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Two Classes of Implicit Runge-Kutta Methods Based on Gauss-Kronrod-Radau Quadrature Formulae

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ABSTRACT

In this paper, two new classes of implicit Runge-Kutta methods which based on 4 points Gauss-Kronrod-Radau I quadrature formula and 4 points Gauss-Kronrod-Radau II quadrature formula were developed. The resulting implicit methods from the 4 points Gauss-Kronrod-Radau I quadrature formula were 4-stage sixth order Gauss-Kronrod-Radau I and 4-stage sixth order Gauss-Kronrod-Radau IA; while the resulting implicit methods from the 4 points Gauss-Kronrod-Radau II quadrature formula were 4-stage sixth order Gauss-Kronrod-Radau II and 4-stage sixth order Gauss-Kronrod-Radau IIA. Each of these methods required 4 function of evaluations at each integration step and gave accuracy of order 6. Numerical experiments compared the accuracy of these four implicit methods and the classical 3-stage sixth order Gauss-Legendre method in solving some test problems. Numerical results revealed that, 4-stage sixth order Gauss-Kronrod-Radau I and 4-stage sixth order Gauss-Kronrod-Radau IIA were more accurate than the 3-stage sixth order Gauss-Legendre method in solving a scalar stiff problem, whereas 4-stage sixth order Gauss-Kronrod-Radau I and 4-stage sixth order Gauss-Kronrod-Radau II were more accurate than the 3-stage sixth order Gauss-Legendre method in solving a two-dimensional stiff problem.

Keywords: Initial value problem, Gauss-Kronrod-Radau I, Gauss-Kronrod-Radau IA, Gauss-Kronrod-Radau II, Gauss-Kronrod-Radau IIA

INTRODUCTION

One-step Runge-Kutta method which is a self-starting numerical method gains tremendous popularity for the computations of numerical solutions of first order initial value problems given by

$$y'(x) = f(x, y), \; y(x_0) = \eta. \tag{1}$$

According to Alexander (1977) and Alexander (2003), the rationale behind the Runge-Kutta method is to approximate the integral in

$$y(x_{n+1}) = y(x_n) + \int_{x_n}^{x_{n+1}} f(x, y(x))\,dx, \tag{2}$$

by a qudrature formula as follows:

$$y_{n+1} = y_n + h\sum_{i=1}^{s} b_i f(x_n + c_i h, Y_i), \tag{3}$$

where the numbers $b_1, b_2, \ldots, b_s$ and $c_1, c_2, \ldots, c_s$ which are independent of the function *f*, are called the quadrature weights and nodes respectively. The functions Y_i are the stage values which are the approximations to $y\left(x_n + c_i h\right),\ i = 1, \ldots, s$, computed by some other quadrature formulae on the intervals $\left[x_n, x_n + c_i h\right]$ as follows:

$$Y_i = y_n + h\sum_{j=1}^{s} a_{ij} f\left(x_n + c_j h, Y_j\right),\ i = 1, \ldots, s. \tag{4}$$

In most cases, explicit Runge-Kutta method is preferable because it allows explicit stage-by-stage implementation which is very easy to program using computer. However, numerical analysts also aware that the computational costs involving function evaluations increases rapidly as higher order requirements are imposed (Hall and Watt, 1976). Another disadvantage of explicit Runge-Kutta method is that it has relatively small interval of absolute stability, which is not suitable to solve stiff initial value problems (Fatunla, 1988). In view of this, we are thus taking interest in implicit Runge-Kutta method. In an implicit Runge-Kutta method, the explicit stage-by-stage implementation scheme enjoyed by explicit Runge-Kutta method is no longer available and needs to be replaced by an iterative computation (Butcher, 2003). Other than this computational difficulty, implicit Runge-Kutta method is an appealing method where higher accuracy can be obtained with fewer function evaluations, and it has relatively bigger interval of absolute stability. For excellent surveys and various perspectives of implicit Runge-Kutta methods, see, for example, Dekker and Verwer (1984), Butcher (1987), Lambert (1991), Hairer and Wanner (1991), Butcher (1992), Hairer et al. (1993), Iserles (1996) and Butcher (2003).

According to Dekker and Verwer (1984), Butcher (1987), Lambert (1991), Hairer and Wanner (1991), Iserles (1996), Butcher (2003) and many others, there are three classes of Gauss-Legendre type implicit Runge-Kutta methods that are based on three different Gauss-Legendre type quadrature formulae, namely Gauss-Legendre methods that are based on Gauss-Legendre quadrature formulae; Radau I, Radau IA, Radau II and Radau IIA methods that are based on Gauss-Radau quadrature formulae; and Lobatto III, Lobatto IIIA, Lobatto IIIB and Lobatto IIIC methods that are based on Gauss-Lobatto quadrature formulae. At this moment, it is natural to ask whether we can devise other types of quadrature formulae in order to develop some new implicit Runge-Kutta methods that will perform equally well or even better than the Gauss-Legendre type implicit Runge-Kutta methods mentioned above. Hence, in this study, we have considered Gauss-Kronrod-Radau I quadrature formula and Gauss-Kronrod-Radau II quadrature formula in constructing two new classes of Kronrod type implicit Runge-Kutta methods.

An *n*-point Gauss-Radau I quadrature formula for the integral

$$I\left(f\right) = \int_a^b f\left(x\right)dx, \tag{5}$$

is a formula of the form

$$G_n f = \sum_{k=1}^{n} w_k f\left(x_k\right), \tag{6}$$

with the nodes $a = x_1 < x_2 < x_3 < \cdots < x_n < b$ and positive weights w_k are chosen so that $G_n f = I(f)$, $\forall f \in \mathrm{P}_{2n-2}$ where P_{2n-2} denotes the set of polynomials of degree $2n-2$ (Davis and Rabinowitz, 1984; Kythe and Schäferkotter, 2005). The associated Gauss-Kronrod-Radau I quadrature formula is given by

$$K_{2n} f = \sum_{k=1}^{n} \hat{w}_k f(\hat{x}_k) + \sum_{k=1}^{n} \tilde{w}_k f(\tilde{x}_k), \tag{7}$$

where $\{\hat{x}_k = x_k\}$ are precisely the one used in equation (6), while all the other 3*n* parameters $\{\hat{w}_k\}$, $\{\tilde{w}_k\}$ and $\{\tilde{x}_k\}$ are chosen in such a way that (Calvetti et al., 2000)

$$K_{2n} f = I(f), \ \forall f \in \mathrm{P}_{3n-1}. \tag{8}$$

According to Calvetti et al. (2000), the nodes in the Gauss-Kronrod-Radau I quadrature formula are ordered so that the following interlacing property is satisfied:

$$a = \hat{x}_1 < \tilde{x}_1 < \hat{x}_2 < \tilde{x}_2 < \hat{x}_3 < \tilde{x}_3 < \cdots < \hat{x}_{n-1} < \tilde{x}_{n-1} < \hat{x}_n < \tilde{x}_n < b.$$

The *n*-point Gauss-Radau II quadrature formula for the integral in equation (5) is a formula of the form

$$H_n f = \sum_{k=1}^{n} w_k f(x_k), \tag{9}$$

with the nodes $a < x_1 < x_2 < x_3 < \cdots < x_n = b$ and positive weights w_k are chosen so that $H_n f = I(f)$, $\forall f \in \mathrm{P}_{2n-2}$ (Davis and Rabinowitz, 1984; Kythe and Schäferkotter, 2005). The associated Gauss-Kronrod-Radau II quadrature formula is given by

$$L_{2n} f = \sum_{k=1}^{n} \hat{w}_k f(\hat{x}_k) + \sum_{k=1}^{n} \tilde{w}_k f(\tilde{x}_k), \tag{10}$$

where $\{\hat{x}_k = x_k\}$ are precisely the one used in equation (9), while all the other 3*n* parameters $\{\hat{w}_k\}$, $\{\tilde{w}_k\}$ and $\{\tilde{x}_k\}$ are chosen in such a way that (Calvetti et al., 2000)

$$L_{2n} f = I(f), \ \forall f \in \mathrm{P}_{3n-1}. \tag{11}$$

According to Calvetti et al. (2000), the nodes in the Gauss-Kronrod-Radau II quadrature formula are ordered so that the following interlacing property is satisfied:

$$a < \tilde{x}_1 < \hat{x}_1 < \tilde{x}_2 < \hat{x}_2 < \tilde{x}_3 < \hat{x}_3 < \cdots < \tilde{x}_{n-1} < \hat{x}_{n-1} < \tilde{x}_n < \hat{x}_n = b.$$

This paper is organized as follows. Section 2 presents the developments of 4-stage sixth order Gauss-Kronrod-Radau I and 4-stage sixth order Gauss-Kronrod-Radau IA. Section 3 presents the developments of 4-stage sixth order Gauss-Kronrod-Radau II and 4-stage sixth order Gauss-Kronrod-Radau IIA. Numerical comparisons among these new methods and the 3-stage sixth order Gauss-Legendre method are presented in Section 4. Lastly, some discussions and conclusions will be given in Section 5.

4-STAGE IMPLICIT RUNGE-KUTTA METHODS BASED ON 4 POINTS GAUSS-KRONROD-RADAU I QUADRATURE FORMULA

In this section, we have developed two implicit Runge-Kutta methods based on 4 points Gauss-Kronrod-Radau I quadrature formula which consists of two fixed nodes from the 2 points Gauss-Radau I quadrature formula, and 2 additional nodes. The weights and nodes of a 2 points Gauss-Radau I quadrature formula are well known, and these values are given by (Butcher, 2003)

$$\left\{ w_1 = \frac{1}{4}, w_2 = \frac{3}{4}, x_1 = 0, x_2 = \frac{2}{3} \right\}. \tag{12}$$

The weights of a 2 points Gauss-Radau I quadrature formula as shown in (12) will not be reused in constructing a 4 points Gauss-Kronrod-Radau I quadrature formula.

For the derivation of the 4 points Gauss-Kronrod-Radau I quadrature formula, we considered the following function given by

$$f\left(x\right) = a_0 + a_1 x + a_2 x^2 + a_3 x^3 + a_4 x^4 + a_5 x^5 . \tag{13}$$

On substituting (5), (7) and (13) into (8) with $n = 2$, $a = 0$ and $b = 1$, then we obtain the following result:

$$\int_0^1 \left(a_0 + a_1 x + a_2 x^2 + a_3 x^3 + a_4 x^4 + a_5 x^5 \right) dx = \sum_{k=1}^{2} \hat{w}_k f\left(\hat{x}_k\right) + \sum_{k=1}^{2} \tilde{w}_k f\left(\tilde{x}_k\right). \tag{14}$$

The integration of integral in (14) yields the following result,

$$\int_0^1 \left(a_0 + a_1 x + a_2 x^2 + a_3 x^3 + a_4 x^4 + a_5 x^5 \right) dx = a_0 + \frac{a_1}{2} + \frac{a_2}{3} + \frac{a_3}{4} + \frac{a_4}{5} + \frac{a_5}{6}. \tag{15}$$

On substituting the result in (15) and $\left\{ \hat{x}_1 = x_1 = 0, \hat{x}_2 = x_2 = 2/3 \right\}$ into (14), we obtain the following expression:

$$\hat{w}_1 f\left(0\right) + \tilde{w}_1 f\left(\tilde{x}_1\right) + \hat{w}_2 f\left(\frac{2}{3}\right) + \tilde{w}_2 f\left(\tilde{x}_2\right) = a_0 + \frac{a_1}{2} + \frac{a_2}{3} + \frac{a_3}{4} + \frac{a_4}{5} + \frac{a_5}{6} . \tag{16}$$

Finally, we have to rearrange the left-hand side of (16) in terms of a_i for $i=0(1)5$ and match these coefficients a_i with those on the right-hand side of (16) in order to obtain a system of six equations. On solving these six equations simultaneously using *MATHEMATICA 5.0*, we have obtained the following weights and quadrature nodes of a 4 points Gauss-Kronrod-Radau I quadrature formula:

$$\left\{\hat{w}_1=\frac{11}{114},\tilde{w}_1=\frac{125\left(4+\sqrt{3}\right)}{1872},\hat{w}_2=\frac{81}{208},\tilde{w}_2=\frac{125\left(4-\sqrt{3}\right)}{1872},\right.$$
$$\left.\hat{x}_1=0,\tilde{x}_1=\frac{3-\sqrt{3}}{5},\hat{x}_2=\frac{2}{3},\tilde{x}_2=\frac{3+\sqrt{3}}{5}\right\},$$

or in the sense of the weights and abscissas of an implicit Runge-Kutta method is

$$\left\{b_1=\frac{11}{114},b_2=\frac{125\left(4+\sqrt{3}\right)}{1872},b_3=\frac{81}{208},b_4=\frac{125\left(4-\sqrt{3}\right)}{1872},\right.$$
$$\left.c_1=0,c_2=\frac{3-\sqrt{3}}{5},c_3=\frac{2}{3},c_4=\frac{3+\sqrt{3}}{5}\right\}. \tag{17}$$

4-stage Sixth Order Gauss-Kronrod-Radau I Method

In order to complete the development of the 4-stage sixth order Gauss-Kronrod-Radau I method, the choice of a_{ij} for $i,j=1(1)4$ is to satisfy all the 16 order conditions of (Butcher, 2003; Hairer and Wanner, 1991)

$$C(4)=\sum_{j=1}^{4}a_{ij}c_j^{k-1}=\frac{c_i^k}{k} \text{ for } i=1(1)4 \text{ and } k=1(1)4. \tag{18}$$

On substituting the abscissas in (17) into (18) and solve these 16 equations simultaneously using *MATHEMATICA 5.0*, yield the solution of the parameters a_{ij}, $i,j=1(1)4$ as shown below:

$$\left\{a_{11}=0,a_{12}=0,a_{13}=0,a_{14}=0,a_{21}=\frac{27+2\sqrt{3}}{300},a_{22}=\frac{102+19\sqrt{3}}{780},a_{23}=\frac{81\left(3-2\sqrt{3}\right)}{1300},\right.$$
$$a_{24}=\frac{150-83\sqrt{3}}{780},a_{31}=\frac{16}{243},a_{32}=\frac{25\left(25+16\sqrt{3}\right)}{3159},a_{33}=\frac{8}{39},a_{34}=\frac{25\left(25-16\sqrt{3}\right)}{3159}, \tag{19}$$
$$\left.a_{41}=\frac{27-2\sqrt{3}}{300},a_{42}=\frac{150+83\sqrt{3}}{780},a_{43}=\frac{81\left(3+2\sqrt{3}\right)}{1300},a_{44}=\frac{102-19\sqrt{3}}{780}\right\}.$$

On substituting the values in (17) and (19) with $s=4$ into (3) and (4), we obtained the 4-stage sixth order Gauss-Kronrod-Radau I method, or in brief as GKRM(4,6)-I. GKRM(4,6)-I has proved to possess sixth order of accuracy because the parameters in (17) satisfy all the order conditions in (Butcher, 2003; Hairer and Wanner, 1991)

$$B(6)=\sum_{i=1}^{4} b_i c_i^{k-1}=\frac{1}{k} \text{ for } k=1(1)6. \tag{20}$$

In addition, the parameters in (17) and (19) also satisfy all the order conditions in (Butcher, 2003; Hairer and Wanner, 1991)

$$D(2)=\sum_{i=1}^{4} b_i c_i^{k-1} a_{ij}=\frac{b_j}{k}\left(1-c_j^k\right) \text{ for } j=1(1)4 \text{ and } k=1(1)2. \tag{21}$$

Since GKRM(4,6)-I satisfies $C(4)$, then we can claim that GKRM(4,6)-I has stage order 4.

The stability function for GKRM(4,6)-I can be easily obtained by using the following formula (Dekker and Verwer, 1984)

$$R(z)=\frac{\det\left[\mathbf{I}-z\mathbf{A}+\mathbf{e}\mathbf{b}^{\mathrm{T}}\right]}{\det\left[\mathbf{I}-z\mathbf{A}\right]}, \tag{22}$$

where in the case of a 4-stage Runge-Kutta method, **I** is a 4×4 identity matrix, **A** is a matrix containing the elements a_{ij} for $i,j=1(1)4$, $e=\begin{pmatrix}1 & 1 & 1 & 1\end{pmatrix}^{\mathrm{T}}$ and **b** is a row vector containing the elements b_i for $i=1(1)4$. Upon these substitutions from (17) and (19), the stability function for GKRM(4,6)-I is given by

$$R(z)_{\text{GKRM(4,6)-I}}=\frac{1800+960z+216z^2+24z^3+z^4}{1800-840z+156z^2-12z^3}. \tag{23}$$

Figure 1 is the plot of stability function (23). The shaded region in Figure 1 is the region of absolute stability of GKRM(4,6)-I where the conditions $\left|R(z)\right|\le 1$ is satisfied.

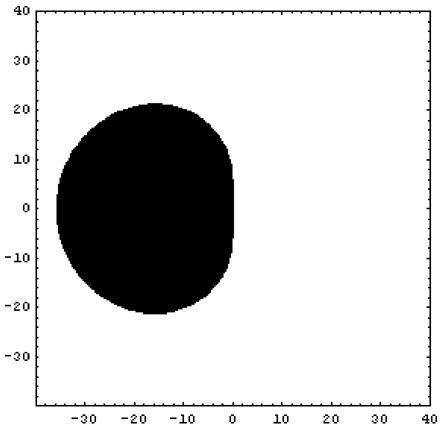

Figure 1: Stability region of GKRM(4,6)-I

Observe that the region of absolute stability of GKRM(4,6)-I is a bounded region which suggest that GKRM(4,6)-I is not *A*-stable.

4-stage Sixth Order Gauss-Kronrod-Radau IA Method

As for the 4-stage sixth order Gauss-Kronrod-Radau IA method, the choice of a_{ij} for $i, j = 1(1)4$ is to satisfy all the 16 order conditions of (Butcher, 2003; Hairer and Wanner, 1991)

$$D(4) = \sum_{i=1}^{4} b_i c_i^{k-1} a_{ij} = \frac{b_i}{k}\left(1 - c_j^k\right) \text{ for } j = 1(1)4 \text{ and } k = 1(1)4. \tag{24}$$

On substituting the weights and abscissas in (17) into (24) and solve these 16 equations simultaneously using *MATHEMATICA 5.0*, yield the solution of the parameters a_{ij}, $i, j = 1(1)4$ as shown below:

$$\begin{Bmatrix} a_{11} = \frac{11}{144}, a_{12} = \frac{5\left(-268-145\sqrt{3}\right)}{20592}, a_{13} = \frac{123}{2288}, a_{14} = \frac{5\left(-268+145\sqrt{3}\right)}{20592}, a_{21} = \frac{11}{144}, \\ a_{22} = \frac{1276+397\sqrt{3}}{9360}, a_{23} = \frac{3\left(71-48\sqrt{3}\right)}{1040}, a_{24} = \frac{7\left(244-139\sqrt{3}\right)}{9360}, a_{31} = \frac{11}{144}, \\ a_{32} = \frac{5\left(76+45\sqrt{3}\right)}{1872}, a_{33} = \frac{115}{624}, a_{34} = \frac{5\left(76-45\sqrt{3}\right)}{1872}, a_{41} = \frac{11}{144}, a_{42} = \frac{7\left(244+139\sqrt{3}\right)}{9360}, \\ a_{43} = \frac{3\left(71+48\sqrt{3}\right)}{1040}, a_{44} = \frac{1276-397\sqrt{3}}{9360} \end{Bmatrix}. \tag{25}$$

On substituting the values in (17) and (25) with $s = 4$ into (3) and (4), we obtained the 4-stage sixth order Gauss-Kronrod-Radau IA method, or in brief as GKRM(4,6)-IA. GKRM(4,6)-IA has proved to possess sixth order of accuracy because the parameters in (17) satisfy all the order conditions in equation (20). In addition, the parameters in (17) and (25) also satisfy all the order conditions in (Butcher, 2003; Hairer and Wanner, 1991)

$$C(2) = \sum_{j=1}^{4} a_{ij} c_j^{k-1} = \frac{c_i^k}{k} \text{ for } i = 1(1)4 \text{ and } k = 1(1)2. \tag{26}$$

Since GKRM(4,6)-IA satisfies $C(2)$, then we can say that GKRM(4,6)-IA has stage order 2.

The stability function for GKRM(4,6)-IA can be easily obtained by substituting the values in (17) and (25) into (22). Upon these substitutions, the stability function for GKRM(4,6)-IA is given by

$$R(z)_{\text{GKRM(4,6)-IA}} = \frac{1800 + 840z + 156z^2 + 12z^3}{1800 - 960z + 216z^2 - 24z^3 + z^4}. \quad (27)$$

Figure 2 is the plot of stability function (27). The shaded region in Figure 2 is the region of absolute stability of GKRM(4,6)-IA where the conditions $|R(z)| \le 1$ is satisfied.

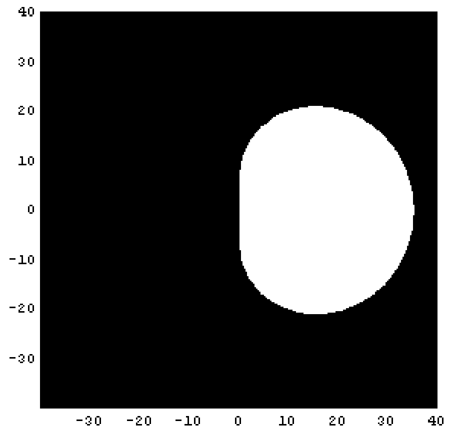

Figure 2: Stability region of GKRM(4,6)-IA

Observe that the region of absolute stability of GKRM(4,6)-IA contains the whole left-half complex plane, which suggest that GKRM(4,6)-IA is *A*-stable. In addition, the condition: $\left|R(z)_{\text{GKRM(4,6)-IA}}\right| \to 0$ as $\text{Re}(z) \to -\infty$ is also satisfied. Therefore, GKRM(4,6)-IA is *L*-stable.

4-STAGE IMPLICIT RUNGE-KUTTA METHODS BASED ON 4 POINTS GAUSS-KRONROD-RADAU II QUADRATURE FORMULA

The discussion for this section is very much similar to the discussion presented in the previous section. In this section, we have developed two implicit Runge-Kutta methods based on 4 points Gauss-Kronrod-Radau II quadrature formula which consists of two fixed nodes from the 2 points Gauss-Radau II quadrature formula, and 2 additional nodes. The weights and nodes of a 2 points Gauss-Radau II quadrature formula are well known, and these values are given by (Butcher, 2003)

$$\left\{ w_1 = \frac{3}{4}, w_2 = \frac{1}{4}, x_1 = \frac{1}{3}, x_2 = 1 \right\}. \quad (28)$$

The weights of a 2 points Gauss-Radau II quadrature formula as shown in (28) will not be reused in constructing a 4 points Gauss-Kronrod-Radau II quadrature formula.

For the derivation of the 4 points Gauss-Kronrod-Radau II quadrature formula, we considered the same function shown in equation (13). On substituting (5), (10) and (13) into (11) with $n = 2$, $a = 0$ and $b = 1$, then we obtain the following result:

$$\int_0^1 \left(a_0 + a_1 x + a_2 x^2 + a_3 x^3 + a_4 x^4 + a_5 x^5\right) dx = \sum_{k=1}^{2} \hat{w}_k f\left(\hat{x}_k\right) + \sum_{k=1}^{2} \tilde{w}_k f\left(\tilde{x}_k\right). \tag{29}$$

The integration of integral in (29) yields the same result as in equation (15). On substituting the result in (15) and $\left\{\hat{x}_1 = x_1 = 1/3, \hat{x}_2 = x_2 = 1\right\}$ into (29), we obtain the following expression:

$$\tilde{w}_1 f\left(\tilde{x}_1\right) + \hat{w}_2 f\left(\frac{1}{3}\right) + \tilde{w}_2 f\left(\tilde{x}_2\right) + \hat{w}_2 f\left(1\right) = a_0 + \frac{a_1}{2} + \frac{a_2}{3} + \frac{a_3}{4} + \frac{a_4}{5} + \frac{a_5}{6}. \tag{30}$$

Finally, we have to rearrange the left-hand side of (30) in terms of a_i for $i = 0(1)5$ and match these coefficients a_i with those on the right-hand side of (30) in order to obtain a system of six equations. On solving these six equations simultaneously using *MATHEMATICA 5.0*, we have obtained the following weights and quadrature nodes of a 4 points Gauss-Kronrod-Radau II quadrature formula:

$$\left\{\tilde{w}_1 = \frac{125\left(4-\sqrt{3}\right)}{1872}, \hat{w}_1 = \frac{81}{208}, \tilde{w}_2 = \frac{125\left(4+\sqrt{3}\right)}{1872}, \hat{w}_2 = \frac{11}{144}, \right.$$
$$\left. \tilde{x}_1 = \frac{2-\sqrt{3}}{5}, \hat{x}_1 = \frac{1}{3}, \tilde{x}_2 = \frac{2+\sqrt{3}}{5}, \hat{x}_2 = 1\right\},$$

or in the sense of the weights and abscissas of an implicit Runge-Kutta method is

$$\left\{b_1 = \frac{125\left(4-\sqrt{3}\right)}{1872}, b_2 = \frac{81}{208}, b_3 = \frac{125\left(4+\sqrt{3}\right)}{1872}, b_4 = \frac{11}{144}, \right.$$
$$\left. c_1 = \frac{2-\sqrt{3}}{5}, c_2 = \frac{1}{3}, c_3 = \frac{2+\sqrt{3}}{5}, c_4 = 1\right\}. \tag{31}$$

4-stage Sixth Order Gauss-Kronrod-Radau II Method

In order to construct the 4-stage sixth order Gauss-Kronrod-Radau II method, the choice of a_{ij} for $i, j = 1(1)4$ is to satisfy all the 16 order conditions of $D(4)$ as given in equation (24). On substituting the weights and abscissas in (31) into (24) and solve these 16 equations simultaneously using *MATHEMATICA 5.0*, yield the solution of the parameters a_{ij}, $i, j = 1(1)4$ as shown below:

$$\left\{a_{11}=\frac{102-19\sqrt{3}}{780},a_{12}=\frac{3\left(4-3\sqrt{3}\right)}{65},a_{13}=\frac{66-29\sqrt{3}}{780},a_{14}=0,a_{21}=\frac{5\left(6+5\sqrt{3}\right)}{468},\right.$$

$$a_{22}=\frac{8}{39},a_{23}=\frac{5\left(6-5\sqrt{3}\right)}{468},a_{24}=0,a_{31}=\frac{66+29\sqrt{3}}{780},a_{32}=\frac{3\left(4+3\sqrt{3}\right)}{65}, \tag{32}$$

$$\left.a_{33}=\frac{102+19\sqrt{3}}{780},a_{34}=0,a_{41}=\frac{5\left(114-35\sqrt{3}\right)}{1716},a_{42}=\frac{48}{143},a_{43}=\frac{5\left(114+35\sqrt{3}\right)}{1716},a_{44}=0\right\}.$$

On substituting the values in (31) and (32) with $s=4$ into (3) and (4), we obtained the 4-stage sixth order Gauss-Kronrod-Radau II method, or in brief as GKRM(4,6)-II. GKRM(4,6)-II has proved to possess sixth order of accuracy because the parameters in (31) satisfy all the order conditions in $B(6)$ as given in equation (20). In addition, the parameters in (31) and (32) also satisfy all the order conditions in $C(2)$ as shown by equation (26). Since GKRM(4,6)-II satisfies $C(2)$, then we can claim that GKRM(4,6)-II has stage order 2.

On substituting the values given in (31) and (32) into equation (22), the stability function for GKRM(4,6)-II is given by

$$R(z)_{\text{GKRM(4,6)-II}}=\frac{1800+960z+216z^2+24z^3+z^4}{1800-840z+156z^2-12z^3}. \tag{33}$$

We note that both GKRM(4,6)-II and GKRM(4,6)-I possess the same stability function. Therefore, Figure 1 also represents the plot of stability function (33). It follows that, the shaded region in Figure 1 is the region of absolute stability of GKRM(4,6)-II where the conditions $\left|R(z)\right|\le 1$ is satisfied. Observe that the region of absolute stability of GKRM(4,6)-II is a bounded region which suggest that GKRM(4,6)-II is not *A*-stable.

4-stage Sixth Order Gauss-Kronrod-Radau IIA Method

As for the 4-stage sixth order Gauss-Kronrod-Radau IIA method, the choice of a_{ij} for $i,j=1(1)4$ is to satisfy all the 16 order conditions of $C(4)$ as given in equation (18). On substituting the abscissas in (31) into (18) and solve these 16 equations simultaneously using *MATHEMATICA 5.0*, yield the solution of the parameters a_{ij}, $i,j=1(1)4$ as shown below:

$$\begin{Bmatrix} a_{11}=\frac{1276-397\sqrt{3}}{9360}, a_{12}=\frac{81\left(13-8\sqrt{3}\right)}{5200}, a_{13}=\frac{7\left(100-53\sqrt{3}\right)}{9360}, a_{14}=\frac{-49+24\sqrt{3}}{3600}, \\ a_{21}=\frac{25\left(140+121\sqrt{3}\right)}{50544}, a_{22}=\frac{115}{624}, a_{23}=\frac{25\left(140-121\sqrt{3}\right)}{50544}, a_{24}=\frac{41}{3888}, \\ a_{31}=\frac{7\left(100+53\sqrt{3}\right)}{9360}, a_{32}=\frac{81\left(13+8\sqrt{3}\right)}{5200}, a_{33}=\frac{1276+397\sqrt{3}}{9360}, a_{34}=\frac{-49-24\sqrt{3}}{3600}, \\ a_{41}=\frac{125\left(4-\sqrt{3}\right)}{1872}, a_{42}=\frac{81}{208}, a_{43}=\frac{125\left(4+\sqrt{3}\right)}{1872}, a_{44}=\frac{11}{144} \end{Bmatrix}. \tag{34}$$

On substituting the values in (31) and (34) with $s=4$ into (3) and (4), we obtained the 4-stage sixth order Gauss-Kronrod-Radau IIA method, or in brief as GKRM(4,6)-IIA. GKRM(4,6)-IIA has also proved to possess sixth order of accuracy because the parameters in (31) satisfy all the order conditions in equation (20). In addition, the parameters in (31) and (34) also satisfy all the order conditions in $D(2)$ as shown in equation (21). Since GKRM(4,6)-IIA satisfies $C(4)$, then we can say that GKRM(4,6)-IIA has stage order 4.

The stability function for GKRM(4,6)-IIA can be easily obtained by substituting the values in (31) and (34) into (22). Upon these substitutions, the stability function for GKRM(4,6)-IIA is given by

$$R(z)_{\text{GKRM(4,6)-IIA}}=\frac{1800+840z+156z^2+12z^3}{1800-960z+216z^2-24z^3+z^4}. \tag{35}$$

We note that both GKRM(4,6)-IIA and GKRM(4,6)-IA possess the same stability function. Therefore, Figure 2 also represents the plot of stability function (35). It follows that, the shaded region in Figure 2 is the region of absolute stability of GKRM(4,6)-IIA where the conditions $\left|R(z)\right|\le 1$ is satisfied. Observe that the region of absolute stability of GKRM(4,6)-IIA contains the whole left-half complex plane, which suggest that GKRM(4,6)-IIA is *A*-stable. In addition, the condition: $\left|R(z)_{\text{GKRM(4,6)-IIA}}\right|\to 0$ as $\text{Re}(z)\to -\infty$ is also satisfied. Therefore, GKRM(4,6)-IIA is *L*-stable.

NUMERICAL EXPERIMENTS AND COMPARISONS

In this section, some test problems are used to check the accuracy of GKRM(4,6)-I, GKRM(4,6)-IA, GKRM(4,6)-II and GKRM(4,6)-IIA using different number of integration steps. We presented the maximum absolute errors over the integration interval given by $\max_{0\le n\le N}\left\{\left|y(x_n)-y_n\right|\right\}$ where *N* is the number of integration steps. We note that $y(x_n)$ and y_n represent the theoretical and numerical solutions of a test problem at point x_n, respectively.

The numerical results obtained from these Kronrod-Radau methods are compared with the numerical results obtained from the 3-stage sixth order Gauss-Legendre method as shown in Hairer et al. (1993). The 3-stage sixth order Gauss-Legendre method consists of the formulae in (3) and (4) with the following values:

$$\Big\{ b_1 = b_3 = \frac{5}{18}, b_2 = \frac{4}{9}, c_1 = \frac{5-\sqrt{15}}{10}, c_2 = \frac{1}{2}, c_3 = \frac{5+\sqrt{15}}{10}, a_{11} = a_{33} = \frac{5}{36}, a_{12} = \frac{80-24\sqrt{15}}{360},$$

$$a_{13} = \frac{50-12\sqrt{15}}{360}, a_{21} = \frac{50+15\sqrt{15}}{360}, a_{22} = \frac{2}{9}, a_{23} = \frac{50-15\sqrt{15}}{360}, a_{31} = \frac{50+12\sqrt{15}}{360},$$

$$a_{32} = \frac{80+24\sqrt{15}}{360} \Big\}.$$

Problem 1 (Ramos, 2007)

$$y'(x) = -100y(x) + 99e^{2x},\ y(0) = 0,\ x \in [0,10].$$

The theoretical solution is given by $y(x) = 33/34(e^{2x} - e^{-100x})$. The maximum absolute errors for each method appeared in Table 1.

Table 1: Maximum absolute errors with respect to number of integration steps, *N* (*Problem 1*)

N	3-stage sixth order Gauss-Legendre method	GKRM(4,6)-I	GKRM(4,6)-IA	GKRM(4,6)-II	GKRM(4,6)-IIA
160	4.50361(+01)	1.62929(-01)	1.24304(+03)	1.86364(+03)	4.83810(-01)
320	1.02504(+00)	6.45554(-03)	3.23311(+01)	3.99111(+01)	1.01077(-02)
640	1.80772(-02)	1.35124(-04)	6.10190(-01)	6.79162(-01)	1.67310(-04)

Problem 2 (Yaakub and Evans, 2003)

$$y''(x) + 101y'(x) + 100y(x) = 0,\ y(0) = 1.01,\ y'(0) = -2,\ x \in [0,10].$$

The theoretical solution is given by $y(x) = 0.01e^{-100x} + e^{-x}$. *Problem 2* can also be written as a system, i.e.

$$y_1'(x) = y_2(x),\ y_1(0) = 1.01,\ x \in [0,10].$$

$$y_2'(x) = -100y_1(x) - 101y_2(x),\ y_2(0) = -2,\ x \in [0,10].$$

The theoretical solutions of this system are given by $y_1(x) = y(x) = 0.01e^{-100x} + e^{-x}$, $y_2(x) = y'(x) = -e^{-100x} - e^{-x}$. The maximum absolute errors for each method appeared in Table 2.

Table 2: Maximum absolute errors with respect to number of integration steps, *N* (*Problem 2*)

N	3-stage sixth order Gauss-Legendre method	GKRM(4,6)-I	GKRM(4,6)-IA	GKRM(4,6)-II	GKRM(4,6)-IIA
160	2.70905(-04)	7.90280(-05)	1.40348(-04)	7.90280(-05)	1.40348(-04)
320	1.82422(-05)	8.11721(-06)	9.97874(-06)	8.11721(-06)	9.97874(-06)
640	5.19273(-07)	2.59024(-07)	2.84600(-07)	2.59024(-07)	2.84600(-07)

From Table 1, we could see that, both GKRM(4,6)-I and GKRM(4,6)-IIA with stage order 4 generate smaller absolute errors compare to the absolute errors generated by the 3-stage sixth order Gauss-Legendre method with stage order 3, and both GKRM(4,6)-IA and GKRM(4,6)-IIA with stage order 2. Although both GKRM(4,6)-IA and GKRM(4,6)-IIA possessed sixth order of accuracy but they were not as accurate as GKRM(4,6)-I and GKRM(4,6)-IIA because they had lower stage order. If the stage order was significantly lower than the order of the Runge-Kutta method, then the values Y_i from (4) were much less accurate due to lower stage order, and affecting the accuracy of the final results computed via formula (3).

From Table 2, the effects of stage order were not apparent, but all four Kronrod-Radau methods were more accurate than the classical 3-stage sixth order Gauss-Legendre method for $N = 160$ and $N = 320$. All methods were found to have comparable accuracy for $N = 640$. *Problem 2* could be expressed in the form of $y' = \lambda y$, $\mathrm{Re}(\lambda) < 0$, which is exactly the Dahlquist's test equation. All stability functions for Runge-Kutta methods could be derived from the application of the Dahlquist's test equation to the Runge-Kutta methods. Since the stability functions for GKRM(4,6)-I and (GKRM(4,6)-II were identical (as in equations (23) and (33)), therefore the results in Table 2 were found to be identical. The same pattern could be observed for GKRM(4,6)-IA and GKRM (4,6)-IIA where both stability functions were found to be identical (as in equations (27) and (35)).

CONCLUSION

In this paper, we have developed two implicit Runge-Kutta methods based on a 4 points Gauss-Kronrod-Radau I quadrature formula, and also two implicit Runge-Kutta methods based on a 4 points Gauss-Kronrod-Radau II quadrature formula.

The resulting implicit methods from the 4 points Gauss-Kronrod-Radau I quadrature formula are 4-stage sixth order Gauss-Kronrod-Radau I (GKRM(4,6)-I) and 4-stage sixth order Gauss-Kronrod-Radau IA (GKRM(4,6)-IA). Both methods possess sixth order of accuracy, but the former possesses stage order 4 while the latter possesses stage order 2. On the other hand, the resulting implicit methods from the 4 points Gauss-Kronrod-Radau II quadrature formula are 4-stage sixth order Gauss-Kronrod-Radau II (GKRM(4,6)-II) and 4-stage sixth order Gauss-Kronrod-Radau IIA (GKRM(4,6)-IIA). Both methods also possess sixth order of accuracy, but the former possesses stage order 2 while the latter possesses stage order 4. In terms of absolute stability analyses, GKRM(4,6)-I and GKRM(4,6)-II shared the same stability function, but they are not *A*-stable. GKRM(4,6)-IA and GKRM(4,6)-IIA shared the same stability function and they are found to be *L*-stable.

Numerical experiments and comparisons showed that implicit Runge-Kutta methods based on Gauss-Kronrod-Radau quadrature formulae worked well for the numerical solution of first order initial value problem (1). In addition, some Kronrod-Radau-type implicit Runge-Kutta methods with higher stage order give more accurate numerical solution. In view of this, a study which focus on the developments of implicit Runge-Kutta methods based on Gauss-Kronrod-Lobatto quadrature formula is now in progress.

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