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A highly efficient implicit Runge-Kutta method for first order ordinary differential equations

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In this paper we develop a more efficient three-stage implicit Runge-Kutta method of order 6 for solving first order initial value problems of ordinary differential equations. Collocation method is used to derive Continuous schemes in which both the interpolation and collocation points are at perturbed Gaussian points. This gives a higher order scheme, which is more efficient and stable than the existing similar ones. Simple linear problems are used to check its level of accuracy and stability.

Key words: Implicit, more efficient, stable, collocation methods, Perturbed Gaussian points and error estimates.

INTRODUCTION

Implicit Runge-Kutta methods are A-stable and hence, very efficient for solving both Stiff and non- Stiff problems of ordinary differential equations (ODEs). Implicit Runge-Kutta methods were earlier developed by Kuntzmann (Butcher, 1964, 1988) etc.

There are different types of implicit Runge-Kutta methods, examples are Singly implicit methods (Butcher and Jackiewicz, 1997) with order $p = s, (s = stages)$; Diagonal implicit methods (Butcher and Jackiewicz, 1998; Kuntzmann, 1961) and Multiply implicit method with order $p = 2s.$

The construction of multiply or full implicit methods are based on the theory of Gauss quadrature, where the nodes of integration are the transformed zeros of Legendre polynomial from (-1, 1) onto (0,1). At the moment we have schemes up to order Six. The existing Sixth order scheme (Press et al., 2007) is given as follows:

$$y_{n+1} = y_n + \frac{5}{18}hk_1 + \frac{4}{9}hk_2 + \frac{5}{18}hk_3 \qquad (1)$$

Where

$$k_1 = y_n + \frac{5}{36}hk_1 + \left(\frac{2}{9} - \frac{\sqrt{15}}{15}\right)hk_2 + \left(\frac{5}{36} - \frac{\sqrt{15}}{30}\right)hk_3$$

$$k_2 = y_n + \left(\frac{5}{36} + \frac{\sqrt{24}}{24}\right)hk_1 + \frac{2}{9}hk_2 + \left(\frac{5}{36} - \frac{\sqrt{15}}{24}\right)hk_3$$

$$k_3 = y_n + \left(\frac{5}{36} + \frac{\sqrt{15}}{30}\right)hk_1 + \left(\frac{2}{9} + \frac{\sqrt{15}}{15}\right)hk_2 + \frac{5}{36}hk_3$$

(Agam, 2014).

Construction of schemes higher than 6 is very tedious and almost impossible to derive because the zeros of

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Legendre polynomials of order 4 and above are very complex. Alternative methods are the Radau and Lobatto method (Yakubu, 2010), Diagonal implicit methods (Butcher and Jackiewicz, 1998; Kuntzmann, 1961). These are good but have low order reduction. Other methods include efficient numerical methods for highly Oscillatory ODEs (Petzol, 1981), method for solving ODEs II (Hairer and Warmer, 1996) etc.

In this work, we shall improve on the 6th order implicit Runge-Kutta method by adding a perturbation on the Gaussian points of the third order Legendre polynomial and using Collocation method (Onumanyi et al., 1994), to derive a new higher order scheme.

DERIVATION OF IMPLICIT RUNGE-KUTTA METHOD FOR FIRST ODEs

Given a differential equation

$$y' = f(x,y) \quad y(x_0) = y_0, a \le x \le b \tag{2}$$

We consider a polynomial of the form

$$y(x) = \sum_{j=0}^{t-1} \alpha_j(x) y_{n+j} + h \sum_{j=0}^{m-1} \beta_j(x) f(\bar{x}, y(\bar{x})) \tag{3}$$

where t denotes the number of interpolation points $x_{n+j}, j = 0,1, \dots m-1, m$ is the distinct collocation points $\bar{x}_j, j = 0,1 \dots .m-1,$ y and f are smooth root vector functions.

We can represent $\alpha_j(x)$ and $\beta_j(x)$ by polynomial of form

$$\alpha_j(x) = \sum_{j=0}^{t+m-1} \alpha_{j,i+1} x^i, j = 0,1 \ t-1 \tag{4}$$

$$h\beta_j(x) = \sum_{j=0}^{t+m-1} \beta_{j,i+1} x^i, t = 0,1 \ ..m-1 \tag{5}$$

with constant coefficients $\alpha_{j,t+1}$ and $\beta_{j,t+1}$ to be determined.

Substituting Equations (4 and 5) into (3), we have

$$y(x) = \sum_{j=0}^{t-1}\left(\sum_{j=0}^{t-1} \alpha_{j,i+1} y_{n+j} + \sum_{j=0}^{m-1} h\beta_{j,i+1} f_{n+j}\right) x^i = \sum_{j=0}^{t+m-1} a_j x^i \tag{6}$$

where

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

Now we assume a power series of q or $p = 2s$, of the form

$$y(x_n) = \sum_{j=0}^{3} a_j x^j$$

as a basis solution for Equation (2), interpolating Equation (6) at $x = x_n$ and collocating at $x = x_{n+\mu}, x_{n+\omega}, x_{n+v}$, we have the following system of equations:

$$y(x) = \sum_{j=0}^{3} a_j x_n^j$$

$$y'(x) = \sum_{j=1}^{3} j a_j x_{n+\lambda}^{j-1} \quad \lambda = (u, \omega, v) \tag{7}$$

Equation (7) yields a system of simultaneous equation of the form:

$$\begin{aligned} a_0 + a_1 x_n + a_2 x_n^2 + a_3 x_n^3 &= y_n \\ a_1 + 2a_2 x_{n+u} + 3a_3 x_{n+u}^2 &= f_{n+u} \\ a_1 + 2a_2 x_{n+\omega} + 3a_3 x_{n+\omega}^2 &= f_{n+\omega} \\ a_1 + 2a_2 x_{n+v} + 3a_3 x_{n+v}^2 &= f_{n+v} \end{aligned} \tag{8}$$

where

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

are the parameters to be determined.
When Equation (8) is arranged in matrix equation form we have

$$\begin{bmatrix} 1 & x_n & x_n^2 & x_n^3 \\ 0 & 1 & 2x_{n+u} & 3x_{n+u}^2 \\ 0 & 1 & 2x_{n+\omega} & 3x_{n+\omega}^2 \\ 0 & 1 & 2x_{n+v} & 3x_{n+v}^2 \end{bmatrix} \begin{bmatrix} a_0 \\ a_1 \\ a_2 \\ a_3 \end{bmatrix} = \begin{vmatrix} y_n \\ f_{n+u} \\ f_{n+\omega} \\ f_{n+v} \end{vmatrix} \tag{9}$$

That is, $DA = Y$

Our D matrix is

$$D = \begin{bmatrix} 1 & x_n & x_n^2 & x_n^3 \\ 0 & 1 & 2x_{n+u} & 3x_{n+u}^2 \\ 0 & 1 & 2x_{n+w} & 3x_{n+w}^2 \\ 0 & 1 & 2x_{n+v} & 3x_{n+v}^2 \end{bmatrix} \quad (10)$$

The D matrix is non-singular and has inverse $D^{-1} = C$, using Maple mathematical software to determine the value of C and solving for $a_j, j = (0,1,2,3)$.

We obtain Continuous scheme as

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

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

$$+\left[\left(\frac{(uh)(wh)}{h^2(-uw+uv-v^2+wv)}\right)x + \frac{1}{2}\left(\frac{uh+wh}{h^2(-uw+uv-v^2+wv)}\right)x^2 - \frac{1}{3}\left(\frac{x^3}{h^2(-uw+uv-v^2+wv)}\right)\right]f_{n+v} \quad (11)$$

Evaluating Equation (11) at $x = x_{n+u}, x_{n+w}, x_{n+v}$, with

$$u = \left(\frac{1}{2} - \frac{3\sqrt{7042}}{680}\right), w = \frac{1}{2}, v = \left(\frac{1}{2} + \frac{3\sqrt{7042}}{680}\right).$$

These are perturbed Quassian points (approximate zero of Legendre polynomial of order 3 on (0, 1)), which gives the following discrete schemes:

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

$$y_{n+w} = y_n + \left(\frac{105625}{760536} + \frac{325\sqrt{7042}}{169008}\right)hf_{n+u} + \frac{84509}{380268}hf_{n+w} + \left(\frac{105625}{760536} - \frac{325\sqrt{7042}}{169008}\right)hf_{n+v}$$

$$y_{n+v} = y_n + \left(\frac{105625}{760536} + \frac{84499\sqrt{7042}}{54927600}\right)hf_{n+u} + \left(\frac{84509}{380268} + \frac{\sqrt{7042}}{325}\right)hf_{n+w} + \left(\frac{105625}{760536} + \frac{\sqrt{7042}}{10985520}\right)hf_{n+v} \quad (12)$$

To convert to Runge-Kutta the three discrete schemes must satisfy Equation (2) that is

$f_{n+u} = k_1, f_{n+w} = k_2, f_{n+v} = k_3$ also

$y'_{n+u} = k_1, y'_{n+w} = k_2, y'_{n+v} = k_3$, we therefore have:

$$y'_{n+u} = f(x+uh, y_{n+u}) = f\left(x + \left(\frac{1}{2} + \frac{3\sqrt{7042}}{650}\right)h, y_n + \left(\frac{105625}{760536} - \frac{\sqrt{7042}}{10985520}\right)hf_{n+u}\right.$$

$$\left. + \left(\frac{84509}{380268} - \frac{\sqrt{7042}}{325}\right)hf_{n+w} + \left(\frac{105625}{760536} - \frac{84499\sqrt{7042}}{54927600}\right)hf_{n+v}\right)$$

$$y'_{n+w} = f(x+wh, y_{n+w}) = f\left(x + \frac{1}{2}h, y_n + \left(\frac{105625}{760536} + \frac{325\sqrt{7042}}{169008}\right)hf_{n+u}\right.$$

$$\left. + \frac{84509}{380268}hf_{n+w} + \left(\frac{105625}{760536} - \frac{325\sqrt{7042}}{169008}\right)hf_{n+v}\right)$$

$$y'_{n+v} = f(x+vh, y_{n+v}) = f\left(x + \left(\frac{1}{2} + \frac{3\sqrt{7042}}{650}\right)h, y_n + \left(\frac{105625}{760536} + \frac{84499\sqrt{7042}}{54927600}\right)hf_{n+u}\right.$$

$$\left. + \left(\frac{84509}{380268} + \frac{\sqrt{7042}}{325}\right)hf_{n+w} + \left(\frac{105625}{760536} + \frac{\sqrt{7042}}{10985520}\right)hf_{n+v}\right) \quad (13)$$

In substituting for

$y'_{n+u} = f_{n+u} = k_1, y'_{n+w} = f_{n+w} = k_2, y'_{n+v} = f_{n+w} = k_3$,

we obtain the following:

$$k_1 = f\left(x + \left(\frac{1}{2} + \frac{3\sqrt{7042}}{650}\right)h, y_n + \left(\frac{105625}{760536} - \frac{\sqrt{7042}}{10985520}\right)hk_1 + \left(\frac{84509}{380268} - \frac{\sqrt{7042}}{325}\right)hk_2\right.$$

$$\left. + \left(\frac{105625}{760536} - \frac{84499\sqrt{7042}}{54927600}\right)hk_3\right)$$

$$k_2 = f\left(x + \frac{1}{2}h, y_n + \left(\frac{105625}{760536} + \frac{325\sqrt{7042}}{169008}\right)hk_1 + \left(\frac{84509}{380268}\right)hk_2\right.$$

$$\left. + \left(\frac{105625}{760536} - \frac{325\sqrt{7042}}{169008}\right)hk_3\right)$$

$$k_3 = f\left(x + \left(\frac{1}{2} + \frac{3\sqrt{7042}}{650}\right)h, y_n + \left(\frac{105625}{760536} + \frac{84499\sqrt{7042}}{54927600}\right)hk_1 + \left(\frac{84509}{380268} + \frac{\sqrt{7042}}{325}\right)hk_2\right.$$

$$\left. + \left(\frac{105625}{760536} + \frac{\sqrt{7042}}{10985520}\right)hk_3\right)$$

Hence the general Runge-Kutta scheme for Equation (2) is given as

$$y_{n+1} = y_n + b_1 hk_1 + b_2 hk_2 + b_3 hk_3.$$

$b_i = i = 1, \ldots 3$ are the weights of the Gauss quadrature and

$$\sum_{i=1}^{3} b_i = 1$$

Now from Equation (11), choose

$u = \left(\frac{1}{2} - \frac{3\sqrt{7042}}{650}\right), w = \frac{1}{2}, v = \left(\frac{1}{2} + \frac{3\sqrt{7042}}{650}\right)$ to obtain the values of b_i at $x = x_{n+1}$ to obtain

$$b_1 = \frac{106626}{380268},\ b_2 = \frac{84509}{190134},\ b_3 = \frac{106626}{380268}$$

Thus, our general solution is

$$y_{n+1} = y_n + \frac{106625}{380268}hk_1 + \frac{84509}{190134}hk_2 + \frac{106623}{380268}hk_3 \qquad (14)$$

where $k_i\ i = 1,..3$ are defined in Equation (13).

ANALYSIS OF THE SCHEME

(1) Order, Consistency and Stability of the schemes. The following Press et al. (2007), Implicit Runge-Kutta methods, based on Gaussian quadrature have order $p = 2s$ for an S stage method. Thus, the order of our proposed scheme is $p = 2s = 6$

(2) The proposed scheme is consistent because it satisfies the Runge-Kutta conditions:

$$\sum_{j=0}^{3} a_{ij} = C_i \quad and \sum_{i=1}^{3} b_i = 1$$ (Press et al., 2007).

(3) The stability test proportion weight was used; $y' = qy$ where q is a constant and we used the stability function $R(z)$.

$$R(z) = I + zb^T(i - ZA)^{-1}e$$

Where $e = (1,1,1)^T$

The domain of $R(z)$ is:

Dim $(R(z)) = \{z: R(x) < 0 \; and \; R(z) \leq 1\}$

Since our method is based on Gaussian quadrature method and related methods, A- stability is achievable, (Press et al., 2007).

ERROR ESTIMATIONS

There are many different ways of error estimations, e.g Adaptive methods; Taylor's series methods etc. However adaptive method for implicit scheme is too complicated and almost impossible to derive, the Taylor's series expansion and Richardson interpolation approach was used to obtain a local or global error bound, by choosing too different step lengths $h \; and \; \frac{h}{2}$ respectively. We obtained the error.

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

where $y^{\left(\frac{h}{2}\right)}$ and $y^{(h)}$ are the solutions of the method with step size $h \; and \; \frac{h}{2}$ respectively.

NUMERICAL EXPERIMENTS

Here, we shall use one linear problem and stiff problem with exact solutions to compare and contrast with the existing 6th order method and our new implicit 6th order method to determine efficiency and stability of our new scheme.

Example 1:

$$y' = y - y^2 \quad y(0) = 0.5 \quad h = 0.1$$

Theoretical solution: $y(x) = \frac{1}{1+e^{-x}}$,

the approximate solutions and Error graph of Problem 1, are shown in Table 1 and Figure 1 respectively.

Example 2

$$y(x) = -8y + 8x + 1 \quad y(0) = 2 \quad h = 0.1$$

Theoretical solution: $y(x) = x + 2e^{-8x}$,

the approximate solutions and error graph of Problem 2, are shown in Table 2 and Figure 2 respectively.

DISCUSSION

The second problem is the stiff problem yet the solution is still better than the existing method, Figure 2. Also in this paper we derived an improved 6th order implicit Runge-Kutta method for solution of first order ODEs. This method is more efficient and stable than the existing 6th order implicit method (1.01).

In the two problems, we observed that our new method is more efficient, stable and less costly in the implementation. Also, the new scheme suggests the best method of calculating local error bounds by using Richardson interpolation approach. This method is

Table 1. Approximate solution to problem 1.

χ	Exact solution	Method (1.01)	Error of method (1.01)	Present method	Absolute error of new method
0.1	0.524979187478940	0.524979187478863	5.4 E(-14)	0.524979187478924	1.60 E(-14)
0.2	0.549833997312478	0.549833997312478	1.53E(-13)	0.549833997312448	3.00E(-14)
0.3	0.574442516811658	0.574442516811432	2.26E(-13)	0.574442516811616	4.2E(-14)
0.4	0.598687660112452	0.598687660112155	2.97E(-13)	0.598687660112399	5.30E(-14)
0.5	0.622459331201856	0.622459331201492	3.64E(-13)	0.622459331201795	6.10E(-14)

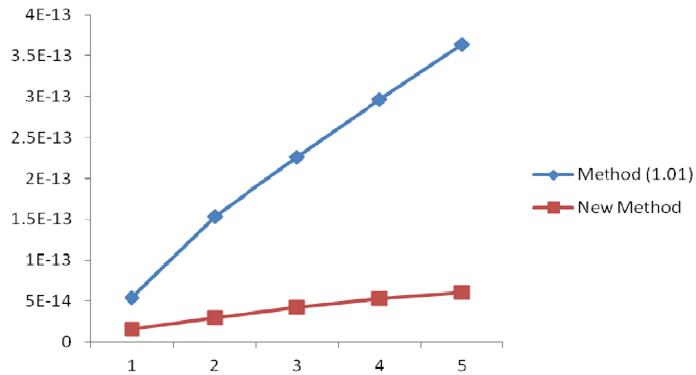

Figure 1. Error graph of problem1.

Table 2. Approximate solution to problem 2.

χ	Exact solution	Method (1.01)	Error of method (1.01)	Present method	Absolute error of new method
0.1	0.998657928234444	0.998656011623680	7.82 E(-06)	0.998656041603738	1.89 E(-06)
0.2	0.603793035989310	0.603791313613691	1.72E(-06)	0.603791340555450	1.69E(-06)
0.3	0.481435906578825	0.481434745710183	1.16E(-06)	0.48143476388714	1.14E(-06)
0.4	0.481524407956732	0.481523712474935	6.95E(-07)	0.481523723353784	6.80E(-07)
0.5	0.536631277777468	0.536630887152740	3.91E(-07)	0.536630893262955	3.85E(-07)

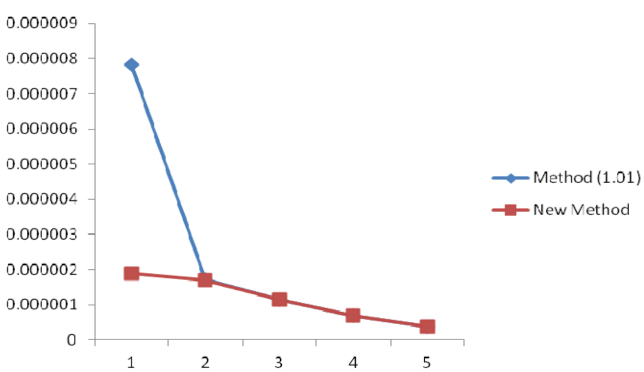

Figure 2. Error graph of problem 2.

simpler than other methods which require a derivative method which are very tedious.

Conflict of Interest

The author(s) have not declared any conflict of interest.

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