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Numerical Integration of Stiff System of Ordinary Differential Equations with a New K-step Rational Runge-Kutta Method

P.O. Babatola, R.A Ademiluyi and E.A Areo

Mathematical Sciences Department
Federal University of Technology,
Akure, Ondo State,
Nigeria.

Abstract

The goal of this work is to develop, analyse and implement a K-step Implicit Rational Runge-Kutta schemes for Integration of Stiff system of Ordinary differential Equations. Its development adopted Taylor and Binomial series expansion Techniques to generate its parameters. The analysis of its basic properties adopted Dahlquist, A-stability model test equation and the results show that the scheme is Consistent, Convergent and A-stable. Numerical results show that the method is accurate and effective

Keywords: Rational, Runge-Kutta, Convergent, Consistent , Effective, Error bound, Implementation, Development, A-stable.

1.0 Introduction:

Consider a differential equation of the form

$$y' = f(x,y),\ y(x_o) = y_o \quad a \le x \le b \tag{1}$$

whose Jacobian $\partial f / \partial y$ possesses eigen values

$$\lambda_j = U_j + iV_j,\ j = 1(1)n \tag{2}$$

where $i = \sqrt{-1}$, and such that

(a). $U_j < < 0,\ j = 1(1)n$

(b). $\text{Max}\left|U_j(x)\right| >> \min\left|U_j(x)\right|$

$$\text{or} \qquad r(x) = \left|\frac{Max\left|U_j(x)\right|}{\min\left|U_j(x)\right|}\right| >> 1 \tag{3}$$

r(x) is said to be the stiffness ratio of the equations..

Next consider the following stiff system of ODEs:

(1). The system of differential equations of the form

$$y' = \begin{bmatrix} -0.00005 & 100 \\ -100 & -0.00005 \end{bmatrix} y \tag{4}$$

with $y^{(0)} = [1,\ \ 1]^T,\ 0 \le x \le 10\pi$

whose solution is obtained as

$$y(x) = e^{-0.00005x}\begin{bmatrix} Sin100x + & Cos100x \\ Cos100x - & Sin100x \end{bmatrix} \tag{5}$$

(2) $$y' = \lambda(y-E(x)) + E'(x),\ y(x_o) = y_o \tag{6}$$

where E(x) is continuously differentiable, λ is a complex constant with Re(λ) <<0, with the Exact solution

$$y(x) = E(x) + y_o e^{\lambda x} \tag{7}$$

Corresponding authors: ***P.O. Babatola: E-mail:*** pobabatola@yahoo.com, Tel. +2347037290018

consisting of two components E(x) which is slowly varying in the interval of integration (x_o, b), and the second component $y_o e^{\lambda x}$ decaying rapidly in the transient phase at the rate of $-1/\lambda$.

Most of the conventional Runge-Kutta schemes cannot effectively solve them because they have small region of absolute stability.

This perhaps motivated Hong Yuanfu (1982) to introduce a Rationalized Runge-Kutta scheme of the form

$$y_{n+1} = \frac{y_n + \sum_{j=1}^{R} W_i K_i}{1 + y_n \sum_{I=1}^{R} V_i H_i} \tag{8}$$

where,

$$K_1 = hf\left(x_n + C_1 h, y_n + \sum_{j=1}^{i} a_{ij} K_j \right)$$

$$H_1 = hg\left(x_n + d_1 h, \ Z_n + \sum_{j=1}^{i} b_{ij} H_j \right) \tag{9}$$

With $$g(x_n, \ Z_n) = -Z^2{}_n f(x_n \ y_n)$$

subject to the constraints $C_i = \sum_{j=1}^{R} a_{ij}$

$$d_i = \sum_{j=1}^{R} b_{ij} \tag{10}$$

Since the method possesses adequate stability property for solution of Stiff ODEs, this paper consider the extension of the scheme to a general step process so that it can serve as a general purpose prediction for Multistep schemes.

$$y_{n+m} = \frac{y_{n+m-1} + \sum_{i=1}^{R} W_i K_i}{1 + y_{n+m-1} \sum_{i=1}^{R} V_i H_i} \tag{11}$$

where

$$K_i = hf\left(x_{n+m-1} + C_i h, y_{n+m-1} + \sum_{j=1}^{R} a_{ij} K_j\right)$$

$$H_i = hg\left(x_{n+m-1} + d_i h, \ Z_{n+m-1} + \sum_{j=1}^{R} b_{ij} H_j\right) \tag{12}$$

In the spirit of Ademiluyi and Babatola (2000) the scheme is classified into:

(i) Explicit, $a_{ij} = 0$, $b_{ij} = 0$ for $j \geq i$.

(ii) Semi-implicit, if $a_{ij} = 0$, $b_{ij} = 0$ for $j > i$.

(iii) Implicit, if $a_{ij} \neq 0$, $b_{ij} \neq$ for at least one $j > i$.

Derivation of the Method

In determining the parameters V_i, W_i, d_i, c_i, a_{ij}, b_{ij} from the system of non-linear equations generated the following steps has been adopted

(1) Obtained the Taylor series expansion of K_i's and H_i's about point (x_{n+m-1}, y_{n+m-1}) for i =1(1)R, following Babatola(1999)

(2) Insert the series expansion into equation (11)

(3) Combine terms in equal powers of h, and compare the final expansion with the Taylor series expansion of y_{n+m-1} about (x_{n+m-1}, y_{n+m-1}) in the power series of h.

The number of parameters normally exceeds the number of equations, but in the spirit of King (1966), Gill (1951) and Blum (1952), these parameters are chosen as to ensure that the resultant computation method has:

i) Adequate order of accuracy

ii) Minimum local truncation error bound.

iii) Large interval of absolute stability.

iv) Minimum computer storage facilities requirement.

One-step one-stage schemes

By setting M = 1 and R = 1,in equation (11) the general one-step one-stage scheme is of the form

$$y_{n+1} = \frac{y_n + W_1 K_1}{1 + y_n V_1 H_1} \tag{14}$$

where, $K_1 = hf\,(x_n + c_1 h,\ y_n + a_{11}K_1)$

$$H_1 = hg\,(x_n + d_1 h,\ z_n + b_{11}H_1) \tag{15}$$

$$g\,(x_n\ z_n) = -Z_n^2 f(x_n, y_n) \tag{16}$$

And $$Z_n = 1/y_n \tag{17}$$

with the constraints $c_1 = a_{11}$, $d_1 = b_{11}$ (18)

The binomial expansion theorem of order one on the right hand sides of equation (11) yield

$$y_{n+1} = y_n + W_1 k_1 - y_n^2 V_1 H_1 + \text{(higher order terms)} \tag{19}$$

While the Taylor series expansion of y_{n+1} about y_n gives

$$y_{n+1} = y_n + hy'_n + \frac{h^2}{2!}y'' + \frac{h^3}{6}y_n^{(3)} + \frac{h^4}{2!}y_n^{(4)} + 0h^5 \tag{20}$$

Adopting differential notations

$$y'_n = f_n, \qquad y''_n = f_x + f_n f_y = Df_n$$

$$y_n^{(3)} = f_{xx} + 2f_n f_{xy} + f_n^2 f_{yy} + f_y(f_x + f_n f_y) = D^2 f_n + f_y Df_n$$

$$y_n^{(4)} = f_{xx} + D^3 f_n + f_y D^2 f_n + 3Df_n Df_y Df_y + f_y^2 Df_n \tag{21}$$

substitute (21) into (20), to get

$$y_{n+1} = y_n + hf_n + \frac{h^2}{2!}Df_n + \frac{h^3}{6}\left(D^2 f_n + f_y Df_n\right)$$
$$+ \frac{h^4}{24}\left(D^3 f_n + f_y D^2 f_n + 3Df_n Df_y + f_y^2 Df_n\right) + 0h^5 \tag{22}$$

Similarly the Taylor series expansion of K_1 about $(x_n y_n)$ is

$$K_1 = h\left(f_n + \left(c_1 hf_x + a_{11}k_1 f_y\right) + \tfrac{1}{2}\left(c_1^2 h^2 f_{xx} + 2c_1 ha_{11}k_1 f_{xy}\right) + a_{11}k_1^2 f_{yy}\right) + 0h^2 \tag{23}$$

Collecting coefficients of equal powers of h, equation (23) can be rewritten in the form

$$K_1 = hA_1 + h^2B_1 + h^3D_1 + 0h^4 \tag{24}$$

where, $A_1 = f_n$,, $B_1 = C_1\,Df_n$

$$D_1 = C_1 B_1 f_y + \tfrac{1}{2}\,C_1^2\,D^2 f_n \tag{25}$$

In a similar manner, expansion of H_1 about (x_n, z_n) yield

$$H_1 = hN_1 + h^2M_1 + h^3R_1 + 0h^4 \tag{26}$$

where,

$$N_1 = g(x_n, z_n) = g_n \quad M_1 = d_1 Dg_n \tag{27}$$

$$R_1 = d_1^2\left(g_z Dg_n + \tfrac{1}{2}D^2 g_n\right)$$

With

$$\left.\begin{aligned}
g_n &= \frac{-f_n}{y_n^2},\ g_x = \frac{-f_x}{y_n^2},\ g_{xx} = \frac{-f_{xx}}{y_n^2}\\
g_z &= \frac{-2f_n}{y_n} + f_y,\ g_{xz} = \frac{-2f_x}{y_n} + f_{xy}\\
g_{xxz} &= \frac{-2f_{xx}}{y_n} + f_{xxy},\quad g_{zz} = -2f_n - y_n^2 f_{yy}\\
g_{xzz} &= -2f_x - 2y_n^2 f_{xyy},\\
g_{zzz} &= 4y_n^2 f_y + 6y_n^2 f_{yy} + y_n^2 f_{yyy}
\end{aligned}\right\} \tag{28}$$

Substitute equation (28) into (27), to get

$$N_1 = \frac{-f_n}{y_n^2}, \quad M_1 = \frac{-d_1}{y_n^2}\left(Df_n + \frac{2f_n^2}{y_n}\right)$$

$$R_1 = \frac{d_1^2}{y_n^2}\left[\left(\frac{-2f_n}{y_n} + f_y\right)\left(Df_n + \frac{f_n^2}{y_n}\right)\right] + ½\left(D^2 f_n - \frac{2f_n}{y_n}\left(\frac{f_n^2}{y_n} + f_x\right)\right] \quad (29)$$

Adopting equation (25) and (26) in (19), to get

$$y_{n+1} = y_n + W_1\left(hA_1 + h^2B_1 + h^3D_1 + 0h^4\right) - y_n^2\left(V_1\left(hN_1 + h^2M_1 + h^3R_1 + 0h^4\right)\right]$$

$$= y_n\left(W_1A_1 - y_n^2V_1N_1\right)h + \left(W_1B_1 - y_n^2V_1M_1\right)h^2 + \left(W_1D_1 - y_n^2V_1R_1\right)h^3 + 0h^4 \quad (30)$$

Comparing the coefficients of the powers of h, h^2 and h^3 in equations (22) and (30), and adopting the values of A_1, B_1, M_1, D_1, R_1. and N_1, we obtained a system of Non-linear simultaneous equation

$$W_1 + V_1 = 1, \qquad W_1c_1 + V_1d_1 = ½ \quad (31)$$

And with the constraints in equation (18) and local truncation error

$$T_{n+1} = \frac{1}{6}\left(D^2 f_n + f_y Df_n\right)\left(-\tfrac{1}{2}C_1 W^2_1 - \tfrac{1}{2}V_1 d_1^2\left(\frac{2f_n}{y_n} - \frac{2f_n}{y_n}\right)\right) \quad (32)$$

And the above conditions we obtained family of one-step one-stage schemes with

(i) $V_1 = W_1 = ½$ $\quad c_1 = a_{11} = ¾,\quad d_1 = b_{11} = ¼$

equation (14) yields

$$y_{n+1} = \frac{y_n + \frac{1}{2}K_1}{1 + \frac{y_n}{2}H_1} \quad (33)$$

where

$$K_1 = hf\,(x_n + ¾\,h,\ y_n + ¾\,K_1)$$
$$H_1 = hg(x_n + ¼\,h,\ z_n + ¼\,H_1) \quad (34)$$

Also with

(ii) $V_1 = ¾$, $W_1 = ¼$, $d_1 = c_1 = ½$, $a_{11} = b_{11} = ¼$ equation (14) becomes

$$y_{n+1} = \frac{y_n + \frac{1}{4}K_1}{1 + \frac{3y_n}{4}H_1} \quad (35)$$

where

$$K_1 = hf\,(x_n + ½h,\ y_n + ½\,K_1)$$
$$H_1 = hf(x_n + ½\,h,\ z_n + ½\,H_1) \quad (36)$$

Similarly with

$W_1 = 1/3$, $V_1 = 2/3$, $a_{11} = C_1 = 1/3$, $b_{11} = d_1 = 7/12$

(14) yields

$$y_{n+1} = \frac{y_n + \frac{1}{3}K_1}{1 + \frac{2y_n}{3}H_1} \quad (37)$$

where

$$K_1 = hf\,(x_n + \tfrac{1}{3}h,\ y_n + \tfrac{1}{3}K_1)$$
$$H_1 = hg(x_n + \tfrac{7}{12}h,\ z_n + \tfrac{7}{12}H_1) \quad (38)$$

Two step One-stage schemes

By setting m = 2 and R = 2, we obtained two step schemes of the general form.

$$y_{n+2} = \frac{y_{n+1} + W_1K_1}{1 + y_{n+1}V_1H_1} \quad (39)$$

where,

$$K_1 = hf(x_{n+1} + c_1 h,\quad y_{n+1} + a_{11} K_1)$$
$$H_1 = hg(x_{n+1} + d_1 h,\quad z_{n+1} + b_{11} H_1) \qquad (40)$$

Adopting the same method as above we obtain family of method of two-step, one-stage schemes as

(i) $V_1 = W_1 = ½$, $C_1 = d_1 = ½$, $a_{11} = b_{11} = ½$ equation (39) becomes

$$y_{n+2} = \frac{y_{n+1} + \frac{1}{2}K_1}{1 + \frac{y_{n+1}}{2}H_1} \qquad (41)$$

where,

$$K_1 = hf\left(x_{n+1} + \tfrac{1}{2}h,\ \ y_{n+1} + \tfrac{1}{2}K_1\right)$$
$$H_1 = hg\left(x_{+1n} + \tfrac{1}{2}h,\ \ z_{n+1} + \tfrac{1}{2}H_1\right) \qquad (42)$$

(ii) with

$V_1 = ¼$, $W_1 = ¾$, $C_1 = ½$, $d_1 = ½$, $a_{11} = b_{11} = 7/12$

$$y_{n+2} = \frac{y_{n+1} + \frac{3}{4}K_1}{1 + \frac{y_{n+1}}{4}H_1} \qquad (43)$$

where,

$$K_1 = hf\left(x_{n+1} + \tfrac{1}{2}h,\ \ y_{n+1} + \tfrac{7}{2}K_1\right) \qquad (44)$$
$$H_1 = hg\left(x_{n+1} + \tfrac{1}{2}h,\ z_{n+1} + \tfrac{7}{2}H_1\right)$$

Next, we access the basic properties of this family of methods.

3.0 The Analysis of Basic Properties of the Methods

The basic properties required of a good computational method for stiff ODEs includes consistency, convergence and A-stability.

(3.1) Consistency

A scheme is said to be consistent, if the difference equation of the computation formula exactly approximate the differential equation it intends to solve (Ademiluyi, 2001).

To prove that equation (11) is consistent

Recall that

$$y_{n+m} = \frac{y_{n+m-1} + \sum_{i=1}^{R} W_i K_i}{1 + y_{n+m-1}\sum_{i=1}^{R} V_{ii} H_i} \qquad (45)$$

subtract y_{n+m-1} on both sides of equation (45)

$$y_{n+m} - y_{n+m-1} = \frac{y_{n+m-1} + \sum_{i=1}^{R} W_i K_i}{1 + y_{n+m-1}\sum_{i=1}^{R} V_i H_i} - y_{n+m-1} \qquad (46)$$

$$= \frac{y_{n+m-1} + \sum_{i=1}^{R} W_i K_i - y_{n+m-1}\left(1 + y_{n+m-1}\sum_{i=1}^{R} V_i H_i\right)}{1 + y_{n+m-1}} \qquad (47)$$

$$= \frac{\sum_{i=1}^{R} W_i K_i - y_{n+m-1}^2}{1 + y_{n+m-1}\sum_{i=1}^{R} V_i H_i} \qquad (48)$$

But

$$K_i = hf\left(x_{n+m-1} + c_i h, y_{n+m-1} \sum_{j=1}^{i} a_{ij} k_j \right)$$

$$H_i = hg\left(x_{n+m-1} + d_i h,\ \ z_{n+m-1} \sum_{j=1}^{i} b_{ij} H_j \right) \quad (49)$$

$$\frac{y_{n+m} - y_{n+m-1} = \sum_{i=1}^{R} hW_i f\left(x_{n+m-1} + c_i h,\ y_{n+m-1} + \sum_{j=1}^{i} a_{ij}\ k_j \right) - y^2_{n+m-1} \sum_{i=1}^{R} V_i hg\left(x_{n+m-1} + d_{ii} h,\ z_{n+m-1} + \sum_{j=1}^{i} b_{ij}\ H_j \right)}{1 + y_{n+m-1} \sum V_i hg(x_{n+m-1} + d_i h,\ z_{n+m-1} \sum_{j=1}^{R} b_{ij} H_j}$$

(50)

Dividing all through by h and taking limit ash tends to zero on both sides to have

$$\lim_{h\to o} \frac{y_{n+m-1} - y_{n+m-1}}{h} = \sum_{i=1}^{R} W_i f\left(x_{n+m-1},\ y_{n+m-1} \right) \quad (51)$$

But $$g(x_{n+m-1},\ z_{n+m-1}) = \frac{1}{y^2_{n+m-1}} f\left(x_{n+m-1,}\ y_{n+m-1} \right) \quad (52)$$

then

$$\begin{matrix} Lim \\ h \to o \end{matrix} \frac{y_{n+m} - y_{n+m-1}}{h} = \sum_{i=1}^{R} (W_i + V_i) f(x_{n+m-1,}\ \ y_{n+m-1}) \quad (53)$$

but $$\sum_{i=1}^{R} W_i + V_i = 1 \quad (54)$$

$$y'_{n+m-1} = f\left(x_{n+m-1,ast},\ y_{n+m-1} \right) \quad (55)$$

Hence the method is consistent.

Convergence: Since the proposed scheme is one-step and it has been proved to be consistent, then it is convergent by Lambert (1973).

Stability properties

To examine the stability property of this scheme, we apply scheme (11) to Dahlquist (1963) stability scalar test initial value problem

$$y' = \lambda y_1\ y(x_o) = y_o \quad (56)$$

To obtain a difference equation

$$y_{n+m} = \mu(p)\, y_{n+m-1} \quad (57)$$

with the stability function

$$\frac{1 + pW^T (I - pA)^{-1} e}{1\ 1pV^T (I - PB)^{-1} e} \quad (58)$$

Where $W^T = (w_1, w_2, w_3 \ldots\ldots W_T)$

$V^t = (v_1, v_2, v_3 \ldots\ldots\ldots v_t)$

Where $p = \lambda h$

To illustrate this with example, we consider two-step one-stage scheme

$$y_{n+2} = \frac{y_{n+1} + W_1 K_1}{1 + y_{n+1} V_1 H_1} \quad (59)$$

where

$$K_1 = hf(x_{n11} + C_1 h_1 \quad y_{n+1} + a_{11} K_1)$$
$$H_1 = hg(x_{n11} + d_1 h_1 \quad z_{n+1} + a_{11} + b_{11} H_1) \quad (60)$$

with relation

$$y_{n+2} = \mu(p)\, y_{n+1} \quad (61)$$

where $$\mu(p) = \frac{1 + W_1 P(1 - a_{11}P)}{1 - V_1 P(1 + b_{11}P)} \qquad (62)$$

The difference equation (62) produce a convergent and A-stable approximation to equation if

$$|\mu(P)| < 1 \qquad (63)$$

Simplifying the inequality (63). Hence the scheme is A-stable because the interval of Absolute stability is $(-\infty, 0)$

Numerical Computations and Results

In order to access the performance of the schemes, the following sample problems were solved.

Problem 1: Consider the stiff system of ODEs.

$$Y' = AY \qquad (64)$$

where

$$A = \begin{bmatrix} 1.0 & -4.99 & 0 \\ 0 & -5.0 & 0 \\ 0 & 2.0 & 12 \end{bmatrix} \qquad (65)$$

with the initial condition y(o) = $[2 \quad 1 \quad 2]$, $0 \le x \le 1$ and theoretical solution

$$y_1(x) = e^{-x} + e^{-5x}$$
$$y_2(x) = e^{-5x} \qquad (66)$$
$$y_3(x) = e^{-5x} + e^{-12x}$$

Using step size h = 0.01. The method is implemented and the results are shown in Table 1.

Problem 2: The second sample problem considered is the stiff system of initial values problems of ODEs shown in Table 2.

$$y' = \begin{bmatrix} -0.5 & 0 & 0 & 0 \\ 0 & -1.0 & 0 & 0 \\ 0 & 0 & -9.0 & 0 \\ 0 & 0 & 0 & -10.0 \end{bmatrix} \begin{bmatrix} y_1 \\ y_2 \\ y_3 \\ y_4 \end{bmatrix}, \; y(o) = [1, \quad 1, \quad 1, \quad 1] \qquad (67)$$

TABLE 1:

Numerical Result Of K-Step Implicit Rational Runge-Kutta Schemes For Solving Stiff Systems Of Ordinary Differential Equations

		Y1	**Y2**	**Y3**
X	**CONTROL STEP SIZE (h)**	**E1**	**E2**	**E3**
		.1980099667D+01	.9706425830D+00	.8869204674D+00
.3000000000D – 01	.3000000000D – 01	.8291942688D-09	.3281419103D-07	.8161313500D-05
		.1885147337D+01	.8379203859D+00	.4917945068D+00
.1774236000D+00	.1771470000D-01	.9577894033D-01	.3422855333D-08	.5357828618D-06
		.1791235536D+01	.7191953586D+00	.2663621637D+00
.3307246652D+00	.1046033532D-01	.11050933794D-10	.35587255336D-09	.3474808041D-07
		.1694213422D+01	6088845946D+00	.1365392880D+00
.4977858155D+00	.6176733963D-02	.1269873096D-11	.3655098446D-10	.2146555961D-08
		.1556933815D+01	.4729421983D+00	.4953161076D-01
.7512863895D+00	.3647299638D-01	.1425978891D-08	.3505060447D-07	.1010194837D-05
		.1435390902D+01	.3709037123D+00	.1867601194D-01
.9951298893D+00	.2153693963D-01	.1594313570D-09	.3316564301D-08	.4481540687D-07

TABLE 2:

Numerical Result Of K-Step Implicit Rational Runge-Kutta Schemes For Solving Stiff Systems Of Ordinary Differential Equations

		Y1	**Y2**	**Y3**	**Y4**
X	**CONTROL STEP SIZE**	**E1**	**E2**	**E3**	**E4**
		.9950124792D+00	.9900498337D+00	.9139311928+00	.9048374306D+00
.3000000000D – 01	.3000000000D – 01	.2597677629D-10	.4145971344D-09	.2617874150D-05	.3971726602D-05
		.9708623323D+00	.9425736684D+00	.5872698932D+00	.5535451450D+00
.1774236000D+00	.1771470000D-01	.3078315380D-11	.4788947017D-10	.2005591107D-06	.2890213078D-06
		.9402798026D+00	.8841261072D+00	.3300866691D+00	.2918382654D+00
.3694667141D+00	.1046033532D-01	.3621547506D-12	.5454525720D-11	.1355160001D-07	.1829417523D-07
		.9144602205D+00	.8362374949D+00	.1999708940D+00	.1672231757D+00
.5365278644D+00	.6176733963D-02	.4285460875D+13	.6268319197D-12	.9915873955D-09	.1265158728D-08
		.8693495443D+00	.7557686301D+00	.8044517344D-01	.6079796167D-01
.8400599835D+00	.3647299638D-01	.4961209221D-10	.6922001861D-09	.5087490103D-06	.5899525189D-06

Conclusion

K-step Rational Runge-Kutta schemes for the Integration of Stiff System of ODEs has been proposed. Theoretically it has been showed that the scheme is consistent, convergent and A-stable. Numerical results and theoretical showed that the schemes are accurate, and effective. Also from the above results the error is very minimal, this implies that the scheme is very accurate.

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