 9/4$ (39)

(34) becomes: $4A^2 + 2D^2 = 9/4$ (40)

From (36), $A = 1/4$ (41)

Putting A into (38), (39) and (40), we get:

$D = 1, A = a_{21} = \frac{1}{4}, B = a_{31} + a_{32} = \frac{3}{4}, a_{31} = -\frac{3}{4}, a_{32} = \frac{3}{2},$ (42)

Also, $D = a_{41} + a_{42} + a_{43} = 1,$ but $a_{42} = -6, a_{43} = 2, a_{41} = 5,$

The parameters put together are:

$C_1 = 0, c_2 = \frac{1}{4}, c_3 = \frac{3}{4}, c_4 = 1, b_1 = \frac{1}{18}, b_2 = \frac{4}{9}, b_3 = \frac{4}{9}, b_4 = \frac{4}{9}$ (43)

Putting (43) into (3), the fourth order method becomes:

$$\begin{aligned}
 y_{n+1} &= y_n + \frac{h}{18} (k_1 + 8k_2 + 8k_3 + k_4) \\
 k_1 &= f(x_n, y_n) \\
 k_2 &= f(x_n + \frac{h}{4}, y_n + \frac{h}{4}k_1) \\
 k_3 &= f(x_n + \frac{3h}{4}, y_n + \frac{h}{4}(-3k_1 + 6k_2)) \\
 k_4 &= f(x_n + h, y_n + h(5k_1 - 6k_2 + 2k_3))
 \end{aligned}
 \tag{44}$$

The Butcher's tableau for the parameters in (44) is:

0				
1/4	1/4			
3/4	-3/4	3/2		
1	5	-6	2	
	1/18	4/9	4/9	1/18

4.0 Implementation of the Formulas and Results

The formula is implemented on the initial – value problems below with the aid of FORTRAN programming language:

- (i) $y^1 = -y, y(0) = 1, 0 \leq x \leq 1, y(x_n) = \frac{1}{e^{xn}}$
- (ii) $y^1 = y, y(0) = 1, 0 \leq x \leq 1, y(x_n) = e^{xn}$
- (iii) $y^1 = 1 + y^2, y(0) = 1, 0 \leq x \leq 1, y(x_n) = \tan(x_n + \pi/4), h = 0.1$

TABLE 2

TABLE OF RESULTS

PROBLEM 1

XN	YN	TSOL	ERROR
.1D+00	0.9048375000000D+00	0.9048374180360D+00	-.8196404044369D-07
.2D+00	0.8187309014063D+00	0.8187307530780D+00	-.1483282683346D-06
.3D+00	0.7408184220012D+00	0.7408182206817D+00	-.2013194597694D-06
.4D+00	0.6703202889175D+00	0.6703200460356D+00	-.2428818514089D-06
.5D+00	0.6065309344234D+00	0.6065306597126D+00	-.2747107467060D-06
.6D+00	0.5488119343763D+00	0.5488116360940D+00	-.2982822888686D-06
.7D+00	0.4965856186712D+00	0.4965853037914D+00	-.3148798197183D-06
.8D+00	0.4493292897344D+00	0.4493289641172D+00	-.3256172068089D-06
.9D+00	0.4065699912001D+00	0.4065696597406D+00	-.3314594766990D-06
.1D+01	0.3678797744125D+00	0.3678794411714D+00	-.3332410563051D-06

PROBLEM 2

XN	YN	TSOL	ERROR
.1D+00	0.1105170833333D+01	0.1105170918076D+01	0.8474231405486D-07
.2D+00	0.1221402570851D+01	0.1221402758160D+01	0.1873094752636D-06
.3D+00	0.1349858497063D+01	0.1349858807576D+01	0.3105134649406D-06
.4D+00	0.1491824240081D+01	0.1491824697641D+01	0.4575605843105D-06
.5D+00	0.1648720638597D+01	0.1648721270700D+01	0.6321032899326D-06
.6D+00	0.1822117962092D+01	0.1822118800391D+01	0.8382985758892D-06
.7D+00	0.2013751626597D+01	0.2013752707470D+01	0.1080873699877D-05
.8D+00	0.2225539563292D+01	0.2225540928492D+01	0.1365200152481D-05
.9D+00	0.2459601413780D+01	0.2459603111157D+01	0.1697376878607D-05
.1D+01	0.2718279744135D+01	0.2718281828459D+01	0.2084323879270D-05

PROBLEM 3

XN	YN	TSOL	ERROR
.1D+00	0.1223051005569D+01	0.1223048880450D+01	-.2125119075158D-05
.2D+00	0.1508502732390D+01	0.1508497647121D+01	-.5085268468541D-05
.3D+00	0.1895771003842D+01	0.1895765122854D+01	-.5880987590245D-05
.4D+00	0.2464942965339D+01	0.2464962756723D+01	0.1979138375674D-04
.5D+00	0.3407951033347D+01	0.3408223442336D+01	0.2724089890727D-03
.6D+00	0.5328707710968D+01	0.5331855223459D+01	0.3147512490389D-02
.7D+00	0.1159500710295D+02	0.1168137380031D+02	0.8636669735614D-01
.8D+00	0.2841447010395D+03	-.6847966834558D+02	-.3526243693850D+03
.9D+00	0.8635045424394D+20	-.8687629546482D+01	-.8635045424394D+20
.1D+01	0.1640237043432+300	-.4588037824984D+01	-.1640237043432+300

5.0 Conclusion

After our implementation, it shows from the tables of numerical results that the method compared favourably well. It also revealed the fact that when the f(x,y) functional derivatives are considered alone it can generate a formula that can improve performance on results. As a result, this will make it less stressful in deriving a formula because the f(Y) functional derivatives were discarded for simplicity sake. Table 1 also revealed how the equations and their individual f(x,y) functional derivatives were represented on Butcher’s rooted trees. Since $\sum_{i=1}^4 b_i = 1$, this shows that the formula is consistent.

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APPENDIX

FORTRAN PROGRAM THAT GENERATED THE RESULTS

PROBLEM 1

```

C PRO
C FOURTH ORDER FOURTH STAGE RUNGE KUTTA METHOD
C OUR PROBLEM IS :Y'=-Y, Y(0)=1
C THEORETICAL SOLUTION:Y(XN)= 1/EXP(XN)
1  DOUBLE PRECISION XN,YN,H,ONE,TWO,EIGHT,EIT,FIV,THREE

```



```

2  DOUBLE PRECISION TSOL,ERROR,K1,K2,K3,K4,SIX,FOUR
3  OPEN(6,FILE='RUNG2.OUT')
4  H=0.1D0
5  YN=1.0D0
6  XN=0.1D0
7  TWO=2.0D0
8  EIGHT=18.0D0
9  EIT=8.0D0
10 THREE=3.0D0
11 FIV=5.0D0
12 FOUR=4.0D0
13 SIX=6.0D0
14 ONE=1.0D0
15 WRITE(6,101)
16 3  K1=-YN
17   K2=- (YN+ONE/FOUR*(H*K1))
18   K3=- (YN+H/FOUR*(-THREE*K1+SIX*K2))
19   K4=- (YN+H*(FIV*K1-SIX*K2+TWO*K3))
20   YN=YN+H/EIGHT*(K1+EIT*K2+EIT*K3+K4)
21   TSOL=ONE/EXP(XN)
22   ERROR=TSOL-YN
23   WRITE(6,100)XN,YN,TSOL,ERROR
24   XN=XN+H
25   IF(XN.LE.ONE) GOTO 3
26 100 FORMAT(D6.1,1X,3(3X,D19.13))
27 101 FORMAT(2X,'XN',13X,'YN',16X,'TSOL',16X,'ERROR')
28   END

```

PROBLEM 2

C PRO

```

C FOURTH ORDER FOURTH STAGE RUNGE KUTTA METHOD
C OUR PROBLEM IS :Y'=Y, Y(0)=1
C THEORETICAL SOLUTION:Y(XN)=EXP(XN)
1  DOUBLE PRECISION XN,YN,H,ONE,THREE,TWO,EIGHT,EIT,FOUR
2  DOUBLE PRECISION TSOL,ERROR,K1,K2,K3,K4,FIVE,SIX
3  OPEN(6,FILE='RUNG2.OUT')
4  H=0.1D0
5  YN=1.0D0
6  XN=0.1D0
7  TWO=2.0D0
8  THREE=3.0D0
9  FOUR=4.0D0
10 SIX=6.0D0
11 ONE=1.0D0
12 EIT=8.0D0
13 EIGHT=18.0D0
14 FIVE=5.0D0
15 WRITE(6,101)
16 3  K1=YN
17   K2=YN+ONE/FOUR*(H*K1)
18   K3=YN+H/FOUR*(-THREE*K1+SIX*K2)
19   K4=YN+H*(FIVE*K1-SIX*K2+TWO*K3)
20   YN=YN+H/EIGHT*(K1+EIT*K2+EIT*K3+K4)
21   TSOL=EXP(XN)
22   ERROR=TSOL-YN
23   WRITE(6,100)XN,YN,TSOL,ERROR
24   XN=XN+H
25   IF(XN.LE.ONE) GOTO 3

```

```

26 100 FORMAT(D6.1,1X,3(3X,D19.13))
27 101 FORMAT(2X,'XN',13X,'YN',16X,'TSOL',16X,'ERROR')
28     END

```

PROBLEM 3

```

C PRO
C FOURTH ORDER FOURTH STAGE RUNGE KUTTA METHOD
C OUR PROBLEM IS :Y'=1+Y**2, Y(0)=1
C THEORETICAL SOLUTION:Y(XN)=TAN(XN+PI/4)
1  DOUBLE PRECISION XN,YN,H,ONE,TWO,EIGHT,PI,THREE,EIT
2  DOUBLE PRECISION TSOL,ERROR,K1,K2,K3,K4,SIX,FOUR,FIV
3  OPEN(6,FILE='RUNG2.OUT')
4  H=0.1D0
5  YN=1.0D0
6  ONE=1.0D0
7  FOUR=4.0D0
8  XN=0.1D0
9  TWO=2.0D0
10 EIGHT=18.0D0
11 EIT=8.0D0
12 THREE=3.0D0
13 FIV=5.0D0
14 SIX=6.0D0
15 PI=FOUR*DATAN(ONE)
16 WRITE(6,101)
17 3  K1=ONE+YN*YN
18     K2=ONE+(YN+(H/FOUR)*K1)**TWO
19     K3=ONE+(YN+(H/FOUR)*(-THREE*K1+SIX*K2))**TWO
20     K4=ONE+(YN+H*(FIV*K1-SIX*K2+TWO*K3))**TWO
21     YN=YN+H/EIGHT*(K1+EIT*K2+EIT*K3+K4)
22     TSOL=TAN(XN+(PI/FOUR))
23     ERROR=TSOL-YN
24     WRITE(6,100)XN,YN,TSOL,ERROR
25     XN=XN+H
26     IF(XN.LE.ONE) GOTO 3
27 100 FORMAT(D6.1,1X,3(3X,D19.13))
28 101 FORMAT(2X,'XN',13X,'YN',16X,'TSOL',16X,'ERROR')
29     END

```