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Fourth Order Four-Stage Diagonally Implicit Runge-Kutta Method for Linear Ordinary Differential Equations

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ABSTRACT

A new fourth order four-stage Diagonally Implicit Runge-Kutta (DIRK) method which is specially designed for the integration of Linear Ordinary Differential Equations (LODEs) is constructed. In the derivation, Butcher's error equations are used but one of the error equations can be eliminated due to the property of the LODE itself. The stability aspect of the method is investigated and it is found to have a bigger region of stability compared to explicit Runge-Kutta (ERK) method of the same type (designed for the integration of LODE). A set of test problems are used to validate the method and numerical results show that the method produced smaller global error compared to ERK method.

INTRODUCTION

In this paper, we consider the numerical integration of linear inhomogeneous systems of ordinary differential equations (ODEs) of the form

$$y' = Ay + g(x) \tag{1.1}$$

where A is a square matrix whose entries does not depend on y or x, and y and $g(x)$ are vectors. Such systems arise in the numerical solution of partial differential equations (PDEs) governing wave and heat phenomena after application of a spatial discretization such as finite-difference method.

Explicit Runge-Kutta method is very popular for simulations of wave equations; (see Zingg and Chisholm (1999) and Ferracina and Spijker (2007), due to their high accuracy and low memory requirements.

In the derivation of Runge-Kutta (RK) methods, certain order equations or sometimes called error equations need to be satisfied; see Dormand (1996). These order equations resulted from the derivatives of the function $y' = f(x, y)$ itself. If the function is linear then some of the error equations resulted by the nonlinearity in the derivative function can be removed, thus less order equations need to be satisfied, hence a more efficient method in some respect than the classical method can be produced or derived. In this paper, we construct diagonally implicit Runge-Kutta method specifically for linear ODEs with constant coefficients, then the stability aspect of the method is looked into and a set of test equations are used to validate the new method.

DERIVATION OF THE METHOD

We consider the following scalar ODE

$$y' = f(x, y). \tag{2.1}$$

When a general s-stage diagonally implicit Runge-Kutta method is applied to the ODE, the following equations are obtained,

$$y_{n+1} = y_n + h\sum_{i=1}^{s} b_i k_i \tag{2.2a}$$

where $$k_i = f(x_n + c_i h, y_n + h\sum_{j=1}^{i} a_{ij} k_j). \tag{2.2b}$$

We shall always assume that the row-sum condition holds $c_i = \sum_{j=1}^{s} a_{ij}$, where $i = 1, 2..s$. According to Dormand(1996) and Butcher (2003), the following eight order equations are equations needed to be satisfied by fourth order four-stage DIRK method.

TABLE 1: Runge-Kutta order equations for fourth order

1.	$\tau_1^{(1)} = \sum_i b_i - 1$
2.	$\tau_1^{(2)} = \sum_i b_i c_i - \frac{1}{2}$
3.	$\tau_1^{(3)} = \sum_i b_i c_i^2 - \frac{1}{3}$
4.	$\tau_2^{(3)} = \sum_{ij} b_i a_{ij} c_j - \frac{1}{6}$
5.	$\tau_1^{(4)} = \sum_i b_i c_i^3 - \frac{1}{4}$
6.	$\tau_2^{(4)} = \sum_{ij} b_i c_i a_{ij} c_j - \frac{1}{8}$
7.	$\tau_3^{(4)} = \sum_{ij} b_i a_{ij} c_j^2 - \frac{1}{12}$
8.	$\tau_4^{(4)} = \sum_{ijk} b_i a_{ij} a_{jk} c_k - \frac{1}{24}$

The restriction to linear ODEs reduces the number of equations which the coefficients of the RK method must satisfy in Table 1. Zingg and Chisholm (1999) have derived new explicit RK methods which are suitable for linear ODEs that are more efficient than the conventional RK methods.

For this new fourth order DIRK method suitable for linear ODEs, equation 6 in Table 1 can be eliminated, see paper Zingg and Chisholm (1999). This condition is eliminated by exploiting the fact that, for linear ODEs,

$$\frac{\partial^2 f}{\partial y^2} = \frac{\partial^2 f}{\partial y \partial x} = 0 .$$

After equation 6 in Table 1 has been eliminated, we have seven equations to be solved with 11 unknowns. So we have four free parameters which are chosen to be $\gamma = 0.20, c_2 = 0.05, c_3 = 0.40$ and $c_4 = 0.80$. All the equations in Table 1 (except equation 6) are solved using MAPLE package. The coefficients obtained are written in Butcher's array as follows:

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

$$\begin{array}{c|llll} 0.20 & 0.20 & & & \\ 0.05 & -0.15 & 0.20 & & \\ 0.40 & -0.78518518518519 & 0.98518518518519 & 0.20 & \\ 0.80 & 0.70671936758894 & -0.19819311123659 & 0.091473743647652 & 0.20 \\ \hline & 0.40740740740741 & 0.016931216931217 & 0.10714285714286 & 0.46851851851852 \end{array}$$

Applying all the parameters into the general form of RK method, we have the new fourth order four-stage DIRK method which is suitable for linear ODEs,

$$y_{n+1} = y_n + h(0.40740...k_1 + 0.01693...k_2 + 0.10714...k_3 + 0.46851...k_4)$$

where

$$\begin{aligned} k_1 &= f(x_n + 0.20h, y_n + h(0.20k_1)). \\ k_2 &= f(x_n + 0.05h, y_n + h(-0.15k_1 + 0.20k_2)). \\ k_3 &= f(x_n + 0.40h, y_n + h(-0.78518...k_1 + 0.98518...k_2 + 0.20k_3)). \\ k_4 &= f(x_n + 0.80h, y_n + h(0.70671...k_1 + (-0.19819...)k_2 + 0.09147...k_3 + 0.20k_4)). \end{aligned}$$

STABILITY

One of the practical criteria for a good method to be useful is that it must have a region of absolute stability. When an s-stage Runge-Kutta method (equations (2.2a) and (2.2b)) is applied to

$$\begin{aligned} y' &= f(x, y) \\ &= \lambda y \end{aligned}$$

the following equations are obtained

$$y_{n+1} = R(h\lambda)\, y_n$$

where $\quad R(h\lambda) = R(\hat{h}) = 1 + \hat{h} b^T (I - \hat{h}A)^{-1} e$

and A is (m x m), e is (m x 1) are obtained from the coefficients of the method itself. $R(\hat{h})$ is called the stability polynomial of the method and for this method it is given as

$$\begin{aligned}
R(\hat{h}) = 1 + \hat{h}\Bigg[& \frac{0.468519\left(-0.198193\hat{h} + 0.169396\hat{h}^2 - 0.0259514\hat{h}^3\right)}{1 - 0.8\hat{h} + 0.24\hat{h}^2 - 0.032\hat{h}^3 + 0.0016\hat{h}^4} + \\
& \frac{1.\left(1 - 0.6\hat{h} + 0.12\hat{h}^2 - 0.008\hat{h}^3\right)}{1 - 0.8\hat{h} + 0.24\hat{h}^2 - 0.032\hat{h}^3 + 0.0016\hat{h}^4} + \\
& \frac{0.0169312(-0.15\hat{h} + 0.06\hat{h}^2 - 0.006\hat{h}^3)}{1 - 0.8\hat{h} + 0.24\hat{h}^2 - 0.032\hat{h}^3 + 0.0016\hat{h}^4} + \\
& \frac{0.107143(-0.785185\hat{h} + 0.166296\hat{h}^2 - 0.00185185\hat{h}^3}{1 - 0.8\hat{h} + 0.24\hat{h}^2 - 0.032\hat{h}^3 + 0.0016\hat{h}^4} + \\
& \frac{0.468519(0.0914737\hat{h} - 0.0365895\hat{h}^2 + 0.00365895\hat{h}^3)}{1 - 0.8\hat{h} + 0.24\hat{h}^2 - 0.032\hat{h}^3 + 0.0016\hat{h}^4} + \\
& \frac{0.468519(0.706719\hat{h} - 0.324783\hat{h}^2 + 0.02317\hat{h}^3}{1 - 0.8\hat{h} + 0.24\hat{h}^2 - 0.032\hat{h}^3 + 0.0016\hat{h}^4} + \\
& \frac{0.107143(0.985185\hat{h} - 0.394074\hat{h}^2 + 0.0394074\hat{h}^3)}{1 - 0.8\hat{h} + 0.24\hat{h}^2 - 0.032\hat{h}^3 + 0.0016\hat{h}^4}\Bigg].
\end{aligned}$$

The stability region is obtained by taking $R(\hat{h}) = 1 = \cos\theta + i\sin\theta$ and solve for $\hat{h}$ using Mathematica package (see Torrence (1999)). The stability region for new fourth order four-stage DIRK is shown in Figure 1.

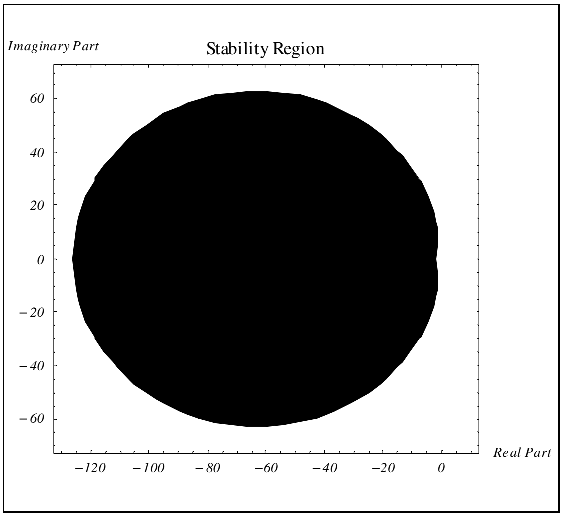

Figure 1: The stability region for new 4^{th} order 4-stage DIRK

We also find the stability polynomial and the stability region for the fourth order four-stage explicit Runge-Kutta method (ERK) in Zingg and Chisholm (1999), and it is shown in Figure 2 below.

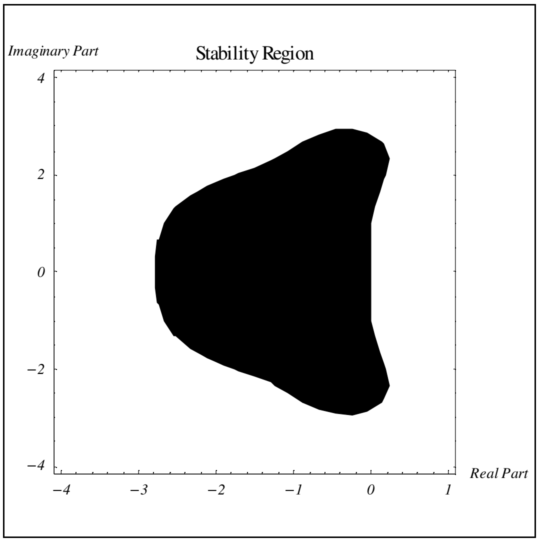

Figure 2: The stability region for 4^{th} order 4-stage ERK

PROBLEMS TESTED AND NUMERICAL RESULTS

The following are some of the problems tested. All the problems are linear ordinary differential equations.

PROBLEM 1:

$$y'(t) = -y$$
$$y(t) = e^{-t}$$
$$0 \le t \le 1, y(0) = 1$$

Source: Richard L.Burden and J.Douglas Faires (2001)

PROBLEM 2:

$$y'(t) = te^{3t} - 2y$$
$$y(t) = \frac{1}{5}te^{3t} - \frac{1}{25}e^{3t} + \frac{1}{25}e^{-2t}$$
$$0 \le t \le 3, y(0) = 0$$

Source: Richard L.Burden and J.Douglas Faires (2001)

PROBLEM 3:

$$y'(t) = -y \tan t - \frac{1}{\cos t}$$
$$y(t) = \cos t - \sin t$$
$$0 \le t \le 1, y(0) = 1$$

Source: J. C. Butcher (2003)

PROBLEM 4:

$$y'(t) = y - t^2 + 1$$
$$y(t) = (t+1)^2 - 0.5e^t$$
$$0 \le t \le 1, y(0) = 0.5$$

Source: Richard L.Burden and J.Douglas Faires (2001)

PROBLEM 5:

$$y'(t) = \frac{2}{t} y + t^2 e^t$$

$$y(t) = t^2 (e^t - e)$$

$$1 \le t \le 5, y(1) = 0$$

Source: Richard L.Burden and J.Douglas Faires (2001)

The numerical results are tabulated and compared with the existing method and below are the notations used:

H	~	Step size used
MTHD	~	Method employed
MAXE	~	Maximum error $\left\| y(x_i) - y_i \right\|$
ERK4	~	Fourth order four-stage explicit RK method – Zingg and Chisholm (1999)
DIRK4	~	New fourth order four-stage DIRK method

TABLE 2: Comparison between ERK4 and DIRK4 for solving Problem 1

	MTHD	H	MAXE
1.	ERK4	0.1	3.33241e-007
	DIRK4		1.77061e-007
2.	ERK4	0.05	1.99761e-008
	DIRK4		1.08176e-008
3.	ERK4	0.025	1.22274e-009
	DIRK4		6.68505e-010
4.	ERK4	0.01	3.09133e-011
	DIRK4		1.69965e-011
5.	ERK4	0.005	1.92441e-012
	DIRK4		1.05727e-012
6.	ERK4	0.0025	1.16185e-013
	DIRK4		5.98965e-014
7.	ERK4	0.001	5.10703e-015
	DIRK4		9.99201e-016

TABLE 3: Comparison between ERK4 and DIRK4 for solving problem 2

	MTHD	H	MAXE
1.	ERK4	0.1	1.94502e-001
	DIRK4		1.59881e-002
2.	ERK4	0.05	1.21124e-002
	DIRK4		1.28593e-003
3.	ERK4	0.025	7.54212e-004
	DIRK4		7.68321e-005
4.	ERK4	0.01	1.92521e-005
	DIRK4		1.91374e-006
5.	ERK4	0.005	1.20159e-006
	DIRK4		1.18587e-007
6.	ERK4	0.0025	7.48842e-008
	DIRK4		7.45786e-009
7.	ERK4	0.001	2.12640e-009
	DIRK4		5.23869e-010

TABLE 4: Comparison between ERK4 and DIRK4 for solving problem 3

	MTHD	H	MAXE
1.	ERK4	0.1	9.88164e-006
	DIRK4		2.05409e-007
2.	ERK4	0.05	1.22646e-006
	DIRK4		5.68730e-009
3.	ERK4	0.025	1.52419e-007
	DIRK4		3.59977e-010
4.	ERK4	0.01	9.72342e-009
	DIRK4		9.26598e-012
5.	ERK4	0.005	1.21412e-009
	DIRK4		5.75096e-013
6.	ERK4	0.0025	1.51681e-010
	DIRK4		1.96509e-014
7.	ERK4	0.001	9.70071e-012
	DIRK4		5.35683e-015

TABLE 5: Comparison between ERK4 and DIRK4 for solving problem 4

	MTHD	H	MAXE
1.	ERK4	0.1	3.69800e-006
	DIRK4		1.47459e-006
2.	ERK4	0.05	2.35953e-007
	DIRK4		8.09916e-008
3.	ERK4	0.025	1.48980e-008
	DIRK4		5.07423e-009
4.	ERK4	0.01	3.83624e-010
	DIRK4		1.30068e-010
5.	ERK4	0.005	2.39861e-011
	DIRK4		8.11218e-012
6.	ERK4	0.0025	1.44684e-012
	DIRK4		4.55636e-013
7.	ERK4	0.001	3.24185e-014
	DIRK4		8.43769e-015

TABLE 6: Comparison between ERK4 and DIRK4 for solving problem 5

	MTHD	H	MAXE
1.	ERK4	0.1	3.53422e-002
	DIRK4		7.26397e-004
2.	ERK4	0.05	4.58145e-003
	DIRK4		4.63550e-005
3.	ERK4	0.025	5.83708e-004
	DIRK4		2.89688e-006
4.	ERK4	0.01	3.77980e-005
	DIRK4		7.53589e-008
5.	ERK4	0.005	4.74347e-006
	DIRK4		4.57658e-009
6.	ERK4	0.0025	5.93553e-007
	DIRK4		7.41693e-010
7.	ERK4	0.001	3.71388e-008
	DIRK4		8.64475e-010

CONCLUSION

The new fourth order four-stage DIRK method has been presented for the integration of linear systems of ODEs. It has a bigger stability region compared to explicit RK method (of the same order), and hence the formula is more stable. From the numerical results in Tables 2 to 6, we can conclude that the new fourth order four-stage DIRK method which is suitable for linear ODEs performs better in terms of accuracy compared to fourth order four-stage ERK method.

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