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Design of New Diagonally Implicit Runge–Kutta Methods for Stiff Problems

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Abstract

This paper presents new fifth-order diagonally implicit Runge-Kutta integration formulas for stiff initial value problems, designed to be L-stable method. The stability of the method is analyzed and numerical results are shown to verify the conclusions.

Mathematics Subject Classifications: 51N20, 62J05, 70F99

Keywords: ODE solver; Runge-Kutta method; L-stable; Stiff problems

1 Introduction

The initial value problem(IVP) for a system of first order ordinary differential equations(ODEs) is defined by

$$y' = f(x, y), \qquad y(a) = y_0, \qquad x \in [a, b]. \tag{1}$$

The general s-stage Runge-Kutta method is defined by

$$y_{n+1} = y_n + h \sum_{i=1}^{s} b_i k_i \tag{2}$$

where

$$k_i = f(x_n + c_i h, y_n + h \sum_{j=1}^{i-1} a_{ij} k_j), i = 1, 2, ..., s$$

such formula can be represented conveniently by Butcher array

$$\begin{array}{c|ccccc} c_1 & a_{11} & a_{12} & a_{13} & \dots & a_{1s} \\ c_2 & a_{21} & a_{22} & a_{23} & \dots & a_{2s} \\ c_3 & \vdots & \vdots & \vdots & & \vdots \\ c_4 & . & . & . & & . \\ c_5 & a_{s1} & a_{s2} & a_{s3} & \dots & a_{ss} \\ \hline & b_1 & b_2 & b_3 & b_4 & b_s \end{array}$$

or simply as

$$\begin{array}{c|c} c & A \\ \hline & b^T \end{array}$$

If matrix A is strictly lower triangular (i.e., the internal stages can be calculated without depending on later stages),then the method is called an explicit method otherwise the internal stages depend not only on the previous stages but also on the current stage and later stages, this method is called an implicit method.

The importance of the implicit methods is due to its high orders of accuracy which is superior to the explicit methods.This makes it more suitable for solving stiff problems.

Stiff equations have proved to be too important to be ignored and too expensive to overpower.They are too important because they occur rather frequently in physical problems.They are too expensive to overpower because of their size and the difficulty they present to classical methods no matter how great an improvement in computing capability becomes available. Stiff differential equations arise in a variety of applications, such as network analysis, chemical or nuclear kinetics [1]

The stiff problem had attracted the attention of many numerical analysts, which led to surveys of methods for stiff problems produced by Bjurel, Dahlquist, Lindberg, Linde and Oden [2].

Because of the excessive cost in evaluating the stages in a fully implicit Runge-Kutta method, many researchers have opted for the diagonally implicit Runge-Kutta (DIRK) method, as called by Alexander [3] for these methods, the coefficient matrix A has lower triangular structure with equal elements on the diagonal and sometimes these methods are referred to as singly equal diagonals.

These methods has been identified as quite popular for solving stiff ODEs. In this paper, we construct a novel method that can be used for solving stiff problems.

2 Diagonally Implicit Runge Kutta Methods

Rosenbrock [4] Butcher [5] showed that the degree of implicitness can be reduced by ensuring that the Runge-kutta matrix is a lower triangular.The first studies of this method appeared in the works of $N\phi rsett$ [6] and Alexander [3].This method is named by "semi-implicit" ," semi-explicit" and "diagonally implicit " or "DIRK".Common usage favors using " singly diagonally implicit " or "SDIRK" in the more restricted sense. The idea here is to restrict the method to the form

$$\begin{array}{c|ccccc} c_1 & \lambda & & & & \\ c_2 & a_{21} & \lambda & & & \\ c_3 & a_{31} & a_{32} & \lambda & & \\ c_4 & \vdots & \vdots & \vdots & \ddots & \\ c_5 & a_{s1} & a_{s2} & a_{s3} & a_{s4} & \lambda \\ \hline & b_1 & b_2 & b_3 & b_4 & b_s \end{array} .$$

In [7–12] various effective DIRK methods have been presented.

3 Derivation of Fifth Order Five stages Diagonally Implicit Runge Kutta Method

In this paper we will introduce a new diagonally implicit Runge Kutta methods which have the following form

$$\begin{array}{c|ccccc} \lambda & \lambda & & & & \\ c_1 & a_{21} & \lambda & & & \\ c_2 & a_{31} & a_{32} & \lambda & & \\ \vdots & \vdots & \vdots & \vdots & \ddots & \\ c_s & b_1 & b_2 & b_3 & \dots & \lambda \\ \hline & b_1 & b_2 & b_3 & \dots & \lambda \end{array} .$$

In order to derive a fifth order diagonally implicit Runge-Kutta (DIRK5)method, seventeen equations have to be satisfied. The equations associated with the order of the method are given in Table 1.

Table 1: Equations of order conditions for Runge Kutta Methods of order5

order	Elementary weights	
1	$\sum b_i = 1$	(3.1)
2	$\sum b_i c_i = \frac{1}{2}$	(3.2)
3	$\sum b_i c_i^2 = \frac{1}{3}$	(3.3)
3	$\sum b_i a_{ij} c_j = \frac{1}{6}$	(3.4)
4	$\sum b_i c_i^3 = \frac{1}{4}$	(3.5)
4	$\sum b_i c_i a_{ij} c_j = \frac{1}{8}$	(3.6)
4	$\sum b_i a_{ij} c_j^2 = \frac{1}{12}$	(3.7)
4	$\sum b_i a_{ij} a_{jk} c_k = \frac{1}{24}$	(3.8)
5	$\sum b_i c_i^4 = \frac{1}{5}$	(3.9)
5	$\sum b_i c_i^2 a_{ij} c_j = \frac{1}{10}$	(3.10)
5	$\sum b_i a_{ij} c_j a_{ik} c_k = \frac{1}{20}$	(3.11)
5	$\sum b_i c_i a_{ij} c_j^2 = \frac{1}{15}$	(3.12)
5	$\sum b_i a_{ij} c_j^3 = \frac{1}{20}$	(3.13)
5	$\sum b_i c_i a_{ij} a_{jk} c_k = \frac{1}{30}$	(3.14)
5	$\sum b_i a_{ij} c_j a_{jk} c_k = \frac{1}{40}$	(3.15)
5	$\sum b_i a_{ij} a_{jk} c_k^2 = \frac{1}{60}$	(3.16)
5	$\sum b_i a_{ij} a_{jk} a_{kl} c_l = \frac{1}{120}$	(3.17)

We use two simplifying assumptions to reduce and simplify the equations.The two assumptions are,

$$\sum_i b_i a_{ij} = b_j(1 - c_j), \quad for j = 1, 2, ..., s. \tag{3.18}$$

$$\sum_j a_{ij} c_j = \frac{1}{2} c_i^2 \quad , \qquad for i = 1, 2, ..., s. \tag{3.19}$$

Consider the condition

$$B(\eta) : \sum_{i=1}^{s} b_i c_i^{k-1} = k^{-1}, \quad k = 1, 2, ..., \eta \quad [13]. \tag{3.20}$$

Therefore equations (3.1),(3.2),(3.3),(3.5)and(3.9) have to be satisfied. Consider equation(3.4),by using (3.18)we can write

$\sum_{ij} b_i a_{ij} c_j = \sum_j b_j(1-c_j)c_j = \sum_j b_j c_j - \sum_j b_j c_j^2 = (3.2) - (3.3).$

So we can remove equation(3.4) because(3.2)and(3.3)hold,the same procedure is used on (3.7),(3.8),(3.13),(3.15),(3.16)and(3.17).

Consider equation(3.6)and(3.5)we have

$$\sum_{ij} b_i c_i a_{ij} c_j = \frac{1}{2}\sum_j b_i c_i^3$$

$$\Rightarrow \sum_{ij} b_i c_i a_{ij} c_j - \frac{1}{2}\sum_j b_i c_i^3 = 0$$

$$\Rightarrow \sum_{ij} b_i c_i \left[\sum_i a_{ij}\, c_j - \frac{c_i^2}{2}\right] = 0.$$

For this method we found that for i=1 (3.19) is not true since for i=1 we have $a_{11}c_1 = \frac{c_1^2}{2} \Rightarrow c_1^2 = \frac{c_1^2}{2}$ which give us $c_1 = 0$,but $c_1 = \lambda \neq 0$, there fore we assign b_1 to be zero,so we can remove equation(3.6), then we implement the same procedure on (3.10), (3.11) and (3.12),(3,14).

The values of a_{i1} for i=1,2,...,5 are obtained by the relationship

$$a_{i1} = c_i - \sum_{j=2}^{i} a_{ij}.$$

Now, we just choose the suitable element of λ, for fifth order five stage take$\lambda = \frac{1}{4}$, this was chosen for simplicity, taking into account the need for A-stable behavior.

We solve the system of equations using the MATHEMATICA software[14]. The coefficients for the method described under these choices are obtained and given by

$$\begin{array}{c|cccccc}
\frac{1}{4} & \frac{1}{4} & & & & & \\
\frac{1}{6} & \frac{-1}{12} & \frac{1}{4} & & & & \\
\frac{49+\sqrt{41}}{60} & \frac{73+12\sqrt{41}}{150} & \frac{24-19\sqrt{41}}{300} & \frac{1}{4} & & & \\
\frac{49-\sqrt{41}}{60} & a_{41} & a_{42} & a_{43} & \frac{1}{4} & & \\
1 & 0 & \frac{15}{37} & \frac{2091-879\sqrt{41}}{12136} & \frac{2091+879\sqrt{41}}{12136} & \frac{1}{4} \\
\hline
1 & 0 & \frac{15}{37} & \frac{2091-879\sqrt{41}}{12136} & \frac{2091+879\sqrt{41}}{12136} & \frac{1}{4}
\end{array}$$

where $a_{41} = \frac{59765462671-2469071899\sqrt{41}}{269065110000}$

$a_{42} = \frac{26775007261+244199891\sqrt{41}}{89286180000}$

$a_{43} = \frac{889326089143-203592224167\sqrt{41}}{19910818140000}$

4 Stability of the DIRK5 method

Consider a scalar test equation

$$y' = \lambda y, \quad \lambda \in C, \quad \mathrm{Re}(\lambda) < 0.$$

Write (2) as

$$\left.\begin{array}{l} y_{n+1} = y_n + h \sum\limits_{i=1}^{s} b_i f(x_n + c_i h, Y_i), \\ where \\ Y_i = y_n + h \sum\limits_{j}^{s} a_{ij} f(x_n + c_j h, Y_j), i = 1, 2, ..., s. \end{array}\right\} \tag{3}$$

The forms(2) and (3) are seen to be equivalent if we make the interpretation

$$k_i = f(x_n + c_j h, Y_i), \quad i = 1, 2, ..., s. \tag{4}$$

Applying (3) to the test equation yields

$$\left.\begin{array}{l} Y_i = y_n + z \sum\limits_{j=1}^{s} a_{ij} Y_j, i = 1, 2, ..., s \\ y_{n+1} = y_n + z \sum\limits_{i=1}^{s} b_i Y_i. \\ z = h\lambda. \\ . \end{array}\right\} \tag{5}$$

Define $Y, e \in R^s$ by $Y = [Y_1, Y_2, ..., Y_s]^T$ and $e = [1, 1, ..., 1]^T$then (5) can be written in the form

$$Y = y_n e + zAY, \quad y_{n+1} = y_n + zb^T Y, \quad where \;\; z = h\lambda. \tag{6}$$

Solving for the first of these for Y and substituting in the second gives

$$y_{n+1} = y_n[1 + zb^T (I - zA)^{-1} e], \tag{7}$$

where I is an identity matrix of size $s \times s$. These steps are explained in [15]. Now we have a one step difference equation of the form

$$y_{n+1} = R(z)y_n \tag{8}$$

$$R(z) = 1 + zb^T(I - zA)^{-1}e. \tag{9}$$

where *R(z)* is the stability function or stability polynomial of the method. Clearly $y_n \to 0$ as $n \to \infty$ if and only if

$$|R(z)| < 1 \tag{10}$$

and the method is absolutely stable for those values of z for which (10) holds.The stability region is defined as $\{z \in C : |R(z)| \leq 1\}$ or the set of points in the complex plane such that the computed solution remains bounded after many steps of computation [14].

Lemma: Let *(A,B,C)*denote a Runge-Kutta method. Then its stability function is given by

$$R(z) = \frac{\det(I + z(eb^T - A)}{\det(I - zA)}. \tag{11}$$

We obtain the stability function for the new method as

$$R(z) = \frac{-1024 + 256z + 128z^2 - 13.5495z^3 - 4.2449z^4}{(-4 + z)^5}. \tag{12}$$

The stability region for the above formula in 2 and 3 dimensions is illustrated in the Figures (1) and (2) below:
Definition:[16] A Runge-Kutta method is said to be A-stable if its stability region contains C^- ,the non-positive half-plane$\{\lambda h | \text{Re}\,(\lambda h) < 0\}$

Theorem 4.1: The new Fifth-Order Five Stage Diagonally Implicit Runge-Kutta Method (DIRK5)is an A-stable method.

Proof
we obtained that $y_{n+1} = R(z)y_n$ where $z = \lambda h$

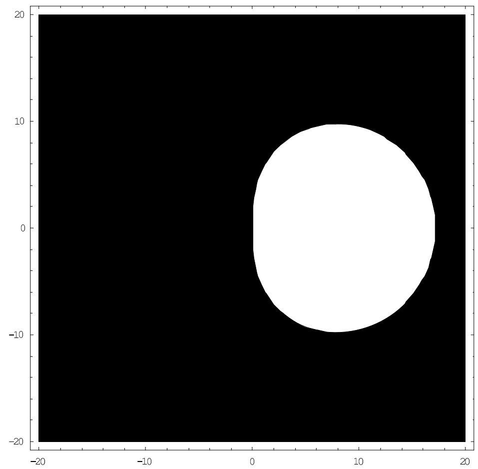

Figure 1: The stability region of the DIRK5 method in 2D.

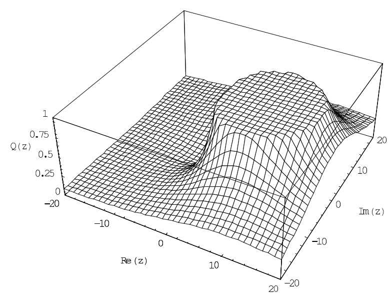

Figure 2: The stability region of the DIRK5 method in 3D.

and $R(z) = \frac{-1024+256z+128z^2-13.5495z^3-4.2449z^4}{(-4+z)^5}$ we have

$$y_{n+1} = \frac{-1024 + 256(\lambda h) + 128(\lambda h)^2 - 13.5495(\lambda h)^3 - 4.2449(\lambda h)^4}{(-4 + (\lambda h))^5} y_n$$

so we have

$$y_1 = \frac{-1024 + 256(\lambda h) + 128(\lambda h)^2 - 13.5495(\lambda h)^3 - 4.2449(\lambda h)^4}{(-4 + (\lambda h))^5} y_0$$

$$y_2 = (\frac{-1024 + 256(\lambda h) + 128(\lambda h)^2 - 13.5495(\lambda h)^3 - 4.2449(\lambda h)^4}{(-4 + (\lambda h))^5})^2 y_0$$

$$y_3 = (\frac{-1024 + 256(\lambda h) + 128(\lambda h)^2 - 13.5495(\lambda h)^3 - 4.2449(\lambda h)^4}{(-4 + (\lambda h))^5})^3 y_0$$

Therefore, for any fixed point n we have

$$y_n = (\frac{-1024 + 256(\lambda h) + 128(\lambda h)^2 - 13.5495(\lambda h)^3 - 4.2449(\lambda h)^4}{(-4 + (\lambda h))^5})^n y_0$$

So for any fixed point $t = t_n = nh$ we have $|R(\lambda nh)^n| \rightarrow 0$ as $n \rightarrow \infty$ for all λh with $\mathrm{Re}(\lambda) < 0$, we get $y_n \rightarrow 0$ as $n \rightarrow \infty$ and consequently the method is A-stable.

For the solution of stiff problems, A-stability is a desirable property, and there is sometimes a preference for methods to be L-stable when the problem is an excessively stiff.

Definition:[17] A method is called L-stable if it is A-stable and if in addition $\lim_{z \rightarrow \infty} R(z) = 0$.

Theorem 4.2: The new Fifth-Order Five Stage Diagonally Implicit Runge-Kutta Method (DIRK5)is an L-stable method.

Proof
According Theorem 4.1 we obtained that DIRK5 method is an A-stable, now if we take $\lim_{z \rightarrow \infty} R(z)$ we get

$$\lim_{z \rightarrow \infty} R(z) = \lim_{z \rightarrow \infty} \frac{-1024 + 256z + 128z^2 - 13.5495z^3 - 4.2449z^4}{(-4 + z)^5} = 0.$$

This implies DIRK5 is L-stable method.

5 Stiff problem

Definition[18]: If a numerical method is forced to use, in an interval of integration, a stepsize is forced to be excessively small relative to dominant time-scale of the solution to get a smooth approximation of the exact solution in that interval,then the problem is said to be stiff in that interval.

According to the definition above, in order to get a smooth approximation of the solution a very small stepsize should be used for stiff problems. In practice a large stepsize is used to reduce computational costs.

6 Problems Tested and Numerical Results

Our aim in this section is to see how well our method compare with other method when solving stiff problems. We then compared the new method with

Cooper and Sayfy method[10].
Cooper and Sayfy have derived many DIRK methods of high order. Their main aim was to minimize the number of implicit stages and not to maximize stability. One of theirs is and we denoted it by Cooper method

$\frac{6-\sqrt{6}}{10}$	$\frac{6-\sqrt{6}}{10}$				
$\frac{6+9\sqrt{6}}{35}$	$\frac{-6+5\sqrt{6}}{14}$	$\frac{6-\sqrt{6}}{10}$			
1	$\frac{888+607\sqrt{6}}{2850}$	$\frac{126-161\sqrt{6}}{1425}$	$\frac{6-\sqrt{6}}{10}$		
$\frac{4-\sqrt{6}}{10}$	$\frac{3153-3082\sqrt{6}}{1425}$	$\frac{3213+1148\sqrt{6}}{28500}$	$\frac{-267+88\sqrt{6}}{500}$	$\frac{6-\sqrt{6}}{10}$	
$\frac{4+\sqrt{6}}{10}$	$\frac{-32583+14638\sqrt{6}}{71250}$	$\frac{-17199+364\sqrt{6}}{36}$	$\frac{1329-544\sqrt{6}}{2500}$	$\frac{-96+131\sqrt{6}}{625}$	$\frac{6-\sqrt{6}}{10}$
1	0	0	$\frac{1}{9}$	$\frac{16-\sqrt{6}}{36}$	$\frac{16+\sqrt{6}}{36}$

To test the accuracy of our new method, problems in ordinary differential equation, which are stiff problem are used.

Problem 1

Consider the stiff ordinary differential equation

$$y'(t) = -200(y(t) - cos(t)); \quad y(0) = 0,$$

with the exact solution $\frac{1}{40001}(200e^{-200t}(-200 + 200e^{200t}\cos(t) + e^{200t}\sin(t))$, which was considered over the range $2 \le t \le 5$, using stepsize $h = 0.01$ and 10 Newton iterations to get the stages values. The results of the error for the methods are plotted in Figure (3).

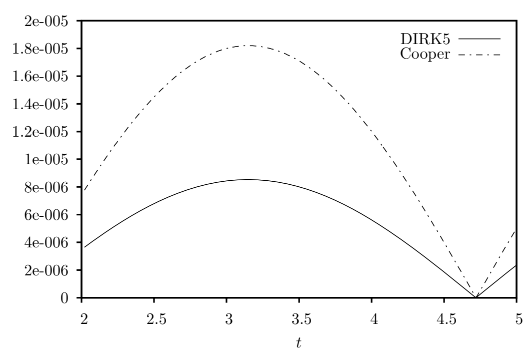

Figure 3: The absolute error of the two methods with h=0.01.

Problem 2 Consider the highly stiff ordinary differential equation

$$y'(t) = -1000y(t) + e^{-2t}; \quad y(0) = 0,$$

with the exact solution $\frac{1}{998}e^{-1000t}(-1 + e^{998})$ which was considered over the range $0 \le t \le 1$ We used 5 Newton iterations to get the stage values. The numerical results for the DIRK5 are compared to those of Cooper in Fig(4) by using h=0.01.The results show an excellent and superior accuracy of the DIRK5 method using two stepsizes namely h=0.01 and h=0.002 which is better than Coopers results.The Cooper method definitely seems to have difficulty of the approximation when h=0.01, so we decrease the step size h.

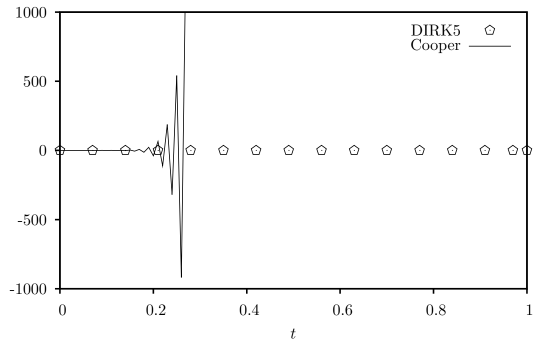

Figure 4: The Solution curves with h=0.01.

Fig(5)shows the absolute errors for the methods when h=0.002. The cooper method performs well with h=0.002. However, the DIRK5 method performs perfectly well with both h=0.01 and h=0.002, and outperforms Cooper method.

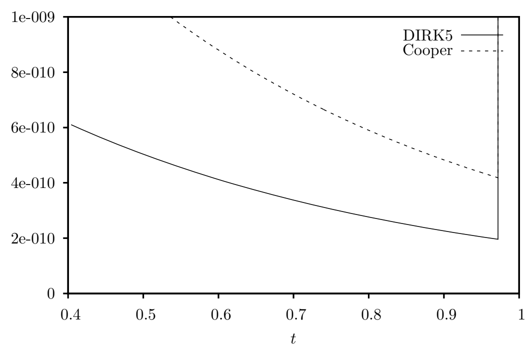

Figure 5: The absolute error of the two methods with h=0.02.

7 Conclusion

The research conducted in this paper shows the possibility of constructing new diagonally implicit Runge-Kutta five-stage fifth order formula with L-stability property.

From the results obtained via the numerical experiment, we verified that the DIRK5 method is appropriate for stiff problems and it outperforms existing methods such as the Cooper method.

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