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DEVELOPMENT OF A NEW CLASS OF BLOCK IMPLICIT RUNGE-KUTTA TYPE METHOD FOR INITIAL VALUE PROBLEMS

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ABSTRACT

In this study, we propose a new class of Runge-Kutta type method with three stages for the solution of initial value problems. The method was developed through the collocation approach and reformulated into a Runge-Kutta type of first order using the Butcher analysis. The first order method was extended to a second order one using the Runge –Kutta Nystrom method. A convergence analysis was carried out in order to determine the order, error constant and stability analysis.Numerical examples carried out on the Initial value problems further substantiate the effectiveness and viability of the methods.

Keywords: *Block, Implicit, Runge-Kutta type, Initial value problems.*

1. INTRODUCTION

Ordinary Differential Equations arise frequently in the study of the physical problems in aspects of science and engineering. Unfortunately, many cannot be solved exactly. 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 methodsKutta methods have provided many satisfactory solutions to many problems that have been regarded as insolvable. The popularity and the 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 & Adegboye, 2011).

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 ordinary differential equations. One way of solving these higher order ordinary differential equations 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,(Agams A S, 2012). The idea in this work is to solve the higher order ODE directly without reduction to first order. This saves computer time and human effort based on the fact that, there is gain in efficiency and accuracy, contains minimal function evaluation and lower computational cost.

In this study, we seek to reformulate the Block Backward Differentiation Formulae (Hybrid and Non-hybrid) for k=1 into Runge Kutta Type Method with three (3) stages for the solution of Initial Value Problems in Ordinary Differential Equations (ODE) of the form

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

$$y'' = f(x,y) \qquad y(x_0) = y \;\; y'(x_0) = \beta \qquad (2)$$

$$y'' = f(x,y,y') \qquad y(x_0) = y \;\; y'(x_0) = \beta \qquad (3)$$

We 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. We 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 enable us to extend the general linear formulation to the high order Runge-Kutta case by considering a polynomial

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

Where t denotes the number of interpolation points $x_{n+j}, j = 0,1 \ldots . t-1$ and m denotes the distinct collocation points $\bar{x}_j \epsilon [x_n, x_{n+k}], j = 0,1 \ldots\ldots m-1$ chosen from the given step $[x_n, x_{n+k}]$(Butcher, 2003).

METHODOLOGY

Butcher (2003) defined an S-stage Runge-Kutta method for the first order differential equation in the form

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

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

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

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

α	β
	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

$$y'' = f(x,y,y') \qquad y(x_0) = y_0 y'(x_0) = y_0' \quad (7)$$

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

$$y_{n+1} = y_n + \alpha_i h y_n' + h^2 \textstyle\sum_{i,j=1}^{s} a_{ij} k_j \qquad (8a)$$

$$y_{n+1}' = y_n' + h \textstyle\sum_{i,j=1}^{s} \bar{a}_{ij}\, k_j \qquad (8b)$$

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

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

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

α	$\bar{A}$	A
	$\bar{b}^T$	b

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

1.1 Construction of the method

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

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

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

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

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

When $K = 1$, we interpolate equation (9) at $j = 0, \frac{1}{2}$ and collocate equation (10) at $j = 1$. Equations (9)& (10)can then be expressed as

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

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

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

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

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

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

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:

$$\left.\begin{aligned} \alpha_1(x) &= C_{11} + C_{21}x + C_{31}x^2 \\ \alpha_2(x) &= C_{12} + C_{22}x + C_{32}x^2 \\ \beta_0(x) &= C_{13} + C_{23}x + C_{33}x^2 \end{aligned}\right\} \qquad (14)$$

The values of the continuous coefficients equation (14) are substituted into equation (13) to give the continuous form of the one step block hybrid Backward Differentiation Formula (BDF) with one off step interpolation point.

$$\bar{y}(x) = \left\{\left(\frac{1}{3}\frac{(2x_n+h)(2x_n+3h)}{h^2} - \frac{8}{3}\frac{x_n+h}{h^2}x + \frac{4}{3h^2}x^2\right)y_n + \left(\frac{-4}{3}\frac{x_n(x_n+2h)}{h^2} + \frac{8}{3}\frac{x_n+h}{h^2}x - \frac{4}{3h^2}x^2\right)y_{n+\frac{1}{2}} + \left(\frac{1}{3}\frac{x_n(2x_n+h)}{h} - \frac{1}{3}\frac{4x_n+h}{h}x + \frac{2}{3h}x^2\right)f_{n+1}\right\} \qquad (15)$$

Evaluating equation (15) at point $x = x_{n+1,}$ and its derivative at $x = x_{n+1/2}$, yields the following two discrete hybrid schemes which are used as a block integrator;

$$y_{n+1} - \frac{4}{3}y_{n+\frac{1}{2}} = -\frac{1}{3}y_n + \frac{1}{3}hf_{n+1}$$

$$(16)$$

$$y_{n+\frac{1}{2}} = y_n + \frac{3}{4}hf_{n+1/2} - \frac{1}{4}hf_{n+1}$$

The equation (16) is of order $[2,2]^T$with error constant $\left[-\frac{1}{36}, -\frac{5}{24}\right]^T$

By rearranging equation (16) simultaneously, equation (17) was obtained

$$y_{n+\frac{1}{2}} = y_n + \frac{h}{4}\left\{3f_{n+\frac{1}{2}} - f_{n+1}\right\}$$

$$(17)$$

$$y_{n+1} = y_n + h\{f_{n+1/2}\}$$

Reformulating equation (17) with the coefficients as characterized by the Butcher array form

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

Where $a_{ij} = \beta$

gives

$$\begin{array}{c|ccc} 0 & 0 & 0 & 0 \\ \frac{1}{2} & 0 & \frac{3}{4} & \frac{-1}{4} \\ 1 & 0 & 1 & 0 \\ \hline & 0 & 1 & 0 \end{array}$$

Using equations (5) and (6), we obtained an implicit 3-stage block Runge-Kutta type method of uniform order two everywhere on the interval of solution

$$y_{n+\frac{1}{2}} = y_n + h(\frac{3}{4}k_2 - \frac{1}{4}k_3)$$

(18)

$$y_{n+1} = y_n + hk_2$$

Where

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

$$k_2 = f(x_n + \frac{1}{2}h, y_n + h\left\{0k_1 + \frac{3}{4}k_2 - \frac{1}{4}k_3\right\})$$

$$k_3 = f(x_n + h, y_n + h\{0k_1 + k_2 + 0k_3)$$

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

α	$\bar{A}$	A
	$\bar{b}^T$	b

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

0	0	0	0	0	0	0
$\frac{1}{2}$	0	$\frac{3}{4}$	$\frac{-1}{4}$	0	$\frac{5}{16}$	$\frac{-3}{16}$
1	0	1	0	0	$\frac{3}{4}$	$\frac{-1}{4}$
	0	1	0	0	$\frac{3}{4}$	$\frac{-1}{4}$

Using equation (8), we obtained an implicit 3 stage block Runge-Kuttatype method of uniform order 2 everywhere on the interval of solution.

$$y_{n+\frac{1}{2}} = y_n + \frac{1}{2}hy_n' + h^2\left(0k_1 + \frac{5}{16}k_2 - \frac{3}{16}k_3\right),$$

$$y'_{n+\frac{1}{2}} = y_n' + h\left(0k_1 + \frac{3}{4}k_2 - \frac{1}{4}k_3\right)$$

(19)

$$y_{n+1} = y_n + hy_n' + h^2\left(0k_1 + \frac{3}{4}k_2 - \frac{1}{4}k_3\right),$$

$$y_{n+1}' = y_n' + h(0k_1 + k_2 + 0k_3)$$

where

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

$$k_2 = f(x_n + \frac{1}{2}h, y_n + \frac{1}{2}hy_n' + h^2\left(0k_1 + \frac{5}{16}k_2 - \frac{3}{16}k_3\right),$$

$$y'_{n+\frac{1}{2}} = y_n' + h\left(0k_1 + \tfrac{3}{4}k_2 - \tfrac{1}{4}k_3\right))$$

$$k_3 = f(x_n + h, y_n + hy_n' + h^2\left(0k_1 + \frac{3}{4}k_2 - \frac{1}{4}k_3\right),$$

$$y_n' + h(0k_1 + k_2 + 0k_3))$$

The derived method was used to solve existing problems by Sunday etal. (2013) and Odigure et al. (2009).

Problem 1: Sunday J etal.(2013)

This is a first order Initial Value Problem with initial conditions, the eigen value (λ), the steplength (h) and the range of solutions given in equation (20) and the exact solution in equation (21).

$$y' = -\lambda y \qquad y(0) = 1,\ \ y'(0) = 1, \qquad \lambda = 1\ ,\ \ h = 0.01, \qquad 0 \le x \le 0.04 \qquad (20)$$

Exact Solution

$$y(x) = e^{-x} \qquad (21)$$

Table 1: $K = 1$ first order $RKTM$

x	Exact solution	Computed solution	Error
0.01	0.9901	0.9900	$-4.10E-08$
0.02	0.9802	0.9802	$-8.11E-08$
0.03	0.9704	0.9704	$-1.205E-07$
0.04	0.9608	0.9608	$-1.590E-07$

Presented in Table1 is the result obtained for exact solution to the problem shown in equation 20. Also presented are the computed results obtained when we applied theRKTM.

It can be observed from the table that the computed solutions are closer to the exact solution with error values in the range $-1.590E-07$to $-4.10E-08$.

Problem 2 :Odigure etal. (2009)

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

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

The quality of CaO produced is dependent on the chemical and microstructure composition, density and burning conditions (temperature, CO_2concentration 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)

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

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

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 equations (26) and (27), respectively;

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

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

$$(D_k)_e = 9.70\times10^3\alpha\left(\frac{T_c}{M_A}\right)^{0.5}$$

$$k_1 = Ae^{-\frac{E}{R_gT}}$$

$$A = 2.01E = 4.062\times10^4 R_g = 8.314J/mol.K\ \rho_A = 2710kg/m^3 k_m = 0.03m/s$$

The performance of the Runge-Kuttatype method (RKTM) 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: $K=1$ second order RKTM

r	$T_o = 600^0C$ T	$T_o = 650^0C$ T	$T_o = 700^0C$ T
0.1	634	684	734
0.2	685	735	785
0.3	736	786	836
0.4	787	837	887
0.5	838	888	938
0.6	889	939	989
0.7	940	990	1040
0.8	991	1041	1091
0.9	1042	1092	1142
1.0	1093	1143	1193

Presented in Table 2 are the solutions to equation 23 using the Runge-Kutta Type Method (RKTM). It can be observed from the table of results that the starting decarbonization temperature and particle size influences the decarbonization temperature.

The time taken and rate of conversion is given in the following Table 3

Table 3: $K = 1$ second order RKTM

r_s	$C_c = 13.204$ C_c	$t(sec)$
0.01	13.2892	0
0.02	13.4169	0.0051
0.03	13.5447	0.0404
0.04	13.6724	0.1351
0.05	13.8002	0.3174
0.06	13.9279	0.6142
0.07	14.0557	1.0517
0.08	14.1834	1.6550
0.09	14.3112	2.4483
0.1	14.4389	3.4552

Based on the obtained simulation results, the rate of conversion $X_A = 0.9\dot{9}$ for the various times and the implication is that there is 99 % conversion of the product.

CONCLUSION

It will be observed that from the table at the initial radius ($r_s = 0.01$), the time taken and the corresponding conversion rate is 0. This means that at that particular point no reaction has taken place. As the radius increases, we have the various times for the conversion with the same conversion rate at 0.99. This implied that the rate of conversion is 99% which means almost all the limestone is converted to quicklime. The various values obtained will help the engineers to make a very good production management decision.

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