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Article

Diagonally Implicit Runge-Kutta Fourth Order Four-Stage Method for Linear Ordinary Differential Equations with Minimized Error Norm

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ABSTRACT

We constructed a new fourth order four-stage diagonally implicit Runge-Kutta (DIRK) method which is specially designed for the integrations of linear ordinary differential equations (LODEs). The method is obtained based on the Butcher's error equations. In the derivation, the error norm is minimized so that the free parameters chosen are obtained from the minimized error norm. Row simplifying assumption is also used so that the number of equations for the method can be reduced and simplified. A set of test problems are used to validate the method and numerical results show that the new method is more efficient in terms of accuracy compared to the existing method.

| Runge-Kutta | Linear ordinary differential equations | Error norm |

1. Introduction

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 [8], due to their high accuracy and low memory requirements.

To derive Runge-Kutta (RK) methods, we need to fulfill certain order equations; see Dormand [3]. 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 derived.

In this paper, we construct diagonally implicit Runge-Kutta method specifically for linear ODEs with constant coefficients. We consider the principal terms of the local truncation error to minimize the error norm. Then, the stability aspect of the method is looked into and a few test equations are used to validate the new method.

2. Materials and Methods

Derivation of the Method

In this section, 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 [3], the following eight order equations (error equations) are equations needed to be satisfied by fourth order four-stage DIRK method.

Table 2.1: 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 2.1. Zingg and Chisholm [8] 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 which is suitable for linear ODEs, equation 6 in table 2.1 can be eliminated, as in [8]. This condition is eliminated by exploiting the fact that, for linear ODEs,

$$\frac{\partial^2 f}{\partial u^2} = \frac{\partial^2 f}{\partial u \partial t} = 0 .$$

Using the simplifying assumption:

$$\sum b_i a_{ij} = b_j (1 - c_j), \qquad j = 2,3,4$$

we can removed several equations, i.e. equation 4 and 7 in table 2.1. This makes the new fourth order four-stage DIRK method different from the classical method. So, the number of order equations can be reduced. Thus, the equations needed to be satisfied are:

$$\begin{aligned} j &= 2 \rightarrow b_2\gamma + b_3 a_{32} + b_4 a_{42} = b_2(1 - c_2) \\ j &= 3 \rightarrow b_3\gamma + b_4 a_{43} = b_3(1 - c_3) \\ j &= 4 \rightarrow c_4 = 1 - \gamma \end{aligned}$$

Altogether there are seven equations to be satisfied and we have 10 unknowns. So, we can take three free parameters which are chosen to be c_2, c_3 and γ. Solving all the related equations, we have all equations in terms of c_2, c_3 and γ.

Table 2.2: Runge-Kutta order equations for fifth order

9.	$\tau_1^{(5)} = \frac{1}{24} \sum_i b_i c_i^4 - \frac{1}{120}$
10.	$\tau_2^{(5)} = \frac{1}{2} \sum_{ij} b_i c_i^2 a_{ij} c_j - \frac{1}{20}$

11.	$\tau_3^{(5)} = \frac{1}{2}\sum_{ijk} b_i a_{ij} c_j a_{ik} c_k - \frac{1}{40}$
12.	$\tau_4^{(5)} = \frac{1}{2}\sum_{ij} b_i c_i a_{ij} c_j^2 - \frac{1}{30}$
13.	$\tau_5^{(5)} = \frac{1}{6}\sum_{ij} b_i a_{ij} c_j^3 - \frac{1}{120}$
14.	$\tau_6^{(5)} = \sum_{ijk} b_i c_i a_{ij} a_{jk} c_k - \frac{1}{30}$
15.	$\tau_7^{(5)} = \sum_{ijk} b_i a_{ij} c_j a_{jk} c_k - \frac{1}{40}$
16.	$\tau_8^{(5)} = \frac{1}{2}\sum_{ijk} b_i a_{ij} a_{jk} c_k^2 - \frac{1}{120}$
17.	$\tau_9^{(5)} = \sum_{ijkm} b_i a_{ij} a_{jk} a_{km} c_m - \frac{1}{120}$

In order to choose the free parameters c_2, c_3 and γ, the principal terms of the local truncation error must be considered. Using the error function $\varphi_p = \sum_{j=1}^{n_{p+1}} \tau_j^{(p+1)} F_j^{(p+1)}$ and RK error coefficients [3], the principal term for fourth order method is

$$\varphi_4 = \sum_{j=1}^{5} \tau_j^{(5)} F_j^{(5)}$$

For case of RK suitable for linear ODEs, we only considered $\Gamma_1^{(5)}, \Gamma_5^{(5)}, \Gamma_8^{(5)}$ and $\Gamma_9^{(5)}$. Here we can eliminated several equations i.e. $\tau_2^{(5)}, \tau_3^{(5)}, \tau_4^{(5)}, \tau_6^{(5)}$ and $\tau_7^{(5)}$. The best strategy for practical purposes would be to choose the free RK parameters is to minimize the error norm, see [3];

$$\mathrm{A}^{(p+1)} = \left\| \tau^{(p+1)} \right\|_2 = \sqrt{\sum_{j=1}^{n_{p+1}} (\tau_j^{(p+1)})^2}$$

So we have the principal error norm for this method;

$$\mathrm{A}^{(5)} = \left\| \tau^{(5)} \right\|_2 = \sqrt{(\tau_1^{(5)})^2 + (\tau_5^{(5)})^2 + (\tau_8^{(5)})^2 + (\tau_9^{(5)})^2}$$

where $\tau_j^{(5)}$ is the error equations associated with the fifth order method, (in table 2.2). Then we get the principal error norm in terms of c_2, c_3 and γ. Minimizing the error norm, we obtained $c_2 = 0.36376391115508, c_3 = 0.62453338645147$ and $\gamma = 0.091291733465251$.

Substituting the values of c_2, c_3 and γ and solving all the equations we finally get all the coefficients as follows;

0.091291733465251			
0.27247217768983	0.091291733465251		
0.18592608940281	0.34731556358341	0.091291733465251	
0.23857907019768	0.20938627024938	0.36945119262243	0.091291733465251
0.22017939484654	0.26923249008354	0.28860138224069	0.22198673282923

Substituting 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 with minimized error norm,

$$y_{n+1} = y_n + h(0.2201...k_1 + 0.2692...k_2 + 0.2886...k_3 + 0.2219...k_4)$$

where

$$\begin{aligned}
k_1 &= f(x_n + 0.0912...h, y_n + h(0.0912...k_1)) \\
k_2 &= f(x_n + 0.3637...h, y_n + h(0.2724...k_1 + 0.0912...k_2)) \\
k_3 &= f(x_n + 0.6245...h, y_n + h(0.1859...k_1 + 0.3473...k_2 + 0.0912...k_3)) \\
k_4 &= f(x_n + 0.9087...h, y_n + h(0.2385...k_1 + 0.2093...k_2 + 0.3694...k_3 + 0.0912...k_4))
\end{aligned}$$

Stability

One of the practical criteria for a good method to be useful is that it must have 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 is obtained

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

with

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

where A is (m x m), e is (m x 1) and $R(\hat{h})$ is called the stability polynomial of the method. The stability region is obtained by taking $R(\hat{h}) = 1 = \cos\theta + i\sin\theta$.

From this Butcher's array,

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

We can solve for $\hat{h}$ using the Mathematica packaged and get the stability polynomial and also the stability region. The stability polynomial for new fourth order four-stage DIRK method is

$$R(\hat{h}) = 1+\hat{h}\left[\frac{0.221987\left(0.209386\hat{h}+0.0900857\hat{h}^2-0.00996914\hat{h}^3\right)}{1-0.365167\hat{h}+0.0500051\hat{h}^2-0.00304337\hat{h}^3+0.0000694586\hat{h}^4}+\right.$$
$$\frac{0.288601\left(0.185926\hat{h}+0.0606868\hat{h}^2-0.00708974\hat{h}^3\right)}{1-0.365167\hat{h}+0.0500051\hat{h}^2-0.00304337\hat{h}^3+0.0000694586\hat{h}^4}+$$
$$\frac{1.(1-0.273875\hat{h}+0.0250025\hat{h}^2-0.000760842\hat{h}^3)}{1-0.365167\hat{h}+0.0500051\hat{h}^2-0.00304337\hat{h}^3+0.0000694586\hat{h}^4}+$$
$$\frac{0.269232(0.272472\hat{h}-0.0497489\hat{h}^2+0.00227083\hat{h}^3}{1-0.365167\hat{h}+0.0500051\hat{h}^2-0.00304337\hat{h}^3+0.0000694586\hat{h}^4}+$$
$$\frac{0.288601(0.347316\hat{h}-0.0634141\hat{h}^2+0.00289459\hat{h}^3)}{1-0.365167\hat{h}+0.0500051\hat{h}^2-0.00304337\hat{h}^3+0.0000694586\hat{h}^4}+$$
$$\frac{0.221987(0.369451\hat{h}-0.0674557\hat{h}^2+0.00307907\hat{h}^3}{1-0.365167\hat{h}+0.0500051\hat{h}^2-0.00304337\hat{h}^3+0.0000694586\hat{h}^4}+$$
$$\left.\frac{0.221987(0.238579\hat{h}+0.082182\hat{h}^2+0.0254717\hat{h}^3)}{1-0.365167\hat{h}+0.0500051\hat{h}^2-0.00304337\hat{h}^3+0.0000694586\hat{h}^4}\right]$$

The stability polynomial is set to zero and solve for $\hat{h}$ which gives the value of $\left|R(\hat{h})\right| \le 1$; this is done by using Mathematica package. The stability region is obtained by tracing the values of $\hat{h}$ and is shown in Figure 2.3. The stability region for new fourth order four-stage DIRK is black in colour.

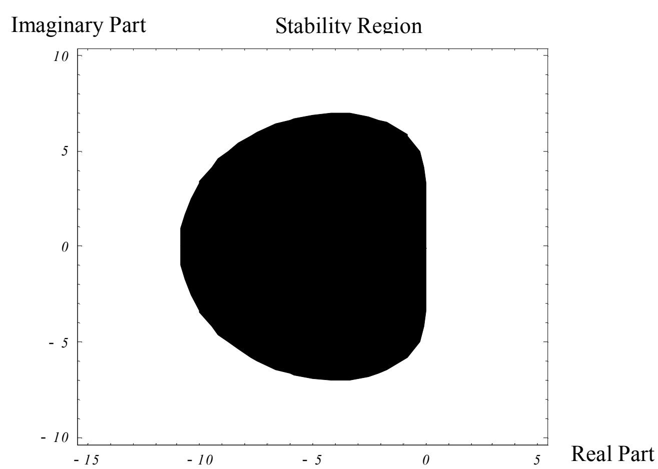

Figure 2.3: The stability region for new 4th order 4-stage DIRK with minimized error norm

3. Results and Discussion

The following are some of the problems tested. All the problems are linear ODEs.

PROBLEM 1:

$$y'(t) = -y$$

$$y(t) = e^{-t} \qquad 0 \le t \le 1,\ y(0) = 1$$

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

PROBLEM 2:

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

$$y(t) = \cos t - \sin t$$

Source: J. C. Butcher (2003)

PROBLEM 3:

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

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

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 $|y(x_i) - y_i|$
- **ERK4** Fourth order four-stage explicit RK method (Zingg and Chisholm, 1999 [8])
- **DIRK4 minimized** New fourth order four-stage DIRK method with minimized error norm
- **SDIRK4,4** Optimal fourth order four-stage singly-DIRK (Ferracina and Spijker,2007 [4])

Table 3.1: Comparison between ERK4 and DIRK4 for solving problem 1

	MTHD	H	MAXE
1.	**ERK4**	0.1	3.33241e-007
	DIRK4 minimized		1.47717e-008
	SDIRK4,4		1.10407e-008
2.	**ERK4**	0.05	1.99761e-008
	DIRK4 minimized		8.98578e-010

	MTHD	H	MAXE
	SDIRK4,4		6.72222e-010
3.	**ERK4**	0.025	1.22274e-009
	DIRK4 minimized		5.54087e-011
	SDIRK4,4		4.14714e-011
4.	**ERK4**	0.01	3.09133e-011
	DIRK4 minimized		1.40699e-012
	SDIRK4,4		1.05449e-012
5.	**ERK4**	0.005	1.92441e-012
	DIRK4 minimized		8.79297e-014
	SDIRK4,4		6.66134e-014
6.	**ERK4**	0.0025	1.16185e-013
	DIRK4 minimized		4.66294e-015
	SDIRK4,4		3.77476e-015
7.	**ERK4**	0.001	5.10703e-015
	DIRK4 minimized		1.88738e-015
	SDIRK4,4		1.99840e-015

Table 3.2: Comparison between ERK4 and DIRK4 for solving problem 2

	MTHD	H	MAXE
1.	**ERK4** **DIRK4 minimized** **SDIRK4,4**	0.1	9.88164e-006 8.60900e-009 1.34285e-008
2.	**ERK4** **DIRK4 minimized** **SDIRK4,4**	0.05	1.22646e-006 1.59223e-010 4.30729e-010
3.	**ERK4** **DIRK4 minimized** **SDIRK4,4**	0.025	1.52419e-007 8.36314e-012 2.58894e-011
4.	**ERK4** **DIRK4 minimized** **SDIRK4,4**	0.01	9.72342e-009 1.88294e-013 6.47565e-013
5.	**ERK4** **DIRK4 minimized** **SDIRK4,4**	0.005	1.21412e-009 1.14908e-014 3.98570e-014
6.	**ERK4** **DIRK4 minimized** **SDIRK4,4**	0.0025	1.51681e-010 1.07692e-014 1.37113e-014
7.	**ERK4** **DIRK4 minimized** **SDIRK4,4**	0.001	9.70071e-012 4.44089e-016 4.44089e-016

Table 3.3: Comparison between ERK4 and DIRK4 for solving problem 3

	MTHD	H	MAXE
1.	**ERK4** **DIRK4 minimized** **SDIRK4,4**	0.1	3.53422e-002 7.04943e-005 4.98821e-006
2.	**ERK4** **DIRK4 minimized** **SDIRK4,4**	0.05	4.58145e-003 4.60092e-006 3.19676e-007
3.	**ERK4** **DIRK4 minimized** **SDIRK4,4**	0.025	5.83708e-004 2.89703e-007 1.89380e-008
4.	**ERK4** **DIRK4 minimized** **SDIRK4,4**	0.01	3.77980e-005 7.51152e-009 4.04270e-010
5.	**ERK4** **DIRK4 minimized** **SDIRK4,4**	0.005	4.74347e-006 3.61979e-010 9.18590e-011
6.	**ERK4** **DIRK4 minimized** **SDIRK4,4**	0.0025	5.93553e-007 5.08408e-010 4.77939e-010
7.	**ERK4** **DIRK4 minimized** **SDIRK4,4**	0.001	3.71388e-008 8.95852e-010 8.92669e-010

4. Conclusion

The new fourth order four-stage DIRK method with minimized error norm has been presented for the integration of linear ODEs. It has a bigger stability region compared to explicit RK method (of the same order), hence more stable. From the numerical results in Table 3.1 to 3.3, we can conclude that the new fourth order four-stage DIRK method which is suitable for linear ODEs performs better in terms of maximum error compared to fourth order four-stage ERK method [8]. This new method is also as good as the optimal fourth order four-stage singly-DIRK [4].

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