Solving Linear Ordinary Differential Equations using Singly Diagonally Implicit Runge-Kutta fifth order five-stage method

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Abstract: - We constructed a new fifth order five-stage singly diagonally implicit Runge-Kutta (DIRK) method which is specially designed for the integrations of linear ordinary differential equations (LODEs). The restriction to linear ordinary differential equations (ODEs) reduces the number of conditions which the coefficients of the Runge-Kutta method must satisfy. The best strategy for practical purposes would be to choose the coefficients of the Runge-Kutta methods such that the error norm is minimized. Thus, here the error norm obtained from the error equations of the sixth order method is minimized so that the free parameters chosen are obtained from the minimized error norm. The stability aspect of the method is also looked into and found to have substantial region of stability, thus it is stable. Then a set of test problems are used to validate the method. Numerical results show that the new method is more efficient in terms of accuracy compared to the existing method.

Key-Words: - Runge-Kutta, Linear ordinary differential equations, Error norm.

1 Introduction

Many algorithms have been proposed for the numerical solution of initial value problem

$$y' = f(x, y),\ y(x_0) = y_0,$$
$$f : \Re \times \Re \to \Re^m \qquad (1)$$

Such algorithm is the Singly Diagonally Implicit Runge-Kutta (SDIRK) method which was introduced to overcome some of the limitations of fully implicit and explicit Runge-Kutta method. Preliminary experiments have shown that these methods are usually more efficient than the standard Singly Implicit Runge-Kutta (SIRK) method and in many cases are competitive with backward differentiation formula. This algorithms can be used by both linear and nonlinear systems of ordinary equations.

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

$$y' = Ay + G(x) \qquad (2)$$

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. This type of partial differential equations can be solved numerically using methods suggested by Rasulov and Kul [7], Rasulov et. al [8] and Zabala and Ramos [12].

Actually there have been several attempts to develop efficient methods for integrating linear systems of ODEs. The basic concept of this method is that the major cost in evaluating the derivative function is in forming the matrix A and vector $G(x)$.

Explicit Runge-Kutta method is very popular for simulations of wave equations; see Zingg and Chisholm [13], due to their high accuracy and low memory requirements.

To derive Runge-Kutta (RK) methods, we need to fulfill certain order equations; see Dormand [4]. 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, a few test equations are used to validate the new method.

2 Materials and Methods

2.1 Derivation of the method

In this section, we consider the following scalar ODE

$$y' = f(x, y) \tag{2}$$

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

$$y_{n+1} = y_n + h\sum_{i=1}^{s} b_i k_i \tag{3}$$

where

$$k_i = f(x_n + c_i h, y_n + h\sum_{j=1}^{i} a_{ij} k_j) \tag{4}$$

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], there are 17 order equations (error equations) needed to be satisfied by the fifth order five-stage RK method. The restriction to linear ODEs reduces the number of equations which the coefficients of the RK method must satisfy see Zingg and Chisholm [13]. The order equations are eliminated by exploiting the fact that, for linear ODEs,

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

Zingg and Chisholm [13] too have derived a new explicit RK methods which are suitable for linear ODEs that are more efficient than the conventional RK methods.

Table 1: Order equations for fifth order Runge-Kutta method suitable for LODEs

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.	$\tau_3^{(4)} = \sum_{ij} b_i a_{ij} c_j^2 - \frac{1}{12}$
7.	$\tau_4^{(4)} = \sum_{ijk} b_i a_{ij} a_{jk} c_k - \frac{1}{24}$
8.	$\tau_1^{(5)} = \frac{1}{24}\sum_i b_i c_i^4 - \frac{1}{120}$
9.	$\tau_5^{(5)} = \frac{1}{6}\sum_{ij} b_i a_{ij} c_j^3 - \frac{1}{120}$
10.	$\tau_8^{(5)} = \frac{1}{2}\sum_{ijk} b_i a_{ij} a_{jk} c_k^2 - \frac{1}{120}$
11.	$\tau_9^{(5)} = \sum_{ijkm} b_i a_{ij} a_{jk} a_{km} c_m - \frac{1}{120}$

Using the simplifying assumption:

$$\sum b_i a_{ij} = b_j(1-c_j), \quad j = 2,...,5 \qquad (5)$$

We have

$$\sum_{ij} b_i a_{ij} c_j = \tfrac{1}{6} \rightarrow (\sum_i b_i c_i = \tfrac{1}{2}) - \ (\sum_i b_i c_i^2 = \tfrac{1}{3}),$$

thus equation 4 can be removed, similarly we can remove equations 6 and 9 in table 1. Thus, using (5) the order equations are replaced by simpler equations. They are:

$$j = 2 \rightarrow b_3 a_{32} + b_4 a_{42} + b_5 a_{52} = b_2(1 - c_2 - \gamma)$$

$$j = 3 \rightarrow b_4 a_{43} + b_5 a_{53} = b_3(1 - c_3 - \gamma)$$

$$j = 4 \rightarrow b_5 a_{54} = b_4(1 - c_4 - \gamma)$$

$$j = 5 \rightarrow c_5 = 1 - \gamma$$

Altogether there are 11 equations needed to be satisfied and we have 15 unknowns. So, we can have four free parameters which are chosen to be c_2, c_3, c_4 and γ. Solving which, we have all equations in terms of c_2, c_3, c_4 and γ.

The order equations for the sixth order method are the 11 order equations in table 1 and the additional order equations given in table 2.2 as obtained by Zingg and Chisholm [13] .

Table 2: Additional order equations for sixth order Runge-Kutta method

12.	$\tau_1^{(6)} = \sum_i b_i c_i^5 - \frac{1}{6}$
13.	$\tau_7^{(6)} = \sum_{ij} b_i a_{ij} c_j^4 - \frac{1}{30}$
14.	$\tau_{15}^{(6)} = \sum_{ijkm} b_i a_{ij} a_{jk} c_k^3 - \frac{1}{120}$
15.	$\tau_{19}^{(6)} = \sum_{ijkm} b_i a_{ij} a_{jk} a_{km} c_m^2 - \frac{1}{360}$
16.	$\tau_{20}^{(6)} = \sum_{ijkmn} b_i a_{ij} a_{jk} a_{km} a_{mn} c_n - \frac{1}{720}$

In order to choose the free parameters c_2, c_3, c_4 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 fifth order method is

$$\varphi_5 = \sum_{j=1}^{6} \tau_j^{(6)} F_j^{(6)}$$

The best strategy for practical purposes would be to choose the free RK parameters is to minimize the error norm, see Dormand [4];

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

So we have the principal error norm for this method;

$$\mathrm{A}^{(6)} = \left\| \tau^{(6)} \right\|_2 = \sqrt{(\tau_1^{(6)})^2 + (\tau_7^{(6)})^2 + (\tau_{15}^{(6)})^2 + (\tau_{19}^{(6)})^2 + (\tau_{20}^{(6)})^2}$$

where $\tau_j^{(6)}$ are the error equations associated with the sixth order method, (in table 2). Substituting the free parameters into $A^{(6)}$, we obtained the principal error norm in terms of c_2, c_3, c_4 and γ.

Minimizing the error norm, we have

$c_2 = 0.2850628601833133$,
$c_3 = 0.4813089538861712$,
$c_4 = 0.7048320137465169$ and
$\gamma = 0.070125720366624$.

Substituting the values of c_2, c_3, c_4 and γ and solving all the equations we finally get all the coefficients of the new SDIRK method for LODEs as follows;

$\gamma = 0.070125720366624$

$c_2 = 0.28506286018331$

$c_3 = 0.48130895388617$

$c_4 = 0.70483201374652$

$c_5 = 0.92987427963338$

$a_{21} = 0.21493713981669$

$a_{31} = 0.14706690123068$

$a_{32} = 0.26411633228886$

$a_{41} = 0.16565616299779$

$a_{42} = 0.18423756277865$

$a_{43} = 0.28481256760346$

$a_{51} = 0.17034709671962$

$a_{52} = 0.26544595147372$

$a_{53} = 0.097698357633858$

$a_{54} = 0.32625715343955$

$b_1 = 0.16938785743399$

$b_2 = 0.21992349463392$

$b_3 = 0.19374055051289$

$b_4 = 0.24674849025278$

$b_5 = 0.17019960716642$

$c_1 = a_{11} = a_{22} = a_{33} = a_{44} = a_{55} = \gamma$

2.2 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 (3) and (4)) is applied to the test equation,

$$y' = f(x, y) = \lambda y$$

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

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

Using the MATHEMATICA package we obtained the stability polynomial and also the stability region. The stability polynomial for new fifth order five-stage SDIRK method is

$$
\begin{aligned}
R(\hat{h}) = \; & 1 + \hat{h}\Bigg[\frac{0.1702\left(0.2654\hat{h} + 0.030\hat{h}^2 + 0.0164\hat{h}^3 - 0.0013\hat{h}^4\right)}{B} + \\
& \frac{0.2467\left(0.1656\hat{h} + 0.0466\hat{h}^2 + 0.0071\hat{h}^3 - 0.00079\hat{h}^4\right)}{B} + \\
& \frac{0.1702\left(0.3262\hat{h} - 0.0686\hat{h}^2 + 0.00481\hat{h}^3 - 0.00011\hat{h}^4\right)}{B} + \\
& \frac{0.24674\left(0.2848\hat{h} - 0.0599\hat{h}^2 + 0.0042\hat{h}^3 - 0.00009\hat{h}^4\right)}{B} + \\
& \frac{0.193741\left(0.2641\hat{h} - 0.0555\hat{h}^2 + 0.00389\hat{h}^3 - 0.00009\hat{h}^4\right)}{B} + \\
& \frac{0.219923\left(0.2149\hat{h} - 0.0452\hat{h}^2 + 0.00317\hat{h}^3 - 0.00007\hat{h}^4\right)}{B} + \\
& \frac{1.\left(1 - 0.2805\hat{h} + 0.0295\hat{h}^2 - 0.0013\hat{h}^3 + 0.000024\hat{h}^4\right)}{B} + \\
& \frac{0.193741\left(0.1470\hat{h} + 0.0258\hat{h}^2 - 0.0057\hat{h}^3 + 0.0002\hat{h}^4\right)}{B} + \\
& \frac{0.246748\left(0.1842\hat{h} + 0.0364\hat{h}^2 - 0.0078\hat{h}^3 + 0.00030\hat{h}^4\right)}{B} + \\
& \frac{0.1702\left(0.0976\hat{h} + 0.0723\hat{h}^2 - 0.0115\hat{h}^3 + 0.00042\hat{h}^4\right)}{B} + \\
& \frac{0.1702\left(0.1703\hat{h} + 0.0896\hat{h}^2 + 0.0170\hat{h}^3 + 0.0035\hat{h}^4\right)}{B} \Bigg]
\end{aligned}
$$

with value of B;

where

$$B = 1 - 0.350629\hat{h} + 0.0491762\hat{h}^2 - 0.00344851\hat{h}^3 + 0.000120915\hat{h}^4 - 1.69585\times 10^{-6}\hat{h}^5.$$

The stability polynomial is solve for $\hat{h}$ which gives the value of $\left|R(\hat{h})\right| \le 1$; this is done by using

Mathematica package (see Torrence [11]). The stability region is obtained by tracing the values of $\hat{h}$ and is shown in Figure 1. Where the vertical axis is the imaginary part and the horizontal axis is the real part.

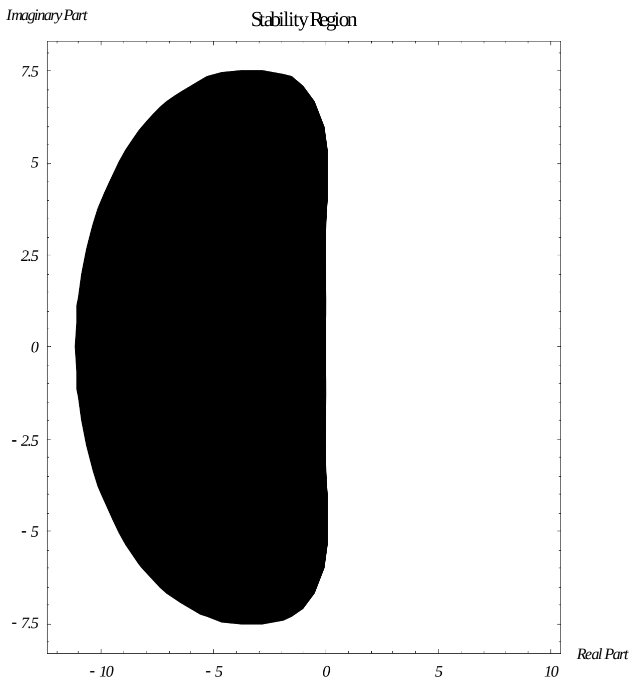

Figure 1: The stability region for the 5th order 5-stage SDIRK method

The stability analysis for fifth order five-stage explicit Runge-Kutta (ERK5) method which has been derived by Zingg and Chisholm [13] is discussed below;

Where the stability polynomial is obtained as in the SDIRK method and the stability polynomial for the explicit method is denoted by $R_1\left(\hat{h}\right)$,

where

$$R_1(\hat{h}) = 1 + \hat{h}(1. + 0.3527\,\hat{h} + 0.41041\,(-0.04418\,\hat{h} + 0.09957\,\hat{h}^2) + 0.3724\,(0.1043\,\hat{h} + 0.2247\,\hat{h}^2) - 0.040921\,(0.13437\,\hat{h} + 0.2706\,\hat{h}^2) - 0.04092\,(-0.02505\,\hat{h} + 0.003002\,\hat{h}^2 + 0.05682\,\hat{h}^3) + 0.372401\,(0.2630\,\hat{h} + 0.10238\,\hat{h}^2 + 0.1065\,\hat{h}^3) + 0.372401\,(0.08886\,\hat{h} + 0.0407\,\hat{h}^2 + 0.01157\,\hat{h}^3 + 0.022377\,\hat{h}^4))$$

Equating $R_1(\hat{h}) = = 1 = \cos\theta + i\sin\theta$

and solving for $\hat{h}$ we have the stabilty regoin of the method.

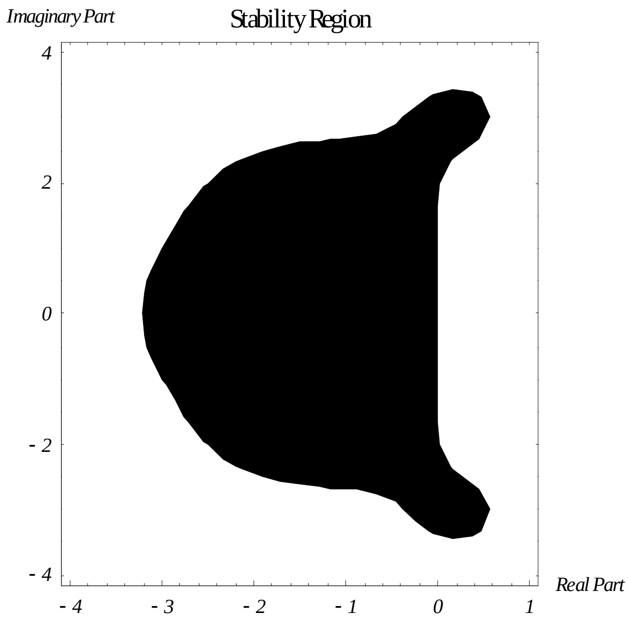

Figure 5.2: The stability region for ERK5 method

Clearly the implicit method has bigger region of stability compared to the explicit method and hence more stable.

3 Results and Discussion

We use the method to obtain the numerical solutions to the following problems, all of them are linear ODEs.

PROBLEM 1:

$$y'(t) = -y\tan t - \frac{1}{\cos t}$$

$$y(t) = \cos t - \sin t \qquad 0 \le t \le 1, y(0) = 1$$

Source: J. C. Butcher [3]

PROBLEM 2:

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

$$y(t) = t^2(e^t - e) \qquad 1 \le t \le 5, y(1) = 0$$

Source: Burden and Faires [2].

PROBLEM 3:

$$y_1' = y_2$$

$$y_2' = y_1$$

$$y_1(0) = 2, \quad y_2(0) = 0, \quad [0,10]$$

Exact Solution:

$$y_1(x) = e^x + e^{-x}$$

$$y_2(x) = e^x - e^{-x}$$

Source: Flowers [6]

PROBLEM 4:

$$y_1' = -Ay_1 - By_2$$

$$y_2' = By_1 - Ay_2$$

$$A = 1, \; B = \sqrt{3}$$

$$y_1(0) = 1, \; y_2(0) = 0, \; [0,20]$$

Exact Solution:

$$y_1(x) = e^{-Ax}\cos Bx$$

$$y_2(x) = e^{-Ax}\sin Bx$$

Source: Tam [10]

PROBLEM 5:

$$y_1' = y_2$$

$$y_2' = -2y_2 - 5y_3 + 3$$

$$y_3' = y_2 + 2y_3$$

$$y_1(0) = 0, \quad y_2(0) = 0$$

$$y_3(0) = 1, \quad [0,4\pi]$$

Exact Solution:

$$y_1(x) = 2\cos(x) + 6\sin(x) - 6x - 2$$

$$y_2(x) = -2\sin(x) + 6\cos(x) - 6$$

$$y_3(x) = 2\sin(x) - 2\cos(x) + 3$$

Source: Suleiman [9]

PROBLEM 6:

$$y_1' = y_2$$

$$y_2' = 2y_2 - y_1$$

$$y_1(0) = 0, \quad y_2(0) = 1, \quad [0,5]$$

Exact Solution:

$$y_1(x) = xe^x$$

$$y_2(x) = (1+x)e^x$$

Source: Bronson [1]

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
The true solution minus the computed solution
: $|y(x_i) - y_i|$

SDIRK5L ~ New fifth order five-stage SDIRK method with minimized error norm for LODEs.

ERK5 ~ Fifth order five-stage explicit RK method for LODEs (Zingg and Chisholm, [13])

SDIRK4(II)~ Optimal fourth order five-stage SDIRK (Ferracina and Spijker, [5])

Table 3: Numerical results for problem 1

	MTHD	H	MAXE
		0.1	
	SDIRK5L		6.12153e-009
1.	ERK5		4.73152e-007
	SDIRK4 (II)		4.90905e-008
	SDIRK5L	0.05	9.68726e-011
2.	ERK5		6.28651e-008
	SDIRK4 (II)		2.04009e-009
	SDIRK5L	0.025	5.51288e-012
3.	ERK5		8.05691e-009
	SDIRK4 (II)		1.24309e-010
	SDIRK5L	0.01	1.32783e-013
4.	ERK5		5.22694e-010
	SDIRK4 (II)		3.97293e-012
	SDIRK5L	0.005	7.76462e-015
5.	ERK5		6.56258e-011
	SDIRK4 (II)		1.06698e-012
	SDIRK5L	0.0025	1.14908e-014
6.	ERK5		8.21701e-012
	SDIRK4 (II)		8.74190e-013
	SDIRK5L	0.001	4.44089e-016
7.	ERK5		5.27051e-013
	SDIRK4 (II)		8.74356e-013

Table 4: Numerical results for problem 2

	MTHD		MAXE
1.	SDIRK5L	0.1	4.69145e-005
	ERK5		2.53931e-003
	SDIRK4 (II)		9.50611e-006
2.	SDIRK5L	0.05	2.99721e-006
	ERK5		2.88897e-004
	SDIRK4 (II)		4.83140e-007
3.	SDIRK5L	0.025	1.86742e-007
	ERK5		3.42545e-005
	SDIRK4 (II)		2.07947e-008
4.	SDIRK5L	0.01	4.77166e-009
	ERK5		2.11933e-006
	SDIRK4 (II)		4.63342e-009
5.	SDIRK5L	0.005	1.89175e-010
	ERK5		2.61750e-007
	SDIRK4 (II)		5.20822e-009
6.	SDIRK5L	0.0025	4.99313e-010
	ERK5		3.30233e-008
	SDIRK4 (II)		5.81076e-009
7.	SDIRK5L	0.001	8.95852e-010
	ERK5		2.97132e-009
	SDIRK4 (II)		6.23004e-009

Table 5: Numerical results for problem 3

	MTHD	H	MAXE
1.	SDIRK5L	0.1	3.06041e-007
	ERK5		3.13452e-003
	SDIRK4 (II)		1.80304e-003
2.	SDIRK5L	0.05	4.60568e-009
	ERK5		9.67696e-005
	SDIRK4 (II)		1.07646e-004
3.	SDIRK5L	0.025	9.82254e-011
	ERK5		3.00577e-006
	SDIRK4 (II)		6.37214e-006
4.	SDIRK5L	0.01	4.72937e-011
	ERK5		3.06609e-008
	SDIRK4 (II)		5.47661e-008
5.	SDIRK5L	0.005	4.72937e-011
	ERK5		9.49512e-010
	SDIRK4 (II)		2.10541e-007
6.	SDIRK5L	0.0025	5.09317e-011
	ERK5		1.01863e-010
	SDIRK4 (II)		2.19814e-007
7.	SDIRK5L	0.001	1.52795e-010
	ERK5		1.45519e-010
	SDIRK4 (II)		2.20294e-007

Table 6: Numerical results for problem 4

	MTHD	H	MAXE
1.	SDIRK5L	0.1	1.20424e-010
	ERK5		3.56188e-007
	SDIRK4 (II)		8.86022e-008
2.	SDIRK5L	0.05	1.77947e-012
	ERK5		1.06522e-008
	SDIRK4 (II)		5.48166e-009
3.	SDIRK5L	0.025	2.70894e-014
	ERK5		3.25603e-010
	SDIRK4 (II)		3.41584e-010
4.	SDIRK5L	0.01	3.33067e-016
	ERK5		3.28926e-012
	SDIRK4 (II)		9.14704e-012
5.	SDIRK5L	0.005	2.22045e-016
	ERK5		1.02029e-013
	SDIRK4 (II)		1.11354e-012
6.	SDIRK5L	0.0025	6.66134e-016
	ERK5		3.66374e-015
	SDIRK4 (II)		7.10959e-013
7.	SDIRK5L	0.001	6.93889e-016
	ERK5		7.21645e-016
	SDIRK4 (II)		6.88338e-013

Table 7: Numerical results for problem 5

	MTHD	H	MAXE
1.	SDIRK5L	0.1	1.20424e-010
	ERK5L		3.56188e-007
	SDIRK4(II)		8.86022e-008
2.	SDIRK5L	0.05	1.77947e-012
	ERK5		1.06522e-008
	SDIRK4(II)		5.48166e-009
3.	SDIRK5L	0.025	2.70894e-014
	ERK5L		3.25603e-010
	SDIRK4(II)		3.41584e-010
4.	SDIRK5l	0.01	3.33067e-016
	ERK5L		3.28926e-012
	SDIRK4(II)		9.14704e-012
5.	SDIRK5L	0.005	2.22045e-016
	ERK5L		1.02029e-013
	SDIRK4(II)		1.11354e-012
6.	SDIRK5L	0.0025	6.66134e-016
	ERK5		3.66374e-015
	SDIRK4(II)		7.10959e-013
7.	SDIRK5L	0.001	6.93889e-016
	ERK5		7.21645e-016
	SDIRK4(II)		6.88338e-013

Table 8: Numerical results for problem 6

	MTHD	H	MAXE
1.	SDIRK5L	0.1	1.22461e-008
	ERK5		1.28130e-004
	SDIRK4 (II)		6.79564e-005
2.	SDIRK5L	0.05	1.82013e-010
	ERK5		3.93399e-006
	SDIRK4 (II)		4.02629e-006
3.	SDIRK5L	0.025	1.81899e-012
	ERK5		1.21854e-007
	SDIRK4 (II)		2.40173e-007
4.	SDIRK5L	0.01	3.63798e-012
	ERK5		1.24066e-009
	SDIRK4 (II)		1.13994e-009
5.	SDIRK5L	0.005	1.81899e-012
	ERK5		3.38787e-011
	SDIRK4 (II)		4.82476e-009
6.	SDIRKL	0.0025	1.47793e-012
	ERK5		2.27374e-012
	SDIRK4 (II)		5.18219e-009
7.	SDIRK5L	0.0001	1.19371e-011
	ERK5		1.20508e-011
	SDIRK4 (II)		5.20674e-009

4 Conclusion

The new fifth order five-stage SDIRK method with minimized error norm has been presented for the integration of linear ODEs. It has a substantial region of stability, thus, it is stable. From the numerical results given in Table 3-8, and for all the problems tested, we can conclude that the new fifth order five-stage SDIRK method which is suitable for linear ODEs performs better in terms of maximum error compared to the fifth order five-stage ERK method and the optimal fourth order five-stage SDIRK method.

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