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An Implicit Runge-Kutta Type Method for the Solution of Initial Value Problems

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Abstract

In this research paper, an implicit block hybrid Backward Differentiation Formula (BDF) for $k = 2$ is reformulated into a Runge-Kutta Type Method (RKTM) of the same step number. The method can be used to solve both first and second order (special or general form) initial value problem in Ordinary Differential Equation (ODE). This method differs from conventional BDF as derivation is done only once. It can also be extended to solve higher order ODE.

Keywords: Implicit, Runge-kutta Type, Initial value problems, Block, Backward Differentiation Formula (BDF)

1. Introduction

Ordinary Differential Equations arise frequently in the study of the physical problems. Unfortunately many cannot be solved exactly (Akinfenwa *et al*, 2011). This is why the ability to solve these equations numerically is important. Traditionally, mathematicians have used one of two classes of methods for solving numerically ordinary differential equations. These are Runge –Kutta methods and Linear Multistep Methods (LMM) (Rattenbury,2005).

Runge Kutta (RK) methods are very popular because of their symmetrical forms, have simple coefficients, very efficient and numerically stable (Agams, 2012). The methods are fairly simple to program, easy to implement and their truncation error can be controlled in a more straight forward manner than multistep methods (Kendall, 1989).

The application of Runge-Kutta methods have provided many satisfactory solutions to many problems that have been regarded as insolvable. The popularity and the explosive growth of these methods coupled with the amount of research effort being undertaken are further evidence that the applications are still the leading source of inspiration for mathematical creativity (Yahaya Y.A. and Adegboye Z.A, 2013).

The significance of numerical solution of Ordinary Differential Equations (ODE) in scientific computation cannot be over emphasized as they are used to solve real life problems such as chemical reactions. Most of these problems come in higher order ODE. One way of solving these higher order ODE is by reduction to a system of first order and then applying any suitable method. This approach has some drawbacks, such as waste of computer time and human efforts (Yahaya, Y.A. & Adegboye, Z.A, 2011). The idea propose in this work is to solve the higher order ODE directly without reduction to first order. This saves computer time and human effort, there is gain in efficiency and accuracy, contains minimal function evaluation and lower computational cost.

This paper seek to reformulate the Block Backward Differentiation Formulae (Hybrid and Non-hybrid) for $k = 2$ into Runge Kutta Type Method for the solution of Initial Value Problems in Ordinary Differential Equations (ODE) of the form

$$y' = f(x, y) \qquad y(x_0) = y \tag{1}$$

$$y'' = f(x, y) \qquad y(x_0) = y \quad y'(x_0) = \beta \tag{2}$$

$$y'' = f(x, y, y') \qquad y(x_0) = y \quad y'(x_0) = \beta \tag{3}$$

Consider the numerical solution of the Initial Value Problem that has benefits such as self-starting, high order, low error constants, satisfactory stability property such as A-stability and low implementation cost. These emphasize the combination of multistep structure with the use of off grid points and seek a method that is both multistage and multivalue. This will help to extend the general linear formulation to the high order Runge Kutta case by considering a polynomial

$$y(x) = \sum_{j=1}^{t-1} \alpha_j(x)\, y_{n+j} + h \sum_{j=1}^{m-1} \beta_j\, f(\bar{x}_j, y(\bar{x}_j)) \tag{4}$$

Where t denotes the number of interpolation points $x_{n+j}, j = 0,1 \dots . t-1$ and m denotes the distinct collocation points $\bar{x}_j \epsilon [x_n, x_{n+k}], j = 0,1 \dots . . m-1$ chosen from the given step $[x_n, x_{n+k}]$.

Butcher defined an S-stage Runge Kutta method for the first order differential equation in the form

$$y_{n+1} = y_n + h \sum_{i,j=1}^{s} a_{ij} k_i \tag{5}$$

where for $i = 1,2 \dots \dots \dots . s$

$$k_i = f(x_i + \alpha_j h, y_n + h \sum_{i,j=1}^{s} a_{ij} k_j) \tag{6}$$

The real parameters α_j, k_i, a_{ij} define the method. The method in Butcher array form can be written as

$$\begin{array}{c|c} \alpha & \beta \end{array}$$

| b^T

Where $a_{ij} = \beta$

The Runge Kutta Nystrom (RKN) method is an extension of Runge Kutta method for second order ODE of the form

$$y'' = f(x, y, y') \qquad y(x_0) = y_0 \quad y'(x_0) = y'_0 \tag{7}$$

An S-stage implicit Runge Kutta Nystrom for direct integration of second order initial value problem is defined in the form

$$y_{n+1} = y_n + \alpha_i h y'_n + h^2 \sum_{i,j=1}^{s} a_{ij} k_j \tag{8a}$$

$$y'_{n+1} = y'_n + h \sum_{i,j=1}^{s} \bar{a}_{ij}\, k_j \tag{8b}$$

where for $i = 1,2 \dots \dots \dots . s$

$$k_i = f(x_i + \alpha_j h, y_n + \alpha_i h y'_n + h^2 \sum_{i,j=1}^{s} a_{ij} k_j \,, y'_n + h \sum_{i,j=1}^{s} \bar{a}_{ij}\, k_j) \tag{8c}$$

The real parameters $\alpha_j, k_j, a_{ij}, \bar{a}_{ij}$ define the method, the method in butcher array form is expressed as

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

$A = a_{ij} = \beta^2 \qquad \bar{A} = \bar{a}_{ij} = \beta \qquad \beta = \beta e$

2. Materials and Method

Consider the approximate solution to (1) in the form of power series

$$y(x) = \sum_{j=0}^{t+m-1} \alpha_j x^j \tag{9}$$

$\alpha \in R, j = 0(1)t + m - 1, y \in C^m(a, b) \subset P(x)$

$$y'(x) = \sum_{j=0}^{t+m-1} j\alpha_j x^{j-1} \tag{10}$$

Where α_j's are the parameters to be determined, t and m are the points of interpolation and collocation respectively.

When $K = 2$, we interpolate $(t = 3)$ at $j = 0, \frac{1}{2}, 1$ and collocate $(m = 1)$ at $j = 2$. The equation can be expressed as

$$y(x) = \sum_{j=0}^{t+m-1} \alpha_j x^j = y_{n+j} \qquad j = 0, \frac{1}{2}, 1 \tag{11}$$

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$$y'(x) = \sum_{j=0}^{t+m-1} j\alpha_j x^{j-1} = f_{n+j} \qquad j = 2 \tag{12}$$

The general form of the method upon addition of one off grid point is expressed as;

$$\bar{y}(x) = \alpha_1(x)y_n + \alpha_2(x)y_{n+1} + \alpha_3 y_{n+\frac{1}{2}} + h\beta_0(x)f_{n+2} \tag{13}$$

The matrix D of dimension $(t+m)*(t+m)$ of the proposed method is expressed as:

$$D = \begin{bmatrix} 1 & x_n & x_n^2 & x_n^3 \\ 1 & x_n + h & (x_n+h)^2 & (x_n+h)^3 \\ 1 & x_n + \frac{1}{2}h & \left(x_n + \frac{1}{2}h\right)^2 & \left(x_n + \frac{1}{2}h\right)^3 \\ 0 & 1 & 2x_n + 4h & 3(x_n+2h)^2 \end{bmatrix}$$

Using the maple software package, we invert the matrix D, to obtain columns which form the matrix C. The elements of C are used to generate the continous coefficients of the method as:

$$\begin{aligned} \alpha_1(x) &= C_{11} + C_{21}x + C_{31}x^2 + C_{41}x^3 \\ \alpha_2(x) &= C_{12} + C_{22}x + C_{32}x^2 + C_{42}x^3 \\ \alpha_3(x) &= C_{13} + C_{23}x + C_{33}x^2 + C_{43}x^3 \\ \beta_0(x) &= C_{14} + C_{24}x + C_{34}x^2 + C_{44}x^3 \end{aligned} \tag{14}$$

The values of the continuous coefficients (14) are substituted into (13) to give

the continuous form of the two step block hybrid BDF with one off step interpolation point.

$$\bar{y}(x) = \Big\{\Big(\frac{1}{13}\frac{13h^3+44x_nh^2+41x_n^2h+10x_n^3}{h^3} - \frac{2}{13}\frac{22h^2+41x_nh+15x_n^2}{h^3}x + \frac{1}{13}\frac{41h+30x_n}{h^3}x^2 + \frac{-10}{13h^3}x^3\Big)y_n + \left(\frac{1}{13}\frac{x_n(20h^2+47x_nh+14x_n^2)}{h^3} - \frac{2}{13}\frac{10h^2+47x_nh+21x_n^2}{h^3}x + \frac{1}{13}\frac{47h+42x_n}{h^3}x^2 - \frac{14}{13h^3}x^3\right)y_{n+1} + \left(\frac{1}{3}\frac{x_n(2x_n+h)}{h} + \frac{8}{13}\frac{9x_n^2+22x_nh+8h^2}{h^3}x + \frac{-8}{13}\frac{9x_n+11h}{h^3}x^2 + \frac{24}{13h^3}x^3\right)y_{n+\frac{1}{2}} + \Big(\frac{-1}{13}\frac{x_n(2x_n^2+3x_nh+h^2)}{h^2} + \frac{1}{13}\frac{6x_n^2+6x_nh+h^2}{h^2}x - \frac{3}{13}\frac{2x_n+h}{h^2}x^2 + \frac{2}{13h^2}x^3\Big)f_{n+2}\Big\} \tag{15}$$

Evaluating (15) at point $x = x_{n+2}$ and its derivative at $x = x_{n+1/2}, x = x_{n+1}$ yields

the following three discrete hybrid schemes which are used as block integrator

$$\frac{-36}{13}y_{n+1} + y_{n+2} + \frac{32}{13}y_{n+\frac{1}{2}} = \frac{9}{13}y_n + \frac{6}{13}hf_{n+2}$$

$$\frac{33}{12}y_{n+1} + y_{n+\frac{1}{2}} = \frac{21}{12}y_n + \frac{26}{12}hf_{n+\frac{1}{2}} + \frac{1}{12}hf_{n+2} \tag{16}$$

$$y_{n+1} - \frac{40}{32}y_{n+\frac{1}{2}} = -\frac{8}{32}y_n + \frac{13}{32}hf_{n+1} - \frac{1}{32}hf_{n+2}$$

The equation is of order $[3,3]^T$ with error constant $\left[-\frac{3}{52}, \frac{17}{832}, -\frac{19}{624}\right]^T$

Rearranging the block hybrid scheme simultaneously we obtained the following block scheme

$$\begin{aligned} y_{n+\frac{1}{2}} &= y_n + \frac{h}{72}(0f_n + 64f_{n+\frac{1}{2}} - 33f_{n+1} + 5f_{n+2}) \\ y_{n+1} &= y_n + \frac{h}{72}\left(0f_n + 80f_{n+\frac{1}{2}} - 12f_{n+1} + 9f_{n+2}\right) \\ y_{n+2} &= y_n + \frac{h}{72}\left(0f_n + 8f_{n+\frac{1}{2}} + 6f_{n+1} + 4f_{n+2}\right) \end{aligned} \tag{17}$$

Reformulating the block hybrid method with the coefficient as characterized by the butcher array form

$$\begin{array}{c|c} \alpha & \beta \\ \hline & b^T \end{array}$$

Where $a_{ij} = \beta$

Gives

$$\begin{array}{c|cccc} 0 & 0 & 0 & 0 & 0 \\ \frac{1}{2} & 0 & \frac{8}{9} & \frac{-11}{24} & \frac{5}{72} \\ 2 & 0 & \frac{8}{9} & \frac{2}{3} & \frac{4}{9} \\ 1 & 0 & \frac{10}{9} & \frac{-1}{6} & \frac{1}{18} \\ \hline & 0 & \frac{10}{9} & \frac{-1}{6} & \frac{1}{18} \end{array}$$

The butcher table is being rearranged with the off grid points appearing first, followed by the $c_{i's}$ in descending order. This is done in order to satisfy the consistency condition.

Using equation (5), gives an implicit 4-stage block Runge Kutta Type method of uniform order three everywhere on the interval of solution

$$y_{n+\frac{1}{2}} = y_n + h(0k_1 + \frac{8}{9}k_2 - \frac{11}{24}k_3 + \frac{5}{72}k_4)$$

$$y_{n+2} = y_n + h\left(0k_1 + \frac{8}{9}k_2 + \frac{2}{3}k_3 + \frac{4}{9}k_4\right) \tag{18}$$

$$y_{n+1} = y_n + h\left(0k_1 + \frac{10}{9}k_2 - \frac{1}{6}k_3 + \frac{1}{18}k_4\right)$$

Where

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

$$k_2 = f(x_n + \frac{1}{2}h, y_n + h\{\frac{8}{9}k_2 - \frac{11}{24}k_3 + \frac{5}{72}k_4\})$$

$$k_3 = f(x_n + h, y_n + h\{\frac{10}{9}k_2 - \frac{1}{6}k_3 + \frac{1}{8}k_4\})$$

$$k_4 = f(x_n + 2h, y_n + h\{\frac{8}{9}k_2 + \frac{2}{3}k_3 + \frac{4}{9}k_4\}))$$

Extending the method (18) with the coefficients as characterized in the butcher array form

α	$\bar{A}$	A
	$\bar{b}^T$	b

$A = a_{ij} = \beta^2$ $\qquad \bar{A} = \bar{a}_{ij} = \beta$ $\qquad \beta = \beta e$

Gives

0	0	0	0	0	0	0	0	0
$\frac{1}{2}$	0	$\frac{8}{9}$	$\frac{-11}{24}$	$\frac{5}{72}$	0	$\frac{37}{108}$	$\frac{-41}{144}$	$\frac{29}{432}$
2	0	$\frac{8}{9}$	$\frac{2}{3}$	$\frac{4}{9}$	0	$\frac{52}{57}$	$\frac{-2}{9}$	$\frac{8}{27}$
1	0	$\frac{10}{9}$	$\frac{-1}{6}$	$\frac{1}{18}$	0	$\frac{23}{27}$	$\frac{-2}{9}$	$\frac{5}{54}$
	0	$\frac{10}{9}$	$\frac{-1}{6}$	$\frac{1}{18}$	0	$\frac{23}{27}$	$\frac{-2}{9}$	$\frac{5}{54}$

The butcher table is being rearranged with the off grid points appearing first, followed by the $c_{i's}$ in descending order. This is done in order to satisfy the consistency condition.

Using equations (8), we obtained an implicit 4 stage block Runge kutta Type method of uniform order 3 everywhere on the interval of solution.

$$y_{n+\frac{1}{2}} = y_n + \frac{1}{2}hy_n' + h^2\left(0k_1 + \frac{37}{108}k_2 - \frac{41}{144}k_3 + \frac{29}{432}k_4\right),$$

$$y'_{n+\frac{1}{2}} = y_n' + h\left(0k_1 + \frac{8}{9}k_2 - \frac{11}{24}k_3 + \frac{5}{72}k_4\right)$$

$$y_{n+2} = y_n + 2hy_n' + h^2\left(0k_1 + \frac{52}{27}k_2 - \frac{2}{9}k_3 + \frac{8}{27}k_4\right),$$

$$y'_{n+2} = y_n' + h\left(0k_1 + \frac{8}{9}k_2 + \frac{2}{3}k_3 + \frac{4}{9}k_4\right)$$

$$y_{n+1} = y_n + hy_n' + h^2\left(0k_1 + \frac{23}{27}k_2 - \frac{4}{9}k_3 + \frac{5}{54}k_4\right), \quad (19)$$

$$y'_{n+1} = y_n' + h\left(0k_1 + \frac{10}{9}k_2 - \frac{1}{6}k_3 + \frac{1}{18}k_4\right)$$

where

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

$$k_2 = f(x_n + \frac{1}{2}h, y_n + \frac{1}{2}hy_n' + h^2\left(0k_1 + \frac{37}{108}k_2 - \frac{41}{144}k_3 + \frac{61}{1728}k_4\right),$$

$$y'_{n+\frac{1}{2}} = y_n' + h\left(0k_1 + \frac{8}{9}k_2 - \frac{11}{24}k_3 + \frac{5}{72}k_4\right))$$

$$k_3 = f(x_n + h, y_n + hy_n' + h^2\left(0k_1 + \frac{23}{27}k_2 - \frac{4}{9}k_3 + \frac{5}{54}k_4\right),$$

$$y'_{n+1} = y_n' + h\left(0k_1 + \frac{10}{9}k_2 - \frac{1}{6}k_3 + \frac{1}{18}k_4\right))$$

$$k_4 = f(x_n + 2h, y_n + 2hy_n' + h^2\left(0k_1 + \frac{52}{27}k_2 - \frac{2}{9}k_3 + \frac{8}{27}k_4\right),$$

$$y_n' + h\left(0k_1 + \frac{8}{9}k_2 + \frac{2}{3}k_3 + \frac{4}{9}k_4\right))$$

3. Results and Discussion

Problem: Odigure et al(2009)

In their study, Odigure etal (2009), developed a mathematical model for the process of limestone decarbonisation to produce quicklime (CaO) according to chemical reaction shown in equation (22)

$$CaCO_3 \rightarrow CaO + CO_2 \quad (22)$$

It has been reported that the quality of CaO produce is dependent on the chemical and microstructure composition, density and burning conditions (temperature, CO_2 concentration and particle size). The mathematical model for the decomposition of calcium carbonate is represented by the relationship presented in Equation (23)

$$\frac{d^2T_C}{dr^2} + \frac{2}{r}\frac{dT_C}{dr} - \frac{\rho_p k_1 C_c \Delta H}{k_e} = 0 \quad (23)$$

$$\frac{dT_c}{dr} = 0 \text{ at } r = 0 \quad (24)$$

Where

$k_e =$ effective thermal conductivities= $3\,W/m.K$

$C_c =$ concentration of CO_2 in the gas stream

$\rho_p = 2710kg/m^3$

The concentration of the CO_2 in the gas stream can be estimated from the relationship presented in equation (4)

$$\frac{d^2C_C}{dr^2} + \frac{2}{r}\frac{dC_C}{dr} - \frac{\rho_p k_1 C_c \Delta H}{(D_k)_e} = 0 \quad (25)$$

$$\frac{dC_c}{dr} = 0 \text{ at } r = 0$$

The time taken to produce quicklime from calcium carbonate and conversion of calcium carbonate to calcium oxide can be estimated from the relationship shown in equation (26) and (27) respectively;

$$t = \frac{\rho_A}{3M_A k_m C_c}\frac{(r_s - r)^3}{r^2} \quad (26)$$

$$X_A = 1 - \frac{3M_A K C_c r^2 t}{\rho_A r_s^3} \quad (27)$$

$$(D_k)_e = 9.70 \times 10^3 \alpha \left(\frac{T_c}{M_A}\right)^{0.5}$$

$$k_1 = Ae^{-\frac{E}{R_g T}}$$

$A = 2.01 \quad E = 4.062 \times 10^4 \quad R_g = 8.314J/mol.K \quad \rho_A = 2710kg/m^3 \quad k_m = 0.03m/s$

The performance of the Runge-Kutta method on this problem will determine the various temperatures of conversions, the time taken to produce quicklime from calcium carbonate and conversion of calcium carbonate to calcium oxide at various values of the step numbers (k_s).

Table 2: $K = 2$ second order RKTM

r	$T_o = 600$ T	$T_o = 650$ T	$T_o = 700$ T
0.1	634	684	734
0.2	736	786	836
0.3	804	854	904
0.4	908	958	1008
0.5	981	1030	1080
0.6	1085	1135	1185
0.7	1184	1234	1284
0.8	1291	1341	1391
0.9	1410	1460	1510
1.0	1518	1568	1618

Presented in Table 2 are the solution to equation (23) using the developed method. It can be observed from the table of results that with each respective initial temperatures, as the particle size increases (r), so does the decarbonization temperature used to decompose it to produce the required final texture of the limestone.

The time taken and rate of conversion is given in the following table below.

Table 3 : $K = 2$ second order RKTM

r_s	$C_c = 13.204$	$t(sec)$
0.01	13.2892	0
0.02	13.5447	0.0051
0.03	13.7150	0.0399
0.04	13.9762	0.1322
0.05	14.1579	0.3093
0.06	14.4198	0.5932
0.07	14.6030	1.0122
0.08	14.8650	1.5791
0.09	15.0484	2.3283
0.1	15.3105	3.2584

Based on the result of simulation obtained, the rate of conversion $X_A = 0.99$ for the various times, it means that there is 99% conversion of the product.

Results also shown the time taken to achieve the decarbonization of limestone as a function of the particle radius. Presented in Table 3 are the solution to equation (25) which indicate that the further the distance from the centre, the higher the concentration of the product obtained, so also the time taken.

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