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Numerical Integration of a new Class of Implicit Schemes for Treatment of Stiff Ordinary Differential Equations.

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Abstract

In this paper, a new class of convergent implicit Rational Runge- Kutta (RR-K) Schemes were developed, analyzed and Computerized to Solve Stiff ODES.The schemes is motivated by the Implicit Conventional Runge-Kutta Schemes and Rational function approximation while its development and analysis make use of Taylor series expansions (Taylor and Binomial) and pade's approximation respectively. The schemes are convergent.

Keywords: Rational, Conventional, Convergent, Implicit,

1.0 Introduction

A differential equation (ODEs) of the general form

$$y' = f(x,y), y(x_0) = y_0 \tag{1}$$

Whose Jacobian poses eigen value

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

Where i = $\sqrt{-1}$, satisfying the following conditions

(a) $U_j << o$, j =1(1)n

(b) Max $(U_j(x)) >>$ Min $(U_j(x))$

In this case, condition (a) show that the system is stable while (b) indicate that the system possesses some components decay very rapidly.The problems associated with numerical solution of stiff ODEs was first recognized by Curtis and Hirschfelder[1]. Other requirements include the necessity for the numerical scheme to be a stable.

These stability criteria require that the numerical schemes must have large stability region, that is it must be A stable. In the present of all these problems, Hong Yuafu [2] proposed a more general form of this scheme called Explicit Rational R.K schemeThe general form of the scheme is given by

$$y_{n+1} = \frac{y_n + \sum_{1=1}^{R} W_i K_i}{1 + y_n \sum_{1=1}^{R} V_i H_i} \tag{3}$$

$$K_1 = hf(x_n, y_n)$$

$$K_i = hf(x_n + c_i h, y_n + \sum_{j=1}^{R} a_i jk_j), \ 1=1(1)R$$

$$H_1 = hg(x_n, z_n)$$

$$H_i = hg(x_n + d_i h, z_n + \sum_{j=1}^{R} b_i jH_j) \tag{4}$$

With $g(x_n, z_n) = -z_n^2 f(x_n, y_n)$ (5)

and $z_n = 1/y_n$ (6)

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In his development $a_{ij} = 0, b_{ij} = 0$ for j > i , he develop families of method of orders one, two and three. During analysis, he discovers that the schemes are A stable. This expectation is the chief mover of the present consideration.

2.0 The Development of The Proposed Scheme

An R-stage IRR-K schemes is of the form

$$y_{n+1} = \frac{y_n + \sum_{1=1}^{R} W_i K_i}{1 + y_n \sum_{1=1}^{R} V_i H_i} \tag{7}$$

Where

$$K_i = hf(x_n + c_i h, y_n + \sum_{1=1}^{R} a_{ij} K_j)$$

$$H_i = hg(x_n + d_i h, z_n + \sum_{i=1}^{R} b_{ij} H_j) \tag{8}$$

And $g(x_n, z_n) = -z_n^2 f(x_n, y_n)$

With the constraints

$$C_i = \sum_{j=1}^{R} a_{ij}, d_i = \sum_{j=1}^{R} b_{ij} \tag{9}$$

The paraments V_i, W_i, C_i, d_i, a_{ij} and b_{ij} are to be determined from the system of non-linear equation generated by adopting that following step.

i. Obtained the Taylor series of K_i, H_i about point $(x_n y_n)$ for i=1 (1) R
ii. Insert the series expansion into (7)
iii. Compare the final expansion with Taylor series expansion of y_{n+1} about (x_n,y_n) in the power of h.

The number of parameter normally exceeds the number of equations but these parameter are chosen to ensure that one or more of the following conditions are satisfied.

i. Adequate order of accuracy of the scheme [3].
ii. Minimum bound of local truncation error [4].
iii. The scheme has maximum interval Region of Absolute Stability [5].
iv. Minimum computer storage facilities.

2.1 <u>One Stage Scheme</u>

The general one stage implicit RR-K scheme is of the form.

$$y_{n+1} = \frac{y_n + W_1 K_1}{1 + y_n V_1 H_1} \tag{10}$$

Where

$$K_i = hf(x_n + c_i h, y_n + a_{11} k_1)$$

$$H_i = hg(x_n + d_i h, z_n + b_{11} k_1 \tag{11}$$

$$g(x_n, z_n) = -z_n^2 f(x_n, y_n) \tag{12}$$

$C_1 = a_{11}$

$d_1 = b_{11}$ (13)

Adopting binomial expansion theorem on the RHS of equation (10) and ignoring higher order terms, yields.

$$y_{n+1} = y_n + W_1 K_1 - y_n^2 V_1 H_1 + \text{(higher order terms)} \tag{14}$$

The Taylor series expansion of y_{n+1} gives

$$y_{n+1} = y_n + hf_n + \frac{h^2}{2} Df_n + \frac{h^3}{31}(D^2 f_n + f_y Df_n)$$

$$+ \frac{h^4}{41}(D^3 f_n + f_y D^2 f_n - 3Df_n Df_y + fy^2 Df_n) + 0h^5 \tag{15}$$

Where

$$Df_n = f_x + f_n f_y$$

$$D^2 f_n = f_{xx} + 2 f_n f_{xy} + f^2{}_n f_{yy}$$

$$D^3 f_n = f_{xxx} + 3 f_{xxy} f_n + 3 f_{xyy} f^2{}_n + f^3{}_n fyyy$$

Similarly expand K_1 about (x_n, y_n), we have

$K_1 = hA_1 + h^2 B_1 + h^3 D_1 + 0h^4$ (16)

Where

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

$$D_1 = C^2{}_1 (Df_n f_y + \frac{1}{2} D^2 f_n) \quad (17)$$

In a similar manner, expand H_1 about $(x_{n,} z_n)$ yields

$$H_1 = hN_1 + h^2 M_1 + h^3 R_1 + oh^4 \quad (18)$$

Where

$$N_1 = -\frac{f_n}{y^2{}_n}, M_1 = -\frac{d_1}{y^2{}_n}(Df_n + \frac{2 f^2{}_n}{y_n})$$

$$R_1 - \frac{d^2{}_1}{y^2{}_n}(-\frac{2 fn}{y_n} + f_y)(Df_n + \frac{f_n{}^2}{y_n}) + \tfrac{1}{2}(D^2 f_n - \frac{2 f_n}{y_n}(f_n{}^2 + f_x) \quad (19)$$

Adopting (16) and (18) in (14)

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

$$= y_n + (W_1 A_1 - y_n{}^2 V_1 H_1)h + (W_1 B_1 - y_n{}^2 V_1 M_1)h^2 \quad + (W_1 D_1 - y_n{}^2 V_1 R_1)h^3 + 0h^4$$

(20)

Comparing the coefficient of the powers of h and h^2 in (15) and (20) and substitute (17) and (19) to get

$W_1 + V_1 = 1$

$W_1 c_1 + V_1 d_1 = 1/2$ (21)

With constraints (13), we obtained family of one – stage scheme of order two

(i) $W_1 = 0, V_1 = 1, c_1 = d_1 = \tfrac{1}{2}, a_{11} = b_{11} = \tfrac{1}{2}$ scheme (11) yield

$$y_{n+1} = \frac{y_n}{1 + y_n H_1} \quad (22)$$

Where $H_1 = hg(x_n + \tfrac{1}{2}h, z_n + \tfrac{1}{2}H,)$ (23)

(ii) Also with

$$V_1 = W_1 = \tfrac{1}{2}, c_1 = a_{11} = \tfrac{3}{4}, d_1 = b_{11} = \tfrac{1}{4}$$

The scheme (11) result into

$$y_{n+1} = \frac{y_n + \tfrac{1}{2} K_1}{1 + \frac{y_n}{2} H_1} \quad (24)$$

where

$$K_1 = hf(x_n + \tfrac{3}{4}h, y_n + \tfrac{3}{4}K_1)$$

$$H_1 = hg(x_n + \tfrac{1}{4}h, z_n + \tfrac{1}{4}H_1) \quad (25)$$

Also with

$$W_1 = 1, V_1 = 0, c_1 = d_1 = \tfrac{1}{2}, a_{11} = b_{11} = \tfrac{1}{2}$$

Scheme (10) result into

$$y_{n+1} = y_n + K_1 \tag{26}$$

Where

$$K_1 = hf\,(x_n + \tfrac{1}{2}h, y_n + \tfrac{1}{2}K_1) \tag{27}$$

Which coincide with implicit Euler scheme of order 2.

Next section analyzed the error, consistency, convergence and stability properties of these schemes.

3.0 Error, Convergence and Stability Properties

In this section, we shall consider the error, convergence, consistency and stability properties of these schemes.

3.1 Error analysis

Error of numerical approximation for stiff ODEs arise from different causes that can majorly classified into truncation, discretization and round off error

Truncation error is the error introduced as a result of ignoring some of the higher terms of the power series during development of the new scheme.

Discretization error e_{n+1} associated with the formula (11) is the difference between the exact solution $y(x_{n+1})$ and the numerical solution y_{n+1} generated by (11) at point x_{n+1}

That is $$e_{n+1} = y_{n+1} - y(x_{n+1}) \tag{28}$$

Round off error is an error introduced as a result of the computing device mathematically it can expressed as

$$r_{n+1} = y_{n+1} - p_{n+1} \tag{29}$$

Where y_{n+1} is the expected solution of the difference equation (10) while

p_{n+1} is the computer output at $(n+1)^{th}$ iteration.

Consistency Property

One step schemes is said to be consistent if

$$\text{Lim}\, h \to 0\left(\frac{y_{n+1} - y_n}{h}\right) = f(x_n, y_n) \tag{30}$$

To show the consistency, we recall that

$y_{n+1} = y_n - y_n^{\,2}\sum_{1=1}^{R} V_i H_i + \sum_{1=1}^{R} W_1 K_1 +$ higher order terms

subtract y_n from both sides and ignoring higher order terms. (31)

$$y_{n+1} = y_n - \sum_{1=1}^{R} W_i K_i - y_n^{\,2}\sum_{1=1}^{R} V_i H_i \tag{32}$$

Substituting the expression for H_i and K_i in equation (8)

$$y_{n+1} - y_n = \sum_{1=1}^{j} W_i hf(x_n + c_i h, y_n + \sum_{j=1}^{i} \overrightarrow{a_{ij} k_j)} - y_n^{\,2}\sum_{1=1}^{R} V_i hg(a_n + d_i h, z_n \sum_{1=1}^{R} a_{ij} H_j) \tag{33}$$

Dividing by h and taking limit as h tends to 0

$$Limh \to 0\left(\frac{y_{n+1} - y_n}{h}\right) = \sum_{1=1}^{R} W_i f(x_n, z_n) - y_n^{\,2}\sum V_i g(x_n, z_n) \tag{34}$$

$$Limh \to 0\left(\frac{y_{n+1} - y_n}{h}\right) = \sum_{1=1}^{R} (W_i + V_i) f(x_n y_n) \tag{35}$$

But $$\sum_{1=1}^{R} (W_i + V_i) = 1 \tag{36}$$

$$Lim h \to 0\left(\frac{y_{n+1}-y_n}{h}\right)= f(x_n, y_n) \quad (37)$$

Equation 37 showing that implicit Rational R-K schemes is consistent.

Convergence Property

The numerical schemes (10) of solution of stiff ODEs will be convergent if the numerical approximation y_{n+1} that is generated tends to the exact solution $y(x_{n+1})$ as the step size tend to zero

That is

$$Lim h \to 0\left(y(x_{n+1}) - y_{n+1}\right)= 0 \quad (38)$$

To Analyzed the convergence of the schemes, the theorem stated below will be considered.

Theorem 1

Let $\{e_j\}$, j=0(1)n be the set of real numbers. If there exist finite constant R and S such that

$$\left|e_j, \right| < R\left|e_{j+1}\right| + S,\ j = 0(1)n-1 \quad 39)$$

$$\left|e_j\right| \le \left(\frac{R^j}{R-1} - 1\right) S + R^j\left|e_0\right| \quad (40)$$

Let e_{n+1} and T_{n+1} denote the discretization and truncation error generated by schemes (7) respectively.

Adopting binomial expansion and ignoring higher terms in (7)

$$y_{n+1} = y_n + \sum_{1=1}^{R} W_i K_i - y_n^2 \sum_{1=1}^{R} V_i H_i \quad (41)$$

Also

$$y(x_{n+1}) = y(x_n) + \sum_{T_{n+1}} W_i K_i(x_n) - y_n^2(x_n)\sum V_i H_i(x_n) \quad (42)$$

Subtract (41) from (42) and adopt equation (28) leads to

$$e_{n+1} = e_n + \sum_{1=1}^{R} W_i K_i(x_n) - \sum_{1=1}^{R} W_i K_i$$

$$- y_n^2\left(\sum_{1=1}^{R} V_i H_i(x_n) - \sum_{1=1}^{R} V_1 H_i\right) + T_{n+1} \quad (43)$$

Let $\sum_{1=1}^{R} W_i K_i(x_n) - \sum_{1=1}^{R} W_i K_i = \psi_1(x_n, y_n; h) - \psi_1(x_n, y(x_n); h) = \psi_2(x_n, y_n; h)$

$$y_n^2\left(\sum_{1=1}^{R} V_i H_i(x_n) - \sum_{1=1}^{R} V_1 H_i\right) = \phi_1(x_n, z_n; h) = \phi_1(x_n, z_n; h)$$

$$e_{n+1} = e_n + h\psi_1(x_n, y_n) - \phi_1(x_n, z_n) + T_{n+1} \quad (44)$$

Taking the absolute value on both sides of equation (44)

$$\left|e_{n+1}\right| \le e_n + kh\left|e_n\right| + hL\left|e_n\right| + T \quad (45)$$

Where L and K are lipschtz constant for $\psi_1(x.y; h) and \phi_1(x, y; h)$

respectively and $T = \sup_{a \le x \le b} \left|T_{n+1}\right|$ (46)

By setting N= L+K

Inequality (45) becomes

$$\left|e_{n+1}\right| \le \left|e_n\right|(1 + hN) + T \quad (47)$$

From theorem 1 expression (47) becomes

$$\left|e_n\right| \le \left(\frac{(1+hN)^n - 1}{hN}\right) T + (1+hN)^n\left|e_0\right| \quad (48)$$

Since $(1+hN)^n = e^{nhN} = e^{N(x_{n-a})}$ (49)

And $x_n \le b$ then $x_n - a \le b - a$ consequently $e^{N(x_{n-a})} \le e^{N(b-a)}$

$$e_n \le \left(\frac{e^{N(b-a)} - 1}{hN} \right) T + e^{N(b-a)} |e_0| \quad (50)$$

Also

$$T_{n+1} = [\psi_1(x_n, +\theta h, y(x_n+\theta h) - \psi_1(x_n, y(x_n)] + h[\phi_1(x_n+\theta h) - \phi_1(x_n, y(x_n]$$

$$= h[\psi_1(x_n+\theta h), y(x_n+\theta h) - \psi_1(x_n+\theta h, y(x_n) + \psi_1(x_n+\theta h, y(x_n)]$$

$$+ h\phi_1(x_n+\theta h, y(x_n+\theta h) - \phi_1(x_n+\theta h, y(x_n)) + \phi_1(x_n+\theta h, y(x_n) + \phi(x_n, y(x_n)] \quad (51)$$

By taking the absolute value of (51) by taking equation (45) into consideration

$$T = hL|y(x_n+\theta h) - y(x_n)| - Jh^2\theta + hK|y(x_n+\theta h) - y(x_n)| + mh^2\theta$$

$$T + h^2\theta N y^1(E_1) + (J+M)h^2\theta, x_n \le E_1 \le x_{n+1} \quad (52)$$

Where M and J are partial derivative of ψ_1 and ϕ_1 with respect to x respectively by setting Q = J + M and

Y= sup $|y'(x)|$

$$a \le x \le b \quad (53)$$

$$T = h^2\theta(NY + Q) \quad (54)$$

By substituting (54) into (50), we have

$$|e_n| \le \frac{h^2\theta e^{N(b-a)}|NY + Q|}{hN} + e^{N(b-a)}|e_o| \quad (55)$$

Assuming no error in the input data,

that is $|e_o|$ = 0 then in the limit as h $\to$ 0

We obtain

$\lim |e_n| = 0$ *as* h tends to zero and as n tends to infinity.

Which implies $\lim y_n = y(x_n)$ as h tends to zero and as n tends to infinity

STABILITY PROPERTY

To analyze the stability property

Recall that general one stage implicit RR-K Scheme is

$$y_{n+1} = \frac{y_n + w_1 k_1}{1 + y_n v_1 H_1} \quad (56)$$

Where

$$K_1 = hf(x_n + c_1 h, y_n + a_{11} K_1)$$
$$H_1 = hg(x_n + d_1 h, z_n + b_{11} H_1) \quad (56)$$

Applying (56) to the stability test equation $y' = \lambda y, y(x_0) = y_0$ (59)

obtain recurrent relation equation

$$y_{n+1} = \frac{1 + w_1{}^T (1 - a_{11} p)^{-1}}{1 - v_1{}^T (1 + b_{11} p)^{-1}} y_n \quad (60)$$

That is $y_{n+1} = \mu(p)\, y_n$ (61)

For example, the associated stability function for scheme (22) – (26) is

$$\mu(p) = \frac{1 + \frac{1}{2} p}{1 - \frac{1}{2} p} \tag{62}$$

Which implies
that it is A-stable since $|\mu(p)| < 1$ at $p \varepsilon [-\infty, o]$

4.0 Numerical Computation and Results

In order to demonstrate the accuracy of this scheme some sample problems were considered
Problems 1: considered initial value problem

$$y^{t} = -100\ (y - x^{3}) + 3x^{2}, y(0) = 1 \tag{63}$$

The theoretical solution is

$$y(x) = x^{3} + e^{-100\ x} \tag{64}$$

The results are shown table 1
Problem 2: consider the initial value problem
$y^1 = 2x + y$, y (0) =1
whose theoretical solution is
$y(x) = - 2(x+1) 3e^x$ (65)
the numerical result is shown in
Table 2: compared with R-K scheme of the same stage
Table 1: Results of One-Stage Implicit Rational R-K scheme and Euler's Schem

Table 1: Results of One-Stage Implicit Rational R-K scheme and Euler's Scheme

H	YEXACT	PROPOSED ONE STAGE R-K METHOD OF ORDER TWO Y_N	El	EULER'S SCHEME OF Y_N	E2
.10000000D+00	.368879440D+00	.36940452D+00	.525081720D-02	.376031250D+00	.71518088D-02
.50000000D-01	.60665566D+00	.606681970D+00	.263095840D-04	.60689665 D+00	.240987420D-03
.25000000D-01	.77881 64 1D+00	.778817430D+00	.102349440D-06	.77882424D0+00	,783356680D-05
.12500000D-01	.88249886D+00	.88249889D+00	.36809087D-07	.882499 11D+00	.24978363D-06
.62500000D-01	.96923326D+00	.969413310+00	.122975660D-08	.9694133 1D+00	.788572420-08
.31250000D-02	.98449644D+00	.96923326D+00	.23411650D-09	.96923326D+00	.24769542D-09
.15625000D-02	.99221794D+00	.98449644D+00	.752897740D-11	.98449644D+00	.776034790D-11
.78125000D-02	.99619137D+00	.99221794D+00	.15305257D-13	.99221794D+00	.24280578D-11
.39062500D-03	.998048780D+00	.99610137D+00	.963329420D-14	.996101370D+00	.75495 166D-14
.19531250D-03	.999023910+00	.99804878D+00	.604183370D-15	.998048780D+00	.222044600D-12
.97656250D-04	.99951184D+00	.9990239 1D+00	.15495538D-09	.9990239 1D+00	.0000000D+00
.48828 125D-04	.99951184D+00	.99951184D+00	.193859370D-15	.99951184D+00	.11102230D-10
.24414063D-04	.99975589D+00	.99975589D+00	.24242830D-11	.99975589D+00	00000000+00
.1220703 ID-04	.99987794D+00	.99987794D+00	.30320191D-15	.99987794D+00	.11102230D-12

Table 2:
Numerical Solutions Of Problem2 Using Implicit Rational Runge-Kutta Schemes And Euler's Scheme

H	**YEXACT** **y(xn)**	**IMPLICIT** **yn**	**EULER'S** **yn**
.10000000D-01	0.10101515D+01	0.10101514D+01	0.10101511D+01
.50000000D-02	0.10050386D+01	0.10050385D+01	0. 1005038 1D+01
.25000000D-02	0.10025096D+01	0.10025095D+01	0.10025094D+01
.12500000D-02	0.10012527D+01	0.10012526D+01	0.10012521D+01
.62500000D-03	0.10006267D+01	0.10006266D+01	0.10006266D+01
.31250000D-03	0. 10003 138D+01	0.1 0003 137D+01	0. 10003 134D+01
.15625000D-03	0.10001568D+01	0.10001567D+01	0.10001561D+01
.78125000D-04	0.10000788D+01	0.10000787D+01	0.10000784D+01
.39062500D-04	0.10000399D+01	0.10000398D+01	0.10000396D+01
.19531250D-04	0.10000209D+01	0.10000208D+01	0.1000206D+01
.976562500-05	0.10000109D+01	0.10000108D+01	0.1000105D+01
.48828 120D-05	0.10000059D+01	0.1000058D+01	0.1000054D+01
.24414060D-05	0.10000029D+01	0.10000028D+01	0.1000021D+01
.-12207030D-05	0.1 00000 19D+01	0.1 0000 18DD+01	0.10000015D+01

Discussion

A cursory observation of result in table 1 and 2 show that the new schemes produce more accurate results than those produced by R-K schemes of the same stage .

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