



A new three stage implicit Runge-Kutta type method with error estimation for first order ordinary differential equations

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ABSTRACT

This paper presents a new three stage implicit Runge-Kutta type method for solving initial value problems of first order ordinary differential equations (ODEs). Collocation approach is used to derive a method of Continuous coefficient system and when evaluated at special Gaussian points gives three different discrete schemes. These schemes were further reformulated to three stage Runge-Kutta type method and when tested with numerical experiments, it demonstrates highly efficient, stable and low implementation cost when compared with existing methods. This scheme can handled both Stiff and non Stiff ODEs.

Keywords: Implicit, Runge-Kutta type method, Collocation approach, Special Gaussian point and error bounds.

1. INTRODUCTION

A number of Mathematical models are formulated into ordinary differential equations with large Eigen values for example, $y' = -100y + 999e^{-x}$. Such problems are found in Kinetic, Chemical reactions, Electric Circuit theory, Control theory, Mechanics and Medicine to mention a few. These models are described as Stiff equations. There are many different approximating methods for solving Stiff equations. Our interest is to develop a method that is simple, efficient with low implementation cost. Researchers have developed implicit Runge-kutta methods among them are Kuntzmann [1], Butcher [2] etc. Their Schemes were derived from Gaussian quadrature formulae with the order $p = 2s$ for an S-stage method. Also variety of alternative methods are Radau, Labato [3], Singl, Diagonal Implicit Runge-Kutta methods (SDIRK) [4], Efficient numerical methods for highly Oscillatory ODES [5]. These methods are quite good but there is need to improve on them for efficiency and stability. We shall use collocation methods [7] to derive an Implicit scheme for solution and error estimation of order $p = 2s$.

2. DERIVATION METHOD

We find the general S-stage implicit Runge-Kutta type method of first order equations of the form $y' = f(x, y)$ $y(x_0) = y_0$ $a \leq x \leq b$ 2.01

By considering a polynomial of the form

$$y(x) = \sum_{j=0}^{t-1} \alpha_j(x) y_{n+j} + h \sum_{j=0}^{m-1} \beta_j(x) f(c_j, y(c_j)) \quad (2.02)$$

where t denotes the number of interpolation points $x_{n+j}, (j = 0, 1, \dots, t-1)$ and m denotes the distinct collocation points $c_j, (j = 0, \dots, m-1)$, y and f are smooth functions

The constant coefficients of α_j, β_j are element of $(t+m) \times (t+m)$ matrix. They are selected so that high accurate approximation of the solution of (2.01) is obtained. Also h can be a constant or variable in the integration process see [7].

The function $\alpha_j(x)$ and $\beta_j(x)$ in (2.02) can be represented by polynomial of the form

$$\alpha_j(x) = \sum_{i=0}^{t-1} \alpha_{j,i+1} x^i \quad j \in [0, 1, \dots, t-1] \quad 2.03$$

$$h \beta_j(x) = \sum_{i=0}^{m-1} h \beta_{j,i+1} x^i \quad j \in [0, 1, \dots, m-1] \quad 2.04$$

The coefficients $\alpha_{j,i+1}$ and $h \beta_{j,i+1}$ are to be determined

Substituting (2.03) and (2.04) in (2.02), we have

$$y(x) = \sum_{i=0}^{m+t-1} \left\{ \sum_{j=0}^{t-1} \alpha_{j,i+1} y_{n+j} + h \sum_{j=0}^{m-1} \beta_{j,i+1} f_{n+j} \right\} x^i = \sum_{i=0}^{m+t-1} a_j x^i \quad 2.05$$

where

$$a_j = \left(\sum_{j=0}^{t-1} \alpha_{j,i+1} y_{n+j} + h \sum_{j=0}^{m-1} \beta_{j,i+1} f_{n+j} \right)$$

$$a_j \in R^j, j \in [0, 1, \dots, t+m-1], y \in C^m(a, b)$$

This can be expressed in matrix form as

$$y(x) = (y_n, \dots, y_{n+t-1}, f_n, \dots, f_{n+m-1}) C^T (1, x_n, \dots, x_n^{t+m-1})^T$$

where

$$C = \begin{bmatrix} \alpha_{01} & \cdot & \cdot & \alpha_{t-1,1} & h\beta_{0,1} & \cdot & \cdot & \cdot & h\beta_{m-1,1} \\ \alpha_{02} & \cdot & \cdot & \alpha_{t-1,2} & h\beta_{0,2} & \cdot & \cdot & \cdot & h\beta_{m-1,2} \\ \alpha_{03} & \cdot & \cdot & \alpha_{t-1,3} & h\beta_{0,3} & \cdot & \cdot & \cdot & h\beta_{m-1,3} \\ \alpha_{04} & \cdot & \cdot & \alpha_{t-1,4} & h\beta_{0,4} & \cdot & \cdot & \cdot & h\beta_{m-1,4} \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \alpha_{0,t+m} & \cdot & \cdot & \alpha_{t-1,t+m} & h\beta_{0,t+m} & \cdot & \cdot & \cdot & h\beta_{m-1,t+m} \end{bmatrix} = D^{-1} \quad (2.06)$$

$$D = \begin{bmatrix} 1 & x_n & x_n^2 & \cdot & \cdot & x_n^{t+m-1} \\ 0 & 1 & 2x_{n+q_1} & \cdot & \cdot & (t+m-1)x_{n+q_1}^{t+m-2} \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ 0 & 1 & 2x_{n+q_{m-1}} & \cdot & \cdot & (t+m-1)x_{n+q_{m-1}}^{t+m-2} \end{bmatrix} \quad 2.07$$

q_i are collocation points

THEOREM 1.0

Let I denote the identity Matrix of dimension $(m+t) \times (m+t)$ and Matrices C and D defined by (2.06) and (2.07) satisfies

$$i) \quad DC = I$$

$$y(x) = \sum_{i=0}^{m+t-1} \left\{ \sum_{j=0}^{t-1} \alpha_{j,i+1} y_{n+j} + \sum_{j=0}^{m-1} h \beta_{j,i+1} f_{n+j} \right\} x^i \quad 2.08$$

(For proof see Onumanyi et al [7])

Also, we assume a solution of the form

$$y(x) = \sum_{j=0}^3 a_j x^j, \quad y'(x) = \sum_{j=0}^3 j a_j x^{j-1} \quad 2.09$$

We interpolate at $x = x_n$, and collocate at $x = x_{n+u}, x_{n+w}$ and x_{n+v} ,

where $u = \lambda_1 + \epsilon, w = \frac{1}{2}, v = \lambda_2 + \epsilon$ that is $\lambda_1, \frac{1}{2}, \lambda_2$ are the gaussian points of Legendre polynomial of degree 3, ϵ is a small perturbation to increase the efficiency of the scheme of order $p = 2s$

Equation (2.09) gives the following system of non linear equations of the form

$$\begin{aligned} a_0 + a_1 x_n + a_2 x_n^2 + a_3 x_n^3 &= y_n \\ a_1 + 2a_2 x_{n+u} + 3a_3 x_{n+u}^2 &= f_{n+u} \\ a_1 + 2a_2 x_{n+w} + 3a_3 x_{n+w}^2 &= f_{n+w} \\ a_1 + 2a_2 x_{n+v} + 3a_3 x_{n+v}^2 &= f_{n+v} \end{aligned} \quad 2.10$$

where $a_j, j = 0, 1, 2, 3$ are parameters to be determined. When equation (2.10) is written in matrix equation form we have

$$\begin{bmatrix} 1 & x_n & x_n^2 & x_n^3 \\ 0 & 1 & 2x_{n+u} & 3x_{n+u}^2 \\ 0 & 1 & 2x_{n+w} & 3x_{n+w}^2 \\ 0 & 1 & 2x_{n+v} & 3x_{n+v}^2 \end{bmatrix} \begin{bmatrix} a_0 \\ a_1 \\ a_2 \\ a_3 \end{bmatrix} = \begin{bmatrix} y_n \\ f_{n+u} \\ f_{n+w} \\ f_{n+v} \end{bmatrix} \quad 2.11$$

By using Maple 11 Mathematical software to find $D^{-1} = C$, we obtain the Continuous formulation of the form

$$y(x) = \alpha_0(x) y_n + h \{ \beta_{n+u}(x) f_{n+u} + \beta_{n+w}(x) f_{n+w} + \beta_{n+v}(x) f_{n+v} \} \quad 2.12$$

When solving for parameters in equation (2.12) we obtain our Continuous formula as follows

$$y(x) = y_n + \left[\frac{(h^2 w v) x}{h^2 (-v+u)(-w+u)} - \left(\frac{v h + w h}{h^2 (-w+u)(-v+u)} \right) \frac{x^2}{2} + \frac{1}{3} \left(\frac{x^3}{h^2 (-v+u)(-w+u)} \right) \right] f_{n+u}$$

$$\begin{aligned}
& + \left[\frac{x(uvh^2)}{h^2(-w+v)(-v+u)} - \left(\frac{uh+vh}{h^2(-w+u)(-w+v)} \right) \frac{x^2}{2} + \frac{1}{3} \left(\frac{x^3}{h^2(-w+v)(-w+u)} \right) \right] f_{n+w} \\
& + \left[\frac{-x(uwh^2)}{h^2(-uw+uv-v^2+wv)} + \left(\frac{uh+wh}{h^2(-uw+uv-v^2+wv)} \right) \frac{x^2}{2} - \frac{1}{3} \left(\frac{x^3}{h^2(-uw+uv-v^2+wv)} \right) \right] f_{n+v}
\end{aligned}
\tag{2.13}$$

Evaluating (2.13) at $x = x_{n+j}, j = (u, w, v)$ and $u = \left(\frac{1}{2} - \frac{3\sqrt{7042}}{650}\right), w = \frac{1}{2}, v = \left(\frac{1}{2} + \frac{3\sqrt{7042}}{650}\right)$.

We have the following discrete schemes.

$$\begin{aligned}
y_{n+u} &= y_n + \left(\frac{105625}{760536} - \frac{\sqrt{7042}}{10985520} \right) hf_{n+u} + \left(\frac{84509}{380268} - \frac{\sqrt{7042}}{325} \right) hf_{n+w} \\
& + \left(\frac{105625}{760536} - \frac{84499\sqrt{7042}}{54927600} \right) hf_{n+v} \\
y_{n+w} &= y_n + \left(\frac{105625}{760536} + \frac{325\sqrt{7042}}{169008} \right) hf_{n+u} + \frac{84509}{380268} hf_{n+w} + \left(\frac{105625}{760536} - \frac{325\sqrt{7042}}{169008} \right) hf_{n+v} \\
y_{n+v} &= y_n + \left(\frac{105625}{760536} - \frac{84499\sqrt{7042}}{54927600} \right) hf_{n+u} + \left(\frac{84509}{380268} + \frac{\sqrt{7042}}{325} \right) hf_{n+w} \\
& + \left(\frac{105625}{760536} + \frac{\sqrt{7042}}{10985520} \right) hf_{n+v}
\end{aligned}
\tag{2.14}$$

Differentiating (2.13) we obtain

$$\begin{aligned}
y'_{n+u} &= f \left[x + uh, y_n + \left(\frac{105625}{760536} - \frac{\sqrt{7042}}{10985520} \right) hf_{n+u} + \left(\frac{84509}{380268} - \frac{\sqrt{7042}}{325} \right) hf_{n+w} + \left(\frac{105625}{760536} - \frac{84499\sqrt{7042}}{54927600} \right) hf_{n+v} \right] \\
y'_{n+w} &= f \left[x + uh, y_n + \left(\frac{105625}{760536} + \frac{325\sqrt{7042}}{10985520} \right) hf_{n+u} + \frac{84509}{380268} hf_{n+w} + \left(\frac{105625}{760536} - \frac{325\sqrt{7042}}{169008} \right) hf_{n+v} \right] \\
y'_{n+v} &= f \left[x + uh, y_n + \left(\frac{105625}{760536} + \frac{84499\sqrt{7042}}{54927600} \right) hf_{n+u} + \left(\frac{84509}{380268} + \frac{\sqrt{7042}}{325} \right) hf_{n+w} \right. \\
& \quad \left. + \left(\frac{105625}{760536} + \frac{\sqrt{7042}}{10985520} \right) hf_{n+v} \right]
\end{aligned}
\tag{2.15}$$

Substituting $k_1 = y'_{n+u}, k_2 = y'_{n+w}, k_3 = y'_{n+v}$ and $f_{n+u} = k_1, f_{n+w} = k_2, f_{n+v} = k_3$, when substituting the values of u, w , and v we obtain the Runge- Kutta type scheme as

$$y_{n+1} = y_n + b_1 k_1 + b_2 k_2 + b_3 k_3.$$

Also evaluating the Continuous (2.13) at $x = 1$, we obtain $b_1 = \frac{105625}{380268}, b_2 = \frac{84509}{1901348}, b_3 = \frac{105625}{380268}$

Thus the Runge-kutta methods is put in a Butcher.s Tableau

C	A	
$\frac{1}{2} - \frac{3\sqrt{7042}}{650}$	$\left(\frac{105625}{760536} - \frac{\sqrt{7042}}{10985520} \right)$	$\left(\frac{84509}{380268} - \frac{\sqrt{7042}}{325} \right)$
		$\left(\frac{105625}{760536} - \frac{84499\sqrt{7042}}{54927600} \right)$

$\frac{1}{2}$	$\left(\frac{105625}{760536} + \frac{325\sqrt{7042}}{10985520}\right)$	$\frac{84509}{380268}$	$\left(\frac{105625}{760536} - \frac{325\sqrt{7042}}{169008}\right)$
$\frac{1}{2} + \frac{3\sqrt{7042}}{650}$	$\left(\frac{105625}{760536} + \frac{84499\sqrt{7042}}{54927600}\right)$	$\left(\frac{84509}{380268} + \frac{\sqrt{7042}}{325}\right)$	$\left(\frac{105625}{760536} + \frac{\sqrt{7042}}{10985520}\right)$
b^T	$\frac{105625}{380268}$	$\frac{84509}{190134}$	$\frac{105625}{380268}$

2.16

3. ERROR ESTIMATION

In this section we derived a local error bound for new scheme and compare this error estimate with some exact solutions to check our level of accuracy, most especially problems without analytic solutions.

Now let $y^{(h)}$ and $y^{(\frac{h}{2})}$ be approximate solutions to (2.01), with step size h and $\frac{h}{2}$ respectively. Every Runge-kutta method of order p agrees with Taylor's series expansion up to the p terms. Since exact solution y_{n+1} is unique, we can write

$$y_{n+1} = y_{n+1}^{(h)} + ch^{p+1} + \mathfrak{R}_n(x) \quad 3.01$$

and

$$y_{n+1} = y_{n+1}^{(\frac{h}{2})} + c\left(\frac{h}{2}\right)^{p+1} + \mathfrak{R}_n(x) \quad 3.02$$

as $p \rightarrow \infty$, $\mathfrak{R}_n(x) \rightarrow 0$, $\mathfrak{R}_n(x)$ can be ignored.

Subtracting (3.02) from (3.01) we have

$$0 = y_{n+1}^{(h)} - y_{n+1}^{(\frac{h}{2})} + Ch^{p+1} \left[\frac{2^{p+1}-1}{2^{p+1}} \right]$$

$$\Rightarrow Ch^{p+1} = \frac{2^{p+1}}{2^{p+1}-1} \left[y_{n+1}^{(\frac{h}{2})} - y_{n+1}^{(h)} \right] \quad (\text{Global error}) \quad 3.03$$

$$\frac{2^{p+4}-7}{2^{p+4}-8} \leq \frac{2^{p+1}}{2^{p+1}-1}, p \geq 1$$

We take our local error as

$$E = \frac{2^{p+4}-7}{2^{p+4}-8} \left[y_{n+1}^{(\frac{h}{2})} - y_{n+1}^{(h)} \right] \quad 3.04$$

Hence, our scheme is of Order 6 (3.04) reduces to

$$E = \frac{1017}{1016} \left[y_{n+1}^{(\frac{h}{2})} - y_{n+1}^{(h)} \right] \quad (\text{local error}) \quad 3.05$$

4. NUMERICAL EXPERIMENTS

In this section we use some problems with exact solutions to check their efficiencies and stability of our methods.

Example 1

$$y' = -4y + 20 \quad y(0) = 2 \quad 0 \leq x \leq 0.25, \text{ with } h = 0.05$$

Exact solution is $y(x) = 5 - 3e^{-4x}$

Example 2

$$y' = -3y + 20 + \sin x, \quad y\left(\frac{\pi}{2}\right) = 3 \quad \frac{\pi}{2} \leq x \leq \frac{3\pi}{5}, \text{ with } h = \frac{\pi}{50}$$

$$\text{Exact solution is } = -\frac{1}{10}\text{Cos}x + \frac{3}{10}\text{Sin}x + \frac{27}{10}\frac{e^{-3x}}{e^{-\frac{3\pi}{2}}}$$

Table 1
Comparison of Approximate solution with exact solution of problem 1

x	Exact Solution	Approximate Solution $h = 0.05$	Absolute Error $h = 0.05$
0.05	2.54387740766050	2.54387741000770	2.35 E (-10)
0.1	2.989039861893080	2.989039862277420	3.84 E (-10)
0.15	3.353565091717920	3.353565092189920	4.72 E (-10)
0.2	3.652013107648330	3.652013108163590	5.15 (-10)
0.25	3.896361676485670	3.896361677012990	5.27 E (-10)

Table 2
Error estimation by method 3.05 for Example 1

x	Approximate Solution $y^{(h)}$	Approximate Solution $y^{(\frac{h}{2})}$	Calculated error method (3.05)
0.05	2.54387741000770	2.543807740766090	2.35 E (-10)
0.1	2.989039862277420	2.989039861893140	3.85 E (-10)
0.15	3.353565092189920	3.353565091717990	4.72 E (-10)
0.2	3.652013108163590	3.652013107648410	5.16 (-10)
0.25	3.896361677012990	3.896361676485750	5.28 E (-10)

Table 3
Comparison of Approximate solution with exact solution of problem 2

x	Exact Solution	Approximate Solution $y^{(h)}$	Absolute Error $h = \frac{\pi}{50}$
$\frac{3\pi}{25}$	0.305687070481413	0.305687070480996	4.17 E (-13)
$\frac{27\pi}{50}$	0.310167733750774	0.310167733750011	7.63 E (-13)
$\frac{14\pi}{25}$	0.313424306677179	0.313424306676131	1.04 E (-12)
$\frac{29\pi}{50}$	0.315443937055075	0.315443937053793	1.28 (-12)
$\frac{3\pi}{5}$	0.316218654326041	0.316218654324570	1.47 E (-12)

Table 4
Error estimation by method 3.05 for Example 2

x	Approximate Solution $h = \frac{\pi}{50}$	Approximate Solution $\frac{h}{2} = \frac{\pi}{100}$	Error method (3.0.5)
$\frac{3\pi}{25}$	0.305687070480996	0.305687070481411	4.15 E (-13)
$\frac{27\pi}{50}$	0.310167733750011	0.310167733750771	7.62 E (-13)
$\frac{14\pi}{25}$	0.313424306676131	0.3134243066777175	1.05 E (-12)
$\frac{29\pi}{50}$	0.315443937053793	0.315443937055070	1.28 (-12)
$\frac{3\pi}{5}$	0.316218654324570	0.316218654326036	1.47 E (-12)

5. CONCLUDING REMARK

We have derived a 3-stage special sixth order implicit Runge-kutta method for first order stiff differential equations alongside we derived its local error bound (3.0.5). The schemes are efficient and stable. Implementation cost is minimal also the error estimate (3.0.5) is exact. We want to conclude that for problem without exact solution, we can use this method together with local error to determine its exact solution or efficiency of any first order ODEs.

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