ISSN 0965-5425, Computational Mathematics and Mathematical Physics, 2006, Vol. 46, No. 12, pp. 2110–2123. © MAIK "Nauka/Interperiodica" (Russia), 2006.
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Diagonally Implicit Runge–Kutta Methods for Stiff Problems

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Received March 27, 2006; in final form, April 30, 2006

Abstract—Diagonally implicit Runge–Kutta methods are examined. It is shown that, for stiff problems, the methods based on the minimization of certain error functions have advantages over other methods; these functions are determined in terms of the errors for simplest model equations. Methods of orders three, four, five, and six are considered.

DOI: 10.1134/S0965542506120098

Keywords: ODE, stiff problems, diagonally implicit Runge–Kutta methods, SDIRK, ESDIRK

INTRODUCTION

The general description of an s-stage Runge–Kutta method for solving the Cauchy problem

$$\mathbf{y}' = \mathbf{f}(t, \mathbf{y}), \quad \mathbf{y}(t_0) = \mathbf{y}_0$$

is given by the formulas

$$\mathbf{y}_{n+1} = \mathbf{y}_n + h\sum_{i=1}^{s} b_i\mathbf{k}_i, \quad \mathbf{k}_i = \mathbf{f}\left(t_n + c_i h, \mathbf{y}_n + h\sum_{j=1}^{s} a_{ij}\mathbf{k}_j\right), \quad i = 1, 2, \ldots, s,$$

which can be represented as the Butcher table

$$\begin{array}{c|c} \mathbf{c} & \mathbf{A} \\ \hline & \mathbf{b}^{\mathrm{T}} \end{array} = \begin{array}{c|ccc} c_1 & a_{11} & \ldots & a_{1s} \\ \vdots & \vdots & \ldots & \vdots \\ c_s & a_{s1} & \ldots & a_{ss} \\ \hline & b_1 & \ldots & b_s \end{array}.$$

It is assumed that the coefficients of the method satisfy the following condition of stage order one: $\mathbf{c} = \mathbf{Ae}$, and $\mathbf{b}^{\mathrm{T}}\mathbf{e} = 1$, where $\mathbf{e} = [1, \ldots, 1]^{\mathrm{T}}$.

Among the implicit Runge–Kutta methods, the diagonally implicit ones (DIRK, meaning Diagonally Implicit Runge–Kutta), whose matrix $\mathbf{A}$ has a lower triangular form, are most easily implemented. A usual requirement is also that the nonzero diagonal entries of $\mathbf{A}$ be identical, which makes it possible to perform at most one LU decomposition per integration step. There are two popular types of such methods, namely, SDIRK (Singly DIRK) and ESDIRK (Explicit first stage Singly DIRK) methods. The SDIRK methods do not have any explicit stages, whereas the ESDIRK methods have an explicit first stage, which explains their name.

The stiffly accurate methods for which the last row in $\mathbf{A}$ is identical to $\mathbf{b}^{\mathrm{T}}$ are advantageous in solving stiff problems (see [1]). Only this kind of methods is considered in this paper. In the subsequent presentation, it is convenient to denote by r the number of implicit stages. Then, for the stiffly accurate SDIRK methods, the Butcher table has the form

$$\begin{array}{c|cccc} c_1 & \gamma & & & \\ \vdots & \vdots & \ddots & & \\ c_{r-1} & a_{r-1,1} & \ldots & \gamma & \\ 1 & b_1 & \ldots & b_{r-1} & \gamma \\ \hline & b_1 & \ldots & b_{r-1} & \gamma \end{array}.$$

Methods of this type were studied in [1–3].

The stiffly accurate ESDIRK methods have the Butcher table

$$\begin{array}{c|ccccc} 0 & 0 & & & & \\ c_2 & a_{21} & \gamma & & & \\ \vdots & \vdots & \vdots & \ddots & & \\ c_r & a_{r1} & a_{r2} & \dots & \gamma & \\ 1 & b_1 & b_2 & \dots & b_r & \gamma \\ \hline & b_1 & b_2 & \dots & b_r & \gamma \end{array}.$$

(In what follows, we drop the last row of the table.) Methods of this type were analyzed in [4–13]. The explicit stage involves no calculations, because its result coincides with that of the last stage in the previous step. This explains the other name for stiffly accurate methods with an explicit first stage, namely, FSAL (First Same As Last) methods (see [4, 6]). ESDIRK methods can have the stage order two, which is their advantage over SDIRK methods whose only stage order is one.

The order reduction is a phenomenon observed in solving stiff problems by Runge–Kutta methods (see [1, 14]); it can be explained using the Prothero–Robinson model equation. Other simple equations modeling the behavior of the errors in solving stiff problems were examined in [9]. Based on these equations, error functions were derived whose minimization makes it possible to improve the accuracy of solving stiff problems by Runge–Kutta methods (see [8, 9, 15]). In [15], the author succeeded in obtaining simple expressions for the error functions of explicit methods. In this paper, analogous expressions are derived for SDIRK and ESDIRK methods. This allows us to justify the choice of the coefficients in methods with improved accuracy for stiff problems.

1. STABILITY FUNCTION

The numerical solution to the problem

$$y' = \lambda y, \quad y(t_0) = y_0 \tag{1.1}$$

obtained by a Runge–Kutta method is given by the formula $y_{n+1} = R(h\lambda)y_n$, where $R(z) = 1 + z\mathbf{b}^{\mathrm{T}}(\mathbf{I} - z\mathbf{A})^{-1}\mathbf{e}$ is the stability function and $\mathbf{I} = \mathrm{diag}(\mathbf{e})$. A method is said to be $A(\alpha)$-stable if its stability domain specified by the inequality $|R(z)| \le 1$ contains the sector $|\arg(-z)| \le \alpha$. A method is called $L(\alpha)$-stable if, in addition, $R(\infty) = 0$. $A(90°)$-stable and $L(90°)$-stable methods are called simply A-stable and L-stable, respectively. The choice of the optimal stability function for DIRK and Rosenbrock methods is the subject of [16–18].

Suppose that the method under discussion as applied to solving (1.1) has the order p. Then, for $z \longrightarrow 0$, we have $e^z - R(z) = Cz^{p+1} + O(z^{p+2})$, where C is the error constant. The normalized error constant $C \times (p + 1)!$, which coincides with a coefficient in the expression for the error of the method, is thereafter used as an accuracy indicator for the stability function.

If the matrix $\mathbf{A}$ of an implicit method is invertible, then its stability function can be written as

$$R(z) = 1 - \mathbf{b}^{\mathrm{T}}\mathbf{A}^{-1}\mathbf{e} + \mathbf{b}^{\mathrm{T}}\mathbf{A}^{-1}(\mathbf{I} - z\mathbf{A})^{-1}\mathbf{e}. \tag{1.2}$$

For an SDIRK method, we set $\bar{\mathbf{A}} = \mathbf{A} - \gamma\mathbf{I}$; then,

$$(\mathbf{I} - z\mathbf{A})^{-1} = \frac{1}{1-\gamma z}\left[\mathbf{I} - \frac{z}{1-\gamma z}\bar{\mathbf{A}}\right]^{-1} = \sum_{i=0}^{r-1}\frac{z^i}{(1-\gamma z)^{i+1}}\bar{\mathbf{A}}^i. \tag{1.3}$$

Substituting (1.3) in (1.2), we obtain

$$R(z) = 1 - d_0 + \sum_{i=0}^{r-1} d_i \frac{z^i}{(1-\gamma z)^{i+1}}, \tag{1.4}$$

where $d_i = \mathbf{b}^{\mathrm{T}}\mathbf{A}^{-1}\bar{\mathbf{A}}^i\mathbf{e}$ $(i = 0, 1, \dots, r-1)$. The stiff accuracy condition yields $\mathbf{b}^{\mathrm{T}}\mathbf{A}^{-1} = \mathbf{e}_r^{\mathrm{T}} = [0, \dots, 0, 1]$; then, $d_0 = 1$, and $d_i = \mathbf{e}_r^{\mathrm{T}}\bar{\mathbf{A}}^i\mathbf{e}$ $(i = 1, 2, \dots, r-1)$.

For an ESDIRK method, we write the coefficient matrix and vectors as

$$\mathbf{A} = \begin{bmatrix} 0 & \mathbf{0} \\ \tilde{\mathbf{a}} & \tilde{\mathbf{A}} \end{bmatrix}, \quad \mathbf{b} = \begin{bmatrix} b_1 \\ \tilde{\mathbf{b}} \end{bmatrix}, \quad \mathbf{c} = \begin{bmatrix} 0 \\ \tilde{\mathbf{c}} \end{bmatrix},$$

which yields

$$R(z) = 1 + zb_1 + z^2\tilde{\mathbf{b}}^{\mathrm{T}}(\mathbf{I} - z\tilde{\mathbf{A}})^{-1}\tilde{\mathbf{a}} + z\tilde{\mathbf{b}}^{\mathrm{T}}(\mathbf{I} - z\tilde{\mathbf{A}})^{-1}\mathbf{e}. \tag{1.5}$$

Using the condition of stage order one and the stiff accuracy condition, we deduce from (1.5) that $R(z) = 1 - \mathbf{e}_r^{\mathrm{T}}\tilde{\mathbf{A}}^{-1}\tilde{\mathbf{c}} + \mathbf{e}_r^{\mathrm{T}}\tilde{\mathbf{A}}^{-1}(\mathbf{I} - z\tilde{\mathbf{A}})^{-1}\tilde{\mathbf{c}}$. Setting $\bar{\mathbf{A}} = \tilde{\mathbf{A}} - \gamma\mathbf{I}$, we obtain the stability function of the ESDIRK method in form (1.4), where

$$d_i = \mathbf{e}_r^{\mathrm{T}}\tilde{\mathbf{A}}^{-1}\bar{\mathbf{A}}^i\tilde{\mathbf{c}}, \quad i = 0, 1, \dots, r-1. \tag{1.6}$$

We examine the methods with $d_0 = 1$, which is a necessary condition for the $L(\alpha)$-stability. For this condition to hold, it is sufficient that an SDIRK method be stiffly accurate, while, for a stiffly accurate ESDIRK method, the additional equality

$$d_0 = \mathbf{e}_r^{\mathrm{T}}\tilde{\mathbf{A}}^{-1}\tilde{\mathbf{c}} = 1 \tag{1.7}$$

must be fulfilled. For $d_0 = 1$, we obtain

$$R(z) = \frac{1}{(1-\gamma z)} + \sum_{i=1}^{r-1} d_i \frac{z^i}{(1-\gamma z)^{i+1}}, \tag{1.8}$$

where the coefficients d_i of a pth-order method satisfy the conditions

$$d_i = D_i(\gamma) = \sum_{j=0}^{i} (-1)^j \binom{i}{j} \frac{\gamma^j}{(i-j)!}, \quad i = 1, 2, \dots, p. \tag{1.9}$$

If $p = r$, then γ must be equal to a root of the equation

$$D_p(\gamma) = 0. \tag{1.10}$$

For $p = r - 1$, the stability function is uniquely determined by γ. The error constant is given by

$$C = \begin{cases} D_{p+1}(\gamma), & p \ge r-1, \\ D_{p+1}(\gamma) - d_{p+1}, & p < r-1. \end{cases}$$

If $p = r$, then, for a given p ($3 \le p \le 6$), only one of the values γ satisfying (1.10) ensures the L-stability (see [1]). Often, the L-stability is an excessive requirement; therefore, we also consider $L(\alpha)$-stable methods with $\alpha \ge 72.3°$. The values γ_a for which the method is L-stable and the values γ_b ensuring the $L(\alpha)$-stability and the minimal error constant are presented in Table 1. The normalized error constants are shown for all of these values γ, and the angle α of the stability sector is given for γ_b.

For $p = r - 1$, we have a wider choice for γ. The graphs depicted in the figure show the normalized error constant and the angle α as functions of γ for $r = 5$, $p = 4$ (the solid curve) and $r = 6$, $p = 5$ (the dotted curve).

2. ERROR FUNCTIONS

The error functions were proposed in [9] and were defined there in terms of the local errors of stiff model equations. Here are some of these equations:

$$\begin{aligned} x_1' &= 1, \quad x_{21}' = x_1, \quad y_{21}' = \lambda(y_{21} - x_1^2) + 2t, \\ y_{31}' &= \lambda(y_{31} - x_1^3) + 3t^2, \quad y_{32}' = \lambda(y_{32} - x_1x_{21}) + \frac{3}{2}t^3. \end{aligned} \tag{2.1}$$

For the zero initial conditions, we have $y_{21}(t) = t^2$, $y_{31}(t) = t^3$, and $y_{32}(t) = t^3/2$. It is easy to obtain the numerical solutions $\tilde{y}_{ij}$ to Eqs. (2.1) for an integration step; then, the local errors can be written as

$$\delta_h(y_{ij}) = y_{ij}(h) - \tilde{y}_{ij}(h) = e_{ij}(z)y_{ij}(h), \quad z = h\lambda,$$

Table 1

$p = r$	γ_a	$\lvert C_a\rvert \times (p+1)!$	γ_b	$\lvert C_b\rvert \times (p+1)!$	α, deg
3	0.435867	6.2×10^{-1}	0.158984	9.4×10^{-2}	75.6
4	0.572816	3.3×10^{0}	0.220428	1.3×10^{-1}	89.56
5	0.278054	3.8×10^{-1}	0.141127	4.2×10^{-2}	72.3
6	0.334142	1.7×10^{0}	0.173156	7.9×10^{-2}	85.6

where the error functions $e_{ij}(z)$ can be expressed by the formulas

$$e_{21}(z) = z\mathbf{b}^{\mathrm{T}}(\mathbf{I} - z\mathbf{A})^{-1}(\mathbf{c}^2 - 2\mathbf{Ac}) + (1 - 2\mathbf{b}^{\mathrm{T}}\mathbf{c}),$$

$$e_{31}(z) = z\mathbf{b}^{\mathrm{T}}(\mathbf{I} - z\mathbf{A})^{-1}(\mathbf{c}^3 - 3\mathbf{Ac}^2) + (1 - 3\mathbf{b}^{\mathrm{T}}\mathbf{c}^2),$$

$$e_{32}(z) = z\mathbf{b}^{\mathrm{T}}(\mathbf{I} - z\mathbf{A})^{-1}(2\mathbf{c} \cdot \mathbf{Ac} - 3\mathbf{Ac}^2) + (1 - 3\mathbf{b}^{\mathrm{T}}\mathbf{c}^2).$$

Here and in the subsequent formulas, we assume that the operations of multiplying vectors and raising a vector to a power are performed componentwise.

In [9], the error functions $e_{4j}(z)$ ($j = 1, \ldots, 5$) were also given. For a method of stage order q, all the functions $e_{ij}(z)$ with $i \le q$ are identically equal to zero. Note that the functions $e_{i1}(z)$ are identical to the functions $e_i(z)$ obtained in [8] by decomposing the error of the Prothero–Robinson equation into the Taylor series; however, the other error functions cannot be derived from this equation. We set $e_i(z) = e_{i1}(z)$, $i = 2, 3, \ldots$.

The SDIRK methods have the stage order one; therefore, the stiff component of the error is mainly determined by $e_2(z)$. For a stiffly accurate method of order $p \ge 2$, this function can be represented as

$$e_2(z) = \mathbf{e}_r^{\mathrm{T}}(\mathbf{I} - z\mathbf{A})^{-1}(\mathbf{c}^2 - 2\mathbf{Ac}) = \sum_{i=p-1}^{r-1} \mathbf{e}_r^{\mathrm{T}}\overline{\mathbf{A}}^i(\mathbf{c}^2 - 2\mathbf{Ac})\frac{z^i}{(1-\gamma z)^{i+1}}. \tag{2.2}$$

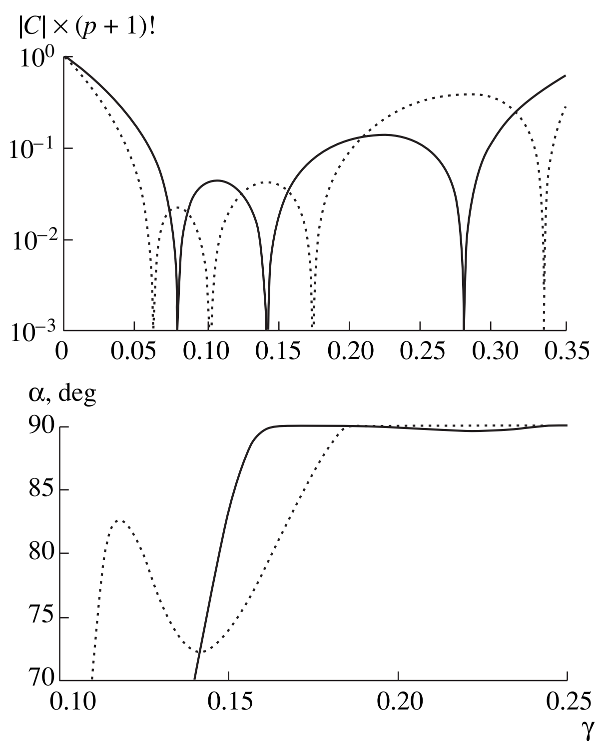

Figure.

(Here, the order conditions $\mathbf{e}_r^{\mathrm{T}}\overline{\mathbf{A}}^i(\mathbf{c}^2 - 2\mathbf{A}\mathbf{c}) = 0$ $(0 \le i \le p-2)$ were used.)

Consider the stiffly accurate SDIRK methods of order $p = r - 1$. In this case, using the relations $c_1 = \gamma$ and $a_{21} = c_2 - \gamma$, we obtain

$$\mathbf{e}_r^{\mathrm{T}}\overline{\mathbf{A}}^{r-2}(\mathbf{c}^2 - \mathbf{A}\mathbf{c}) = b_{r-1}a_{r-1,r-2}\dots a_{32}(c_2-\gamma)^2 = b_{r-1}a_{r-1,r-2}\dots a_{32}a_{21}(c_2-\gamma) = d_{r-1}(c_2-\gamma),$$

$$\mathbf{e}_r^{\mathrm{T}}\overline{\mathbf{A}}^{r-2}\mathbf{A}\mathbf{c} = \mathbf{e}_r^{\mathrm{T}}\overline{\mathbf{A}}^{r-2}(\overline{\mathbf{A}} + \gamma\mathbf{I})^2\mathbf{e} = 2d_{r-1}\gamma + d_{r-2}\gamma^2,$$

$$\mathbf{e}_r^{\mathrm{T}}\overline{\mathbf{A}}^{r-1}(\mathbf{c}^2 - 2\mathbf{A}\mathbf{c}) = b_{r-1}a_{r-1,r-2}\dots a_{32}a_{21}(-\gamma^2) = -d_{r-1}\gamma^2.$$

Substituting these expressions in (2.2), we have

$$e_2(z) = [d_{r-1}(c_2 - 3\gamma) - d_{r-2}\gamma^2]\frac{z^{r-2}}{(1-\gamma z)^{r-1}} - d_{r-1}\gamma^2\frac{z^{r-1}}{(1-\gamma z)^r}.$$

Taking into account (1.9) and assuming that $D_{r-1}(\gamma) \ne 0$, we finally obtain

$$\begin{gathered} e_2(z) = \frac{z^{r-2}}{(1-\gamma z)^r}D_{r-1}(\gamma)[c_2 - (c_2^* + \gamma) - \gamma z(c_2 - c_2^*)], \\ c_2^* = 2\gamma + \gamma^2\frac{D_{r-2}(\gamma)}{D_{r-1}(\gamma)}. \end{gathered} \tag{2.3}$$

For the ESDIRK methods, we require the stage order two; that is, the condition

$$\tilde{\mathbf{c}}^2 = 2\tilde{\mathbf{A}}\tilde{\mathbf{c}} \tag{2.4}$$

must be satisfied. In this case, $e_2(z) \equiv 0$, and the stiff component of the error is determined by $e_3(z) = e_{31}(z) = e_{32}(z)$. For a stiffly accurate method of order $p \ge 3$, this function can be represented as

$$e_3(z) = \mathbf{e}_r^{\mathrm{T}}(\mathbf{I} - z\tilde{\mathbf{A}})^{-1}(\tilde{\mathbf{c}}^3 - 3\tilde{\mathbf{A}}\tilde{\mathbf{c}}^2) = \sum_{i=p-2}^{r-1}\mathbf{e}_r^{\mathrm{T}}\overline{\mathbf{A}}^i(\tilde{\mathbf{c}}^3 - 3\tilde{\mathbf{A}}\tilde{\mathbf{c}}^2)\frac{z^i}{(1-\gamma z)^{i+1}}. \tag{2.5}$$

We first consider the case $p = r$. By analogy with the SDIRK methods, we derive from (2.4) and (2.5) that

$$e_3(z) = [2d_{r-1}\gamma(c_3 - 5\gamma) - 2d_{r-2}\gamma^3]\frac{z^{r-2}}{(1-\gamma z)^{r-1}} - 2d_{r-1}\gamma^3\frac{z^{r-1}}{(1-\gamma z)^r}.$$

If (1.10) is fulfilled, then

$$\begin{gathered} e_3(z) = \frac{z^{r-2}}{(1-\gamma z)^r}2\gamma D_{r-1}(\gamma)[c_3 - (c_3^* + \gamma) - \gamma z(c_3 - c_3^*)], \\ c_3^* = 4\gamma + \gamma^2\frac{D_{r-2}(\gamma)}{D_{r-1}(\gamma)}. \end{gathered} \tag{2.6}$$

Now, for $p = r - 1$, we find the function $e_3(z)$ under the additional condition

$$\tilde{\mathbf{b}}^{\mathrm{T}}\tilde{\mathbf{A}}^{-2}\tilde{\mathbf{c}}^3 = \mathbf{e}_r^{\mathrm{T}}\tilde{\mathbf{A}}^{-1}\tilde{\mathbf{c}}^3 = 3, \tag{2.7}$$

which guarantees the decay of $e_3(z)$ at the rate $O(z^{-2})$ as $z \longrightarrow \infty$. Relation (2.7) is also one of the order conditions for differential algebraic equations (DAE) of index 2 (see [1, 3, 7]). Omitting the intermediate calculations, we give the final formula

$$e_3(z) = [2d_{r-1}(c_3 - 4\gamma) - 2d_{r-2}\gamma^2]\frac{z^{r-3}}{(1-\gamma z)^{r-1}} - 2d_{r-1}\gamma^2\frac{z^{r-2}}{(1-\gamma z)^r}.$$

If a method is $L(\alpha)$-stable and $D_{r-1}(\gamma) \neq 0$, this formula can be written in the form

$$
\begin{aligned}
e_3(z) &= \frac{z^{r-3}}{(1-\gamma z)^r} 2D_{r-1}(\gamma)[c_3 - (c_3^* + \gamma) - \gamma z(c_3 - c_3^*)], \\
c_3^* &= 3\gamma + \gamma^2 \frac{D_{r-2}(\gamma)}{D_{r-1}(\gamma)}.
\end{aligned}
\tag{2.8}
$$

In expressions (2.3), (2.6), and (2.8), the error function depends only on two parameters, namely, on γ and c_2 (or c_3). Denote by $\varepsilon(z, c_2)$ the modulus of error function (2.3) for a given positive γ. Then, the following assertions are valid:

(1) if $c_2 < c_2^*$ and $\mathrm{Re}\, z < 0$, then $\varepsilon(z, c_2) > \varepsilon(z, c_2^*)$;

(2) if $c_2 > c_2^* + \gamma$ and $\mathrm{Re}\, z < 0$, then $\varepsilon(z, c_2) > \varepsilon(z, c_2^* + \gamma)$;

(3) if $c_2^* \le c_2 < c_2' \le c_2^* + \gamma$, then there exist z and z' such that $\mathrm{Re}\, z < 0$, $\varepsilon(z, c_2) < \varepsilon(z, c_2')$ and $\mathrm{Re}\, z' < 0$, $\varepsilon(z', c_2) > \varepsilon(z'\ c_2')$.

Thus, the inequality

$$c_2^* \le c_2 \le c_2^* + \gamma \tag{2.9}$$

describes the set of all the values of c_2 whose modification cannot simultaneously decrease the modulus of function (2.3) at all the points of the left half-plane. The optimal value of c_2 must be sought on interval (2.9). For very stiff problems, it is shifted to the left endpoint of this interval, and, for weakly stiff problems, it is shifted to the right endpoint. The analogous inequality for functions (2.6) and (2.8) can be written as

$$c_3^* \le c_3 \le c_3^* + \gamma. \tag{2.10}$$

3. ORDER CONDITIONS

The basic difficulty in the construction of high-order methods is the necessity of ensuring that a great number of algebraic conditions are fulfilled. The diagonal form of **A** makes it possible to simplify these conditions; as a result, they become nearly as simple as those for explicit methods. Simplified order conditions for SDIRK methods were derived in [1]. Here, we obtain analogous conditions for stiffly accurate ESDIRK methods of stage order two.

From the condition of stage order one, we have

$$a_{i1} = c_i - \sum_{j=2}^{i-1} a_{ij} - \gamma, \quad i = 2, 3, \ldots, r, \quad b_1 = 1 - \sum_{j=2}^{r} b_j - \gamma. \tag{3.1}$$

The coefficients determined by (3.1) do not appear in the other order conditions; therefore, they are calculated lastly. From the condition of stage order two (see (2.4)), we obtain

$$c_2 = 2\gamma, \quad a_{i2} = \frac{1}{4\gamma}\left[c_i^2 - 2\left(\sum_{j=3}^{i-1} a_{ij} c_j + \gamma c_i\right)\right], \quad i = 3, 4, \ldots, r. \tag{3.2}$$

Define $\bar{\mathbf{b}} = \tilde{\mathbf{b}} - \gamma \mathbf{e}_r = (\mathbf{e}_r^{\mathrm{T}} \bar{\mathbf{A}})^{\mathrm{T}}$. Then, the quadrature conditions ensuring the order p in the solution of the equation $y' = f(t)$ take the form

$$\bar{\mathbf{b}}^{\mathrm{T}} \tilde{\mathbf{c}}^{i-1} = \sum_{j=2}^{r} b_j c_j^{i-1} = \frac{1}{i} - \gamma, \quad i = 2, 3, \ldots, p. \tag{3.3}$$

One of the third-order conditions appears in (3.3); the second condition can be written as

$$\tilde{\mathbf{b}}^{\mathrm{T}} \tilde{\mathbf{A}} \tilde{\mathbf{c}} = (\bar{\mathbf{b}} + \gamma \mathbf{e}_r)^{\mathrm{T}} (\bar{\mathbf{A}} + \gamma \mathbf{I}) \tilde{\mathbf{c}} = \frac{1}{6}.$$

Taking into account (3.3), we obtain

$$\bar{\mathbf{b}}^{\mathrm{T}}\bar{\mathbf{A}}\tilde{\mathbf{c}} = \frac{1}{6} - \gamma + \gamma^2. \tag{3.4}$$

For the construction of a third-order method, it suffices to ensure that conditions (3.1)–(3.3) are fulfilled; then, these conditions imply (3.4). However, relation (3.4) is also needed in the derivation of higher order conditions.

A fourth-order method must additionally satisfy four conditions. Since the stage order is two, the number of additional conditions can be reduced to two of which one appears in (3.3) and the other has the form

$$\tilde{\mathbf{b}}^{\mathrm{T}}\tilde{\mathbf{A}}^2\tilde{\mathbf{c}} = (\bar{\mathbf{b}} + \gamma\mathbf{e}_r)^{\mathrm{T}}(\bar{\mathbf{A}} + \gamma\mathbf{I})^2\tilde{\mathbf{c}} = \bar{\mathbf{b}}^{\mathrm{T}}\bar{\mathbf{A}}^2\tilde{\mathbf{c}} + 3\gamma\bar{\mathbf{b}}^{\mathrm{T}}\bar{\mathbf{A}}\tilde{\mathbf{c}} + 3\gamma^2\bar{\mathbf{b}}^{\mathrm{T}}\tilde{\mathbf{c}} + \gamma^3 = \frac{1}{24}.$$

Using this condition and relations (3.3) and (3.4), we obtain

$$\bar{\mathbf{b}}^{\mathrm{T}}\bar{\mathbf{A}}^2\tilde{\mathbf{c}} = \frac{1}{24} - \frac{1}{2}\gamma + \frac{3}{2}\gamma^2 - \gamma^3. \tag{3.5}$$

With the growth of the order, the number of additional conditions is rapidly increasing. For a fifth-order method, it is equal to nine; however, it reduces to four if the condition of stage order two is fulfilled. One of these additional conditions appears in (3.3); using a similar reasoning, the three remaining conditions are reduced to the form

$$\begin{aligned} \bar{\mathbf{b}}^{\mathrm{T}}(\tilde{\mathbf{c}} \cdot \bar{\mathbf{A}}^2\tilde{\mathbf{c}}) &= \frac{1}{30} - \frac{5}{12}\gamma + \frac{4}{3}\gamma^2 - \gamma^3, \\ \bar{\mathbf{b}}^{\mathrm{T}}\bar{\mathbf{A}}(\tilde{\mathbf{c}} \cdot \bar{\mathbf{A}}\tilde{\mathbf{c}}) &= \frac{1}{40} - \frac{1}{3}\gamma + \frac{7}{6}\gamma^2 - \gamma^3, \\ \bar{\mathbf{b}}^{\mathrm{T}}\bar{\mathbf{A}}^3\tilde{\mathbf{c}} &= \frac{1}{120} - \frac{1}{6}\gamma + \gamma^2 - 2\gamma^3 + \gamma^4. \end{aligned} \tag{3.6}$$

In addition to the order conditions, we require that equality (1.7) be fulfilled to ensure the $L(\alpha)$-stability. For $p = r$, (1.7) is fulfilled if γ is a root of Eq. (1.10). For $p = r - 1$, we write (1.7) in the form

$$\mathbf{e}_r^{\mathrm{T}}\tilde{\mathbf{A}}^{-1}\tilde{\mathbf{c}} = \frac{1}{\gamma}\mathbf{e}_r^{\mathrm{T}}\left(\mathbf{I} + \frac{1}{\gamma}\bar{\mathbf{A}}\right)^{-1}\tilde{\mathbf{c}} = \frac{1}{\gamma} + \sum_{i=0}^{r-2}\frac{(-1)^{i+1}}{\gamma^{i+2}}\bar{\mathbf{b}}^{\mathrm{T}}\bar{\mathbf{A}}^i\tilde{\mathbf{c}} = 1. \tag{3.7}$$

Let us substitute in (3.7) the values $\bar{\mathbf{b}}^{\mathrm{T}}\bar{\mathbf{A}}^i\tilde{\mathbf{c}}$ ($i = 0, 1, \ldots, r - 1$) appearing in order conditions (3.3)–(3.6). For $r = 5$, $p = 4$, this yields

$$\bar{\mathbf{b}}^{\mathrm{T}}\bar{\mathbf{A}}^3\tilde{\mathbf{c}} = b_5a_{54}a_{43}a_{32}c_2 = \gamma\left(\frac{1}{24} - \frac{2}{3}\gamma + 3\gamma^2 - 4\gamma^3 + \gamma^4\right). \tag{3.8}$$

For $r = 6$, $p = 5$, we have

$$\bar{\mathbf{b}}^{\mathrm{T}}\bar{\mathbf{A}}^4\tilde{\mathbf{c}} = b_6a_{65}a_{54}a_{43}a_{32}c_2 = \gamma\left(\frac{1}{120} - \frac{5}{24}\gamma + \frac{5}{3}\gamma^2 - 5\gamma^3 + 5\gamma^4 - \gamma^5\right). \tag{3.9}$$

Formulas (3.8) and (3.9) can be extended. Indeed, if $i = p = r - 1$, we deduce from (1.6) and (1.9) that

$$d_p = \mathbf{e}_r^{\mathrm{T}}\tilde{\mathbf{A}}^{-1}\bar{\mathbf{A}}^p\tilde{\mathbf{c}} = \frac{1}{\gamma}\mathbf{e}_r^{\mathrm{T}}\left(\mathbf{I} + \frac{1}{\gamma}\bar{\mathbf{A}}\right)^{-1}\bar{\mathbf{A}}^p\tilde{\mathbf{c}} = \frac{1}{\gamma}\bar{\mathbf{b}}^{\mathrm{T}}\bar{\mathbf{A}}^{p-1}\tilde{\mathbf{c}} = D_p(\gamma),$$

whence $\bar{\mathbf{b}}^{\mathrm{T}}\bar{\mathbf{A}}^{p-1}\tilde{\mathbf{c}} = \gamma D_p(\gamma)$.

For $p = r - 1$, we additionally require that (2.7) be fulfilled. This condition can be written as

$$\mathbf{e}_r^{\mathrm{T}}\tilde{\mathbf{A}}^{-1}\tilde{\mathbf{c}}^3 = \frac{1}{\gamma} + \sum_{i=0}^{r-2}\frac{(-1)^{i+1}}{\gamma^{i+2}}\bar{\mathbf{b}}^{\mathrm{T}}\bar{\mathbf{A}}^i\tilde{\mathbf{c}}^3 = 3. \tag{3.10}$$

4. THIRD-ORDER METHODS

For $r = p = 3$, the stiffly accurate methods were studied in [2]. They are specified by the table

$$\begin{array}{c|ccc} \gamma & \gamma & & \\ \dfrac{1+\gamma}{2} & \dfrac{1-\gamma}{2} & \gamma & \\ 1 & 1-b_2-\gamma & b_2 & \gamma \end{array},$$

where $b_2 = \dfrac{1}{4}(5 - 20\gamma + 6\gamma^2)$ and γ is a root of the equation

$$D_3(\gamma) = \frac{1}{6} - \frac{3}{2}\gamma + 3\gamma^2 - \gamma^3 = 0. \tag{4.1}$$

The method for which $\gamma = 0.435866521508$ is L-stable. We call it S33a (here, the first digit indicates the number r of implicit stages, and the second digit indicates the order p). The method for which $\gamma = 0.158983899989$ is $L(\alpha)$-stable and has small error coefficients; it is denoted by S33b.

The analogous ESDIRK methods of stage order two with $r = p = 3$ were analyzed in [7, 8, 10–13]. They are given by the table

$$\begin{array}{c|cccc} 0 & 0 & & & \\ 2\gamma & \gamma & \gamma & & \\ c_3 & c_3 - a_{32} - \gamma & a_{32} & \gamma & \\ 1 & 1 - b_2 - b_3 - \gamma & b_2 & b_3 & \gamma \end{array}.$$

From (3.2) and (3.3), we have

$$a_{32} = \frac{c_3(c_3 - 2\gamma)}{4\gamma}, \quad b_2 = \frac{2 - 6\gamma - 3c_3 + 6\gamma c_3}{12\gamma(2\gamma - c_3)}, \quad b_3 = \frac{1 - 6\gamma + 6\gamma^2}{3c_3(c_3 - 2\gamma)}.$$

The diagonal entry of any $L(\alpha)$-stable method must satisfy Eq. (4.1), while c_3 is a free parameter. For a third-order method of stage order two, the minimization of the error function $e_3(z)$ yields no tangible benefits; therefore, we choose c_3 using different considerations. The minimum condition for the error coefficients $e(t_{41})$ and $e(t_{42})$ leads to the equation $1 - 4(b_2c_2^3 + b_3c_3^3 + \gamma) = 0$ (see [19]), whence

$$c_3 = 1/2 + \gamma/4. \tag{4.2}$$

For $\gamma = 0.435\ldots$, this method, which we denote by ES33a, was proposed in [10]. Another method with the parameters $\gamma = 0.158\ldots$ and $c_3 = (2 + \sqrt{2})\gamma$ was proposed in [9]. In this method, which we call ES33b, the value of c_3 is not too different from (4.2). The L-stability of the inner stage and the convenient implementation are also ensured.

The basic characteristics of the third-order methods are presented in Table 2. There, $\|e(t_i)\|_2 = \sqrt{\sum_j e(t_{ij})^2}$ is the norm of the ith-order error coefficients, $\|e_{q+1}(z)\|_\infty = \max\limits_{\mathrm{Re}\, z \le 0} |e_{q+1}(z)|$ is the norm of the error function, and q is the stage order.

5. FOURTH-ORDER METHODS

There are no stiffly accurate SDIRK methods for $r = p = 4$ (see [2]). The fourth-order SDIRK methods having five stages were examined in [1]. For a given γ, they constitute a two-parameter family governed by the abscissas c_2 and c_3. The minimization of the error coefficients results in the method called SDIRK4 for which $\gamma = 0.25$, $c_2 = 0.75$, and $c_3 = 0.55$. (We denote this method by S54a.)

We show a different approach to the choice of the parameters that is based on the minimization of the error function. According to (2.3) and (2.9), the optimal value of c_2 for $\gamma = 0.25$ belongs to the interval

Table 2

Method	γ	α, deg	$\|e(t_4)\|_2$	$\|e_{q+1}(z)\|_\infty$
S33a	0.435867	90.0	6.9×10^{-1}	7.0×10^{-2}
S33b	0.158984	75.6	1.0×10^{-1}	8.0×10^{-2}
ES33a	0.435867	90.0	8.8×10^{-1}	1.5×10^{-1}
ES33b	0.158984	75.6	1.3×10^{-1}	6.1×10^{-2}

[−1/12, 1/6]. Setting $c_2 = 0$ and $c_3 = 1/2$, we obtain the coefficient table for the method S54b:

$$\begin{array}{c|ccccc} 1/4 & 1/4 & & & & \\ 0 & -1/4 & 1/4 & & & \\ 1/2 & 1/8 & 1/8 & 1/4 & & \\ 1 & -3/2 & 3/4 & 3/2 & 1/4 & \\ 1 & 0 & 1/6 & 2/3 & -1/12 & 1/4 \end{array}.$$

This method proved to be the most accurate among the SDIRK methods.

To further improve the accuracy, we use ESDIRK methods. It is possible to construct $L(\alpha)$-stable methods for $r = p = 4$ if the diagonal entry is set to a root of the equation

$$D_4(\gamma) = \frac{1}{24} - \frac{2}{3}\gamma + 3\gamma^2 - 4\gamma^3 + \gamma^4 = 0 \qquad (5.1)$$

different from 0.106…. Such methods were considered in [8, 13]. If all the abscissas c_2, c_3, and c_4 are distinct, then, for a given γ, these methods constitute a two-parameter family governed by c_3 and c_4. The weights b_2, b_3, and b_4 are found from Eqs. (3.3). From (3.5), we obtain

$$a_{43} = \frac{1 - 12\gamma + 36\gamma^2 - 24\gamma^3}{12 b_4 c_3 (c_3 - 2\gamma)}.$$

The other coefficients are determined from (3.1) and (3.2).

The method with the parameters $\gamma = 0.220428410259$, $c_3 = (2 + \sqrt{2})\gamma = 0.752589667839$, and $c_4 = 0.610097451414$ was proposed in [8]; we denote this method by ES44. These values of the parameters ensure the L-stability of two inner stages. Since $c_3^* = 0.701$, inequality (2.10) is also fulfilled.

Now, we consider the fourth-order ESDIRK methods with five implicit stages satisfying conditions (3.8) and (3.10). Regarding γ, c_3, c_4, c_5, and b_5 as free parameters, we find b_2, b_3, and b_4 from Eqs. (3.3). Taking into account (3.2), we deduce from (3.5), (3.8), and (3.10) that

$$a_{43} = \frac{(1 - 16\gamma + 72\gamma^2 - 96\gamma^3 + 24\gamma^4) c_4 (c_4 - c_3)(c_4 - 2\gamma)}{c_3 (c_3 - 2\gamma)[3 - 32\gamma + 84\gamma^2 - 48\gamma^3 - c_3(4 - 36\gamma + 72\gamma^2 - 24\gamma^3)]},$$

$$a_{54} = \gamma \frac{1 - 16\gamma + 72\gamma^2 - 96\gamma^3 + 24\gamma^4}{12 b_5 a_{43} c_3 (c_3 - 2\gamma)}, \qquad (5.2)$$

$$a_{53} = \frac{1 - 12\gamma + 36\gamma^2 - 24\gamma^3 - 12 b_4 a_{43} c_3 (c_3 - 2\gamma) - 12 b_5 a_{54} c_4 (c_4 - 2\gamma)}{12 b_5 c_3 (c_3 - 2\gamma)}.$$

The remaining coefficients are found from (3.1) and (3.2).

Let us discuss the choice of γ. In [1, 6, 8, 11], γ was set to 1/4, which ensures the L-stability and a small error constant. If we also admit $L(\alpha)$-stable methods, then, for $0.164 \le \gamma \le 0.191$, the error constant is small and the angle α of the stability sector is greater than 89.9° (see figure). The most convenient value in this interval is $\gamma = 1/6$.

The optimal values of c_3 are given by formulas (2.8) and (2.10). They yield $1/6 \le c_3 \le 5/12$ for $\gamma = 1/4$ and $8/15 \le c_3 \le 7/10$ for $\gamma = 1/6$. The method with the parameters $\gamma = c_3 = 1/4$, $c_4 = 3/4$, $c_5 = 1$, and $b_5 = -31/180$ was proposed in [8]. Here, we examine the method ES54 with the coefficient table

$$
\begin{array}{c|cccccc}
0 & 0 & & & & & \\
1/3 & 1/6 & 1/6 & & & & \\
2/3 & 1/6 & 1/3 & 1/6 & & & \\
1 & 11/24 & -1/4 & 5/8 & 1/6 & & \\
1 & 11/36 & -1/6 & 11/12 & -2/9 & 1/6 & \\
1 & 1/8 & 3/8 & 3/8 & -1/12 & 1/24 & 1/6
\end{array}.
$$

The penultimate stage of this method has the unit abscissa and the third order. This makes it possible to use ES54 as an embedded method as proposed in [13]. A similar property has the method specified by the parameters $\gamma = c_3 = 1/4$, $c_4 = c_5 = 1$, and $b_5 = -1/4$.

Among the methods given by formulas (3.1)–(3.3) and (5.2), we also mention the one-parameter family with the coefficients $\gamma = 1/6$, $c_3 = 8/15$, $c_5 = 1/2$, and $b_5 = 2/3$; c_4 is a free parameter. The methods in this family satisfy a number of order conditions for DAE systems of indices two and three (see [1, 3]) and have a higher accuracy for such problems.

The basic characteristics of the fourth-order methods are presented in Table 3.

6. FIFTH- AND SIXTH-ORDER METHODS

It is possible to construct $L(\alpha)$-stable ESDIRK methods for $r = p = 5$ if γ is set to a root of the equation

$$D_5(\gamma) = \frac{1}{120} - \frac{5}{24}\gamma + \frac{5}{3}\gamma^2 - 5\gamma^3 + 5\gamma^4 - \gamma^5 = 0 \qquad (6.1)$$

different from 0.0791…. For a given γ, there exists the two-parameter family of such methods determined by Eqs. (3.1)– (3.3), (3.5), and (3.6). Regarding c_3 and c_4 as free parameters, we obtain

$$c_5 = \frac{4\gamma - 64\gamma^2 + 368\gamma^3 - 848\gamma^4 + 720\gamma^5 - c_3(1 - 18\gamma + 120\gamma^2 - 336\gamma^3 + 360\gamma^4)}{4\gamma - 56\gamma^2 + 288\gamma^3 - 600\gamma^4 + 480\gamma^5 - c_3(1 - 16\gamma + 96\gamma^2 - 240\gamma^3 + 240\gamma^4)}.$$

The weights b_2, b_3, b_4, and b_5 are found from Eqs. (3.3). Then, we have

$$a_{43} = \frac{4 - 50\gamma + 160\gamma^2 - 120\gamma^3 - c_5(5 - 60\gamma + 180\gamma^2 - 120\gamma^3)}{60 b_4 c_3 (c_4 - c_5)(c_3 - 2\gamma)},$$

$$a_{54} = \frac{1 - 20\gamma + 120\gamma^2 - 240\gamma^3 + 120\gamma^4}{60 b_5 a_{43} c_3 (c_3 - 2\gamma)},$$

$$a_{53} = \frac{1 - 12\gamma + 36\gamma^2 - 24\gamma^3}{12 b_5 c_3 (c_3 - 2\gamma)} - \frac{b_4}{b_5} a_{43} - \frac{c_4(c_4 - 2\gamma)}{c_3(c_3 - 2\gamma)} a_{54}.$$

The remaining coefficients are found from (3.1) and (3.2). For the method called ES55, we set $\gamma = 0.141127125789$, $c_3 = 0.55$, and $c_4 = 0.75$. This ensures small error coefficients. Since $c_3^* = 0.497$, inequality (2.10) is also fulfilled.

We also examined ESDIRK methods for $r = 6$ and $p = 5$ satisfying conditions (3.9) and (3.10). In this case, we again were able to derive expressions for the coefficients of the method; however, they are too cumbersome and are not given here. Instead, we outline the construction of such methods.

The value of γ uniquely determines the stability function and can be chosen using the figure. We regard c_3, c_4, c_5, c_6, and b_6 as free parameters. Having chosen their values, we find b_2, b_3, b_4, and b_5 from (3.3). Substituting expressions (3.2) for a_{i2} in (3.5), (3.6), (3.9), and (3.10), we obtain a system of equations from which a_{43}, a_{53}, a_{54}, a_{63}, a_{64}, and a_{65} are determined. Finally, the remaining coefficients are found from (3.1) and (3.2). For this method called ES65, we choose the values $\gamma = c_6 = 1/5$, $c_3 = 3/5$, $c_4 = 1$, $c_5 = 4/5$, and $b_6 = 25/96$. Inequality (2.10) is fulfilled because $c_3^* = 0.518$. The coefficients of this method are given in [8].

Table 3

Method	γ	α, deg	$\|e(t_5)\|_2$	$\|e_{q+1}(z)\|_\infty$
S54a	0.25	90.0	1.3×10^{-1}	6.3×10^{-2}
S54b	0.25	90.0	2.0×10^{-1}	9.3×10^{-3}
ES44	0.220428	89.56	2.5×10^{-1}	1.2×10^{-2}
ES54	1/6	89.95	1.2×10^{-1}	7.0×10^{-3}

Now, we consider the ESDIRK methods constructed using the condition

$$e_3(z) \equiv 0. \tag{6.2}$$

A similar approach was used for the construction of explicit Runge–Kutta methods in [15]. Condition (6.2) is satisfied if

$$\begin{gathered} \mathbf{e}_r^{\mathrm{T}} \tilde{\mathbf{A}}^i = [0, *, \ldots, *], \quad i = 0, 1, \ldots, r-1, \\ \tilde{\mathbf{c}}^3 - 3\tilde{\mathbf{A}}\tilde{\mathbf{c}}^2 = [*, 0, \ldots, 0]^{\mathrm{T}}, \end{gathered} \tag{6.3}$$

where the asterisks denote nonzero components. In turn, (6.3) is ensured if we set

$$\begin{gathered} c_2 = 2\gamma, \quad c_3 = (3-\sqrt{3})\gamma, \quad c_4 = (3+\sqrt{3})\gamma, \quad c_5 = 0, \\ a_{32} = \frac{c_3(c_3 - 2\gamma)}{4\gamma}, \quad a_{42} = \frac{c_4(c_4 - 2\gamma)}{4\gamma}, \quad a_{43} = 0, \quad b_2 = 0 \end{gathered} \tag{6.4}$$

and require that conditions (3.3) with $p \ge 3$ and the conditions

$$\sum_{j=3}^{i-1} a_{ij} a_{j2} = 0, \quad \sum_{j=2}^{i-1} a_{ij} c_j = \frac{c_i^2}{2} - \gamma c_i, \quad \sum_{j=2}^{i-1} a_{ij} c_j^2 = \frac{c_i^3}{3} - \gamma c_i^2, \quad i = 5, 6, \ldots, r, \tag{6.5}$$

$$\sum_{i=3}^{r} b_i a_{i2} = 0 \tag{6.6}$$

be fulfilled.

The $L(\alpha)$-stable method based on relations (6.4)–(6.6) has stability function (1.8) with $d_{r-2} = d_{r-1} = 0$; therefore, a method of order p must have at least $p + 2$ implicit stages. To construct a fifth-order method, we additionally require that

$$\sum_{i=3}^{r} b_i c_i a_{i2} = 0. \tag{6.7}$$

This ensures the validity of the relation $\mathbf{b}^{\mathrm{T}}(\mathbf{c} \cdot \mathbf{A}^{-1}\mathbf{c}^3) = 3/4$, which is one of the order conditions for DAE systems of index two (see [3]). Let us describe how the method called ES75 is constructed.

We set $\gamma = 0.141127125789$; with this value, Eq. (6.1) is satisfied. We assign the values $c_6 = 0.8$, $c_7 = 1$, $a_{72} = 0$, and $b_5 = 0.02$ to the free parameters. Note that the value of c_6 is chosen so as to minimize the error function $e_4(z)$. We calculate coefficients (6.4) and then find b_3, b_4, b_6, and b_7 from Eqs. (3.3). From (6.6) and (6.7), we determine a_{52} and a_{62}. Setting $i = 5$ in the first two equations (6.5), we calculate a_{53} and a_{54}. From (6.5) with $i = 6$, we find a_{63}, a_{64}, and a_{65}. Using the last condition in (3.6), we calculate

$$a_{76} = \frac{1 - 20\gamma + 120\gamma^2 - 240\gamma^3 + 120\gamma^4}{120 b_7 a_{65}(a_{53}c_3 + a_{54}c_4)}.$$

Finally, (6.5) with $i = 7$ yields a_{73}, a_{74}, and a_{75}.

Table 4

Method	γ	α, deg	$\lVert e(t_6)\rVert_2$	$\lVert e_3(z)\rVert_\infty$
ES55	0.141127	72.3	1.1×10^{-1}	7.4×10^{-3}
ES65	0.2	90.0	3.4×10^{-1}	4.6×10^{-3}
ES75	0.141127	72.3	1.1×10^{-1}	0
ES86	1/6	88.7	0	7.5×10^{-4}

Table 5

Method	μ				
	10^1	10^2	10^3	10^4	10^5
S33a	5.7×10^{-5}	$\mathbf{7.4 \times 10^{-5}}$	2.5×10^{-5}	8.5×10^{-6}	6.5×10^{-6}
S33b	1.3×10^{-5}	$\mathbf{7.9 \times 10^{-5}}$	7.8×10^{-5}	8.3×10^{-6}	1.7×10^{-6}
ES33a	$\mathbf{2.6 \times 10^{-5}}$	1.3×10^{-5}	7.4×10^{-5}	6.4×10^{-6}	6.3×10^{-6}
ES33b	5.1×10^{-6}	$\mathbf{5.8 \times 10^{-6}}$	2.8×10^{-6}	1.1×10^{-6}	1.0×10^{-6}
S54a	1.5×10^{-5}	$\mathbf{1.7 \times 10^{-4}}$	7.2×10^{-5}	7.9×10^{-6}	8.7×10^{-7}
S54b	4.6×10^{-7}	$\mathbf{1.1 \times 10^{-5}}$	9.4×10^{-6}	1.2×10^{-6}	1.9×10^{-7}
ES44	8.4×10^{-7}	$\mathbf{8.5 \times 10^{-7}}$	1.4×10^{-7}	2.2×10^{-8}	4.2×10^{-8}
ES54	4.4×10^{-7}	$\mathbf{4.5 \times 10^{-7}}$	2.4×10^{-8}	5.3×10^{-8}	4.8×10^{-8}
ES55	8.5×10^{-8}	3.1×10^{-7}	$\mathbf{5.6 \times 10^{-7}}$	9.5×10^{-8}	1.0×10^{-8}
ES65	$\mathbf{3.3 \times 10^{-7}}$	2.4×10^{-7}	9.0×10^{-8}	1.7×10^{-8}	4.1×10^{-9}
ES75	$\mathbf{1.0 \times 10^{-7}}$	4.3×10^{-8}	6.4×10^{-8}	8.9×10^{-9}	1.7×10^{-9}
ES86	3.3×10^{-8}	$\mathbf{6.1 \times 10^{-8}}$	2.7×10^{-8}	4.1×10^{-9}	4.1×10^{-10}

We also managed to construct sixth-order ESDIRK methods for which the function $e_3(z)$ has a small norm. Here are the coefficients of the method called ES86:

$$\gamma = \frac{1}{6},\quad c_2 = \frac{1}{3},\quad c_3 = c_8 = \frac{1}{4},\quad c_4 = c_7 = \frac{1}{2},\quad c_5 = \frac{3}{4},\quad c_6 = 1,\quad a_{32} = -\frac{1}{32},\quad a_{42} = -\frac{1}{4},$$

$$a_{43} = \frac{1}{2},\quad a_{52} = -\frac{6987}{5024},\quad a_{53} = \frac{3271}{1884},\quad a_{54} = \frac{175}{471},\quad a_{62} = -\frac{114988}{31871},\quad a_{63} = \frac{1208156}{286839},$$

$$a_{64} = \frac{132950}{286839},\quad a_{65} = \frac{68}{203},\quad a_{72} = -\frac{480525599}{416107776},\quad a_{73} = \frac{2240951089}{1404363744},$$

$$a_{74} = \frac{394951619}{2808727488},\quad a_{75} = -\frac{5160553}{26834976},\quad a_{76} = \frac{35815}{352512},\quad a_{82} = \frac{9786099235}{14425069568},$$

$$a_{83} = -\frac{34306812733}{48684609792},\quad a_{84} = -\frac{15985588007}{97369219584},\quad a_{85} = \frac{37652437}{930279168},$$

$$a_{86} = -\frac{340747}{12220416},\quad a_{87} = \frac{1}{26},\quad b_2 = b_3 = b_4 = 0,\quad b_5 = b_8 = \frac{16}{45},\quad b_6 = -\frac{4}{45},\quad b_7 = \frac{2}{15}.$$

(The coefficients $a_{21}, a_{31}, \ldots, a_{81}$, and b_1 can easily be found from (3.1).) The characteristics of the fifth- and sixth-order methods are presented in Table 4.

Table 6

Method	Error	Method	Error	Method	Error
S33a	7.4×10^{-4}	S54a	1.9×10^{-3}	ES55	8.3×10^{-6}
S33b	1.9×10^{-3}	S54b	1.5×10^{-4}	ES65	2.5×10^{-6}
ES33a	1.3×10^{-4}	ES44	1.2×10^{-5}	ES75	7.7×10^{-7}
ES33b	6.7×10^{-5}	ES54	7.9×10^{-6}	ES86	1.2×10^{-6}

Table 7

Problem	Method	scd	Nf	NJ	NLU
VDPOL	ES33b	3.99	2221	75	278
	ES44	4.08	2711	94	242
	RADAU	4.44	2214	165	231
OREGO	ES33b	2.36	2396	149	317
	ES44	3.66	3160	157	350
	RADAU	3.12	3416	200	267

6. RESULTS OF SOLVING TEST PROBLEMS

For the constant step integration, the accuracy of the methods was estimated for two problems. One of them is the Kaps problem

$$y_1' = -(\mu+2)y_1 + \mu y_2^2, \quad y_1(0) = 1,$$

$$y_2' = y_1 - y_2 - y_2^2, \quad y_2(0) = 1, \quad 0 \le t \le 1,$$

which has the smooth solution $y_1(t) = \exp(-2t)$, $y_2(t) = \exp(-t)$, which is independent of the stiffness parameter μ. To balance the computational cost of all the methods, the step size h was set to $h = r/60$. For $r \le 6$, this corresponds to executing 60 implicit stages on the integration interval. For $r = 7$, nine steps were executed, and, for $r = 8$, the number of steps was eight. (In both cases, the integration interval is slightly greater than 1.) The maximal relative error with respect to the entire interval was calculated. The results for five values of μ are presented in Table 5, where the maximal relative error is given in bold.

The second problem (which is the test problem PLATE given in [1]) consists of 80 equations; its Jacobian matrix has a complex spectrum. For $h = r/120$, the maximal relative error was calculated at the endpoint of the interval. The corresponding results are shown in Table 6.

The results presented here and in [8] demonstrate the superiority of ESDIRK methods, which is explained by their higher stage order. Among the SDIRK methods, the best one was S54b, in which the error function $e_2(z)$ is minimized. It was shown in [8, 9] that the most advantageous ESDIRK methods are those with the error function $e_3(z)$ minimized; therefore, here, we considered only such methods.

Implementations of ES33b and ES44 were included in the software package MVTU (see [20, 21]). These implementations were used for solving the stiff problems VDPOL and OREGO (see [1, 22]) under the conditions stated in [22] with the prescribed accuracy Tol $= 10^{-4}$. The actual accuracy was estimated by the formula scd $= -\log(\text{err})$, where err is the maximal relative error at the endpoint of the integration interval maximized over all the components. Thus, scd is the number of correct significant digits in the numerical solution. To estimate the computational effort, the following characteristics were used: the number Nf of function evaluations, the number NJ of Jacobian matrix evaluations, and the number NLU of LU decompositions. The results are presented in Table 7. For comparison purposes, we also show in this table the results obtained by RADAU, which is one of the best solvers for stiff problems (see [1, 22]).

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