Adamawa State University Journal of Scientific Research
ISSN: 2251-0702 (P)
Volume 6 Number 2, August, 2018; Article no. ADSUJSR 0602032
http://www.adsujsr.com

Implicit Second-Derivative Runge-Kutta Collocation Methods of Uniformly Accurate Order 3 and 4 for the Solution of Systems of Initial Value Problems

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Abstract

We consider the construction of a new class of implicit Second-derivative Runge-Kutta collocation methods based on intra-step nodal points of Chebyshev-Gauss-Lobatto type, designed for the numerical solution of systems of initial value equations and show how they have been implemented in an efficient parallel computing environment. We also discuss the difficulty associated with large systems and how, in this case, one must take advantage of the second derivative terms in the methods. We involve the introduction of collocation at the two end points of the integration interval in addition to the Gaussian interior collocation points and also the introduction of a different class of basic second derivative methods. With these modifications, fewer function evaluations per step are achieved. The stability properties of these methods are investigated and numerical results are given for each method.

Keywords: Block hybrid discrete scheme; Continuous scheme; System of equations; Second-derivative Runge-Kutta methods

Introduction

In this paper, we present a new class of implicit second-derivative Runge-Kutta (SDRK) collocation methods for the numerical solution of initial value problems for systems of ordinary differential equations (ODEs),

$$\begin{aligned} y'(x) &= f(x, y(x)), \quad x \in [x_o, T], \\ y(0) &= y(x_o). \end{aligned} \tag{1}$$

Here $y:[x_o,T] \to \Re^d$ *and* $f:[x_o,T]\, x\, \Re^d \to \Re^d$ is assumed to be sufficiently smooth and $y_o \in \Re^d$ is the given initial value. Let $h > 0$ be a constant step-size and define the grid by $x_n = x_o + nh,\ n = 0,1,2,\ldots,N$ where $Nh = T - x_o$ and a set of equally spaced points on the integration interval is defined by $x_o < x_1 < x_2 < x_3 <,\ldots,x_{n+1} = T$. The motivation for studying the implicit second-derivative Runge-Kutta collocation methods, particularly, the Gauss–Runge–Kutta collocation family, is that, collocation at the Gauss points leads to Runge-Kutta methods which are symmetric and algebraically stable, Burrage and Butcher (1979). It was also shown in Yakubu (2003, 2010, 2011, 2015, 2016) and Donald, Skwame and Dominic (2015) that the only symmetric algebraically stable collocation methods are those based on Gauss points. The inclusion of the two end points of the integration interval as collocation points in addition to the Gaussian interior collocation points make them more advantageous, because this minimizes the number of internal function evaluations necessary to achieve a given order of accuracy. Secondly, a substantial increase in efficiency maybe achieved by the numerical integration methods which utilize the second-derivative terms. Thirdly, the relatively good stability properties enjoyed by these methods make them more efficient for the numerical integration of system shaving Jacobians with eigenvalues lying close to the imaginary axis Adesanya, Fotta and Onsachi (2016) and Akinfenwa, Abdulganiy, Akinnukawe ,Okunuga and Rufai (2017).

In this paper, we follow the approach of Yakubu, Kumleng and Markus (2017) to derive a class of efficient implicit second-derivative Runge-Kutta collocation methods of high order accuracy, which converge rapidly to the required solutions. We hope that our study can stimulate further interest which will lead to a thorough investigation of the new class of methods.

A General Approach to the Derivation of the SDRK Collocation Methods

In this section, we shall carryout the general derivation of the special class of implicit second-derivative Runge-Kutta collocation methods for direct integration of initial value problems of the form (1). We consider the multistep collocation approach of Onumanyi *et al.,* [1994] and now extends to second derivative of the form,

$$y(x)=\sum_{j=0}^{r-1}\alpha_j(x)y_{n+j}+h\sum_{j=0}^{s-1}\beta_j(x)\bar{y}'_{n+j}+h^2\sum_{j=0}^{t-1}\gamma_j(x)\bar{y}''_{n+j} \quad (2)$$

We set the sum $p=r+s+t$ where, r denotes the number of interpolation points used, and $s>0, t>0$ are distinct collocation points.

Here $\alpha_j(x)$, $\beta_j(x)$ and $\gamma_j(x)$ are parameters of the methods which are to be determined. They are assumed to be polynomials of the form

$$\alpha_j(x)=\sum_{i=0}^{p-1}\alpha_{j,i+1}x^i,\quad h\beta_j(x)=\sum_{i=0}^{p-1}h\beta_{j,i+1}x^i,\quad h^2\gamma_j(x)=\sum_{i=0}^{p-1}h^2\gamma_{j,i+1}x^i \quad (3)$$

We find it convenient to introduce the following polynomials

$$\rho(\xi)=\sum_{i=0}^{p-1}\alpha_i\xi^i,\quad \sigma(\xi)=\sum_{i=0}^{p-1}\beta_i\xi^i,\quad \tau(\xi)=\sum_{i=0}^{p-1}\gamma_i\xi^i$$

which we shall call the first, second and third characteristic polynomials respectively of (2).

Here, our aim is to utilize not only the interpolation points $\{x_j\}$ but also several collocation points on the interpolation interval of (2). This means that we employ a special type of Hermite interpolation for $y(x)$. Substituting (3) into (2) we have

$$y(x)=\sum_{j=0}^{r-1}\sum_{i=0}^{p-1}\alpha_{j,i+1}x^i y_{n+j}+h\sum_{j=0}^{s-1}\sum_{i=0}^{p-1}\beta_{j,i+1}x^i\ \bar{y}'^{\,i}_{n+j}+h^2\sum_{j=0}^{t-1}\sum_{i=0}^{p-1}\gamma_{j,i+1}+x^i\ \bar{y}''_{n+j}$$

$$=\sum_{i=0}^{p-1}\left\{\sum_{j=0}^{r-1}\alpha_{j,i+1}y_{n+j}+h\sum_{j=0}^{s-1}\beta_{j,i+1}\bar{y}'_{n+j}+h^2\sum_{j=0}^{t-1}\gamma_{j,i+1}y''_{n+j}\right\}x^i. \quad (4)$$

writing

$$\phi_i=\sum_{i=0}^{p-1}\left\{\sum_{j=0}^{r-1}\alpha_{j,i+1}y_{n+j}+h\sum_{j=0}^{s-1}\beta_{j,i+1}\bar{y}'_{n+j}+h^2\sum_{j=0}^{t-1}\gamma_{j,i+1}y''_{n+j}\right\}$$

Equation (4) reduces to

$$y(x)=\sum_{i=0}^{p-1}\phi_i x^i. \quad (5)$$

Here $\{c_{n+j}\}$ are collocation points distributed on the step-points array, y_{n+j} is the interpolation data of $y(x)$ on $x_{n+j}, and\ \bar{y}'_{n+j}\ and\ \bar{y}''_{n+j}$ are the collocation data of $y'(x)\ and\ y''(x)$, respectively, on $\{c_{n+j}\}$. We set the sum $r+s+t$ to be equal to p so as to be able to determine $\{\alpha_i\}$ in (2) uniquely.

To fix the parameters $\alpha_i(i=0,1,\cdots,p-1),$ we impose the following conditions:

$$\alpha(x_{n+j})=y_{n+j},\qquad (j=0,1,2,\cdots,r-1) \quad (6)$$

$$\beta'(c_{n+j})=\bar{y}'_{n+j}\qquad (j=0,1,2,\cdots s-1) \quad (7)$$

$$\gamma''(c_{n+j})=\bar{y}''_{n+j}\qquad (j=0,1,2,\cdots t-1) \quad (8)$$

In fact, equations (6) to (8) can be expressed in the matrix-vector form by

$V\alpha = y$ (9)

where the $p-square\ matrix\ V, the\ p-vectors\ \alpha\ and\ y$ are defined as follows:

$$V = \begin{pmatrix} 1 & x_n & x_n^2 & x_n^3 & x_n^4 & x_n^5 & \cdots & x_n^{p-1} \\ 0 & x_{n+1} & x^2{}_{n+1} & x_{n+1}^3 & x_{n+1}^4 & x_{n+1}^5 & \cdots & x_{n+1}^{p-1} \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & x_{n+s-1} & x_{n+s-1}^2 & x_{n+s-1}^3 & x_{n+s-1}^4 & x_{n+s-1}^5 & \cdots & x_{n+s-1}^{p-1} \\ 0 & 1 & 2c_n & 3cx_n^2 & 4cx_n^3 & 5cx_n^4 & \cdots & D'c_n^{p-2} \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 1 & 2c_{n+s-1} & 3c_{n+s-1}^2 & 4c_{n+s-1}^3 & 5x_{n+s-1}^4 & \cdots & D'c_{n+s-1}^{p-2} \\ 0 & 0 & 2 & 6c_n & 12c_n^2 & 20c_n^3 & \cdots & D''c_n^{p-3} \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 2 & 6c_{n+s-1} & 12c_{n+s-1}^2 & 20c_{n+s-1}^3 & \cdots & D''x_{n+s-1}^{p-3} \end{pmatrix} \quad (10)$$

$$\alpha = (\alpha_0, \alpha_1, \alpha_{2,} \cdots, \alpha_{p-1})^T, \quad y = (y_n, \cdots, y_{n+r-1},\ \bar{y}'_n, \cdots, \bar{y}'_{n+s-1},\ \bar{y}''_n, \cdots, \bar{y}''_{n+s-1})^T$$

where $D' = (p-1)\ and\ D'' = (p-1)(p-2)$ represent first and second derivatives respectively. Similar to the Vandermonde matrix, V in (9) is non-singular. Consequently, equation (9) has the unique solution given by

$$\alpha = Uy,\ \ where\ \ U = V^{-1} \quad (11)$$

The interpolation polynomial $y(x)$ in (5) can now be expressed explicitly as follows:

$$y(x) = \left\{ \sum_{j=0}^{r-1} \alpha_{j,p-1} y_{n+j} + h\sum_{j=0}^{s-1} \beta_{j,p-1} \bar{y}'_{n+j} + h^2 \sum_{j=0}^{t-1} \gamma_{j,p-1} \bar{y}''_{n+j} \right\} (1, x, x^2, \ldots, x^{p-1})^T . \quad (12)$$

Recall that $p+s+t$, such that equation (12) becomes

$$y(x) = \left\{ \sum_{j=0}^{r-1} \alpha_{j,r+s+t-1} y_{n+j} h \sum_{j=0}^{s-1} \beta_{j,r+s+t-1} \bar{y}'_{n+j} + h^2 \sum_{j=0}^{t-1} \gamma_{j,r+s+t-1} y''_{n+j} \right\} (1, x, x^2, \ldots, x^{r+s+t-1})^T . \quad (13)$$

Expanding (13) fully, gives the continuous scheme;

$$y(x) = (y_n, \cdots, y_{n+r-1,}\ \bar{y}'_n, \cdots, \bar{y}'_{n+s-1},\ \bar{y}''_n, \cdots, \bar{y}''_{n+t-1}) U^T (1, x, x^2, \cdots, x^{r+s+t-1})^T .$$

where T denotes transpose of the matrix U in (11) and the vector $(1, x, x^2, \cdots, x^{r+s+t-1})$.

In the second-derivative methods, we see that, in addition to the computation of the f -values at the internal stages in the standard Runge-Kutta methods Butcher (2014), the modified methods involve computing g-values, where g is defined by Butcher and Hojjati (2005) as $y''(x) = g(y(x))$, the component number i of $g(y(x))$ can be written as,

$$g_i(y(x)) = \sum \frac{\partial f_i(y(x))}{\partial y_i} f_j(y(x)), \quad i = 1,2,\ldots,m.$$

According to Chan and Tsai (2010) these methods can be practical if the costs of evaluating g are comparable to those in evaluating f and can even be more efficient than the standard Runge-Kutta methods if the number of function evaluations is fewer. It is convenient to rewrite the coefficients of the defining method (13) evaluated at some points in the block matrix form as

$$Y = e \otimes y_n + h(A \otimes I_N)F(Y) + h^2(\hat{A} \otimes I_N)G(Y), \quad (14)$$

$$y_{n+1} = y_n + h\left(b^T \otimes I_N\right)F(Y) + h^2\left(\hat{b}^T \otimes I_N\right)G(Y),$$

where $A = \lfloor a_{ij} \rfloor_{sxs}$, $\hat{A} = [\hat{a}_{ij}]_{s\times s}$ indicate the dependence of the stages on the derivatives found at the other stages and $b = [b_i]_{s\times 1}$, $\hat{b} = \lfloor \hat{b}_i \rfloor_{s\times 1}$ are

$$Y = y_n + hAF(Y) + h^2 \hat{A} G(Y), \qquad (15)$$

$$y_{n+1} = y_n + hb^T F(Y) + h^2 \hat{b}^T G(Y),$$

vectors of quadrature weights showing how the final result depends on the derivatives computed at the various stages, I is the identity matrix of size equal to the differential equation system to be solved and N is the dimension of the system. Also $\otimes$ is the Kronecker product of two matrices and e is the s×1 vector of units. For simplicity, we write the method in Yakubu (2017) as follows:

and the block vectors in $\Re^{sN}$ are defined by

$$Y = \begin{bmatrix} Y_1 \\ Y_2 \\ \vdots \\ Y_s \end{bmatrix}, \qquad F(Y) = \begin{bmatrix} f(Y_1) \\ f(Y_2) \\ \vdots \\ f(Y_s) \end{bmatrix}, \qquad G(Y) = \begin{bmatrix} g(Y_1) \\ g(Y_2) \\ \vdots \\ g(Y_s) \end{bmatrix}. \qquad (16)$$

where s denotes stage values used in the computation of the step $Y_1, Y_2, \ldots, Y_s$.

The coefficients of the Implicit Two-Derivative Runge-Kutta methods can be conveniently represented more compactly in an extended partitioned Butcher Tableau, of the form

$$\begin{array}{c|c||c} c & A & \hat{A} \\ \hline & b^T & \hat{b}^T \end{array} \qquad (17)$$

where $c = [1]_{s\times 1}$ is the abscissa vectors which indicates the position within the step of the stage values.

Methods

Third Order Implicit Second-Derivative Runge-Kutta Collocation Method

For the first implicit second-derivative Runge-Kutta collocation method we define $\xi = (x - x_n)$ and consider the zeros of Legendre polynomial of degree two in the symmetric interval $[-1,1]$, which were transformed into the standard interval $[x_n, x_{n+1}]$. The proposed continuous scheme in (13) can now be written as,

$$y(x) = \alpha_o(x) y_n + h[\beta_1(x) f_{n+u} + \beta_2(x) f_{n+v}] + h^2[\gamma_1(x) g_{n+v}] \qquad (18)$$

where

$$\alpha_0(x) = 1$$

$$\beta_1(x) = \frac{h}{12}\left(-9 - 6\sqrt{2} + 6\sqrt{2}\, t + 12t - 8t^2\right)t$$

$$\beta_2(x) = \frac{h}{12}\left(-6\sqrt{2} + 3 + 6\sqrt{2}\, t + 12t - 8t^2\right)t$$

$$\gamma_1(x) = \frac{\sqrt{2}}{24}\left(3 - 12t + 8t^2\right)th^2$$

Evaluating the continuous scheme $y(x)$ in (18) at the points $x = x_{n+1}, x_{n+u}$ and x_{n+v} (where u and v are the zeros of Legendre polynomial of degree 2) we obtain the implicit second- derivative Runge-Kutta collocation method of uniformly order 3 with only 2-stages with the following block hybrid discrete scheme:

$$y_{n+1} = y_n + \frac{h}{24}[10 f_{n+u} + 14 f_{n+v}] - \frac{h^2}{24}\sqrt{2} g_{n+v}$$

$$order\ p = 3, \quad C_4 = \frac{1}{6} - \frac{\sqrt{2}}{15}$$

$$y_{n+u} = y_n - \frac{h}{48}\left[\left(\sqrt{2} - 10\right) f_{n+u} + \left(11\sqrt{2} - 14\right) f_{n+v}\right] - \frac{h^2}{48}\left[\left(-2 + \sqrt{2}\right) g_{n+v}\right]$$

$$order\ p = 3, \quad C_4 = \frac{-3}{53} - \frac{\sqrt{2}}{45}$$

$$y_{n+v} = y_n + \frac{h}{48}\left[\left(10 + 7\sqrt{2}\right) f_{n+u} + \left(-14 - 5\sqrt{2}\right) f_{n+v}\right] - \frac{h^2}{48}\left[\left(2 + \sqrt{2}\right) g_{n+v}\right]$$

$$order\ p = 3, \quad C_4 = \frac{-3}{53} + \frac{\sqrt{2}}{45}$$

Converting the block hybrid discrete scheme to implicit second-derivative Runge-Kutta method and using (16) we write the method as,

$$y_n = y_{n-1} + h\left(\frac{5}{12}\right)F_1 + h\left(\frac{7}{12}\right)F_2 + h^2\left(\frac{\sqrt{2}}{24}\right)G_1 \tag{19}$$

where the internal stage values at the n^{th} step are computed as:

$$Y_1 = y_{n-1},$$

$$Y_2 = y_{n-1} + h\left(\frac{245}{1176} - \frac{\sqrt{2}}{48}\right)F_1 + h\left(-\frac{343}{1176} - \frac{539\sqrt{2}}{2352}\right)F_2 - h^2\left(-\frac{\sqrt{2}}{48}\right)G_1$$

$$Y_3 = y_{n-1} + h\left(\frac{5}{24} + \frac{7\sqrt{2}}{48}\right)F_1 + h\left(\frac{-7}{24} - \frac{5\sqrt{2}}{48}\right)F_2 + h^2\left(\frac{1}{24} - \frac{\sqrt{2}}{48}\right)G_1$$

$$Y_4 = y_{n-1} + h\left(\frac{5}{12}\right)F_1 + h\left(\frac{7}{12}\right)F_2 + h^2\left(\frac{\sqrt{2}}{24}\right)G_1$$

with the stage derivatives calculated as follows:

$$F_1 = f\left(x_{n-1} + h(0), Y_1\right),$$

$$F_2 = f\left(x_{n-1} + h\left(\frac{1}{2} - \frac{\sqrt{2}}{4}\right), Y_2\right),$$

$$F_3 = f\left(x_{n-1} + h\left(\frac{1}{2} + \frac{\sqrt{2}}{4}\right), Y_3\right),$$

$$F_4 = f\left(x_{n-1} + h(1), Y_4\right).$$

The implicit second-derivative Runge-Kutta collocation method has order p = 3. Writing the method in an extended Butcher Tableau (16), we have

$\frac{2-\sqrt{2}}{4}$	$\frac{-(-490+49\sqrt{2})}{2352}$	$\frac{(-686-532\sqrt{2})}{2352}$	0	0	$\frac{(-686-532\sqrt{2})}{2352}$	0
$\frac{2+\sqrt{2}}{4}$	$\frac{(10+7\sqrt{2})}{48}$	$\frac{(-14+5\sqrt{2})}{48}$	0	0	$-\frac{(-2+\sqrt{2})}{48}$	0
1	$\frac{10}{24}$	$\frac{14}{24}$	0	0	$\frac{-\sqrt{2}}{24}$	0
	$\frac{10}{24}$	$\frac{14}{24}$	0	0	$\frac{-\sqrt{2}}{24}$	0

A Fourth Order Implicit Second-Derivative Runge-Kutta Collocation Method

Next, as the order of the method being sought for increases, the algebraic conditions on the coefficients of the method become increasingly complicated. However, we consider again the two end points of the integration interval as collocation points in addition to the Gaussian interior collocation points, obtained in the same manner as in method (18) with the same $p_2(x)=0$, Legendre polynomial of degree 2. Thus, the proposed continuous scheme in (13) takes the following form:

$$y(x)=\alpha_o(x)y_n+h[\beta_1(x)f_{n+u}+\beta_2(x)f_{n+v}]+h^2[\gamma_1(x)g_{n+u}+\gamma_2(x)g_{n+v}] \tag{19}$$

where

$$\alpha_0(x)=1$$

$$\beta_1(x)=\frac{\sqrt{2}}{4}t\,h\left(\sqrt{2}+1+3t-8t^2+4t^3\right)$$

$$\beta_2(x)=\frac{\sqrt{2}\,h}{4}\left(\sqrt{2}-1-3t+8t^2-4t^3\right)t$$

$$\gamma_1(x)=-\frac{h^2}{48}\left(6+3\sqrt{2}-12t\sqrt{2}-30t-8t^2\sqrt{2}+48t^2-24t^3\right)t$$

$$\gamma_2(x)=\frac{h^2}{48}\left(-6+3\sqrt{2}-12t\sqrt{2}+30t+8t^2\sqrt{2}-48t^2+24t^3\right)t$$

Evaluating the proposed continuous scheme $y(x)$ in (19) at the points $x=x_{n+1},x_{n+u}\ and\ x_{n+v}$ (where u and v are the zeros of Legendre polynomial of degree 2) we obtain the block hybrid discrete scheme as follows:

$$y_{n+1}=y_n+\frac{h}{48}[24f_{n+u}+24f_{n+v}]+\frac{h^2}{48}[\sqrt{2}g_{n+u}-\sqrt{2}g_{n+v}]$$

$$y_{n+u}=y_n+\frac{h}{384}[(96-30\sqrt{2})f_{n+u}+(96-66\sqrt{2})f_{n+v}]+\frac{h^2}{384}[-(11-4\sqrt{2})g_{n+u}+(5-4\sqrt{2})g_{n+v}]$$

$$y_{n+v}=y_n+\frac{h}{384}[(96+66\sqrt{2})f_{n+u}+(96+30\sqrt{2})f_{n+v}]+\frac{h^2}{384}[(5+4\sqrt{2})g_{n+u}-(11+4\sqrt{2})g_{n+v}]$$

Solving the block hybrid discrete scheme simultaneously, we obtain the higher order implicit second-derivative Runge-Kutta collocation method written in the formalism of (15) as follows:

$$y_n = y_{n-1} + h\left(\frac{1}{2}\right)F_1 + h\left(\frac{1}{2}\right)F_2 + h^2\left(\frac{\sqrt{2}}{48}\right)G_1 - h^2\left(\frac{\sqrt{2}}{48}\right)G_2 \qquad (20a)$$

where the internal stage values at the n^{th} step are computed as:

$$Y_1 = y_{n-1},$$

$$Y_2 = y_{n-1} + h\left(\frac{1}{4} - \frac{5\sqrt{2}}{64}\right)F_1 + h\left(\frac{1}{4} - \frac{11\sqrt{2}}{64}\right)F_2 - h^2\left(\frac{11}{384} - \frac{\sqrt{2}}{96}\right)G_1 + h^2\left(\frac{5}{384} - \frac{\sqrt{2}}{96}\right)G_2$$

$$Y_3 = y_{n-1} + h\left(\frac{1}{4} + \frac{5\sqrt{2}}{64}\right)F_1 + h\left(\frac{1}{4} + \frac{5\sqrt{2}}{64}\right)F_2 + h^2\left(\frac{5}{384} + \frac{\sqrt{2}}{96}\right)G_1 - h^2\left(\frac{11}{384} + \frac{\sqrt{2}}{96}\right)G_2$$

$$Y_4 = y_{n-1} + h\left(\frac{1}{2}\right)F_1 + h\left(\frac{1}{2}\right)F_2 + h^2\left(\frac{\sqrt{2}}{48}\right)G_1 - h^2\left(\frac{\sqrt{2}}{48}\right)G_2$$

where the stage derivatives are calculated as follows:

$$F_1 = f\left(x_{n-1} + h(0), Y_1\right),$$

$$F_2 = f\left(x_{n-1} + h\left(\frac{1}{2} - \frac{\sqrt{2}}{4}\right), Y_2\right),$$

$$F_3 = f\left(x_{n-1} + h\left(\frac{1}{2} + \frac{\sqrt{2}}{4}\right), Y_3\right),$$

$$F_4 = f\left(x_{n-1} + h(1), Y_4\right).$$

The implicit second-derivative Runge-Kutta collocation method has order p = 4. Writing the method in an extended Butcher Tableau (16), we have

$$\begin{array}{c|ccc|ccc}
\frac{2-\sqrt{2}}{4} & \frac{(96-30\sqrt{2})}{384} & \frac{(96-66\sqrt{2})}{384} & 0 & -\frac{(11-4\sqrt{2})}{384} & \frac{(5-4\sqrt{2})}{384} & 0 \\
\frac{2+\sqrt{2}}{4} & \frac{(96+66\sqrt{2})}{384} & \frac{(96+30\sqrt{2})}{384} & 0 & \frac{(5+4\sqrt{2})}{384} & -\frac{(11+4\sqrt{2})}{384} & 0
\end{array}$$

1	$\frac{1}{2}$	$\frac{1}{2}$	0	$\frac{\sqrt{2}}{48}$	$\frac{-\sqrt{2}}{48}$	0
	$\frac{1}{2}$	$\frac{1}{2}$	0	$\frac{\sqrt{2}}{48}$	$\frac{-\sqrt{2}}{48}$	0

Analysis of the Second Derivative Runge-Kutta Collocation Methods

Order, Consistency, Zero-stability and Convergence of SDRKC Methods

With the multistep collocation formula (2) we associate the linear difference operator ℓ defined by

$$\ell[y(x);h] = \sum_{j=0}^{r} \alpha_j(x) y(x+jh) + h\sum_{j=0}^{s} \beta_j(x) y'(x+jh) + h^2 \sum_{j=0}^{t} \gamma_j(x) y''(x+jh) \qquad (20b)$$

where $y(x)$ is an arbitrary function, continuously differentiable on $[a,b]$, following Yakubu (2010), we can write the terms in (20b) as a Taylor series expansion about the point x to obtain the expression,

$$\ell[y(x);h] = C_0 y(x) + C_1 h y'(x) + C_2 h^2 y''(x) + \cdots + C_p h^p y^{(p)}(x) + \cdots$$

Where the constant coefficients $C_p,\ p = 0, 1, 2, \ldots$ are given as follows:

$$C_{0:} = \sum_{j=0}^{r} \alpha_j$$

$$C_1 = \sum_{j=1}^{r} j\alpha_j$$

$$C_2 = \sum_{j=1}^{r} j\alpha_j - \sum_{j=0}^{s} \beta_j$$

$$C_3 = \frac{1}{3!}\left(\sum_{j=0}^{r} j^2 \alpha_j - 2\sum_{j=1}^{s} j\beta_j - \sum_{j=0}^{t} \gamma_j \right)$$

$$\vdots \qquad \vdots \qquad \vdots \qquad \vdots$$

$$C_p = \frac{1}{p!}\left(\sum_{j=0}^{r} j\alpha_j - \frac{2}{(p-1)!}\sum_{j=1}^{s} j^{p-1}\beta_j - \frac{1}{(p-2)!}\sum_{j=0}^{t} j^{p-2}\gamma_j \right), p = 3, 4, \cdots$$

According to [24], the multistep collocation formula (2) has order p if

$$\ell[y(x);h] = O\left(h^{(p+1)}\right), C_0 = C_1 = \cdots C_p = 0, C_{p+1} \neq 0.$$

Therefore C_{p+1} is the error constant and $C_{p+1} h^{p+1} y^{(p+1)}$ is the principal local truncation error at the point x_n (Chan and Tai [2010]).

Therefore, the order and the error constants for the two methods constructed are represented in Table1.

Table1: Order and error constants of SDRK collocation methods

Method	Order	Error constant

Method (18)	$p=3$	$C_4 = 7.2383x10^{-2}$
	$p=3$	$C_4 = -8.597x10^{-2}$
	$p=3$	$C_4 = 3.7617x10^{-2}$
Method (20)	$p=4$	$C_5 = 1.4583x10^{-2}$
	$p=4$	$C_5 = 1.1193x10^{-2}$
	$p=4$	$C_5 = 1.0547x10^{-2}$

Definition 1: Yakubu and Kwami (2015) The implicit second-derivative Runge-Kutta collocation (18) and (20) are said to be consistent if the order of the individual method is greater than or equal to one, that is, if $p \geq 1$.

$(i)\quad \rho(1)=0$ *and*

$(ii)\quad \rho'(1)=\sigma(1)$, *where* $\rho(z)$ *and* $\sigma(z)$ *are respectively the* 1*st and* 2*nd characteristic polynomials*.

Definition 2:. Yakubu *et. al.,* (2010) The second derivative Runge-Kutta collocation methods (18) and (20) are said to be zero-stable if the roots

$$\rho(\lambda)=\det\left[\sum_{i=0}^{k} A^i \lambda^{k-1}\right]=0$$

Satisfies $|\lambda_j| \leq 1,\ j=1,2,\ldots,k$ and for those roots with $|\lambda_j|=1$, the multiplicity does not exceed 2.

Definition 3: Yakubu *et al.,* (2010) The necessary and sufficient conditions for the SDRK collocation methods (18) and (20) to be convergent are that they must be consistent and zero-stable.

Stability regions of the SDRK collocation methods

In this paper stability properties of the methods are discussed by reformulating the block hybrid discrete schemes as general linear methods by Butcher (2014) and Butcher and Hojjati (2005). Hence, we use the notations introduced by Butcher and Hojjati (2005), where a general linear method is represented by a partitioned $(s+r)x(s+r)$ matrix (containing A,U, B and V),

$$\begin{bmatrix} Y^{[n]} \\ y^{(n-1)} \end{bmatrix} = \begin{bmatrix} A & U \\ B & V \end{bmatrix} \begin{bmatrix} hf\left(Y^{[n]}\right) \\ y^{[n]} \end{bmatrix}, \quad n=1,2,\ldots,N \qquad (21)$$

where

$$Y^{[n]}=\begin{bmatrix} Y_1^{[n]} \\ Y_2^{[n]} \\ \vdots \\ Y_s^{[n]} \end{bmatrix},\quad y^{[n-1]}=\begin{bmatrix} y_1^{[n-1]} \\ y_2^{[n-1]} \\ \vdots \\ y_r^{[n-1]} \end{bmatrix},\quad f\left(Y^{[n]}\right)=\begin{bmatrix} f\left(Y_1^{[n]}\right) \\ f\left(Y_2^{[n]}\right) \\ \vdots \\ f\left(Y_s^{[n]}\right) \end{bmatrix},\quad y^{[n]}=\begin{bmatrix} y_1^{[n]} \\ y_2^{[n]} \\ \vdots \\ y_r^{[n]} \end{bmatrix},$$

$$A=\begin{bmatrix} 0 & 0 \\ A & B \end{bmatrix},\quad U=\begin{bmatrix} 1 & 0 & 0 \\ 0 & u & c-u \end{bmatrix},\quad B=\begin{bmatrix} A & B \\ 0 & 0 \\ v^T & \omega^T \end{bmatrix},\quad V=\begin{bmatrix} I & \mu & e-\mu \\ 0 & 0 & I \\ 0 & 0 & I-\theta \end{bmatrix},$$

and $e=[1,\ldots,1]$.

Hence (21) takes the form

$$\begin{bmatrix} Y_1^{[n]} \\ Y_2^{[n]} \\ \vdots \\ Y_s^{[n]} \\ ---- \\ y_1^{[n]} \\ y_2^{[n]} \\ \vdots \\ y_r^{[n]} \end{bmatrix} = \begin{bmatrix} A & U \\ --- & \\ B & V \end{bmatrix} \begin{bmatrix} hf\left(Y_1^{[n]}\right) \\ hf\left(Y_2^{[n]}\right) \\ \vdots \\ hf\left(Y_s^{[n]}\right) \\ ---- \\ y_1^{[n-1]} \\ y_2^{[n-1]} \\ \vdots \\ y_r^{[n-1]} \end{bmatrix} \qquad (22)$$

Where r denotes quantities as output from each step and input to the next step and s denotes stage values used in the computation of the step $y_1, y_2, \ldots, y_s$. The coefficients of these matrices $A, U, B, and\ V$ indicate the relationship between the various numerical quantities that arise in the computation of stability regions. The elements of the matrices $A, U, B, and\ V$ are substituted into the stability matrix which leads to the recurrent equation

$$y^{[n-1]} = M(z)y^{[n]}, n = 1,2,3,\ldots, N-1, Z = \lambda h$$

where the stability matrix

$$M(z) = V + zB(I - zA)^{-1}U$$

and the stability polynomial of the method can easily be obtained as follows:

$$\rho(\eta, z) = \det\left(r\left(A - Uz - Vz^2\right) - B\right).$$

The absolute stability region of the method is defined as

$$\Re = x \in C : \rho(\eta, z) = 1 \Rightarrow |\eta| \leq 1.$$

Computing the stability functions gives the stability polynomials of the methods, which are plotted to produce the required graphs of the absolute stability regions of the methods as displayed in Fig. 1.

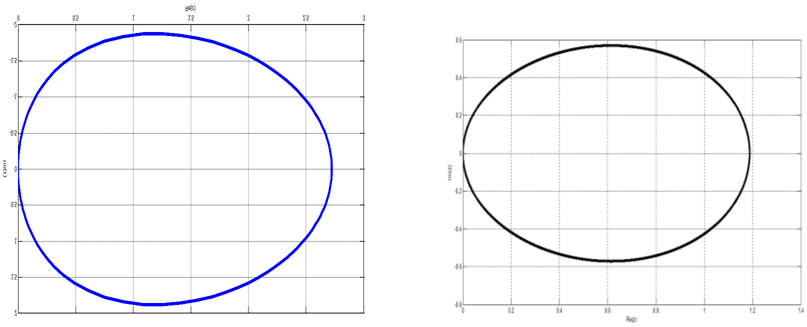

Fig1: Regions of absolute stability of method (18) and method (20) respectively

Remark: The regions of absolute stability of methods (18) and (20) are $A-stable$ since the region consists of the complex plane outside the enclosed figures.

Numerical Results

Preliminary numerical experiments have been carried out using a constant step size implementation in Matlab. The test examples are some systems of ordinary differential equations written as first order initial value problems. We solved these systems and compared the obtained results side by side in Tables.

Example 1:

We consider a well-known classical system which is a mildly stiff problem composed of two first order equations,

$$\begin{bmatrix} y_1'(x) \\ y_2'(x) \end{bmatrix} = \begin{bmatrix} 998+1998 \\ -999-1999 \end{bmatrix} \begin{bmatrix} y_1(x) \\ y_2(x) \end{bmatrix}, \qquad \begin{bmatrix} y_1(0) \\ y_2(0) \end{bmatrix} = \begin{bmatrix} 1 \\ 1 \end{bmatrix},$$

and the exact solutions given by the sum of two decaying exponential components

$$\begin{bmatrix} y_1(x) \\ y_2(x) \end{bmatrix} = \begin{bmatrix} 4e^{-x} - 3e^{-1000x} \\ -2e^{-x} + 3e^{-1000x} \end{bmatrix} \text{ or } \begin{cases} y_1(x) = 4e^{-x} - 3e^{-1000x} \\ y_2(x) = -2e^{-x} + 3e^{-1000x} \end{cases}.$$

The stiffness ratio is R = 1000 and the problem is solved numerically on the interval [10,100]. We have solve the problem using the newly derived Gauss-Radau-Runge-Kutta collocation methods and Continuous General Linear methods of Yakubu (2017) The numerical results obtained are shown in Table 1, while the region of absolute stability shown in Fig.1.

Table 1: Absolute errors of numerical solutions of example 1 within the interval 10≤x≤100

x	Error in Method (18)		Error in Method (20)		Error in Yakubu (2010)	
	Y1	Y2	Y1	Y2	Y1	Y2
10.0	4.684×10^{-4}	4.4075×10^{-3}	3.452×10^{-6}	4.607×10^{-5}	4.642×10^{-3}	4.754×10^{-3}
20.0	5.558×10^{-6}	4.2692×10^{-6}	4.522×10^{-7}	2.728×10^{-6}	6.808×10^{-5}	9.838×10^{-5}
30.0	5.689×10^{-6}	2.5522×10^{-5}	6.344×10^{-8}	8.572×10^{-8}	5.356×10^{-6}	2.078×10^{-5}
40.0	3.895×10^{-6}	1.2500×10^{-6}	4.255×10^{-8}	2.029×10^{-8}	3.476×10^{-7}	3.705×10^{-6}
50.0	1.125×10^{-7}	5.7196×10^{-6}	3.232×10^{-9}	4.464×10^{-11}	2.107×10^{-8}	6.173×10^{-7}
60.0	3.223×10^{-9}	2.5080×10^{-7}	3.553×10^{-11}	9.412×10^{-12}	1.223×10^{-9}	9.854×10^{-8}
70.0	6.023×10^{-10}	1.0681×10^{-6}	5.801×10^{-12}	1.927×10^{-14}	6.899×10^{-10}	1.528×10^{-8}
80.0	3.457×10^{-13}	4.4538×10^{-7}	3.422×10^{-14}	3.864×10^{-16}	3.801×10^{-12}	2.320×10^{-9}
90.0	3.470×10^{-14}	1.8272×10^{-8}	2.070×10^{-16}	7.622×10^{-18}	2.070×10^{-13}	3.465×10^{-10}
100	2.441×10^{-16}	7.4021×10^{-8}	1.110×10^{-20}	1.485×10^{-18}	1.110×10^{-14}	5.110×10^{-11}

Example 2:

Consider the system of mildly stiff linear initial value problem

$$y_1' = -8y_1 + 7y_2, \qquad y_1(0) = 1$$
$$y_2' = 42y_1 - 43y_2, \qquad y_2(0) = 8$$

Whose exact solution is giving by

$$y_1(x) = 2\exp(-x) - \exp(-50x)$$
$$y_2(x) = 2\exp(-x) + 6\exp(-50x).$$

This problem shows that to solve stiff equations the stability of a good method should impose no limitation on the step size, and hence it requires a large stability region. The solution of this example is shown in Table 2, while the region of absolute stability is shown in Fig.1

Table 2: Absolute errors of numerical solutions of example 2 within the interval 10≤x≤100

x	Error in Method (18)		Error in Method (20)		Error in Yakubu (2010)	
	Y1	Y2	Y1	Y2	Y1	Y2
10.0	3.7762×10^{-4}	1.241×10^{-5}	3.4026×10^{-8}	2.781×10^{-7}	2.8477×10^{-5}	1.7827×10^{-6}
20.0	7.7285×10^{-4}	2.843×10^{-6}	4.6957×10^{-8}	1.843×10^{-7}	2.2959×10^{-5}	3.7246×10^{-6}
30.0	2.9815×10^{-4}	6.048×10^{-7}	2.6505×10^{-8}	3.248×10^{-8}	1.2762×10^{-5}	7.7960×10^{-7}
40.0	5.0360×10^{-6}	3.701×10^{-6}	2.3947×10^{-11}	4.766×10^{-8}	6.2503×10^{-6}	1.6317×10^{-7}
50.0	9.2208×10^{-6}	3.688×10^{-8}	3.2812×10^{-12}	2.482×10^{-9}	2.8598×10^{-6}	3.4155×10^{-8}
60.0	2.6744×10^{-6}	6.266×10^{-9}	2.3141×10^{-11}	5.251×10^{-10}	1.2540×10^{-6}	7.1490×10^{-9}
70.0	2.4106×10^{-7}	3.022×10^{-8}	5.0340×10^{-13}	2.722×10^{-11}	5.3409×10^{-7}	1.4963×10^{-9}
80.0	4.9468×10^{-7}	4.154×10^{-10}	2.2382×10^{-14}	3.121×10^{-12}	2.2269×10^{-7}	3.1321×10^{-10}
90.0	2.4149×10^{-8}	5.524×10^{-12}	4.8010×10^{-16}	3.884×10^{-15}	9.1364×10^{-8}	6.5558×10^{-11}
100	3.8820×10^{-9}	3.652×10^{-15}	8.1667×10^{-16}	2.781×10^{-17}	3.7010×10^{-8}	1.3722×10^{-13}

Conclusion

The purpose of the present paper has been to introduce a special class of implicit second-derivative Runge-Kutta collocation methods suitable for the approximate numerical integration of systems of ordinary differential equations. The derived methods provide an efficient way to find numerical solutions to systems of initial value problems when the second derivative terms are cheap to evaluate. We present two new methods of orders three and four. We also presented summary of numerical comparisons between the new methods on a set of two systems of initial value problems. The numerical comparisons as well as establishing the efficiency of the new methods show that the order three method and the order four method shows more accuracy on all the problems considered in the paper.

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